Full wwPDB EM Validation Report

Mar 7, 2026 – 03:44 AM UTC

PDB ID	:	8JZE / pdb_00008jze
EMDB ID	:	EMD-36742
Title	:	PSI-AcpPCI supercomplex from Symbiodinium
Authors	:	Li, Z.H.; Li, X.Y.; Wang, W.D.
Deposited on	:	2023-07-05
Resolution	:	2.99 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:

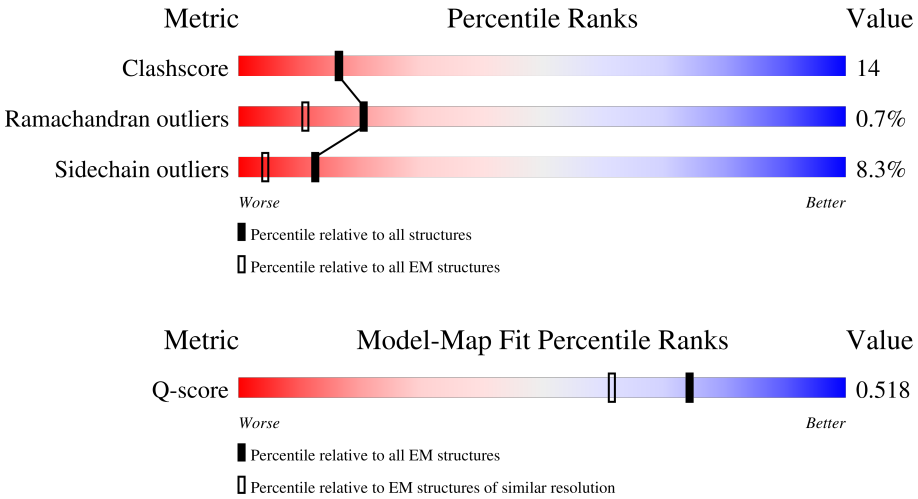
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.99 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	13287 (2.49 - 3.49)

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	I	200	6%, 71%, 26%, ·
2	K	177	·, 67%, 31%, ·
3	z	78	92%, 8%
4	y	131	·, 97%, ·

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Mol	Chain	Length	Quality of chain
5	G	224	65% 29%
6	A	189	73% 22%
7	c	86	72% 28%
8	d	218	76% 22%
9	e	73	75% 25%
10	f	184	79% 20%
11	h	131	69% 31%
12	i	119	73% 27%
13	j	98	74% 24%
14	l	250	69% 28%
15	m	79	76% 24%
16	a	670	70% 27%
17	b	663	70% 29%
18	B	192	65% 32%
19	D	165	57% 32% 8%
20	F	176	6% 64% 26% 5%
21	H	160	66% 61% 34% 5%
22	J	220	72% 25%
23	L	185	63% 30% 7%
24	M	173	62% 28% 8%
25	N	160	36% 55% 32% 8%
26	O	161	7% 66% 30%
27	P	160	59% 28% 12%

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
30	CLA	A	307	X	-	-	-
30	CLA	A	308	X	-	-	-
30	CLA	A	309	X	-	-	-
30	CLA	A	310	X	-	-	-
30	CLA	A	311	X	-	-	-
30	CLA	A	312	X	-	-	-
30	CLA	A	313	X	-	-	-
30	CLA	A	315	X	-	-	-
30	CLA	A	316	X	-	-	-
30	CLA	A	317	X	-	-	-
30	CLA	A	319	X	-	-	-
30	CLA	A	320	X	-	-	-
30	CLA	B	301	X	-	-	-
30	CLA	B	307	X	-	-	-
30	CLA	B	308	X	-	-	-
30	CLA	B	309	X	-	-	-
30	CLA	B	310	X	-	-	-
30	CLA	B	311	X	-	-	-
30	CLA	B	312	X	-	-	-
30	CLA	B	313	X	-	-	-
30	CLA	B	315	X	-	-	-
30	CLA	B	316	X	-	-	-
30	CLA	B	317	X	-	-	-
30	CLA	D	308	X	-	-	-
30	CLA	D	309	X	-	-	-
30	CLA	D	311	X	-	-	-
30	CLA	D	312	X	-	-	-
30	CLA	D	313	X	-	-	-
30	CLA	D	314	X	-	-	-
30	CLA	D	316	X	-	-	-
30	CLA	F	307	X	-	-	-
30	CLA	F	308	X	-	-	-
30	CLA	F	310	X	-	-	-
30	CLA	F	311	X	-	-	-
30	CLA	F	312	X	-	-	-
30	CLA	F	313	X	-	-	-
30	CLA	F	315	X	-	-	-
30	CLA	G	509	X	-	-	-
30	CLA	G	510	X	-	-	-
30	CLA	G	511	X	-	-	-
30	CLA	G	512	X	-	-	-
30	CLA	G	513	X	-	-	-
30	CLA	G	514	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	G	516	X	-	-	-
30	CLA	G	517	X	-	-	-
30	CLA	G	518	X	-	-	-
30	CLA	G	519	X	-	-	-
30	CLA	G	520	X	-	-	-
30	CLA	H	304	X	-	-	-
30	CLA	H	305	X	-	-	-
30	CLA	H	307	X	-	-	-
30	CLA	H	308	X	-	-	-
30	CLA	H	309	X	-	-	-
30	CLA	H	312	X	-	-	-
30	CLA	I	306	X	-	-	-
30	CLA	I	307	X	-	-	-
30	CLA	I	308	X	-	-	-
30	CLA	I	309	X	-	-	-
30	CLA	I	310	X	-	-	-
30	CLA	I	311	X	-	-	-
30	CLA	I	312	X	-	-	-
30	CLA	I	313	X	-	-	-
30	CLA	I	315	X	-	-	-
30	CLA	I	316	X	-	-	-
30	CLA	I	319	X	-	-	-
30	CLA	I	321	X	-	-	-
30	CLA	J	301	X	-	-	-
30	CLA	J	306	X	-	-	-
30	CLA	J	307	X	-	-	-
30	CLA	J	308	X	-	-	-
30	CLA	J	309	X	-	-	-
30	CLA	J	310	X	-	-	-
30	CLA	J	311	X	-	-	-
30	CLA	J	312	X	-	-	-
30	CLA	J	314	X	-	-	-
30	CLA	J	315	X	-	-	-
30	CLA	K	306	X	-	-	-
30	CLA	K	307	X	-	-	-
30	CLA	K	308	X	-	-	-
30	CLA	K	309	X	-	-	-
30	CLA	K	310	X	-	-	-
30	CLA	K	311	X	-	-	-
30	CLA	K	312	X	-	-	-
30	CLA	K	313	X	-	-	-
30	CLA	K	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	K	316	X	-	-	-
30	CLA	L	308	X	-	-	-
30	CLA	L	309	X	-	-	-
30	CLA	L	310	X	-	-	-
30	CLA	L	311	X	-	-	-
30	CLA	L	312	X	-	-	-
30	CLA	L	313	X	-	-	-
30	CLA	L	314	X	-	-	-
30	CLA	L	316	X	-	-	-
30	CLA	L	317	X	-	-	-
30	CLA	L	318	X	-	-	-
30	CLA	M	308	X	-	-	-
30	CLA	M	309	X	-	-	-
30	CLA	M	310	X	-	-	-
30	CLA	M	311	X	-	-	-
30	CLA	M	312	X	-	-	-
30	CLA	M	313	X	-	-	-
30	CLA	M	315	X	-	-	-
30	CLA	M	316	X	-	-	-
30	CLA	M	317	X	-	-	-
30	CLA	M	318	X	-	-	-
30	CLA	N	304	X	-	-	-
30	CLA	N	305	X	-	-	-
30	CLA	N	307	X	-	-	-
30	CLA	N	309	X	-	-	-
30	CLA	N	310	X	-	-	-
30	CLA	O	308	X	-	-	-
30	CLA	O	309	X	-	-	-
30	CLA	O	311	X	-	-	-
30	CLA	O	313	X	-	-	-
30	CLA	O	314	X	-	-	-
30	CLA	O	316	X	-	-	-
30	CLA	P	209	X	-	-	-
30	CLA	P	210	X	-	-	-
30	CLA	P	212	X	-	-	-
30	CLA	P	214	X	-	-	-
30	CLA	P	215	X	-	-	-
30	CLA	P	217	X	-	-	-
30	CLA	a	701	X	-	-	-
30	CLA	a	702	X	-	-	-
30	CLA	a	703	X	-	-	-
30	CLA	a	704	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	a	705	X	-	-	-
30	CLA	a	706	X	-	-	-
30	CLA	a	707	X	-	-	-
30	CLA	a	708	X	-	-	-
30	CLA	a	709	X	-	-	-
30	CLA	a	710	X	-	-	-
30	CLA	a	711	X	-	-	-
30	CLA	a	712	X	-	-	-
30	CLA	a	713	X	-	-	-
30	CLA	a	714	X	-	-	-
30	CLA	a	715	X	-	-	-
30	CLA	a	716	X	-	-	-
30	CLA	a	717	X	-	-	-
30	CLA	a	718	X	-	-	-
30	CLA	a	719	X	-	-	-
30	CLA	a	720	X	-	-	-
30	CLA	a	721	X	-	-	-
30	CLA	a	722	X	-	-	-
30	CLA	a	723	X	-	-	-
30	CLA	a	724	X	-	-	-
30	CLA	a	725	X	-	-	-
30	CLA	a	726	X	-	-	-
30	CLA	a	727	X	-	-	-
30	CLA	a	728	X	-	-	-
30	CLA	a	729	X	-	-	-
30	CLA	a	730	X	-	-	-
30	CLA	a	731	X	-	-	-
30	CLA	a	735	X	-	-	-
30	CLA	a	738	X	-	-	-
30	CLA	b	701	X	-	-	-
30	CLA	b	703	X	-	-	-
30	CLA	b	704	X	-	-	-
30	CLA	b	705	X	-	-	-
30	CLA	b	706	X	-	-	-
30	CLA	b	707	X	-	-	-
30	CLA	b	708	X	-	-	-
30	CLA	b	709	X	-	-	-
30	CLA	b	710	X	-	-	-
30	CLA	b	711	X	-	-	-
30	CLA	b	712	X	-	-	-
30	CLA	b	713	X	-	-	-
30	CLA	b	714	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	b	715	X	-	-	-
30	CLA	b	716	X	-	-	-
30	CLA	b	717	X	-	-	-
30	CLA	b	718	X	-	-	-
30	CLA	b	719	X	-	-	-
30	CLA	b	720	X	-	-	-
30	CLA	b	721	X	-	-	-
30	CLA	b	722	X	-	-	-
30	CLA	b	723	X	-	-	-
30	CLA	b	724	X	-	-	-
30	CLA	b	725	X	-	-	-
30	CLA	b	726	X	-	-	-
30	CLA	b	727	X	-	-	-
30	CLA	b	728	X	-	-	-
30	CLA	f	301	X	-	-	-
30	CLA	f	302	X	-	-	-
30	CLA	f	303	X	-	-	-
30	CLA	h	202	X	-	-	-
30	CLA	j	104	X	-	-	-
30	CLA	j	106	X	-	-	-
30	CLA	l	303	X	-	-	-
30	CLA	l	304	X	-	-	-
30	CLA	l	305	X	-	-	-
30	CLA	l	308	X	-	-	-
30	CLA	l	309	X	-	-	-
30	CLA	l	311	X	-	-	-
30	CLA	l	312	X	-	-	-
30	CLA	l	313	X	-	-	-
30	CLA	m	202	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 55927 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-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	200	Total	C	N	O	S	0	0
			1480	961	250	259	10		

- Molecule 2 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	177	Total	C	N	O	S	0	0
			1349	872	227	238	12		

- Molecule 3 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	z	78	Total	C	N	O	0	0
			390	234	78	78		

- Molecule 4 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	y	131	Total	C	N	O	0	0
			655	393	131	131		

- Molecule 5 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	217	Total	C	N	O	S	0	0
			1572	1004	269	289	10		

- Molecule 6 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	186	Total	C	N	O	S	0	0
			1346	870	225	242	9		

- Molecule 7 is a protein called Photosystem I PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	86	Total	C	N	O	S	0	0
			653	403	109	132	9		

- Molecule 8 is a protein called Photosystem I PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	218	Total	C	N	O	S	0	0
			1731	1096	307	315	13		

- Molecule 9 is a protein called Photosystem I PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	e	73	Total	C	N	O	0	0
			587	384	99	104		

- Molecule 10 is a protein called Photosystem I PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	184	Total	C	N	O	S	0	0
			1450	930	252	260	8		

- Molecule 11 is a protein called Photosystem I PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	h	131	Total	C	N	O	S	0	0
			1066	704	165	193	4		

- Molecule 12 is a protein called Photosystem I PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	119	Total	C	N	O	S	0	0
			964	620	167	175	2		

- Molecule 13 is a protein called Photosystem I PsaJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	j	98	Total 783	C 505	N 125	O 153	0	0

- Molecule 14 is a protein called Photosystem I PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	250	Total 1943	C 1267	N 312	O 354	S 10	0	0

- Molecule 15 is a protein called Photosystem I PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m	79	Total 582	C 373	N 100	O 107	S 2	0	0

- Molecule 16 is a protein called Photosystem I PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	670	Total 5194	C 3393	N 875	O 910	S 16	0	0

- Molecule 17 is a protein called Photosystem I PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	663	Total 5199	C 3408	N 851	O 928	S 12	0	0

- Molecule 18 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	192	Total 1452	C 934	N 241	O 265	S 12	0	0

- Molecule 19 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D	160	Total 1158	C 728	N 195	O 228	S 7	0	0

- Molecule 20 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2,

acpPCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	169	Total	C	N	O	S	0	0
			1237	777	209	239	12		

- Molecule 21 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	160	Total	C	N	O	S	0	0
			1202	769	198	228	7		

- Molecule 22 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	J	220	Total	C	N	O	S	0	0
			1496	938	261	290	7		

- Molecule 23 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	185	Total	C	N	O	S	0	0
			1427	924	239	258	6		

- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	168	Total	C	N	O	S	0	0
			1211	773	208	225	5		

- Molecule 25 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	153	Total	C	N	O	S	0	0
			993	607	179	202	5		

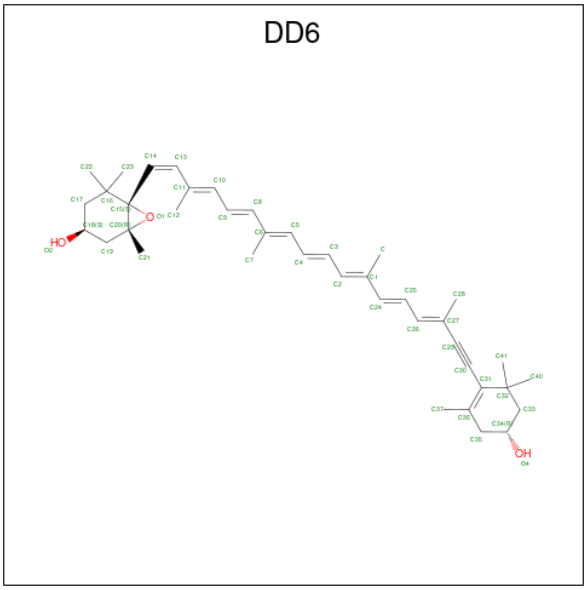
- Molecule 26 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	161	Total	C	N	O	S	0	0
			1073	670	189	207	7		

- Molecule 27 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	159	Total	C	N	O	S	0	0
			1113	693	191	223	6		

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	I	1	Total	C	O		0
			43	40	3		
28	I	1	Total	C	O		0
			43	40	3		
28	I	1	Total	C	O		0
			43	40	3		
28	I	1	Total	C	O		0
			43	40	3		
28	K	1	Total	C	O		0
			43	40	3		
28	K	1	Total	C	O		0
			43	40	3		

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Mol	Chain	Residues	Atoms	AltConf
28	K	1	Total C O 43 40 3	0
28	K	1	Total C O 43 40 3	0
28	K	1	Total C O 43 40 3	0
28	G	1	Total C O 43 40 3	0
28	G	1	Total C O 43 40 3	0
28	G	1	Total C O 43 40 3	0
28	G	1	Total C O 43 40 3	0
28	A	1	Total C O 43 40 3	0
28	A	1	Total C O 43 40 3	0
28	A	1	Total C O 43 40 3	0
28	A	1	Total C O 43 40 3	0
28	h	1	Total C O 43 40 3	0
28	b	1	Total C O 43 40 3	0
28	B	1	Total C O 42 39 3	0
28	B	1	Total C O 43 40 3	0
28	B	1	Total C O 43 40 3	0
28	B	1	Total C O 43 40 3	0
28	D	1	Total C O 43 40 3	0
28	F	1	Total C O 43 40 3	0
28	F	1	Total C O 43 40 3	0
28	H	1	Total C O 43 40 3	0

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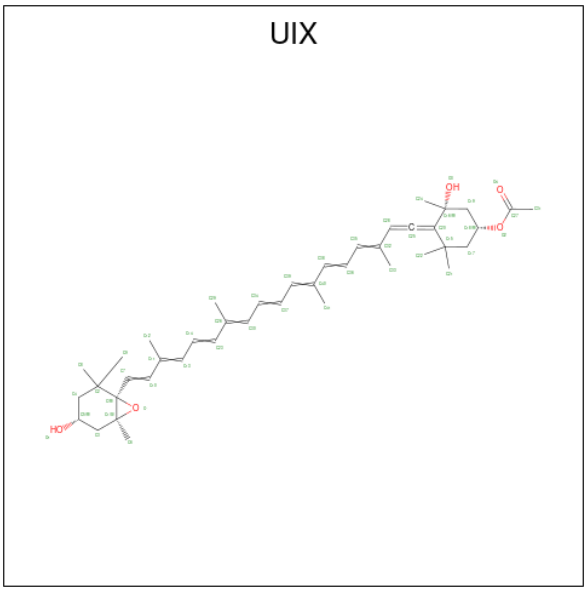
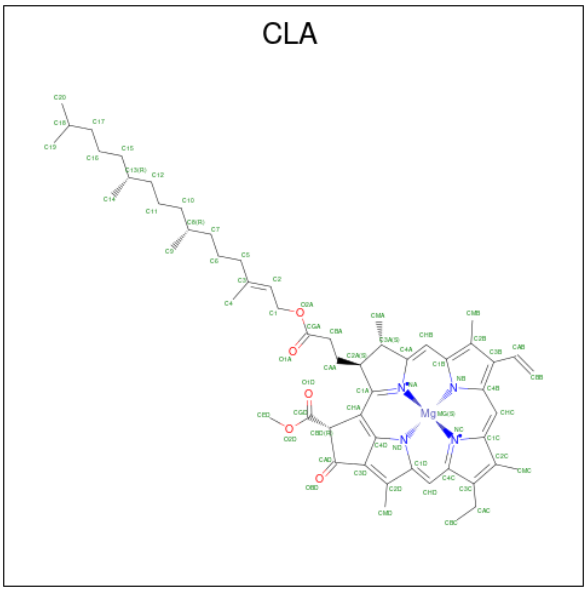
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			43	40	3	
28	J	1	Total	C	O	0
			43	40	3	
28	J	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	N	1	Total	C	O	0
			43	40	3	
28	O	1	Total	C	O	0
			43	40	3	
28	P	1	Total	C	O	0
			43	40	3	

- Molecule 29 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (CCD ID: UIX) (formula: $C_{42}H_{58}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
29	I	1	Total C O 47 42 5	0
29	K	1	Total C O 47 42 5	0
29	G	1	Total C O 47 42 5	0
29	A	1	Total C O 47 42 5	0
29	h	1	Total C O 47 42 5	0
29	B	1	Total C O 47 42 5	0
29	J	1	Total C O 47 42 5	0
29	O	1	Total C O 47 42 5	0
29	P	1	Total C O 47 42 5	0

- Molecule 30 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
30	I	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	K	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
30	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms	AltConf
30	l	1	Total C N O 45 36 4 5	0
30	l	1	Total C Mg N O 65 55 1 4 5	0
30	l	1	Total C Mg N O 46 36 1 4 5	0
30	l	1	Total C Mg N O 65 55 1 4 5	0
30	m	1	Total C Mg N O 60 50 1 4 5	0
30	a	1	Total C Mg N O 45 35 1 4 5	0
30	a	1	Total C Mg N O 65 55 1 4 5	0
30	a	1	Total C Mg N O 55 45 1 4 5	0
30	a	1	Total C Mg N O 65 55 1 4 5	0
30	a	1	Total C Mg N O 55 45 1 4 5	0
30	a	1	Total C Mg N O 58 48 1 4 5	0
30	a	1	Total C Mg N O 65 55 1 4 5	0
30	a	1	Total C Mg N O 51 41 1 4 5	0
30	a	1	Total C Mg N O 65 55 1 4 5	0
30	a	1	Total C Mg N O 55 45 1 4 5	0
30	a	1	Total C Mg N O 45 35 1 4 5	0
30	a	1	Total C Mg N O 60 50 1 4 5	0
30	a	1	Total C Mg N O 60 50 1 4 5	0
30	a	1	Total C Mg N O 45 35 1 4 5	0
30	a	1	Total C Mg N O 45 35 1 4 5	0
30	a	1	Total C Mg N O 47 37 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			47	39	1	4	3	
30	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	M	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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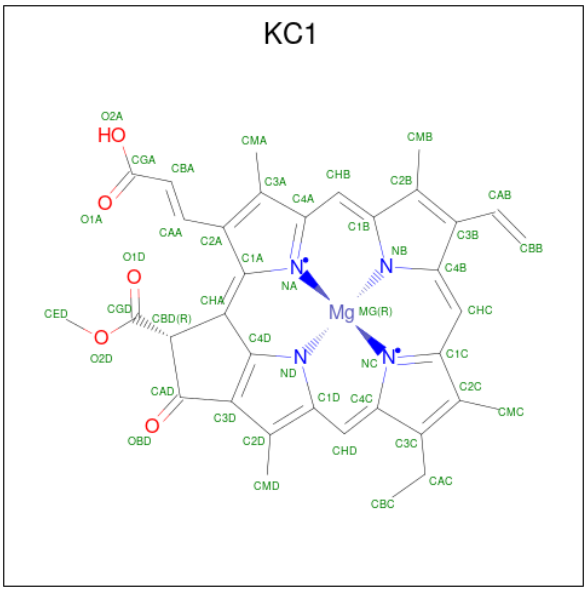
Mol	Chain	Residues	Atoms					AltConf
30	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 31 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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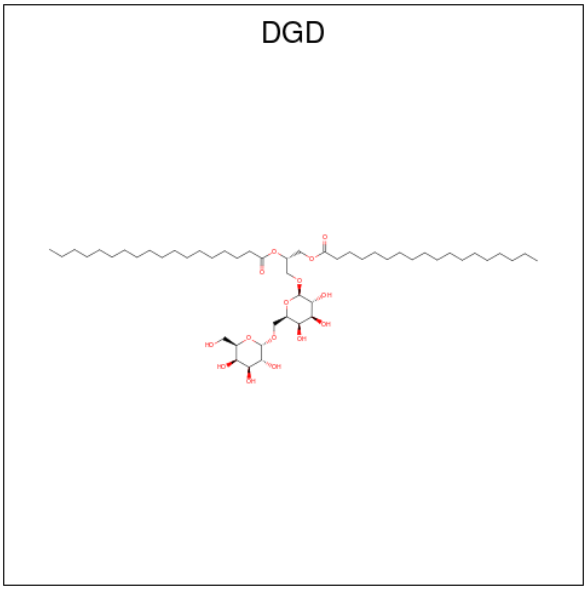
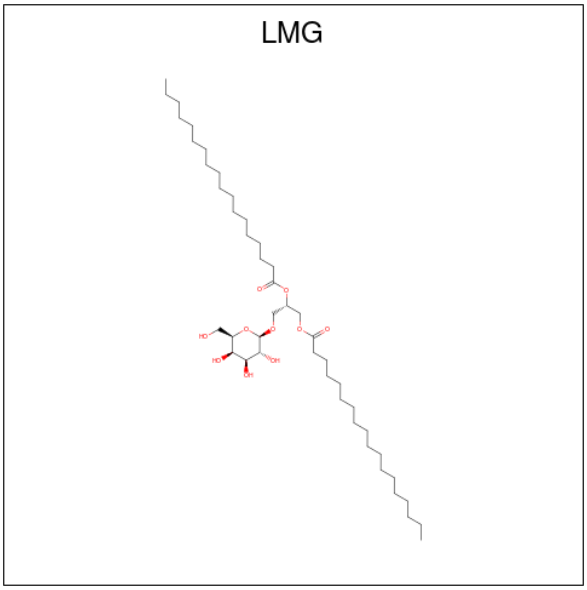
Mol	Chain	Residues	Atoms					AltConf
31	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 32 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
32	I	1	Total C O 39 24 15	0
32	y	1	Total C O 54 39 15	0
32	G	1	Total C O 45 30 15	0
32	G	1	Total C O 44 29 15	0
32	j	1	Total C O 41 26 15	0
32	l	1	Total C O 50 35 15	0
32	L	1	Total C O 38 23 15	0

- Molecule 33 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
33	I	1	Total C O 36 26 10	0
33	I	1	Total C O 38 28 10	0
33	K	1	Total C O 43 33 10	0
33	j	1	Total C O 35 25 10	0

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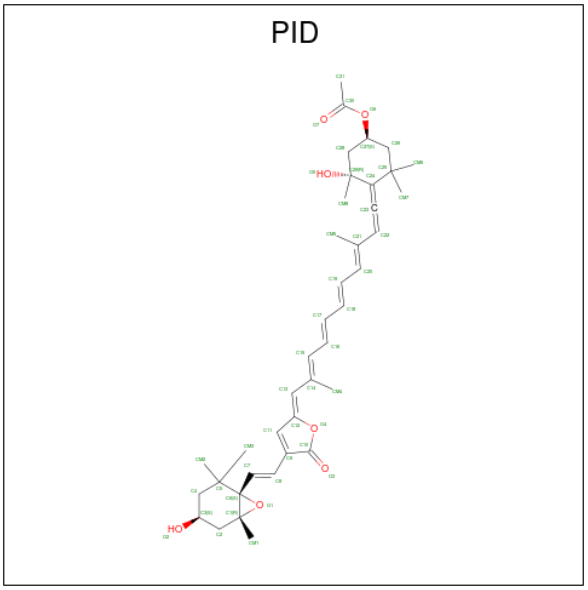
Mol	Chain	Residues	Atoms	AltConf
33	b	1	Total C O 44 34 10	0
33	b	1	Total C O 31 21 10	0
33	B	1	Total C O 37 27 10	0
33	D	1	Total C O 49 39 10	0
33	P	1	Total C O 27 17 10	0

- Molecule 34 is PERIDININ (CCD ID: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
34	G	1	Total C O 46 39 7	0
34	G	1	Total C O 46 39 7	0
34	j	1	Total C O 46 39 7	0
34	D	1	Total C O 46 39 7	0
34	D	1	Total C O 46 39 7	0
34	D	1	Total C O 46 39 7	0

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Mol	Chain	Residues	Atoms			AltConf
34	D	1	Total	C	O	0
			46	39	7	
34	D	1	Total	C	O	0
			46	39	7	
34	D	1	Total	C	O	0
			46	39	7	
34	F	1	Total	C	O	0
			46	39	7	
34	F	1	Total	C	O	0
			46	39	7	
34	F	1	Total	C	O	0
			46	39	7	
34	F	1	Total	C	O	0
			46	39	7	
34	H	1	Total	C	O	0
			46	39	7	
34	H	1	Total	C	O	0
			46	39	7	
34	M	1	Total	C	O	0
			46	39	7	
34	N	1	Total	C	O	0
			46	39	7	
34	N	1	Total	C	O	0
			46	39	7	
34	O	1	Total	C	O	0
			46	39	7	
34	O	1	Total	C	O	0
			46	39	7	
34	O	1	Total	C	O	0
			46	39	7	
34	O	1	Total	C	O	0
			46	39	7	
34	O	1	Total	C	O	0
			46	39	7	
34	P	1	Total	C	O	0
			46	39	7	
34	P	1	Total	C	O	0
			46	39	7	
34	P	1	Total	C	O	0
			46	39	7	
34	P	1	Total	C	O	0
			46	39	7	

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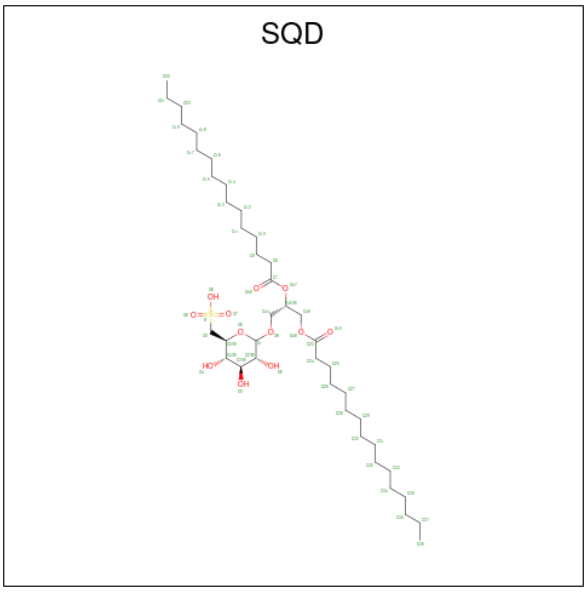
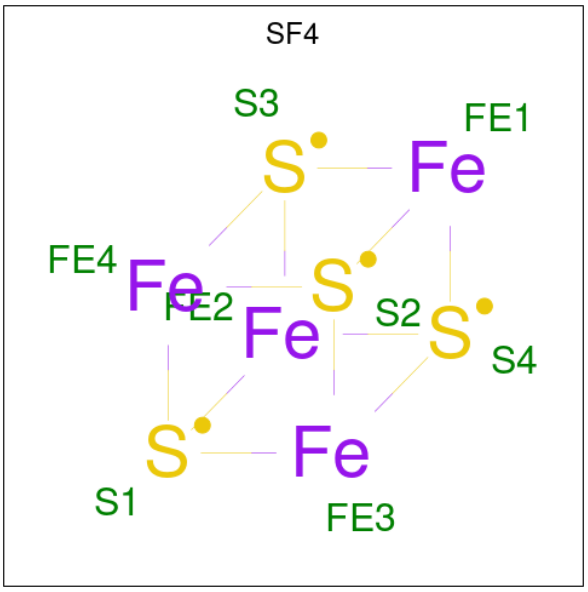
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	P	1	46	39	7	0

- Molecule 35 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).



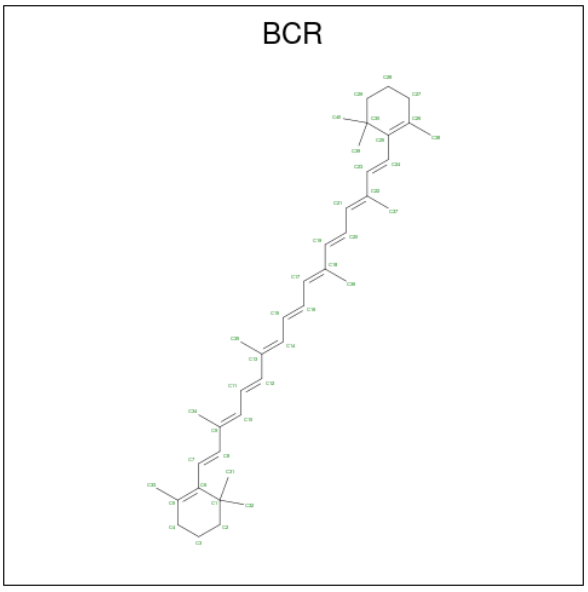
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
35	A	1	50	37	12	1	0

- Molecule 36 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
36	c	1	Total Fe S 8 4 4	0
36	c	1	Total Fe S 8 4 4	0
36	a	1	Total Fe S 8 4 4	0

- Molecule 37 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
37	f	1	Total C 40 40	0

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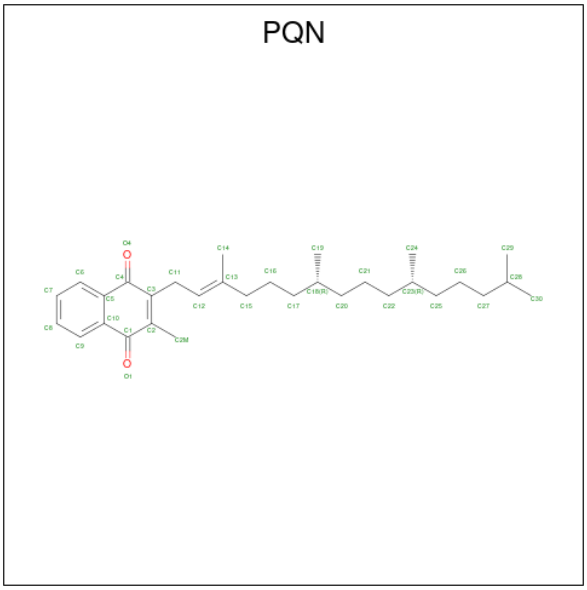
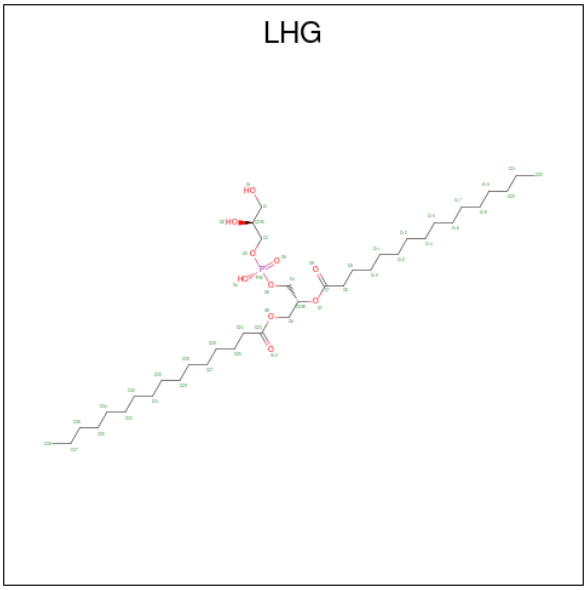
Mol	Chain	Residues	Atoms	AltConf
37	i	1	Total C 40 40	0
37	j	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	m	1	Total C 40 40	0
37	a	1	Total C 40 40	0
37	a	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	b	1	Total C 40 40	0

- Molecule 38 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
38	a	1	Total 33	C 31	O 2	0
38	b	1	Total 33	C 31	O 2	0

- Molecule 39 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

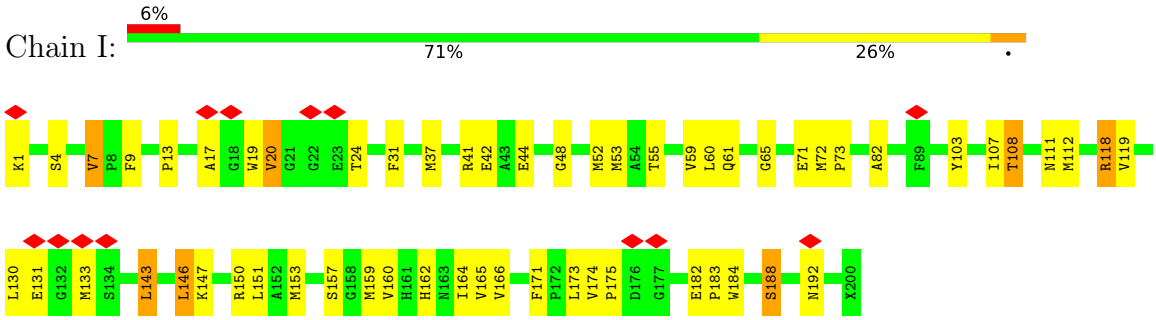


Mol	Chain	Residues	Atoms				AltConf
39	a	1	Total 48	C 37	O 10	P 1	0

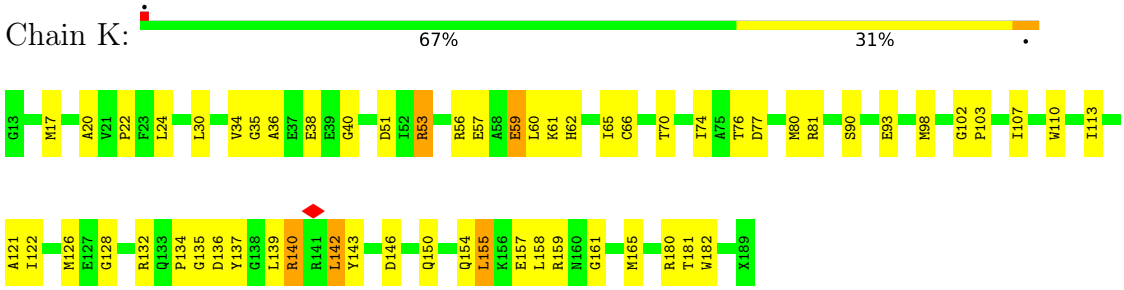
3 Residue-property plots (i)

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

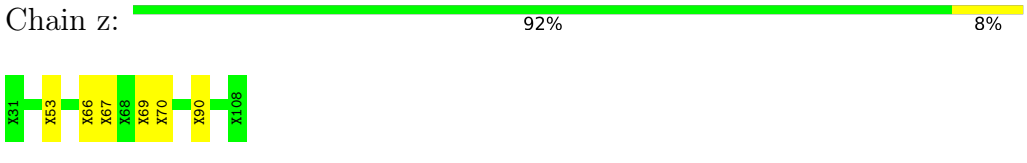
• Molecule 1: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7



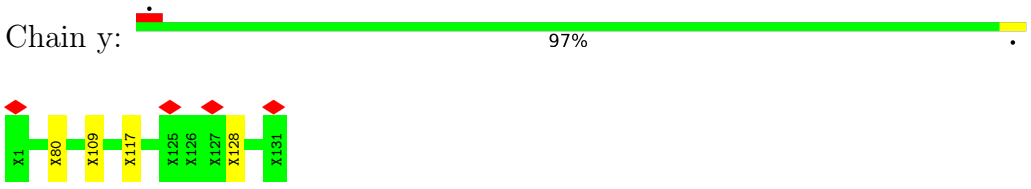
• Molecule 2: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6



• Molecule 3: Photosystem I unk

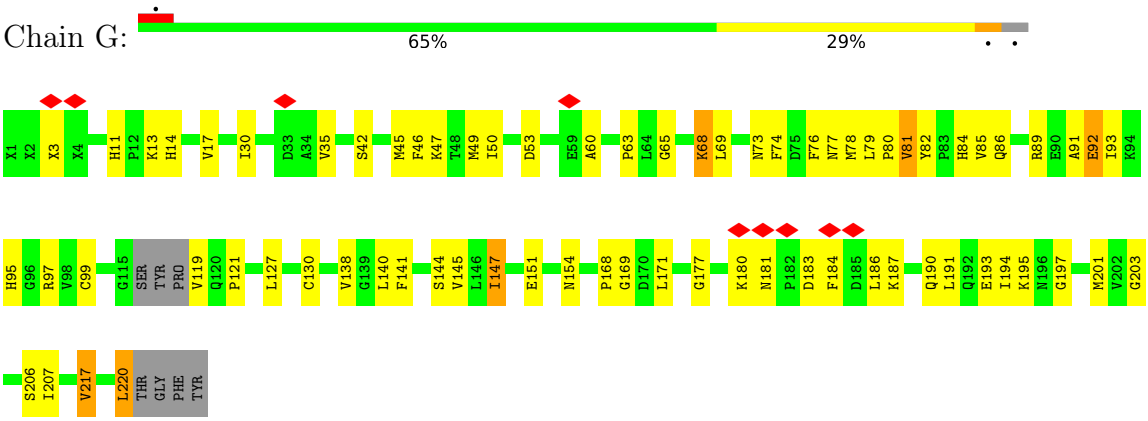


• Molecule 4: Photosystem I unk



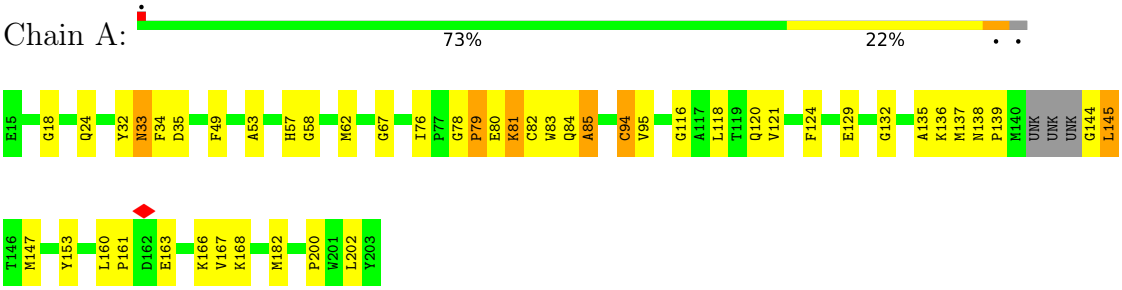
• Molecule 5: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8

Chain G:



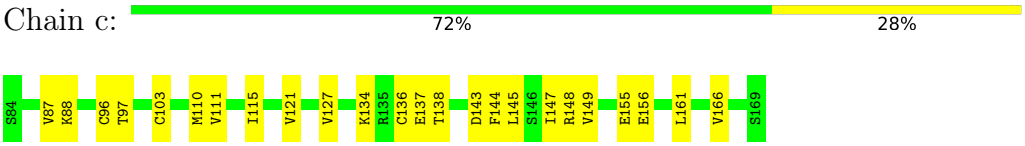
• Molecule 6: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10

Chain A:



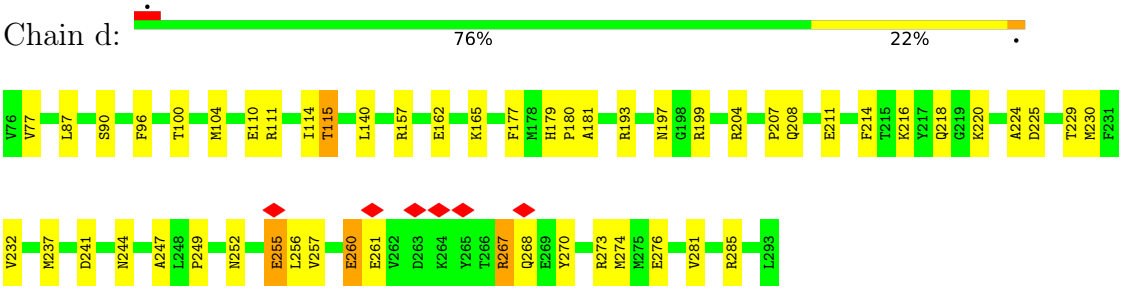
• Molecule 7: Photosystem I PsaC

Chain c:



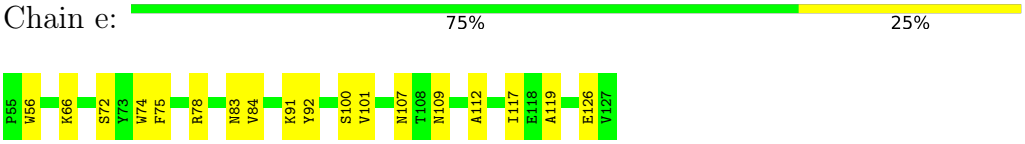
• Molecule 8: Photosystem I PsaD

Chain d:



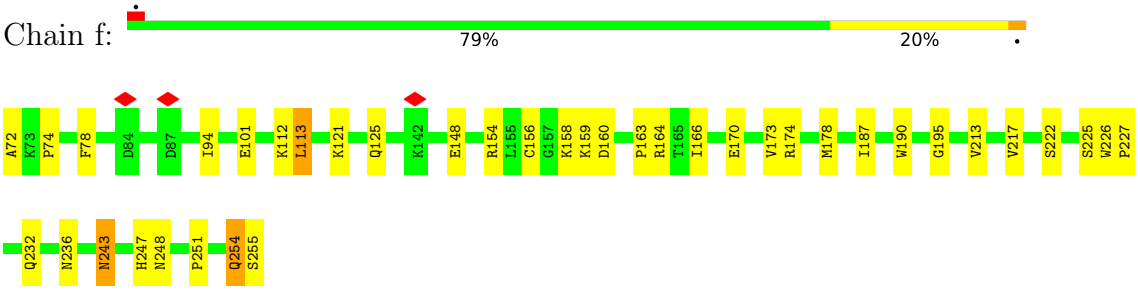
• Molecule 9: Photosystem I PsaE

Chain e:



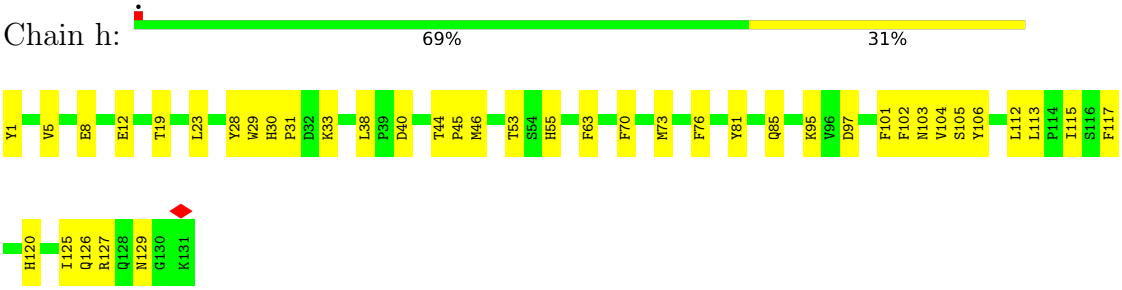
• Molecule 10: Photosystem I PsaF

Chain f:



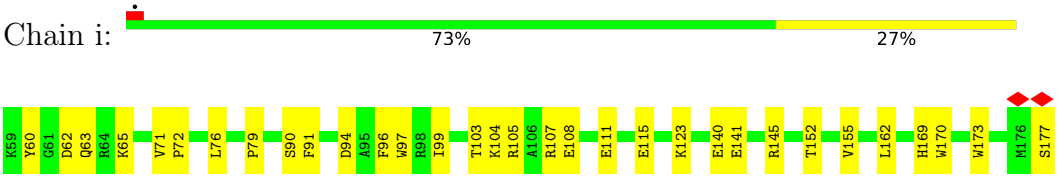
• Molecule 11: Photosystem I PsaR

Chain h:



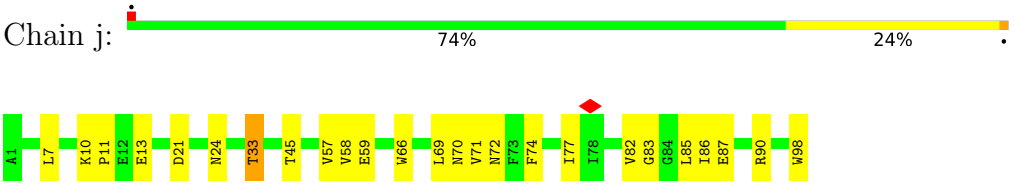
• Molecule 12: Photosystem I PsaI

Chain i:



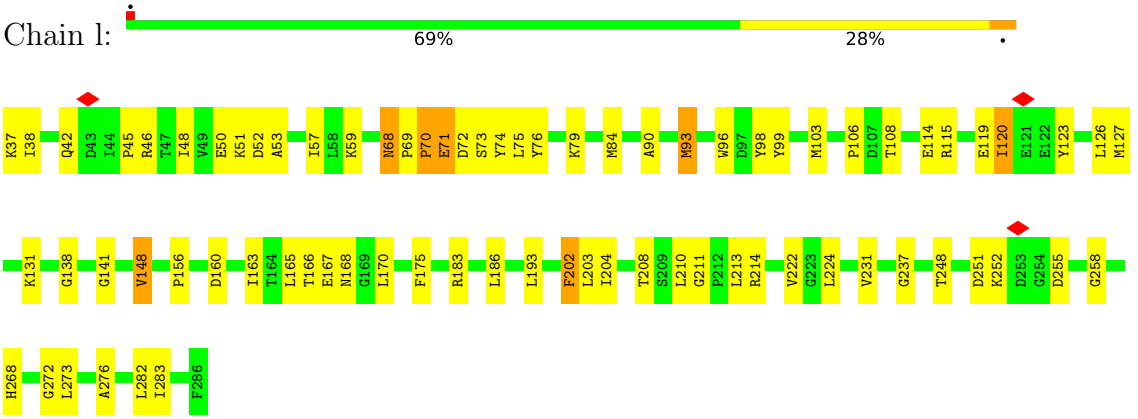
• Molecule 13: Photosystem I PsaJ

Chain j:



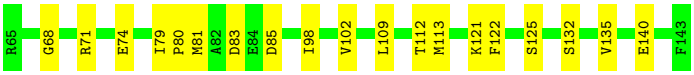
• Molecule 14: Photosystem I PsaL

Chain l:



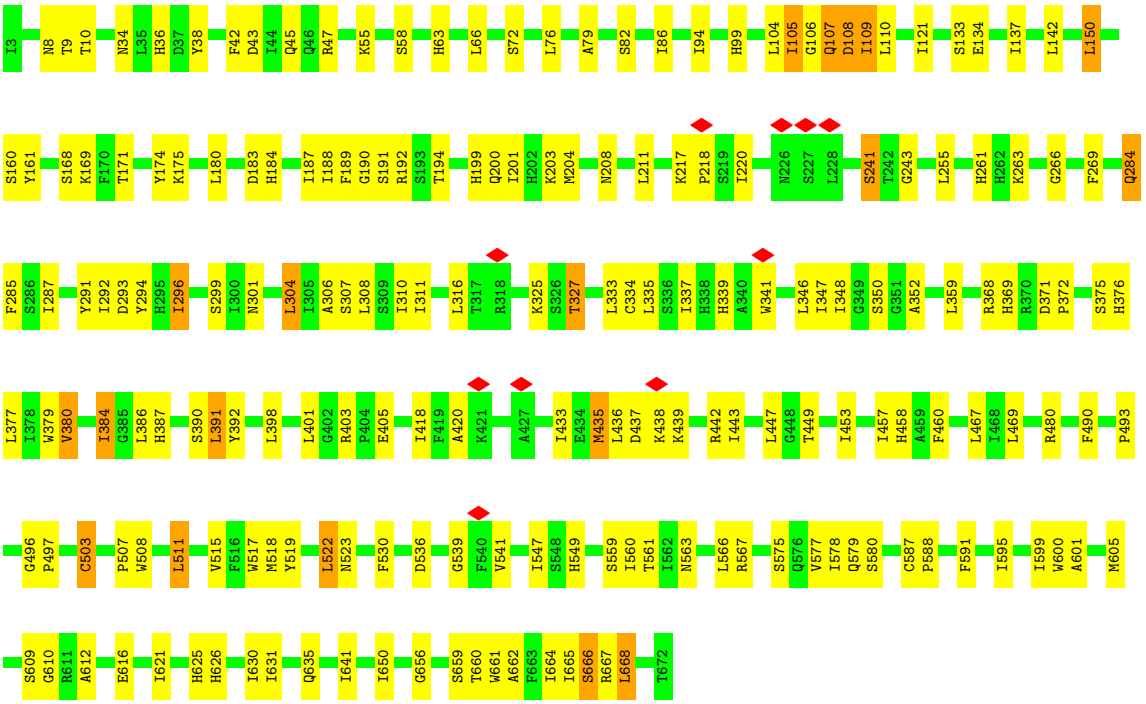
• Molecule 15: Photosystem I PsaM

Chain m:



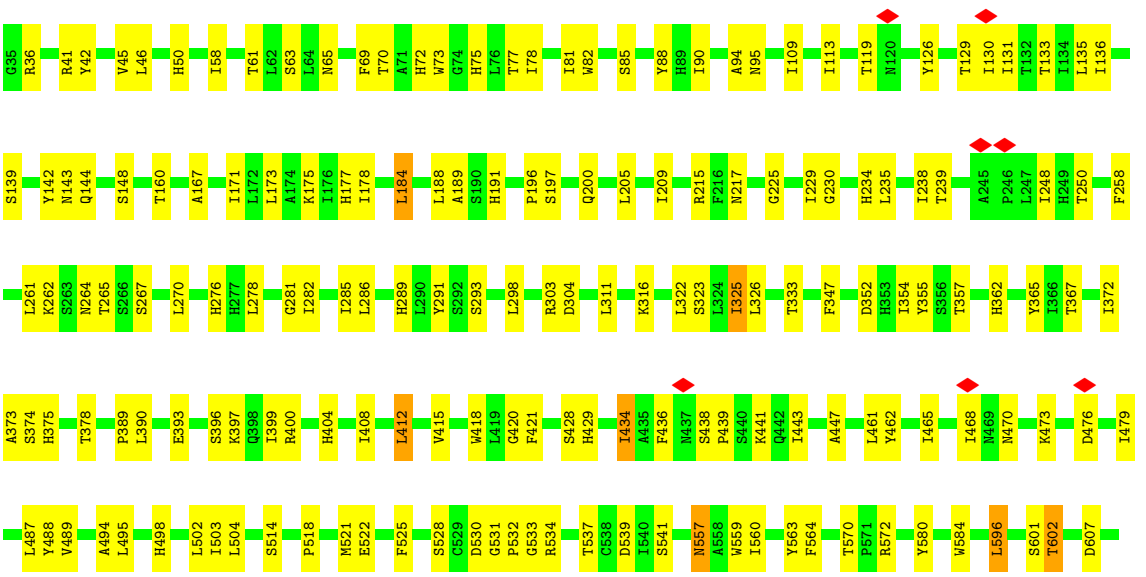
• Molecule 16: Photosystem I PsaA

Chain a:



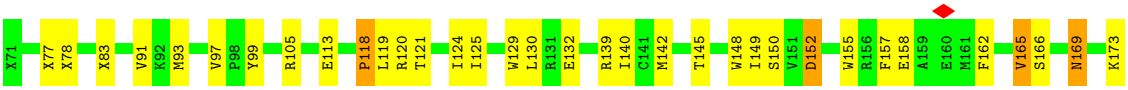
• Molecule 17: Photosystem I PsaB

Chain b:



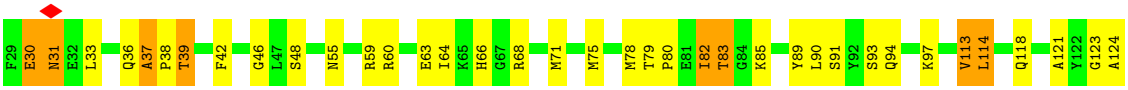
• Molecule 18: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11

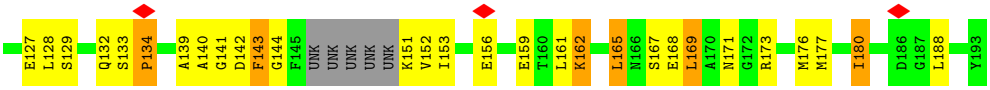
Chain B:



• Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9

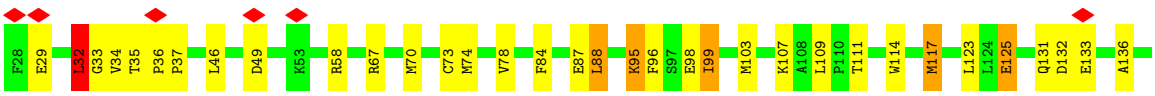
Chain D:

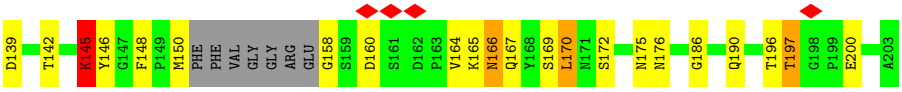




• Molecule 20: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2

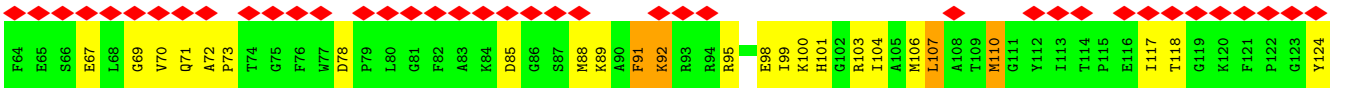
Chain F:

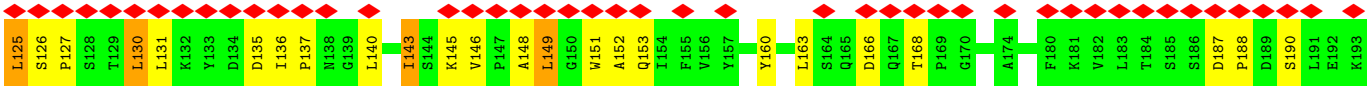


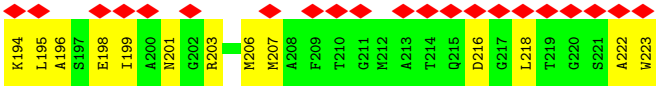


• Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12

Chain H:

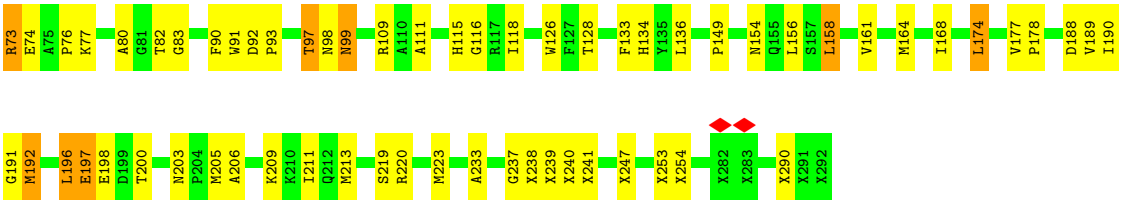






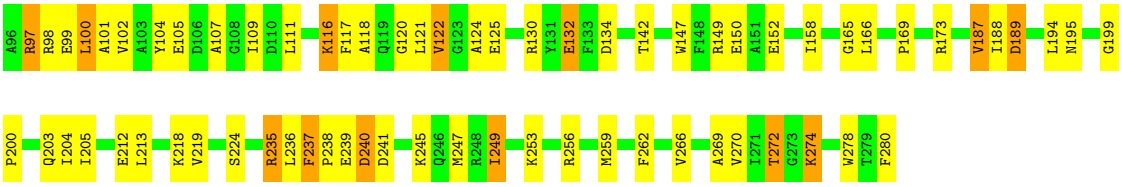
• Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3

Chain J:



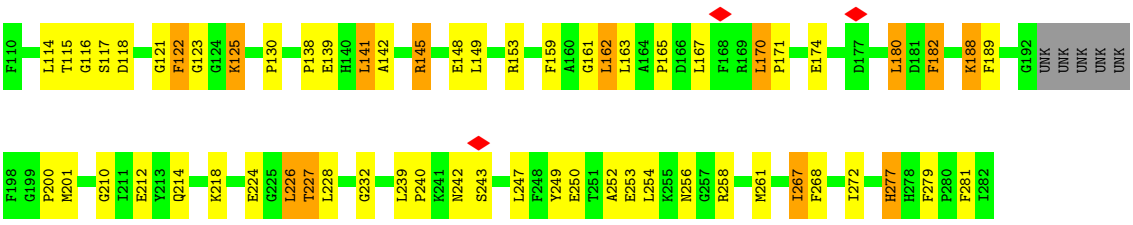
• Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5

Chain L:



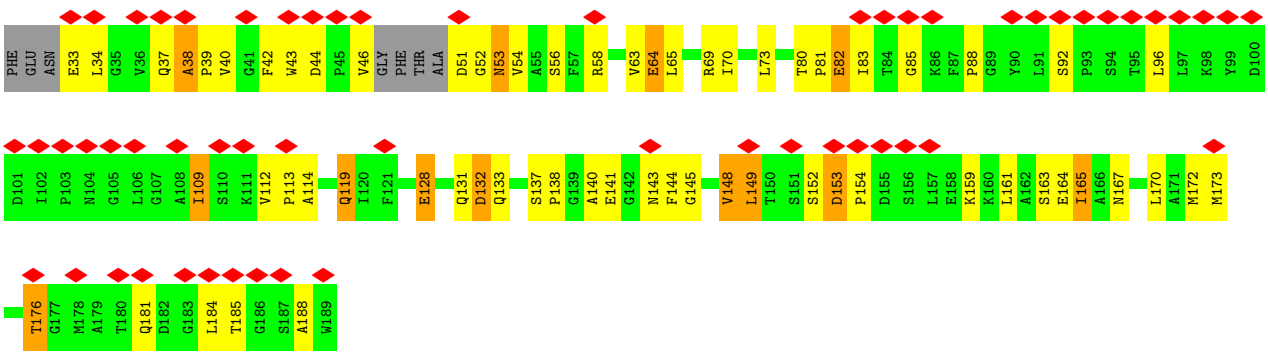
• Molecule 24: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4

Chain M:



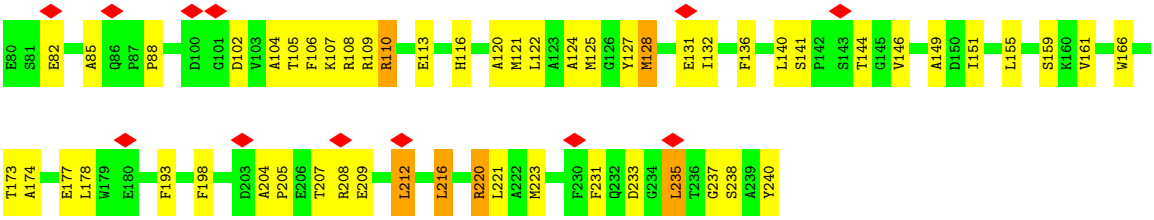
• Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13

Chain N:



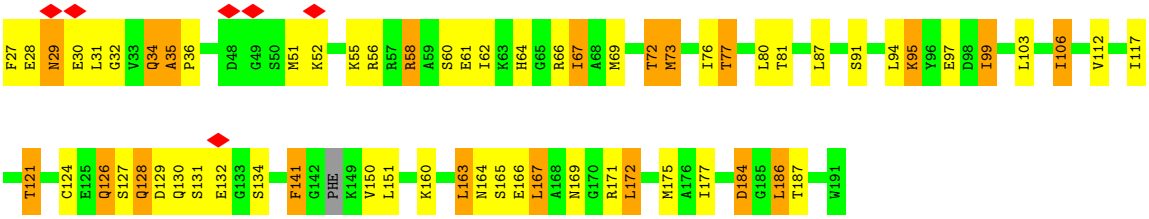
• Molecule 26: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15

Chain O:



• Molecule 27: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46321	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	1.690	Depositor
Minimum map value	-0.344	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.235	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, DGD, DD6, LMG, PID, LHG, SF4, CLA, SQD, KC1, PQN, UIX

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	I	0.13	0/1484	0.33	0/2019
2	K	0.14	0/1357	0.33	1/1838 (0.1%)
5	G	0.35	0/1562	0.52	1/2122 (0.0%)
6	A	0.37	0/1276	0.53	0/1725
7	c	0.12	0/663	0.31	0/902
8	d	0.11	0/1767	0.30	0/2375
9	e	0.24	0/608	0.29	0/833
10	f	0.16	0/1489	0.33	0/2016
11	h	0.12	0/1101	0.27	0/1493
12	i	0.17	0/992	0.32	0/1346
13	j	0.14	0/801	0.31	0/1092
14	l	0.20	0/1998	0.35	0/2706
15	m	0.13	0/590	0.29	0/793
16	a	0.26	0/5344	0.41	2/7280 (0.0%)
17	b	0.19	0/5362	0.33	0/7335
18	B	0.17	0/1382	0.36	1/1862 (0.1%)
19	D	0.25	0/1178	0.47	0/1592
20	F	0.24	0/1263	0.54	4/1708 (0.2%)
21	H	0.19	0/1232	0.42	1/1665 (0.1%)
22	J	0.17	0/1246	0.39	0/1699
23	L	0.24	0/1462	0.43	0/1985
24	M	0.20	0/1241	0.35	0/1681
25	N	0.23	0/1005	0.51	0/1370
26	O	0.12	0/1091	0.40	0/1491
27	P	0.28	0/1128	0.45	0/1523
All	All	0.22	0/38622	0.39	10/52451 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	145	LYS	N-CA-C	8.92	123.26	112.38
16	a	391	LEU	N-CA-C	-6.93	103.78	111.82
21	H	110	MET	N-CA-C	-6.54	104.15	111.28
20	F	148	PHE	CA-C-N	-6.02	113.74	119.76
20	F	148	PHE	C-N-CA	-6.02	113.74	119.76
20	F	146	TYR	N-CA-C	-5.99	104.42	113.89
16	a	82	SER	N-CA-C	5.82	118.03	109.24
2	K	38	GLU	N-CA-C	-5.74	108.08	114.62
18	B	118	PRO	N-CA-C	-5.54	101.05	112.47
5	G	68	LYS	N-CA-C	5.47	119.44	112.87

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	I	1480	0	1381	53	0
2	K	1349	0	1323	54	0
3	z	390	0	87	4	0
4	y	655	0	136	3	0
5	G	1572	0	1440	51	0
6	A	1346	0	1242	40	0
7	c	653	0	629	22	0
8	d	1731	0	1741	42	0
9	e	587	0	575	17	0
10	f	1450	0	1437	30	0
11	h	1066	0	1018	33	0
12	i	964	0	941	25	0
13	j	783	0	774	22	0
14	l	1943	0	1919	65	0
15	m	582	0	603	15	0
16	a	5194	0	5023	159	0
17	b	5199	0	5053	172	0
18	B	1452	0	1368	40	0
19	D	1158	0	1114	53	0
20	F	1237	0	1188	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	H	1202	0	1182	47	0
22	J	1496	0	1233	47	0
23	L	1427	0	1392	51	0
24	M	1211	0	1090	43	0
25	N	993	0	844	39	0
26	O	1073	0	956	37	0
27	P	1113	0	1050	49	0
28	A	172	0	0	2	0
28	B	171	0	0	1	0
28	D	43	0	0	0	0
28	F	86	0	0	1	0
28	G	172	0	0	5	0
28	H	43	0	0	1	0
28	I	172	0	0	2	0
28	J	129	0	0	5	0
28	K	215	0	0	0	0
28	L	215	0	0	2	0
28	M	215	0	0	2	0
28	N	43	0	0	0	0
28	O	43	0	0	0	0
28	P	43	0	0	0	0
28	b	43	0	0	0	0
28	h	43	0	0	0	0
29	A	47	0	0	1	0
29	B	47	0	0	0	0
29	G	47	0	0	0	0
29	I	47	0	0	2	0
29	J	47	0	0	1	0
29	K	47	0	0	1	0
29	O	47	0	0	0	0
29	P	47	0	0	0	0
29	h	47	0	0	0	0
30	A	597	0	493	23	0
30	B	587	0	532	20	0
30	D	317	0	229	18	0
30	F	317	0	227	22	0
30	G	592	0	530	22	0
30	H	343	0	278	15	0
30	I	637	0	554	31	0
30	J	552	0	456	29	0
30	K	496	0	398	18	0
30	L	503	0	411	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	M	481	0	370	19	0
30	N	256	0	216	10	0
30	O	297	0	245	14	0
30	P	297	0	245	18	0
30	a	1870	0	1786	110	0
30	b	1563	0	1526	106	0
30	f	147	0	115	10	0
30	h	55	0	49	0	0
30	j	113	0	104	8	0
30	l	493	0	471	25	0
30	m	60	0	59	2	0
31	A	90	0	0	0	0
31	B	45	0	0	0	0
31	D	90	0	0	1	0
31	F	90	0	0	2	0
31	G	45	0	0	0	0
31	H	90	0	0	1	0
31	I	45	0	0	0	0
31	J	45	0	0	0	0
31	K	45	0	0	0	0
31	L	90	0	0	0	0
31	M	90	0	0	1	0
31	N	135	0	0	1	0
31	O	135	0	0	4	0
31	P	135	0	0	1	0
32	G	89	0	94	2	0
32	I	39	0	36	0	0
32	L	38	0	34	2	0
32	j	41	0	40	3	0
32	l	50	0	58	0	0
32	y	54	0	66	1	0
33	B	37	0	44	1	0
33	D	49	0	64	5	0
33	I	74	0	88	2	0
33	K	43	0	56	0	0
33	P	27	0	24	0	0
33	b	75	0	90	5	0
33	j	35	0	40	4	0
34	D	276	0	300	12	0
34	F	184	0	200	13	0
34	G	92	0	100	6	0
34	H	92	0	100	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	M	46	0	50	1	0
34	N	92	0	100	4	0
34	O	230	0	250	23	0
34	P	230	0	250	17	0
34	j	46	0	50	4	0
35	A	50	0	64	8	0
36	a	8	0	0	1	0
36	c	16	0	0	2	0
37	a	80	0	112	5	0
37	b	120	0	168	15	0
37	f	40	0	56	4	0
37	i	40	0	56	7	0
37	j	40	0	56	5	0
37	l	120	0	168	10	0
37	m	40	0	56	4	0
38	a	33	0	46	5	0
38	b	33	0	46	4	0
39	a	48	0	69	3	0
All	All	55927	0	49064	1485	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 14.

All (1485) 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)
10:f:72:ALA:N	17:b:462:TYR:HH	1.46	1.12
30:K:308:CLA:H2A	30:K:308:CLA:HED3	1.53	0.88
17:b:468:ILE:HG22	17:b:470:ASN:H	1.36	0.87
30:b:712:CLA:H12	18:B:124:ILE:HD11	1.56	0.87
26:O:221:LEU:HG	34:O:305:PID:H13	1.56	0.87
34:O:305:PID:HM52	30:O:314:CLA:HHC	1.58	0.85
6:A:144:GLY:N	35:A:318:SQD:HO3	1.75	0.84
18:B:124:ILE:HG21	30:B:301:CLA:HHB	1.61	0.82
30:a:707:CLA:HBB1	30:a:723:CLA:HAB	1.60	0.80
22:J:116:GLY:HA3	22:J:219:SER:HB2	1.62	0.80
34:O:305:PID:HM52	30:O:314:CLA:CHC	2.13	0.79
30:a:714:CLA:H3A	37:a:734:BCR:H332	1.64	0.78
16:a:359:LEU:HD13	16:a:490:PHE:HA	1.65	0.78
6:A:144:GLY:N	35:A:318:SQD:HO2	1.82	0.78
24:M:115:THR:HG21	24:M:250:GLU:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:160:LEU:HD13	30:A:313:CLA:HAA2	1.66	0.77
10:f:159:LYS:HD3	17:b:572:ARG:HH12	1.50	0.77
30:G:517:CLA:HBB1	11:h:76:PHE:HE2	1.49	0.77
5:G:130:CYS:HB3	5:G:140:LEU:HD21	1.68	0.76
1:I:20:VAL:HG21	1:I:146:LEU:HG	1.69	0.75
30:a:730:CLA:HAB	30:a:730:CLA:H122	1.68	0.74
1:I:159:MET:HG2	29:I:304:UIX:C9	2.18	0.74
26:O:125:MET:HA	26:O:128:MET:HE2	1.70	0.73
30:b:709:CLA:HBB1	30:b:709:CLA:HHC	1.71	0.73
27:P:124:CYS:O	27:P:129:ASP:HB2	1.89	0.73
10:f:94:ILE:HG12	10:f:166:ILE:HD12	1.71	0.72
30:G:519:CLA:O1D	11:h:127:ARG:NH2	2.23	0.72
14:l:160:ASP:O	17:b:649:LYS:NZ	2.22	0.72
6:A:76:ILE:HB	6:A:83:TRP:CZ3	2.25	0.71
34:G:507:PID:HM83	34:G:507:PID:HM51	1.72	0.71
9:e:91:LYS:HA	11:h:5:VAL:HG21	1.72	0.71
7:c:97:THR:HA	7:c:110:MET:HE3	1.72	0.71
30:b:704:CLA:CGA	30:b:704:CLA:H3A	2.20	0.71
27:P:127:SER:C	27:P:129:ASP:H	1.98	0.71
6:A:79:PRO:O	6:A:83:TRP:HD1	1.74	0.70
22:J:83:GLY:HA2	22:J:220:ARG:HH12	1.56	0.70
2:K:180:ARG:NH1	2:K:181:THR:OG1	2.24	0.70
25:N:149:LEU:HD13	25:N:149:LEU:H	1.55	0.70
18:B:221:PRO:HB2	18:B:226:LYS:HB3	1.73	0.70
19:D:55:ASN:HD21	19:D:59:ARG:HE	1.40	0.69
22:J:98:ASN:O	22:J:99:ASN:ND2	2.24	0.69
24:M:162:LEU:HD13	24:M:267:ILE:HG21	1.74	0.69
8:d:257:VAL:HG13	17:b:191:HIS:HA	1.75	0.69
17:b:610:VAL:HG22	30:b:710:CLA:HAC1	1.74	0.69
21:H:100:LYS:HG3	34:H:302:PID:H41	1.72	0.69
30:a:716:CLA:CGA	30:a:721:CLA:HBB2	2.23	0.69
18:B:129:TRP:HE1	18:B:202:LEU:HD22	1.58	0.69
28:G:504:DD6:C24	30:G:510:CLA:HAB	2.23	0.68
16:a:110:LEU:HD22	16:a:588:PRO:HG3	1.75	0.68
2:K:53:ARG:HH21	2:K:126:MET:HA	1.58	0.68
21:H:218:LEU:HB3	30:H:311:CLA:HED1	1.73	0.68
27:P:165:SER:O	27:P:169:ASN:ND2	2.23	0.68
8:d:214:PHE:H	8:d:218:GLN:HG2	1.57	0.68
18:B:233:LYS:O	18:B:237:ASN:ND2	2.23	0.68
34:F:305:PID:H17	34:F:305:PID:HM41	1.76	0.68
15:m:79:ILE:HD11	17:b:109:ILE:HG12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:209:ILE:O	17:b:215:ARG:NH2	2.27	0.68
19:D:30:GLU:O	19:D:31:ASN:ND2	2.27	0.68
8:d:204:ARG:NH2	17:b:522:GLU:OE2	2.26	0.67
16:a:306:ALA:HB2	16:a:346:LEU:HB2	1.75	0.67
8:d:157:ARG:NH1	8:d:162:GLU:OE1	2.27	0.67
23:L:147:TRP:HH2	30:L:313:CLA:HAA2	1.58	0.67
8:d:211:GLU:HG2	8:d:232:VAL:HB	1.76	0.67
13:j:87:GLU:OE1	13:j:90:ARG:NH2	2.28	0.67
18:B:243:LEU:HD13	28:B:302:DD6:C26	2.24	0.67
16:a:563:ASN:OD1	16:a:567:ARG:NH1	2.27	0.67
17:b:530:ASP:OD2	17:b:534:ARG:NH2	2.27	0.67
18:B:124:ILE:HG23	18:B:125:ILE:HG13	1.75	0.67
34:F:304:PID:H7	30:F:315:CLA:HMB2	1.77	0.67
28:J:304:DD6:C24	30:J:307:CLA:HAB	2.25	0.67
30:b:704:CLA:H43	30:b:704:CLA:HMB3	1.77	0.67
30:a:735:CLA:HHB	30:b:703:CLA:H192	1.75	0.67
8:d:256:LEU:HD21	18:B:78:UNK:HA	1.75	0.66
30:b:712:CLA:H42	18:B:124:ILE:HG12	1.76	0.66
13:j:24:ASN:ND2	23:L:105:GLU:OE2	2.27	0.66
12:i:141:GLU:OE2	12:i:145:ARG:NH2	2.28	0.66
16:a:72:SER:HB2	16:a:150:LEU:HD22	1.77	0.66
25:N:163:SER:O	25:N:167:ASN:ND2	2.27	0.66
6:A:82:CYS:SG	6:A:83:TRP:N	2.68	0.66
25:N:92:SER:H	25:N:96:LEU:HA	1.61	0.66
17:b:528:SER:HB3	17:b:669:ILE:HD12	1.78	0.66
20:F:88:LEU:HG	20:F:109:LEU:HD11	1.76	0.66
22:J:97:THR:HG22	30:J:307:CLA:HBA1	1.77	0.66
5:G:97:ARG:NH1	5:G:193:GLU:OE2	2.29	0.66
9:e:101:VAL:HG12	9:e:107:ASN:HB3	1.78	0.66
24:M:252:ALA:O	24:M:256:ASN:ND2	2.22	0.66
2:K:76:THR:O	2:K:81:ARG:NH1	2.28	0.66
11:h:95:LYS:NZ	11:h:101:PHE:O	2.25	0.66
30:a:704:CLA:H193	30:b:710:CLA:H2	1.77	0.66
23:L:149:ARG:NH1	23:L:152:GLU:OE1	2.28	0.66
22:J:82:THR:HG21	22:J:109:ARG:HH12	1.61	0.65
34:O:305:PID:H16	31:O:315:KC1:CAB	2.26	0.65
26:O:140:LEU:HD21	26:O:161:VAL:HG13	1.79	0.65
5:G:181:ASN:HB2	5:G:184:PHE:HB2	1.79	0.65
22:J:128:THR:HG21	30:J:309:CLA:HAC2	1.78	0.65
8:d:100:THR:O	16:a:480:ARG:NH2	2.30	0.65
5:G:50:ILE:O	5:G:89:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:307:SER:O	16:a:311:ILE:HG12	1.97	0.65
30:l:313:CLA:H51	30:a:720:CLA:HBB2	1.79	0.65
16:a:519:TYR:O	16:a:523:ASN:ND2	2.21	0.65
21:H:100:LYS:HZ3	34:H:302:PID:H42	1.62	0.65
25:N:112:VAL:O	25:N:114:ALA:N	2.26	0.65
5:G:177:GLY:HA2	5:G:180:LYS:HG3	1.77	0.65
22:J:233:ALA:HA	22:J:237:GLY:O	1.97	0.65
24:M:227:THR:OG1	24:M:228:LEU:N	2.30	0.65
35:A:318:SQD:H241	35:A:318:SQD:H91	1.78	0.65
16:a:379:TRP:HB2	30:b:701:CLA:HED2	1.79	0.65
17:b:72:HIS:ND1	30:b:713:CLA:OBD	2.29	0.65
27:P:60:SER:O	27:P:64:HIS:ND1	2.27	0.65
17:b:286:LEU:HD23	37:b:730:BCR:H14C	1.79	0.64
34:P:202:PID:HM22	30:P:210:CLA:HAC2	1.78	0.64
30:A:319:CLA:HAB	17:b:230:GLY:HA2	1.80	0.64
16:a:86:ILE:HG13	16:a:94:ILE:HG13	1.79	0.64
30:b:703:CLA:H41	30:b:703:CLA:H102	1.79	0.64
24:M:161:GLY:O	24:M:165:PRO:HD2	1.97	0.64
8:d:252:ASN:ND2	8:d:255:GLU:OE1	2.20	0.64
18:B:118:PRO:C	18:B:120:ARG:H	2.06	0.64
19:D:33:LEU:O	19:D:60:ARG:NH2	2.31	0.64
2:K:57:GLU:OE1	2:K:132:ARG:NH2	2.31	0.63
30:A:312:CLA:H12	35:A:318:SQD:H322	1.78	0.63
16:a:293:ASP:HB3	16:a:296:ILE:HG22	1.80	0.63
24:M:142:ALA:HB1	24:M:226:LEU:HD22	1.79	0.63
6:A:160:LEU:HG	6:A:167:VAL:HG12	1.81	0.63
17:b:50:HIS:ND1	30:b:707:CLA:O1A	2.32	0.63
2:K:53:ARG:NH1	32:j:103:DGD:O5E	2.31	0.63
13:j:90:ARG:HD3	34:j:105:PID:H41	1.80	0.63
23:L:256:ARG:HA	23:L:259:MET:HE3	1.80	0.63
24:M:182:PHE:HE2	24:M:268:PHE:HA	1.63	0.63
10:f:72:ALA:N	17:b:462:TYR:OH	2.26	0.63
21:H:135:ASP:O	21:H:145:LYS:NZ	2.31	0.63
1:I:65:GLY:HA2	30:I:310:CLA:HMD1	1.81	0.63
30:b:709:CLA:H43	30:b:720:CLA:H11	1.80	0.63
21:H:151:TRP:HB3	30:H:312:CLA:HMC1	1.80	0.63
2:K:70:THR:O	2:K:74:ILE:HG12	1.99	0.63
16:a:591:PHE:O	16:a:595:ILE:HG12	1.99	0.63
16:a:201:ILE:HD13	30:J:301:CLA:HBC2	1.81	0.62
2:K:132:ARG:NH1	2:K:136:ASP:O	2.30	0.62
17:b:270:LEU:HD11	17:b:347:PHE:HZ	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:626:PHE:HB3	30:b:704:CLA:HMC2	1.81	0.62
25:N:132:ASP:OD1	25:N:132:ASP:N	2.28	0.62
16:a:334:CYS:HB3	30:a:722:CLA:HMA1	1.81	0.62
14:l:204:ILE:HD12	14:l:224:LEU:HA	1.82	0.62
23:L:240:ASP:OD1	23:L:240:ASP:N	2.32	0.62
16:a:377:LEU:HD22	30:a:729:CLA:HBB1	1.82	0.62
14:l:53:ALA:HB2	14:l:108:THR:HG22	1.82	0.62
18:B:246:SER:HB2	30:B:315:CLA:HMC2	1.81	0.62
14:l:126:LEU:HD22	14:l:131:LYS:HB2	1.80	0.62
22:J:73:ARG:HG2	22:J:76:PRO:HB2	1.80	0.62
24:M:117:SER:HB2	24:M:125:LYS:HG3	1.82	0.62
18:B:220:LEU:HD12	18:B:221:PRO:HD2	1.81	0.62
16:a:458:HIS:HB3	30:a:727:CLA:HAB	1.82	0.61
30:l:303:CLA:HAA2	30:F:312:CLA:HBA1	1.81	0.61
19:D:66:HIS:NE2	31:D:310:KC1:ND	2.48	0.61
30:l:311:CLA:H201	22:J:174:LEU:HD12	1.83	0.61
30:b:704:CLA:HBC3	30:b:704:CLA:HHD	1.82	0.61
19:D:167:SER:O	19:D:171:ASN:ND2	2.27	0.61
23:L:122:VAL:O	23:L:149:ARG:NH2	2.32	0.61
24:M:159:PHE:HA	24:M:162:LEU:HD12	1.83	0.61
1:I:108:THR:HG23	10:f:222:SER:HB3	1.83	0.61
2:K:159:ARG:NH1	30:K:307:CLA:O1D	2.34	0.61
30:G:511:CLA:HBC1	30:G:513:CLA:HAC1	1.83	0.61
15:m:122:PHE:HB2	17:b:189:ALA:HB2	1.82	0.61
18:B:174:MET:HB3	18:B:180:MET:HG2	1.82	0.61
16:a:243:GLY:O	16:a:442:ARG:NH2	2.32	0.61
6:A:32:TYR:O	6:A:33:ASN:C	2.44	0.61
16:a:104:LEU:HG	16:a:105:ILE:HG23	1.82	0.61
16:a:107:GLN:O	16:a:110:LEU:HG	2.01	0.61
30:a:702:CLA:NA	30:b:703:CLA:HAB	2.16	0.60
20:F:131:GLN:NE2	20:F:132:ASP:O	2.34	0.60
22:J:220:ARG:HA	22:J:223:MET:HE3	1.82	0.60
13:j:59:GLU:HB3	33:j:101:LMG:HC61	1.84	0.60
17:b:610:VAL:HG11	30:b:709:CLA:HAC1	1.83	0.60
25:N:141:GLU:HG3	25:N:143:ASN:H	1.67	0.60
30:I:316:CLA:CHA	30:I:316:CLA:HBA1	2.32	0.60
14:l:210:LEU:HD11	30:a:725:CLA:HBB2	1.83	0.60
17:b:412:LEU:HG	17:b:502:LEU:HB2	1.83	0.60
20:F:88:LEU:HD23	20:F:99:ILE:HD13	1.83	0.60
5:G:127:LEU:HD23	34:G:507:PID:HM23	1.83	0.60
5:G:138:VAL:HB	19:D:113:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:309:CLA:HAC1	30:A:316:CLA:HAB	1.82	0.60
11:h:38:LEU:O	17:b:303:ARG:NH2	2.34	0.60
16:a:433:ILE:HB	16:a:443:ILE:HG22	1.84	0.60
17:b:333:THR:HB	17:b:367:THR:HB	1.84	0.60
18:B:253:ASN:HB2	30:B:317:CLA:HMA3	1.84	0.60
1:I:55:THR:HA	1:I:159:MET:HE1	1.84	0.60
15:m:81:MET:HE1	17:b:131:ILE:HG21	1.82	0.60
18:B:239:ARG:HA	18:B:242:MET:HE3	1.83	0.60
30:l:313:CLA:H193	37:a:736:BCR:H271	1.81	0.60
15:m:80:PRO:O	17:b:95:ASN:ND2	2.35	0.60
6:A:24:GLN:OE1	6:A:168:LYS:NZ	2.34	0.60
13:j:86:ILE:HD13	30:a:710:CLA:HMA3	1.83	0.60
25:N:181:GLN:NE2	25:N:188:ALA:O	2.35	0.60
14:l:103:MET:HE1	30:a:711:CLA:H2A	1.84	0.60
15:m:132:SER:HB2	15:m:135:VAL:HG23	1.82	0.60
16:a:76:LEU:HD13	30:a:708:CLA:HAC2	1.84	0.60
21:H:124:TYR:O	21:H:126:SER:N	2.34	0.59
16:a:316:LEU:O	16:a:325:LYS:NZ	2.34	0.59
24:M:121:GLY:HA3	31:M:307:KC1:O1D	2.02	0.59
27:P:128:GLN:HE22	27:P:141:PHE:HB2	1.67	0.59
8:d:241:ASP:OD2	8:d:244:ASN:ND2	2.35	0.59
18:B:183:MET:HG2	30:B:316:CLA:HBC1	1.83	0.59
34:F:305:PID:H22	31:F:309:KC1:CAA	2.33	0.59
17:b:373:ALA:HB2	30:b:722:CLA:HMC2	1.84	0.59
12:i:140:GLU:HA	12:i:155:VAL:HG21	1.84	0.59
17:b:173:LEU:O	17:b:177:HIS:ND1	2.30	0.59
17:b:258:PHE:O	17:b:473:LYS:NZ	2.34	0.59
34:D:305:PID:HM81	30:D:314:CLA:HBC3	1.84	0.59
1:I:41:ARG:NH2	30:I:308:CLA:O1D	2.33	0.59
30:b:709:CLA:HAB	30:b:710:CLA:H11	1.84	0.59
21:H:67:GLU:HG2	21:H:91:PHE:CZ	2.38	0.59
1:I:184:TRP:CE2	30:I:316:CLA:HBA2	2.37	0.59
17:b:415:VAL:HG23	30:b:725:CLA:HBB1	1.84	0.59
20:F:172:SER:O	20:F:176:ASN:ND2	2.30	0.59
2:K:56:ARG:NH1	2:K:59:GLU:OE2	2.36	0.59
27:P:127:SER:C	27:P:129:ASP:N	2.60	0.59
6:A:137:MET:HG2	6:A:145:LEU:HD22	1.85	0.58
16:a:621:ILE:HD13	30:a:730:CLA:HMD1	1.85	0.58
34:G:507:PID:HM31	30:G:517:CLA:HED3	1.86	0.58
11:h:103:ASN:OD1	11:h:105:SER:OG	2.20	0.58
30:l:303:CLA:H101	37:l:307:BCR:H363	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:99:GLU:HG3	23:L:101:ALA:H	1.69	0.58
23:L:147:TRP:CH2	30:L:313:CLA:HAA2	2.37	0.58
8:d:252:ASN:HB3	8:d:256:LEU:HD23	1.85	0.58
9:e:78:ARG:NH2	9:e:126:GLU:OE2	2.36	0.58
25:N:109:ILE:HA	25:N:114:ALA:HB3	1.85	0.58
5:G:97:ARG:NH2	5:G:169:GLY:O	2.37	0.58
14:l:120:ILE:HG12	16:a:285:PHE:CE2	2.38	0.58
11:h:117:PHE:O	11:h:120:HIS:ND1	2.36	0.58
20:F:88:LEU:HD21	30:F:310:CLA:HBA2	1.84	0.58
15:m:68:GLY:N	17:b:607:ASP:OD1	2.37	0.58
19:D:39:THR:HG21	19:D:42:PHE:HD1	1.67	0.58
24:M:189:PHE:HB2	24:M:201:MET:HG2	1.85	0.58
17:b:689:PRO:HG2	30:b:720:CLA:H2	1.86	0.58
25:N:128:GLU:CD	34:N:302:PID:HM32	2.29	0.58
5:G:46:PHE:HB2	5:G:85:VAL:HG21	1.86	0.58
20:F:170:LEU:HG	30:F:313:CLA:HMA1	1.85	0.58
25:N:172:MET:O	25:N:176:THR:OG1	2.21	0.58
26:O:106:PHE:O	26:O:110:ARG:HB3	2.03	0.58
6:A:84:GLN:O	6:A:85:ALA:HB3	2.04	0.57
10:f:78:PHE:CG	17:b:479:ILE:HD11	2.39	0.57
14:l:46:ARG:HH22	23:L:142:THR:H	1.51	0.57
30:l:312:CLA:HAB	30:a:729:CLA:HAB	1.86	0.57
20:F:125:GLU:HG2	30:F:312:CLA:C1B	2.34	0.57
30:N:310:CLA:HED2	30:N:310:CLA:HBA1	1.85	0.57
6:A:35:ASP:OD1	28:A:303:DD6:O2	2.22	0.57
15:m:121:LYS:HE2	15:m:125:SER:HB2	1.87	0.57
25:N:148:VAL:O	25:N:154:PRO:HD2	2.04	0.57
25:N:159:LYS:O	25:N:163:SER:N	2.34	0.57
26:O:131:GLU:HG3	26:O:240:TYR:HE2	1.69	0.57
5:G:92:GLU:HG2	30:G:510:CLA:C1B	2.34	0.57
16:a:390:SER:HB2	30:a:726:CLA:HHC	1.86	0.57
16:a:460:PHE:CE1	30:b:704:CLA:HBA2	2.40	0.57
20:F:145:LYS:HA	30:F:313:CLA:HAA1	1.86	0.57
30:I:311:CLA:H62	32:G:501:DGD:HG12	1.86	0.57
16:a:503:CYS:HB3	36:a:737:SF4:S4	2.44	0.57
19:D:173:ARG:HA	19:D:176:MET:HE3	1.85	0.57
30:J:301:CLA:HBA2	32:L:301:DGD:HD61	1.85	0.57
1:I:20:VAL:HG11	1:I:146:LEU:HD23	1.85	0.57
25:N:65:LEU:O	25:N:69:ARG:HG2	2.04	0.57
25:N:170:LEU:HD23	34:N:301:PID:HM31	1.86	0.57
2:K:143:TYR:CD1	30:K:313:CLA:HAA2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:138:THR:HG22	17:b:533:GLY:HA3	1.87	0.57
16:a:433:ILE:HD13	16:a:547:ILE:HD11	1.85	0.57
20:F:186:GLY:O	20:F:190:GLN:HG2	2.05	0.57
1:I:153:MET:HE1	30:I:308:CLA:HHC	1.87	0.57
2:K:107:ILE:HG22	30:K:316:CLA:HBC1	1.87	0.57
13:j:74:PHE:HA	13:j:77:ILE:HG22	1.87	0.57
34:D:305:PID:H20	30:D:314:CLA:HBB1	1.87	0.57
26:O:233:ASP:HA	26:O:238:SER:O	2.05	0.57
11:h:45:PRO:O	11:h:53:THR:OG1	2.20	0.57
16:a:294:TYR:HB3	30:a:706:CLA:HAC1	1.87	0.57
18:B:220:LEU:HD13	30:B:313:CLA:HAA2	1.87	0.57
12:i:99:ILE:HD12	17:b:45:VAL:HG13	1.85	0.57
26:O:136:PHE:HB3	26:O:149:ALA:HA	1.87	0.57
14:l:204:ILE:HD11	14:l:276:ALA:HB1	1.87	0.56
30:l:304:CLA:HAC2	37:l:306:BCR:H24C	1.87	0.56
17:b:640:ILE:HD11	37:b:732:BCR:H282	1.86	0.56
1:I:4:SER:HB3	1:I:13:PRO:HD3	1.86	0.56
2:K:62:HIS:HB3	2:K:165:MET:HE3	1.87	0.56
14:l:127:MET:HE3	16:a:368:ARG:HH12	1.68	0.56
16:a:304:LEU:HD22	30:a:719:CLA:HAA1	1.87	0.56
30:A:317:CLA:CBB	30:A:320:CLA:HBB1	2.35	0.56
16:a:335:LEU:O	16:a:339:HIS:ND1	2.35	0.56
16:a:610:GLY:N	17:b:539:ASP:OD2	2.38	0.56
17:b:525:PHE:O	17:b:541:SER:OG	2.23	0.56
20:F:46:LEU:HB3	20:F:58:ARG:HH12	1.70	0.56
22:J:177:VAL:HB	22:J:178:PRO:HD3	1.87	0.56
23:L:189:ASP:OD1	23:L:189:ASP:N	2.34	0.56
5:G:13:LYS:HG3	9:e:117:ILE:HG12	1.87	0.56
13:j:7:LEU:HD23	13:j:21:ASP:HA	1.86	0.56
20:F:74:MET:HB2	30:F:310:CLA:HMC2	1.87	0.56
26:O:220:ARG:HA	26:O:223:MET:HE3	1.88	0.56
27:P:29:ASN:OD1	27:P:29:ASN:N	2.39	0.56
27:P:30:GLU:O	27:P:58:ARG:NH2	2.39	0.56
27:P:66:ARG:HA	27:P:69:MET:HE3	1.88	0.56
16:a:333:LEU:HD21	16:a:664:ILE:HB	1.87	0.56
17:b:139:SER:HA	30:b:720:CLA:HMA2	1.88	0.56
30:b:712:CLA:C4D	30:b:712:CLA:H11	2.36	0.56
30:b:712:CLA:H92	30:B:301:CLA:HMB3	1.87	0.56
34:O:302:PID:HM12	30:O:314:CLA:HAC2	1.86	0.56
11:h:28:TYR:HB3	11:h:33:LYS:HZ1	1.71	0.56
11:h:125:ILE:O	11:h:129:ASN:ND2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:118:ALA:HB3	30:L:309:CLA:HED1	1.88	0.56
27:P:117:ILE:O	27:P:121:THR:OG1	2.20	0.56
39:a:733:LHG:O2	39:a:733:LHG:O4	2.22	0.56
23:L:158:ILE:HD12	30:L:313:CLA:HMD3	1.88	0.56
30:b:707:CLA:H161	30:b:721:CLA:HBB2	1.87	0.56
19:D:33:LEU:HD13	19:D:165:LEU:HG	1.88	0.56
5:G:183:ASP:O	5:G:186:LEU:N	2.39	0.56
6:A:53:ALA:O	6:A:57:HIS:ND1	2.24	0.56
30:J:307:CLA:H61	30:J:308:CLA:HBA2	1.88	0.56
24:M:254:LEU:O	24:M:258:ARG:HD3	2.05	0.56
17:b:610:VAL:HG22	30:b:710:CLA:HHD	1.88	0.55
23:L:134:ASP:OD1	28:L:304:DD6:O4	2.24	0.55
14:l:57:ILE:HD11	14:l:106:PRO:HG2	1.88	0.55
26:O:105:THR:HG22	26:O:108:ARG:HH12	1.70	0.55
17:b:113:ILE:HB	17:b:133:THR:HB	1.88	0.55
23:L:212:GLU:HG2	30:L:313:CLA:NB	2.20	0.55
30:K:312:CLA:HED2	30:K:312:CLA:H2A	1.88	0.55
5:G:63:PRO:C	5:G:65:GLY:H	2.15	0.55
37:j:102:BCR:HC31	16:a:66:LEU:HD11	1.88	0.55
15:m:109:LEU:HG	15:m:113:MET:HE2	1.88	0.55
17:b:94:ALA:HB1	17:b:142:TYR:OH	2.06	0.55
30:G:513:CLA:H161	30:G:513:CLA:HMC3	1.89	0.55
30:G:517:CLA:HBB1	11:h:76:PHE:CE2	2.36	0.55
11:h:28:TYR:HB3	11:h:33:LYS:NZ	2.20	0.55
16:a:183:ASP:OD1	16:a:184:HIS:N	2.39	0.55
16:a:518:MET:HG2	16:a:522:LEU:HD21	1.87	0.55
1:I:173:LEU:HG	1:I:174:VAL:HG23	1.89	0.55
16:a:530:PHE:HE1	16:a:668:LEU:HD23	1.72	0.55
28:J:303:DD6:C5	30:J:310:CLA:HAC1	2.36	0.55
5:G:86:GLN:HG3	5:G:168:PRO:HG3	1.88	0.55
30:G:520:CLA:HBC3	37:f:304:BCR:H362	1.89	0.55
22:J:111:ALA:O	22:J:115:HIS:ND1	2.39	0.55
12:i:94:ASP:CG	12:i:105:ARG:HE	2.14	0.55
21:H:103:ARG:NE	21:H:198:GLU:OE2	2.36	0.55
21:H:188:PRO:HD2	21:H:190:SER:HB3	1.89	0.55
25:N:53:ASN:OD1	25:N:53:ASN:N	2.40	0.55
16:a:662:ALA:O	16:a:666:SER:OG	2.25	0.55
30:b:713:CLA:H171	30:b:717:CLA:HBB2	1.88	0.55
11:h:1:TYR:HD2	12:i:152:THR:HG22	1.72	0.55
14:l:138:GLY:N	14:l:141:GLY:O	2.29	0.55
25:N:70:ILE:HG12	34:N:302:PID:HM22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:34:GLN:NE2	34:P:202:PID:O2	2.40	0.55
27:P:127:SER:O	27:P:129:ASP:N	2.36	0.55
1:I:147:LYS:NZ	28:I:301:DD6:O4	2.39	0.54
5:G:154:ASN:HB3	5:G:171:LEU:HD22	1.89	0.54
35:A:318:SQD:H192	30:b:718:CLA:HBB1	1.89	0.54
7:c:143:ASP:OD2	9:e:72:SER:OG	2.24	0.54
8:d:274:MET:HE1	17:b:197:SER:HB3	1.88	0.54
27:P:94:LEU:HD11	27:P:99:ILE:HG22	1.90	0.54
4:y:80:UNK:N	16:a:433:ILE:O	2.40	0.54
24:M:212:GLU:HG2	30:M:312:CLA:CHB	2.37	0.54
37:i:201:BCR:H382	37:i:201:BCR:H23C	1.90	0.54
30:a:707:CLA:H122	30:a:707:CLA:HMA3	1.89	0.54
30:O:314:CLA:HED2	30:O:314:CLA:HBA1	1.89	0.54
2:K:126:MET:HB3	33:j:101:LMG:HC72	1.89	0.54
5:G:93:ILE:O	5:G:97:ARG:HG3	2.06	0.54
30:l:313:CLA:H201	16:a:296:ILE:HD13	1.90	0.54
16:a:449:THR:O	16:a:453:ILE:HG13	2.07	0.54
20:F:87:GLU:HA	20:F:95:LYS:HA	1.88	0.54
20:F:136:ALA:HB3	20:F:139:ASP:HB2	1.90	0.54
14:l:93:MET:HE2	23:L:111:LEU:HD11	1.90	0.54
16:a:560:ILE:HG13	16:a:561:THR:HG23	1.90	0.54
17:b:389:PRO:HD2	17:b:399:ILE:HD11	1.88	0.54
27:P:72:THR:HG23	27:P:177:ILE:HB	1.88	0.54
34:P:202:PID:HM31	30:P:209:CLA:HAC2	1.90	0.54
1:I:108:THR:HG22	1:I:111:ASN:H	1.72	0.54
1:I:118:ARG:HG3	1:I:119:VAL:H	1.73	0.54
13:j:11:PRO:HB3	14:l:84:MET:SD	2.47	0.54
37:l:302:BCR:H10C	30:b:728:CLA:H191	1.89	0.54
16:a:188:ILE:O	16:a:192:ARG:HB2	2.08	0.54
17:b:217:ASN:ND2	17:b:291:TYR:O	2.40	0.54
19:D:114:LEU:O	19:D:118:GLN:NE2	2.41	0.54
1:I:143:LEU:O	1:I:147:LYS:HG2	2.07	0.54
4:y:109:UNK:HA	16:a:217:LYS:HA	1.90	0.54
30:b:701:CLA:H141	30:b:728:CLA:H151	1.89	0.54
19:D:89:TYR:HA	19:D:97:LYS:HA	1.88	0.54
20:F:125:GLU:HG2	30:F:312:CLA:CHB	2.37	0.54
34:P:206:PID:HM52	30:P:215:CLA:HHC	1.89	0.54
1:I:1:LYS:NZ	2:K:128:GLY:O	2.31	0.54
1:I:188:SER:OG	30:I:319:CLA:OBD	2.21	0.54
30:a:703:CLA:O1A	17:b:420:GLY:HA3	2.08	0.54
19:D:121:ALA:HB2	33:D:317:LMG:H182	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:F:306:PID:HM51	34:F:306:PID:HM83	1.89	0.54
24:M:163:LEU:HD22	24:M:279:PHE:HB2	1.89	0.54
26:O:109:ARG:HD3	30:O:309:CLA:H43	1.90	0.54
34:G:506:PID:H21	34:G:507:PID:HM22	1.90	0.54
16:a:517:TRP:HE1	30:b:704:CLA:C1D	2.21	0.54
19:D:114:LEU:HD23	30:D:312:CLA:HED2	1.90	0.54
17:b:627:MET:HB3	30:b:704:CLA:C1C	2.38	0.53
24:M:122:PHE:HD1	24:M:123:GLY:H	1.56	0.53
24:M:138:PRO:HA	24:M:141:LEU:HD22	1.90	0.53
2:K:136:ASP:OD1	2:K:140:ARG:NH2	2.41	0.53
6:A:78:GLY:O	6:A:79:PRO:C	2.50	0.53
8:d:207:PRO:HA	10:f:255:SER:HA	1.90	0.53
30:f:302:CLA:HMB1	13:j:85:LEU:HD11	1.90	0.53
26:O:121:MET:HG2	34:O:305:PID:H17	1.90	0.53
16:a:327:THR:HG21	16:a:436:LEU:HD23	1.91	0.53
34:D:304:PID:H22	30:D:312:CLA:CHB	2.37	0.53
25:N:64:GLU:HG3	25:N:165:ILE:HD11	1.89	0.53
30:a:703:CLA:HMD3	17:b:503:ILE:HG12	1.90	0.53
30:b:715:CLA:C1D	30:b:716:CLA:HBB2	2.38	0.53
18:B:149:ILE:HG12	18:B:260:PHE:HB2	1.90	0.53
23:L:249:ILE:HD12	23:L:253:LYS:HE3	1.89	0.53
27:P:67:ILE:HD11	34:P:203:PID:HM22	1.90	0.53
15:m:112:THR:OG1	17:b:175:LYS:NZ	2.41	0.53
16:a:187:ILE:HA	16:a:191:SER:HB2	1.89	0.53
17:b:276:HIS:HB2	30:b:716:CLA:C1B	2.38	0.53
19:D:37:ALA:HB2	30:D:308:CLA:HMA2	1.89	0.53
30:j:104:CLA:H72	38:a:732:PQN:H243	1.90	0.53
23:L:166:LEU:HA	23:L:187:VAL:HG21	1.91	0.53
17:b:326:LEU:HD13	17:b:373:ALA:HB1	1.90	0.53
22:J:200:THR:HG23	22:J:206:ALA:HB2	1.91	0.53
26:O:128:MET:SD	34:O:307:PID:H11	2.48	0.53
26:O:221:LEU:CG	34:O:305:PID:H13	2.33	0.53
27:P:32:GLY:N	27:P:164:ASN:OD1	2.34	0.53
9:e:83:ASN:OD1	9:e:84:VAL:N	2.42	0.53
12:i:62:ASP:O	12:i:65:LYS:NZ	2.32	0.53
19:D:133:SER:HB2	19:D:134:PRO:HD3	1.90	0.53
21:H:148:ALA:O	21:H:152:ALA:N	2.41	0.53
27:P:91:SER:OG	31:P:213:KC1:O1A	2.26	0.53
1:I:103:TYR:HD2	1:I:107:ILE:HG22	1.72	0.53
37:f:304:BCR:H333	30:b:724:CLA:H142	1.90	0.53
25:N:65:LEU:HD12	25:N:140:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:N:69:ARG:NE	25:N:164:GLU:OE2	2.41	0.53
27:P:166:GLU:HA	30:P:215:CLA:HBB1	1.91	0.53
2:K:51:ASP:OD1	32:j:103:DGD:O5E	2.24	0.53
21:H:140:LEU:N	21:H:216:ASP:OD2	2.39	0.53
10:f:154:ARG:HD2	10:f:163:PRO:HB2	1.91	0.52
17:b:270:LEU:HD11	17:b:347:PHE:CZ	2.43	0.52
22:J:116:GLY:CA	22:J:219:SER:HB2	2.34	0.52
27:P:58:ARG:NH1	27:P:61:GLU:OE1	2.42	0.52
27:P:73:MET:O	27:P:77:THR:OG1	2.27	0.52
7:c:96:CYS:N	36:c:202:SF4:S1	2.81	0.52
8:d:104:MET:SD	14:l:160:ASP:HB3	2.50	0.52
30:a:725:CLA:HBB1	30:a:726:CLA:H2	1.91	0.52
30:b:717:CLA:H142	30:b:717:CLA:HBC2	1.91	0.52
25:N:119:GLN:NE2	31:N:308:KC1:O2D	2.40	0.52
12:i:104:LYS:HG3	12:i:108:GLU:OE1	2.09	0.52
30:a:702:CLA:C1A	30:b:703:CLA:HAB	2.39	0.52
19:D:141:GLY:O	30:D:314:CLA:HAA2	2.10	0.52
20:F:73:CYS:HB3	34:F:304:PID:HM43	1.91	0.52
13:j:66:TRP:O	13:j:72:ASN:ND2	2.42	0.52
11:h:63:PHE:O	11:h:126:GLN:NE2	2.38	0.52
16:a:36:HIS:HB3	39:a:733:LHG:H121	1.91	0.52
37:b:702:BCR:HC41	30:b:724:CLA:HBB2	1.91	0.52
22:J:82:THR:HA	22:J:213:MET:SD	2.49	0.52
34:O:305:PID:H8	30:O:316:CLA:HBB1	1.91	0.52
15:m:79:ILE:HD12	17:b:136:ILE:HG12	1.92	0.52
30:a:725:CLA:H91	30:b:704:CLA:H171	1.91	0.52
19:D:79:THR:HB	19:D:80:PRO:HD3	1.92	0.52
34:O:307:PID:HM51	34:O:307:PID:HM83	1.91	0.52
16:a:612:ALA:HB2	17:b:537:THR:HA	1.91	0.52
16:a:630:ILE:HD13	30:a:730:CLA:HMB2	1.91	0.52
30:a:703:CLA:HMB1	30:a:703:CLA:HBB1	1.92	0.52
23:L:116:LYS:HB2	23:L:120:GLY:H	1.74	0.52
1:I:20:VAL:HG12	1:I:143:LEU:HD22	1.92	0.52
1:I:108:THR:O	1:I:112:MET:N	2.42	0.52
16:a:386:LEU:O	30:a:726:CLA:HBB2	2.09	0.52
17:b:225:GLY:HA2	17:b:281:GLY:HA2	1.90	0.52
17:b:235:LEU:HA	17:b:239:THR:HB	1.91	0.52
34:H:301:PID:H20	30:H:311:CLA:HBC2	1.92	0.52
23:L:122:VAL:HG12	23:L:249:ILE:HG12	1.90	0.52
24:M:117:SER:H	30:M:309:CLA:HED2	1.74	0.52
6:A:62:MET:SD	30:A:313:CLA:HAB	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:200:PRO:O	29:A:304:UIX:O1	2.29	0.52
11:h:44:THR:HG23	11:h:55:HIS:HB3	1.91	0.52
13:j:69:LEU:HB3	13:j:72:ASN:HD22	1.75	0.52
17:b:622:TRP:HB2	17:b:683:GLY:HA3	1.92	0.52
21:H:69:GLY:HA3	21:H:203:ARG:HH22	1.75	0.52
21:H:124:TYR:HD2	21:H:127:PRO:HA	1.75	0.52
21:H:216:ASP:OD1	21:H:222:ALA:N	2.42	0.52
2:K:132:ARG:NH2	2:K:134:PRO:O	2.43	0.51
2:K:161:GLY:O	2:K:165:MET:HG3	2.10	0.51
14:l:115:ARG:O	14:l:119:GLU:HG2	2.10	0.51
16:a:659:SER:HB3	30:a:702:CLA:O1D	2.09	0.51
17:b:126:TYR:OH	17:b:610:VAL:HG23	2.10	0.51
21:H:73:PRO:HB3	30:H:304:CLA:HBB1	1.92	0.51
21:H:103:ARG:HB3	34:H:302:PID:HM13	1.92	0.51
23:L:235:ARG:HH21	23:L:236:LEU:HD21	1.75	0.51
28:M:303:DD6:C35	30:M:309:CLA:H2	2.40	0.51
34:O:307:PID:H15	31:O:315:KC1:CBB	2.40	0.51
30:A:320:CLA:HBB1	30:A:320:CLA:HHC	1.92	0.51
10:f:195:GLY:HA2	30:a:730:CLA:H172	1.93	0.51
17:b:354:ILE:HG12	17:b:697:SER:HB3	1.91	0.51
17:b:647:HIS:CE1	30:b:727:CLA:HAC1	2.46	0.51
24:M:122:PHE:HD1	24:M:123:GLY:N	2.08	0.51
25:N:81:PRO:HG3	30:N:307:CLA:C3D	2.41	0.51
5:G:97:ARG:HD3	30:G:514:CLA:CHD	2.40	0.51
14:l:167:GLU:HB2	30:l:311:CLA:HBA2	1.92	0.51
30:a:730:CLA:HED3	30:a:730:CLA:H2A	1.93	0.51
30:I:306:CLA:HAB	2:K:137:TYR:O	2.10	0.51
5:G:53:ASP:OD2	5:G:195:LYS:NZ	2.32	0.51
21:H:95:ARG:NH2	30:H:305:CLA:O1D	2.42	0.51
21:H:135:ASP:OD1	21:H:135:ASP:N	2.42	0.51
27:P:126:GLN:HG2	30:P:214:CLA:HMA1	1.91	0.51
2:K:17:MET:CE	23:L:101:ALA:HA	2.40	0.51
6:A:137:MET:HE2	6:A:145:LEU:HD13	1.93	0.51
14:l:193:LEU:HD11	37:l:307:BCR:H381	1.92	0.51
16:a:42:PHE:CD2	30:a:706:CLA:HMC2	2.46	0.51
16:a:203:LYS:HB3	16:a:204:MET:HE2	1.93	0.51
19:D:114:LEU:HD12	33:D:317:LMG:H111	1.92	0.51
25:N:148:VAL:O	25:N:152:SER:HB2	2.09	0.51
27:P:67:ILE:HG12	34:P:203:PID:HM13	1.91	0.51
18:B:139:ARG:HA	18:B:142:MET:HE3	1.93	0.51
24:M:253:GLU:HG2	30:M:313:CLA:C1B	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:237:MET:HG2	17:b:390:LEU:HD21	1.92	0.51
16:a:180:LEU:HD23	30:a:713:CLA:HBC2	1.92	0.51
30:a:704:CLA:HBB2	30:b:704:CLA:HBA1	1.92	0.51
17:b:322:LEU:HD11	30:b:722:CLA:HBB1	1.93	0.51
24:M:149:LEU:O	24:M:153:ARG:HG2	2.11	0.51
14:l:170:LEU:HB3	22:J:191:GLY:HA3	1.93	0.51
17:b:396:SER:HB2	17:b:399:ILE:HG12	1.93	0.51
24:M:180:LEU:HD11	24:M:188:LYS:HG2	1.93	0.51
5:G:73:ASN:ND2	5:G:80:PRO:HA	2.26	0.51
8:d:274:MET:HE2	8:d:274:MET:HA	1.93	0.51
17:b:438:SER:HB3	17:b:441:LYS:HG3	1.93	0.51
17:b:626:PHE:CB	30:b:704:CLA:HMC2	2.40	0.51
24:M:242:ASN:CG	24:M:243:SER:H	2.19	0.51
16:a:301:ASN:ND2	30:a:706:CLA:OBD	2.42	0.50
16:a:496:GLY:HA2	17:b:532:PRO:HD3	1.92	0.50
26:O:231:PHE:O	26:O:235:LEU:HB2	2.12	0.50
5:G:47:LYS:HZ3	5:G:60:ALA:H	1.58	0.50
8:d:220:LYS:HD3	12:i:170:TRP:HE1	1.76	0.50
16:a:387:HIS:O	16:a:391:LEU:HG	2.11	0.50
19:D:93:SER:OG	19:D:94:GLN:OE1	2.26	0.50
20:F:78:VAL:HG21	30:F:310:CLA:HAC2	1.93	0.50
20:F:84:PHE:HB2	20:F:96:PHE:CD2	2.46	0.50
23:L:280:PHE:H	30:L:316:CLA:HED3	1.75	0.50
30:a:703:CLA:CGA	30:a:703:CLA:H3A	2.41	0.50
37:a:734:BCR:H351	30:L:317:CLA:H42	1.93	0.50
7:c:143:ASP:HB2	9:e:109:ASN:CG	2.35	0.50
14:l:283:ILE:HG12	30:l:305:CLA:H12	1.91	0.50
1:I:130:LEU:HG	1:I:131:GLU:H	1.77	0.50
30:G:510:CLA:H42	30:G:510:CLA:C2B	2.42	0.50
30:f:301:CLA:HAB	38:a:732:PQN:H161	1.94	0.50
14:l:268:HIS:CD2	37:l:306:BCR:H291	2.47	0.50
16:a:79:ALA:HB2	16:a:142:LEU:HB3	1.93	0.50
17:b:113:ILE:HD12	17:b:133:THR:HG22	1.94	0.50
17:b:447:ALA:HB2	17:b:487:LEU:HB2	1.93	0.50
22:J:77:LYS:HA	22:J:80:ALA:HB2	1.94	0.50
23:L:205:ILE:HG12	30:L:317:CLA:HBC2	1.93	0.50
24:M:149:LEU:HD13	24:M:232:GLY:HA3	1.94	0.50
27:P:34:GLN:HG3	27:P:36:PRO:HD2	1.91	0.50
21:H:104:ILE:HD12	30:H:308:CLA:HMD3	1.93	0.50
21:H:117:ILE:HG13	21:H:118:THR:H	1.76	0.50
27:P:128:GLN:O	27:P:141:PHE:HD1	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:380:VAL:HG22	30:a:728:CLA:HBB2	1.94	0.50
30:a:704:CLA:H71	17:b:617:LEU:HD13	1.93	0.50
17:b:372:ILE:HG13	17:b:504:LEU:HD11	1.92	0.50
11:h:19:THR:O	11:h:23:LEU:HG	2.11	0.50
11:h:106:TYR:HH	33:D:317:LMG:HO4	1.55	0.50
16:a:293:ASP:OD1	16:a:294:TYR:N	2.44	0.50
18:B:186:ILE:HG22	30:B:311:CLA:H121	1.93	0.50
21:H:78:ASP:OD1	28:H:303:DD6:O2	2.30	0.50
24:M:148:GLU:OE2	24:M:258:ARG:NH1	2.31	0.50
27:P:87:LEU:HA	27:P:95:LYS:HA	1.92	0.50
7:c:88:LYS:HD3	8:d:197:ASN:HB3	1.94	0.50
11:h:40:ASP:OD1	17:b:303:ARG:NH1	2.35	0.50
14:l:99:TYR:OH	30:a:711:CLA:O1A	2.30	0.50
23:L:107:ALA:HA	23:L:224:SER:HB3	1.94	0.50
25:N:63:VAL:HG22	30:N:309:CLA:HED1	1.94	0.50
27:P:62:ILE:O	27:P:66:ARG:HG3	2.12	0.50
1:I:133:MET:SD	1:I:133:MET:N	2.85	0.49
14:l:231:VAL:HG11	14:l:272:GLY:HA3	1.93	0.49
21:H:195:LEU:O	21:H:199:ILE:HG12	2.11	0.49
5:G:147:ILE:O	5:G:151:GLU:HG2	2.12	0.49
30:b:727:CLA:HAB	38:b:729:PQN:H151	1.94	0.49
30:K:306:CLA:O1A	27:P:127:SER:HB2	2.12	0.49
24:M:153:ARG:HD2	30:M:313:CLA:C4C	2.43	0.49
24:M:189:PHE:HB3	24:M:200:PRO:HD2	1.93	0.49
25:N:137:SER:HB2	25:N:138:PRO:HD3	1.92	0.49
5:G:89:ARG:O	5:G:93:ILE:HG12	2.12	0.49
13:j:13:GLU:N	13:j:13:GLU:OE1	2.45	0.49
17:b:281:GLY:O	17:b:285:ILE:HG12	2.11	0.49
30:K:309:CLA:H2	30:K:309:CLA:HED3	1.95	0.49
10:f:232:GLN:O	10:f:236:ASN:ND2	2.46	0.49
17:b:686:LEU:HD23	30:b:720:CLA:H42	1.93	0.49
20:F:35:THR:HG21	20:F:175:ASN:HD21	1.77	0.49
20:F:36:PRO:N	20:F:37:PRO:HD2	2.27	0.49
14:l:74:TYR:CD2	14:l:106:PRO:HG3	2.48	0.49
16:a:200:GLN:HA	16:a:204:MET:HG2	1.95	0.49
16:a:304:LEU:HD13	30:a:719:CLA:HHB	1.95	0.49
19:D:139:ALA:N	30:D:314:CLA:HED3	2.28	0.49
20:F:95:LYS:N	20:F:98:GLU:OE2	2.39	0.49
29:J:305:UIX:C35	30:J:312:CLA:HAB	2.43	0.49
6:A:138:ASN:HB2	6:A:139:PRO:HD3	1.95	0.49
16:a:261:HIS:HB2	30:a:716:CLA:C1B	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:664:ILE:HG13	16:a:665:ILE:N	2.27	0.49
17:b:461:LEU:O	17:b:465:ILE:HG12	2.12	0.49
20:F:49:ASP:OD1	20:F:49:ASP:N	2.41	0.49
8:d:110:GLU:C	8:d:111:ARG:HD2	2.38	0.49
8:d:204:ARG:HG3	10:f:254:GLN:HG3	1.94	0.49
21:H:166:ASP:HB2	21:H:168:THR:HG23	1.94	0.49
22:J:93:PRO:HD2	28:J:304:DD6:O4	2.13	0.49
1:I:61:GLN:O	1:I:72:MET:HE1	2.13	0.49
9:e:101:VAL:O	16:a:635:GLN:NE2	2.45	0.49
16:a:63:HIS:CE1	30:a:706:CLA:HMA2	2.48	0.49
16:a:168:SER:N	16:a:171:THR:OG1	2.33	0.49
30:a:721:CLA:H11	30:a:721:CLA:H143	1.95	0.49
20:F:67:ARG:HA	20:F:70:MET:HE3	1.95	0.49
22:J:240:UNK:O	22:J:241:UNK:CB	2.61	0.49
7:c:143:ASP:N	9:e:109:ASN:OD1	2.46	0.49
16:a:650:ILE:HD13	30:a:724:CLA:H101	1.95	0.49
37:b:702:BCR:H323	30:b:724:CLA:HBB1	1.94	0.49
2:K:53:ARG:HG3	2:K:134:PRO:HG3	1.95	0.48
6:A:82:CYS:O	6:A:83:TRP:C	2.55	0.48
30:A:317:CLA:HBB1	30:A:320:CLA:HBB1	1.95	0.48
30:j:106:CLA:HMC1	17:b:428:SER:HB2	1.95	0.48
30:l:312:CLA:HBA1	30:l:312:CLA:H3A	1.54	0.48
16:a:380:VAL:O	16:a:384:ILE:HG12	2.12	0.48
17:b:421:PHE:HZ	37:b:702:BCR:H372	1.78	0.48
19:D:144:GLY:HA3	19:D:152:VAL:HG21	1.94	0.48
20:F:170:LEU:HG	30:F:313:CLA:CMA	2.42	0.48
22:J:238:UNK:O	22:J:239:UNK:C	2.61	0.48
1:I:143:LEU:HB3	30:I:307:CLA:HED3	1.95	0.48
2:K:57:GLU:HG2	2:K:122:ILE:HD11	1.95	0.48
12:i:99:ILE:HD11	30:b:705:CLA:HED1	1.95	0.48
14:l:183:ARG:NH1	14:l:186:LEU:HD11	2.27	0.48
16:a:184:HIS:ND1	30:a:719:CLA:OBD	2.46	0.48
17:b:375:HIS:HB3	17:b:504:LEU:HB3	1.94	0.48
30:b:717:CLA:H3A	30:b:717:CLA:HBA2	1.54	0.48
18:B:178:GLY:HA2	18:B:181:GLN:HE22	1.77	0.48
19:D:38:PRO:HG2	34:D:301:PID:H22A	1.94	0.48
34:P:203:PID:HM52	34:P:205:PID:H17	1.94	0.48
1:I:48:GLY:O	1:I:52:MET:HG3	2.13	0.48
5:G:13:LYS:HG2	5:G:14:HIS:H	1.78	0.48
7:c:136:CYS:HB2	7:c:147:ILE:HD13	1.96	0.48
14:l:45:PRO:HD2	14:l:48:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:262:LYS:HE3	17:b:264:ASN:HD21	1.77	0.48
30:b:709:CLA:O1A	30:b:720:CLA:HBD	2.13	0.48
27:P:103:LEU:HB3	27:P:184:ASP:OD1	2.13	0.48
2:K:60:LEU:HD13	2:K:135:GLY:HA3	1.95	0.48
5:G:190:GLN:O	5:G:194:ILE:HG13	2.13	0.48
7:c:134:LYS:O	7:c:138:THR:HG23	2.14	0.48
16:a:386:LEU:HD23	30:b:704:CLA:H71	1.95	0.48
19:D:124:ALA:HB2	30:D:313:CLA:CAB	2.44	0.48
23:L:97:ARG:NH2	23:L:100:LEU:HD13	2.27	0.48
3:z:66:UNK:HA	3:z:70:UNK:HA	1.95	0.48
5:G:203:GLY:O	5:G:207:ILE:HG13	2.13	0.48
7:c:111:VAL:HG12	8:d:193:ARG:HB3	1.95	0.48
10:f:113:LEU:HD22	10:f:148:GLU:HB2	1.94	0.48
18:B:118:PRO:C	18:B:120:ARG:N	2.71	0.48
6:A:118:LEU:O	6:A:121:VAL:N	2.46	0.48
6:A:163:GLU:OE1	6:A:166:LYS:N	2.44	0.48
8:d:115:THR:HG22	8:d:140:LEU:HD13	1.96	0.48
15:m:83:ASP:OD1	15:m:83:ASP:N	2.45	0.48
16:a:420:ALA:HB1	16:a:447:LEU:HD12	1.95	0.48
22:J:253:UNK:O	22:J:254:UNK:C	2.61	0.48
26:O:141:SER:HB3	26:O:146:VAL:HB	1.95	0.48
26:O:161:VAL:HB	26:O:166:TRP:NE1	2.28	0.48
5:G:50:ILE:HG21	5:G:187:LYS:HG3	1.96	0.48
16:a:566:LEU:HD22	17:b:616:LEU:HD21	1.95	0.48
30:a:709:CLA:H8	30:a:709:CLA:H122	1.60	0.48
17:b:70:THR:HG21	17:b:178:ILE:HD11	1.96	0.48
30:J:301:CLA:HBB1	32:L:301:DGD:HB41	1.95	0.48
25:N:51:ASP:OD1	25:N:52:GLY:N	2.46	0.48
25:N:144:PHE:CB	25:N:149:LEU:HD11	2.44	0.48
1:I:42:GLU:OE1	1:I:118:ARG:NH2	2.47	0.48
30:I:311:CLA:OBD	32:G:501:DGD:O2D	2.32	0.48
30:G:520:CLA:HMB2	30:a:730:CLA:HAA2	1.95	0.48
7:c:166:VAL:HG11	17:b:663:THR:OG1	2.14	0.48
9:e:74:TRP:NE1	9:e:100:SER:O	2.37	0.48
16:a:304:LEU:HD13	30:a:719:CLA:H3A	1.96	0.48
16:a:403:ARG:HG3	17:b:119:THR:HG22	1.95	0.48
17:b:73:TRP:CE2	30:b:713:CLA:HED1	2.49	0.48
18:B:130:LEU:HD13	30:B:309:CLA:H11	1.95	0.48
30:M:315:CLA:HBC1	30:M:317:CLA:HAB	1.96	0.48
1:I:188:SER:O	1:I:192:ASN:N	2.40	0.48
30:I:311:CLA:HBC1	10:f:225:SER:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:h:102:PHE:HB2	30:b:715:CLA:H12	1.94	0.48
14:l:204:ILE:O	14:l:208:THR:HG22	2.14	0.48
30:l:313:CLA:HED3	30:a:720:CLA:H72	1.95	0.48
34:H:301:PID:HM22	30:H:305:CLA:HAC2	1.95	0.48
30:L:314:CLA:H12	30:L:314:CLA:H51	1.71	0.48
2:K:61:LYS:HE2	29:K:302:UIX:O1	2.14	0.48
30:K:311:CLA:HBA1	30:K:311:CLA:H3A	1.52	0.48
5:G:74:PHE:HA	5:G:78:MET:HA	1.95	0.48
14:l:46:ARG:NH2	23:L:142:THR:H	2.12	0.48
16:a:601:ALA:HB3	30:a:703:CLA:HBB2	1.96	0.48
1:I:59:VAL:HG13	1:I:171:PHE:CE2	2.49	0.47
2:K:61:LYS:O	2:K:65:ILE:HG12	2.14	0.47
12:i:71:VAL:HG22	30:b:708:CLA:HAA1	1.96	0.47
15:m:98:ILE:O	15:m:102:VAL:HG23	2.14	0.47
16:a:359:LEU:HD11	16:a:507:PRO:HG2	1.95	0.47
16:a:493:PRO:HB3	16:a:641:ILE:HB	1.95	0.47
30:a:724:CLA:H203	30:a:731:CLA:H121	1.96	0.47
18:B:166:SER:HB3	18:B:169:ASN:HD21	1.79	0.47
21:H:107:LEU:HD13	30:H:309:CLA:HAC1	1.95	0.47
23:L:272:THR:HG22	23:L:274:LYS:HG3	1.94	0.47
24:M:114:LEU:HB3	24:M:145:ARG:NH2	2.29	0.47
6:A:120:GLN:NE2	30:A:311:CLA:O1D	2.47	0.47
17:b:129:THR:OG1	17:b:130:ILE:N	2.47	0.47
22:J:92:ASP:CG	22:J:97:THR:HG23	2.39	0.47
30:L:317:CLA:HHC	30:L:317:CLA:HBB1	1.96	0.47
6:A:84:GLN:O	6:A:85:ALA:CB	2.62	0.47
8:d:96:PHE:CZ	14:l:156:PRO:HB2	2.49	0.47
14:l:73:SER:O	14:l:76:TYR:N	2.46	0.47
16:a:199:HIS:HB2	30:a:714:CLA:C1C	2.45	0.47
5:G:89:ARG:HD2	5:G:93:ILE:HD11	1.95	0.47
30:A:310:CLA:H171	30:A:310:CLA:H111	1.96	0.47
11:h:30:HIS:CG	11:h:31:PRO:HD2	2.49	0.47
19:D:63:GLU:HB2	30:D:309:CLA:C1B	2.44	0.47
25:N:64:GLU:HG2	30:N:305:CLA:C1B	2.44	0.47
26:O:174:ALA:HB2	30:O:313:CLA:CAB	2.44	0.47
2:K:142:LEU:HB2	30:K:313:CLA:H2	1.96	0.47
6:A:83:TRP:CH2	30:A:310:CLA:O1A	2.67	0.47
11:h:73:MET:HG2	33:D:317:LMG:H221	1.97	0.47
16:a:519:TYR:OH	16:a:656:GLY:HA3	2.14	0.47
17:b:36:ARG:NH1	17:b:41:ARG:HH22	2.12	0.47
17:b:77:THR:HG23	17:b:167:ALA:HB1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:701:CLA:HBC1	38:b:729:PQN:H193	1.96	0.47
25:N:149:LEU:HD13	25:N:149:LEU:N	2.27	0.47
10:f:170:GLU:HG2	10:f:173:VAL:HG13	1.97	0.47
16:a:58:SER:O	16:a:160:SER:OG	2.31	0.47
30:a:706:CLA:H61	30:a:706:CLA:H41	1.61	0.47
30:a:731:CLA:H193	30:a:735:CLA:H191	1.96	0.47
17:b:278:LEU:O	17:b:282:ILE:HG12	2.14	0.47
2:K:17:MET:HE3	23:L:101:ALA:HA	1.96	0.47
2:K:36:ALA:O	2:K:40:GLY:N	2.45	0.47
2:K:66:CYS:SG	2:K:165:MET:HG2	2.55	0.47
30:K:309:CLA:HED1	32:j:103:DGD:HA31	1.97	0.47
8:d:165:LYS:HB3	8:d:177:PHE:HE1	1.79	0.47
16:a:375:SER:HB2	17:b:646:ILE:CG1	2.45	0.47
30:a:717:CLA:H91	30:a:721:CLA:HBA2	1.97	0.47
30:B:309:CLA:C2B	30:B:309:CLA:H42	2.45	0.47
30:F:313:CLA:HAA2	30:F:313:CLA:HED2	1.97	0.47
21:H:127:PRO:HD3	34:H:302:PID:HM61	1.97	0.47
22:J:133:PHE:CD2	30:J:316:CLA:HBA2	2.50	0.47
28:J:303:DD6:C22	30:J:310:CLA:HAA1	2.44	0.47
24:M:261:MET:HE1	30:M:309:CLA:HAB	1.97	0.47
25:N:128:GLU:O	25:N:132:ASP:HB3	2.14	0.47
26:O:124:ALA:CB	34:O:305:PID:HM43	2.45	0.47
27:P:35:ALA:H	27:P:36:PRO:HD2	1.79	0.47
10:f:156:CYS:HB3	10:f:163:PRO:HA	1.97	0.47
13:j:33:THR:HB	16:a:169:LYS:HE3	1.96	0.47
16:a:577:VAL:O	16:a:580:SER:OG	2.25	0.47
30:a:702:CLA:H162	30:a:702:CLA:H122	1.71	0.47
30:L:312:CLA:HBA1	30:L:312:CLA:H3A	1.38	0.47
24:M:148:GLU:HB2	30:M:309:CLA:C1B	2.45	0.47
6:A:182:MET:HE1	30:A:308:CLA:HHC	1.96	0.47
11:h:70:PHE:HB2	19:D:128:LEU:HD12	1.97	0.47
28:F:301:DD6:C40	30:F:307:CLA:HAC2	2.44	0.47
23:L:165:GLY:O	23:L:169:PRO:HD2	2.15	0.47
23:L:247:MET:HE1	30:L:314:CLA:H2	1.96	0.47
1:I:17:ALA:H	1:I:19:TRP:HZ3	1.63	0.47
1:I:31:PHE:HB2	30:I:308:CLA:O1A	2.15	0.47
30:f:301:CLA:H2	30:j:104:CLA:HED2	1.97	0.47
16:a:371:ASP:HB2	16:a:372:PRO:HD3	1.96	0.47
17:b:184:LEU:HD21	17:b:205:LEU:HD22	1.97	0.47
17:b:239:THR:HG22	17:b:270:LEU:HD13	1.97	0.47
17:b:316:LYS:HA	17:b:316:LYS:HD3	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:703:CLA:H102	30:b:703:CLA:H62	1.67	0.47
30:B:308:CLA:H3A	30:B:308:CLA:HBA2	1.61	0.47
25:N:65:LEU:HD23	25:N:65:LEU:HA	1.79	0.47
10:f:174:ARG:NH2	13:j:98:TRP:O	2.44	0.46
37:m:201:BCR:H11C	37:m:201:BCR:H341	1.73	0.46
17:b:69:PHE:HE2	17:b:177:HIS:CD2	2.33	0.46
30:b:723:CLA:HBA2	30:b:723:CLA:H3A	1.43	0.46
1:I:60:LEU:HD22	30:I:310:CLA:HAC2	1.97	0.46
1:I:130:LEU:HB2	30:I:313:CLA:HAA2	1.96	0.46
5:G:195:LYS:NZ	30:G:509:CLA:O1D	2.47	0.46
30:A:313:CLA:H41	30:A:313:CLA:H61	1.66	0.46
8:d:230:MET:HE1	12:i:162:LEU:HD13	1.97	0.46
30:j:104:CLA:H51	38:a:732:PQN:H243	1.97	0.46
16:a:204:MET:O	16:a:208:ASN:N	2.40	0.46
30:a:723:CLA:H141	30:a:723:CLA:H162	1.69	0.46
17:b:264:ASN:OD1	17:b:265:THR:N	2.48	0.46
17:b:418:TRP:CZ2	30:b:725:CLA:HMC3	2.50	0.46
18:B:118:PRO:O	18:B:120:ARG:N	2.48	0.46
19:D:165:LEU:HD13	19:D:165:LEU:HA	1.84	0.46
20:F:145:LYS:HZ3	20:F:145:LYS:HG2	1.57	0.46
21:H:91:PHE:CD2	21:H:92:LYS:HG2	2.49	0.46
30:J:311:CLA:HBA1	30:J:311:CLA:H3A	1.63	0.46
24:M:253:GLU:HG2	30:M:313:CLA:NB	2.31	0.46
4:y:117:UNK:N	4:y:128:UNK:O	2.48	0.46
6:A:49:PHE:CD1	35:A:318:SQD:H242	2.51	0.46
7:c:115:ILE:HD11	7:c:121:VAL:HG11	1.97	0.46
19:D:68:ARG:HB3	34:D:302:PID:HM32	1.97	0.46
23:L:121:LEU:HD12	23:L:121:LEU:HA	1.77	0.46
2:K:103:PRO:HB3	30:K:311:CLA:CAD	2.45	0.46
28:G:505:DD6:C24	30:G:514:CLA:HAB	2.46	0.46
7:c:97:THR:HG22	7:c:110:MET:HG3	1.96	0.46
8:d:261:GLU:OE1	8:d:261:GLU:N	2.47	0.46
11:h:81:TYR:CZ	11:h:85:GLN:HG3	2.50	0.46
30:j:106:CLA:HBA1	30:j:106:CLA:H3A	1.43	0.46
14:l:96:TRP:CE2	30:a:711:CLA:HED2	2.50	0.46
37:m:201:BCR:HC42	30:b:705:CLA:H72	1.97	0.46
17:b:143:ASN:ND2	17:b:347:PHE:O	2.41	0.46
19:D:168:GLU:HB2	30:D:314:CLA:C1B	2.45	0.46
34:H:301:PID:HM41	34:H:301:PID:H16	1.61	0.46
30:J:307:CLA:C1B	30:J:307:CLA:H42	2.46	0.46
30:M:309:CLA:H71	30:M:310:CLA:HMB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:MET:HE3	30:I:313:CLA:HMC3	1.96	0.46
16:a:371:ASP:O	16:a:375:SER:HB3	2.14	0.46
16:a:605:MET:O	16:a:609:SER:OG	2.26	0.46
17:b:615:PHE:CZ	17:b:619:HIS:HE1	2.34	0.46
31:F:309:KC1:CBC	30:F:312:CLA:HAC1	2.45	0.46
5:G:99:CYS:SG	28:G:504:DD6:C6	3.04	0.46
7:c:166:VAL:HG13	17:b:660:ASP:HA	1.97	0.46
10:f:178:MET:HA	10:f:178:MET:HE2	1.97	0.46
14:l:148:VAL:HG22	22:J:205:MET:CB	2.46	0.46
16:a:105:ILE:HD12	30:a:710:CLA:C2B	2.45	0.46
16:a:137:ILE:HD11	16:a:211:LEU:HD11	1.97	0.46
26:O:208:ARG:HH22	26:O:212:LEU:HD13	1.80	0.46
2:K:136:ASP:CG	2:K:140:ARG:HH22	2.23	0.46
5:G:99:CYS:SG	28:G:504:DD6:C5	3.03	0.46
16:a:348:ILE:HG21	16:a:515:VAL:HG22	1.96	0.46
17:b:144:GLN:NE2	17:b:148:SER:OG	2.49	0.46
18:B:145:THR:HG23	18:B:248:ILE:HD12	1.98	0.46
20:F:32:LEU:HD22	20:F:170:LEU:HB3	1.97	0.46
30:N:309:CLA:H2A	30:N:309:CLA:O1D	2.16	0.46
27:P:166:GLU:HG3	30:P:215:CLA:C4B	2.46	0.46
30:l:312:CLA:O2A	30:l:313:CLA:HBB2	2.15	0.46
16:a:110:LEU:HD21	17:b:436:PHE:CE1	2.51	0.46
30:a:728:CLA:H41	30:a:728:CLA:H62	1.65	0.46
38:a:732:PQN:H161	38:a:732:PQN:H141	1.64	0.46
17:b:82:TRP:O	17:b:85:SER:OG	2.21	0.46
17:b:262:LYS:N	17:b:267:SER:O	2.49	0.46
30:b:709:CLA:H2	30:b:709:CLA:H61	1.75	0.46
37:b:730:BCR:H341	37:b:730:BCR:H11C	1.73	0.46
22:J:73:ARG:O	22:J:76:PRO:HD2	2.16	0.46
26:O:240:TYR:CZ	34:O:307:PID:HM32	2.51	0.46
34:j:105:PID:H11	30:a:710:CLA:HAA2	1.98	0.46
16:a:600:TRP:HZ3	30:a:735:CLA:HMD3	1.81	0.46
30:a:726:CLA:H203	30:a:726:CLA:H162	1.74	0.46
21:H:201:ASN:ND2	30:H:304:CLA:OBD	2.48	0.46
22:J:203:ASN:C	22:J:205:MET:H	2.22	0.46
34:O:304:PID:H22	31:O:312:KC1:CMB	2.46	0.46
8:d:247:ALA:O	8:d:285:ARG:NH1	2.35	0.46
14:l:148:VAL:HG21	22:J:200:THR:HG21	1.98	0.46
16:a:390:SER:OG	30:a:726:CLA:HAB	2.16	0.46
30:a:709:CLA:H3A	30:a:709:CLA:HBA2	1.37	0.46
30:b:715:CLA:H3A	30:b:715:CLA:HBA2	1.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:D:165:LEU:HD22	30:D:314:CLA:HMA3	1.98	0.46
34:F:304:PID:H16	34:F:304:PID:HM41	1.64	0.46
26:O:136:PHE:HD2	26:O:149:ALA:HA	1.80	0.46
26:O:220:ARG:H	26:O:220:ARG:HG2	1.52	0.46
1:I:37:MET:HE2	1:I:37:MET:HB2	1.81	0.45
6:A:58:GLY:O	6:A:62:MET:HG3	2.16	0.45
34:j:105:PID:HM52	30:a:731:CLA:H142	1.97	0.45
14:l:123:TYR:O	14:l:127:MET:HG2	2.16	0.45
16:a:661:TRP:O	16:a:665:ILE:HG12	2.16	0.45
30:B:315:CLA:HBC1	30:B:317:CLA:HAB	1.98	0.45
22:J:164:MET:O	22:J:168:ILE:HG12	2.16	0.45
34:P:206:PID:HM41	34:P:206:PID:H16	1.51	0.45
30:A:313:CLA:CHB	30:A:313:CLA:H11	2.47	0.45
30:j:106:CLA:H41	30:j:106:CLA:H62	1.65	0.45
30:a:702:CLA:HBD	30:a:702:CLA:HED2	1.45	0.45
17:b:46:LEU:HB3	33:b:733:LMG:H162	1.97	0.45
17:b:276:HIS:HB2	30:b:716:CLA:CHB	2.47	0.45
30:b:707:CLA:H91	33:b:733:LMG:H391	1.98	0.45
30:B:313:CLA:H111	30:B:313:CLA:H151	1.74	0.45
14:l:46:ARG:HH22	23:L:142:THR:N	2.14	0.45
14:l:175:PHE:HE2	22:J:174:LEU:HD11	1.81	0.45
16:a:110:LEU:HD21	17:b:436:PHE:HE1	1.80	0.45
26:O:136:PHE:HA	30:O:311:CLA:OBD	2.17	0.45
34:P:205:PID:HM41	34:P:205:PID:H16	1.56	0.45
30:I:306:CLA:HMB3	2:K:139:LEU:HD23	1.98	0.45
6:A:81:LYS:HE2	6:A:82:CYS:HB2	1.98	0.45
11:h:8:GLU:O	11:h:12:GLU:HG2	2.16	0.45
11:h:81:TYR:CE1	19:D:114:LEU:HD11	2.52	0.45
14:l:37:LYS:HG2	14:l:38:ILE:H	1.80	0.45
14:l:165:LEU:HD11	22:J:190:ILE:HG22	1.97	0.45
16:a:109:ILE:HD13	16:a:587:CYS:SG	2.55	0.45
30:a:706:CLA:H61	30:a:706:CLA:H92	1.77	0.45
17:b:88:TYR:HB2	17:b:160:THR:HG21	1.98	0.45
22:J:133:PHE:CE2	30:J:316:CLA:HBA2	2.52	0.45
24:M:116:GLY:H	24:M:145:ARG:HH22	1.64	0.45
30:I:312:CLA:H142	30:I:312:CLA:H111	1.71	0.45
9:e:75:PHE:HB3	10:f:247:HIS:CD2	2.51	0.45
10:f:251:PRO:HD2	17:b:518:PRO:HB3	1.99	0.45
30:f:302:CLA:HBB1	13:j:85:LEU:HD21	1.99	0.45
12:i:90:SER:HB3	17:b:662:TYR:OH	2.16	0.45
37:a:736:BCR:H11C	37:a:736:BCR:H341	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:713:CLA:H112	30:b:717:CLA:H92	1.99	0.45
19:D:60:ARG:NH1	19:D:63:GLU:OE1	2.49	0.45
20:F:160:ASP:OD1	20:F:160:ASP:N	2.46	0.45
1:I:4:SER:OG	1:I:7:VAL:O	2.35	0.45
30:I:308:CLA:H91	30:I:308:CLA:H111	1.74	0.45
13:j:82:VAL:HG13	37:j:102:BCR:H373	1.98	0.45
14:l:120:ILE:HD13	14:l:120:ILE:HA	1.81	0.45
16:a:189:PHE:HB3	16:a:269:PHE:CD2	2.52	0.45
30:a:731:CLA:HBA1	30:a:731:CLA:H3A	1.58	0.45
17:b:323:SER:OG	17:b:378:THR:OG1	2.33	0.45
20:F:150:MET:O	20:F:158:GLY:N	2.50	0.45
21:H:146:VAL:HB	21:H:151:TRP:NE1	2.32	0.45
22:J:211:ILE:HG12	30:J:312:CLA:HHB	1.99	0.45
30:M:308:CLA:H41	30:M:308:CLA:H61	1.63	0.45
30:M:318:CLA:HBA2	30:M:318:CLA:H3A	1.34	0.45
26:O:88:PRO:HG3	30:O:308:CLA:CHB	2.46	0.45
1:I:61:GLN:HE21	30:I:310:CLA:HED1	1.82	0.45
2:K:30:LEU:HD23	2:K:40:GLY:HA2	1.97	0.45
32:y:201:DGD:HA22	32:y:201:DGD:HA51	1.75	0.45
5:G:99:CYS:SG	5:G:201:MET:HG2	2.56	0.45
14:l:50:GLU:OE1	14:l:50:GLU:N	2.49	0.45
16:a:161:TYR:HB2	30:a:712:CLA:HMC2	1.98	0.45
17:b:674:PHE:HZ	30:b:722:CLA:H61	1.82	0.45
18:B:150:SER:HB2	18:B:155:TRP:HE3	1.82	0.45
19:D:123:GLY:O	19:D:127:GLU:HG2	2.16	0.45
30:J:311:CLA:HMB1	30:J:311:CLA:HBB1	1.98	0.45
24:M:170:LEU:HD23	24:M:171:PRO:HD2	1.98	0.45
26:O:216:LEU:O	26:O:220:ARG:HG2	2.17	0.45
30:P:210:CLA:H41	30:P:210:CLA:H61	1.52	0.45
1:I:73:PRO:HG3	1:I:82:ALA:HB3	1.98	0.45
2:K:157:GLU:HB2	30:K:313:CLA:CHB	2.46	0.45
6:A:95:VAL:O	6:A:116:GLY:HA2	2.17	0.45
11:h:97:ASP:OD2	17:b:468:ILE:HA	2.16	0.45
14:l:273:LEU:HD21	30:l:308:CLA:C3D	2.46	0.45
16:a:460:PHE:HE1	30:b:704:CLA:HBA2	1.80	0.45
30:a:705:CLA:H11	30:a:705:CLA:H51	1.73	0.45
30:a:705:CLA:H92	30:a:705:CLA:H61	1.75	0.45
17:b:113:ILE:HD11	17:b:135:LEU:HG	1.98	0.45
17:b:323:SER:OG	17:b:374:SER:O	2.34	0.45
18:B:77:UNK:CB	18:B:83:UNK:HA	2.47	0.45
23:L:132:GLU:H	23:L:132:GLU:HG2	1.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:P:202:PID:H22	30:P:217:CLA:HMD2	1.99	0.45
2:K:34:VAL:HG11	2:K:154:GLN:HB3	1.99	0.45
6:A:160:LEU:HD12	6:A:161:PRO:HD2	1.98	0.45
8:d:267:ARG:HH21	8:d:268:GLN:HB2	1.81	0.45
11:h:30:HIS:CD2	11:h:31:PRO:HD2	2.52	0.45
30:b:727:CLA:H3A	38:b:729:PQN:H293	1.98	0.45
19:D:71:MET:HE3	19:D:171:ASN:HB3	1.99	0.45
21:H:143:ILE:HG22	21:H:151:TRP:CZ2	2.52	0.45
1:I:151:LEU:HD13	30:I:307:CLA:HBC1	1.97	0.45
1:I:166:VAL:HG13	1:I:175:PRO:HG3	1.99	0.45
5:G:92:GLU:HG2	30:G:510:CLA:CHB	2.47	0.45
6:A:138:ASN:OD1	35:A:318:SQD:H101	2.16	0.45
30:A:308:CLA:HBB1	30:A:308:CLA:HMB3	1.99	0.45
30:a:718:CLA:CHA	30:a:718:CLA:HBA1	2.46	0.45
17:b:389:PRO:HD2	17:b:399:ILE:CD1	2.47	0.45
21:H:160:TYR:CD2	30:N:309:CLA:HBA2	2.52	0.45
27:P:163:LEU:HD13	30:P:215:CLA:HMA2	1.98	0.45
27:P:175:MET:O	30:P:217:CLA:HMC2	2.17	0.45
2:K:102:GLY:N	2:K:103:PRO:HD2	2.32	0.44
6:A:135:ALA:O	6:A:139:PRO:HD2	2.17	0.44
30:A:309:CLA:H2	30:A:309:CLA:H61	1.62	0.44
30:A:312:CLA:H92	30:A:312:CLA:H61	1.79	0.44
12:i:63:GLN:NE2	15:m:85:ASP:O	2.31	0.44
17:b:81:ILE:HD13	17:b:81:ILE:HA	1.88	0.44
19:D:85:LYS:HE2	30:D:311:CLA:HED3	1.99	0.44
19:D:176:MET:O	19:D:180:ILE:HG22	2.17	0.44
30:M:315:CLA:H2A	30:M:315:CLA:CED	2.47	0.44
27:P:32:GLY:HA2	27:P:171:ARG:HH12	1.82	0.44
6:A:34:PHE:HB3	30:A:308:CLA:HMD2	1.99	0.44
30:f:301:CLA:HAC1	16:a:625:HIS:CD2	2.52	0.44
13:j:45:THR:HG23	14:l:90:ALA:HB1	1.98	0.44
38:a:732:PQN:H172	37:b:702:BCR:H382	2.00	0.44
18:B:132:GLU:OE2	18:B:208:ARG:NH2	2.39	0.44
34:F:305:PID:HM41	34:F:305:PID:C17	2.43	0.44
25:N:53:ASN:CG	25:N:56:SER:HB3	2.42	0.44
26:O:104:ALA:O	26:O:108:ARG:N	2.50	0.44
30:I:321:CLA:O1D	13:j:90:ARG:NH1	2.45	0.44
8:d:208:GLN:HG3	10:f:255:SER:HB3	1.99	0.44
16:a:307:SER:O	16:a:310:ILE:HG22	2.17	0.44
16:a:392:TYR:HE2	16:a:457:ILE:HG13	1.82	0.44
17:b:420:GLY:N	17:b:495:LEU:HD13	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:J:309:CLA:HBC1	30:J:316:CLA:C4B	2.47	0.44
24:M:139:GLU:H	24:M:139:GLU:CD	2.25	0.44
27:P:172:LEU:HD22	34:P:206:PID:H11	1.99	0.44
2:K:122:ILE:HD11	30:K:312:CLA:HED3	1.99	0.44
3:z:67:UNK:O	3:z:69:UNK:N	2.49	0.44
30:l:313:CLA:H162	30:l:313:CLA:H203	1.73	0.44
30:b:725:CLA:H41	30:b:725:CLA:H61	1.57	0.44
18:B:178:GLY:HA2	18:B:181:GLN:NE2	2.32	0.44
30:F:311:CLA:H2A	30:F:311:CLA:O1D	2.17	0.44
30:J:307:CLA:H3A	30:J:307:CLA:HBA2	1.34	0.44
30:J:307:CLA:O1D	30:J:307:CLA:H2A	2.18	0.44
30:J:307:CLA:H111	30:J:307:CLA:H71	1.55	0.44
30:J:307:CLA:H93	30:J:308:CLA:HMA1	1.98	0.44
23:L:237:PHE:CD1	23:L:238:PRO:HD2	2.52	0.44
30:M:308:CLA:HAA2	25:N:145:GLY:O	2.16	0.44
30:I:312:CLA:H92	30:I:312:CLA:H61	1.71	0.44
2:K:98:MET:HG3	30:K:310:CLA:HAA2	1.99	0.44
8:d:216:LYS:HG3	12:i:123:LYS:O	2.18	0.44
12:i:97:TRP:HA	12:i:103:THR:HG21	1.99	0.44
30:a:713:CLA:H91	30:a:723:CLA:H71	2.00	0.44
17:b:293:SER:OG	30:b:718:CLA:OBD	2.23	0.44
30:b:715:CLA:H61	30:b:715:CLA:H41	1.70	0.44
30:J:309:CLA:H41	30:J:316:CLA:HMC3	2.00	0.44
24:M:267:ILE:HD12	24:M:281:PHE:CD2	2.52	0.44
2:K:146:ASP:O	2:K:150:GLN:HG3	2.17	0.44
8:d:177:PHE:CZ	8:d:180:PRO:HG2	2.53	0.44
11:h:23:LEU:HD22	11:h:28:TYR:CG	2.52	0.44
13:j:83:GLY:O	13:j:87:GLU:HG2	2.18	0.44
16:a:306:ALA:CB	16:a:347:ILE:HG13	2.48	0.44
16:a:539:GLY:HA3	16:a:549:HIS:HA	2.00	0.44
30:a:735:CLA:H41	30:a:735:CLA:H62	1.57	0.44
17:b:234:HIS:HB2	30:b:714:CLA:CHC	2.47	0.44
17:b:443:ILE:O	17:b:488:TYR:OH	2.22	0.44
17:b:494:ALA:O	17:b:498:HIS:ND1	2.38	0.44
30:b:704:CLA:H202	30:b:704:CLA:H161	1.61	0.44
33:b:734:LMG:H171	33:b:734:LMG:H292	2.00	0.44
20:F:95:LYS:H	20:F:98:GLU:CD	2.25	0.44
26:O:125:MET:HE1	34:O:305:PID:H22	1.99	0.44
26:O:128:MET:HE3	26:O:128:MET:HB2	1.75	0.44
27:P:186:LEU:HD21	30:P:217:CLA:HMD1	1.99	0.44
1:I:42:GLU:HG2	1:I:112:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:157:SER:HB3	30:I:315:CLA:HBC2	1.98	0.44
14:l:52:ASP:OD1	14:l:52:ASP:N	2.50	0.44
16:a:348:ILE:HD13	16:a:469:LEU:HD11	2.00	0.44
16:a:375:SER:HB2	17:b:646:ILE:HG12	1.98	0.44
16:a:435:MET:SD	16:a:541:VAL:HG11	2.58	0.44
30:a:713:CLA:H61	30:a:713:CLA:H41	1.56	0.44
30:b:701:CLA:H62	30:b:701:CLA:H41	1.49	0.44
34:F:304:PID:HM53	30:F:313:CLA:HAB	2.00	0.44
26:O:198:PHE:CB	34:O:305:PID:H312	2.47	0.44
11:h:104:VAL:HG13	30:b:715:CLA:H72	2.00	0.44
14:l:98:TYR:CG	23:L:109:ILE:HG21	2.53	0.44
30:a:707:CLA:H143	30:a:707:CLA:H111	1.76	0.44
30:b:725:CLA:HBB1	30:b:725:CLA:HMB1	2.00	0.44
19:D:78:MET:SD	34:D:306:PID:H11	2.57	0.44
23:L:200:PRO:O	23:L:204:ILE:HG13	2.17	0.44
26:O:177:GLU:HG2	30:O:313:CLA:CHB	2.47	0.44
10:f:164:ARG:HA	10:f:164:ARG:HD3	1.86	0.44
16:a:8:ASN:HB3	16:a:10:THR:HG22	1.99	0.44
30:a:717:CLA:H3A	30:a:717:CLA:HBA2	1.37	0.44
30:B:309:CLA:CHB	30:B:309:CLA:H12	2.47	0.44
19:D:89:TYR:C	19:D:91:SER:H	2.26	0.44
21:H:100:LYS:NZ	34:H:302:PID:H42	2.29	0.44
22:J:90:PHE:CD2	30:J:307:CLA:HED3	2.52	0.44
22:J:126:TRP:CE2	22:J:149:PRO:HG2	2.52	0.44
34:O:305:PID:HM82	34:O:305:PID:O6	2.18	0.44
30:f:301:CLA:HAA2	13:j:74:PHE:CE2	2.53	0.43
37:l:306:BCR:H20C	30:b:701:CLA:HBB2	2.00	0.43
16:a:204:MET:HB3	16:a:255:LEU:HD23	1.99	0.43
16:a:341:TRP:HB3	30:a:722:CLA:HMC2	2.00	0.43
16:a:616:GLU:OE2	17:b:514:SER:OG	2.33	0.43
30:a:721:CLA:H143	30:a:721:CLA:H161	1.85	0.43
19:D:143:PHE:HB2	34:D:305:PID:O5	2.18	0.43
34:F:302:PID:HM41	34:F:302:PID:H16	1.75	0.43
22:J:209:LYS:O	22:J:213:MET:HG2	2.18	0.43
30:I:313:CLA:H62	30:I:313:CLA:H41	1.53	0.43
5:G:144:SER:O	5:G:147:ILE:HG22	2.19	0.43
7:c:166:VAL:HG21	17:b:663:THR:HG23	2.00	0.43
14:l:51:LYS:H	14:l:51:LYS:HD2	1.83	0.43
16:a:86:ILE:HG23	16:a:94:ILE:HG21	2.00	0.43
17:b:36:ARG:HA	17:b:36:ARG:NE	2.33	0.43
17:b:596:LEU:HD21	17:b:615:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:131:LEU:HD22	21:H:136:ILE:HD11	2.00	0.43
23:L:199:GLY:O	23:L:203:GLN:HG3	2.18	0.43
34:O:305:PID:HM22	30:O:316:CLA:HMB1	1.99	0.43
14:l:210:LEU:CD1	30:a:725:CLA:HBB2	2.46	0.43
16:a:497:PRO:HD3	17:b:531:GLY:HA2	2.00	0.43
30:a:722:CLA:HBB1	30:a:722:CLA:HMB3	2.00	0.43
17:b:248:ILE:O	17:b:250:THR:N	2.48	0.43
30:b:707:CLA:H111	30:b:707:CLA:H72	1.46	0.43
34:F:302:PID:HM12	30:F:313:CLA:HAC2	1.99	0.43
22:J:196:LEU:HD22	22:J:197:GLU:H	1.83	0.43
23:L:97:ARG:HG3	23:L:237:PHE:HE2	1.83	0.43
1:I:160:VAL:O	1:I:164:ILE:HG13	2.18	0.43
13:j:10:LYS:HD2	13:j:10:LYS:HA	1.86	0.43
16:a:341:TRP:CE3	16:a:522:LEU:HD12	2.53	0.43
16:a:377:LEU:HG	16:a:467:LEU:HB2	2.01	0.43
30:a:722:CLA:O1D	30:a:723:CLA:HHB	2.18	0.43
18:B:199:LYS:O	18:B:203:LEU:HG	2.18	0.43
20:F:117:MET:H	20:F:117:MET:HG2	1.49	0.43
21:H:98:GLU:OE2	21:H:203:ARG:NE	2.35	0.43
21:H:149:LEU:O	21:H:153:GLN:N	2.40	0.43
30:O:314:CLA:HBA1	30:O:314:CLA:H11	1.81	0.43
5:G:45:MET:HG2	5:G:84:HIS:CE1	2.53	0.43
8:d:179:HIS:HB3	8:d:180:PRO:HD3	2.00	0.43
10:f:248:ASN:OD1	10:f:248:ASN:N	2.51	0.43
37:f:304:BCR:H371	37:f:304:BCR:H24C	1.84	0.43
37:j:102:BCR:H15C	37:j:102:BCR:H351	1.78	0.43
30:b:704:CLA:H61	30:b:704:CLA:H41	1.81	0.43
37:b:732:BCR:H15C	37:b:732:BCR:H351	1.83	0.43
18:B:142:MET:SD	30:B:313:CLA:HAB	2.59	0.43
30:L:308:CLA:HBA2	30:L:308:CLA:H3A	1.42	0.43
1:I:41:ARG:NH1	1:I:44:GLU:OE1	2.51	0.43
2:K:20:ALA:O	2:K:22:PRO:HD3	2.18	0.43
16:a:45:GLN:OE1	16:a:55:LYS:NZ	2.40	0.43
16:a:104:LEU:O	16:a:105:ILE:HG12	2.18	0.43
30:a:731:CLA:H141	30:a:731:CLA:H161	1.83	0.43
17:b:285:ILE:HD12	30:b:718:CLA:HAC1	2.01	0.43
19:D:139:ALA:H	30:D:314:CLA:HED3	1.84	0.43
25:N:64:GLU:HG2	30:N:305:CLA:NB	2.32	0.43
1:I:130:LEU:HA	1:I:133:MET:HE1	2.00	0.43
33:I:320:LMG:O5	33:I:320:LMG:O4	2.29	0.43
7:c:137:GLU:HB3	7:c:145:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:f:121:LYS:HG2	10:f:125:GLN:OE1	2.18	0.43
16:a:503:CYS:HB2	17:b:632:TRP:HB3	1.99	0.43
17:b:489:VAL:HG11	17:b:563:TYR:HB2	2.00	0.43
18:B:221:PRO:HG2	18:B:227:ALA:HA	1.99	0.43
19:D:68:ARG:HB3	30:D:314:CLA:HAC2	2.00	0.43
20:F:196:THR:OG1	20:F:197:THR:N	2.51	0.43
34:G:506:PID:H16	34:G:506:PID:HM41	1.71	0.43
30:G:518:CLA:HBA2	30:G:518:CLA:H3A	1.33	0.43
6:A:67:GLY:HA3	30:A:310:CLA:C1C	2.48	0.43
30:l:304:CLA:H111	30:l:304:CLA:H91	1.63	0.43
15:m:81:MET:HE3	15:m:81:MET:HB2	1.77	0.43
30:a:706:CLA:H12	30:a:707:CLA:HAB	2.01	0.43
30:a:721:CLA:H143	30:a:721:CLA:H111	1.82	0.43
37:a:734:BCR:H351	37:a:734:BCR:H15C	1.73	0.43
17:b:389:PRO:CB	17:b:393:GLU:HB2	2.49	0.43
18:B:173:LYS:O	18:B:177:MET:HG2	2.19	0.43
19:D:162:LYS:HE3	19:D:162:LYS:HB2	1.89	0.43
34:O:301:PID:HM41	34:O:301:PID:H16	1.64	0.43
5:G:206:SER:HB3	5:G:217:VAL:HG21	2.00	0.43
8:d:225:ASP:O	8:d:229:THR:HG23	2.19	0.43
14:l:202:PHE:CZ	30:l:304:CLA:HBB1	2.54	0.43
30:l:303:CLA:H2A	30:l:303:CLA:O2D	2.18	0.43
16:a:284:GLN:HE21	16:a:284:GLN:HB2	1.62	0.43
16:a:437:ASP:C	16:a:439:LYS:H	2.26	0.43
17:b:229:ILE:HD13	37:b:730:BCR:H373	2.01	0.43
20:F:114:TRP:HA	20:F:117:MET:HG3	2.00	0.43
24:M:261:MET:HE1	30:M:309:CLA:HHC	2.00	0.43
34:M:301:PID:HM41	34:M:301:PID:H16	1.62	0.43
34:O:307:PID:H8	34:O:307:PID:HM31	2.01	0.43
12:i:94:ASP:OD2	12:i:105:ARG:NE	2.50	0.43
14:l:213:LEU:HD12	14:l:222:VAL:HG21	2.01	0.43
16:a:106:GLY:C	16:a:108:ASP:N	2.75	0.43
30:a:704:CLA:HBB1	30:a:704:CLA:HMB3	2.00	0.43
30:b:701:CLA:HMD3	37:b:732:BCR:H383	2.01	0.43
37:b:702:BCR:H20C	37:b:702:BCR:H361	1.86	0.43
22:J:196:LEU:HD23	22:J:196:LEU:HA	1.87	0.43
23:L:237:PHE:CD1	30:L:314:CLA:HAA2	2.54	0.43
24:M:182:PHE:CE1	24:M:277:HIS:HA	2.54	0.43
26:O:146:VAL:HG12	26:O:151:ILE:HD11	2.01	0.43
34:O:302:PID:HM41	34:O:302:PID:H16	1.85	0.43
27:P:32:GLY:HA3	27:P:171:ARG:HH22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:e:66:LYS:HB3	9:e:117:ILE:HG22	2.00	0.42
14:l:68:ASN:O	14:l:69:PRO:C	2.61	0.42
16:a:595:ILE:HG22	30:a:709:CLA:H191	2.01	0.42
17:b:559:TRP:CD1	30:b:703:CLA:H43	2.54	0.42
19:D:80:PRO:HG3	30:D:311:CLA:C2D	2.49	0.42
21:H:124:TYR:CZ	21:H:130:LEU:HA	2.54	0.42
25:N:164:GLU:HB2	30:N:310:CLA:C1B	2.48	0.42
30:I:321:CLA:HBC3	30:I:321:CLA:HHD	2.02	0.42
30:G:513:CLA:H102	30:G:517:CLA:HMA2	2.01	0.42
17:b:75:HIS:CE1	30:b:706:CLA:HMA2	2.54	0.42
23:L:213:LEU:HG	30:L:313:CLA:HMB2	2.01	0.42
30:L:313:CLA:H11	30:L:313:CLA:H51	1.77	0.42
34:P:202:PID:H16	34:P:202:PID:HM41	1.72	0.42
33:I:320:LMG:H131	33:I:320:LMG:H162	1.76	0.42
30:I:321:CLA:HBC2	34:j:105:PID:C12	2.49	0.42
2:K:30:LEU:O	2:K:36:ALA:HB1	2.19	0.42
5:G:197:GLY:O	5:G:201:MET:HG3	2.19	0.42
35:A:318:SQD:H272	17:b:298:LEU:HD21	1.99	0.42
8:d:177:PHE:HZ	8:d:180:PRO:HG2	1.84	0.42
10:f:213:VAL:O	10:f:217:VAL:HG22	2.19	0.42
14:l:203:LEU:HD11	30:b:727:CLA:H192	2.01	0.42
37:l:302:BCR:H24C	37:l:302:BCR:H371	1.74	0.42
16:a:308:LEU:HD11	30:a:723:CLA:H172	2.00	0.42
30:a:717:CLA:H61	30:a:717:CLA:H41	1.82	0.42
17:b:362:HIS:HB2	30:b:720:CLA:C1B	2.49	0.42
19:D:173:ARG:HB2	34:D:301:PID:HM23	2.01	0.42
23:L:117:PHE:CG	23:L:132:GLU:HB3	2.54	0.42
23:L:150:GLU:HG2	23:L:219:VAL:HG13	2.02	0.42
30:O:309:CLA:CGA	30:O:309:CLA:H3A	2.49	0.42
34:P:203:PID:HM12	30:P:215:CLA:HAC1	2.01	0.42
1:I:162:HIS:HA	1:I:165:VAL:HG22	2.00	0.42
28:I:305:DD6:C4	30:I:309:CLA:HBB2	2.50	0.42
2:K:90:SER:HB3	2:K:93:GLU:OE1	2.20	0.42
5:G:89:ARG:HA	5:G:92:GLU:HB2	2.01	0.42
30:G:513:CLA:H121	30:G:517:CLA:HED2	2.01	0.42
6:A:32:TYR:OH	28:A:305:DD6:O2	2.31	0.42
10:f:112:LYS:NZ	10:f:160:ASP:O	2.42	0.42
30:f:302:CLA:HMB1	30:f:302:CLA:HBB1	2.02	0.42
37:i:201:BCR:H383	37:l:302:BCR:H353	2.00	0.42
14:l:59:LYS:HZ2	14:l:114:GLU:N	2.17	0.42
14:l:214:ARG:NH2	16:a:405:GLU:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:508:TRP:NE1	30:a:724:CLA:HMD3	2.34	0.42
24:M:272:ILE:HD13	30:M:317:CLA:O1D	2.20	0.42
3:z:90:UNK:HA	8:d:181:ALA:HB1	2.01	0.42
30:G:520:CLA:H3A	30:G:520:CLA:HBA2	1.63	0.42
9:e:66:LYS:HB2	9:e:119:ALA:HB2	2.01	0.42
30:f:301:CLA:CGA	30:j:104:CLA:H43	2.48	0.42
37:i:201:BCR:H272	30:a:725:CLA:HMA2	2.01	0.42
16:a:418:ILE:HD13	16:a:418:ILE:HA	1.85	0.42
30:a:722:CLA:H93	30:a:722:CLA:H62	1.83	0.42
30:b:717:CLA:H203	30:b:721:CLA:CAD	2.50	0.42
33:b:734:LMG:HC2	33:b:734:LMG:HC71	1.63	0.42
18:B:174:MET:HG2	30:B:311:CLA:HAA2	2.00	0.42
19:D:37:ALA:HB3	19:D:38:PRO:HD3	2.01	0.42
19:D:85:LYS:HD3	19:D:85:LYS:HA	1.93	0.42
30:D:314:CLA:HED2	30:D:314:CLA:HBD	1.78	0.42
21:H:100:LYS:HD2	30:H:308:CLA:C3D	2.49	0.42
30:M:310:CLA:HAC1	30:M:316:CLA:CBB	2.48	0.42
5:G:49:MET:HG2	5:G:89:ARG:HH21	1.84	0.42
30:l:303:CLA:HAA1	30:F:312:CLA:H3A	2.01	0.42
16:a:104:LEU:O	16:a:107:GLN:HB2	2.20	0.42
16:a:190:GLY:HA2	16:a:266:GLY:HA2	2.00	0.42
30:B:310:CLA:H92	30:B:310:CLA:H61	1.68	0.42
26:O:109:ARG:O	26:O:113:GLU:N	2.48	0.42
26:O:124:ALA:HB3	34:O:305:PID:HM43	2.01	0.42
27:P:184:ASP:HA	27:P:187:THR:HG22	2.01	0.42
29:I:304:UIX:C9	29:I:304:UIX:C3	2.97	0.42
14:l:282:LEU:HD13	30:l:305:CLA:H93	2.02	0.42
16:a:352:ALA:HB2	16:a:511:LEU:HD13	2.00	0.42
17:b:77:THR:HG21	17:b:171:ILE:HD11	2.02	0.42
17:b:90:ILE:O	17:b:94:ALA:HB3	2.20	0.42
17:b:261:LEU:HG	17:b:476:ASP:HB2	2.01	0.42
30:b:724:CLA:H93	30:b:724:CLA:H111	1.85	0.42
38:b:729:PQN:H212	38:b:729:PQN:H171	1.66	0.42
19:D:46:GLY:C	19:D:48:SER:H	2.27	0.42
21:H:187:ASP:N	21:H:188:PRO:HD3	2.35	0.42
22:J:158:LEU:HD23	22:J:158:LEU:HA	1.91	0.42
25:N:128:GLU:HG2	30:N:309:CLA:HMA3	2.00	0.42
34:O:305:PID:H16	31:O:315:KC1:C3B	2.49	0.42
30:G:511:CLA:H12	30:G:511:CLA:H51	1.81	0.42
12:i:60:TYR:HB3	17:b:131:ILE:HD11	2.01	0.42
13:j:70:ASN:ND2	30:j:104:CLA:OBD	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:l:163:ILE:HG22	14:l:168:ASN:ND2	2.35	0.42
16:a:291:TYR:CG	16:a:296:ILE:HG12	2.55	0.42
30:a:721:CLA:H62	30:a:721:CLA:H102	1.81	0.42
30:b:713:CLA:H112	30:b:713:CLA:H71	1.86	0.42
18:B:157:PHE:HB2	18:B:162:PHE:CD2	2.55	0.42
20:F:95:LYS:O	20:F:99:ILE:HD12	2.20	0.42
21:H:101:HIS:HB3	21:H:206:MET:SD	2.60	0.42
21:H:222:ALA:HB1	21:H:223:TRP:HE3	1.85	0.42
22:J:290:UNK:N	30:J:301:CLA:OBD	2.53	0.42
24:M:153:ARG:NH2	24:M:232:GLY:O	2.53	0.42
27:P:56:ARG:HE	27:P:56:ARG:HB3	1.68	0.42
5:G:220:LEU:HD22	5:G:220:LEU:HA	1.89	0.42
10:f:190:TRP:CE3	30:f:302:CLA:HBA1	2.55	0.42
12:i:91:PHE:HE2	17:b:661:ILE:HG21	1.85	0.42
16:a:99:HIS:ND1	16:a:121:ILE:HD12	2.34	0.42
30:a:704:CLA:H92	30:a:704:CLA:H62	1.88	0.42
30:a:723:CLA:H142	30:a:723:CLA:H111	1.78	0.42
17:b:61:THR:O	17:b:65:ASN:ND2	2.29	0.42
30:b:707:CLA:H51	30:b:722:CLA:H52	2.02	0.42
30:b:718:CLA:H43	30:B:301:CLA:C2D	2.50	0.42
30:b:723:CLA:HAB	30:b:726:CLA:HBB2	2.02	0.42
18:B:182:GLN:O	18:B:186:ILE:HG12	2.20	0.42
34:F:304:PID:HM52	30:F:313:CLA:HHC	2.01	0.42
21:H:69:GLY:HA3	30:H:305:CLA:O1D	2.20	0.42
21:H:137:PRO:HD2	21:H:145:LYS:HG3	2.02	0.42
30:L:308:CLA:HBC3	30:L:308:CLA:HHD	2.01	0.42
34:P:203:PID:H16	34:P:203:PID:HM41	1.90	0.42
16:a:575:SER:HA	16:a:578:ILE:HG22	2.02	0.42
16:a:595:ILE:O	16:a:599:ILE:HG12	2.20	0.42
30:b:709:CLA:C1A	30:b:709:CLA:CGA	2.98	0.42
30:H:304:CLA:HBD	31:H:310:KC1:OBD	2.20	0.42
24:M:239:LEU:N	24:M:240:PRO:HD2	2.35	0.42
1:I:146:LEU:HD13	1:I:146:LEU:HA	1.81	0.41
30:K:308:CLA:H62	30:K:308:CLA:H41	1.56	0.41
5:G:91:ALA:O	5:G:95:HIS:ND1	2.42	0.41
7:c:137:GLU:OE1	7:c:148:ARG:NH1	2.52	0.41
10:f:243:ASN:OD1	10:f:243:ASN:N	2.52	0.41
12:i:123:LYS:HA	12:i:123:LYS:HD3	1.75	0.41
37:i:201:BCR:H15C	37:i:201:BCR:H351	1.78	0.41
14:l:37:LYS:HD3	14:l:42:GLN:OE1	2.20	0.41
14:l:73:SER:O	14:l:74:TYR:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:l:74:TYR:CG	14:l:106:PRO:HG3	2.55	0.41
16:a:133:SER:HB2	30:a:717:CLA:HED1	2.02	0.41
16:a:134:GLU:O	30:a:714:CLA:HED1	2.20	0.41
17:b:352:ASP:HB3	17:b:355:TYR:HB2	2.01	0.41
17:b:489:VAL:HG11	17:b:563:TYR:CG	2.54	0.41
19:D:127:GLU:OE2	34:D:302:PID:H22A	2.20	0.41
20:F:165:LYS:HE2	20:F:165:LYS:HB3	1.78	0.41
30:H:305:CLA:H162	30:H:305:CLA:H141	1.77	0.41
23:L:269:ALA:HB2	23:L:278:TRP:CD1	2.55	0.41
26:O:235:LEU:HD12	26:O:235:LEU:HA	1.83	0.41
30:I:311:CLA:HBA1	30:I:311:CLA:H3A	1.64	0.41
10:f:74:PRO:HG3	17:b:462:TYR:CE1	2.55	0.41
16:a:372:PRO:O	16:a:376:HIS:ND1	2.29	0.41
17:b:42:TYR:HE2	30:b:727:CLA:HMA1	1.85	0.41
17:b:131:ILE:HD12	17:b:131:ILE:HA	1.86	0.41
17:b:429:HIS:C	17:b:429:HIS:CD2	2.97	0.41
17:b:616:LEU:HD23	17:b:616:LEU:HA	1.86	0.41
37:b:730:BCR:H351	37:b:730:BCR:H15C	1.70	0.41
22:J:76:PRO:HB3	22:J:90:PHE:CZ	2.55	0.41
27:P:66:ARG:HB3	30:P:215:CLA:HAC1	2.02	0.41
34:G:507:PID:HM41	34:G:507:PID:H16	1.80	0.41
12:i:96:PHE:CD1	17:b:45:VAL:HG11	2.56	0.41
17:b:646:ILE:HD13	17:b:646:ILE:HA	1.94	0.41
37:b:732:BCR:H11C	37:b:732:BCR:H341	1.97	0.41
23:L:235:ARG:HB2	28:L:305:DD6:O4	2.19	0.41
1:I:71:GLU:OE1	1:I:71:GLU:N	2.44	0.41
2:K:77:ASP:HB3	2:K:182:TRP:H	1.85	0.41
8:d:100:THR:OG1	16:a:371:ASP:OD1	2.37	0.41
8:d:249:PRO:HG3	8:d:281:VAL:HG11	2.01	0.41
37:j:102:BCR:H24C	37:j:102:BCR:H371	1.86	0.41
16:a:530:PHE:HZ	16:a:667:ARG:HD3	1.85	0.41
30:a:707:CLA:H41	39:a:733:LHG:H271	2.02	0.41
17:b:404:HIS:CE1	17:b:408:ILE:HD11	2.55	0.41
18:B:223:GLU:C	18:B:225:ASP:H	2.27	0.41
20:F:88:LEU:HD13	20:F:88:LEU:HA	1.81	0.41
22:J:92:ASP:HA	28:J:304:DD6:O4	2.20	0.41
30:J:307:CLA:H52	30:J:308:CLA:HBA2	2.03	0.41
1:I:182:GLU:N	1:I:183:PRO:HD3	2.35	0.41
30:I:316:CLA:H42	30:I:319:CLA:HMC1	2.02	0.41
30:G:514:CLA:H61	30:G:514:CLA:H41	1.71	0.41
10:f:101:GLU:HB2	10:f:158:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:174:TYR:CE2	16:a:175:LYS:HG3	2.55	0.41
16:a:438:LYS:HB3	16:a:438:LYS:HE2	1.74	0.41
17:b:357:THR:HA	17:b:564:PHE:HE2	1.85	0.41
17:b:400:ARG:NE	30:b:723:CLA:OBD	2.34	0.41
30:b:701:CLA:H71	30:b:727:CLA:H102	2.03	0.41
19:D:82:ILE:HG23	19:D:83:THR:OG1	2.21	0.41
19:D:114:LEU:HD22	19:D:114:LEU:H	1.85	0.41
34:D:301:PID:H16	34:D:301:PID:HM41	1.82	0.41
22:J:133:PHE:HE1	22:J:247:UNK:CB	2.34	0.41
26:O:85:ALA:HB3	30:O:309:CLA:O1D	2.21	0.41
27:P:51:MET:O	27:P:55:LYS:HB2	2.19	0.41
27:P:167:LEU:HD13	27:P:167:LEU:HA	1.88	0.41
2:K:56:ARG:HH11	2:K:59:GLU:HG2	1.86	0.41
2:K:139:LEU:O	30:K:313:CLA:HBD	2.21	0.41
30:A:312:CLA:H52	30:A:312:CLA:H11	1.79	0.41
7:c:155:GLU:OE2	12:i:173:TRP:HD1	2.04	0.41
10:f:226:TRP:CD1	10:f:227:PRO:HD3	2.56	0.41
37:j:102:BCR:H11C	37:j:102:BCR:H341	1.94	0.41
14:l:70:PRO:HB2	14:l:71:GLU:H	1.66	0.41
14:l:251:ASP:OD2	14:l:258:GLY:N	2.40	0.41
30:l:305:CLA:H3A	30:l:305:CLA:HBA1	1.84	0.41
30:a:709:CLA:CHC	30:a:710:CLA:HMD2	2.50	0.41
17:b:434:ILE:HG21	17:b:580:TYR:CD2	2.56	0.41
17:b:678:VAL:HG11	30:b:728:CLA:HED3	2.02	0.41
19:D:118:GLN:HG2	33:D:317:LMG:H332	2.03	0.41
34:D:301:PID:HM22	30:D:309:CLA:HAC2	2.03	0.41
22:J:192:MET:HB2	22:J:192:MET:HE3	1.65	0.41
22:J:213:MET:HB2	30:J:306:CLA:HED2	2.02	0.41
1:I:9:PHE:HD2	2:K:121:ALA:HB2	1.86	0.41
2:K:180:ARG:HH12	2:K:181:THR:HG1	1.67	0.41
6:A:124:PHE:HD1	33:B:318:LMG:H381	1.85	0.41
7:c:87:VAL:HG22	7:c:149:VAL:HG22	2.03	0.41
9:e:92:TYR:HA	9:e:112:ALA:HA	2.03	0.41
14:l:237:GLY:HA3	37:l:306:BCR:H19C	2.03	0.41
30:l:310:CLA:H3A	30:l:310:CLA:HBA1	1.85	0.41
16:a:352:ALA:HB2	16:a:511:LEU:CD1	2.50	0.41
17:b:365:TYR:HA	17:b:557:ASN:OD1	2.21	0.41
18:B:148:TRP:O	18:B:152:ASP:HB2	2.21	0.41
34:D:304:PID:H16	34:D:304:PID:HM41	1.75	0.41
20:F:109:LEU:HB3	20:F:114:TRP:NE1	2.36	0.41
24:M:258:ARG:HG2	30:M:309:CLA:C4C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:N:82:GLU:O	25:N:85:GLY:N	2.50	0.41
2:K:59:GLU:HB2	30:K:308:CLA:C1B	2.51	0.41
3:z:53:UNK:O	14:l:248:THR:OG1	2.39	0.41
5:G:69:LEU:HB3	5:G:82:TYR:CG	2.55	0.41
12:i:72:PRO:O	12:i:76:LEU:HB2	2.20	0.41
12:i:76:LEU:C	12:i:79:PRO:HD2	2.46	0.41
37:i:201:BCR:H332	30:b:705:CLA:H143	2.02	0.41
30:l:303:CLA:H72	30:l:303:CLA:H112	1.77	0.41
37:m:201:BCR:HC8	17:b:78:ILE:HG12	2.02	0.41
37:m:201:BCR:H15C	37:m:201:BCR:H351	1.65	0.41
16:a:241:SER:HA	30:a:738:CLA:O1D	2.21	0.41
16:a:578:ILE:HG23	16:a:579:GLN:HG3	2.03	0.41
16:a:626:HIS:CE1	16:a:631:ILE:HG22	2.56	0.41
30:a:708:CLA:HMB3	30:a:709:CLA:H3A	2.02	0.41
30:a:731:CLA:H18	30:a:735:CLA:H201	2.01	0.41
17:b:389:PRO:HB3	17:b:393:GLU:HB2	2.03	0.41
37:b:702:BCR:H11C	37:b:702:BCR:H341	1.82	0.41
30:b:716:CLA:HBA1	30:b:716:CLA:H3A	1.80	0.41
34:F:306:PID:H16	34:F:306:PID:HM41	1.77	0.41
23:L:97:ARG:NH2	23:L:99:GLU:HA	2.35	0.41
26:O:136:PHE:CD2	26:O:149:ALA:HA	2.56	0.41
27:P:67:ILE:HD12	30:P:214:CLA:HHD	2.02	0.41
27:P:103:LEU:HD12	27:P:106:ILE:HD11	2.02	0.41
1:I:59:VAL:HG13	1:I:171:PHE:HE2	1.82	0.41
1:I:107:ILE:HD11	30:I:311:CLA:CHD	2.50	0.41
2:K:35:GLY:H	2:K:155:LEU:HD22	1.84	0.41
2:K:110:TRP:O	2:K:113:ILE:HG22	2.21	0.41
5:G:3:UNK:N	9:e:56:TRP:O	2.53	0.41
5:G:47:LYS:HD2	5:G:47:LYS:HA	1.75	0.41
8:d:199:ARG:NH2	8:d:224:ALA:O	2.42	0.41
37:f:304:BCR:H12C	37:f:304:BCR:H15C	1.85	0.41
11:h:112:LEU:HD23	11:h:115:ILE:HD12	2.03	0.41
12:i:107:ARG:NH1	12:i:177:SER:O	2.54	0.41
37:i:201:BCR:H11C	37:i:201:BCR:H341	1.89	0.41
33:j:101:LMG:HC92	33:j:101:LMG:H292	1.78	0.41
14:l:69:PRO:HD2	14:l:79:LYS:HD3	2.01	0.41
14:l:211:GLY:H	14:l:214:ARG:HB3	1.86	0.41
30:m:202:CLA:H42	30:b:705:CLA:H11	2.01	0.41
30:m:202:CLA:HBA1	30:m:202:CLA:H3A	1.75	0.41
16:a:261:HIS:HB2	30:a:716:CLA:CHB	2.51	0.41
16:a:263:LYS:HE3	16:a:263:LYS:HB3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:707:CLA:H141	30:a:723:CLA:HBB2	2.03	0.41
30:a:707:CLA:H2	30:a:707:CLA:H61	1.69	0.41
17:b:560:ILE:HD13	33:b:734:LMG:H112	2.03	0.41
17:b:610:VAL:HG21	30:b:710:CLA:HMD3	2.03	0.41
30:b:706:CLA:HBA1	30:b:706:CLA:H3A	1.62	0.41
18:B:99:TYR:CE1	30:B:307:CLA:HBB1	2.55	0.41
30:H:307:CLA:H3A	30:H:307:CLA:HBA2	1.85	0.41
23:L:152:GLU:OE2	23:L:256:ARG:NE	2.33	0.41
23:L:247:MET:CE	30:L:314:CLA:H2	2.51	0.41
30:L:313:CLA:HBA1	30:L:313:CLA:H3A	1.67	0.41
30:L:317:CLA:HHC	30:L:317:CLA:CBB	2.51	0.41
24:M:130:PRO:HD2	28:M:303:DD6:C33	2.51	0.41
25:N:82:GLU:O	25:N:83:ILE:C	2.63	0.41
27:P:80:LEU:HD13	34:P:208:PID:HM22	2.03	0.41
5:G:191:LEU:O	5:G:195:LYS:HG2	2.21	0.41
8:d:204:ARG:NH2	17:b:521:MET:HE2	2.35	0.41
8:d:270:TYR:HB3	17:b:196:PRO:HD3	2.03	0.41
8:d:273:ARG:HA	8:d:276:GLU:CD	2.45	0.41
30:l:311:CLA:CHA	30:l:311:CLA:HBA1	2.49	0.41
16:a:299:SER:OG	16:a:350:SER:O	2.34	0.41
30:B:309:CLA:H41	30:B:309:CLA:H61	1.71	0.41
19:D:55:ASN:ND2	19:D:59:ARG:HE	2.14	0.41
34:F:304:PID:HM52	30:F:313:CLA:CHC	2.51	0.41
22:J:192:MET:O	22:J:196:LEU:HB2	2.21	0.41
23:L:100:LEU:HG	23:L:104:TYR:CZ	2.56	0.41
23:L:262:PHE:O	23:L:266:VAL:HG22	2.22	0.41
25:N:69:ARG:HD2	30:N:310:CLA:C4C	2.51	0.41
27:P:67:ILE:HD13	30:P:214:CLA:HBC3	2.03	0.41
27:P:128:GLN:O	27:P:141:PHE:CD1	2.74	0.41
34:P:208:PID:H16	34:P:208:PID:HM41	1.77	0.41
2:K:66:CYS:SG	2:K:165:MET:HA	2.61	0.40
2:K:180:ARG:HH11	2:K:181:THR:H	1.68	0.40
5:G:99:CYS:SG	5:G:201:MET:HA	2.61	0.40
5:G:141:PHE:O	5:G:145:VAL:HG13	2.21	0.40
28:G:508:DD6:C	30:G:517:CLA:HBB2	2.51	0.40
11:h:28:TYR:CE2	11:h:30:HIS:HB2	2.56	0.40
14:l:69:PRO:HG3	14:l:75:LEU:HG	2.03	0.40
15:m:71:ARG:HA	15:m:74:GLU:HG2	2.03	0.40
16:a:392:TYR:HE1	16:a:559:SER:O	2.04	0.40
30:a:726:CLA:H141	30:a:726:CLA:H161	1.75	0.40
30:a:728:CLA:H52	30:a:728:CLA:H11	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:708:CLA:HAA2	30:b:710:CLA:HED1	2.04	0.40
30:b:713:CLA:H141	30:b:713:CLA:H161	1.80	0.40
30:F:310:CLA:H2A	30:F:310:CLA:O2D	2.20	0.40
21:H:95:ARG:O	21:H:99:ILE:HG13	2.21	0.40
27:P:172:LEU:CD2	34:P:206:PID:H11	2.51	0.40
1:I:162:HIS:CE1	1:I:166:VAL:HG21	2.56	0.40
6:A:202:LEU:HD21	30:A:315:CLA:HMA1	2.04	0.40
7:c:156:GLU:HB3	7:c:161:LEU:HG	2.03	0.40
11:h:29:TRP:HZ3	17:b:200:GLN:HB2	1.87	0.40
16:a:398:LEU:HD23	16:a:401:LEU:HD12	2.02	0.40
30:b:717:CLA:H143	30:b:717:CLA:H162	1.81	0.40
30:b:720:CLA:H11	30:b:720:CLA:H52	1.93	0.40
20:F:34:VAL:HG23	30:F:308:CLA:HED2	2.02	0.40
21:H:194:LYS:C	30:H:309:CLA:HMA1	2.46	0.40
22:J:91:TRP:CE2	22:J:93:PRO:HG3	2.56	0.40
23:L:124:ALA:HB3	23:L:130:ARG:NH2	2.36	0.40
23:L:204:ILE:HG22	30:L:317:CLA:HBC1	2.03	0.40
24:M:210:GLY:O	24:M:214:GLN:HG2	2.21	0.40
25:N:38:ALA:HB3	25:N:39:PRO:HD3	2.03	0.40
26:O:116:HIS:O	26:O:120:ALA:N	2.39	0.40
30:P:210:CLA:H2	30:P:210:CLA:C1B	2.52	0.40
30:I:310:CLA:H3A	30:I:310:CLA:HBA2	1.69	0.40
30:K:313:CLA:HBB1	30:K:313:CLA:HMB3	2.03	0.40
5:G:46:PHE:CZ	5:G:60:ALA:HB1	2.55	0.40
6:A:136:LYS:HD2	6:A:153:TYR:CE1	2.56	0.40
37:i:201:BCR:H20C	37:i:201:BCR:H361	1.91	0.40
14:l:70:PRO:O	14:l:76:TYR:CD1	2.75	0.40
16:a:194:THR:HG23	16:a:266:GLY:HA3	2.03	0.40
17:b:434:ILE:HD12	17:b:439:PRO:HA	2.03	0.40
19:D:140:ALA:HB3	30:D:314:CLA:CAD	2.52	0.40
21:H:71:GLN:OE1	21:H:196:ALA:HB1	2.21	0.40
21:H:163:LEU:HD11	30:J:307:CLA:H101	2.03	0.40
22:J:164:MET:HA	30:J:310:CLA:CBC	2.51	0.40
30:J:301:CLA:H62	30:J:301:CLA:H92	1.78	0.40
27:P:36:PRO:HB3	30:P:209:CLA:C3B	2.52	0.40
1:I:147:LYS:HZ2	1:I:150:ARG:HH11	1.69	0.40
2:K:126:MET:HG3	33:j:101:LMG:O2	2.21	0.40
5:G:11:HIS:HB2	9:e:117:ILE:HD13	2.03	0.40
5:G:73:ASN:HB3	5:G:79:LEU:O	2.21	0.40
5:G:77:ASN:HD21	5:G:81:VAL:HG11	1.85	0.40
6:A:18:GLY:HA3	6:A:147:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:103:CYS:HA	36:c:201:SF4:S4	2.61	0.40
7:c:144:PHE:CZ	17:b:518:PRO:HD2	2.55	0.40
30:f:303:CLA:HBA1	30:f:303:CLA:H3A	1.41	0.40
11:h:46:MET:HE3	17:b:304:ASP:HB3	2.03	0.40
16:a:34:ASN:HB3	16:a:38:TYR:CE2	2.55	0.40
16:a:287:ILE:HG23	16:a:291:TYR:CD2	2.56	0.40
16:a:369:HIS:O	16:a:372:PRO:HD2	2.21	0.40
16:a:443:ILE:HD11	16:a:536:ASP:O	2.21	0.40
17:b:390:LEU:H	17:b:390:LEU:HD22	1.87	0.40
17:b:397:LYS:HD3	17:b:397:LYS:HA	1.88	0.40
17:b:601:SER:OG	17:b:602:THR:N	2.54	0.40
30:F:310:CLA:CHA	30:F:310:CLA:HBA1	2.51	0.40
27:P:76:ILE:HG13	27:P:77:THR:N	2.36	0.40
2:K:34:VAL:HG12	2:K:158:LEU:HD12	2.02	0.40
6:A:94:CYS:SG	30:A:310:CLA:HAA2	2.62	0.40
30:A:319:CLA:HBB1	37:b:730:BCR:H271	2.03	0.40
8:d:87:LEU:HG	8:d:90:SER:HB2	2.03	0.40
8:d:260:GLU:OE1	17:b:191:HIS:N	2.54	0.40
9:e:117:ILE:HD12	9:e:117:ILE:HA	1.91	0.40
12:i:111:GLU:O	12:i:115:GLU:HG3	2.22	0.40
37:l:307:BCR:H342	30:l:311:CLA:H143	2.02	0.40
16:a:325:LYS:HB3	16:a:325:LYS:HE3	1.76	0.40
16:a:380:VAL:HG21	30:a:729:CLA:C2C	2.51	0.40
17:b:325:ILE:HD12	30:b:706:CLA:OBD	2.22	0.40
17:b:563:TYR:HA	17:b:584:TRP:HH2	1.85	0.40
17:b:627:MET:O	17:b:631:SER:OG	2.25	0.40
30:b:720:CLA:H62	30:b:720:CLA:H41	1.82	0.40
30:B:313:CLA:H141	30:B:313:CLA:H162	1.89	0.40
19:D:169:LEU:HA	19:D:169:LEU:HD13	1.77	0.40
20:F:166:ASN:ND2	20:F:169:SER:HB2	2.36	0.40
21:H:88:MET:HG3	21:H:92:LYS:NZ	2.37	0.40
21:H:125:LEU:HB3	21:H:131:LEU:HB2	2.03	0.40
24:M:258:ARG:HG2	30:M:309:CLA:C3C	2.51	0.40
34:N:302:PID:H16	34:N:302:PID:HM41	1.78	0.40
30:P:210:CLA:HBB1	30:P:210:CLA:HMB3	2.03	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	I	191/200 (96%)	163 (85%)	28 (15%)	0	100	100
2	K	171/177 (97%)	160 (94%)	11 (6%)	0	100	100
5	G	204/224 (91%)	175 (86%)	27 (13%)	2 (1%)	12	45
6	A	162/189 (86%)	144 (89%)	14 (9%)	4 (2%)	4	23
7	c	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
8	d	216/218 (99%)	197 (91%)	19 (9%)	0	100	100
9	e	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	f	182/184 (99%)	177 (97%)	4 (2%)	1 (0%)	24	60
11	h	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
12	i	117/119 (98%)	105 (90%)	12 (10%)	0	100	100
13	j	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
14	l	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	30	65
15	m	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
16	a	668/670 (100%)	622 (93%)	43 (6%)	3 (0%)	30	65
17	b	661/663 (100%)	613 (93%)	47 (7%)	1 (0%)	43	76
18	B	171/192 (89%)	153 (90%)	15 (9%)	3 (2%)	6	31
19	D	156/165 (94%)	131 (84%)	22 (14%)	3 (2%)	6	30
20	F	165/176 (94%)	153 (93%)	10 (6%)	2 (1%)	10	40
21	H	158/160 (99%)	140 (89%)	16 (10%)	2 (1%)	9	38
22	J	164/220 (74%)	146 (89%)	17 (10%)	1 (1%)	21	56
23	L	183/185 (99%)	161 (88%)	22 (12%)	0	100	100
24	M	164/173 (95%)	151 (92%)	13 (8%)	0	100	100
25	N	149/160 (93%)	119 (80%)	24 (16%)	6 (4%)	2	14
26	O	159/161 (99%)	130 (82%)	25 (16%)	4 (2%)	4	23
27	P	155/160 (97%)	135 (87%)	19 (12%)	1 (1%)	21	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4901/5113 (96%)	4446 (91%)	421 (9%)	34 (1%)	20 53

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	121	PRO
6	A	85	ALA
14	l	70	PRO
16	a	47	ARG
16	a	218	PRO
19	D	134	PRO
21	H	72	ALA
25	N	88	PRO
25	N	109	ILE
25	N	113	PRO
25	N	153	ASP
26	O	159	SER
26	O	205	PRO
27	P	35	ALA
5	G	76	PHE
21	H	125	LEU
26	O	204	ALA
6	A	79	PRO
10	f	254	GLN
19	D	156	GLU
16	a	220	ILE
18	B	119	LEU
20	F	33	GLY
22	J	74	GLU
18	B	93	MET
20	F	32	LEU
25	N	82	GLU
6	A	33	ASN
17	b	311	LEU
19	D	37	ALA
6	A	132	GLY
18	B	165	VAL
25	N	38	ALA
26	O	237	GLY

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	I	139/155 (90%)	131 (94%)	8 (6%)	18 51
2	K	133/138 (96%)	126 (95%)	7 (5%)	20 54
5	G	147/171 (86%)	136 (92%)	11 (8%)	12 41
6	A	122/129 (95%)	117 (96%)	5 (4%)	27 61
7	c	76/76 (100%)	75 (99%)	1 (1%)	61 81
8	d	182/184 (99%)	176 (97%)	6 (3%)	33 67
9	e	63/63 (100%)	63 (100%)	0	100 100
10	f	148/148 (100%)	145 (98%)	3 (2%)	48 76
11	h	112/114 (98%)	111 (99%)	1 (1%)	70 85
12	i	100/101 (99%)	99 (99%)	1 (1%)	68 84
13	j	88/89 (99%)	84 (96%)	4 (4%)	24 59
14	l	199/201 (99%)	189 (95%)	10 (5%)	22 56
15	m	60/63 (95%)	59 (98%)	1 (2%)	53 78
16	a	540/592 (91%)	517 (96%)	23 (4%)	26 60
17	b	557/581 (96%)	540 (97%)	17 (3%)	35 68
18	B	142/146 (97%)	123 (87%)	19 (13%)	4 18
19	D	116/123 (94%)	91 (78%)	25 (22%)	1 6
20	F	126/140 (90%)	106 (84%)	20 (16%)	2 13
21	H	123/123 (100%)	111 (90%)	12 (10%)	7 30
22	J	124/136 (91%)	107 (86%)	17 (14%)	3 17
23	L	140/145 (97%)	115 (82%)	25 (18%)	2 10
24	M	106/128 (83%)	86 (81%)	20 (19%)	1 9
25	N	80/124 (64%)	52 (65%)	28 (35%)	0 1
26	O	89/124 (72%)	70 (79%)	19 (21%)	1 6
27	P	105/123 (85%)	72 (69%)	33 (31%)	0 1
All	All	3817/4117 (93%)	3501 (92%)	316 (8%)	12 37

All (316) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	7	VAL
1	I	20	VAL
1	I	24	THR
1	I	108	THR
1	I	118	ARG
1	I	143	LEU
1	I	146	LEU
1	I	188	SER
2	K	24	LEU
2	K	53	ARG
2	K	59	GLU
2	K	80	MET
2	K	140	ARG
2	K	142	LEU
2	K	155	LEU
5	G	17	VAL
5	G	30	ILE
5	G	35	VAL
5	G	42	SER
5	G	68	LYS
5	G	81	VAL
5	G	92	GLU
5	G	119	VAL
5	G	147	ILE
5	G	217	VAL
5	G	220	LEU
6	A	80	GLU
6	A	81	LYS
6	A	94	CYS
6	A	129	GLU
6	A	145	LEU
7	c	127	VAL
8	d	77	VAL
8	d	114	ILE
8	d	115	THR
8	d	255	GLU
8	d	260	GLU
8	d	267	ARG
10	f	113	LEU
10	f	187	ILE
10	f	243	ASN
11	h	113	LEU

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Mol	Chain	Res	Type
12	i	169	HIS
13	j	33	THR
13	j	57	VAL
13	j	58	VAL
13	j	71	VAL
14	l	68	ASN
14	l	71	GLU
14	l	72	ASP
14	l	93	MET
14	l	120	ILE
14	l	148	VAL
14	l	166	THR
14	l	202	PHE
14	l	252	LYS
14	l	255	ASP
15	m	140	GLU
16	a	9	THR
16	a	43	ASP
16	a	105	ILE
16	a	107	GLN
16	a	108	ASP
16	a	109	ILE
16	a	150	LEU
16	a	241	SER
16	a	284	GLN
16	a	292	ILE
16	a	296	ILE
16	a	304	LEU
16	a	327	THR
16	a	337	ILE
16	a	380	VAL
16	a	384	ILE
16	a	435	MET
16	a	503	CYS
16	a	511	LEU
16	a	522	LEU
16	a	660	THR
16	a	666	SER
16	a	668	LEU
17	b	58	ILE
17	b	63	SER
17	b	184	LEU

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Mol	Chain	Res	Type
17	b	188	LEU
17	b	238	ILE
17	b	289	HIS
17	b	325	ILE
17	b	412	LEU
17	b	434	ILE
17	b	557	ASN
17	b	570	THR
17	b	596	LEU
17	b	602	THR
17	b	650	THR
17	b	651	PRO
17	b	652	ILE
17	b	667	LEU
18	B	91	VAL
18	B	97	VAL
18	B	105	ARG
18	B	113	GLU
18	B	121	THR
18	B	140	ILE
18	B	152	ASP
18	B	158	GLU
18	B	165	VAL
18	B	169	ASN
18	B	176	GLU
18	B	179	VAL
18	B	215	ILE
18	B	222	LYS
18	B	224	GLU
18	B	226	LYS
18	B	228	LYS
18	B	230	MET
18	B	253	ASN
19	D	30	GLU
19	D	31	ASN
19	D	36	GLN
19	D	39	THR
19	D	64	ILE
19	D	75	MET
19	D	82	ILE
19	D	83	THR
19	D	90	LEU

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Mol	Chain	Res	Type
19	D	113	VAL
19	D	114	LEU
19	D	129	SER
19	D	132	GLN
19	D	142	ASP
19	D	143	PHE
19	D	151	LYS
19	D	153	ILE
19	D	159	GLU
19	D	161	LEU
19	D	162	LYS
19	D	165	LEU
19	D	169	LEU
19	D	177	MET
19	D	180	ILE
19	D	188	LEU
20	F	29	GLU
20	F	32	LEU
20	F	88	LEU
20	F	95	LYS
20	F	99	ILE
20	F	103	MET
20	F	107	LYS
20	F	111	THR
20	F	117	MET
20	F	123	LEU
20	F	125	GLU
20	F	133	GLU
20	F	142	THR
20	F	145	LYS
20	F	164	VAL
20	F	166	ASN
20	F	167	GLN
20	F	170	LEU
20	F	197	THR
20	F	200	GLU
21	H	70	VAL
21	H	85	ASP
21	H	89	LYS
21	H	91	PHE
21	H	92	LYS
21	H	106	MET

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Mol	Chain	Res	Type
21	H	107	LEU
21	H	110	MET
21	H	130	LEU
21	H	143	ILE
21	H	149	LEU
21	H	207	MET
22	J	73	ARG
22	J	97	THR
22	J	99	ASN
22	J	118	ILE
22	J	134	HIS
22	J	136	LEU
22	J	154	ASN
22	J	156	LEU
22	J	158	LEU
22	J	161	VAL
22	J	174	LEU
22	J	188	ASP
22	J	189	VAL
22	J	192	MET
22	J	196	LEU
22	J	197	GLU
22	J	198	GLU
23	L	97	ARG
23	L	98	ARG
23	L	100	LEU
23	L	102	VAL
23	L	116	LYS
23	L	122	VAL
23	L	125	GLU
23	L	132	GLU
23	L	173	ARG
23	L	187	VAL
23	L	188	ILE
23	L	189	ASP
23	L	194	LEU
23	L	195	ASN
23	L	218	LYS
23	L	235	ARG
23	L	237	PHE
23	L	239	GLU
23	L	240	ASP

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Mol	Chain	Res	Type
23	L	241	ASP
23	L	245	LYS
23	L	249	ILE
23	L	270	VAL
23	L	272	THR
23	L	274	LYS
24	M	118	ASP
24	M	122	PHE
24	M	125	LYS
24	M	141	LEU
24	M	145	ARG
24	M	162	LEU
24	M	167	LEU
24	M	170	LEU
24	M	174	GLU
24	M	180	LEU
24	M	182	PHE
24	M	188	LYS
24	M	218	LYS
24	M	224	GLU
24	M	226	LEU
24	M	227	THR
24	M	247	LEU
24	M	249	TYR
24	M	267	ILE
24	M	277	HIS
25	N	33	GLU
25	N	34	LEU
25	N	37	GLN
25	N	40	VAL
25	N	42	PHE
25	N	43	TRP
25	N	44	ASP
25	N	46	VAL
25	N	53	ASN
25	N	54	VAL
25	N	58	ARG
25	N	64	GLU
25	N	73	LEU
25	N	80	THR
25	N	119	GLN
25	N	128	GLU

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Mol	Chain	Res	Type
25	N	131	GLN
25	N	132	ASP
25	N	133	GLN
25	N	148	VAL
25	N	149	LEU
25	N	153	ASP
25	N	161	LEU
25	N	165	ILE
25	N	173	MET
25	N	176	THR
25	N	184	LEU
25	N	185	THR
26	O	82	GLU
26	O	102	ASP
26	O	107	LYS
26	O	110	ARG
26	O	122	LEU
26	O	127	TYR
26	O	128	MET
26	O	132	ILE
26	O	144	THR
26	O	155	LEU
26	O	173	THR
26	O	178	LEU
26	O	193	PHE
26	O	207	THR
26	O	209	GLU
26	O	212	LEU
26	O	216	LEU
26	O	220	ARG
26	O	235	LEU
27	P	27	PHE
27	P	28	GLU
27	P	29	ASN
27	P	31	LEU
27	P	34	GLN
27	P	52	LYS
27	P	58	ARG
27	P	67	ILE
27	P	72	THR
27	P	73	MET
27	P	77	THR

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Mol	Chain	Res	Type
27	P	81	THR
27	P	95	LYS
27	P	97	GLU
27	P	99	ILE
27	P	106	ILE
27	P	112	VAL
27	P	121	THR
27	P	126	GLN
27	P	128	GLN
27	P	130	GLN
27	P	131	SER
27	P	132	GLU
27	P	134	SER
27	P	141	PHE
27	P	150	VAL
27	P	151	LEU
27	P	160	LYS
27	P	163	LEU
27	P	167	LEU
27	P	172	LEU
27	P	184	ASP
27	P	186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	61	GLN
1	I	191	ASN
2	K	95	HIS
2	K	124	ASN
2	K	154	GLN
5	G	109	GLN
5	G	210	ASN
6	A	33	ASN
8	d	190	ASN
9	e	76	GLN
10	f	247	HIS
13	j	72	ASN
14	l	280	HIS
16	a	46	GLN
16	a	163	HIS
16	a	208	ASN

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Mol	Chain	Res	Type
16	a	284	GLN
16	a	456	HIS
16	a	546	HIS
16	a	579	GLN
16	a	625	HIS
17	b	44	GLN
17	b	67	GLN
17	b	75	HIS
17	b	219	HIS
18	B	163	GLN
18	B	169	ASN
19	D	55	ASN
20	F	166	ASN
20	F	191	ASN
22	J	163	GLN
22	J	232	GLN
23	L	268	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

342 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	$\#\|Z\|>2$
30	CLA	b	721	28	50,54,73	1.37	8 (16%)	59,90,113	1.34	4 (6%)
30	CLA	b	723	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	7 (10%)
31	KC1	M	314	24	49,53,53	1.34	5 (10%)	61,89,89	1.73	14 (22%)
30	CLA	P	209	-	51,55,73	1.37	6 (11%)	60,91,113	1.39	5 (8%)
30	CLA	P	210	-	69,73,73	1.17	6 (8%)	82,113,113	1.31	6 (7%)
28	DD6	I	302	-	40,45,45	1.61	2 (5%)	51,67,67	2.17	18 (35%)
30	CLA	P	214	-	50,54,73	1.34	8 (16%)	59,90,113	1.34	4 (6%)
30	CLA	a	701	-	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
33	LMG	j	101	-	35,35,55	0.88	1 (2%)	43,43,63	1.23	4 (9%)
30	CLA	B	317	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
28	DD6	G	502	-	40,45,45	1.54	2 (5%)	51,67,67	1.87	11 (21%)
28	DD6	h	203	-	40,45,45	1.55	2 (5%)	51,67,67	1.86	12 (23%)
28	DD6	M	305	-	40,45,45	1.56	3 (7%)	51,67,67	1.88	16 (31%)
30	CLA	M	309	24	59,63,73	1.28	6 (10%)	70,101,113	1.31	5 (7%)
31	KC1	D	315	19	49,53,53	1.32	6 (12%)	61,89,89	1.73	15 (24%)
29	UIX	J	305	-	43,49,49	1.35	4 (9%)	53,74,74	2.37	18 (33%)
28	DD6	I	301	-	40,45,45	1.57	2 (5%)	51,67,67	2.17	17 (33%)
30	CLA	D	309	-	50,54,73	1.36	7 (14%)	59,90,113	1.42	4 (6%)
34	PID	O	304	-	43,49,49	1.23	3 (6%)	52,76,76	1.70	11 (21%)
30	CLA	a	716	-	51,55,73	1.35	7 (13%)	60,91,113	1.40	5 (8%)
28	DD6	F	301	-	40,45,45	1.53	2 (5%)	51,67,67	2.31	16 (31%)
30	CLA	J	310	-	50,54,73	1.39	8 (16%)	59,90,113	1.36	3 (5%)
28	DD6	O	303	-	40,45,45	1.60	3 (7%)	51,67,67	2.02	13 (25%)
28	DD6	A	305	31	40,45,45	1.52	2 (5%)	51,67,67	1.89	14 (27%)
30	CLA	m	202	-	64,68,73	1.22	7 (10%)	76,107,113	1.33	6 (7%)
30	CLA	j	106	-	62,66,73	1.24	8 (12%)	73,104,113	1.32	6 (8%)
28	DD6	B	302	-	39,44,45	1.74	2 (5%)	49,65,67	2.08	17 (34%)
30	CLA	K	308	2	58,62,73	1.27	6 (10%)	68,99,113	1.34	6 (8%)
30	CLA	L	318	-	50,54,73	1.37	8 (16%)	59,90,113	1.42	4 (6%)
28	DD6	b	731	30	40,45,45	1.61	2 (5%)	51,67,67	1.98	17 (33%)
30	CLA	G	518	-	50,54,73	1.39	8 (16%)	59,90,113	1.44	5 (8%)
30	CLA	a	711	-	49,53,73	1.38	6 (12%)	58,89,113	1.45	7 (12%)
30	CLA	b	708	-	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
30	CLA	A	311	6	50,54,73	1.37	6 (12%)	59,90,113	1.38	4 (6%)
30	CLA	A	309	-	59,63,73	1.27	6 (10%)	70,101,113	1.32	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	G	513	5	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
31	KC1	D	310	-	49,53,53	1.34	6 (12%)	61,89,89	1.73	13 (21%)
28	DD6	M	304	-	40,45,45	1.59	3 (7%)	51,67,67	1.92	14 (27%)
30	CLA	b	714	-	50,54,73	1.37	7 (14%)	59,90,113	1.42	5 (8%)
30	CLA	a	715	-	49,53,73	1.39	8 (16%)	58,89,113	1.45	4 (6%)
31	KC1	P	211	-	49,53,53	1.33	5 (10%)	61,89,89	1.73	14 (22%)
34	PID	D	305	-	43,49,49	1.26	3 (6%)	52,76,76	1.46	9 (17%)
30	CLA	l	308	-	45,49,73	1.43	7 (15%)	54,84,113	1.45	5 (9%)
33	LMG	D	317	-	48,48,55	0.76	1 (2%)	55,55,63	1.28	5 (9%)
34	PID	D	304	-	43,49,49	1.23	3 (6%)	52,76,76	1.72	7 (13%)
30	CLA	D	308	-	51,55,73	1.36	6 (11%)	60,91,113	1.37	5 (8%)
30	CLA	b	727	-	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
37	BCR	m	201	-	41,41,41	0.68	0	56,56,56	2.35	17 (30%)
30	CLA	B	313	18	69,73,73	1.17	6 (8%)	82,113,113	1.27	4 (4%)
34	PID	F	302	-	43,49,49	1.24	3 (6%)	52,76,76	1.59	7 (13%)
33	LMG	b	733	-	44,44,55	0.81	1 (2%)	52,52,63	1.31	7 (13%)
30	CLA	h	202	-	59,63,73	1.28	7 (11%)	70,101,113	1.33	5 (7%)
34	PID	O	307	-	43,49,49	1.26	3 (6%)	52,76,76	1.28	5 (9%)
30	CLA	l	311	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	5 (6%)
28	DD6	P	204	-	40,45,45	1.53	2 (5%)	51,67,67	2.04	15 (29%)
30	CLA	B	311	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	5 (6%)
30	CLA	A	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.47	5 (9%)
30	CLA	a	720	-	66,70,73	1.21	7 (10%)	78,109,113	1.29	6 (7%)
30	CLA	J	312	-	57,61,73	1.28	8 (14%)	67,98,113	1.42	7 (10%)
30	CLA	H	312	-	50,54,73	1.38	7 (14%)	59,90,113	1.39	4 (6%)
30	CLA	F	311	-	50,54,73	1.37	8 (16%)	59,90,113	1.45	5 (8%)
28	DD6	M	303	-	40,45,45	1.75	4 (10%)	51,67,67	2.19	18 (35%)
34	PID	P	206	-	43,49,49	1.24	3 (6%)	52,76,76	1.82	11 (21%)
30	CLA	b	722	-	69,73,73	1.18	8 (11%)	82,113,113	1.31	6 (7%)
34	PID	P	203	-	43,49,49	1.26	3 (6%)	52,76,76	1.32	6 (11%)
30	CLA	b	711	-	59,63,73	1.27	5 (8%)	70,101,113	1.31	6 (8%)
30	CLA	L	312	-	50,54,73	1.36	7 (14%)	59,90,113	1.39	4 (6%)
30	CLA	H	304	-	51,55,73	1.36	7 (13%)	60,91,113	1.38	5 (8%)
30	CLA	N	304	-	51,55,73	1.36	7 (13%)	60,91,113	1.40	5 (8%)
30	CLA	M	318	-	50,54,73	1.38	8 (16%)	59,90,113	1.37	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DD6	I	303	-	40,45,45	1.82	5 (12%)	51,67,67	2.02	16 (31%)
28	DD6	K	305	-	40,45,45	1.51	2 (5%)	51,67,67	1.86	15 (29%)
30	CLA	N	305	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
34	PID	F	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.91	9 (17%)
30	CLA	D	314	-	50,54,73	1.40	8 (16%)	59,90,113	1.45	6 (10%)
30	CLA	a	735	-	69,73,73	1.18	6 (8%)	82,113,113	1.21	5 (6%)
31	KC1	M	307	30	49,53,53	1.36	6 (12%)	61,89,89	1.79	14 (22%)
38	PQN	a	732	-	34,34,34	1.61	2 (5%)	43,45,45	1.15	5 (11%)
30	CLA	a	708	-	55,59,73	1.32	7 (12%)	64,96,113	1.39	6 (9%)
34	PID	H	302	-	43,49,49	1.29	3 (6%)	52,76,76	1.39	9 (17%)
30	CLA	G	517	-	50,54,73	1.36	7 (14%)	59,90,113	1.38	4 (6%)
33	LMG	B	318	-	37,37,55	0.84	0	45,45,63	1.33	6 (13%)
34	PID	G	506	-	43,49,49	1.29	3 (6%)	52,76,76	1.35	7 (13%)
30	CLA	F	308	-	50,54,73	1.35	8 (16%)	59,90,113	1.40	4 (6%)
28	DD6	L	304	-	40,45,45	1.55	2 (5%)	51,67,67	1.81	12 (23%)
34	PID	N	301	-	43,49,49	1.25	3 (6%)	52,76,76	1.44	6 (11%)
30	CLA	a	725	-	65,69,73	1.21	7 (10%)	77,108,113	1.30	6 (7%)
33	LMG	I	318	-	36,36,55	0.89	1 (2%)	44,44,63	1.25	3 (6%)
30	CLA	N	309	25	50,54,73	1.36	7 (14%)	59,90,113	1.42	4 (6%)
30	CLA	P	212	-	55,59,73	1.32	7 (12%)	64,96,113	1.38	5 (7%)
30	CLA	J	309	-	60,64,73	1.25	9 (15%)	71,102,113	1.40	6 (8%)
30	CLA	a	738	22	50,54,73	1.37	7 (14%)	59,90,113	1.44	5 (8%)
30	CLA	H	311	-	45,49,73	1.44	7 (15%)	54,84,113	1.45	5 (9%)
30	CLA	H	305	-	69,73,73	1.18	6 (8%)	82,113,113	1.29	6 (7%)
30	CLA	J	308	-	50,54,73	1.38	8 (16%)	59,90,113	1.41	6 (10%)
28	DD6	I	305	-	40,45,45	1.80	4 (10%)	51,67,67	2.24	17 (33%)
35	SQD	A	318	-	48,50,54	0.41	1 (2%)	58,61,65	0.58	0
30	CLA	a	729	-	60,64,73	1.26	6 (10%)	71,102,113	1.30	5 (7%)
28	DD6	K	304	-	40,45,45	1.56	2 (5%)	51,67,67	1.99	15 (29%)
30	CLA	O	311	-	55,59,73	1.31	7 (12%)	64,96,113	1.34	5 (7%)
34	PID	O	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.47	5 (9%)
28	DD6	D	303	-	40,45,45	1.49	2 (5%)	51,67,67	1.83	14 (27%)
30	CLA	a	704	-	69,73,73	1.18	7 (10%)	82,113,113	1.17	2 (2%)
30	CLA	b	706	-	52,56,73	1.36	6 (11%)	61,92,113	1.37	6 (9%)
34	PID	M	301	-	43,49,49	1.22	3 (6%)	52,76,76	1.68	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	PID	P	208	-	43,49,49	1.25	3 (6%)	52,76,76	1.42	6 (11%)
30	CLA	a	709	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
30	CLA	A	320	-	50,54,73	1.37	7 (14%)	59,90,113	1.41	4 (6%)
30	CLA	a	728	-	59,63,73	1.27	8 (13%)	70,101,113	1.34	6 (8%)
30	CLA	a	705	30	59,63,73	1.28	7 (11%)	70,101,113	1.37	7 (10%)
28	DD6	B	304	-	40,45,45	1.54	2 (5%)	51,67,67	1.88	11 (21%)
37	BCR	l	307	-	41,41,41	0.67	0	56,56,56	2.02	19 (33%)
28	DD6	L	303	-	40,45,45	1.50	2 (5%)	51,67,67	1.94	14 (27%)
33	LMG	P	201	-	27,27,55	0.99	1 (3%)	35,35,63	1.19	4 (11%)
30	CLA	J	316	-	50,54,73	1.37	7 (14%)	59,90,113	1.37	4 (6%)
30	CLA	l	305	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	4 (4%)
30	CLA	F	310	-	50,54,73	1.36	6 (12%)	59,90,113	1.46	5 (8%)
30	CLA	b	716	-	54,58,73	1.32	7 (12%)	64,95,113	1.40	5 (7%)
30	CLA	f	301	-	59,63,73	1.27	7 (11%)	70,101,113	1.32	5 (7%)
30	CLA	b	726	-	51,55,73	1.36	7 (13%)	60,91,113	1.36	5 (8%)
30	CLA	L	313	-	59,63,73	1.27	8 (13%)	70,101,113	1.30	5 (7%)
31	KC1	A	314	6	49,53,53	1.33	6 (12%)	61,89,89	1.73	14 (22%)
28	DD6	K	301	-	40,45,45	1.52	2 (5%)	51,67,67	1.93	15 (29%)
28	DD6	G	505	-	40,45,45	1.83	3 (7%)	51,67,67	2.32	19 (37%)
37	BCR	a	734	-	41,41,41	0.65	0	56,56,56	2.08	20 (35%)
28	DD6	K	303	-	40,45,45	1.65	3 (7%)	51,67,67	1.73	12 (23%)
30	CLA	P	215	-	51,55,73	1.36	8 (15%)	60,91,113	1.52	7 (11%)
31	KC1	A	306	30,28	49,53,53	1.34	6 (12%)	61,89,89	1.71	13 (21%)
30	CLA	O	308	-	51,55,73	1.36	6 (11%)	60,91,113	1.39	5 (8%)
30	CLA	K	307	-	50,54,73	1.34	7 (14%)	59,90,113	1.42	5 (8%)
30	CLA	L	310	-	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
30	CLA	B	315	-	45,49,73	1.41	7 (15%)	54,84,113	1.52	5 (9%)
30	CLA	H	307	-	55,59,73	1.32	7 (12%)	64,96,113	1.40	6 (9%)
30	CLA	A	316	-	51,55,73	1.35	7 (13%)	60,91,113	1.39	5 (8%)
30	CLA	K	312	-	52,56,73	1.34	8 (15%)	61,92,113	1.38	5 (8%)
34	PID	P	205	-	43,49,49	1.24	3 (6%)	52,76,76	1.64	8 (15%)
30	CLA	a	731	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
29	UIX	I	304	-	43,49,49	1.42	6 (13%)	53,74,74	2.50	16 (30%)
31	KC1	P	216	27	49,53,53	1.33	6 (12%)	61,89,89	1.70	12 (19%)
38	PQN	b	729	-	34,34,34	1.58	2 (5%)	43,45,45	1.28	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	G	520	-	53,57,73	1.32	7 (13%)	61,93,113	1.35	7 (11%)
34	PID	G	507	-	43,49,49	1.25	3 (6%)	52,76,76	1.34	7 (13%)
33	LMG	I	320	-	38,38,55	0.81	0	46,46,63	1.29	6 (13%)
31	KC1	O	315	26	49,53,53	1.34	5 (10%)	61,89,89	1.68	13 (21%)
37	BCR	l	302	-	41,41,41	0.68	0	56,56,56	2.20	22 (39%)
30	CLA	I	310	-	52,56,73	1.34	6 (11%)	61,92,113	1.42	6 (9%)
30	CLA	G	512	-	64,68,73	1.22	7 (10%)	76,107,113	1.31	5 (6%)
30	CLA	b	710	-	56,60,73	1.32	8 (14%)	65,97,113	1.36	5 (7%)
30	CLA	G	516	5	45,49,73	1.44	6 (13%)	54,84,113	1.48	5 (9%)
34	PID	F	306	-	43,49,49	1.24	3 (6%)	52,76,76	1.43	5 (9%)
29	UIX	h	201	-	43,49,49	1.41	4 (9%)	53,74,74	2.48	20 (37%)
30	CLA	a	717	-	61,65,73	1.26	7 (11%)	72,103,113	1.31	7 (9%)
30	CLA	B	312	-	55,59,73	1.32	7 (12%)	64,96,113	1.36	5 (7%)
30	CLA	G	510	-	69,73,73	1.16	6 (8%)	82,113,113	1.28	7 (8%)
30	CLA	j	104	-	59,63,73	1.29	7 (11%)	70,101,113	1.31	6 (8%)
30	CLA	L	309	-	57,61,73	1.29	6 (10%)	67,98,113	1.36	6 (8%)
30	CLA	b	715	-	64,68,73	1.22	5 (7%)	76,107,113	1.31	5 (6%)
31	KC1	O	312	-	49,53,53	1.33	5 (10%)	61,89,89	1.73	14 (22%)
28	DD6	J	304	-	40,45,45	1.80	4 (10%)	51,67,67	2.14	19 (37%)
28	DD6	A	303	-	40,45,45	1.49	2 (5%)	51,67,67	1.79	13 (25%)
37	BCR	b	702	-	41,41,41	0.66	0	56,56,56	2.19	16 (28%)
32	DGD	j	103	-	42,42,67	1.06	2 (4%)	56,56,81	1.01	3 (5%)
30	CLA	b	701	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)
30	CLA	I	308	-	64,68,73	1.22	8 (12%)	76,107,113	1.28	7 (9%)
30	CLA	A	307	31	49,53,73	1.41	6 (12%)	58,89,113	1.44	4 (6%)
30	CLA	b	718	-	55,59,73	1.33	7 (12%)	64,96,113	1.42	6 (9%)
30	CLA	b	707	-	69,73,73	1.18	5 (7%)	82,113,113	1.28	6 (7%)
28	DD6	H	303	-	40,45,45	1.54	3 (7%)	51,67,67	1.92	14 (27%)
30	CLA	I	321	30	56,60,73	1.31	6 (10%)	65,97,113	1.47	7 (10%)
30	CLA	N	307	-	55,59,73	1.32	8 (14%)	64,96,113	1.34	5 (7%)
34	PID	N	302	-	43,49,49	1.31	3 (6%)	52,76,76	1.64	10 (19%)
31	KC1	F	309	20	49,53,53	1.35	6 (12%)	61,89,89	1.79	14 (22%)
29	UIX	O	306	-	43,49,49	1.39	4 (9%)	53,74,74	2.89	20 (37%)
28	DD6	K	318	-	40,45,45	1.54	2 (5%)	51,67,67	2.05	12 (23%)
30	CLA	O	316	-	45,49,73	1.44	7 (15%)	54,84,113	1.50	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	M	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.55	8 (14%)
30	CLA	b	712	-	58,62,73	1.36	9 (15%)	71,100,113	1.38	7 (9%)
28	DD6	A	302	-	40,45,45	1.60	3 (7%)	51,67,67	2.10	15 (29%)
30	CLA	B	309	18	69,73,73	1.17	6 (8%)	82,113,113	1.26	6 (7%)
28	DD6	L	306	-	40,45,45	1.54	2 (5%)	51,67,67	2.03	15 (29%)
32	DGD	I	317	-	40,40,67	1.10	2 (5%)	54,54,81	1.01	4 (7%)
30	CLA	I	315	-	56,60,73	1.31	7 (12%)	65,97,113	1.37	7 (10%)
30	CLA	a	719	-	51,55,73	1.36	8 (15%)	60,91,113	1.35	5 (8%)
30	CLA	J	315	-	50,54,73	1.37	6 (12%)	59,90,113	1.41	4 (6%)
30	CLA	F	315	-	45,49,73	1.43	6 (13%)	54,84,113	1.53	6 (11%)
28	DD6	L	302	-	40,45,45	1.48	2 (5%)	51,67,67	1.97	16 (31%)
30	CLA	L	317	-	56,60,73	1.32	7 (12%)	65,97,113	1.37	6 (9%)
30	CLA	J	306	-	50,54,73	1.37	8 (16%)	59,90,113	1.42	4 (6%)
30	CLA	a	706	16	62,66,73	1.23	7 (11%)	73,104,113	1.31	5 (6%)
30	CLA	K	316	-	50,54,73	1.37	8 (16%)	59,90,113	1.41	5 (8%)
30	CLA	a	724	-	69,73,73	1.19	8 (11%)	82,113,113	1.29	8 (9%)
28	DD6	M	302	-	40,45,45	1.75	3 (7%)	51,67,67	2.23	19 (37%)
30	CLA	P	217	-	45,49,73	1.43	8 (17%)	54,84,113	1.49	5 (9%)
30	CLA	l	304	-	64,68,73	1.22	6 (9%)	76,107,113	1.34	5 (6%)
31	KC1	I	314	1	49,53,53	1.33	6 (12%)	61,89,89	1.74	15 (24%)
28	DD6	F	303	-	40,45,45	1.55	2 (5%)	51,67,67	2.03	14 (27%)
31	KC1	N	308	-	49,53,53	1.43	6 (12%)	61,89,89	2.04	15 (24%)
31	KC1	F	314	20	49,53,53	1.35	5 (10%)	61,89,89	1.72	13 (21%)
30	CLA	b	728	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)
30	CLA	M	308	31	57,61,73	1.29	7 (12%)	67,98,113	1.38	6 (8%)
30	CLA	l	313	14	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
30	CLA	a	721	-	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
36	SF4	c	202	7	0,12,12	-	-	-		
30	CLA	I	312	-	69,73,73	1.18	8 (11%)	82,113,113	1.21	5 (6%)
30	CLA	I	313	-	59,63,73	1.26	7 (11%)	70,101,113	1.35	7 (10%)
30	CLA	a	727	-	50,54,73	1.38	7 (14%)	59,90,113	1.38	4 (6%)
34	PID	H	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.58	7 (13%)
31	KC1	K	314	2	49,53,53	1.33	6 (12%)	61,89,89	1.69	12 (19%)
30	CLA	B	316	-	50,54,73	1.37	6 (12%)	59,90,113	1.35	4 (6%)
30	CLA	F	312	-	50,54,73	1.32	8 (16%)	59,90,113	1.37	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	l	310	-	39,50,73	2.85	11 (28%)	32,76,113	1.72	6 (18%)
31	KC1	O	310	-	49,53,53	1.33	6 (12%)	61,89,89	1.73	14 (22%)
30	CLA	D	311	-	50,54,73	1.36	6 (12%)	59,90,113	1.41	4 (6%)
30	CLA	l	309	-	45,49,73	1.42	5 (11%)	54,84,113	1.47	5 (9%)
30	CLA	J	314	-	45,49,73	1.43	6 (13%)	54,84,113	1.47	6 (11%)
30	CLA	I	307	-	50,54,73	1.37	6 (12%)	59,90,113	1.39	4 (6%)
30	CLA	F	313	-	50,54,73	1.37	7 (14%)	59,90,113	1.47	6 (10%)
31	KC1	B	314	18	49,53,53	1.33	5 (10%)	61,89,89	1.71	13 (21%)
30	CLA	M	316	-	56,60,73	1.31	8 (14%)	65,97,113	1.36	4 (6%)
30	CLA	l	312	-	50,54,73	1.37	7 (14%)	59,90,113	1.34	4 (6%)
30	CLA	O	314	-	51,55,73	1.36	8 (15%)	60,91,113	1.48	6 (10%)
30	CLA	f	303	10	50,54,73	1.36	9 (18%)	59,90,113	1.39	4 (6%)
39	LHG	a	733	-	47,47,48	0.27	0	50,53,54	0.33	0
30	CLA	H	309	-	51,55,73	1.36	7 (13%)	60,91,113	1.40	5 (8%)
31	KC1	H	306	-	49,53,53	1.33	5 (10%)	61,89,89	1.72	13 (21%)
30	CLA	a	710	16	59,63,73	1.28	8 (13%)	70,101,113	1.36	7 (10%)
30	CLA	b	713	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	6 (7%)
28	DD6	M	306	-	40,45,45	1.70	2 (5%)	51,67,67	2.22	20 (39%)
30	CLA	K	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.50	7 (12%)
30	CLA	B	307	18	53,57,73	1.35	7 (13%)	61,93,113	1.37	5 (8%)
31	KC1	P	213	-	49,53,53	1.34	6 (12%)	61,89,89	1.75	14 (22%)
29	UIX	K	302	-	43,49,49	1.40	4 (9%)	53,74,74	2.71	22 (41%)
37	BCR	b	732	-	41,41,41	0.72	0	56,56,56	1.90	18 (32%)
30	CLA	A	313	-	59,63,73	1.26	6 (10%)	70,101,113	1.32	6 (8%)
31	KC1	N	306	-	49,53,53	1.33	5 (10%)	61,89,89	1.72	13 (21%)
30	CLA	a	703	-	59,63,73	1.25	10 (16%)	70,101,113	1.44	8 (11%)
30	CLA	a	723	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	5 (6%)
34	PID	D	307	-	43,49,49	1.22	4 (9%)	52,76,76	1.37	5 (9%)
30	CLA	M	310	-	52,56,73	1.35	7 (13%)	61,92,113	1.39	5 (8%)
30	CLA	b	709	-	64,68,73	1.22	7 (10%)	76,107,113	1.32	7 (9%)
30	CLA	J	301	-	64,68,73	1.22	7 (10%)	76,107,113	1.29	5 (6%)
30	CLA	a	726	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	8 (9%)
30	CLA	b	720	-	57,61,73	1.28	7 (12%)	67,98,113	1.32	5 (7%)
28	DD6	G	508	-	40,45,45	1.55	2 (5%)	51,67,67	2.02	14 (27%)
30	CLA	b	703	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	DGD	l	301	-	51,51,67	0.96	2 (3%)	65,65,81	0.89	2 (3%)
28	DD6	G	504	-	40,45,45	1.83	6 (15%)	51,67,67	2.12	20 (39%)
30	CLA	G	509	5	55,59,73	1.32	6 (10%)	64,96,113	1.38	5 (7%)
34	PID	F	305	-	43,49,49	1.24	4 (9%)	52,76,76	1.83	8 (15%)
30	CLA	b	704	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	6 (7%)
30	CLA	J	311	22	51,55,73	1.36	5 (9%)	60,91,113	1.41	6 (10%)
30	CLA	b	717	-	69,73,73	1.18	9 (13%)	82,113,113	1.22	5 (6%)
30	CLA	l	303	14	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
33	LMG	b	734	-	31,31,55	0.98	1 (3%)	39,39,63	1.18	4 (10%)
30	CLA	A	319	-	50,54,73	1.36	7 (14%)	59,90,113	1.34	4 (6%)
34	PID	D	306	-	43,49,49	1.25	3 (6%)	52,76,76	1.37	5 (9%)
30	CLA	K	306	2	53,57,73	1.34	7 (13%)	61,93,113	1.41	6 (9%)
28	DD6	L	305	-	40,45,45	1.54	2 (5%)	51,67,67	1.93	14 (27%)
30	CLA	a	722	-	62,66,73	1.23	7 (11%)	73,104,113	1.29	8 (10%)
31	KC1	H	310	-	49,53,53	1.35	5 (10%)	61,89,89	1.72	13 (21%)
32	DGD	G	521	-	45,45,67	1.03	2 (4%)	59,59,81	1.46	8 (13%)
29	UIX	A	304	-	43,49,49	1.36	4 (9%)	53,74,74	2.42	22 (41%)
30	CLA	a	707	-	69,73,73	1.18	6 (8%)	82,113,113	1.21	5 (6%)
30	CLA	D	312	19	50,54,73	1.37	8 (16%)	59,90,113	1.36	4 (6%)
31	KC1	G	515	5	49,53,53	1.35	6 (12%)	61,89,89	1.70	14 (22%)
30	CLA	G	514	-	57,61,73	1.28	8 (14%)	67,98,113	1.38	6 (8%)
36	SF4	c	201	7	0,12,12	-	-	-		
31	KC1	J	313	-	49,53,53	1.34	6 (12%)	61,89,89	1.71	12 (19%)
30	CLA	H	308	-	50,54,73	1.38	7 (14%)	59,90,113	1.40	4 (6%)
31	KC1	L	315	-	49,53,53	1.35	5 (10%)	61,89,89	1.75	14 (22%)
31	KC1	N	311	25	49,53,53	1.33	5 (10%)	61,89,89	1.72	13 (21%)
37	BCR	b	730	-	41,41,41	0.70	0	56,56,56	2.27	20 (35%)
30	CLA	a	702	-	69,73,73	1.19	9 (13%)	82,113,113	1.32	5 (6%)
28	DD6	B	303	-	40,45,45	1.51	1 (2%)	51,67,67	1.89	13 (25%)
30	CLA	J	307	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	4 (4%)
30	CLA	O	313	-	50,54,73	1.34	6 (12%)	59,90,113	1.36	5 (8%)
29	UIX	P	207	-	43,49,49	1.40	5 (11%)	53,74,74	2.79	21 (39%)
30	CLA	G	511	-	59,63,73	1.28	7 (11%)	70,101,113	1.32	5 (7%)
37	BCR	f	304	-	41,41,41	0.68	0	56,56,56	2.08	17 (30%)
34	PID	O	305	-	43,49,49	1.31	4 (9%)	52,76,76	1.52	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	K	313	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	7 (10%)
30	CLA	A	312	-	59,63,73	1.27	7 (11%)	70,101,113	1.29	5 (7%)
32	DGD	L	301	-	39,39,67	0.96	2 (5%)	53,53,81	0.99	3 (5%)
30	CLA	A	310	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	5 (6%)
28	DD6	A	301	-	40,45,45	1.52	2 (5%)	51,67,67	2.05	14 (27%)
30	CLA	f	302	-	50,54,73	1.37	7 (14%)	59,90,113	1.39	5 (8%)
30	CLA	a	718	-	50,54,73	1.36	5 (10%)	59,90,113	1.41	4 (6%)
30	CLA	L	308	31	49,55,73	1.37	6 (12%)	62,91,113	1.39	7 (11%)
29	UIX	B	305	-	43,49,49	1.36	4 (9%)	53,74,74	2.39	17 (32%)
30	CLA	G	519	-	63,67,73	1.23	7 (11%)	74,105,113	1.30	4 (5%)
30	CLA	K	311	-	56,60,73	1.31	7 (12%)	65,97,113	1.34	6 (9%)
37	BCR	j	102	-	41,41,41	0.66	0	56,56,56	2.03	17 (30%)
37	BCR	l	306	-	41,41,41	0.68	0	56,56,56	1.92	12 (21%)
30	CLA	K	310	-	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
33	LMG	K	317	-	43,43,55	0.81	1 (2%)	51,51,63	1.32	6 (11%)
30	CLA	b	725	-	69,73,73	1.17	6 (8%)	82,113,113	1.25	6 (7%)
30	CLA	M	317	-	50,54,73	1.36	6 (12%)	59,90,113	1.43	5 (8%)
30	CLA	A	317	-	45,49,73	1.42	8 (17%)	54,84,113	1.48	6 (11%)
28	DD6	J	303	-	40,45,45	1.86	3 (7%)	51,67,67	2.45	16 (31%)
30	CLA	O	309	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	6 (7%)
28	DD6	J	302	-	40,45,45	1.55	1 (2%)	51,67,67	2.06	14 (27%)
30	CLA	I	316	-	59,63,73	1.25	5 (8%)	70,101,113	1.34	6 (8%)
30	CLA	a	714	-	49,53,73	1.40	6 (12%)	58,89,113	1.43	5 (8%)
34	PID	D	302	-	43,49,49	1.26	3 (6%)	52,76,76	1.40	9 (17%)
30	CLA	D	313	19	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
31	KC1	L	307	30	49,53,53	1.33	5 (10%)	61,89,89	1.73	15 (24%)
30	CLA	a	712	30	64,68,73	1.21	8 (12%)	76,107,113	1.30	6 (7%)
28	DD6	N	303	-	40,45,45	1.54	2 (5%)	51,67,67	2.07	17 (33%)
30	CLA	A	308	-	59,63,73	1.26	6 (10%)	70,101,113	1.33	6 (8%)
34	PID	O	302	-	43,49,49	1.27	3 (6%)	52,76,76	1.27	6 (11%)
30	CLA	b	719	-	50,54,73	1.37	8 (16%)	59,90,113	1.44	4 (6%)
30	CLA	M	312	-	52,56,73	1.35	8 (15%)	61,92,113	1.40	6 (9%)
34	PID	P	202	-	43,49,49	1.23	3 (6%)	52,76,76	1.53	6 (11%)
30	CLA	B	310	-	59,63,73	1.28	7 (11%)	70,101,113	1.32	7 (10%)
37	BCR	a	736	-	41,41,41	0.70	0	56,56,56	2.04	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	I	311	1	59,63,73	1.28	6 (10%)	70,101,113	1.34	6 (8%)
30	CLA	B	308	-	49,53,73	1.40	5 (10%)	58,89,113	1.45	4 (6%)
34	PID	D	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.44	7 (13%)
30	CLA	a	713	-	64,68,73	1.22	7 (10%)	76,107,113	1.28	6 (7%)
34	PID	j	105	-	43,49,49	1.28	4 (9%)	52,76,76	1.54	11 (21%)
30	CLA	b	705	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
28	DD6	B	306	-	40,45,45	1.55	2 (5%)	51,67,67	1.95	19 (37%)
30	CLA	M	313	-	50,54,73	1.37	7 (14%)	59,90,113	1.37	4 (6%)
36	SF4	a	737	16,17	0,12,12	-	-	-		
30	CLA	L	314	-	57,61,73	1.29	7 (12%)	67,98,113	1.36	6 (8%)
32	DGD	G	501	-	46,46,67	1.03	2 (4%)	60,60,81	1.01	4 (6%)
30	CLA	F	307	-	50,54,73	1.37	8 (16%)	59,90,113	1.43	4 (6%)
30	CLA	L	311	-	59,63,73	1.27	6 (10%)	70,101,113	1.34	5 (7%)
30	CLA	D	316	-	45,49,73	1.42	7 (15%)	54,84,113	1.46	5 (9%)
30	CLA	I	319	30	49,53,73	1.39	7 (14%)	58,89,113	1.46	7 (12%)
30	CLA	I	306	1	53,57,73	1.33	7 (13%)	61,93,113	1.43	6 (9%)
30	CLA	I	309	-	59,63,73	1.28	8 (13%)	70,101,113	1.33	6 (8%)
30	CLA	M	311	-	50,54,73	1.37	8 (16%)	59,90,113	1.38	4 (6%)
37	BCR	i	201	-	41,41,41	0.78	2 (4%)	56,56,56	2.14	21 (37%)
30	CLA	B	301	-	64,68,73	1.23	7 (10%)	76,107,113	1.25	5 (6%)
29	UIX	G	503	-	43,49,49	1.33	4 (9%)	53,74,74	2.33	19 (35%)
30	CLA	N	310	-	51,55,73	1.37	7 (13%)	60,91,113	1.50	6 (10%)
30	CLA	b	724	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	4 (4%)
30	CLA	L	316	-	45,49,73	1.43	7 (15%)	54,84,113	1.49	5 (9%)
30	CLA	a	730	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
30	CLA	K	309	-	54,58,73	1.31	7 (12%)	64,95,113	1.40	7 (10%)
32	DGD	y	201	-	55,55,67	0.93	2 (3%)	69,69,81	0.97	3 (4%)

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
30	CLA	b	721	28	1/1/11/20	1/17/93/115	-
30	CLA	b	723	-	1/1/12/20	9/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	KC1	M	314	24	-	9/15/71/71	-
30	CLA	P	209	-	1/1/11/20	6/18/94/115	-
30	CLA	P	210	-	1/1/15/20	13/39/115/115	-
30	CLA	P	214	-	1/1/11/20	3/17/93/115	-
28	DD6	I	302	-	-	5/26/80/80	0/3/3/3
30	CLA	a	701	-	1/1/11/20	2/15/91/115	-
33	LMG	j	101	-	-	14/30/50/70	0/1/1/1
30	CLA	B	317	-	1/1/11/20	7/15/91/115	-
28	DD6	G	502	-	-	6/26/80/80	0/3/3/3
28	DD6	h	203	-	-	1/26/80/80	0/3/3/3
30	CLA	M	309	24	1/1/13/20	5/27/103/115	-
28	DD6	M	305	-	-	1/26/80/80	0/3/3/3
31	KC1	D	315	19	-	4/15/71/71	-
29	UIX	J	305	-	-	11/31/87/87	0/3/3/3
28	DD6	I	301	-	-	3/26/80/80	0/3/3/3
30	CLA	D	309	-	1/1/11/20	7/17/93/115	-
34	PID	O	304	-	-	3/24/93/93	0/4/4/4
30	CLA	a	716	-	1/1/11/20	6/18/94/115	-
28	DD6	F	301	-	-	2/26/80/80	0/3/3/3
30	CLA	J	310	-	1/1/11/20	8/17/93/115	-
28	DD6	O	303	-	-	0/26/80/80	0/3/3/3
30	CLA	m	202	-	1/1/14/20	10/33/109/115	-
28	DD6	A	305	31	-	1/26/80/80	0/3/3/3
30	CLA	j	106	-	1/1/13/20	11/31/107/115	-
28	DD6	B	302	-	-	3/24/78/80	0/3/3/3
30	CLA	K	308	2	1/1/12/20	10/26/102/115	-
30	CLA	L	318	-	1/1/11/20	8/17/93/115	-
28	DD6	b	731	30	-	3/26/80/80	0/3/3/3
30	CLA	G	518	-	1/1/11/20	7/17/93/115	-
30	CLA	a	711	-	1/1/11/20	6/15/91/115	-
30	CLA	b	708	-	1/1/15/20	10/39/115/115	-
30	CLA	A	311	6	1/1/11/20	5/17/93/115	-
30	CLA	A	309	-	1/1/13/20	5/27/103/115	-
30	CLA	G	513	5	1/1/15/20	7/39/115/115	-
31	KC1	D	310	-	-	10/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DD6	M	304	-	-	0/26/80/80	0/3/3/3
30	CLA	b	714	-	1/1/11/20	3/17/93/115	-
30	CLA	a	715	-	1/1/11/20	7/15/91/115	-
31	KC1	P	211	-	-	9/15/71/71	-
34	PID	D	305	-	-	2/24/93/93	0/4/4/4
30	CLA	l	308	-	1/1/10/20	3/10/86/115	-
33	LMG	D	317	-	-	17/41/61/70	0/1/1/1
34	PID	D	304	-	-	3/24/93/93	0/4/4/4
30	CLA	D	308	-	1/1/11/20	4/18/94/115	-
30	CLA	b	727	-	1/1/15/20	7/39/115/115	-
37	BCR	m	201	-	-	5/29/63/63	0/2/2/2
30	CLA	B	313	18	1/1/15/20	9/39/115/115	-
34	PID	F	302	-	-	2/24/93/93	0/4/4/4
33	LMG	b	733	-	-	18/39/59/70	0/1/1/1
30	CLA	h	202	-	1/1/13/20	9/27/103/115	-
34	PID	O	307	-	-	4/24/93/93	0/4/4/4
30	CLA	l	311	-	1/1/15/20	14/39/115/115	-
28	DD6	P	204	-	-	1/26/80/80	0/3/3/3
30	CLA	B	311	-	1/1/15/20	21/39/115/115	-
30	CLA	A	315	-	1/1/10/20	4/10/86/115	-
30	CLA	a	720	-	1/1/14/20	7/36/112/115	-
30	CLA	J	312	-	1/1/12/20	6/25/101/115	-
30	CLA	H	312	-	1/1/11/20	9/17/93/115	-
30	CLA	F	311	-	1/1/11/20	7/17/93/115	-
28	DD6	M	303	-	-	2/26/80/80	0/3/3/3
34	PID	P	206	-	-	3/24/93/93	0/4/4/4
30	CLA	b	722	-	1/1/15/20	7/39/115/115	-
34	PID	P	203	-	-	2/24/93/93	0/4/4/4
30	CLA	b	711	-	1/1/13/20	11/27/103/115	-
30	CLA	L	312	-	1/1/11/20	7/17/93/115	-
30	CLA	H	304	-	1/1/11/20	6/18/94/115	-
30	CLA	N	304	-	1/1/11/20	4/18/94/115	-
30	CLA	M	318	-	1/1/11/20	9/17/93/115	-
28	DD6	I	303	-	-	2/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DD6	K	305	-	-	4/26/80/80	0/3/3/3
30	CLA	N	305	-	1/1/15/20	9/39/115/115	-
34	PID	F	304	-	-	3/24/93/93	0/4/4/4
30	CLA	D	314	-	1/1/11/20	8/17/93/115	-
30	CLA	a	735	-	1/1/15/20	18/39/115/115	-
31	KC1	M	307	30	-	6/15/71/71	-
38	PQN	a	732	-	-	8/23/43/43	0/2/2/2
30	CLA	a	708	-	1/1/12/20	5/23/99/115	-
34	PID	H	302	-	-	2/24/93/93	0/4/4/4
30	CLA	G	517	-	1/1/11/20	4/17/93/115	-
33	LMG	B	318	-	-	15/32/52/70	0/1/1/1
34	PID	G	506	-	-	3/24/93/93	0/4/4/4
30	CLA	F	308	-	1/1/11/20	3/17/93/115	-
28	DD6	L	304	-	-	0/26/80/80	0/3/3/3
34	PID	N	301	-	-	6/24/93/93	0/4/4/4
30	CLA	a	725	-	1/1/14/20	13/35/111/115	-
33	LMG	I	318	-	-	21/31/51/70	0/1/1/1
30	CLA	N	309	25	1/1/11/20	4/17/93/115	-
30	CLA	P	212	-	1/1/12/20	9/23/99/115	-
30	CLA	J	309	-	1/1/13/20	10/29/105/115	-
30	CLA	a	738	22	1/1/11/20	4/17/93/115	-
30	CLA	H	311	-	-	6/10/86/115	-
30	CLA	H	305	-	1/1/15/20	8/39/115/115	-
30	CLA	J	308	-	1/1/11/20	9/17/93/115	-
28	DD6	I	305	-	-	5/26/80/80	0/3/3/3
35	SQD	A	318	-	-	5/45/65/69	0/1/1/1
30	CLA	a	729	-	1/1/13/20	8/29/105/115	-
28	DD6	K	304	-	-	1/26/80/80	0/3/3/3
30	CLA	O	311	-	1/1/12/20	4/23/99/115	-
34	PID	O	301	-	-	4/24/93/93	0/4/4/4
28	DD6	D	303	-	-	6/26/80/80	0/3/3/3
30	CLA	a	704	-	1/1/15/20	6/39/115/115	-
30	CLA	b	706	-	1/1/11/20	4/19/95/115	-
34	PID	M	301	-	-	1/24/93/93	0/4/4/4
34	PID	P	208	-	-	2/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	a	709	-	1/1/15/20	16/39/115/115	-
30	CLA	A	320	-	1/1/11/20	6/17/93/115	-
30	CLA	a	728	-	1/1/13/20	8/27/103/115	-
30	CLA	a	705	30	1/1/13/20	8/27/103/115	-
28	DD6	B	304	-	-	0/26/80/80	0/3/3/3
37	BCR	l	307	-	-	0/29/63/63	0/2/2/2
28	DD6	L	303	-	-	0/26/80/80	0/3/3/3
33	LMG	P	201	-	-	9/22/42/70	0/1/1/1
30	CLA	J	316	-	-	3/17/93/115	-
30	CLA	l	305	-	1/1/15/20	12/39/115/115	-
30	CLA	F	310	-	1/1/11/20	8/17/93/115	-
30	CLA	b	716	-	1/1/12/20	4/21/97/115	-
30	CLA	f	301	-	1/1/13/20	11/27/103/115	-
30	CLA	b	726	-	1/1/11/20	2/18/94/115	-
30	CLA	L	313	-	1/1/13/20	11/27/103/115	-
31	KC1	A	314	6	-	5/15/71/71	-
28	DD6	K	301	-	-	5/26/80/80	0/3/3/3
28	DD6	G	505	-	-	4/26/80/80	0/3/3/3
37	BCR	a	734	-	-	2/29/63/63	0/2/2/2
28	DD6	K	303	-	-	0/26/80/80	0/3/3/3
30	CLA	P	215	-	1/1/11/20	7/18/94/115	-
31	KC1	A	306	30,28	-	7/15/71/71	-
30	CLA	O	308	-	1/1/11/20	6/18/94/115	-
30	CLA	K	307	-	1/1/11/20	2/17/93/115	-
30	CLA	L	310	-	1/1/13/20	0/27/103/115	-
30	CLA	B	315	-	1/1/10/20	4/10/86/115	-
30	CLA	H	307	-	1/1/12/20	5/23/99/115	-
30	CLA	A	316	-	1/1/11/20	4/18/94/115	-
30	CLA	K	312	-	1/1/11/20	5/19/95/115	-
34	PID	P	205	-	-	3/24/93/93	0/4/4/4
30	CLA	a	731	-	1/1/15/20	13/39/115/115	-
29	UIX	I	304	-	-	4/31/87/87	0/3/3/3
31	KC1	P	216	27	-	8/15/71/71	-
38	PQN	b	729	-	-	4/23/43/43	0/2/2/2
30	CLA	G	520	-	1/1/11/20	5/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PID	G	507	-	-	0/24/93/93	1/4/4/4
33	LMG	I	320	-	-	14/33/53/70	0/1/1/1
31	KC1	O	315	26	-	6/15/71/71	-
37	BCR	l	302	-	-	3/29/63/63	0/2/2/2
30	CLA	I	310	-	1/1/11/20	8/19/95/115	-
30	CLA	G	512	-	1/1/14/20	11/33/109/115	-
30	CLA	b	710	-	1/1/12/20	4/24/100/115	-
30	CLA	G	516	5	1/1/10/20	6/10/86/115	-
34	PID	F	306	-	-	0/24/93/93	0/4/4/4
29	UIX	h	201	-	-	2/31/87/87	0/3/3/3
30	CLA	a	717	-	1/1/13/20	13/30/106/115	-
30	CLA	B	312	-	1/1/12/20	4/23/99/115	-
30	CLA	G	510	-	1/1/15/20	10/39/115/115	-
30	CLA	j	104	-	1/1/13/20	6/27/103/115	-
30	CLA	L	309	-	1/1/12/20	7/25/101/115	-
30	CLA	b	715	-	1/1/14/20	12/33/109/115	-
31	KC1	O	312	-	-	9/15/71/71	-
28	DD6	J	304	-	-	2/26/80/80	0/3/3/3
28	DD6	A	303	-	-	1/26/80/80	0/3/3/3
37	BCR	b	702	-	-	2/29/63/63	0/2/2/2
32	DGD	j	103	-	-	8/30/70/95	0/2/2/2
30	CLA	b	701	-	1/1/15/20	13/39/115/115	-
30	CLA	I	308	-	1/1/14/20	12/33/109/115	-
30	CLA	A	307	31	1/1/11/20	1/15/91/115	-
30	CLA	b	718	-	1/1/12/20	3/23/99/115	-
30	CLA	b	707	-	1/1/15/20	18/39/115/115	-
30	CLA	I	321	30	1/1/12/20	8/24/100/115	-
28	DD6	H	303	-	-	1/26/80/80	0/3/3/3
30	CLA	N	307	-	1/1/12/20	3/23/99/115	-
34	PID	N	302	-	-	2/24/93/93	0/4/4/4
31	KC1	F	309	20	-	9/15/71/71	-
29	UIX	O	306	-	-	4/31/87/87	0/3/3/3
28	DD6	K	318	-	-	4/26/80/80	0/3/3/3
30	CLA	O	316	-	1/1/10/20	4/10/86/115	-
30	CLA	M	315	-	1/1/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	712	-	1/1/13/20	9/25/101/115	-
30	CLA	B	309	18	1/1/15/20	19/39/115/115	-
28	DD6	A	302	-	-	3/26/80/80	0/3/3/3
28	DD6	L	306	-	-	3/26/80/80	0/3/3/3
32	DGD	I	317	-	-	3/28/68/95	0/2/2/2
30	CLA	I	315	-	1/1/12/20	8/24/100/115	-
30	CLA	a	719	-	1/1/11/20	7/18/94/115	-
30	CLA	J	315	-	1/1/11/20	3/17/93/115	-
30	CLA	F	315	-	1/1/10/20	4/10/86/115	-
28	DD6	L	302	-	-	4/26/80/80	0/3/3/3
30	CLA	L	317	-	1/1/12/20	11/24/100/115	-
30	CLA	J	306	-	1/1/11/20	6/17/93/115	-
30	CLA	a	706	16	1/1/13/20	15/31/107/115	-
30	CLA	K	316	-	1/1/11/20	3/17/93/115	-
30	CLA	a	724	-	1/1/15/20	13/39/115/115	-
30	CLA	P	217	-	1/1/10/20	4/10/86/115	-
28	DD6	M	302	-	-	3/26/80/80	0/3/3/3
30	CLA	l	304	-	1/1/14/20	9/33/109/115	-
31	KC1	I	314	1	-	9/15/71/71	-
28	DD6	F	303	-	-	2/26/80/80	0/3/3/3
31	KC1	N	308	-	-	8/15/71/71	-
31	KC1	F	314	20	-	5/15/71/71	-
30	CLA	b	728	-	1/1/15/20	9/39/115/115	-
30	CLA	M	308	31	1/1/12/20	10/25/101/115	-
30	CLA	l	313	14	1/1/15/20	20/39/115/115	-
30	CLA	a	721	-	1/1/15/20	18/39/115/115	-
36	SF4	c	202	7	-	-	0/6/5/5
30	CLA	I	312	-	1/1/15/20	15/39/115/115	-
30	CLA	I	313	-	1/1/13/20	11/27/103/115	-
30	CLA	a	727	-	1/1/11/20	9/17/93/115	-
34	PID	H	301	-	-	4/24/93/93	0/4/4/4
31	KC1	K	314	2	-	9/15/71/71	-
30	CLA	B	316	-	1/1/11/20	9/17/93/115	-
30	CLA	F	312	-	1/1/11/20	3/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	l	310	-	-	10/15/65/115	0/5/5/9
31	KC1	O	310	-	-	7/15/71/71	-
30	CLA	D	311	-	1/1/11/20	3/17/93/115	-
30	CLA	l	309	-	1/1/10/20	3/10/86/115	-
30	CLA	J	314	-	1/1/10/20	2/10/86/115	-
30	CLA	I	307	-	1/1/11/20	7/17/93/115	-
30	CLA	F	313	-	1/1/11/20	5/17/93/115	-
31	KC1	B	314	18	-	7/15/71/71	-
30	CLA	M	316	-	1/1/12/20	10/24/100/115	-
30	CLA	l	312	-	1/1/11/20	6/17/93/115	-
30	CLA	O	314	-	1/1/11/20	8/18/94/115	-
30	CLA	f	303	10	1/1/11/20	8/17/93/115	-
39	LHG	a	733	-	-	16/52/52/53	-
30	CLA	H	309	-	1/1/11/20	8/18/94/115	-
31	KC1	H	306	-	-	4/15/71/71	-
30	CLA	a	710	16	1/1/13/20	6/27/103/115	-
30	CLA	b	713	-	1/1/15/20	8/39/115/115	-
28	DD6	M	306	-	-	5/26/80/80	0/3/3/3
30	CLA	K	315	-	1/1/10/20	2/10/86/115	-
30	CLA	B	307	18	1/1/11/20	3/20/96/115	-
31	KC1	P	213	-	-	8/15/71/71	-
29	UIX	K	302	-	-	5/31/87/87	0/3/3/3
37	BCR	b	732	-	-	0/29/63/63	0/2/2/2
30	CLA	A	313	-	1/1/13/20	10/27/103/115	-
31	KC1	N	306	-	-	6/15/71/71	-
30	CLA	a	703	-	1/1/13/20	6/27/103/115	-
30	CLA	a	723	-	1/1/15/20	13/39/115/115	-
34	PID	D	307	-	-	4/24/93/93	0/4/4/4
30	CLA	M	310	-	1/1/11/20	8/19/95/115	-
30	CLA	b	709	-	1/1/14/20	8/33/109/115	-
30	CLA	J	301	-	1/1/14/20	12/33/109/115	-
30	CLA	a	726	-	1/1/15/20	13/39/115/115	-
30	CLA	b	720	-	1/1/12/20	9/25/101/115	-
28	DD6	G	508	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	703	-	1/1/15/20	12/39/115/115	-
32	DGD	l	301	-	-	8/39/79/95	0/2/2/2
28	DD6	G	504	-	-	5/26/80/80	0/3/3/3
30	CLA	G	509	5	1/1/12/20	4/23/99/115	-
34	PID	F	305	-	-	8/24/93/93	0/4/4/4
30	CLA	b	704	-	1/1/15/20	19/39/115/115	-
30	CLA	J	311	22	1/1/11/20	7/18/94/115	-
30	CLA	b	717	-	1/1/15/20	18/39/115/115	-
30	CLA	l	303	14	1/1/15/20	14/39/115/115	-
33	LMG	b	734	-	-	12/26/46/70	0/1/1/1
30	CLA	A	319	-	1/1/11/20	9/17/93/115	-
34	PID	D	306	-	-	8/24/93/93	0/4/4/4
30	CLA	K	306	2	1/1/11/20	4/20/96/115	-
28	DD6	L	305	-	-	3/26/80/80	0/3/3/3
30	CLA	a	722	-	1/1/13/20	8/31/107/115	-
31	KC1	H	310	-	-	6/15/71/71	-
32	DGD	G	521	-	-	18/33/73/95	0/2/2/2
29	UIX	A	304	-	-	0/31/87/87	0/3/3/3
30	CLA	a	707	-	1/1/15/20	17/39/115/115	-
30	CLA	D	312	19	1/1/11/20	7/17/93/115	-
31	KC1	G	515	5	-	6/15/71/71	-
30	CLA	G	514	-	1/1/12/20	11/25/101/115	-
36	SF4	c	201	7	-	-	0/6/5/5
31	KC1	J	313	-	-	7/15/71/71	-
30	CLA	H	308	-	1/1/11/20	4/17/93/115	-
31	KC1	L	315	-	-	8/15/71/71	-
31	KC1	N	311	25	-	7/15/71/71	-
37	BCR	b	730	-	-	6/29/63/63	0/2/2/2
30	CLA	a	702	-	1/1/15/20	11/39/115/115	-
28	DD6	B	303	-	-	2/26/80/80	0/3/3/3
30	CLA	J	307	-	1/1/15/20	19/39/115/115	-
30	CLA	O	313	-	1/1/11/20	3/17/93/115	-
29	UIX	P	207	-	-	8/31/87/87	0/3/3/3
30	CLA	G	511	-	1/1/13/20	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	BCR	f	304	-	-	2/29/63/63	0/2/2/2
34	PID	O	305	-	-	16/24/93/93	0/4/4/4
30	CLA	K	313	-	1/1/13/20	7/27/103/115	-
30	CLA	A	312	-	1/1/13/20	6/27/103/115	-
32	DGD	L	301	-	-	1/26/66/95	0/2/2/2
30	CLA	A	310	-	1/1/15/20	15/39/115/115	-
30	CLA	f	302	-	1/1/11/20	6/17/93/115	-
28	DD6	A	301	-	-	3/26/80/80	0/3/3/3
30	CLA	a	718	-	1/1/11/20	9/17/93/115	-
30	CLA	L	308	31	1/1/11/20	9/15/91/115	-
29	UIX	B	305	-	-	2/31/87/87	0/3/3/3
30	CLA	G	519	-	1/1/13/20	13/32/108/115	-
30	CLA	K	311	-	1/1/12/20	11/24/100/115	-
37	BCR	j	102	-	-	5/29/63/63	0/2/2/2
37	BCR	l	306	-	-	7/29/63/63	0/2/2/2
30	CLA	K	310	-	1/1/13/20	5/27/103/115	-
33	LMG	K	317	-	-	19/38/58/70	0/1/1/1
30	CLA	b	725	-	1/1/15/20	9/39/115/115	-
30	CLA	M	317	-	1/1/11/20	8/17/93/115	-
30	CLA	A	317	-	1/1/10/20	0/10/86/115	-
28	DD6	J	303	-	-	2/26/80/80	0/3/3/3
30	CLA	O	309	-	1/1/15/20	1/39/115/115	-
30	CLA	a	714	-	1/1/11/20	4/15/91/115	-
30	CLA	I	316	-	1/1/13/20	13/27/103/115	-
28	DD6	J	302	-	-	3/26/80/80	0/3/3/3
34	PID	D	302	-	-	3/24/93/93	0/4/4/4
30	CLA	D	313	19	1/1/11/20	2/15/91/115	-
31	KC1	L	307	30	-	6/15/71/71	-
30	CLA	a	712	30	1/1/14/20	8/33/109/115	-
30	CLA	A	308	-	1/1/13/20	4/27/103/115	-
28	DD6	N	303	-	-	0/26/80/80	0/3/3/3
34	PID	O	302	-	-	2/24/93/93	0/4/4/4
30	CLA	b	719	-	1/1/11/20	9/17/93/115	-
30	CLA	M	312	-	1/1/11/20	5/19/95/115	-
34	PID	P	202	-	-	3/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	B	310	-	1/1/13/20	8/27/103/115	-
37	BCR	a	736	-	-	2/29/63/63	0/2/2/2
30	CLA	I	311	1	1/1/13/20	10/27/103/115	-
30	CLA	B	308	-	1/1/11/20	5/15/91/115	-
34	PID	D	301	-	-	2/24/93/93	0/4/4/4
30	CLA	a	713	-	1/1/14/20	11/33/109/115	-
34	PID	j	105	-	-	4/24/93/93	0/4/4/4
30	CLA	b	705	-	1/1/15/20	11/39/115/115	-
28	DD6	B	306	-	-	2/26/80/80	0/3/3/3
30	CLA	M	313	-	1/1/11/20	2/17/93/115	-
36	SF4	a	737	16,17	-	-	0/6/5/5
30	CLA	L	314	-	1/1/12/20	6/25/101/115	-
32	DGD	G	501	-	-	10/34/74/95	0/2/2/2
30	CLA	F	307	-	1/1/11/20	3/17/93/115	-
30	CLA	L	311	-	1/1/13/20	5/27/103/115	-
30	CLA	D	316	-	1/1/10/20	0/10/86/115	-
30	CLA	I	319	30	1/1/11/20	7/15/91/115	-
30	CLA	I	306	1	1/1/11/20	9/20/96/115	-
30	CLA	I	309	-	1/1/13/20	6/27/103/115	-
30	CLA	M	311	-	1/1/11/20	4/17/93/115	-
37	BCR	i	201	-	-	8/29/63/63	0/2/2/2
30	CLA	B	301	-	1/1/14/20	10/33/109/115	-
29	UIX	G	503	-	-	5/31/87/87	0/3/3/3
30	CLA	N	310	-	1/1/11/20	10/18/94/115	-
30	CLA	b	724	-	1/1/15/20	15/39/115/115	-
30	CLA	L	316	-	1/1/10/20	4/10/86/115	-
30	CLA	a	730	-	1/1/15/20	4/39/115/115	-
30	CLA	K	309	-	1/1/12/20	2/21/97/115	-
32	DGD	y	201	-	-	7/43/83/95	0/2/2/2

All (1826) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	l	310	CLA	C1B-C2B	9.21	1.49	1.39
28	J	303	DD6	C30-C31	-9.00	1.25	1.42
28	I	305	DD6	C30-C31	-8.99	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	505	DD6	C30-C31	-8.98	1.25	1.42
28	M	306	DD6	C30-C31	-8.97	1.25	1.42
28	M	303	DD6	C30-C31	-8.90	1.25	1.42
28	b	731	DD6	C30-C31	-8.80	1.25	1.42
28	G	504	DD6	C30-C31	-8.78	1.25	1.42
28	I	303	DD6	C30-C31	-8.75	1.25	1.42
28	B	302	DD6	C30-C31	-8.75	1.25	1.42
28	J	304	DD6	C30-C31	-8.73	1.25	1.42
28	M	302	DD6	C30-C31	-8.72	1.25	1.42
28	O	303	DD6	C30-C31	-8.60	1.25	1.42
28	h	203	DD6	C30-C31	-8.54	1.25	1.42
28	N	303	DD6	C30-C31	-8.53	1.25	1.42
28	B	306	DD6	C30-C31	-8.53	1.25	1.42
28	I	301	DD6	C30-C31	-8.51	1.26	1.42
28	M	304	DD6	C30-C31	-8.51	1.26	1.42
28	A	302	DD6	C30-C31	-8.46	1.26	1.42
28	K	304	DD6	C30-C31	-8.45	1.26	1.42
28	G	508	DD6	C30-C31	-8.45	1.26	1.42
28	I	302	DD6	C30-C31	-8.44	1.26	1.42
28	G	502	DD6	C30-C31	-8.43	1.26	1.42
28	P	204	DD6	C30-C31	-8.42	1.26	1.42
28	K	303	DD6	C30-C31	-8.41	1.26	1.42
28	K	318	DD6	C30-C31	-8.40	1.26	1.42
28	B	303	DD6	C30-C31	-8.40	1.26	1.42
28	F	303	DD6	C30-C31	-8.39	1.26	1.42
28	M	305	DD6	C30-C31	-8.39	1.26	1.42
28	A	301	DD6	C30-C31	-8.39	1.26	1.42
28	F	301	DD6	C30-C31	-8.37	1.26	1.42
28	L	306	DD6	C30-C31	-8.36	1.26	1.42
28	L	305	DD6	C30-C31	-8.35	1.26	1.42
28	A	305	DD6	C30-C31	-8.32	1.26	1.42
28	K	305	DD6	C30-C31	-8.29	1.26	1.42
28	B	304	DD6	C30-C31	-8.28	1.26	1.42
28	L	304	DD6	C30-C31	-8.25	1.26	1.42
28	D	303	DD6	C30-C31	-8.25	1.26	1.42
28	J	302	DD6	C30-C31	-8.25	1.26	1.42
30	l	310	CLA	C1D-C2D	8.23	1.48	1.39
28	H	303	DD6	C30-C31	-8.23	1.26	1.42
28	L	303	DD6	C30-C31	-8.21	1.26	1.42
28	A	303	DD6	C30-C31	-8.21	1.26	1.42
28	K	301	DD6	C30-C31	-8.19	1.26	1.42
28	L	302	DD6	C30-C31	-8.10	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	l	310	CLA	C3B-C4B	8.06	1.49	1.41
38	a	732	PQN	C3-C2	7.68	1.49	1.35
38	b	729	PQN	C3-C2	7.48	1.48	1.35
34	N	302	PID	C13-C14	-6.24	1.33	1.45
34	H	302	PID	C13-C14	-5.98	1.34	1.45
34	G	506	PID	C13-C14	-5.97	1.34	1.45
34	O	302	PID	C13-C14	-5.90	1.34	1.45
34	P	203	PID	C13-C14	-5.89	1.34	1.45
34	O	307	PID	C13-C14	-5.80	1.34	1.45
34	D	302	PID	C13-C14	-5.78	1.34	1.45
34	O	305	PID	C13-C14	-5.78	1.34	1.45
34	D	305	PID	C13-C14	-5.77	1.34	1.45
34	D	306	PID	C13-C14	-5.72	1.34	1.45
34	D	301	PID	C13-C14	-5.70	1.35	1.45
34	j	105	PID	C13-C14	-5.69	1.35	1.45
34	G	507	PID	C13-C14	-5.69	1.35	1.45
34	N	301	PID	C13-C14	-5.65	1.35	1.45
34	O	301	PID	C13-C14	-5.61	1.35	1.45
34	P	208	PID	C13-C14	-5.61	1.35	1.45
34	F	306	PID	C13-C14	-5.58	1.35	1.45
34	H	301	PID	C13-C14	-5.56	1.35	1.45
34	P	205	PID	C13-C14	-5.56	1.35	1.45
34	F	304	PID	C13-C14	-5.46	1.35	1.45
34	P	202	PID	C13-C14	-5.44	1.35	1.45
34	F	302	PID	C13-C14	-5.42	1.35	1.45
34	F	305	PID	C13-C14	-5.42	1.35	1.45
34	P	206	PID	C13-C14	-5.40	1.35	1.45
34	D	307	PID	C13-C14	-5.39	1.35	1.45
34	O	304	PID	C13-C14	-5.37	1.35	1.45
34	D	304	PID	C13-C14	-5.31	1.35	1.45
34	M	301	PID	C13-C14	-5.30	1.35	1.45
31	N	308	KC1	MG-ND	-5.12	1.95	2.05
31	L	315	KC1	MG-ND	-5.05	1.95	2.05
31	F	314	KC1	MG-ND	-5.05	1.95	2.05
31	M	307	KC1	MG-ND	-5.04	1.95	2.05
31	F	309	KC1	MG-ND	-5.04	1.95	2.05
29	B	305	UIX	O2-C27	5.02	1.46	1.35
30	l	310	CLA	C3D-C4D	5.01	1.48	1.41
31	H	310	KC1	MG-ND	-5.01	1.95	2.05
31	O	310	KC1	MG-ND	-4.99	1.95	2.05
31	J	313	KC1	MG-ND	-4.97	1.95	2.05
31	O	315	KC1	MG-ND	-4.97	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	515	KC1	MG-ND	-4.97	1.95	2.05
31	N	311	KC1	MG-ND	-4.97	1.95	2.05
31	O	312	KC1	MG-ND	-4.95	1.96	2.05
31	A	306	KC1	MG-ND	-4.95	1.96	2.05
31	P	213	KC1	MG-ND	-4.94	1.96	2.05
31	M	314	KC1	MG-ND	-4.94	1.96	2.05
38	b	729	PQN	C10-C5	4.91	1.48	1.40
31	I	314	KC1	MG-ND	-4.91	1.96	2.05
31	N	306	KC1	MG-ND	-4.91	1.96	2.05
29	J	305	UIX	O2-C27	4.91	1.46	1.35
31	B	314	KC1	MG-ND	-4.90	1.96	2.05
31	H	306	KC1	MG-ND	-4.89	1.96	2.05
31	P	216	KC1	MG-ND	-4.89	1.96	2.05
29	h	201	UIX	O2-C27	4.88	1.46	1.35
31	D	315	KC1	MG-ND	-4.88	1.96	2.05
31	K	314	KC1	MG-ND	-4.87	1.96	2.05
29	O	306	UIX	O2-C27	4.87	1.46	1.35
31	L	307	KC1	MG-ND	-4.87	1.96	2.05
38	a	732	PQN	C10-C5	4.86	1.48	1.40
29	P	207	UIX	O2-C27	4.86	1.45	1.35
31	A	314	KC1	MG-ND	-4.85	1.96	2.05
29	G	503	UIX	O2-C27	4.83	1.45	1.35
31	D	310	KC1	MG-ND	-4.83	1.96	2.05
31	P	211	KC1	MG-ND	-4.82	1.96	2.05
29	A	304	UIX	O2-C27	4.81	1.45	1.35
29	K	302	UIX	O2-C27	4.81	1.45	1.35
31	M	307	KC1	MG-NB	-4.72	1.96	2.05
31	P	211	KC1	MG-NB	-4.68	1.96	2.05
31	H	310	KC1	MG-NB	-4.68	1.96	2.05
31	F	314	KC1	MG-NB	-4.67	1.96	2.05
31	O	315	KC1	MG-NB	-4.65	1.96	2.05
31	D	310	KC1	MG-NB	-4.65	1.96	2.05
31	M	314	KC1	MG-NB	-4.64	1.96	2.05
31	N	311	KC1	MG-NB	-4.63	1.96	2.05
31	F	309	KC1	MG-NB	-4.63	1.96	2.05
31	P	216	KC1	MG-NB	-4.62	1.96	2.05
31	N	308	KC1	MG-NB	-4.62	1.96	2.05
31	N	306	KC1	MG-NB	-4.62	1.96	2.05
31	H	306	KC1	MG-NB	-4.60	1.96	2.05
31	J	313	KC1	MG-NB	-4.59	1.96	2.05
31	O	310	KC1	MG-NB	-4.58	1.96	2.05
31	A	306	KC1	MG-NB	-4.57	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I	314	KC1	MG-NB	-4.57	1.96	2.05
31	L	315	KC1	MG-NB	-4.57	1.96	2.05
31	A	314	KC1	MG-NB	-4.57	1.96	2.05
31	B	314	KC1	MG-NB	-4.55	1.96	2.05
31	L	307	KC1	MG-NB	-4.55	1.96	2.05
31	O	312	KC1	MG-NB	-4.54	1.96	2.05
31	G	515	KC1	MG-NB	-4.54	1.96	2.05
31	K	314	KC1	MG-NB	-4.53	1.96	2.05
31	P	213	KC1	MG-NB	-4.50	1.96	2.05
31	D	315	KC1	MG-NB	-4.49	1.96	2.05
29	I	304	UIX	O2-C27	4.33	1.44	1.35
32	I	317	DGD	O1G-C1A	4.27	1.45	1.33
32	G	501	DGD	O1G-C1A	4.26	1.45	1.33
29	h	201	UIX	C25-C20	-4.25	1.25	1.30
32	l	301	DGD	O1G-C1A	4.23	1.45	1.33
32	j	103	DGD	O1G-C1A	4.22	1.45	1.33
29	K	302	UIX	C25-C20	-4.20	1.25	1.30
32	y	201	DGD	O1G-C1A	4.20	1.45	1.33
32	G	521	DGD	O2G-C1B	4.19	1.46	1.34
32	G	501	DGD	O2G-C1B	4.14	1.46	1.34
28	J	303	DD6	C19-C20	4.14	1.58	1.52
32	l	301	DGD	O2G-C1B	4.11	1.45	1.34
32	j	103	DGD	O2G-C1B	4.11	1.45	1.34
29	A	304	UIX	C25-C20	-4.10	1.25	1.30
32	y	201	DGD	O2G-C1B	4.06	1.45	1.34
32	I	317	DGD	O2G-C1B	4.04	1.45	1.34
32	L	301	DGD	O2G-C1B	4.03	1.45	1.34
32	G	521	DGD	O1G-C1A	4.01	1.45	1.33
29	I	304	UIX	C25-C20	-4.00	1.25	1.30
29	B	305	UIX	C25-C20	-3.94	1.26	1.30
29	h	201	UIX	C25-C28	-3.83	1.25	1.31
29	P	207	UIX	C25-C20	-3.80	1.26	1.30
29	O	306	UIX	C25-C20	-3.80	1.26	1.30
29	I	304	UIX	C25-C28	-3.79	1.25	1.31
28	G	505	DD6	C19-C20	3.78	1.57	1.52
30	L	317	CLA	C1D-ND	3.76	1.42	1.37
30	J	316	CLA	C1D-ND	3.75	1.42	1.37
29	K	302	UIX	C25-C28	-3.74	1.25	1.31
30	b	718	CLA	C1D-ND	3.73	1.42	1.37
30	H	311	CLA	C1D-ND	3.73	1.42	1.37
30	M	318	CLA	C1D-ND	3.72	1.42	1.37
30	N	310	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	307	CLA	C1D-ND	3.71	1.42	1.37
30	O	316	CLA	C1D-ND	3.71	1.42	1.37
29	A	304	UIX	C25-C28	-3.69	1.25	1.31
30	H	308	CLA	C1D-ND	3.68	1.42	1.37
30	a	738	CLA	C1D-ND	3.67	1.42	1.37
30	H	304	CLA	C1D-ND	3.67	1.42	1.37
30	G	516	CLA	C1D-ND	3.67	1.42	1.37
30	J	311	CLA	C1D-ND	3.66	1.42	1.37
30	G	518	CLA	C1D-ND	3.66	1.42	1.37
30	A	307	CLA	C1D-ND	3.66	1.42	1.37
30	a	717	CLA	C1D-ND	3.66	1.42	1.37
30	F	315	CLA	C1D-ND	3.66	1.42	1.37
30	K	306	CLA	C1D-ND	3.65	1.42	1.37
30	K	316	CLA	C1D-ND	3.64	1.42	1.37
30	B	316	CLA	C1D-ND	3.63	1.42	1.37
30	b	726	CLA	C1D-ND	3.63	1.42	1.37
30	H	312	CLA	C1D-ND	3.63	1.42	1.37
30	a	726	CLA	C1D-ND	3.63	1.42	1.37
30	B	307	CLA	C1D-ND	3.63	1.42	1.37
30	a	728	CLA	C1D-ND	3.63	1.42	1.37
30	J	308	CLA	C1D-ND	3.62	1.42	1.37
30	P	209	CLA	C1D-ND	3.62	1.42	1.37
30	K	312	CLA	C1D-ND	3.62	1.42	1.37
30	G	512	CLA	C1D-ND	3.62	1.42	1.37
30	b	708	CLA	C1D-ND	3.62	1.42	1.37
30	P	215	CLA	C1D-ND	3.62	1.42	1.37
30	J	314	CLA	C1D-ND	3.62	1.42	1.37
29	B	305	UIX	C25-C28	-3.61	1.26	1.31
30	A	316	CLA	C1D-ND	3.61	1.42	1.37
30	h	202	CLA	C1D-ND	3.61	1.42	1.37
30	L	313	CLA	C1D-ND	3.60	1.42	1.37
30	b	711	CLA	C1D-ND	3.60	1.42	1.37
30	M	308	CLA	C1D-ND	3.60	1.42	1.37
30	j	104	CLA	C1D-ND	3.60	1.42	1.37
30	b	705	CLA	C1D-ND	3.60	1.42	1.37
30	b	707	CLA	C1D-ND	3.60	1.42	1.37
30	b	717	CLA	C1D-ND	3.60	1.42	1.37
30	F	313	CLA	C1D-ND	3.60	1.42	1.37
30	M	309	CLA	C1D-ND	3.60	1.42	1.37
30	I	311	CLA	C1D-ND	3.60	1.42	1.37
30	L	318	CLA	C1D-ND	3.59	1.42	1.37
30	I	315	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	l	309	CLA	C1D-ND	3.59	1.42	1.37
30	L	316	CLA	C1D-ND	3.59	1.42	1.37
30	M	315	CLA	C1D-ND	3.59	1.42	1.37
30	F	310	CLA	C1D-ND	3.59	1.42	1.37
30	l	303	CLA	C1D-ND	3.59	1.42	1.37
30	a	721	CLA	C1D-ND	3.58	1.42	1.37
30	B	312	CLA	C1D-ND	3.58	1.42	1.37
30	A	311	CLA	C1D-ND	3.58	1.42	1.37
30	m	202	CLA	C1D-ND	3.58	1.42	1.37
30	b	706	CLA	C1D-ND	3.58	1.42	1.37
30	K	307	CLA	C1D-ND	3.58	1.42	1.37
30	O	314	CLA	C1D-ND	3.58	1.42	1.37
29	O	306	UIX	C25-C28	-3.58	1.26	1.31
30	a	705	CLA	C1D-ND	3.58	1.42	1.37
30	A	312	CLA	C1D-ND	3.58	1.42	1.37
30	O	308	CLA	C1D-ND	3.58	1.42	1.37
30	G	509	CLA	C1D-ND	3.58	1.42	1.37
30	l	305	CLA	C1D-ND	3.58	1.42	1.37
30	K	310	CLA	C1D-ND	3.58	1.42	1.37
30	F	311	CLA	C1D-ND	3.58	1.42	1.37
30	D	314	CLA	C1D-ND	3.57	1.42	1.37
30	H	307	CLA	C1D-ND	3.57	1.42	1.37
30	f	301	CLA	C1D-ND	3.57	1.42	1.37
30	a	731	CLA	C1D-ND	3.57	1.42	1.37
30	G	513	CLA	C1D-ND	3.57	1.42	1.37
30	l	308	CLA	C1D-ND	3.57	1.42	1.37
30	N	304	CLA	C1D-ND	3.57	1.42	1.37
30	G	511	CLA	C1D-ND	3.57	1.42	1.37
30	a	714	CLA	C1D-ND	3.57	1.42	1.37
30	H	305	CLA	C1D-ND	3.57	1.42	1.37
30	a	715	CLA	C1D-ND	3.57	1.42	1.37
30	N	305	CLA	C1D-ND	3.57	1.42	1.37
30	a	707	CLA	C1D-ND	3.57	1.42	1.37
30	I	307	CLA	C1D-ND	3.57	1.42	1.37
30	F	307	CLA	C1D-ND	3.57	1.42	1.37
29	P	207	UIX	C25-C28	-3.56	1.26	1.31
30	f	302	CLA	C1D-ND	3.56	1.42	1.37
30	M	311	CLA	C1D-ND	3.56	1.42	1.37
28	G	504	DD6	C19-C20	3.56	1.57	1.52
30	a	720	CLA	C1D-ND	3.56	1.42	1.37
30	D	316	CLA	C1D-ND	3.56	1.42	1.37
29	G	503	UIX	C25-C20	-3.56	1.26	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	315	CLA	C1D-ND	3.56	1.42	1.37
30	D	311	CLA	C1D-ND	3.56	1.42	1.37
30	I	306	CLA	C1D-ND	3.56	1.42	1.37
30	A	309	CLA	C1D-ND	3.56	1.42	1.37
30	D	309	CLA	C1D-ND	3.56	1.42	1.37
30	l	311	CLA	C1D-ND	3.55	1.42	1.37
30	a	716	CLA	C1D-ND	3.55	1.42	1.37
30	b	714	CLA	C1D-ND	3.55	1.42	1.37
30	a	722	CLA	C1D-ND	3.55	1.42	1.37
30	b	715	CLA	C1D-ND	3.55	1.42	1.37
30	b	716	CLA	C1D-ND	3.55	1.42	1.37
30	O	309	CLA	C1D-ND	3.55	1.42	1.37
30	P	217	CLA	C1D-ND	3.55	1.42	1.37
30	G	517	CLA	C1D-ND	3.55	1.42	1.37
30	b	719	CLA	C1D-ND	3.55	1.42	1.37
30	G	510	CLA	C1D-ND	3.55	1.42	1.37
30	A	317	CLA	C1D-ND	3.55	1.42	1.37
30	B	308	CLA	C1D-ND	3.55	1.42	1.37
30	B	313	CLA	C1D-ND	3.55	1.42	1.37
30	L	311	CLA	C1D-ND	3.55	1.42	1.37
30	K	311	CLA	C1D-ND	3.54	1.42	1.37
30	a	723	CLA	C1D-ND	3.54	1.42	1.37
30	b	701	CLA	C1D-ND	3.54	1.42	1.37
30	M	310	CLA	C1D-ND	3.54	1.42	1.37
30	O	311	CLA	C1D-ND	3.54	1.42	1.37
30	I	310	CLA	C1D-ND	3.53	1.42	1.37
30	J	315	CLA	C1D-ND	3.53	1.42	1.37
30	a	709	CLA	C1D-ND	3.53	1.42	1.37
30	B	301	CLA	C1D-ND	3.53	1.42	1.37
30	b	728	CLA	C1D-ND	3.53	1.42	1.37
30	J	301	CLA	C1D-ND	3.53	1.42	1.37
28	K	303	DD6	C28-C27	-3.53	1.48	1.50
30	I	312	CLA	C1D-ND	3.53	1.42	1.37
30	M	313	CLA	C1D-ND	3.53	1.42	1.37
30	b	724	CLA	C1D-ND	3.53	1.42	1.37
30	K	315	CLA	C1D-ND	3.53	1.42	1.37
30	a	708	CLA	C1D-ND	3.52	1.42	1.37
30	N	309	CLA	C1D-ND	3.52	1.42	1.37
30	D	312	CLA	C1D-ND	3.52	1.42	1.37
30	H	309	CLA	C1D-ND	3.52	1.42	1.37
30	f	303	CLA	C1D-ND	3.52	1.42	1.37
30	b	720	CLA	C1D-ND	3.52	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	J	310	CLA	C1D-ND	3.52	1.42	1.37
30	j	106	CLA	C1D-ND	3.52	1.42	1.37
30	l	313	CLA	C1D-ND	3.52	1.42	1.37
30	B	317	CLA	C1D-ND	3.52	1.42	1.37
30	P	212	CLA	C1D-ND	3.52	1.42	1.37
30	a	718	CLA	C1D-ND	3.52	1.42	1.37
30	M	317	CLA	C1D-ND	3.51	1.42	1.37
30	B	310	CLA	C1D-ND	3.51	1.42	1.37
30	B	309	CLA	C1D-ND	3.51	1.42	1.37
30	a	704	CLA	C1D-ND	3.51	1.42	1.37
30	A	319	CLA	C1D-ND	3.50	1.42	1.37
30	a	729	CLA	C1D-ND	3.50	1.42	1.37
30	L	314	CLA	C1D-ND	3.50	1.42	1.37
30	L	310	CLA	C1D-ND	3.50	1.42	1.37
30	I	308	CLA	C1D-ND	3.50	1.42	1.37
30	a	706	CLA	C1D-ND	3.50	1.42	1.37
30	D	313	CLA	C1D-ND	3.50	1.42	1.37
30	A	313	CLA	C1D-ND	3.50	1.42	1.37
30	L	308	CLA	C1D-ND	3.49	1.42	1.37
30	J	306	CLA	C1D-ND	3.49	1.42	1.37
30	a	711	CLA	C1D-ND	3.49	1.42	1.37
30	b	727	CLA	C1D-ND	3.49	1.42	1.37
30	L	309	CLA	C1D-ND	3.49	1.42	1.37
30	D	308	CLA	C1D-ND	3.49	1.42	1.37
30	I	309	CLA	C1D-ND	3.49	1.42	1.37
30	I	319	CLA	C1D-ND	3.49	1.42	1.37
30	L	312	CLA	C1D-ND	3.48	1.42	1.37
30	a	725	CLA	C1D-ND	3.48	1.42	1.37
30	P	210	CLA	C1D-ND	3.48	1.42	1.37
30	b	723	CLA	C1D-ND	3.48	1.42	1.37
29	J	305	UIX	C25-C20	-3.48	1.26	1.30
30	a	727	CLA	C1D-ND	3.48	1.42	1.37
30	K	309	CLA	C1D-ND	3.47	1.42	1.37
30	a	701	CLA	C1D-ND	3.47	1.42	1.37
30	b	710	CLA	C1D-ND	3.47	1.42	1.37
30	K	308	CLA	C1D-ND	3.47	1.42	1.37
30	b	725	CLA	C1D-ND	3.47	1.42	1.37
30	b	713	CLA	C1D-ND	3.47	1.42	1.37
30	M	316	CLA	C1D-ND	3.47	1.42	1.37
30	l	304	CLA	C1D-ND	3.46	1.42	1.37
30	F	308	CLA	C1D-ND	3.46	1.42	1.37
30	M	312	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	I	316	CLA	C1D-ND	3.46	1.42	1.37
30	G	519	CLA	C1D-ND	3.46	1.42	1.37
30	A	308	CLA	C1D-ND	3.45	1.42	1.37
30	J	309	CLA	C1D-ND	3.45	1.42	1.37
30	A	310	CLA	C1D-ND	3.44	1.42	1.37
30	a	735	CLA	C1D-ND	3.44	1.42	1.37
30	I	321	CLA	C1D-ND	3.44	1.42	1.37
30	K	313	CLA	C1D-ND	3.43	1.42	1.37
30	b	712	CLA	C1D-ND	3.43	1.42	1.37
30	b	722	CLA	C1D-ND	3.43	1.42	1.37
30	G	520	CLA	C1D-ND	3.43	1.42	1.37
30	I	313	CLA	C1D-ND	3.43	1.42	1.37
30	l	312	CLA	C1D-ND	3.43	1.42	1.37
30	G	514	CLA	C1D-ND	3.43	1.42	1.37
30	B	315	CLA	C1D-ND	3.41	1.42	1.37
30	b	703	CLA	C1D-ND	3.41	1.42	1.37
30	J	307	CLA	C1D-ND	3.41	1.42	1.37
30	a	719	CLA	C1D-ND	3.41	1.42	1.37
30	a	730	CLA	C1D-ND	3.41	1.42	1.37
29	G	503	UIX	C25-C28	-3.40	1.26	1.31
30	a	710	CLA	C1D-ND	3.40	1.42	1.37
30	b	709	CLA	C1D-ND	3.39	1.42	1.37
30	J	312	CLA	C1D-ND	3.39	1.42	1.37
30	O	313	CLA	C1D-ND	3.39	1.42	1.37
30	a	724	CLA	C1D-ND	3.38	1.42	1.37
30	a	713	CLA	C1D-ND	3.37	1.42	1.37
30	a	712	CLA	C1D-ND	3.36	1.42	1.37
28	J	303	DD6	O1-C20	-3.35	1.41	1.46
30	A	320	CLA	C1D-ND	3.35	1.42	1.37
29	J	305	UIX	C25-C28	-3.34	1.26	1.31
30	b	721	CLA	C1D-ND	3.34	1.42	1.37
30	P	214	CLA	C1D-ND	3.32	1.42	1.37
30	B	311	CLA	C1D-ND	3.31	1.42	1.37
30	A	320	CLA	C4B-NB	3.31	1.42	1.37
30	I	311	CLA	C4B-NB	3.28	1.42	1.37
30	B	307	CLA	C4B-NB	3.27	1.42	1.37
30	j	104	CLA	C4B-NB	3.27	1.42	1.37
30	l	303	CLA	C4B-NB	3.27	1.42	1.37
30	b	719	CLA	C4B-NB	3.26	1.42	1.37
30	b	709	CLA	C4B-NB	3.26	1.42	1.37
30	G	518	CLA	C4B-NB	3.25	1.42	1.37
30	b	718	CLA	C4B-NB	3.24	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	727	CLA	C4B-NB	3.24	1.42	1.37
28	J	304	DD6	O1-C20	-3.23	1.42	1.46
30	N	307	CLA	C4B-NB	3.23	1.42	1.37
30	A	307	CLA	C4B-NB	3.21	1.42	1.37
30	a	707	CLA	C4B-NB	3.21	1.42	1.37
30	J	310	CLA	C4B-NB	3.21	1.42	1.37
30	G	516	CLA	C4B-NB	3.19	1.42	1.37
30	a	735	CLA	C4B-NB	3.19	1.42	1.37
30	a	731	CLA	C4B-NB	3.18	1.42	1.37
30	H	311	CLA	C4B-NB	3.18	1.42	1.37
30	L	316	CLA	C4B-NB	3.18	1.42	1.37
30	L	309	CLA	C4B-NB	3.18	1.42	1.37
30	K	316	CLA	C4B-NB	3.17	1.42	1.37
30	b	706	CLA	C4B-NB	3.17	1.42	1.37
30	b	726	CLA	C4B-NB	3.17	1.42	1.37
30	O	308	CLA	C4B-NB	3.16	1.42	1.37
30	I	307	CLA	C4B-NB	3.16	1.42	1.37
30	a	738	CLA	C4B-NB	3.16	1.42	1.37
30	b	728	CLA	C4B-NB	3.16	1.42	1.37
30	M	313	CLA	C4B-NB	3.16	1.42	1.37
30	N	304	CLA	C4B-NB	3.16	1.42	1.37
30	b	723	CLA	C4B-NB	3.15	1.42	1.37
30	D	308	CLA	C4B-NB	3.15	1.42	1.37
30	B	308	CLA	C4B-NB	3.15	1.42	1.37
30	L	317	CLA	C4B-NB	3.15	1.42	1.37
30	M	316	CLA	C4B-NB	3.15	1.42	1.37
30	a	716	CLA	C4B-NB	3.15	1.42	1.37
28	M	302	DD6	C19-C20	3.15	1.56	1.52
30	b	712	CLA	CAB-C3B	-3.14	1.44	1.50
30	l	308	CLA	C4B-NB	3.14	1.42	1.37
30	F	311	CLA	C4B-NB	3.14	1.42	1.37
30	M	318	CLA	C4B-NB	3.13	1.42	1.37
30	A	319	CLA	C4B-NB	3.13	1.42	1.37
30	a	724	CLA	C4B-NB	3.13	1.42	1.37
30	b	710	CLA	C4B-NB	3.13	1.42	1.37
30	l	310	CLA	C4D-ND	-3.13	1.33	1.38
28	I	303	DD6	O1-C20	-3.13	1.42	1.46
30	l	309	CLA	C4B-NB	3.13	1.42	1.37
30	b	711	CLA	C4B-NB	3.13	1.42	1.37
30	a	719	CLA	C4B-NB	3.13	1.42	1.37
30	A	317	CLA	C4B-NB	3.13	1.42	1.37
30	H	312	CLA	C4B-NB	3.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	311	CLA	C4B-NB	3.13	1.42	1.37
30	I	321	CLA	C4B-NB	3.12	1.42	1.37
30	a	710	CLA	C4B-NB	3.12	1.42	1.37
30	a	718	CLA	C4B-NB	3.12	1.42	1.37
29	O	306	UIX	O-C1	-3.12	1.42	1.46
30	a	714	CLA	C4B-NB	3.12	1.42	1.37
30	H	304	CLA	C4B-NB	3.12	1.42	1.37
30	M	310	CLA	C4B-NB	3.12	1.42	1.37
30	A	316	CLA	C4B-NB	3.12	1.42	1.37
30	J	316	CLA	C4B-NB	3.12	1.42	1.37
30	a	704	CLA	C4B-NB	3.12	1.42	1.37
30	b	721	CLA	C4B-NB	3.11	1.42	1.37
30	B	317	CLA	C4B-NB	3.11	1.42	1.37
29	P	207	UIX	O-C1	-3.11	1.42	1.46
30	I	315	CLA	C4B-NB	3.11	1.41	1.37
30	l	311	CLA	C4B-NB	3.11	1.41	1.37
30	H	308	CLA	C4B-NB	3.11	1.41	1.37
30	l	304	CLA	C4B-NB	3.11	1.41	1.37
30	b	712	CLA	C4B-NB	3.11	1.41	1.37
30	J	306	CLA	C4B-NB	3.11	1.41	1.37
30	P	217	CLA	C4B-NB	3.11	1.41	1.37
30	b	722	CLA	C4B-NB	3.10	1.41	1.37
30	L	311	CLA	C4B-NB	3.10	1.41	1.37
30	a	709	CLA	C4B-NB	3.10	1.41	1.37
30	I	309	CLA	C4B-NB	3.10	1.41	1.37
30	F	310	CLA	C4B-NB	3.10	1.41	1.37
30	P	210	CLA	C4B-NB	3.10	1.41	1.37
30	D	314	CLA	C4B-NB	3.10	1.41	1.37
30	D	316	CLA	C4B-NB	3.10	1.41	1.37
30	B	301	CLA	C4B-NB	3.09	1.41	1.37
30	b	716	CLA	C4B-NB	3.09	1.41	1.37
30	D	312	CLA	C4B-NB	3.09	1.41	1.37
30	K	306	CLA	C4B-NB	3.09	1.41	1.37
30	O	316	CLA	C4B-NB	3.09	1.41	1.37
30	D	311	CLA	C4B-NB	3.09	1.41	1.37
30	I	308	CLA	C4B-NB	3.09	1.41	1.37
30	j	106	CLA	C4B-NB	3.09	1.41	1.37
30	b	701	CLA	C4B-NB	3.09	1.41	1.37
30	A	311	CLA	C4B-NB	3.09	1.41	1.37
30	G	511	CLA	C4B-NB	3.09	1.41	1.37
30	m	202	CLA	C4B-NB	3.09	1.41	1.37
30	l	312	CLA	C4B-NB	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	J	314	CLA	C4B-NB	3.09	1.41	1.37
30	B	316	CLA	C4B-NB	3.08	1.41	1.37
30	P	209	CLA	C4B-NB	3.08	1.41	1.37
30	a	712	CLA	C4B-NB	3.08	1.41	1.37
30	h	202	CLA	C4B-NB	3.08	1.41	1.37
34	N	302	PID	C8-C9	-3.08	1.39	1.46
30	G	519	CLA	C4B-NB	3.08	1.41	1.37
30	a	717	CLA	C4B-NB	3.08	1.41	1.37
30	M	315	CLA	C4B-NB	3.08	1.41	1.37
30	J	315	CLA	C4B-NB	3.08	1.41	1.37
30	H	309	CLA	C4B-NB	3.07	1.41	1.37
30	a	705	CLA	C4B-NB	3.07	1.41	1.37
30	a	708	CLA	C4B-NB	3.07	1.41	1.37
30	L	308	CLA	C4B-NB	3.07	1.41	1.37
30	I	306	CLA	C4B-NB	3.07	1.41	1.37
30	B	315	CLA	C4B-NB	3.07	1.41	1.37
30	J	312	CLA	C4B-NB	3.07	1.41	1.37
30	M	308	CLA	C4B-NB	3.07	1.41	1.37
30	K	311	CLA	C4B-NB	3.07	1.41	1.37
34	G	506	PID	C8-C9	-3.07	1.39	1.46
30	b	713	CLA	C4B-NB	3.07	1.41	1.37
30	l	305	CLA	C4B-NB	3.06	1.41	1.37
30	B	311	CLA	C4B-NB	3.06	1.41	1.37
30	K	315	CLA	C4B-NB	3.06	1.41	1.37
30	O	314	CLA	C4B-NB	3.06	1.41	1.37
30	F	315	CLA	C4B-NB	3.06	1.41	1.37
30	l	313	CLA	C4B-NB	3.06	1.41	1.37
30	F	307	CLA	C4B-NB	3.06	1.41	1.37
30	J	308	CLA	C4B-NB	3.06	1.41	1.37
30	B	310	CLA	C4B-NB	3.06	1.41	1.37
30	L	312	CLA	C4B-NB	3.05	1.41	1.37
30	b	707	CLA	C4B-NB	3.05	1.41	1.37
30	L	310	CLA	C4B-NB	3.05	1.41	1.37
30	a	713	CLA	C4B-NB	3.05	1.41	1.37
30	I	316	CLA	C4B-NB	3.05	1.41	1.37
30	K	310	CLA	C4B-NB	3.05	1.41	1.37
30	b	714	CLA	C4B-NB	3.05	1.41	1.37
30	b	715	CLA	C4B-NB	3.05	1.41	1.37
30	b	724	CLA	C4B-NB	3.05	1.41	1.37
30	I	319	CLA	C4B-NB	3.05	1.41	1.37
30	J	307	CLA	C4B-NB	3.05	1.41	1.37
30	A	315	CLA	C4B-NB	3.04	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	308	CLA	C4B-NB	3.04	1.41	1.37
30	H	305	CLA	C4B-NB	3.04	1.41	1.37
30	b	727	CLA	C4B-NB	3.04	1.41	1.37
30	I	312	CLA	C4B-NB	3.04	1.41	1.37
30	D	309	CLA	C4B-NB	3.04	1.41	1.37
30	I	313	CLA	C4B-NB	3.04	1.41	1.37
30	a	701	CLA	C4B-NB	3.04	1.41	1.37
30	M	309	CLA	C4B-NB	3.03	1.41	1.37
30	b	703	CLA	C4B-NB	3.03	1.41	1.37
30	J	301	CLA	C4B-NB	3.03	1.41	1.37
30	a	722	CLA	C4B-NB	3.03	1.41	1.37
30	a	725	CLA	C4B-NB	3.03	1.41	1.37
30	f	301	CLA	C4B-NB	3.03	1.41	1.37
30	b	725	CLA	C4B-NB	3.03	1.41	1.37
30	G	509	CLA	C4B-NB	3.02	1.41	1.37
30	A	312	CLA	C4B-NB	3.02	1.41	1.37
30	M	317	CLA	C4B-NB	3.02	1.41	1.37
30	a	715	CLA	C4B-NB	3.02	1.41	1.37
30	K	313	CLA	C4B-NB	3.02	1.41	1.37
30	P	212	CLA	C4B-NB	3.02	1.41	1.37
30	K	308	CLA	C4B-NB	3.01	1.41	1.37
30	O	309	CLA	C4B-NB	3.01	1.41	1.37
30	H	307	CLA	C4B-NB	3.01	1.41	1.37
30	B	312	CLA	C4B-NB	3.01	1.41	1.37
30	G	517	CLA	C4B-NB	3.00	1.41	1.37
30	a	706	CLA	C4B-NB	3.00	1.41	1.37
30	f	303	CLA	C4B-NB	3.00	1.41	1.37
30	I	310	CLA	C4B-NB	3.00	1.41	1.37
30	G	514	CLA	C4B-NB	3.00	1.41	1.37
30	a	711	CLA	C4B-NB	3.00	1.41	1.37
28	I	305	DD6	O1-C20	-3.00	1.42	1.46
30	f	302	CLA	C4B-NB	3.00	1.41	1.37
30	O	311	CLA	C4B-NB	3.00	1.41	1.37
30	B	309	CLA	C4B-NB	3.00	1.41	1.37
30	a	723	CLA	C4B-NB	2.99	1.41	1.37
30	N	310	CLA	C4B-NB	2.99	1.41	1.37
30	b	717	CLA	C4B-NB	2.99	1.41	1.37
30	G	520	CLA	C4B-NB	2.99	1.41	1.37
30	a	720	CLA	C4B-NB	2.99	1.41	1.37
30	F	308	CLA	C4B-NB	2.99	1.41	1.37
30	G	512	CLA	C4B-NB	2.99	1.41	1.37
30	A	309	CLA	C4B-NB	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	P	215	CLA	C4B-NB	2.98	1.41	1.37
30	L	318	CLA	C4B-NB	2.98	1.41	1.37
30	N	305	CLA	C4B-NB	2.98	1.41	1.37
28	G	505	DD6	O1-C20	-2.98	1.42	1.46
30	M	312	CLA	C4B-NB	2.97	1.41	1.37
30	J	311	CLA	C4B-NB	2.97	1.41	1.37
30	L	313	CLA	C4B-NB	2.97	1.41	1.37
30	L	314	CLA	C4B-NB	2.97	1.41	1.37
30	J	309	CLA	C4B-NB	2.97	1.41	1.37
30	K	312	CLA	C4B-NB	2.96	1.41	1.37
30	K	309	CLA	C4B-NB	2.96	1.41	1.37
30	a	721	CLA	C4B-NB	2.96	1.41	1.37
30	A	310	CLA	C4B-NB	2.96	1.41	1.37
30	b	720	CLA	C4B-NB	2.96	1.41	1.37
30	B	313	CLA	C4B-NB	2.96	1.41	1.37
30	a	729	CLA	C4B-NB	2.95	1.41	1.37
30	a	726	CLA	C4B-NB	2.95	1.41	1.37
30	G	510	CLA	C4B-NB	2.95	1.41	1.37
30	A	313	CLA	C4B-NB	2.94	1.41	1.37
30	D	313	CLA	C4B-NB	2.94	1.41	1.37
30	P	214	CLA	C4B-NB	2.94	1.41	1.37
30	b	708	CLA	C4B-NB	2.93	1.41	1.37
30	b	705	CLA	C4B-NB	2.93	1.41	1.37
29	K	302	UIX	O-C1	-2.91	1.42	1.46
30	F	313	CLA	C4B-NB	2.91	1.41	1.37
28	J	304	DD6	C19-C20	2.91	1.56	1.52
30	a	728	CLA	C4B-NB	2.91	1.41	1.37
30	B	301	CLA	C1B-C2B	2.90	1.49	1.43
34	O	307	PID	C8-C9	-2.90	1.39	1.46
30	a	730	CLA	C4B-NB	2.90	1.41	1.37
30	O	313	CLA	C4B-NB	2.89	1.41	1.37
30	N	309	CLA	C4B-NB	2.89	1.41	1.37
30	O	309	CLA	C1B-C2B	2.88	1.49	1.43
34	O	302	PID	C8-C9	-2.86	1.39	1.46
34	P	203	PID	C8-C9	-2.86	1.39	1.46
30	b	703	CLA	C1B-C2B	2.86	1.49	1.43
30	P	210	CLA	C1B-C2B	2.86	1.49	1.43
30	G	513	CLA	C4B-NB	2.85	1.41	1.37
30	B	309	CLA	C1B-C2B	2.85	1.49	1.43
30	G	512	CLA	C1B-C2B	2.84	1.49	1.43
30	B	313	CLA	C1B-C2B	2.83	1.49	1.43
30	h	202	CLA	C1B-C2B	2.83	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	O	301	PID	C8-C9	-2.83	1.39	1.46
28	I	305	DD6	C36-C31	-2.82	1.31	1.35
30	G	511	CLA	C1B-C2B	2.82	1.49	1.43
30	P	217	CLA	C1B-C2B	2.82	1.49	1.43
30	F	307	CLA	C1B-C2B	2.82	1.49	1.43
30	O	314	CLA	C1B-C2B	2.82	1.49	1.43
34	H	302	PID	C8-C9	-2.82	1.39	1.46
30	F	315	CLA	C1B-C2B	2.81	1.49	1.43
30	b	707	CLA	C1B-C2B	2.81	1.49	1.43
30	K	312	CLA	C1B-C2B	2.81	1.49	1.43
30	N	304	CLA	C1B-C2B	2.81	1.49	1.43
30	b	714	CLA	C1B-C2B	2.81	1.49	1.43
30	l	305	CLA	C1B-C2B	2.81	1.49	1.43
30	A	308	CLA	C1B-C2B	2.81	1.49	1.43
30	a	729	CLA	C1B-C2B	2.80	1.49	1.43
30	b	720	CLA	C1B-C2B	2.80	1.49	1.43
30	J	309	CLA	C1B-C2B	2.80	1.49	1.43
30	F	308	CLA	C1B-C2B	2.80	1.49	1.43
34	D	302	PID	C8-C9	-2.80	1.39	1.46
30	J	314	CLA	C1B-C2B	2.80	1.49	1.43
30	a	720	CLA	C1B-C2B	2.79	1.49	1.43
31	N	308	KC1	C4A-C3A	-2.79	1.38	1.44
34	D	304	PID	C13-C12	2.79	1.44	1.36
30	a	715	CLA	C1B-C2B	2.79	1.49	1.43
30	D	313	CLA	C1B-C2B	2.79	1.49	1.43
30	M	315	CLA	C1B-C2B	2.79	1.49	1.43
30	l	309	CLA	C1B-C2B	2.79	1.49	1.43
30	D	308	CLA	C1B-C2B	2.79	1.49	1.43
30	M	309	CLA	C1B-C2B	2.79	1.49	1.43
30	l	304	CLA	C1B-C2B	2.79	1.49	1.43
30	L	309	CLA	C1B-C2B	2.79	1.49	1.43
30	G	519	CLA	C1B-C2B	2.79	1.49	1.43
30	L	311	CLA	C1B-C2B	2.79	1.49	1.43
30	M	308	CLA	C1B-C2B	2.79	1.49	1.43
30	L	308	CLA	C1B-C2B	2.79	1.49	1.43
30	I	310	CLA	C1B-C2B	2.78	1.49	1.43
34	O	304	PID	C8-C9	-2.78	1.39	1.46
30	f	303	CLA	C1B-C2B	2.78	1.49	1.43
30	a	714	CLA	C1B-C2B	2.78	1.49	1.43
30	D	311	CLA	C1B-C2B	2.78	1.49	1.43
30	K	311	CLA	C1B-C2B	2.78	1.49	1.43
30	b	706	CLA	C1B-C2B	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	O	316	CLA	C1B-C2B	2.78	1.49	1.43
30	P	214	CLA	C1B-C2B	2.78	1.49	1.43
30	H	308	CLA	C1B-C2B	2.78	1.49	1.43
30	P	209	CLA	C1B-C2B	2.78	1.49	1.43
30	G	509	CLA	C1B-C2B	2.78	1.49	1.43
30	A	315	CLA	C1B-C2B	2.78	1.49	1.43
30	B	308	CLA	C1B-C2B	2.78	1.49	1.43
30	b	728	CLA	C1B-C2B	2.78	1.49	1.43
30	b	727	CLA	C1B-C2B	2.77	1.49	1.43
30	G	517	CLA	C1B-C2B	2.77	1.49	1.43
30	J	315	CLA	C1B-C2B	2.77	1.49	1.43
30	I	319	CLA	C1B-C2B	2.77	1.49	1.43
30	M	317	CLA	C1B-C2B	2.77	1.49	1.43
30	A	309	CLA	C1B-C2B	2.77	1.49	1.43
30	M	310	CLA	C1B-C2B	2.77	1.49	1.43
30	b	716	CLA	C1B-C2B	2.77	1.49	1.43
28	M	303	DD6	O1-C20	-2.77	1.42	1.46
29	h	201	UIX	O-C1	-2.77	1.42	1.46
30	a	707	CLA	C1B-C2B	2.77	1.49	1.43
29	G	503	UIX	O-C1	-2.77	1.42	1.46
30	F	311	CLA	C1B-C2B	2.77	1.49	1.43
30	L	314	CLA	C1B-C2B	2.77	1.49	1.43
34	F	304	PID	C13-C12	2.76	1.44	1.36
30	D	309	CLA	C1B-C2B	2.76	1.49	1.43
30	b	725	CLA	C1B-C2B	2.76	1.49	1.43
30	J	306	CLA	C1B-C2B	2.76	1.49	1.43
30	I	307	CLA	C1B-C2B	2.76	1.49	1.43
30	b	711	CLA	C1B-C2B	2.76	1.49	1.43
30	a	706	CLA	C1B-C2B	2.76	1.49	1.43
30	D	316	CLA	C1B-C2B	2.76	1.49	1.43
30	F	310	CLA	C1B-C2B	2.76	1.49	1.43
30	H	309	CLA	C1B-C2B	2.76	1.49	1.43
30	b	726	CLA	C1B-C2B	2.76	1.49	1.43
34	F	306	PID	C8-C9	-2.76	1.39	1.46
30	a	728	CLA	C1B-C2B	2.76	1.49	1.43
30	K	315	CLA	C1B-C2B	2.76	1.49	1.43
30	a	725	CLA	C1B-C2B	2.76	1.49	1.43
34	O	305	PID	C8-C9	-2.75	1.39	1.46
30	f	301	CLA	C1B-C2B	2.75	1.49	1.43
30	H	305	CLA	C1B-C2B	2.75	1.49	1.43
30	H	307	CLA	C1B-C2B	2.75	1.49	1.43
34	M	301	PID	C13-C12	2.75	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	316	CLA	C1B-C2B	2.75	1.49	1.43
30	a	730	CLA	C1B-C2B	2.75	1.49	1.43
30	b	705	CLA	C1B-C2B	2.75	1.49	1.43
30	b	723	CLA	C1B-C2B	2.75	1.49	1.43
34	F	302	PID	C8-C9	-2.75	1.39	1.46
34	P	206	PID	C13-C12	2.75	1.44	1.36
30	H	311	CLA	C1B-C2B	2.75	1.49	1.43
30	B	312	CLA	C1B-C2B	2.75	1.49	1.43
30	K	307	CLA	C1B-C2B	2.75	1.49	1.43
30	l	308	CLA	C1B-C2B	2.75	1.49	1.43
30	O	308	CLA	C1B-C2B	2.75	1.49	1.43
30	b	715	CLA	C1B-C2B	2.75	1.49	1.43
30	a	718	CLA	C1B-C2B	2.75	1.49	1.43
30	A	312	CLA	C1B-C2B	2.75	1.49	1.43
30	K	307	CLA	C4B-NB	2.74	1.41	1.37
34	D	306	PID	C8-C9	-2.74	1.39	1.46
30	H	304	CLA	C1B-C2B	2.74	1.49	1.43
30	a	738	CLA	C1B-C2B	2.74	1.49	1.43
30	A	319	CLA	C1B-C2B	2.74	1.49	1.43
30	P	212	CLA	C1B-C2B	2.74	1.49	1.43
30	L	318	CLA	C1B-C2B	2.74	1.49	1.43
34	P	205	PID	C8-C9	-2.74	1.39	1.46
30	H	312	CLA	C1B-C2B	2.74	1.49	1.43
30	J	311	CLA	C1B-C2B	2.74	1.49	1.43
30	a	710	CLA	C1B-C2B	2.74	1.49	1.43
30	G	520	CLA	C1B-C2B	2.73	1.49	1.43
30	A	307	CLA	C1B-C2B	2.73	1.49	1.43
34	G	507	PID	C8-C9	-2.73	1.39	1.46
34	F	305	PID	C8-C9	-2.73	1.39	1.46
30	b	721	CLA	C1B-C2B	2.73	1.49	1.43
30	l	310	CLA	C4D-CHA	2.73	1.43	1.39
30	G	514	CLA	C1B-C2B	2.73	1.49	1.43
30	D	312	CLA	C1B-C2B	2.73	1.49	1.43
30	G	516	CLA	C1B-C2B	2.73	1.49	1.43
30	L	317	CLA	C1B-C2B	2.73	1.49	1.43
30	O	313	CLA	C1B-C2B	2.73	1.49	1.43
30	B	311	CLA	C1B-C2B	2.73	1.49	1.43
30	a	731	CLA	C1B-C2B	2.73	1.49	1.43
30	j	106	CLA	C1B-C2B	2.73	1.49	1.43
30	a	722	CLA	C1B-C2B	2.73	1.49	1.43
34	D	305	PID	C8-C9	-2.73	1.39	1.46
30	J	301	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	313	CLA	C1B-C2B	2.72	1.49	1.43
30	J	307	CLA	C1B-C2B	2.72	1.49	1.43
34	P	206	PID	C8-C9	-2.72	1.39	1.46
30	N	310	CLA	C1B-C2B	2.72	1.49	1.43
30	a	702	CLA	C1D-ND	2.72	1.41	1.37
30	I	306	CLA	C1B-C2B	2.72	1.49	1.43
30	L	312	CLA	C1B-C2B	2.72	1.49	1.43
30	G	513	CLA	C1B-C2B	2.72	1.49	1.43
30	b	701	CLA	C1B-C2B	2.72	1.49	1.43
30	B	315	CLA	C1B-C2B	2.72	1.49	1.43
30	K	309	CLA	C1B-C2B	2.72	1.49	1.43
30	j	104	CLA	C1B-C2B	2.72	1.49	1.43
30	a	727	CLA	C1B-C2B	2.72	1.49	1.43
30	N	309	CLA	C1B-C2B	2.72	1.49	1.43
30	A	310	CLA	C1B-C2B	2.71	1.49	1.43
30	B	316	CLA	C1B-C2B	2.71	1.49	1.43
34	F	302	PID	C13-C12	2.71	1.44	1.36
30	L	316	CLA	C1B-C2B	2.71	1.49	1.43
30	a	701	CLA	C1B-C2B	2.71	1.49	1.43
30	f	302	CLA	C1B-C2B	2.70	1.49	1.43
30	M	318	CLA	C1B-C2B	2.70	1.49	1.43
30	F	313	CLA	C1B-C2B	2.70	1.49	1.43
34	H	301	PID	C8-C9	-2.70	1.40	1.46
30	K	310	CLA	C1B-C2B	2.70	1.49	1.43
30	B	317	CLA	C1B-C2B	2.70	1.49	1.43
30	b	724	CLA	C1B-C2B	2.70	1.49	1.43
30	b	713	CLA	C1B-C2B	2.70	1.49	1.43
30	A	311	CLA	C1B-C2B	2.70	1.49	1.43
30	I	313	CLA	C1B-C2B	2.70	1.49	1.43
30	l	311	CLA	C1B-C2B	2.70	1.49	1.43
30	O	311	CLA	C1B-C2B	2.70	1.49	1.43
30	K	308	CLA	C1B-C2B	2.69	1.49	1.43
30	B	310	CLA	C1B-C2B	2.69	1.49	1.43
28	G	504	DD6	O1-C20	-2.69	1.42	1.46
30	a	702	CLA	MG-NB	-2.69	2.00	2.05
30	K	306	CLA	C1B-C2B	2.69	1.49	1.43
30	G	510	CLA	C1B-C2B	2.69	1.49	1.43
30	a	719	CLA	C1B-C2B	2.69	1.49	1.43
34	P	202	PID	C13-C12	2.69	1.43	1.36
30	a	708	CLA	C1B-C2B	2.69	1.49	1.43
34	O	304	PID	C13-C12	2.69	1.43	1.36
31	N	308	KC1	C4B-NB	-2.69	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	J	313	KC1	C4B-NB	-2.69	1.34	1.37
30	N	305	CLA	C1B-C2B	2.69	1.49	1.43
30	F	312	CLA	C1D-ND	2.69	1.41	1.37
30	I	311	CLA	C1B-C2B	2.69	1.49	1.43
30	a	704	CLA	C1B-C2B	2.68	1.49	1.43
30	a	703	CLA	MG-NB	-2.68	2.00	2.05
30	b	712	CLA	C4B-C3B	2.68	1.49	1.43
30	K	316	CLA	C1B-C2B	2.68	1.49	1.43
30	b	717	CLA	C1B-C2B	2.68	1.49	1.43
30	M	311	CLA	C1B-C2B	2.68	1.49	1.43
34	j	105	PID	C8-C9	-2.68	1.40	1.46
30	J	312	CLA	C1B-C2B	2.68	1.49	1.43
30	J	316	CLA	C1B-C2B	2.68	1.49	1.43
30	b	709	CLA	C3B-C4B	2.68	1.50	1.42
30	l	303	CLA	C1B-C2B	2.68	1.49	1.43
30	b	704	CLA	MG-NB	-2.68	2.00	2.05
30	a	705	CLA	C1B-C2B	2.68	1.49	1.43
30	a	716	CLA	C1B-C2B	2.67	1.49	1.43
34	D	307	PID	C13-C12	2.67	1.43	1.36
30	a	717	CLA	C1B-C2B	2.67	1.49	1.43
30	L	310	CLA	C1B-C2B	2.67	1.49	1.43
30	I	315	CLA	C1B-C2B	2.67	1.49	1.43
30	a	711	CLA	C1B-C2B	2.67	1.49	1.43
30	l	313	CLA	C1B-C2B	2.67	1.49	1.43
30	b	708	CLA	C1B-C2B	2.67	1.49	1.43
30	a	712	CLA	C1B-C2B	2.67	1.49	1.43
28	M	302	DD6	O1-C20	-2.67	1.42	1.46
30	a	723	CLA	C1B-C2B	2.66	1.49	1.43
30	P	215	CLA	C1B-C2B	2.66	1.49	1.43
30	b	718	CLA	C1B-C2B	2.66	1.49	1.43
31	P	213	KC1	C4B-NB	-2.66	1.34	1.37
30	I	312	CLA	C1B-C2B	2.66	1.49	1.43
30	I	316	CLA	C1B-C2B	2.66	1.49	1.43
30	I	309	CLA	C1B-C2B	2.65	1.49	1.43
34	D	301	PID	C8-C9	-2.65	1.40	1.46
30	a	721	CLA	C1B-C2B	2.65	1.49	1.43
34	F	305	PID	C13-C12	2.65	1.43	1.36
30	I	321	CLA	C1B-C2B	2.65	1.49	1.43
34	P	208	PID	C13-C12	2.65	1.43	1.36
28	K	301	DD6	O1-C20	-2.65	1.42	1.46
30	b	710	CLA	C1B-C2B	2.65	1.49	1.43
30	K	313	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	P	202	PID	C8-C9	-2.65	1.40	1.46
30	a	709	CLA	C1B-C2B	2.65	1.49	1.43
31	M	314	KC1	C4B-NB	-2.64	1.34	1.37
30	A	317	CLA	C1B-C2B	2.64	1.49	1.43
30	a	735	CLA	C1B-C2B	2.64	1.49	1.43
34	H	301	PID	C13-C12	2.64	1.43	1.36
30	l	310	CLA	CMD-C2D	-2.64	1.46	1.51
31	M	307	KC1	C4B-NB	-2.64	1.34	1.37
30	M	316	CLA	C1B-C2B	2.64	1.49	1.43
31	K	314	KC1	CBA-CGA	-2.64	1.41	1.48
34	F	306	PID	C13-C12	2.64	1.43	1.36
34	M	301	PID	C8-C9	-2.64	1.40	1.46
30	N	307	CLA	C1B-C2B	2.63	1.49	1.43
31	L	315	KC1	C4B-NB	-2.63	1.34	1.37
30	b	719	CLA	C1B-C2B	2.63	1.49	1.43
30	I	308	CLA	C1B-C2B	2.63	1.49	1.43
34	P	208	PID	C8-C9	-2.63	1.40	1.46
34	N	301	PID	C13-C12	2.63	1.43	1.36
31	A	306	KC1	CBA-CGA	-2.63	1.41	1.48
30	A	320	CLA	C1B-C2B	2.62	1.49	1.43
31	K	314	KC1	C4B-NB	-2.62	1.34	1.37
30	L	313	CLA	C1B-C2B	2.62	1.49	1.43
31	O	312	KC1	C4B-NB	-2.62	1.34	1.37
31	D	310	KC1	C4B-NB	-2.62	1.34	1.37
30	l	312	CLA	C1B-C2B	2.61	1.49	1.43
34	j	105	PID	C13-C12	2.61	1.43	1.36
34	P	205	PID	C13-C12	2.61	1.43	1.36
31	F	314	KC1	C4B-NB	-2.61	1.34	1.37
31	N	306	KC1	C4B-NB	-2.61	1.34	1.37
31	P	211	KC1	C4B-NB	-2.61	1.34	1.37
31	G	515	KC1	C4B-NB	-2.60	1.34	1.37
31	H	306	KC1	C4B-NB	-2.60	1.34	1.37
30	M	313	CLA	C3B-C4B	2.60	1.50	1.42
30	F	312	CLA	MG-NB	-2.60	2.00	2.05
30	B	307	CLA	C1B-C2B	2.60	1.49	1.43
30	b	704	CLA	C1D-ND	2.60	1.41	1.37
31	O	315	KC1	C4B-NB	-2.60	1.34	1.37
28	I	305	DD6	C19-C20	2.59	1.55	1.52
30	M	313	CLA	C1B-C2B	2.59	1.49	1.43
31	B	314	KC1	C4B-NB	-2.59	1.34	1.37
31	M	307	KC1	CBA-CGA	-2.59	1.41	1.48
34	D	304	PID	C8-C9	-2.59	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	307	KC1	CBA-CGA	-2.59	1.41	1.48
31	H	310	KC1	C4B-NB	-2.59	1.34	1.37
30	a	703	CLA	CMD-C2D	-2.58	1.45	1.50
31	P	216	KC1	C4B-NB	-2.58	1.34	1.37
30	b	722	CLA	CMB-C2B	-2.58	1.45	1.50
29	B	305	UIX	O-C1	-2.58	1.42	1.46
28	I	302	DD6	O1-C20	-2.58	1.42	1.46
31	L	307	KC1	C4B-NB	-2.58	1.34	1.37
28	L	304	DD6	O1-C20	-2.58	1.42	1.46
34	N	301	PID	C8-C9	-2.57	1.40	1.46
32	L	301	DGD	O1G-C1A	2.57	1.45	1.33
28	B	302	DD6	O1-C20	-2.57	1.42	1.46
30	b	708	CLA	C3B-C4B	2.57	1.50	1.42
31	N	308	KC1	C1B-NB	-2.57	1.34	1.37
30	m	202	CLA	C1B-C2B	2.57	1.49	1.43
31	A	314	KC1	C4B-NB	-2.56	1.34	1.37
34	O	301	PID	C13-C12	2.56	1.43	1.36
28	G	504	DD6	C36-C31	-2.56	1.32	1.35
30	D	314	CLA	C3B-C4B	2.56	1.50	1.42
31	A	314	KC1	CBA-CGA	-2.56	1.42	1.48
30	a	726	CLA	CHC-C1C	2.56	1.43	1.38
31	J	313	KC1	CBA-CGA	-2.56	1.42	1.48
30	A	320	CLA	C3B-C4B	2.55	1.50	1.42
30	j	104	CLA	C3B-C4B	2.55	1.50	1.42
31	A	306	KC1	C4B-NB	-2.55	1.34	1.37
31	B	314	KC1	CBA-CGA	-2.54	1.42	1.48
30	G	518	CLA	C1B-C2B	2.54	1.49	1.43
30	I	311	CLA	C3B-C4B	2.54	1.50	1.42
31	F	309	KC1	C4B-NB	-2.54	1.34	1.37
31	O	310	KC1	C4B-NB	-2.54	1.34	1.37
29	A	304	UIX	O-C1	-2.54	1.42	1.46
30	M	316	CLA	C3B-C4B	2.54	1.50	1.42
30	a	723	CLA	C3B-C4B	2.54	1.50	1.42
30	J	308	CLA	C1B-C2B	2.53	1.49	1.43
28	K	304	DD6	O1-C20	-2.53	1.42	1.46
30	a	735	CLA	CHC-C1C	2.53	1.43	1.38
30	B	307	CLA	C3B-C4B	2.53	1.50	1.42
31	I	314	KC1	C4B-NB	-2.53	1.34	1.37
29	J	305	UIX	O-C1	-2.53	1.43	1.46
31	H	310	KC1	CBA-CGA	-2.53	1.42	1.48
30	J	316	CLA	C3B-C4B	2.52	1.50	1.42
29	I	304	UIX	O-C1	-2.52	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	310	KC1	CBA-CGA	-2.52	1.42	1.48
34	G	507	PID	C13-C12	2.52	1.43	1.36
31	P	216	KC1	CBA-CGA	-2.52	1.42	1.48
31	N	311	KC1	C4B-NB	-2.52	1.34	1.37
30	a	713	CLA	C1B-C2B	2.52	1.49	1.43
31	L	315	KC1	CBA-CGA	-2.52	1.42	1.48
30	l	310	CLA	CMB-C2B	-2.52	1.46	1.51
30	a	735	CLA	C3B-C4B	2.52	1.50	1.42
30	a	702	CLA	CMD-C2D	-2.52	1.45	1.50
30	l	310	CLA	CMC-C2C	-2.52	1.46	1.50
34	D	306	PID	C13-C12	2.52	1.43	1.36
28	O	303	DD6	C28-C27	-2.51	1.49	1.50
30	a	724	CLA	C1B-C2B	2.51	1.49	1.43
31	H	306	KC1	CBA-CGA	-2.51	1.42	1.48
30	l	311	CLA	C3B-C4B	2.51	1.50	1.42
34	D	301	PID	C13-C12	2.51	1.43	1.36
28	B	304	DD6	O1-C20	-2.51	1.43	1.46
30	a	705	CLA	CHC-C1C	2.50	1.43	1.38
30	M	313	CLA	CHC-C1C	2.50	1.43	1.38
30	b	712	CLA	C1B-C2B	2.50	1.49	1.43
30	K	308	CLA	C3B-C4B	2.50	1.50	1.42
34	D	307	PID	C8-C9	-2.50	1.40	1.46
31	N	311	KC1	CBA-CGA	-2.50	1.42	1.48
31	M	314	KC1	CBA-CGA	-2.50	1.42	1.48
28	G	508	DD6	O1-C20	-2.50	1.43	1.46
30	a	731	CLA	C3B-C4B	2.50	1.50	1.42
31	F	314	KC1	CBA-CGA	-2.50	1.42	1.48
28	b	731	DD6	O1-C20	-2.50	1.43	1.46
30	a	726	CLA	C3B-C4B	2.49	1.50	1.42
31	G	515	KC1	CBA-CGA	-2.49	1.42	1.48
30	F	312	CLA	CMD-C2D	-2.49	1.45	1.50
31	N	306	KC1	CBA-CGA	-2.49	1.42	1.48
31	I	314	KC1	CBA-CGA	-2.49	1.42	1.48
31	F	309	KC1	CBA-CGA	-2.48	1.42	1.48
30	L	317	CLA	C3B-C4B	2.48	1.50	1.42
31	P	211	KC1	CBA-CGA	-2.48	1.42	1.48
30	D	314	CLA	C1B-C2B	2.48	1.49	1.43
30	a	705	CLA	C3B-C4B	2.48	1.50	1.42
34	H	302	PID	C13-C12	2.48	1.43	1.36
30	a	711	CLA	C3B-C4B	2.48	1.49	1.42
30	F	312	CLA	CMB-C2B	-2.48	1.45	1.50
31	O	312	KC1	CBA-CGA	-2.47	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	303	DD6	O1-C20	-2.47	1.43	1.46
31	O	310	KC1	CBA-CGA	-2.47	1.42	1.48
30	L	316	CLA	C3B-C4B	2.47	1.49	1.42
30	I	316	CLA	C3B-C4B	2.47	1.49	1.42
31	D	315	KC1	CBA-CGA	-2.47	1.42	1.48
30	a	727	CLA	C3B-C4B	2.47	1.49	1.42
34	D	305	PID	C13-C12	2.47	1.43	1.36
28	K	303	DD6	O1-C20	-2.46	1.43	1.46
30	a	716	CLA	C3B-C4B	2.46	1.49	1.42
30	I	308	CLA	C3B-C4B	2.46	1.49	1.42
30	I	309	CLA	C3B-C4B	2.46	1.49	1.42
30	K	313	CLA	C3B-C4B	2.46	1.49	1.42
30	a	724	CLA	CMB-C2B	-2.46	1.45	1.50
30	a	702	CLA	CMB-C2B	-2.46	1.45	1.50
31	O	315	KC1	CBA-CGA	-2.46	1.42	1.48
30	b	704	CLA	CMB-C2B	-2.46	1.45	1.50
30	M	312	CLA	C1B-C2B	2.46	1.48	1.43
30	A	307	CLA	C3B-C4B	2.46	1.49	1.42
30	b	704	CLA	CMD-C2D	-2.46	1.45	1.50
30	A	313	CLA	C3B-C4B	2.46	1.49	1.42
34	F	304	PID	C8-C9	-2.45	1.40	1.46
30	b	722	CLA	C1B-C2B	2.45	1.48	1.43
30	I	316	CLA	CHC-C1C	2.45	1.43	1.38
31	P	213	KC1	CBA-CGA	-2.44	1.42	1.48
30	I	315	CLA	C3B-C4B	2.44	1.49	1.42
30	F	310	CLA	C3B-C4B	2.44	1.49	1.42
30	I	308	CLA	CHC-C1C	2.44	1.43	1.38
30	G	510	CLA	C3B-C4B	2.44	1.49	1.42
30	a	704	CLA	C3B-C4B	2.44	1.49	1.42
30	J	312	CLA	C3B-C4B	2.44	1.49	1.42
30	I	309	CLA	CHC-C1C	2.44	1.43	1.38
30	b	715	CLA	C3B-C4B	2.44	1.49	1.42
28	H	303	DD6	O1-C20	-2.44	1.43	1.46
28	M	304	DD6	O1-C20	-2.44	1.43	1.46
30	B	309	CLA	C3B-C4B	2.44	1.49	1.42
34	D	302	PID	C13-C12	2.43	1.43	1.36
30	J	301	CLA	C3B-C4B	2.43	1.49	1.42
30	A	317	CLA	C3B-C4B	2.43	1.49	1.42
30	b	709	CLA	C1B-C2B	2.43	1.48	1.43
30	J	310	CLA	CMB-C2B	-2.43	1.45	1.50
30	b	725	CLA	C3B-C4B	2.43	1.49	1.42
28	M	306	DD6	O1-C20	-2.43	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	H	307	CLA	C3B-C4B	2.43	1.49	1.42
30	a	717	CLA	C3B-C4B	2.43	1.49	1.42
30	b	725	CLA	CHC-C1C	2.43	1.43	1.38
30	l	303	CLA	C3B-C4B	2.43	1.49	1.42
30	A	311	CLA	CHC-C1C	2.43	1.43	1.38
30	a	724	CLA	CMD-C2D	-2.43	1.45	1.50
30	J	314	CLA	C3B-C4B	2.43	1.49	1.42
30	a	707	CLA	C3B-C4B	2.43	1.49	1.42
30	M	318	CLA	C3B-C4B	2.43	1.49	1.42
30	L	310	CLA	C3B-C4B	2.42	1.49	1.42
30	K	306	CLA	C3B-C4B	2.42	1.49	1.42
30	A	308	CLA	C3B-C4B	2.42	1.49	1.42
30	L	316	CLA	CHC-C1C	2.42	1.43	1.38
30	J	310	CLA	C1B-C2B	2.42	1.48	1.43
30	L	313	CLA	CHC-C1C	2.42	1.43	1.38
30	b	715	CLA	CHC-C1C	2.42	1.43	1.38
30	O	311	CLA	C3B-C4B	2.42	1.49	1.42
30	I	321	CLA	C3B-C4B	2.42	1.49	1.42
30	D	314	CLA	CHC-C1C	2.42	1.43	1.38
30	a	738	CLA	C3B-C4B	2.41	1.49	1.42
30	A	319	CLA	CHC-C1C	2.41	1.43	1.38
30	G	516	CLA	C3B-C4B	2.41	1.49	1.42
30	K	309	CLA	CHC-C1C	2.41	1.43	1.38
30	I	307	CLA	C3B-C4B	2.41	1.49	1.42
30	a	701	CLA	CHC-C1C	2.41	1.43	1.38
30	K	316	CLA	C3B-C4B	2.41	1.49	1.42
30	a	709	CLA	CHC-C1C	2.41	1.43	1.38
30	b	728	CLA	C3B-C4B	2.41	1.49	1.42
30	b	724	CLA	C3B-C4B	2.41	1.49	1.42
30	L	313	CLA	C3B-C4B	2.40	1.49	1.42
30	a	706	CLA	C3B-C4B	2.40	1.49	1.42
30	G	511	CLA	C3B-C4B	2.40	1.49	1.42
30	b	714	CLA	C3B-C4B	2.40	1.49	1.42
30	I	312	CLA	C3B-C4B	2.40	1.49	1.42
30	L	314	CLA	C3B-C4B	2.40	1.49	1.42
30	O	311	CLA	CHC-C1C	2.40	1.43	1.38
30	G	513	CLA	C3B-C4B	2.40	1.49	1.42
30	I	313	CLA	C3B-C4B	2.40	1.49	1.42
30	P	212	CLA	C3B-C4B	2.40	1.49	1.42
30	P	209	CLA	C3B-C4B	2.40	1.49	1.42
28	B	306	DD6	O1-C20	-2.40	1.43	1.46
30	a	722	CLA	C3B-C4B	2.40	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	O	316	CLA	C3B-C4B	2.40	1.49	1.42
30	a	709	CLA	C3B-C4B	2.40	1.49	1.42
30	a	721	CLA	C3B-C4B	2.40	1.49	1.42
30	a	711	CLA	CHC-C1C	2.40	1.43	1.38
30	B	315	CLA	C3B-C4B	2.40	1.49	1.42
30	H	304	CLA	C3B-C4B	2.40	1.49	1.42
30	a	701	CLA	C3B-C4B	2.40	1.49	1.42
30	L	310	CLA	CHC-C1C	2.40	1.43	1.38
30	L	309	CLA	C3B-C4B	2.40	1.49	1.42
30	O	308	CLA	C3B-C4B	2.40	1.49	1.42
30	b	711	CLA	C3B-C4B	2.40	1.49	1.42
30	b	714	CLA	CHC-C1C	2.40	1.43	1.38
28	O	303	DD6	O1-C20	-2.40	1.43	1.46
30	K	309	CLA	C3B-C4B	2.40	1.49	1.42
30	a	718	CLA	C3B-C4B	2.40	1.49	1.42
30	j	106	CLA	C3B-C4B	2.39	1.49	1.42
30	M	315	CLA	C3B-C4B	2.39	1.49	1.42
30	b	719	CLA	C3B-C4B	2.39	1.49	1.42
30	D	316	CLA	C3B-C4B	2.39	1.49	1.42
30	H	309	CLA	C3B-C4B	2.39	1.49	1.42
30	F	310	CLA	CHC-C1C	2.39	1.43	1.38
30	f	303	CLA	C3B-C4B	2.39	1.49	1.42
30	J	311	CLA	C3B-C4B	2.39	1.49	1.42
30	D	312	CLA	C3B-C4B	2.39	1.49	1.42
30	L	311	CLA	C3B-C4B	2.39	1.49	1.42
30	a	730	CLA	C3B-C4B	2.39	1.49	1.42
30	I	319	CLA	C3B-C4B	2.39	1.49	1.42
30	a	714	CLA	C3B-C4B	2.39	1.49	1.42
30	J	301	CLA	CHC-C1C	2.39	1.43	1.38
30	N	309	CLA	CHC-C1C	2.39	1.43	1.38
30	D	311	CLA	C3B-C4B	2.39	1.49	1.42
30	H	305	CLA	C3B-C4B	2.39	1.49	1.42
30	N	309	CLA	C3B-C4B	2.39	1.49	1.42
30	B	312	CLA	C3B-C4B	2.39	1.49	1.42
30	G	519	CLA	C3B-C4B	2.39	1.49	1.42
28	P	204	DD6	O1-C20	-2.39	1.43	1.46
30	G	520	CLA	C3B-C4B	2.39	1.49	1.42
30	G	518	CLA	C3B-C4B	2.39	1.49	1.42
30	b	704	CLA	C1B-C2B	2.39	1.48	1.43
30	K	315	CLA	C3B-C4B	2.39	1.49	1.42
30	J	312	CLA	CHC-C1C	2.39	1.43	1.38
30	b	704	CLA	CMC-C2C	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	I	313	CLA	CHC-C1C	2.39	1.43	1.38
33	K	317	LMG	O7-C8	-2.39	1.41	1.46
30	b	726	CLA	C3B-C4B	2.38	1.49	1.42
30	A	309	CLA	CHC-C1C	2.38	1.43	1.38
30	K	313	CLA	CHC-C1C	2.38	1.43	1.38
28	L	305	DD6	O1-C20	-2.38	1.43	1.46
30	D	308	CLA	C3B-C4B	2.38	1.49	1.42
30	a	704	CLA	CHC-C1C	2.38	1.43	1.38
30	A	313	CLA	CHC-C1C	2.38	1.43	1.38
30	b	710	CLA	CMB-C2B	-2.38	1.45	1.50
30	b	727	CLA	CHC-C1C	2.38	1.43	1.38
30	K	308	CLA	CHC-C1C	2.38	1.43	1.38
30	L	314	CLA	CHC-C1C	2.38	1.43	1.38
30	A	309	CLA	C3B-C4B	2.38	1.49	1.42
30	J	307	CLA	C3B-C4B	2.38	1.49	1.42
30	K	311	CLA	C3B-C4B	2.38	1.49	1.42
30	H	312	CLA	C3B-C4B	2.38	1.49	1.42
30	M	311	CLA	C3B-C4B	2.38	1.49	1.42
34	O	307	PID	C13-C12	2.38	1.43	1.36
30	B	310	CLA	C3B-C4B	2.38	1.49	1.42
30	N	304	CLA	C3B-C4B	2.38	1.49	1.42
30	b	723	CLA	C3B-C4B	2.38	1.49	1.42
30	a	708	CLA	C3B-C4B	2.38	1.49	1.42
30	A	315	CLA	CHC-C1C	2.37	1.43	1.38
30	b	707	CLA	C3B-C4B	2.37	1.49	1.42
30	J	308	CLA	C3B-C4B	2.37	1.49	1.42
31	N	308	KC1	CBA-CGA	-2.37	1.42	1.48
30	J	315	CLA	C3B-C4B	2.37	1.49	1.42
30	M	309	CLA	C3B-C4B	2.37	1.49	1.42
30	A	311	CLA	C3B-C4B	2.37	1.49	1.42
30	b	706	CLA	C3B-C4B	2.37	1.49	1.42
30	I	321	CLA	CHC-C1C	2.37	1.43	1.38
30	a	703	CLA	C1D-ND	2.37	1.41	1.37
30	B	313	CLA	C3B-C4B	2.37	1.49	1.42
30	f	303	CLA	CHC-C1C	2.37	1.43	1.38
34	G	506	PID	C13-C12	2.37	1.43	1.36
30	A	312	CLA	C3B-C4B	2.37	1.49	1.42
34	O	305	PID	C6-C7	2.37	1.54	1.50
30	G	514	CLA	C3B-C4B	2.37	1.49	1.42
30	A	315	CLA	C3B-C4B	2.37	1.49	1.42
30	b	727	CLA	C3B-C4B	2.37	1.49	1.42
30	a	726	CLA	C1B-C2B	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	I	319	CLA	CHC-C1C	2.37	1.43	1.38
30	B	317	CLA	C3B-C4B	2.37	1.49	1.42
30	b	724	CLA	CHC-C1C	2.37	1.43	1.38
28	A	302	DD6	C26-C27	-2.37	1.32	1.37
31	D	315	KC1	C4B-NB	-2.37	1.34	1.37
30	l	309	CLA	C3B-C4B	2.37	1.49	1.42
30	b	703	CLA	CHC-C1C	2.37	1.43	1.38
30	B	316	CLA	C3B-C4B	2.37	1.49	1.42
30	a	706	CLA	CHC-C1C	2.37	1.43	1.38
30	K	312	CLA	C3B-C4B	2.36	1.49	1.42
30	G	509	CLA	C3B-C4B	2.36	1.49	1.42
30	l	305	CLA	C3B-C4B	2.36	1.49	1.42
30	L	312	CLA	C3B-C4B	2.36	1.49	1.42
30	N	307	CLA	C3B-C4B	2.36	1.49	1.42
30	F	311	CLA	C3B-C4B	2.36	1.49	1.42
30	G	510	CLA	CHC-C1C	2.36	1.43	1.38
30	B	312	CLA	CHC-C1C	2.36	1.43	1.38
30	b	716	CLA	C3B-C4B	2.36	1.49	1.42
30	J	311	CLA	CHC-C1C	2.36	1.43	1.38
30	J	314	CLA	CHC-C1C	2.36	1.43	1.38
30	j	104	CLA	CHC-C1C	2.36	1.43	1.38
30	l	312	CLA	CHC-C1C	2.36	1.43	1.38
30	H	305	CLA	CHC-C1C	2.36	1.43	1.38
30	a	719	CLA	C3B-C4B	2.36	1.49	1.42
30	J	315	CLA	CHC-C1C	2.36	1.43	1.38
30	P	212	CLA	CHC-C1C	2.36	1.43	1.38
30	M	310	CLA	C3B-C4B	2.36	1.49	1.42
30	N	305	CLA	C3B-C4B	2.36	1.49	1.42
30	a	719	CLA	CHC-C1C	2.36	1.43	1.38
30	K	310	CLA	CHC-C1C	2.36	1.43	1.38
30	H	307	CLA	CHC-C1C	2.36	1.43	1.38
30	M	318	CLA	CHC-C1C	2.36	1.43	1.38
30	F	315	CLA	C3B-C4B	2.36	1.49	1.42
34	O	302	PID	C13-C12	2.36	1.43	1.36
30	A	316	CLA	C3B-C4B	2.36	1.49	1.42
28	M	305	DD6	O1-C20	-2.36	1.43	1.46
30	L	318	CLA	C3B-C4B	2.36	1.49	1.42
30	D	316	CLA	CHC-C1C	2.36	1.43	1.38
30	b	718	CLA	C3B-C4B	2.35	1.49	1.42
30	b	713	CLA	C3B-C4B	2.35	1.49	1.42
37	i	201	BCR	C1-C6	-2.35	1.50	1.53
30	G	520	CLA	CHC-C1C	2.35	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	312	CLA	CMB-C2B	-2.35	1.45	1.50
30	K	310	CLA	C3B-C4B	2.35	1.49	1.42
30	A	312	CLA	CHC-C1C	2.35	1.43	1.38
30	l	309	CLA	CHC-C1C	2.35	1.43	1.38
30	a	714	CLA	CHC-C1C	2.35	1.43	1.38
30	a	717	CLA	CHC-C1C	2.35	1.43	1.38
30	a	713	CLA	C3B-C4B	2.35	1.49	1.42
30	l	308	CLA	CHC-C1C	2.35	1.43	1.38
30	l	312	CLA	C3B-C4B	2.35	1.49	1.42
30	l	304	CLA	C3B-C4B	2.35	1.49	1.42
30	L	308	CLA	C3B-C4B	2.35	1.49	1.42
30	a	703	CLA	CMB-C2B	-2.35	1.46	1.50
30	l	308	CLA	C3B-C4B	2.35	1.49	1.42
34	O	305	PID	C13-C12	2.35	1.43	1.36
30	H	308	CLA	C3B-C4B	2.35	1.49	1.42
30	b	705	CLA	C3B-C4B	2.35	1.49	1.42
30	b	712	CLA	CMB-C2B	-2.35	1.46	1.50
30	M	311	CLA	CHC-C1C	2.34	1.43	1.38
30	h	202	CLA	C3B-C4B	2.34	1.49	1.42
30	P	217	CLA	C3B-C4B	2.34	1.49	1.42
30	L	309	CLA	CHC-C1C	2.34	1.43	1.38
30	a	729	CLA	C3B-C4B	2.34	1.49	1.42
30	b	707	CLA	CHC-C1C	2.34	1.43	1.38
30	B	317	CLA	CHC-C1C	2.34	1.43	1.38
30	B	308	CLA	C3B-C4B	2.34	1.49	1.42
30	A	319	CLA	C3B-C4B	2.34	1.49	1.42
30	f	301	CLA	C3B-C4B	2.34	1.49	1.42
30	A	317	CLA	CHC-C1C	2.34	1.43	1.38
30	D	311	CLA	CHC-C1C	2.34	1.43	1.38
30	M	310	CLA	CHC-C1C	2.34	1.43	1.38
30	a	702	CLA	C1B-C2B	2.34	1.48	1.43
30	M	317	CLA	C3B-C4B	2.34	1.49	1.42
30	f	301	CLA	CHC-C1C	2.34	1.43	1.38
28	L	306	DD6	O1-C20	-2.34	1.43	1.46
30	A	310	CLA	C3B-C4B	2.34	1.49	1.42
30	a	710	CLA	C3B-C4B	2.34	1.49	1.42
30	a	722	CLA	CHC-C1C	2.34	1.43	1.38
30	N	310	CLA	C3B-C4B	2.34	1.49	1.42
30	I	306	CLA	C3B-C4B	2.33	1.49	1.42
30	G	517	CLA	C3B-C4B	2.33	1.49	1.42
30	l	313	CLA	C3B-C4B	2.33	1.49	1.42
30	b	701	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	h	203	DD6	O1-C20	-2.33	1.43	1.46
30	b	706	CLA	CHC-C1C	2.33	1.43	1.38
30	B	309	CLA	CHC-C1C	2.33	1.43	1.38
30	f	302	CLA	C3B-C4B	2.33	1.49	1.42
30	M	308	CLA	C3B-C4B	2.33	1.49	1.42
30	l	313	CLA	CHC-C1C	2.33	1.43	1.38
30	a	708	CLA	CHC-C1C	2.33	1.43	1.38
30	L	311	CLA	CHC-C1C	2.33	1.43	1.38
30	a	720	CLA	C3B-C4B	2.33	1.49	1.42
30	M	315	CLA	CHC-C1C	2.33	1.43	1.38
30	F	315	CLA	CHC-C1C	2.33	1.43	1.38
30	a	724	CLA	C3B-C4B	2.33	1.49	1.42
30	b	720	CLA	C3B-C4B	2.33	1.49	1.42
30	O	316	CLA	CHC-C1C	2.33	1.43	1.38
30	P	210	CLA	C3B-C4B	2.33	1.49	1.42
30	B	310	CLA	CHC-C1C	2.33	1.43	1.38
30	a	727	CLA	CHC-C1C	2.33	1.43	1.38
30	b	716	CLA	CHC-C1C	2.33	1.43	1.38
30	m	202	CLA	C3B-C4B	2.33	1.49	1.42
30	B	311	CLA	CMD-C2D	-2.33	1.46	1.50
30	a	723	CLA	CHC-C1C	2.33	1.43	1.38
30	a	725	CLA	CHC-C1C	2.33	1.43	1.38
30	G	513	CLA	CHC-C1C	2.33	1.43	1.38
28	K	305	DD6	O1-C20	-2.32	1.43	1.46
30	G	519	CLA	CHC-C1C	2.32	1.43	1.38
30	D	308	CLA	CHC-C1C	2.32	1.43	1.38
30	L	308	CLA	CHC-C1C	2.32	1.43	1.38
30	a	728	CLA	C3B-C4B	2.32	1.49	1.42
30	f	302	CLA	CHC-C1C	2.32	1.43	1.38
30	a	729	CLA	CHC-C1C	2.32	1.43	1.38
30	a	707	CLA	CHC-C1C	2.32	1.43	1.38
30	a	710	CLA	CMD-C2D	-2.32	1.46	1.50
30	L	312	CLA	CHC-C1C	2.32	1.43	1.38
30	F	313	CLA	C3B-C4B	2.32	1.49	1.42
30	M	309	CLA	CHC-C1C	2.32	1.43	1.38
30	a	730	CLA	CHC-C1C	2.32	1.43	1.38
33	I	318	LMG	C4-C5	2.32	1.58	1.53
34	P	203	PID	C13-C12	2.32	1.42	1.36
30	l	304	CLA	CHC-C1C	2.32	1.43	1.38
30	b	723	CLA	CHC-C1C	2.32	1.43	1.38
28	I	303	DD6	C28-C27	-2.32	1.49	1.50
31	F	309	KC1	C1B-NB	-2.32	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	J	306	CLA	C3B-C4B	2.32	1.49	1.42
30	K	315	CLA	CHC-C1C	2.32	1.43	1.38
30	l	305	CLA	CHC-C1C	2.32	1.43	1.38
30	j	106	CLA	CHC-C1C	2.32	1.43	1.38
30	l	310	CLA	CAC-C3C	-2.32	1.47	1.51
30	b	726	CLA	CHC-C1C	2.32	1.43	1.38
30	P	217	CLA	CHC-C1C	2.32	1.43	1.38
30	F	312	CLA	C4B-NB	2.31	1.40	1.37
30	N	307	CLA	CHC-C1C	2.31	1.43	1.38
30	G	514	CLA	CHC-C1C	2.31	1.43	1.38
30	b	705	CLA	CHC-C1C	2.31	1.43	1.38
30	D	312	CLA	CHC-C1C	2.31	1.43	1.38
30	H	308	CLA	CHC-C1C	2.31	1.43	1.38
30	M	317	CLA	CHC-C1C	2.31	1.43	1.38
30	a	702	CLA	CMC-C2C	-2.31	1.46	1.50
30	O	314	CLA	C3B-C4B	2.31	1.49	1.42
30	I	310	CLA	C3B-C4B	2.31	1.49	1.42
30	K	312	CLA	CHC-C1C	2.31	1.43	1.38
30	b	721	CLA	C3B-C4B	2.31	1.49	1.42
30	D	309	CLA	CHC-C1C	2.31	1.43	1.38
30	a	716	CLA	CHC-C1C	2.30	1.43	1.38
30	a	712	CLA	C3B-C4B	2.30	1.49	1.42
30	A	308	CLA	CHC-C1C	2.30	1.43	1.38
30	G	512	CLA	C3B-C4B	2.30	1.49	1.42
30	a	713	CLA	CHC-C1C	2.30	1.43	1.38
30	I	312	CLA	CHC-C1C	2.30	1.43	1.38
30	B	311	CLA	CHC-C1C	2.30	1.43	1.38
30	D	309	CLA	C3B-C4B	2.30	1.49	1.42
30	a	718	CLA	CHC-C1C	2.30	1.43	1.38
31	D	310	KC1	C1B-NB	-2.30	1.34	1.37
30	A	320	CLA	CHC-C1C	2.30	1.43	1.38
30	P	215	CLA	C3B-C4B	2.30	1.49	1.42
30	b	721	CLA	CMD-C2D	-2.30	1.46	1.50
30	O	313	CLA	CHC-C1C	2.30	1.43	1.38
30	b	717	CLA	C3B-C4B	2.30	1.49	1.42
30	O	313	CLA	C3B-C4B	2.30	1.49	1.42
30	G	517	CLA	CHC-C1C	2.30	1.43	1.38
30	M	316	CLA	CHC-C1C	2.30	1.43	1.38
30	F	311	CLA	CHC-C1C	2.29	1.43	1.38
30	a	710	CLA	CHC-C1C	2.29	1.43	1.38
30	b	713	CLA	CHC-C1C	2.29	1.43	1.38
30	H	312	CLA	CHC-C1C	2.29	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	302	DD6	C28-C27	2.29	1.52	1.50
30	a	731	CLA	CHC-C1C	2.29	1.43	1.38
30	b	712	CLA	CHC-C1C	2.29	1.43	1.38
30	a	712	CLA	CHC-C1C	2.29	1.43	1.38
30	b	720	CLA	CHC-C1C	2.29	1.43	1.38
30	B	308	CLA	CHC-C1C	2.29	1.43	1.38
30	a	715	CLA	C3B-C4B	2.29	1.49	1.42
28	M	304	DD6	C28-C27	-2.29	1.49	1.50
30	b	728	CLA	CHC-C1C	2.29	1.43	1.38
28	H	303	DD6	C28-C27	-2.29	1.49	1.50
30	M	308	CLA	CHC-C1C	2.29	1.43	1.38
30	G	516	CLA	CHC-C1C	2.28	1.43	1.38
30	a	720	CLA	CHC-C1C	2.28	1.43	1.38
30	H	311	CLA	C3B-C4B	2.28	1.49	1.42
30	h	202	CLA	CHC-C1C	2.28	1.43	1.38
30	b	722	CLA	C3B-C4B	2.28	1.49	1.42
28	I	303	DD6	C21-C20	-2.28	1.48	1.51
30	H	311	CLA	CHC-C1C	2.28	1.43	1.38
31	D	315	KC1	C1B-NB	-2.28	1.34	1.37
30	B	301	CLA	C3B-C4B	2.28	1.49	1.42
30	F	308	CLA	C3B-C4B	2.28	1.49	1.42
30	L	318	CLA	CHC-C1C	2.28	1.43	1.38
30	A	310	CLA	CHC-C1C	2.28	1.43	1.38
30	K	311	CLA	CHC-C1C	2.28	1.43	1.38
30	b	701	CLA	CHC-C1C	2.28	1.43	1.38
30	a	703	CLA	CMC-C2C	-2.28	1.46	1.50
30	B	315	CLA	CHC-C1C	2.28	1.43	1.38
30	G	511	CLA	CHC-C1C	2.28	1.43	1.38
30	b	709	CLA	CHC-C1C	2.28	1.43	1.38
31	O	315	KC1	C1B-NB	-2.28	1.34	1.37
30	b	703	CLA	C3B-C4B	2.28	1.49	1.42
30	l	303	CLA	CHC-C1C	2.27	1.43	1.38
30	a	721	CLA	CHC-C1C	2.27	1.43	1.38
30	a	728	CLA	CHC-C1C	2.27	1.43	1.38
30	B	313	CLA	CHC-C1C	2.27	1.43	1.38
33	b	733	LMG	O7-C8	-2.27	1.41	1.46
30	B	316	CLA	CHC-C1C	2.27	1.43	1.38
30	J	308	CLA	CHC-C1C	2.27	1.43	1.38
33	D	317	LMG	O7-C8	-2.27	1.41	1.46
30	I	310	CLA	CHC-C1C	2.27	1.43	1.38
30	a	738	CLA	CHC-C1C	2.27	1.43	1.38
30	G	518	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	722	CLA	CMD-C2D	-2.26	1.46	1.50
28	K	318	DD6	O1-C20	-2.26	1.43	1.46
30	H	309	CLA	CHC-C1C	2.26	1.43	1.38
30	O	308	CLA	CHC-C1C	2.26	1.43	1.38
30	l	311	CLA	CHC-C1C	2.26	1.43	1.38
30	b	711	CLA	CHC-C1C	2.26	1.43	1.38
29	I	304	UIX	C15-C20	-2.26	1.50	1.54
28	N	303	DD6	O1-C20	-2.26	1.43	1.46
30	P	214	CLA	C3B-C4B	2.26	1.49	1.42
30	a	725	CLA	C3B-C4B	2.26	1.49	1.42
30	a	715	CLA	CHC-C1C	2.26	1.43	1.38
30	N	304	CLA	CHC-C1C	2.26	1.43	1.38
30	J	310	CLA	C3B-C4B	2.25	1.49	1.42
30	F	307	CLA	C3B-C4B	2.25	1.49	1.42
34	j	105	PID	C20-C21	2.25	1.41	1.35
30	I	315	CLA	CHC-C1C	2.25	1.43	1.38
31	L	307	KC1	C1B-NB	-2.25	1.34	1.37
30	A	307	CLA	CHC-C1C	2.25	1.43	1.38
30	B	311	CLA	C3B-C4B	2.25	1.49	1.42
30	I	307	CLA	CHC-C1C	2.25	1.43	1.38
30	B	301	CLA	CHC-C1C	2.25	1.43	1.38
30	B	307	CLA	CHC-C1C	2.25	1.43	1.38
30	J	309	CLA	C3B-C4B	2.25	1.49	1.42
30	b	710	CLA	C3B-C4B	2.24	1.49	1.42
30	N	305	CLA	CHC-C1C	2.24	1.43	1.38
30	l	310	CLA	C1D-ND	2.24	1.42	1.38
31	P	211	KC1	C1B-NB	-2.24	1.34	1.37
30	K	306	CLA	CHC-C1C	2.24	1.43	1.38
30	m	202	CLA	CHC-C1C	2.24	1.43	1.38
30	O	309	CLA	CHC-C1C	2.24	1.43	1.38
30	H	304	CLA	CHC-C1C	2.24	1.43	1.38
34	N	302	PID	C13-C12	2.24	1.42	1.36
30	D	313	CLA	C3B-C4B	2.24	1.49	1.42
30	J	307	CLA	CHC-C1C	2.24	1.43	1.38
30	G	509	CLA	CHC-C1C	2.24	1.43	1.38
30	M	312	CLA	CHC-C1C	2.24	1.43	1.38
30	b	710	CLA	CHC-C1C	2.24	1.43	1.38
30	A	320	CLA	CMD-C2D	-2.24	1.46	1.50
30	F	312	CLA	CMC-C2C	-2.23	1.46	1.50
30	J	316	CLA	CHC-C1C	2.23	1.43	1.38
30	a	702	CLA	MG-ND	-2.23	2.01	2.05
30	O	309	CLA	C3B-C4B	2.23	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	515	KC1	C1B-NB	-2.23	1.34	1.37
30	b	708	CLA	CHC-C1C	2.23	1.42	1.38
30	P	209	CLA	CHC-C1C	2.23	1.42	1.38
31	H	310	KC1	C1B-NB	-2.23	1.34	1.37
30	b	721	CLA	CHC-C1C	2.22	1.42	1.38
28	I	301	DD6	O1-C20	-2.22	1.43	1.46
37	i	201	BCR	C30-C25	-2.22	1.50	1.53
30	b	718	CLA	CMB-C2B	-2.22	1.46	1.50
30	b	719	CLA	CHC-C1C	2.22	1.42	1.38
30	b	713	CLA	CMB-C2B	-2.22	1.46	1.50
31	A	306	KC1	C1B-NB	-2.22	1.34	1.37
31	J	313	KC1	C1B-NB	-2.22	1.34	1.37
30	J	308	CLA	CMD-C2D	-2.22	1.46	1.50
30	F	312	CLA	C1B-C2B	2.22	1.48	1.43
30	P	210	CLA	CHC-C1C	2.22	1.42	1.38
30	P	214	CLA	CHC-C1C	2.21	1.42	1.38
28	I	303	DD6	C19-C20	2.21	1.55	1.52
30	I	311	CLA	CHC-C1C	2.21	1.42	1.38
30	J	306	CLA	CHC-C1C	2.21	1.42	1.38
30	M	312	CLA	C3B-C4B	2.21	1.49	1.42
30	M	312	CLA	MG-NB	-2.21	2.01	2.05
30	b	721	CLA	CMB-C2B	-2.21	1.46	1.50
30	a	724	CLA	CHC-C1C	2.21	1.42	1.38
31	O	310	KC1	C1B-NB	-2.21	1.35	1.37
28	L	302	DD6	O1-C20	-2.21	1.43	1.46
30	l	313	CLA	CMB-C2B	-2.21	1.46	1.50
30	G	518	CLA	CMB-C2B	-2.20	1.46	1.50
30	P	212	CLA	CMD-C2D	-2.20	1.46	1.50
30	a	712	CLA	CMB-C2B	-2.20	1.46	1.50
30	b	719	CLA	CMB-C2B	-2.20	1.46	1.50
28	A	301	DD6	O1-C20	-2.20	1.43	1.46
31	I	314	KC1	C1B-NB	-2.20	1.35	1.37
30	l	305	CLA	CMD-C2D	-2.19	1.46	1.50
30	a	711	CLA	CMD-C2D	-2.19	1.46	1.50
28	A	303	DD6	O1-C20	-2.19	1.43	1.46
30	b	709	CLA	CMB-C2B	-2.19	1.46	1.50
30	a	703	CLA	MG-ND	-2.19	2.01	2.05
30	a	703	CLA	C1B-C2B	2.19	1.48	1.43
30	D	313	CLA	CHC-C1C	2.19	1.42	1.38
28	F	301	DD6	O1-C20	-2.19	1.43	1.46
30	b	701	CLA	CMB-C2B	-2.19	1.46	1.50
31	A	314	KC1	C1B-NB	-2.19	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	P	213	KC1	C1B-NB	-2.18	1.35	1.37
30	a	719	CLA	CMC-C2C	-2.18	1.46	1.50
30	I	306	CLA	CHC-C1C	2.18	1.42	1.38
30	b	717	CLA	CHC-C1C	2.18	1.42	1.38
30	N	309	CLA	CMC-C2C	-2.18	1.46	1.50
30	N	309	CLA	CMD-C2D	-2.18	1.46	1.50
28	G	502	DD6	O1-C20	-2.18	1.43	1.46
28	L	303	DD6	O1-C20	-2.18	1.43	1.46
28	M	305	DD6	C28-C27	-2.18	1.49	1.50
28	J	304	DD6	C36-C31	-2.18	1.32	1.35
34	F	305	PID	C20-C21	2.17	1.40	1.35
30	b	710	CLA	CMD-C2D	-2.17	1.46	1.50
30	b	722	CLA	MG-NB	-2.17	2.01	2.05
30	B	311	CLA	MG-NB	-2.17	2.01	2.05
31	M	314	KC1	C1B-NB	-2.17	1.35	1.37
30	b	703	CLA	CMD-C2D	-2.17	1.46	1.50
31	K	314	KC1	C1B-NB	-2.17	1.35	1.37
31	F	314	KC1	C1B-NB	-2.17	1.35	1.37
30	J	308	CLA	MG-NB	-2.17	2.01	2.05
30	b	717	CLA	CMB-C2B	-2.17	1.46	1.50
30	b	704	CLA	C4B-NB	2.17	1.40	1.37
30	a	719	CLA	CMD-C2D	-2.16	1.46	1.50
30	a	724	CLA	MG-NB	-2.16	2.01	2.05
28	M	303	DD6	C36-C31	-2.16	1.32	1.35
30	F	307	CLA	CHC-C1C	2.16	1.42	1.38
30	G	512	CLA	CHC-C1C	2.16	1.42	1.38
30	P	215	CLA	CHC-C1C	2.16	1.42	1.38
31	B	314	KC1	C1B-NB	-2.16	1.35	1.37
30	F	308	CLA	CHC-C1C	2.16	1.42	1.38
30	b	704	CLA	MG-ND	-2.16	2.01	2.05
31	N	311	KC1	C1B-NB	-2.16	1.35	1.37
30	O	313	CLA	CMD-C2D	-2.16	1.46	1.50
30	K	307	CLA	MG-NB	-2.16	2.01	2.05
30	J	309	CLA	CHC-C1C	2.16	1.42	1.38
30	a	719	CLA	CMB-C2B	-2.15	1.46	1.50
31	M	307	KC1	C1B-NB	-2.15	1.35	1.37
30	L	317	CLA	CHC-C1C	2.15	1.42	1.38
30	a	703	CLA	C4B-NB	2.15	1.40	1.37
30	G	512	CLA	CMC-C2C	-2.15	1.46	1.50
30	l	312	CLA	CMB-C2B	-2.15	1.46	1.50
30	b	718	CLA	CHC-C1C	2.15	1.42	1.38
30	K	307	CLA	C3B-C4B	2.15	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	312	KC1	C1B-NB	-2.15	1.35	1.37
30	M	316	CLA	CMD-C2D	-2.15	1.46	1.50
30	K	311	CLA	CMD-C2D	-2.15	1.46	1.50
30	D	313	CLA	CMD-C2D	-2.15	1.46	1.50
30	b	701	CLA	CMD-C2D	-2.15	1.46	1.50
30	j	106	CLA	CMD-C2D	-2.15	1.46	1.50
30	b	713	CLA	MG-NB	-2.15	2.01	2.05
31	F	309	KC1	C4A-C3A	-2.15	1.40	1.44
30	K	316	CLA	CMB-C2B	-2.15	1.46	1.50
30	a	727	CLA	CMD-C2D	-2.15	1.46	1.50
30	J	308	CLA	CMB-C2B	-2.15	1.46	1.50
30	P	214	CLA	CMD-C2D	-2.14	1.46	1.50
30	I	312	CLA	CMB-C2B	-2.14	1.46	1.50
30	K	315	CLA	CMD-C2D	-2.14	1.46	1.50
31	A	306	KC1	C4A-C3A	-2.14	1.40	1.44
30	P	215	CLA	CMB-C2B	-2.14	1.46	1.50
30	A	316	CLA	CHC-C1C	2.14	1.42	1.38
30	J	306	CLA	CMD-C2D	-2.14	1.46	1.50
31	L	315	KC1	C1B-NB	-2.14	1.35	1.37
35	A	318	SQD	O8-S	2.14	1.55	1.47
30	a	712	CLA	MG-NB	-2.14	2.01	2.05
30	a	723	CLA	CMD-C2D	-2.14	1.46	1.50
30	O	314	CLA	CHC-C1C	2.13	1.42	1.38
30	N	307	CLA	CMD-C2D	-2.13	1.46	1.50
31	P	216	KC1	C1B-NB	-2.13	1.35	1.37
28	A	305	DD6	O1-C20	-2.13	1.43	1.46
30	a	713	CLA	MG-NB	-2.13	2.01	2.05
30	F	313	CLA	CHC-C1C	2.13	1.42	1.38
30	K	316	CLA	CHC-C1C	2.13	1.42	1.38
30	b	709	CLA	CMD-C2D	-2.13	1.46	1.50
30	J	310	CLA	CHC-C1C	2.13	1.42	1.38
30	F	313	CLA	CMD-C2D	-2.13	1.46	1.50
30	D	314	CLA	CMB-C2B	-2.13	1.46	1.50
30	a	701	CLA	CMD-C2D	-2.12	1.46	1.50
30	B	301	CLA	CMB-C2B	-2.12	1.46	1.50
30	a	709	CLA	CMB-C2B	-2.12	1.46	1.50
31	A	314	KC1	C4A-C3A	-2.12	1.40	1.44
31	G	515	KC1	C4A-C3A	-2.12	1.40	1.44
30	I	311	CLA	CMB-C2B	-2.12	1.46	1.50
30	P	217	CLA	CMD-C2D	-2.12	1.46	1.50
30	a	702	CLA	C4B-NB	2.11	1.40	1.37
30	b	717	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	H	306	KC1	C1B-NB	-2.11	1.35	1.37
30	G	511	CLA	CMD-C2D	-2.11	1.46	1.50
30	a	706	CLA	CMC-C2C	-2.11	1.46	1.50
30	a	715	CLA	CMD-C2D	-2.11	1.46	1.50
31	N	306	KC1	C1B-NB	-2.11	1.35	1.37
28	M	303	DD6	C21-C20	2.11	1.54	1.51
30	N	310	CLA	CHC-C1C	2.10	1.42	1.38
31	D	310	KC1	C4A-C3A	-2.10	1.40	1.44
30	F	308	CLA	CMC-C2C	-2.10	1.46	1.50
30	J	310	CLA	CMD-C2D	-2.10	1.46	1.50
30	L	312	CLA	CMB-C2B	-2.10	1.46	1.50
30	b	721	CLA	MG-NB	-2.10	2.01	2.05
30	b	723	CLA	CMB-C2B	-2.10	1.46	1.50
30	a	717	CLA	CMB-C2B	-2.09	1.46	1.50
30	P	217	CLA	CMC-C2C	-2.09	1.46	1.50
30	b	710	CLA	MG-NB	-2.09	2.01	2.05
30	J	310	CLA	MG-NB	-2.09	2.01	2.05
30	A	310	CLA	CMB-C2B	-2.09	1.46	1.50
30	H	308	CLA	CMD-C2D	-2.09	1.46	1.50
30	A	319	CLA	CMD-C2D	-2.09	1.46	1.50
30	a	729	CLA	CMD-C2D	-2.09	1.46	1.50
30	b	726	CLA	CMB-C2B	-2.09	1.46	1.50
30	b	712	CLA	MG-NB	-2.09	2.01	2.05
30	K	311	CLA	CMB-C2B	-2.09	1.46	1.50
30	L	318	CLA	CMC-C2C	-2.09	1.46	1.50
30	l	303	CLA	CMB-C2B	-2.09	1.46	1.50
30	B	317	CLA	CMD-C2D	-2.09	1.46	1.50
30	H	311	CLA	CMD-C2D	-2.08	1.46	1.50
30	a	710	CLA	MG-NB	-2.08	2.01	2.05
30	O	314	CLA	CMD-C2D	-2.08	1.46	1.50
28	D	303	DD6	O1-C20	-2.08	1.43	1.46
30	K	310	CLA	CMD-C2D	-2.08	1.46	1.50
30	J	312	CLA	CMD-C2D	-2.08	1.46	1.50
30	L	317	CLA	CMD-C2D	-2.08	1.46	1.50
30	I	308	CLA	CMB-C2B	-2.08	1.46	1.50
30	b	713	CLA	CMD-C2D	-2.08	1.46	1.50
30	a	730	CLA	CMC-C2C	-2.08	1.46	1.50
30	b	706	CLA	CMB-C2B	-2.08	1.46	1.50
30	a	726	CLA	MG-NB	-2.08	2.01	2.05
30	b	727	CLA	CMC-C2C	-2.08	1.46	1.50
30	G	512	CLA	CMB-C2B	-2.08	1.46	1.50
30	A	320	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	F	312	CLA	MG-ND	-2.08	2.01	2.05
30	H	309	CLA	CMB-C2B	-2.08	1.46	1.50
30	L	318	CLA	CMB-C2B	-2.08	1.46	1.50
30	B	316	CLA	CMB-C2B	-2.07	1.46	1.50
30	I	319	CLA	CMD-C2D	-2.07	1.46	1.50
30	K	312	CLA	CMD-C2D	-2.07	1.46	1.50
30	b	724	CLA	CMD-C2D	-2.07	1.46	1.50
30	a	702	CLA	C1B-NB	-2.07	1.35	1.37
30	L	318	CLA	CMD-C2D	-2.07	1.46	1.50
30	M	316	CLA	CMB-C2B	-2.07	1.46	1.50
30	G	518	CLA	MG-NB	-2.07	2.01	2.05
30	f	302	CLA	MG-NB	-2.07	2.01	2.05
30	P	214	CLA	MG-NB	-2.07	2.01	2.05
30	K	310	CLA	MG-NB	-2.07	2.01	2.05
30	D	312	CLA	MG-NB	-2.07	2.01	2.05
30	I	312	CLA	CMD-C2D	-2.07	1.46	1.50
30	N	305	CLA	MG-NB	-2.07	2.01	2.05
30	a	701	CLA	CMB-C2B	-2.07	1.46	1.50
30	b	724	CLA	MG-NB	-2.07	2.01	2.05
30	M	311	CLA	MG-NB	-2.07	2.01	2.05
30	P	209	CLA	CMD-C2D	-2.07	1.46	1.50
30	K	312	CLA	CMC-C2C	-2.07	1.46	1.50
30	F	310	CLA	CMD-C2D	-2.07	1.46	1.50
30	O	309	CLA	CMB-C2B	-2.07	1.46	1.50
30	A	310	CLA	CMD-C2D	-2.07	1.46	1.50
30	a	713	CLA	CMD-C2D	-2.07	1.46	1.50
30	L	310	CLA	MG-NB	-2.07	2.01	2.05
30	A	315	CLA	CMD-C2D	-2.06	1.46	1.50
33	b	734	LMG	O7-C8	-2.06	1.41	1.46
30	I	319	CLA	MG-NB	-2.06	2.01	2.05
30	G	520	CLA	CMD-C2D	-2.06	1.46	1.50
30	a	731	CLA	CMD-C2D	-2.06	1.46	1.50
31	J	313	KC1	C4A-C3A	-2.06	1.40	1.44
30	L	317	CLA	CMB-C2B	-2.06	1.46	1.50
30	A	316	CLA	CMC-C2C	-2.06	1.46	1.50
30	f	301	CLA	CMD-C2D	-2.06	1.46	1.50
30	a	704	CLA	CMD-C2D	-2.06	1.46	1.50
30	a	717	CLA	CMC-C2C	-2.06	1.46	1.50
30	D	316	CLA	CMC-C2C	-2.06	1.46	1.50
30	L	311	CLA	CMD-C2D	-2.06	1.46	1.50
30	F	307	CLA	CMD-C2D	-2.06	1.46	1.50
30	N	305	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	305	CLA	CMD-C2D	-2.06	1.46	1.50
30	J	307	CLA	CMD-C2D	-2.06	1.46	1.50
34	D	307	PID	C20-C21	2.06	1.40	1.35
30	m	202	CLA	MG-NB	-2.06	2.01	2.05
30	B	317	CLA	CMB-C2B	-2.06	1.46	1.50
30	G	514	CLA	CMC-C2C	-2.06	1.46	1.50
30	M	311	CLA	CMB-C2B	-2.06	1.46	1.50
33	P	201	LMG	O7-C8	-2.06	1.41	1.46
30	D	314	CLA	MG-NB	-2.06	2.01	2.05
30	B	315	CLA	CMD-C2D	-2.06	1.46	1.50
30	M	311	CLA	CMD-C2D	-2.06	1.46	1.50
30	a	722	CLA	CMC-C2C	-2.06	1.46	1.50
30	f	301	CLA	CMB-C2B	-2.06	1.46	1.50
30	b	712	CLA	CMD-C2D	-2.06	1.46	1.50
30	b	728	CLA	CMC-C2C	-2.06	1.46	1.50
30	B	310	CLA	MG-NB	-2.06	2.01	2.05
30	J	316	CLA	CMB-C2B	-2.05	1.46	1.50
30	M	318	CLA	CMD-C2D	-2.05	1.46	1.50
30	L	313	CLA	CMD-C2D	-2.05	1.46	1.50
30	D	309	CLA	MG-NB	-2.05	2.01	2.05
30	b	705	CLA	CMB-C2B	-2.05	1.46	1.50
30	L	308	CLA	CMB-C2B	-2.05	1.46	1.50
30	M	317	CLA	CMD-C2D	-2.05	1.46	1.50
30	a	728	CLA	MG-NB	-2.05	2.01	2.05
30	a	712	CLA	CMD-C2D	-2.05	1.46	1.50
30	a	728	CLA	CMB-C2B	-2.05	1.46	1.50
30	G	516	CLA	CMD-C2D	-2.05	1.46	1.50
30	b	726	CLA	CMD-C2D	-2.05	1.46	1.50
30	O	316	CLA	CMC-C2C	-2.05	1.46	1.50
30	G	519	CLA	CMD-C2D	-2.05	1.46	1.50
31	M	307	KC1	C4A-C3A	-2.05	1.40	1.44
30	a	723	CLA	CMC-C2C	-2.05	1.46	1.50
30	J	316	CLA	CMD-C2D	-2.05	1.46	1.50
31	D	315	KC1	C4A-C3A	-2.05	1.40	1.44
30	a	727	CLA	CMB-C2B	-2.05	1.46	1.50
30	I	315	CLA	CMB-C2B	-2.05	1.46	1.50
30	h	202	CLA	CMD-C2D	-2.05	1.46	1.50
30	D	314	CLA	CMD-C2D	-2.05	1.46	1.50
30	J	312	CLA	CMB-C2B	-2.05	1.46	1.50
30	I	312	CLA	MG-NB	-2.05	2.01	2.05
30	b	701	CLA	MG-NB	-2.05	2.01	2.05
30	H	312	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	307	CLA	CMB-C2B	-2.05	1.46	1.50
30	A	317	CLA	CMB-C2B	-2.05	1.46	1.50
30	a	726	CLA	CMB-C2B	-2.05	1.46	1.50
30	M	313	CLA	CMD-C2D	-2.05	1.46	1.50
30	b	722	CLA	CHC-C1C	2.05	1.42	1.38
30	l	308	CLA	CMB-C2B	-2.05	1.46	1.50
30	a	707	CLA	CMD-C2D	-2.05	1.46	1.50
30	L	316	CLA	CMB-C2B	-2.05	1.46	1.50
33	j	101	LMG	O7-C8	-2.05	1.41	1.46
30	b	708	CLA	CMD-C2D	-2.05	1.46	1.50
30	I	310	CLA	CMD-C2D	-2.05	1.46	1.50
30	I	313	CLA	CMD-C2D	-2.05	1.46	1.50
30	L	313	CLA	CMB-C2B	-2.05	1.46	1.50
30	K	310	CLA	CMB-C2B	-2.05	1.46	1.50
30	G	510	CLA	CMC-C2C	-2.05	1.46	1.50
30	a	715	CLA	CMB-C2B	-2.05	1.46	1.50
30	A	316	CLA	CMB-C2B	-2.04	1.46	1.50
30	b	714	CLA	CMD-C2D	-2.04	1.46	1.50
30	J	309	CLA	MG-NB	-2.04	2.01	2.05
30	I	321	CLA	CMC-C2C	-2.04	1.46	1.50
30	A	308	CLA	CMD-C2D	-2.04	1.46	1.50
30	l	303	CLA	CMD-C2D	-2.04	1.46	1.50
30	a	704	CLA	CMB-C2B	-2.04	1.46	1.50
30	a	725	CLA	CMD-C2D	-2.04	1.46	1.50
30	A	319	CLA	CMC-C2C	-2.04	1.46	1.50
30	a	730	CLA	CMD-C2D	-2.04	1.46	1.50
30	B	307	CLA	CMB-C2B	-2.04	1.46	1.50
30	K	313	CLA	CMC-C2C	-2.04	1.46	1.50
30	h	202	CLA	CMB-C2B	-2.04	1.46	1.50
30	b	719	CLA	CMD-C2D	-2.04	1.46	1.50
30	F	308	CLA	CMD-C2D	-2.04	1.46	1.50
29	I	304	UIX	O2-C18	-2.04	1.41	1.46
30	a	708	CLA	CMB-C2B	-2.04	1.46	1.50
30	b	725	CLA	CMC-C2C	-2.04	1.46	1.50
30	F	308	CLA	CMB-C2B	-2.04	1.46	1.50
30	N	304	CLA	CMB-C2B	-2.04	1.46	1.50
30	a	703	CLA	C1B-NB	-2.04	1.35	1.37
30	A	313	CLA	CMD-C2D	-2.04	1.46	1.50
30	b	717	CLA	MG-NB	-2.04	2.01	2.05
30	B	307	CLA	CMD-C2D	-2.04	1.46	1.50
30	O	311	CLA	MG-NB	-2.04	2.01	2.05
30	a	725	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	G	514	CLA	CMD-C2D	-2.04	1.46	1.50
30	N	310	CLA	CMD-C2D	-2.04	1.46	1.50
30	D	313	CLA	MG-NB	-2.04	2.01	2.05
30	b	703	CLA	CMC-C2C	-2.04	1.46	1.50
28	G	504	DD6	C17-C16	-2.04	1.51	1.54
30	H	308	CLA	MG-NB	-2.04	2.01	2.05
30	I	315	CLA	CMD-C2D	-2.04	1.46	1.50
30	K	306	CLA	CMB-C2B	-2.04	1.46	1.50
30	b	728	CLA	CMB-C2B	-2.04	1.46	1.50
30	j	106	CLA	CMC-C2C	-2.04	1.46	1.50
30	A	307	CLA	CMD-C2D	-2.04	1.46	1.50
30	b	705	CLA	CMD-C2D	-2.04	1.46	1.50
30	a	706	CLA	CMD-C2D	-2.04	1.46	1.50
30	b	727	CLA	CMD-C2D	-2.04	1.46	1.50
30	O	308	CLA	CMD-C2D	-2.04	1.46	1.50
30	l	311	CLA	CMD-C2D	-2.03	1.46	1.50
30	B	311	CLA	CMB-C2B	-2.03	1.46	1.50
30	G	513	CLA	CMC-C2C	-2.03	1.46	1.50
30	B	309	CLA	CMD-C2D	-2.03	1.46	1.50
29	P	207	UIX	C15-C20	-2.03	1.51	1.54
30	I	307	CLA	CMD-C2D	-2.03	1.46	1.50
30	G	513	CLA	CMD-C2D	-2.03	1.46	1.50
30	a	714	CLA	CMD-C2D	-2.03	1.46	1.50
30	b	714	CLA	CMC-C2C	-2.03	1.46	1.50
30	P	215	CLA	MG-NB	-2.03	2.01	2.05
30	I	309	CLA	CMD-C2D	-2.03	1.46	1.50
30	a	720	CLA	CMB-C2B	-2.03	1.46	1.50
30	a	726	CLA	CMD-C2D	-2.03	1.46	1.50
30	b	720	CLA	CMC-C2C	-2.03	1.46	1.50
30	M	315	CLA	CMD-C2D	-2.03	1.46	1.50
30	G	518	CLA	CMD-C2D	-2.03	1.46	1.50
30	B	315	CLA	CMC-C2C	-2.03	1.46	1.50
30	F	311	CLA	CMD-C2D	-2.03	1.46	1.50
30	J	301	CLA	MG-NB	-2.03	2.01	2.05
30	K	309	CLA	MG-NB	-2.03	2.01	2.05
31	I	314	KC1	C4A-C3A	-2.03	1.40	1.44
30	G	509	CLA	CMB-C2B	-2.03	1.46	1.50
30	a	716	CLA	CMB-C2B	-2.03	1.46	1.50
31	O	310	KC1	C4A-C3A	-2.03	1.40	1.44
30	K	316	CLA	CMD-C2D	-2.03	1.46	1.50
30	I	309	CLA	MG-NB	-2.03	2.01	2.05
30	F	315	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	730	CLA	MG-NB	-2.03	2.01	2.05
30	b	724	CLA	CMB-C2B	-2.03	1.46	1.50
30	M	318	CLA	CMB-C2B	-2.03	1.46	1.50
30	M	308	CLA	CMD-C2D	-2.03	1.46	1.50
30	F	311	CLA	MG-NB	-2.03	2.01	2.05
30	J	301	CLA	CMD-C2D	-2.03	1.46	1.50
30	L	314	CLA	MG-NB	-2.03	2.01	2.05
30	B	312	CLA	CMB-C2B	-2.03	1.46	1.50
30	M	312	CLA	CMD-C2D	-2.03	1.46	1.50
30	A	312	CLA	CMD-C2D	-2.03	1.46	1.50
30	a	735	CLA	CMD-C2D	-2.03	1.46	1.50
30	L	314	CLA	CMD-C2D	-2.03	1.46	1.50
30	b	720	CLA	CMD-C2D	-2.03	1.46	1.50
31	P	213	KC1	C4A-C3A	-2.03	1.40	1.44
30	N	304	CLA	CMD-C2D	-2.02	1.46	1.50
30	b	718	CLA	MG-NB	-2.02	2.01	2.05
30	B	317	CLA	MG-NB	-2.02	2.01	2.05
30	J	315	CLA	CMD-C2D	-2.02	1.46	1.50
30	I	306	CLA	CMB-C2B	-2.02	1.46	1.50
30	A	312	CLA	CMC-C2C	-2.02	1.46	1.50
30	j	104	CLA	CMD-C2D	-2.02	1.46	1.50
30	a	710	CLA	CMC-C2C	-2.02	1.46	1.50
30	a	738	CLA	CMB-C2B	-2.02	1.46	1.50
30	J	309	CLA	CMB-C2B	-2.02	1.46	1.50
30	G	517	CLA	MG-NB	-2.02	2.01	2.05
30	a	715	CLA	MG-NB	-2.02	2.01	2.05
30	H	304	CLA	MG-NB	-2.02	2.01	2.05
30	a	705	CLA	CMD-C2D	-2.02	1.46	1.50
30	M	310	CLA	CMD-C2D	-2.02	1.46	1.50
30	H	307	CLA	CMD-C2D	-2.02	1.46	1.50
30	l	308	CLA	CMD-C2D	-2.02	1.46	1.50
30	j	106	CLA	MG-NB	-2.02	2.01	2.05
30	I	313	CLA	CMC-C2C	-2.02	1.46	1.50
30	K	308	CLA	CMD-C2D	-2.02	1.46	1.50
30	I	306	CLA	CMD-C2D	-2.02	1.46	1.50
30	J	309	CLA	CMD-C2D	-2.02	1.46	1.50
30	J	314	CLA	CMD-C2D	-2.02	1.46	1.50
30	O	309	CLA	CMD-C2D	-2.02	1.46	1.50
30	G	520	CLA	MG-NB	-2.02	2.01	2.05
30	a	705	CLA	CMC-C2C	-2.02	1.46	1.50
30	F	307	CLA	CMB-C2B	-2.02	1.46	1.50
30	a	728	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	P	215	CLA	CMD-C2D	-2.02	1.46	1.50
30	M	318	CLA	MG-NB	-2.02	2.01	2.05
28	G	504	DD6	C28-C27	-2.02	1.49	1.50
30	H	307	CLA	CMB-C2B	-2.02	1.46	1.50
30	L	313	CLA	MG-NB	-2.02	2.01	2.05
30	a	731	CLA	CMB-C2B	-2.02	1.46	1.50
30	D	316	CLA	CMD-C2D	-2.02	1.46	1.50
30	l	305	CLA	MG-NB	-2.02	2.01	2.05
30	K	307	CLA	CMD-C2D	-2.02	1.46	1.50
30	D	312	CLA	CMB-C2B	-2.02	1.46	1.50
30	D	312	CLA	CMD-C2D	-2.02	1.46	1.50
30	L	310	CLA	CMD-C2D	-2.02	1.46	1.50
30	F	307	CLA	MG-NB	-2.02	2.01	2.05
30	b	705	CLA	CMC-C2C	-2.01	1.46	1.50
30	B	313	CLA	CMB-C2B	-2.01	1.46	1.50
30	I	308	CLA	MG-NB	-2.01	2.01	2.05
30	b	723	CLA	CMD-C2D	-2.01	1.46	1.50
30	J	309	CLA	CMC-C2C	-2.01	1.46	1.50
30	a	721	CLA	MG-NB	-2.01	2.01	2.05
30	K	309	CLA	CMC-C2C	-2.01	1.46	1.50
30	a	709	CLA	CMD-C2D	-2.01	1.46	1.50
30	L	316	CLA	CMD-C2D	-2.01	1.46	1.50
30	G	511	CLA	CMB-C2B	-2.01	1.46	1.50
30	l	312	CLA	CMD-C2D	-2.01	1.46	1.50
30	a	722	CLA	CMD-C2D	-2.01	1.46	1.50
30	B	312	CLA	CMD-C2D	-2.01	1.46	1.50
30	O	311	CLA	CMD-C2D	-2.01	1.46	1.50
30	b	719	CLA	MG-NB	-2.01	2.01	2.05
30	H	312	CLA	MG-NB	-2.01	2.01	2.05
30	a	716	CLA	CMD-C2D	-2.01	1.46	1.50
30	a	720	CLA	CMD-C2D	-2.01	1.46	1.50
30	a	730	CLA	CMB-C2B	-2.01	1.46	1.50
30	B	310	CLA	CMB-C2B	-2.01	1.46	1.50
30	D	311	CLA	CMC-C2C	-2.01	1.46	1.50
30	M	313	CLA	CMB-C2B	-2.01	1.46	1.50
30	a	708	CLA	CMD-C2D	-2.01	1.46	1.50
30	D	308	CLA	CMD-C2D	-2.01	1.46	1.50
30	D	309	CLA	CMC-C2C	-2.01	1.46	1.50
30	L	312	CLA	CMD-C2D	-2.01	1.46	1.50
30	I	309	CLA	CMB-C2B	-2.01	1.46	1.50
30	G	519	CLA	CMB-C2B	-2.01	1.46	1.50
30	f	303	CLA	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	H	311	CLA	CMB-C2B	-2.01	1.46	1.50
30	f	303	CLA	MG-NB	-2.01	2.01	2.05
30	f	303	CLA	CMC-C2C	-2.01	1.46	1.50
30	m	202	CLA	CMD-C2D	-2.01	1.46	1.50
30	N	307	CLA	CMC-C2C	-2.01	1.46	1.50
31	K	314	KC1	C4A-C3A	-2.01	1.40	1.44
30	A	317	CLA	CMC-C2C	-2.01	1.46	1.50
30	b	716	CLA	CMD-C2D	-2.01	1.46	1.50
30	a	709	CLA	MG-NB	-2.01	2.01	2.05
30	J	306	CLA	MG-NB	-2.01	2.01	2.05
30	P	210	CLA	MG-NB	-2.01	2.01	2.05
30	I	308	CLA	CMD-C2D	-2.01	1.46	1.50
30	l	304	CLA	CMD-C2D	-2.01	1.46	1.50
30	b	717	CLA	CMD-C2D	-2.01	1.46	1.50
30	L	309	CLA	CMD-C2D	-2.01	1.46	1.50
30	P	214	CLA	CMC-C2C	-2.01	1.46	1.50
30	J	306	CLA	CMB-C2B	-2.01	1.46	1.50
30	M	309	CLA	CMD-C2D	-2.01	1.46	1.50
30	N	307	CLA	MG-NB	-2.01	2.01	2.05
30	f	302	CLA	CMD-C2D	-2.01	1.46	1.50
30	A	310	CLA	MG-NB	-2.01	2.01	2.05
30	b	708	CLA	CMB-C2B	-2.01	1.46	1.50
30	B	301	CLA	CMD-C2D	-2.01	1.46	1.50
30	A	311	CLA	CMB-C2B	-2.01	1.46	1.50
30	a	738	CLA	CMD-C2D	-2.01	1.46	1.50
30	N	310	CLA	CMB-C2B	-2.01	1.46	1.50
30	j	104	CLA	CMB-C2B	-2.01	1.46	1.50
30	G	517	CLA	CMD-C2D	-2.01	1.46	1.50
30	F	311	CLA	CMB-C2B	-2.01	1.46	1.50
30	H	305	CLA	CMD-C2D	-2.01	1.46	1.50
30	M	310	CLA	MG-NB	-2.01	2.01	2.05
30	P	212	CLA	MG-NB	-2.01	2.01	2.05
30	b	716	CLA	CMC-C2C	-2.01	1.46	1.50
30	a	703	CLA	CAA-C2A	-2.01	1.50	1.54
30	F	313	CLA	CMC-C2C	-2.01	1.46	1.50
30	O	314	CLA	CMC-C2C	-2.01	1.46	1.50
30	O	316	CLA	CMD-C2D	-2.01	1.46	1.50
30	P	217	CLA	MG-NB	-2.01	2.01	2.05
30	a	721	CLA	CMD-C2D	-2.00	1.46	1.50
30	M	308	CLA	CMB-C2B	-2.00	1.46	1.50
30	G	514	CLA	CMB-C2B	-2.00	1.46	1.50
30	D	313	CLA	CMB-C2B	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	O	314	CLA	CMB-C2B	-2.00	1.46	1.50
30	H	304	CLA	CMD-C2D	-2.00	1.46	1.50
30	K	316	CLA	MG-NB	-2.00	2.01	2.05
30	G	513	CLA	MG-NB	-2.00	2.01	2.05
30	A	317	CLA	CMD-C2D	-2.00	1.46	1.50
30	A	309	CLA	MG-NB	-2.00	2.01	2.05
30	J	307	CLA	MG-NB	-2.00	2.01	2.05
30	M	316	CLA	MG-NB	-2.00	2.01	2.05
30	H	309	CLA	MG-NB	-2.00	2.01	2.05
30	K	312	CLA	CMB-C2B	-2.00	1.46	1.50
30	b	723	CLA	MG-NB	-2.00	2.01	2.05
30	O	309	CLA	MG-NB	-2.00	2.01	2.05
30	K	306	CLA	CMD-C2D	-2.00	1.46	1.50
30	f	303	CLA	CMB-C2B	-2.00	1.46	1.50
30	J	312	CLA	MG-NB	-2.00	2.01	2.05
30	K	313	CLA	CMD-C2D	-2.00	1.46	1.50
31	P	216	KC1	C4A-C3A	-2.00	1.40	1.44

All (2771) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	304	UIX	C6-C1-C	-9.10	107.33	122.30
37	m	201	BCR	C7-C8-C9	-8.31	113.94	126.23
29	O	306	UIX	C14-C13-C11	-7.75	116.40	127.28
30	l	304	CLA	C4A-NA-C1A	7.44	110.07	106.68
30	O	314	CLA	C4A-NA-C1A	7.35	110.03	106.68
29	I	304	UIX	O-C1-C3	7.27	120.31	113.49
29	G	503	UIX	C6-C1-C	-7.23	110.41	122.30
28	J	303	DD6	C3-C2-C1	-7.17	117.22	127.28
30	P	215	CLA	C4A-NA-C1A	7.12	109.93	106.68
29	h	201	UIX	C6-C1-C	-7.09	110.64	122.30
30	J	307	CLA	C4A-NA-C1A	7.07	109.91	106.68
29	J	305	UIX	O-C1-C3	7.04	120.09	113.49
30	J	309	CLA	C4A-NA-C1A	7.04	109.89	106.68
30	B	308	CLA	C4A-NA-C1A	7.01	109.88	106.68
30	P	210	CLA	C4A-NA-C1A	7.01	109.88	106.68
30	a	702	CLA	C4A-NA-C1A	7.00	109.87	106.68
30	a	715	CLA	C4A-NA-C1A	6.99	109.87	106.68
30	L	311	CLA	C4A-NA-C1A	6.99	109.87	106.68
29	J	305	UIX	C6-C1-C	-6.98	110.82	122.30
30	N	310	CLA	C4A-NA-C1A	6.97	109.86	106.68
30	b	714	CLA	C4A-NA-C1A	6.97	109.86	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	G	512	CLA	C4A-NA-C1A	6.96	109.85	106.68
30	b	704	CLA	C4A-NA-C1A	6.95	109.85	106.68
30	B	317	CLA	C4A-NA-C1A	6.94	109.85	106.68
29	B	305	UIX	C6-C1-C	-6.94	110.89	122.30
30	L	309	CLA	C4A-NA-C1A	6.94	109.84	106.68
30	M	317	CLA	C4A-NA-C1A	6.93	109.84	106.68
30	b	719	CLA	C4A-NA-C1A	6.93	109.84	106.68
30	b	718	CLA	C4A-NA-C1A	6.93	109.84	106.68
30	L	318	CLA	C4A-NA-C1A	6.92	109.83	106.68
30	D	311	CLA	C4A-NA-C1A	6.90	109.83	106.68
30	J	312	CLA	C4A-NA-C1A	6.90	109.83	106.68
30	a	730	CLA	C4A-NA-C1A	6.87	109.81	106.68
30	a	738	CLA	C4A-NA-C1A	6.87	109.81	106.68
30	A	310	CLA	C4A-NA-C1A	6.87	109.81	106.68
30	M	315	CLA	C4A-NA-C1A	6.86	109.81	106.68
30	h	202	CLA	C4A-NA-C1A	6.86	109.81	106.68
30	G	514	CLA	C4A-NA-C1A	6.83	109.80	106.68
30	b	728	CLA	C4A-NA-C1A	6.83	109.80	106.68
30	N	309	CLA	C4A-NA-C1A	6.83	109.80	106.68
30	M	310	CLA	C4A-NA-C1A	6.83	109.79	106.68
30	B	315	CLA	C4A-NA-C1A	6.79	109.78	106.68
30	A	308	CLA	C4A-NA-C1A	6.79	109.78	106.68
30	P	212	CLA	C4A-NA-C1A	6.78	109.77	106.68
30	l	303	CLA	C4A-NA-C1A	6.78	109.77	106.68
30	K	312	CLA	C4A-NA-C1A	6.77	109.77	106.68
30	A	316	CLA	C4A-NA-C1A	6.77	109.77	106.68
37	b	702	BCR	C24-C23-C22	-6.77	116.22	126.23
30	J	306	CLA	C4A-NA-C1A	6.77	109.77	106.68
37	b	730	BCR	C7-C8-C9	-6.77	116.22	126.23
30	I	307	CLA	C4A-NA-C1A	6.76	109.77	106.68
30	b	720	CLA	C4A-NA-C1A	6.76	109.76	106.68
29	P	207	UIX	C14-C13-C11	-6.76	117.80	127.28
30	B	313	CLA	C4A-NA-C1A	6.76	109.76	106.68
30	I	306	CLA	C4A-NA-C1A	6.76	109.76	106.68
30	A	307	CLA	C4A-NA-C1A	6.74	109.75	106.68
30	a	731	CLA	C4A-NA-C1A	6.74	109.75	106.68
34	P	206	PID	C17-C16-C15	6.74	137.30	123.52
30	a	714	CLA	C4A-NA-C1A	6.73	109.75	106.68
30	F	315	CLA	C4A-NA-C1A	6.72	109.75	106.68
30	J	315	CLA	C4A-NA-C1A	6.72	109.74	106.68
30	b	701	CLA	C4A-NA-C1A	6.72	109.74	106.68
30	a	703	CLA	C4A-NA-C1A	6.71	109.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	F	313	CLA	C4A-NA-C1A	6.71	109.74	106.68
30	F	310	CLA	C4A-NA-C1A	6.71	109.74	106.68
30	P	217	CLA	C4A-NA-C1A	6.71	109.74	106.68
28	M	303	DD6	C9-C10-C11	-6.71	117.87	127.28
30	F	308	CLA	C4A-NA-C1A	6.70	109.74	106.68
30	A	320	CLA	C4A-NA-C1A	6.69	109.73	106.68
30	M	308	CLA	C4A-NA-C1A	6.69	109.73	106.68
30	a	720	CLA	C4A-NA-C1A	6.69	109.73	106.68
30	b	716	CLA	C4A-NA-C1A	6.68	109.73	106.68
30	I	319	CLA	C4A-NA-C1A	6.67	109.72	106.68
30	b	705	CLA	C4A-NA-C1A	6.67	109.72	106.68
30	K	307	CLA	C4A-NA-C1A	6.66	109.72	106.68
30	a	701	CLA	C4A-NA-C1A	6.66	109.72	106.68
30	K	316	CLA	C4A-NA-C1A	6.65	109.71	106.68
30	b	727	CLA	C4A-NA-C1A	6.65	109.71	106.68
30	a	718	CLA	C4A-NA-C1A	6.65	109.71	106.68
30	b	709	CLA	C4A-NA-C1A	6.65	109.71	106.68
30	a	710	CLA	C4A-NA-C1A	6.64	109.71	106.68
30	a	716	CLA	C4A-NA-C1A	6.64	109.71	106.68
30	L	316	CLA	C4A-NA-C1A	6.64	109.71	106.68
30	I	311	CLA	C4A-NA-C1A	6.63	109.71	106.68
30	b	707	CLA	C4A-NA-C1A	6.63	109.70	106.68
30	O	309	CLA	C4A-NA-C1A	6.62	109.70	106.68
29	A	304	UIX	C6-C1-C	-6.62	111.41	122.30
30	B	309	CLA	C4A-NA-C1A	6.62	109.70	106.68
30	G	518	CLA	C4A-NA-C1A	6.61	109.70	106.68
30	a	705	CLA	C4A-NA-C1A	6.61	109.69	106.68
30	N	304	CLA	C4A-NA-C1A	6.61	109.69	106.68
30	K	306	CLA	C4A-NA-C1A	6.60	109.69	106.68
29	O	306	UIX	C7-C10-C11	-6.59	115.31	125.53
30	I	310	CLA	C4A-NA-C1A	6.59	109.68	106.68
30	G	519	CLA	C4A-NA-C1A	6.59	109.68	106.68
30	O	316	CLA	C4A-NA-C1A	6.58	109.68	106.68
30	D	309	CLA	C4A-NA-C1A	6.58	109.68	106.68
30	I	313	CLA	C4A-NA-C1A	6.58	109.68	106.68
29	B	305	UIX	O-C1-C3	6.57	119.65	113.49
30	K	308	CLA	C4A-NA-C1A	6.56	109.67	106.68
30	I	321	CLA	C4A-NA-C1A	6.56	109.67	106.68
30	a	722	CLA	C4A-NA-C1A	6.56	109.67	106.68
30	l	313	CLA	C4A-NA-C1A	6.56	109.67	106.68
30	H	305	CLA	C4A-NA-C1A	6.56	109.67	106.68
30	F	307	CLA	C4A-NA-C1A	6.55	109.67	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	H	312	CLA	C4A-NA-C1A	6.55	109.67	106.68
30	b	724	CLA	C4A-NA-C1A	6.55	109.67	106.68
34	F	305	PID	C17-C16-C15	6.54	136.91	123.52
30	a	727	CLA	C4A-NA-C1A	6.54	109.66	106.68
30	b	712	CLA	C4A-NA-C1A	6.54	109.66	106.68
30	a	725	CLA	C4A-NA-C1A	6.53	109.66	106.68
30	D	316	CLA	C4A-NA-C1A	6.53	109.66	106.68
30	G	517	CLA	C4A-NA-C1A	6.53	109.66	106.68
30	a	711	CLA	C4A-NA-C1A	6.53	109.66	106.68
37	l	302	BCR	C24-C23-C22	-6.53	116.58	126.23
30	l	311	CLA	C4A-NA-C1A	6.52	109.66	106.68
30	G	510	CLA	C4A-NA-C1A	6.52	109.65	106.68
30	H	307	CLA	C4A-NA-C1A	6.52	109.65	106.68
30	f	301	CLA	C4A-NA-C1A	6.52	109.65	106.68
30	a	708	CLA	C4A-NA-C1A	6.51	109.65	106.68
30	B	312	CLA	C4A-NA-C1A	6.51	109.65	106.68
30	F	311	CLA	C4A-NA-C1A	6.51	109.65	106.68
30	A	311	CLA	C4A-NA-C1A	6.51	109.65	106.68
30	K	311	CLA	C4A-NA-C1A	6.50	109.64	106.68
30	L	314	CLA	C4A-NA-C1A	6.49	109.64	106.68
30	L	312	CLA	C4A-NA-C1A	6.49	109.64	106.68
30	G	509	CLA	C4A-NA-C1A	6.48	109.64	106.68
30	b	726	CLA	C4A-NA-C1A	6.48	109.64	106.68
30	f	303	CLA	C4A-NA-C1A	6.48	109.64	106.68
30	H	308	CLA	C4A-NA-C1A	6.48	109.64	106.68
30	G	516	CLA	C4A-NA-C1A	6.47	109.63	106.68
30	a	728	CLA	C4A-NA-C1A	6.47	109.63	106.68
28	F	301	DD6	C9-C10-C11	-6.47	118.20	127.28
28	K	318	DD6	C9-C10-C11	-6.47	118.21	127.28
30	D	313	CLA	C4A-NA-C1A	6.46	109.63	106.68
30	N	305	CLA	C4A-NA-C1A	6.46	109.63	106.68
30	O	313	CLA	C4A-NA-C1A	6.46	109.63	106.68
30	l	308	CLA	C4A-NA-C1A	6.46	109.62	106.68
30	J	311	CLA	C4A-NA-C1A	6.46	109.62	106.68
30	j	106	CLA	C4A-NA-C1A	6.44	109.62	106.68
30	D	312	CLA	C4A-NA-C1A	6.44	109.62	106.68
30	I	315	CLA	C4A-NA-C1A	6.44	109.62	106.68
30	b	715	CLA	C4A-NA-C1A	6.43	109.61	106.68
30	b	723	CLA	C4A-NA-C1A	6.43	109.61	106.68
30	A	313	CLA	C4A-NA-C1A	6.43	109.61	106.68
30	K	315	CLA	C4A-NA-C1A	6.43	109.61	106.68
30	A	315	CLA	C4A-NA-C1A	6.42	109.61	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	M	316	CLA	C4A-NA-C1A	6.42	109.61	106.68
30	a	723	CLA	C4A-NA-C1A	6.42	109.61	106.68
30	D	308	CLA	C4A-NA-C1A	6.42	109.61	106.68
30	b	708	CLA	C4A-NA-C1A	6.41	109.60	106.68
30	b	710	CLA	C4A-NA-C1A	6.41	109.60	106.68
30	f	302	CLA	C4A-NA-C1A	6.40	109.60	106.68
30	G	511	CLA	C4A-NA-C1A	6.39	109.60	106.68
30	a	707	CLA	C4A-NA-C1A	6.39	109.59	106.68
30	J	316	CLA	C4A-NA-C1A	6.39	109.59	106.68
30	A	317	CLA	C4A-NA-C1A	6.39	109.59	106.68
30	L	310	CLA	C4A-NA-C1A	6.39	109.59	106.68
28	A	302	DD6	C9-C10-C11	-6.38	118.33	127.28
30	A	312	CLA	C4A-NA-C1A	6.38	109.59	106.68
30	G	513	CLA	C4A-NA-C1A	6.37	109.59	106.68
30	a	712	CLA	C4A-NA-C1A	6.37	109.58	106.68
30	b	725	CLA	C4A-NA-C1A	6.37	109.58	106.68
34	P	205	PID	C17-C16-C15	6.37	136.55	123.52
30	O	308	CLA	C4A-NA-C1A	6.36	109.58	106.68
28	M	302	DD6	C3-C2-C1	-6.36	118.36	127.28
30	K	310	CLA	C4A-NA-C1A	6.35	109.58	106.68
30	m	202	CLA	C4A-NA-C1A	6.35	109.58	106.68
30	b	722	CLA	C4A-NA-C1A	6.35	109.57	106.68
30	l	309	CLA	C4A-NA-C1A	6.34	109.57	106.68
30	H	309	CLA	C4A-NA-C1A	6.34	109.57	106.68
28	F	301	DD6	C4-C5-C6	-6.34	118.39	127.28
30	A	309	CLA	C4A-NA-C1A	6.34	109.57	106.68
30	a	706	CLA	C4A-NA-C1A	6.34	109.57	106.68
30	M	311	CLA	C4A-NA-C1A	6.33	109.57	106.68
30	a	729	CLA	C4A-NA-C1A	6.33	109.57	106.68
30	a	721	CLA	C4A-NA-C1A	6.33	109.57	106.68
30	K	313	CLA	C4A-NA-C1A	6.33	109.57	106.68
30	K	309	CLA	C4A-NA-C1A	6.33	109.56	106.68
30	B	301	CLA	C4A-NA-C1A	6.33	109.56	106.68
30	J	301	CLA	C4A-NA-C1A	6.33	109.56	106.68
30	P	214	CLA	C4A-NA-C1A	6.32	109.56	106.68
34	F	305	PID	C18-C19-C20	6.32	136.44	123.52
30	b	703	CLA	C4A-NA-C1A	6.31	109.56	106.68
30	P	209	CLA	C4A-NA-C1A	6.31	109.56	106.68
30	A	319	CLA	C4A-NA-C1A	6.30	109.55	106.68
30	B	316	CLA	C4A-NA-C1A	6.30	109.55	106.68
30	M	309	CLA	C4A-NA-C1A	6.29	109.55	106.68
30	I	316	CLA	C4A-NA-C1A	6.28	109.55	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	M	318	CLA	C4A-NA-C1A	6.28	109.55	106.68
30	O	311	CLA	C4A-NA-C1A	6.28	109.54	106.68
30	b	721	CLA	C4A-NA-C1A	6.28	109.54	106.68
30	b	713	CLA	C4A-NA-C1A	6.27	109.54	106.68
29	P	207	UIX	C7-C10-C11	-6.27	115.81	125.53
30	J	314	CLA	C4A-NA-C1A	6.26	109.53	106.68
30	H	304	CLA	C4A-NA-C1A	6.25	109.53	106.68
30	b	717	CLA	C4A-NA-C1A	6.23	109.52	106.68
30	b	711	CLA	C4A-NA-C1A	6.22	109.52	106.68
29	K	302	UIX	C6-C1-C	-6.22	112.07	122.30
30	B	307	CLA	C4A-NA-C1A	6.22	109.52	106.68
30	J	308	CLA	C4A-NA-C1A	6.22	109.52	106.68
30	a	724	CLA	C4A-NA-C1A	6.20	109.51	106.68
30	L	317	CLA	C4A-NA-C1A	6.19	109.50	106.68
30	j	104	CLA	C4A-NA-C1A	6.18	109.50	106.68
30	b	706	CLA	C4A-NA-C1A	6.17	109.49	106.68
30	H	311	CLA	C4A-NA-C1A	6.16	109.49	106.68
30	I	312	CLA	C4A-NA-C1A	6.15	109.48	106.68
30	l	305	CLA	C4A-NA-C1A	6.14	109.48	106.68
30	a	709	CLA	C4A-NA-C1A	6.13	109.48	106.68
30	B	311	CLA	C4A-NA-C1A	6.13	109.48	106.68
30	L	308	CLA	C4A-NA-C1A	6.11	109.47	106.68
30	D	314	CLA	C4A-NA-C1A	6.11	109.47	106.68
30	G	520	CLA	C4A-NA-C1A	6.10	109.46	106.68
34	H	301	PID	C17-C16-C15	6.09	135.98	123.52
30	N	307	CLA	C4A-NA-C1A	6.09	109.46	106.68
30	I	308	CLA	C4A-NA-C1A	6.08	109.45	106.68
30	F	312	CLA	C4A-NA-C1A	6.06	109.45	106.68
30	a	717	CLA	C4A-NA-C1A	6.05	109.44	106.68
29	K	302	UIX	C14-C13-C11	-6.03	118.82	127.28
30	M	313	CLA	C4A-NA-C1A	6.03	109.43	106.68
37	a	736	BCR	C7-C8-C9	-6.01	117.35	126.23
30	I	309	CLA	C4A-NA-C1A	6.01	109.42	106.68
37	m	201	BCR	C15-C14-C13	-6.01	118.85	127.28
29	P	207	UIX	C6-C1-C	-6.00	112.43	122.30
29	O	306	UIX	C6-C1-C	-5.99	112.45	122.30
28	J	304	DD6	C9-C10-C11	-5.98	118.89	127.28
30	M	312	CLA	C4A-NA-C1A	5.98	109.41	106.68
29	G	503	UIX	O-C1-C3	5.97	119.09	113.49
29	P	207	UIX	C34-C30-C26	-5.96	118.91	127.28
30	l	312	CLA	C4A-NA-C1A	5.94	109.39	106.68
30	a	719	CLA	C4A-NA-C1A	5.93	109.38	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	P	207	UIX	C37-C39-C40	-5.92	118.98	127.28
31	N	308	KC1	C1D-ND-C4D	5.91	110.46	106.31
28	A	302	DD6	C14-C13-C11	-5.91	116.36	125.53
31	N	308	KC1	O2D-CGD-CBD	5.90	121.54	111.23
37	j	102	BCR	C16-C17-C18	-5.87	119.04	127.28
28	P	204	DD6	C4-C5-C6	-5.87	119.05	127.28
30	L	313	CLA	C4A-NA-C1A	5.86	109.35	106.68
29	O	306	UIX	C37-C39-C40	-5.84	119.09	127.28
28	A	301	DD6	C21-C20-C19	5.84	120.80	114.24
29	J	305	UIX	C34-C30-C26	-5.84	119.09	127.28
28	M	306	DD6	C3-C2-C1	-5.82	119.11	127.28
28	J	302	DD6	C3-C2-C1	-5.79	119.16	127.28
28	I	305	DD6	C4-C5-C6	-5.78	119.17	127.28
28	G	504	DD6	C4-C5-C6	-5.78	119.17	127.28
30	a	735	CLA	C4A-NA-C1A	5.78	109.32	106.68
34	M	301	PID	C17-C16-C15	5.77	135.34	123.52
30	a	704	CLA	C4A-NA-C1A	5.77	109.31	106.68
37	b	702	BCR	C16-C17-C18	-5.77	119.18	127.28
34	F	304	PID	C17-C16-C15	5.77	135.32	123.52
30	a	726	CLA	C4A-NA-C1A	5.77	109.31	106.68
29	K	302	UIX	C34-C30-C26	-5.73	119.25	127.28
28	I	305	DD6	C3-C2-C1	-5.72	119.26	127.28
29	h	201	UIX	O-C1-C3	5.71	118.84	113.49
28	G	505	DD6	O1-C20-C21	5.71	121.43	115.05
28	J	304	DD6	C3-C2-C1	-5.68	119.31	127.28
28	G	505	DD6	C3-C2-C1	-5.65	119.35	127.28
30	J	310	CLA	C4A-NA-C1A	5.64	109.25	106.68
29	O	306	UIX	C34-C30-C26	-5.64	119.37	127.28
28	O	303	DD6	C4-C5-C6	-5.63	119.38	127.28
30	a	713	CLA	C4A-NA-C1A	5.63	109.25	106.68
34	F	302	PID	C18-C19-C20	5.62	135.02	123.52
34	D	304	PID	C17-C16-C15	5.61	135.01	123.52
29	O	306	UIX	C36-C35-C32	-5.60	119.42	127.28
28	J	303	DD6	C4-C5-C6	-5.57	119.47	127.28
37	i	201	BCR	C24-C23-C22	-5.57	118.00	126.23
34	F	304	PID	C7-C8-C9	5.55	133.05	126.06
37	a	736	BCR	C11-C10-C9	-5.55	119.50	127.28
30	B	310	CLA	C4A-NA-C1A	5.54	109.21	106.68
28	M	305	DD6	C3-C2-C1	-5.54	119.51	127.28
28	F	301	DD6	C21-C20-C19	5.53	120.45	114.24
28	L	306	DD6	C9-C10-C11	-5.52	119.54	127.28
28	A	303	DD6	C21-C20-C19	5.51	120.44	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	N	302	PID	C18-C19-C20	5.51	134.79	123.52
37	b	702	BCR	C20-C21-C22	-5.50	119.57	127.28
28	A	301	DD6	C9-C10-C11	-5.49	119.58	127.28
28	I	301	DD6	C21-C20-C19	5.49	120.40	114.24
28	B	303	DD6	C21-C20-C19	5.48	120.40	114.24
28	I	302	DD6	C9-C10-C11	-5.46	119.62	127.28
28	F	303	DD6	C4-C5-C6	-5.45	119.64	127.28
31	P	213	KC1	O2D-CGD-CBD	5.44	120.74	111.23
28	A	305	DD6	C21-C20-C19	5.44	120.35	114.24
28	G	502	DD6	C21-C20-C19	5.43	120.34	114.24
28	I	301	DD6	C9-C10-C11	-5.40	119.70	127.28
28	J	303	DD6	C9-C10-C11	-5.40	119.71	127.28
37	b	730	BCR	C15-C14-C13	-5.39	119.71	127.28
34	P	202	PID	C17-C16-C15	5.39	134.55	123.52
29	O	306	UIX	O-C1-C6	5.38	121.06	115.05
29	K	302	UIX	O-C1-C3	5.33	118.49	113.49
28	I	301	DD6	C4-C5-C6	-5.30	119.84	127.28
37	b	730	BCR	C3-C4-C5	-5.30	104.61	114.06
37	f	304	BCR	C15-C14-C13	-5.28	119.87	127.28
28	J	302	DD6	C9-C10-C11	-5.28	119.87	127.28
29	O	306	UIX	O-C-C7	-5.28	101.76	116.88
29	I	304	UIX	O-C1-C6	5.27	120.93	115.05
31	M	307	KC1	C1D-ND-C4D	5.26	110.00	106.31
28	K	304	DD6	C21-C20-C19	5.25	120.14	114.24
28	A	302	DD6	C3-C2-C1	-5.23	119.94	127.28
28	J	302	DD6	C14-C13-C11	-5.22	117.43	125.53
34	D	304	PID	C18-C19-C20	5.21	134.19	123.52
29	h	201	UIX	C37-C39-C40	-5.21	119.97	127.28
28	L	302	DD6	C14-C13-C11	-5.21	117.45	125.53
28	B	302	DD6	C3-C2-C1	-5.21	119.98	127.28
29	P	207	UIX	O-C-C7	-5.20	101.98	116.88
28	G	508	DD6	C21-C20-C19	5.20	120.08	114.24
29	B	305	UIX	O2-C27-C31	5.19	120.34	111.09
31	L	307	KC1	O2D-CGD-CBD	5.18	120.29	111.23
37	l	307	BCR	C3-C4-C5	-5.17	104.83	114.06
29	K	302	UIX	O-C1-C6	5.16	120.82	115.05
28	N	303	DD6	C4-C5-C6	-5.16	120.04	127.28
31	M	314	KC1	O2D-CGD-CBD	5.12	120.18	111.23
28	B	306	DD6	C3-C2-C1	-5.11	120.11	127.28
37	a	734	BCR	C15-C14-C13	-5.11	120.11	127.28
31	F	309	KC1	O2D-CGD-CBD	5.11	120.17	111.23
28	P	204	DD6	C21-C20-C19	5.11	119.98	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	730	BCR	C11-C10-C9	-5.11	120.12	127.28
29	A	304	UIX	O-C1-C3	5.10	118.27	113.49
29	A	304	UIX	O-C1-C6	5.10	120.75	115.05
28	K	305	DD6	C3-C2-C1	-5.09	120.14	127.28
28	G	508	DD6	C3-C2-C1	-5.09	120.14	127.28
31	A	306	KC1	O2D-CGD-CBD	5.08	120.11	111.23
28	M	304	DD6	C21-C20-C19	5.08	119.95	114.24
28	G	502	DD6	C4-C5-C6	-5.07	120.17	127.28
28	F	301	DD6	C3-C2-C1	-5.07	120.17	127.28
28	H	303	DD6	C21-C20-C19	5.05	119.91	114.24
28	G	504	DD6	C3-C2-C1	-5.04	120.21	127.28
28	G	508	DD6	C4-C5-C6	-5.04	120.21	127.28
28	K	301	DD6	C21-C20-C19	5.04	119.90	114.24
31	J	313	KC1	O2D-CGD-CBD	5.03	120.03	111.23
31	H	310	KC1	C1D-ND-C4D	5.03	109.84	106.31
28	B	304	DD6	C21-C20-C19	5.03	119.89	114.24
37	f	304	BCR	C11-C10-C9	-5.03	120.22	127.28
28	K	304	DD6	C3-C2-C1	-5.01	120.25	127.28
37	m	201	BCR	C11-C10-C9	-4.99	120.27	127.28
28	B	306	DD6	C21-C20-C19	4.99	119.85	114.24
28	L	306	DD6	C4-C5-C6	-4.98	120.29	127.28
31	F	314	KC1	C1D-ND-C4D	4.98	109.81	106.31
31	O	312	KC1	O2D-CGD-CBD	4.98	119.93	111.23
31	D	315	KC1	O2D-CGD-CBD	4.98	119.93	111.23
28	M	306	DD6	C4-C5-C6	-4.97	120.30	127.28
31	F	309	KC1	C1D-ND-C4D	4.97	109.80	106.31
34	O	301	PID	C17-C16-C15	4.97	133.69	123.52
29	P	207	UIX	O-C1-C6	4.97	120.60	115.05
31	P	213	KC1	C1D-ND-C4D	4.97	109.80	106.31
30	l	310	CLA	C4D-CHA-CBD	-4.97	106.07	108.45
28	K	305	DD6	C21-C20-C19	4.97	119.82	114.24
31	A	306	KC1	C1D-ND-C4D	4.97	109.80	106.31
31	N	311	KC1	O2D-CGD-CBD	4.96	119.91	111.23
31	L	315	KC1	O2D-CGD-CBD	4.96	119.90	111.23
28	N	303	DD6	C21-C20-C19	4.96	119.81	114.24
34	P	206	PID	CM4-C14-C15	-4.95	114.79	122.82
28	L	303	DD6	C21-C20-C19	4.95	119.80	114.24
29	h	201	UIX	O2-C27-C31	4.95	119.92	111.09
28	L	303	DD6	C3-C2-C1	-4.95	120.34	127.28
31	D	310	KC1	C1D-ND-C4D	4.94	109.78	106.31
31	H	310	KC1	O2D-CGD-CBD	4.94	119.87	111.23
28	I	305	DD6	C15-C14-C13	-4.94	115.55	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	h	203	DD6	C21-C20-C19	4.93	119.78	114.24
31	N	306	KC1	C1D-ND-C4D	4.93	109.77	106.31
28	L	305	DD6	C21-C20-C19	4.92	119.77	114.24
31	J	313	KC1	C1D-ND-C4D	4.92	109.76	106.31
31	P	216	KC1	O2D-CGD-CBD	4.90	119.79	111.23
28	K	303	DD6	C21-C20-C19	4.90	119.74	114.24
29	K	302	UIX	C16-C20-C15	4.88	124.54	119.70
28	O	303	DD6	C21-C20-C19	4.88	119.72	114.24
28	L	306	DD6	C21-C20-C19	4.88	119.72	114.24
29	P	207	UIX	C36-C35-C32	-4.87	120.45	127.28
31	G	515	KC1	C1D-ND-C4D	4.86	109.72	106.31
28	G	505	DD6	C4-C5-C6	-4.86	120.46	127.28
31	O	315	KC1	C1D-ND-C4D	4.86	109.72	106.31
28	F	303	DD6	C21-C20-C19	4.86	119.70	114.24
37	a	736	BCR	C16-C17-C18	-4.86	120.47	127.28
31	F	314	KC1	O2D-CGD-CBD	4.85	119.71	111.23
28	L	302	DD6	C21-C20-C19	4.84	119.68	114.24
28	G	505	DD6	C9-C10-C11	-4.84	120.49	127.28
31	M	314	KC1	C1D-ND-C4D	4.83	109.70	106.31
28	I	301	DD6	C3-C2-C1	-4.82	120.52	127.28
37	l	306	BCR	C7-C8-C9	-4.82	119.10	126.23
29	A	304	UIX	O2-C27-C31	4.81	119.67	111.09
29	P	207	UIX	O-C1-C3	4.81	118.00	113.49
31	N	311	KC1	C1D-ND-C4D	4.81	109.69	106.31
34	N	301	PID	C17-C16-C15	4.81	133.35	123.52
31	H	306	KC1	O2D-CGD-CBD	4.80	119.63	111.23
31	A	314	KC1	O2D-CGD-CBD	4.80	119.63	111.23
37	l	306	BCR	C33-C5-C6	-4.80	119.24	124.48
28	M	305	DD6	C21-C20-C19	4.78	119.61	114.24
31	I	314	KC1	O2D-CGD-CBD	4.78	119.59	111.23
29	K	302	UIX	C17-C15-C20	4.78	113.86	109.21
37	i	201	BCR	C20-C21-C22	-4.78	120.58	127.28
31	L	315	KC1	C1D-ND-C4D	4.78	109.66	106.31
28	M	302	DD6	C15-C14-C13	-4.77	115.91	125.99
31	P	211	KC1	C1D-ND-C4D	4.77	109.66	106.31
28	I	302	DD6	C21-C20-C19	4.77	119.59	114.24
28	M	304	DD6	C3-C2-C1	-4.77	120.59	127.28
28	K	318	DD6	C3-C2-C1	-4.76	120.60	127.28
28	M	306	DD6	C9-C10-C11	-4.76	120.60	127.28
31	P	216	KC1	C1D-ND-C4D	4.75	109.65	106.31
37	l	306	BCR	C16-C17-C18	-4.75	120.61	127.28
28	K	318	DD6	C4-C5-C6	-4.74	120.62	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	j	102	BCR	C15-C14-C13	-4.74	120.63	127.28
29	P	207	UIX	O2-C27-C31	4.74	119.54	111.09
28	K	301	DD6	C4-C5-C6	-4.73	120.65	127.28
31	M	307	KC1	O2D-CGD-CBD	4.72	119.49	111.23
31	N	308	KC1	O2D-CGD-O1D	-4.72	114.66	123.85
29	O	306	UIX	O2-C27-C31	4.71	119.49	111.09
31	D	315	KC1	C1D-ND-C4D	4.70	109.61	106.31
37	f	304	BCR	C16-C17-C18	-4.69	120.69	127.28
31	O	312	KC1	C1D-ND-C4D	4.69	109.60	106.31
31	I	314	KC1	C1D-ND-C4D	4.68	109.60	106.31
28	D	303	DD6	C21-C20-C19	4.68	119.50	114.24
31	O	310	KC1	C1D-ND-C4D	4.67	109.59	106.31
31	G	515	KC1	O2D-CGD-CBD	4.67	119.39	111.23
31	B	314	KC1	C1D-ND-C4D	4.67	109.59	106.31
28	A	301	DD6	C3-C2-C1	-4.66	120.75	127.28
28	L	305	DD6	C3-C2-C1	-4.65	120.76	127.28
28	M	303	DD6	C4-C5-C6	-4.65	120.76	127.28
28	N	303	DD6	C9-C10-C11	-4.64	120.77	127.28
31	L	307	KC1	C1D-ND-C4D	4.64	109.57	106.31
31	O	310	KC1	O2D-CGD-CBD	4.64	119.34	111.23
37	i	201	BCR	C15-C14-C13	-4.64	120.77	127.28
28	I	303	DD6	C9-C10-C11	-4.64	120.77	127.28
31	K	314	KC1	O2D-CGD-CBD	4.64	119.34	111.23
31	B	314	KC1	O2D-CGD-CBD	4.64	119.34	111.23
28	J	303	DD6	O1-C15-C14	-4.64	103.59	116.88
37	l	302	BCR	C28-C27-C26	-4.63	105.79	114.06
28	b	731	DD6	C21-C20-C19	4.63	119.44	114.24
34	P	205	PID	CM4-C14-C15	-4.62	115.32	122.82
28	B	302	DD6	C9-C10-C11	-4.62	120.79	127.28
31	N	308	KC1	O1D-CGD-CBD	-4.62	115.41	124.52
29	K	302	UIX	O2-C27-C31	4.62	119.33	111.09
28	I	303	DD6	C21-C20-C19	4.62	119.42	114.24
28	J	303	DD6	O1-C20-C21	4.61	120.20	115.05
28	D	303	DD6	C10-C9-C8	-4.61	109.84	123.20
31	A	314	KC1	C1D-ND-C4D	4.60	109.54	106.31
31	H	306	KC1	C1D-ND-C4D	4.59	109.53	106.31
29	G	503	UIX	O2-C27-C31	4.59	119.27	111.09
28	I	302	DD6	C3-C2-C1	-4.58	120.85	127.28
37	a	736	BCR	C15-C14-C13	-4.57	120.86	127.28
28	G	505	DD6	O1-C15-C14	-4.57	103.79	116.88
37	a	734	BCR	C16-C17-C18	-4.56	120.89	127.28
28	L	304	DD6	C21-C20-C19	4.56	119.36	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	F	304	PID	C6-C7-C8	4.54	135.59	125.99
31	K	314	KC1	C1D-ND-C4D	4.54	109.50	106.31
34	O	304	PID	CM4-C14-C15	-4.54	115.47	122.82
37	l	302	BCR	C16-C17-C18	-4.53	120.93	127.28
29	J	305	UIX	O2-C27-C31	4.53	119.16	111.09
28	b	731	DD6	C4-C5-C6	-4.52	120.94	127.28
28	J	302	DD6	C4-C5-C6	-4.52	120.94	127.28
34	M	301	PID	CM4-C14-C15	-4.52	115.50	122.82
28	M	303	DD6	C3-C2-C1	-4.51	120.95	127.28
28	I	305	DD6	O1-C15-C14	-4.51	103.95	116.88
31	N	306	KC1	O2D-CGD-CBD	4.50	119.10	111.23
29	I	304	UIX	O2-C27-C31	4.50	119.11	111.09
29	B	305	UIX	O-C1-C6	4.50	120.07	115.05
37	l	307	BCR	C15-C14-C13	-4.49	120.98	127.28
29	G	503	UIX	O-C1-C6	4.49	120.06	115.05
37	b	732	BCR	C33-C5-C6	-4.48	119.59	124.48
34	M	301	PID	C12-O4-C10	4.48	109.86	107.68
28	N	303	DD6	C3-C2-C1	-4.48	121.00	127.28
31	O	315	KC1	O2D-CGD-CBD	4.47	119.04	111.23
28	G	502	DD6	C9-C10-C11	-4.47	121.01	127.28
34	D	301	PID	C17-C16-C15	4.47	132.66	123.52
28	G	504	DD6	O1-C20-C19	4.47	117.68	113.49
28	J	303	DD6	O1-C20-C19	4.47	117.68	113.49
29	K	302	UIX	O-C-C7	-4.46	104.09	116.88
34	P	202	PID	CM4-C14-C15	-4.45	115.61	122.82
29	h	201	UIX	O-C1-C6	4.45	120.02	115.05
37	l	306	BCR	C38-C26-C25	-4.45	119.63	124.48
28	M	303	DD6	O1-C15-C14	-4.44	104.16	116.88
37	j	102	BCR	C20-C21-C22	-4.44	121.06	127.28
28	B	304	DD6	C3-C2-C1	-4.43	121.06	127.28
31	D	310	KC1	O2D-CGD-CBD	4.43	118.97	111.23
28	I	305	DD6	C21-C20-C19	4.43	119.21	114.24
34	D	304	PID	CM4-C14-C15	-4.43	115.65	122.82
29	A	304	UIX	C6-C1-C3	4.42	119.21	114.24
28	J	303	DD6	C15-C14-C13	-4.42	116.65	125.99
34	D	304	PID	C12-O4-C10	4.42	109.82	107.68
28	M	302	DD6	O1-C20-C21	4.41	119.98	115.05
29	O	306	UIX	O-C1-C3	4.41	117.62	113.49
28	L	305	DD6	C9-C10-C11	-4.41	121.10	127.28
29	h	201	UIX	C-C7-C10	-4.40	116.70	125.99
29	K	302	UIX	C21-C15-C20	-4.39	106.55	110.47
34	O	305	PID	C17-C16-C15	4.38	132.48	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	F	303	DD6	C9-C10-C11	-4.38	121.14	127.28
28	h	203	DD6	C3-C2-C1	-4.38	121.14	127.28
28	A	301	DD6	O1-C20-C19	-4.37	109.39	113.49
28	H	303	DD6	C4-C5-C6	-4.37	121.16	127.28
28	M	303	DD6	O1-C20-C21	4.37	119.93	115.05
37	b	732	BCR	C16-C17-C18	-4.35	121.17	127.28
38	b	729	PQN	C11-C12-C13	-4.35	119.34	126.83
34	H	301	PID	CM4-C14-C15	-4.35	115.77	122.82
34	F	302	PID	C12-O4-C10	4.34	109.79	107.68
34	P	202	PID	C12-O4-C10	4.34	109.79	107.68
34	D	305	PID	C18-C19-C20	4.34	132.40	123.52
28	L	306	DD6	C3-C2-C1	-4.33	121.20	127.28
28	b	731	DD6	C15-C14-C13	-4.33	116.84	125.99
34	O	305	PID	CM4-C14-C15	-4.32	115.81	122.82
34	O	304	PID	C17-C16-C15	4.32	132.35	123.52
34	O	301	PID	CM4-C14-C15	-4.30	115.84	122.82
28	K	318	DD6	O1-C20-C21	-4.30	110.25	115.05
28	L	304	DD6	C3-C2-C1	-4.29	121.25	127.28
37	i	201	BCR	C16-C17-C18	-4.29	121.25	127.28
34	O	304	PID	C12-O4-C10	4.29	109.76	107.68
28	M	306	DD6	C25-C24-C1	-4.29	114.60	126.36
34	F	304	PID	C12-O4-C10	4.27	109.75	107.68
34	F	304	PID	CM4-C14-C15	-4.26	115.91	122.82
28	K	301	DD6	C15-C14-C13	-4.26	116.98	125.99
37	m	201	BCR	C38-C26-C25	-4.25	119.84	124.48
29	I	304	UIX	C7-C10-C11	-4.25	118.94	125.53
31	P	211	KC1	O2D-CGD-CBD	4.24	118.65	111.23
28	B	303	DD6	C4-C5-C6	-4.24	121.33	127.28
28	A	305	DD6	C4-C5-C6	-4.24	121.33	127.28
28	I	302	DD6	C7-C6-C8	4.22	124.53	118.09
28	O	303	DD6	C3-C2-C1	-4.21	121.37	127.28
28	O	303	DD6	C9-C10-C11	-4.21	121.38	127.28
28	H	303	DD6	C3-C2-C1	-4.20	121.38	127.28
34	D	306	PID	C18-C19-C20	4.20	132.12	123.52
34	P	206	PID	C12-O4-C10	4.19	109.72	107.68
28	L	303	DD6	C9-C10-C11	-4.19	121.41	127.28
34	O	301	PID	C12-O4-C10	4.18	109.71	107.68
29	A	304	UIX	C16-C20-C15	4.17	123.83	119.70
32	G	521	DGD	O2G-C1B-C2B	4.17	120.49	111.48
34	H	301	PID	C12-O4-C10	4.16	109.70	107.68
34	F	302	PID	CM4-C14-C15	-4.16	116.08	122.82
28	L	302	DD6	C3-C2-C1	-4.15	121.46	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	F	301	DD6	O1-C20-C19	-4.15	109.60	113.49
28	K	304	DD6	C15-C14-C13	-4.15	117.22	125.99
28	B	302	DD6	C14-C13-C11	-4.15	119.09	125.53
28	L	305	DD6	C4-C5-C6	-4.14	121.47	127.28
32	j	103	DGD	O2G-C1B-C2B	4.12	120.40	111.48
34	N	301	PID	C12-O4-C10	4.12	109.68	107.68
34	D	306	PID	C17-C16-C15	4.12	131.94	123.52
37	a	734	BCR	C11-C10-C9	-4.11	121.52	127.28
37	a	734	BCR	C33-C5-C6	-4.10	120.01	124.48
34	D	307	PID	C12-O4-C10	4.09	109.67	107.68
34	P	208	PID	C17-C16-C15	4.09	131.89	123.52
32	L	301	DGD	O2G-C1B-C2B	4.09	120.33	111.48
28	L	302	DD6	C9-C10-C11	-4.08	121.56	127.28
28	A	301	DD6	C4-C5-C6	-4.08	121.56	127.28
34	D	301	PID	C18-C19-C20	4.06	131.84	123.52
34	P	203	PID	C18-C19-C20	4.06	131.82	123.52
37	b	732	BCR	C15-C14-C13	-4.06	121.59	127.28
29	h	201	UIX	O-C-C7	-4.06	105.26	116.88
28	K	318	DD6	C14-C13-C11	-4.05	119.25	125.53
28	I	302	DD6	C12-C11-C13	4.05	124.27	118.09
29	J	305	UIX	C34-C37-C39	-4.04	115.26	123.52
28	J	304	DD6	O1-C15-C14	-4.04	105.31	116.88
34	N	301	PID	CM4-C14-C15	-4.03	116.29	122.82
31	D	315	KC1	CHB-C1B-NB	4.03	130.47	124.80
28	O	303	DD6	C15-C14-C13	-4.02	117.49	125.99
28	L	302	DD6	C4-C5-C6	-4.02	121.64	127.28
31	O	312	KC1	CHC-C4B-NB	4.01	130.45	124.80
28	M	306	DD6	O1-C15-C14	-4.01	105.38	116.88
32	y	201	DGD	O2G-C1B-C2B	4.01	120.15	111.48
29	h	201	UIX	C16-C20-C15	4.01	123.67	119.70
37	i	201	BCR	C7-C8-C9	-4.00	120.31	126.23
37	b	730	BCR	C4-C5-C6	-4.00	117.30	122.70
34	F	306	PID	C12-O4-C10	4.00	109.62	107.68
28	I	303	DD6	O1-C15-C14	-4.00	105.43	116.88
31	H	310	KC1	CHB-C1B-NB	3.99	130.43	124.80
37	a	734	BCR	C28-C27-C26	-3.99	106.93	114.06
28	B	303	DD6	O1-C20-C19	-3.99	109.75	113.49
28	M	302	DD6	O1-C20-C19	3.99	117.23	113.49
29	B	305	UIX	C37-C39-C40	-3.99	121.68	127.28
29	h	201	UIX	C6-C1-C3	3.98	118.72	114.24
28	H	303	DD6	C15-C14-C13	-3.98	117.58	125.99
31	P	216	KC1	CHB-C1B-NB	3.98	130.40	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	l	306	BCR	C20-C21-C22	-3.97	121.70	127.28
34	F	305	PID	C12-O4-C10	3.96	109.60	107.68
34	P	208	PID	C12-O4-C10	3.96	109.60	107.68
37	m	201	BCR	C3-C4-C5	-3.96	107.00	114.06
31	D	310	KC1	CHC-C4B-NB	3.96	130.37	124.80
31	F	309	KC1	CHC-C4B-NB	3.96	130.37	124.80
29	A	304	UIX	C34-C30-C26	-3.95	121.73	127.28
28	B	304	DD6	C4-C5-C6	-3.95	121.73	127.28
34	D	301	PID	CM4-C14-C15	-3.95	116.42	122.82
34	D	301	PID	C12-O4-C10	3.94	109.59	107.68
37	j	102	BCR	C24-C23-C22	-3.94	120.41	126.23
28	M	302	DD6	C21-C20-C15	-3.94	115.82	122.30
29	J	305	UIX	O-C1-C6	3.94	119.45	115.05
28	L	304	DD6	C4-C5-C6	-3.93	121.76	127.28
29	G	503	UIX	O-C-C7	-3.93	105.61	116.88
31	M	314	KC1	CHB-C1B-NB	3.93	130.34	124.80
28	I	303	DD6	C4-C5-C6	-3.93	121.77	127.28
37	m	201	BCR	C15-C16-C17	-3.93	115.48	123.52
31	H	306	KC1	CHB-C1B-NB	3.93	130.33	124.80
37	f	304	BCR	C33-C5-C6	-3.93	120.20	124.48
31	F	314	KC1	CHB-C1B-NB	3.92	130.32	124.80
34	F	306	PID	C17-C16-C15	3.92	131.54	123.52
28	B	304	DD6	C15-C14-C13	-3.92	117.71	125.99
31	D	310	KC1	CHB-C1B-NB	3.91	130.30	124.80
31	A	314	KC1	CHB-C1B-NB	3.90	130.30	124.80
28	b	731	DD6	C9-C10-C11	-3.89	121.82	127.28
28	G	508	DD6	C9-C10-C11	-3.89	121.83	127.28
37	l	302	BCR	C33-C5-C6	-3.89	120.24	124.48
28	M	304	DD6	C15-C14-C13	-3.88	117.78	125.99
28	P	204	DD6	C15-C14-C13	-3.88	117.78	125.99
31	L	315	KC1	CHB-C1B-NB	3.88	130.26	124.80
34	F	306	PID	CM4-C14-C15	-3.87	116.54	122.82
28	K	303	DD6	C15-C14-C13	-3.87	117.81	125.99
29	J	305	UIX	C14-C13-C11	-3.87	121.85	127.28
29	G	503	UIX	C-C7-C10	-3.87	117.81	125.99
37	b	730	BCR	C16-C17-C18	-3.87	121.85	127.28
31	P	211	KC1	CHC-C4B-NB	3.87	130.25	124.80
28	M	302	DD6	C4-C5-C6	-3.86	121.87	127.28
37	f	304	BCR	C20-C21-C22	-3.86	121.87	127.28
34	G	506	PID	CM4-C14-C15	-3.86	116.57	122.82
32	I	317	DGD	O2G-C1B-C2B	3.86	119.83	111.48
31	I	314	KC1	CHB-C1B-NB	3.86	130.23	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	G	501	DGD	O2G-C1B-C2B	3.85	119.81	111.48
31	O	310	KC1	CHB-C1B-NB	3.85	130.22	124.80
31	P	213	KC1	CHC-C4B-NB	3.85	130.22	124.80
28	F	303	DD6	C3-C2-C1	-3.85	121.88	127.28
29	I	304	UIX	C14-C13-C11	-3.84	121.89	127.28
28	F	303	DD6	C15-C14-C13	-3.84	117.87	125.99
29	G	503	UIX	C6-C1-C3	3.84	118.56	114.24
28	I	303	DD6	C3-C2-C1	-3.84	121.90	127.28
32	l	301	DGD	O2G-C1B-C2B	3.84	119.78	111.48
31	B	314	KC1	CHB-C1B-NB	3.83	130.20	124.80
28	A	302	DD6	C4-C5-C6	-3.83	121.91	127.28
31	N	311	KC1	CHC-C4B-NB	3.82	130.18	124.80
37	b	702	BCR	C16-C15-C14	-3.82	115.70	123.52
34	O	307	PID	C12-O4-C10	3.82	109.53	107.68
28	K	301	DD6	O1-C20-C21	-3.82	110.78	115.05
31	N	306	KC1	CHB-C1B-NB	3.82	130.17	124.80
31	H	306	KC1	CHC-C4B-NB	3.81	130.17	124.80
31	K	314	KC1	CHC-C4B-NB	3.80	130.16	124.80
37	f	304	BCR	C7-C8-C9	-3.80	120.61	126.23
31	L	307	KC1	CHC-C4B-NB	3.80	130.15	124.80
29	I	304	UIX	C37-C39-C40	-3.80	121.95	127.28
31	N	311	KC1	CHB-C1B-NB	3.80	130.15	124.80
34	G	506	PID	C17-C16-C15	3.79	131.28	123.52
37	f	304	BCR	C28-C27-C26	-3.79	107.30	114.06
34	F	302	PID	C17-C16-C15	3.79	131.27	123.52
34	D	306	PID	C12-O4-C10	3.78	109.51	107.68
28	I	302	DD6	C14-C13-C11	3.78	131.40	125.53
31	L	307	KC1	CHB-C1B-NB	3.78	130.12	124.80
31	F	314	KC1	CHC-C4B-NB	3.77	130.12	124.80
28	A	302	DD6	C21-C20-C19	3.77	118.48	114.24
31	F	309	KC1	CHD-C1D-ND	3.77	129.70	124.05
28	B	302	DD6	O1-C20-C21	3.77	119.26	115.05
31	P	211	KC1	CHB-C1B-NB	3.76	130.10	124.80
31	I	314	KC1	CHC-C4B-NB	3.76	130.10	124.80
31	F	309	KC1	CHB-C1B-NB	3.76	130.09	124.80
31	K	314	KC1	CHB-C1B-NB	3.76	130.09	124.80
31	N	308	KC1	CHD-C1D-ND	3.75	129.68	124.05
28	J	304	DD6	C4-C5-C6	-3.75	122.02	127.28
28	G	502	DD6	C3-C2-C1	-3.75	122.02	127.28
29	O	306	UIX	C6-C1-C3	3.75	118.45	114.24
28	B	302	DD6	C21-C20-C19	3.74	118.45	114.24
31	O	315	KC1	CHB-C1B-NB	3.74	130.07	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	F	303	DD6	O1-C20-C19	-3.74	109.99	113.49
31	N	306	KC1	CHC-C4B-NB	3.74	130.06	124.80
34	P	205	PID	C12-O4-C10	3.73	109.49	107.68
34	P	208	PID	CM4-C14-C15	-3.73	116.77	122.82
31	J	313	KC1	CHB-C1B-NB	3.73	130.05	124.80
29	J	305	UIX	C14-C23-C26	-3.73	116.14	126.36
34	D	307	PID	CM4-C14-C15	-3.73	116.78	122.82
28	M	306	DD6	C21-C20-C19	3.73	118.43	114.24
31	A	314	KC1	CHC-C4B-NB	3.73	130.05	124.80
28	I	301	DD6	O1-C20-C19	-3.72	110.00	113.49
34	G	507	PID	C12-O4-C10	3.72	109.48	107.68
28	M	302	DD6	O1-C15-C14	-3.72	106.23	116.88
30	a	726	CLA	C3B-C4B-NB	-3.71	107.22	110.53
34	D	302	PID	C18-C19-C20	3.71	131.10	123.52
34	D	306	PID	CM4-C14-C15	-3.70	116.82	122.82
31	N	308	KC1	CHB-C1B-NB	3.70	130.01	124.80
31	H	310	KC1	CHC-C4B-NB	3.69	130.00	124.80
31	L	315	KC1	CHC-C4B-NB	3.69	130.00	124.80
34	G	506	PID	C12-O4-C10	3.69	109.47	107.68
29	B	305	UIX	C34-C30-C26	-3.69	122.10	127.28
31	G	515	KC1	CHB-C1B-NB	3.69	129.99	124.80
31	M	314	KC1	CHC-C4B-NB	3.69	129.99	124.80
37	l	306	BCR	C11-C10-C9	-3.68	122.11	127.28
31	B	314	KC1	CHC-C4B-NB	3.68	129.98	124.80
34	N	302	PID	CM4-C14-C15	-3.68	116.86	122.82
29	G	503	UIX	C34-C30-C26	-3.67	122.13	127.28
34	O	305	PID	C18-C19-C20	3.67	131.03	123.52
28	I	301	DD6	C15-C14-C13	-3.66	118.25	125.99
28	G	508	DD6	C15-C14-C13	-3.66	118.25	125.99
28	A	305	DD6	C3-C2-C1	-3.66	122.14	127.28
34	D	305	PID	C12-O4-C10	3.66	109.46	107.68
29	P	207	UIX	C6-C1-C3	3.66	118.35	114.24
31	A	306	KC1	CHB-C1B-NB	3.66	129.95	124.80
28	J	304	DD6	C24-C1-C2	3.66	124.76	119.01
31	D	315	KC1	CHD-C1D-ND	3.65	129.53	124.05
28	L	303	DD6	C4-C5-C6	-3.65	122.17	127.28
29	A	304	UIX	C18-O2-C27	-3.64	111.41	117.85
31	M	307	KC1	CHB-C1B-NB	3.64	129.93	124.80
31	A	306	KC1	CHC-C4B-NB	3.64	129.93	124.80
31	P	216	KC1	CHC-C4B-NB	3.64	129.92	124.80
31	M	307	KC1	CHC-C4B-NB	3.64	129.92	124.80
28	I	303	DD6	C14-C13-C11	-3.63	119.89	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	G	507	PID	CM4-C14-C15	-3.63	116.94	122.82
30	F	311	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
34	H	302	PID	C18-C19-C20	3.62	130.92	123.52
28	K	318	DD6	C21-C20-C19	3.61	118.30	114.24
31	O	312	KC1	CHB-C1B-NB	3.60	129.88	124.80
37	a	734	BCR	C7-C8-C9	-3.60	120.90	126.23
28	J	304	DD6	C21-C20-C19	3.60	118.29	114.24
34	j	105	PID	C12-O4-C10	3.60	109.43	107.68
31	M	307	KC1	O1D-CGD-CBD	-3.60	117.41	124.52
28	L	306	DD6	C14-C13-C11	-3.60	119.94	125.53
34	F	305	PID	C16-C15-C14	3.60	132.32	127.28
37	f	304	BCR	C24-C23-C22	-3.60	120.91	126.23
34	O	302	PID	C18-C19-C20	3.59	130.87	123.52
31	O	310	KC1	CHC-C4B-NB	3.59	129.86	124.80
28	P	204	DD6	C9-C10-C11	-3.59	122.25	127.28
31	M	307	KC1	O2D-CGD-O1D	-3.58	116.89	123.85
29	I	304	UIX	C6-C1-C3	3.56	118.24	114.24
28	h	203	DD6	C4-C5-C6	-3.56	122.28	127.28
31	J	313	KC1	CHC-C4B-NB	3.56	129.81	124.80
28	B	303	DD6	C3-C2-C1	-3.55	122.29	127.28
34	G	507	PID	C18-C19-C20	3.55	130.79	123.52
29	K	302	UIX	C18-O2-C27	-3.55	111.58	117.85
28	K	304	DD6	C9-C10-C11	-3.54	122.31	127.28
37	l	302	BCR	C15-C14-C13	-3.54	122.31	127.28
34	O	304	PID	C29-C24-C25	3.54	123.21	119.70
28	h	203	DD6	C15-C14-C13	-3.53	118.52	125.99
28	L	304	DD6	C15-C14-C13	-3.53	118.53	125.99
37	b	702	BCR	C11-C10-C9	-3.53	122.33	127.28
34	O	307	PID	CM4-C14-C15	-3.53	117.11	122.82
28	F	303	DD6	O1-C15-C14	-3.52	106.78	116.88
28	N	303	DD6	C15-C14-C13	-3.52	118.54	125.99
28	G	505	DD6	C14-C13-C11	-3.52	120.06	125.53
37	b	732	BCR	C21-C20-C19	-3.52	113.00	123.20
37	m	201	BCR	C4-C5-C6	-3.51	117.95	122.70
37	l	307	BCR	C4-C5-C6	-3.51	117.96	122.70
28	K	304	DD6	O1-C15-C14	-3.51	106.82	116.88
29	B	305	UIX	C14-C13-C11	-3.51	122.36	127.28
28	J	302	DD6	C21-C20-C19	3.51	118.18	114.24
28	A	303	DD6	C3-C2-C1	-3.51	122.36	127.28
32	G	521	DGD	C4D-C3D-C2D	3.51	116.99	110.83
28	I	302	DD6	O1-C15-C14	-3.51	106.83	116.88
31	O	315	KC1	CHC-C4B-NB	3.51	129.74	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	P	213	KC1	CHB-C1B-NB	3.50	129.73	124.80
28	N	303	DD6	O1-C20-C19	-3.50	110.21	113.49
31	P	213	KC1	CHD-C1D-ND	3.50	129.30	124.05
31	D	310	KC1	CHD-C1D-ND	3.49	129.29	124.05
28	B	306	DD6	C4-C5-C6	-3.49	122.38	127.28
34	D	302	PID	C12-O4-C10	3.49	109.37	107.68
34	D	307	PID	C17-C16-C15	3.49	130.66	123.52
34	j	105	PID	C17-C16-C15	3.49	130.65	123.52
37	b	702	BCR	C33-C5-C6	-3.48	120.69	124.48
37	l	307	BCR	C7-C8-C9	-3.48	121.09	126.23
31	L	307	KC1	CHD-C1D-ND	3.47	129.26	124.05
28	I	305	DD6	C9-C8-C6	-3.47	116.86	126.36
31	M	314	KC1	CHD-C1D-ND	3.46	129.24	124.05
37	l	307	BCR	C38-C26-C25	-3.45	120.72	124.48
28	J	303	DD6	C21-C20-C15	-3.45	116.62	122.30
34	H	302	PID	C12-O4-C10	3.44	109.35	107.68
31	N	311	KC1	CHD-C1D-ND	3.44	129.21	124.05
28	G	504	DD6	C21-C20-C19	3.43	118.10	114.24
31	N	308	KC1	CHC-C4B-NB	3.43	129.63	124.80
37	l	302	BCR	C20-C21-C22	-3.43	122.47	127.28
37	l	307	BCR	C11-C10-C9	-3.43	122.47	127.28
28	M	304	DD6	C4-C5-C6	-3.43	122.47	127.28
37	j	102	BCR	C33-C5-C6	-3.42	120.75	124.48
29	A	304	UIX	C17-C15-C20	3.42	112.53	109.21
31	I	314	KC1	CHD-C1D-ND	3.42	129.18	124.05
31	O	310	KC1	CHD-C1D-ND	3.42	129.18	124.05
31	F	314	KC1	CHD-C1D-ND	3.41	129.17	124.05
31	O	315	KC1	CHD-C1D-ND	3.41	129.16	124.05
30	l	310	CLA	O2D-CGD-CBD	3.41	114.69	110.95
37	m	201	BCR	C11-C12-C13	-3.41	117.03	126.36
31	L	315	KC1	CHD-C1D-ND	3.40	129.15	124.05
31	G	515	KC1	CHC-C4B-NB	3.40	129.59	124.80
34	P	203	PID	C12-O4-C10	3.40	109.33	107.68
31	N	306	KC1	CHD-C1D-ND	3.39	129.13	124.05
31	O	312	KC1	CHD-C1D-ND	3.39	129.13	124.05
34	F	306	PID	C18-C19-C20	3.39	130.45	123.52
28	B	306	DD6	C15-C14-C13	-3.38	118.84	125.99
28	I	301	DD6	C37-C36-C35	3.38	120.64	114.42
30	F	310	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
31	K	314	KC1	CHD-C1D-ND	3.37	129.11	124.05
34	N	301	PID	C18-C19-C20	3.37	130.41	123.52
31	H	306	KC1	CHD-C1D-ND	3.37	129.10	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	314	KC1	CHD-C1D-ND	3.37	129.10	124.05
37	a	734	BCR	C20-C21-C22	-3.36	122.56	127.28
30	P	215	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
28	b	731	DD6	C3-C2-C1	-3.36	122.56	127.28
28	P	204	DD6	C3-C2-C1	-3.36	122.57	127.28
34	O	302	PID	CM4-C14-C15	-3.36	117.38	122.82
31	G	515	KC1	CHD-C1D-ND	3.36	129.09	124.05
30	J	312	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
28	D	303	DD6	O1-C20-C19	3.35	116.64	113.49
34	O	302	PID	C12-O4-C10	3.34	109.30	107.68
34	P	208	PID	C18-C19-C20	3.34	130.35	123.52
31	P	216	KC1	CHD-C1D-ND	3.34	129.05	124.05
28	F	301	DD6	C14-C13-C11	-3.33	120.36	125.53
30	D	314	CLA	C3B-C4B-NB	-3.33	107.56	110.53
31	A	314	KC1	CHD-C1D-ND	3.33	129.04	124.05
29	O	306	UIX	C14-C23-C26	-3.32	117.25	126.36
37	m	201	BCR	C20-C21-C22	-3.32	122.62	127.28
28	I	305	DD6	C3-C4-C5	-3.32	116.73	123.52
28	G	505	DD6	C24-C1-C2	3.32	124.23	119.01
31	A	306	KC1	CHD-C1D-ND	3.32	129.02	124.05
30	l	310	CLA	C3D-C4D-ND	3.31	111.95	107.71
37	i	201	BCR	C27-C26-C25	-3.31	118.23	122.70
34	D	307	PID	C18-C19-C20	3.30	130.28	123.52
28	M	306	DD6	C25-C26-C27	-3.30	117.38	126.61
30	M	315	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
31	H	310	KC1	CHD-C1D-ND	3.29	128.99	124.05
28	A	303	DD6	C15-C14-C13	-3.29	119.04	125.99
34	N	302	PID	C12-O4-C10	3.29	109.27	107.68
28	B	302	DD6	C21-C20-C15	-3.28	116.90	122.30
31	P	211	KC1	CHD-C1D-ND	3.28	128.97	124.05
34	N	302	PID	C26-C25-C24	3.28	112.40	109.21
37	j	102	BCR	C3-C4-C5	-3.28	108.21	114.06
28	K	304	DD6	C4-C5-C6	-3.28	122.68	127.28
28	G	504	DD6	O1-C20-C21	3.28	118.71	115.05
34	D	302	PID	CM4-C14-C15	-3.28	117.51	122.82
29	K	302	UIX	C34-C37-C39	-3.27	116.82	123.52
29	B	305	UIX	C6-C1-C3	3.27	117.92	114.24
28	I	305	DD6	O1-C20-C21	3.27	118.70	115.05
29	J	305	UIX	C6-C1-C3	3.27	117.91	114.24
38	a	732	PQN	C14-C13-C15	3.27	120.90	115.23
28	G	508	DD6	O1-C20-C21	-3.26	111.40	115.05
28	I	303	DD6	O1-C20-C19	-3.26	110.44	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	I	305	DD6	C37-C36-C35	3.26	120.41	114.42
28	I	303	DD6	C24-C1-C2	3.26	124.13	119.01
28	H	303	DD6	C9-C10-C11	-3.25	122.71	127.28
28	F	301	DD6	C25-C26-C27	-3.25	117.51	126.61
30	N	309	CLA	O2D-CGD-O1D	-3.25	117.51	123.85
30	I	319	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
31	J	313	KC1	CHD-C1D-ND	3.25	128.93	124.05
28	P	204	DD6	O1-C15-C14	-3.25	107.57	116.88
28	L	303	DD6	C21-C20-C15	-3.25	116.96	122.30
37	i	201	BCR	C11-C10-C9	-3.24	122.73	127.28
31	M	307	KC1	CHD-C1D-ND	3.24	128.91	124.05
28	A	305	DD6	O1-C20-C19	-3.24	110.45	113.49
34	O	304	PID	C6-C7-C8	-3.24	119.15	125.99
29	P	207	UIX	C14-C23-C26	-3.23	117.50	126.36
28	L	305	DD6	C15-C14-C13	-3.23	119.16	125.99
28	b	731	DD6	C4-C3-C2	-3.23	116.92	123.52
34	P	203	PID	CM4-C14-C15	-3.22	117.59	122.82
28	J	302	DD6	O1-C20-C21	-3.22	111.45	115.05
34	j	105	PID	CM4-C14-C15	-3.22	117.60	122.82
37	i	201	BCR	C15-C16-C17	-3.22	116.93	123.52
30	a	726	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
34	G	507	PID	C17-C16-C15	3.21	130.09	123.52
28	K	305	DD6	C15-C14-C13	-3.21	119.20	125.99
32	G	521	DGD	C1D-C2D-C3D	3.21	116.76	110.01
28	h	203	DD6	C9-C10-C11	-3.21	122.78	127.28
30	F	312	CLA	C3B-C4B-NB	-3.20	107.67	110.53
28	L	304	DD6	O1-C20-C21	-3.20	111.47	115.05
37	l	302	BCR	C38-C26-C25	-3.20	120.99	124.48
28	G	502	DD6	C14-C13-C11	-3.20	120.57	125.53
28	M	302	DD6	C21-C20-C19	3.20	117.83	114.24
28	B	304	DD6	O1-C20-C21	-3.19	111.48	115.05
28	F	301	DD6	C9-C8-C6	-3.19	117.61	126.36
28	D	303	DD6	C14-C13-C11	3.19	130.48	125.53
28	O	303	DD6	O1-C15-C14	-3.19	107.75	116.88
29	A	304	UIX	O-C-C7	-3.19	107.75	116.88
30	D	314	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
28	J	304	DD6	C25-C24-C1	-3.18	117.63	126.36
37	l	307	BCR	C16-C17-C18	-3.18	122.82	127.28
30	b	724	CLA	C3B-C4B-NB	-3.18	107.69	110.53
34	P	206	PID	C16-C15-C14	-3.18	122.82	127.28
30	b	723	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
28	D	303	DD6	C21-C20-C15	-3.17	117.08	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	307	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
37	m	201	BCR	C23-C24-C25	-3.16	118.55	127.00
34	P	206	PID	C17-C18-C19	3.16	132.03	124.72
30	K	315	CLA	CAA-C2A-C3A	-3.16	108.98	116.23
34	O	307	PID	C17-C16-C15	3.16	129.98	123.52
34	O	301	PID	C18-C19-C20	3.15	129.97	123.52
29	A	304	UIX	C35-C36-C38	-3.15	114.06	123.20
30	H	307	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
34	M	301	PID	C26-C25-C24	3.15	112.27	109.21
34	O	304	PID	C18-C19-C20	3.15	129.96	123.52
30	G	516	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
30	I	311	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
28	M	305	DD6	C4-C5-C6	-3.14	122.87	127.28
28	K	301	DD6	C9-C10-C11	-3.14	122.88	127.28
30	a	702	CLA	C3B-C4B-NB	-3.14	107.73	110.53
30	b	709	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
28	M	306	DD6	C37-C36-C35	3.14	120.19	114.42
28	M	305	DD6	C9-C10-C11	-3.14	122.88	127.28
37	i	201	BCR	C30-C25-C26	-3.13	118.35	122.64
30	l	310	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
28	K	303	DD6	C3-C2-C1	-3.13	122.88	127.28
31	D	315	KC1	CHC-C4B-NB	3.13	129.21	124.80
28	G	504	DD6	C21-C20-C15	-3.13	117.15	122.30
37	b	702	BCR	C28-C27-C26	-3.13	108.47	114.06
29	J	305	UIX	C7-C10-C11	-3.13	120.67	125.53
28	I	305	DD6	C25-C24-C1	-3.13	117.78	126.36
30	F	315	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
28	I	302	DD6	C12-C11-C10	-3.13	117.75	122.82
28	I	302	DD6	O1-C20-C21	-3.13	111.55	115.05
28	A	305	DD6	C37-C36-C35	3.12	120.16	114.42
28	M	306	DD6	C14-C13-C11	-3.12	120.69	125.53
28	J	303	DD6	C32-C33-C34	-3.12	106.75	113.59
29	K	302	UIX	C35-C36-C38	-3.12	114.16	123.20
30	L	309	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
37	b	732	BCR	C8-C7-C6	-3.12	118.67	127.00
28	M	302	DD6	C-C1-C2	-3.12	117.77	122.82
30	b	704	CLA	C3B-C4B-NB	-3.12	107.75	110.53
30	l	303	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
34	D	305	PID	CM4-C14-C15	-3.11	117.77	122.82
28	A	305	DD6	C37-C36-C31	-3.11	118.35	124.16
30	L	308	CLA	CBD-CHA-C1A	3.11	132.07	127.38
30	I	306	CLA	O2D-CGD-O1D	-3.11	117.80	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	K	305	DD6	C4-C5-C6	-3.11	122.92	127.28
29	B	305	UIX	O-C-C7	-3.10	107.99	116.88
37	l	307	BCR	C20-C21-C22	-3.10	122.93	127.28
28	A	303	DD6	C4-C5-C6	-3.10	122.93	127.28
29	K	302	UIX	C6-C1-C3	3.10	117.72	114.24
28	A	302	DD6	C21-C20-C15	-3.10	117.21	122.30
30	a	738	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
31	O	312	KC1	CHC-C4B-C3B	-3.09	119.99	125.21
28	K	304	DD6	O1-C20-C19	-3.09	110.60	113.49
30	M	318	CLA	C3B-C4B-NB	-3.09	107.77	110.53
37	b	732	BCR	C10-C11-C12	-3.09	114.26	123.20
30	b	722	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
28	L	303	DD6	C15-C14-C13	-3.09	119.47	125.99
34	M	301	PID	C17-C18-C19	3.09	131.85	124.72
29	h	201	UIX	C37-C34-C30	-3.08	117.21	123.52
30	H	308	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
28	P	204	DD6	C37-C36-C35	3.08	120.08	114.42
28	K	301	DD6	O1-C15-C14	-3.07	108.07	116.88
34	H	301	PID	C17-C18-C19	3.07	131.82	124.72
29	A	304	UIX	C37-C39-C40	-3.07	122.97	127.28
30	B	310	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
37	l	307	BCR	C24-C23-C22	-3.07	121.69	126.23
30	L	317	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
28	b	731	DD6	C37-C36-C35	3.06	120.05	114.42
30	K	316	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
32	G	501	DGD	O1G-C1A-C2A	3.06	121.15	111.83
30	a	703	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
30	a	729	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
29	B	305	UIX	C-C7-C10	-3.05	119.54	125.99
28	G	504	DD6	C37-C36-C35	3.05	120.03	114.42
30	J	308	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
31	D	310	KC1	CHC-C4B-C3B	-3.05	120.07	125.21
37	l	302	BCR	C29-C30-C25	3.05	114.87	110.44
28	K	303	DD6	O1-C15-C14	-3.05	108.14	116.88
34	P	202	PID	C18-C19-C20	3.05	129.75	123.52
37	b	730	BCR	C21-C20-C19	-3.05	114.37	123.20
37	f	304	BCR	C38-C26-C25	-3.04	121.16	124.48
30	O	309	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
28	b	731	DD6	C32-C33-C34	-3.04	106.92	113.59
30	I	310	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
30	M	316	CLA	C3B-C4B-NB	-3.04	107.81	110.53
28	A	301	DD6	C14-C13-C11	-3.04	120.81	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	303	DD6	O1-C20-C19	-3.04	110.64	113.49
34	P	205	PID	C17-C18-C19	3.04	131.74	124.72
30	I	309	CLA	C3B-C4B-NB	-3.04	107.82	110.53
30	b	719	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
28	B	302	DD6	O1-C15-C14	-3.03	108.18	116.88
30	l	311	CLA	C3B-C4B-NB	-3.03	107.82	110.53
30	a	724	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
37	a	736	BCR	C20-C21-C22	-3.03	123.03	127.28
30	J	314	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
30	a	721	CLA	C3B-C4B-NB	-3.02	107.83	110.53
30	F	313	CLA	CHB-C4A-NA	3.02	128.76	124.40
37	b	702	BCR	C8-C7-C6	-3.02	118.93	127.00
28	P	204	DD6	C4-C3-C2	-3.02	117.34	123.52
29	I	304	UIX	C35-C36-C38	-3.02	114.45	123.20
37	a	734	BCR	C3-C4-C5	-3.02	108.67	114.06
37	b	730	BCR	C28-C27-C26	-3.02	108.67	114.06
30	L	312	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
30	a	716	CLA	C3B-C4B-NB	-3.02	107.84	110.53
30	I	315	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
34	D	304	PID	C17-C18-C19	3.01	131.69	124.72
34	O	305	PID	C7-C8-C9	-3.01	122.26	126.06
28	M	306	DD6	O1-C20-C21	3.01	118.41	115.05
28	J	304	DD6	C14-C13-C11	-3.01	120.86	125.53
29	B	305	UIX	C18-O2-C27	-3.01	112.53	117.85
30	B	311	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
34	F	304	PID	C17-C18-C19	3.01	131.68	124.72
32	G	521	DGD	O6E-C5E-C4E	-3.01	104.28	109.70
28	H	303	DD6	O1-C15-C14	-3.01	108.26	116.88
30	O	314	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
30	J	301	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
30	G	518	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
31	F	309	KC1	CHC-C4B-C3B	-3.00	120.14	125.21
30	L	316	CLA	CAA-C2A-C3A	-3.00	109.34	116.23
28	O	303	DD6	C21-C20-C15	-3.00	117.36	122.30
28	M	304	DD6	O1-C15-C14	-3.00	108.28	116.88
34	H	302	PID	CM4-C14-C15	-3.00	117.95	122.82
30	A	317	CLA	C3B-C4B-NB	-3.00	107.85	110.53
30	a	712	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
30	a	714	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
30	a	727	CLA	C3B-C4B-NB	-3.00	107.86	110.53
30	a	723	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
31	P	213	KC1	CHC-C4B-C3B	-2.99	120.16	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	O	304	PID	C26-C25-C24	2.99	112.12	109.21
30	J	308	CLA	C3B-C4B-NB	-2.99	107.86	110.53
30	K	306	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
30	J	307	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
28	M	305	DD6	C15-C14-C13	-2.99	119.67	125.99
31	P	211	KC1	O1D-CGD-CBD	-2.98	118.63	124.52
30	H	309	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
30	L	316	CLA	C3B-C4B-NB	-2.98	107.87	110.53
29	B	305	UIX	C7-C10-C11	-2.98	120.90	125.53
28	M	306	DD6	C24-C1-C2	2.98	123.70	119.01
37	l	307	BCR	C33-C5-C4	2.98	119.95	113.60
34	j	105	PID	C6-C7-C8	-2.98	119.70	125.99
30	a	725	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
31	N	308	KC1	CHB-C1B-C2B	-2.97	119.30	125.49
29	G	503	UIX	C18-O2-C27	-2.97	112.60	117.85
28	K	303	DD6	C10-C9-C8	-2.97	114.59	123.20
34	F	305	PID	C29-C24-C25	2.97	122.64	119.70
37	b	702	BCR	C3-C4-C5	-2.97	108.76	114.06
30	J	310	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
28	L	304	DD6	O1-C15-C14	-2.97	108.38	116.88
30	J	301	CLA	C3B-C4B-NB	-2.97	107.88	110.53
28	G	508	DD6	C4-C3-C2	-2.96	117.45	123.52
28	N	303	DD6	O1-C15-C14	-2.96	108.39	116.88
28	A	305	DD6	C9-C10-C11	-2.96	123.12	127.28
34	F	302	PID	CM5-C21-C20	-2.96	118.02	122.82
30	O	316	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
34	N	302	PID	CM5-C21-C20	-2.96	118.02	122.82
30	B	315	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
30	G	510	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
29	G	503	UIX	C36-C35-C32	-2.96	123.13	127.28
30	L	313	CLA	C3B-C4B-NB	-2.95	107.89	110.53
31	N	308	KC1	C2D-C1D-ND	-2.95	107.26	110.33
28	B	306	DD6	C25-C26-C27	-2.95	118.36	126.61
30	a	702	CLA	C1-C2-C3	-2.95	121.36	126.20
34	H	302	PID	C17-C16-C15	2.95	129.56	123.52
31	M	307	KC1	C2D-C1D-ND	-2.95	107.27	110.33
30	a	717	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
30	H	311	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
37	a	734	BCR	C8-C7-C6	-2.95	119.13	127.00
30	a	703	CLA	C3B-C4B-NB	-2.94	107.90	110.53
29	h	201	UIX	C13-C14-C23	-2.94	114.69	123.20
28	L	303	DD6	C37-C36-C31	-2.94	118.67	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	I	308	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
37	b	732	BCR	C24-C23-C22	-2.94	121.89	126.23
30	B	307	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
37	i	201	BCR	C10-C11-C12	-2.93	114.70	123.20
34	F	305	PID	C19-C20-C21	2.93	131.39	127.28
30	H	304	CLA	C3B-C4B-NB	-2.93	107.91	110.53
28	B	303	DD6	C37-C36-C31	-2.93	118.68	124.16
28	J	302	DD6	C25-C24-C1	-2.93	118.32	126.36
33	P	201	LMG	O6-C1-O1	-2.93	103.12	110.04
31	D	310	KC1	C2D-C1D-ND	-2.93	107.29	110.33
30	B	309	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
28	B	304	DD6	O1-C15-C14	-2.93	108.50	116.88
30	b	716	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
30	D	309	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
30	M	313	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
31	L	307	KC1	CHC-C4B-C3B	-2.92	120.28	125.21
28	B	304	DD6	C37-C36-C31	-2.92	118.69	124.16
30	I	309	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
30	B	310	CLA	C1-C2-C3	-2.92	121.41	126.20
28	K	304	DD6	C3-C4-C5	-2.92	117.54	123.52
30	M	313	CLA	C3B-C4B-NB	-2.92	107.92	110.53
30	A	315	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
28	G	505	DD6	O1-C20-C15	-2.92	56.61	58.93
30	K	309	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
30	l	309	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
30	P	217	CLA	CAA-C2A-C3A	-2.92	109.54	116.23
28	P	204	DD6	O1-C20-C19	-2.92	110.76	113.49
30	J	315	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
37	b	702	BCR	C10-C11-C12	-2.92	114.75	123.20
28	L	302	DD6	C28-C27-C26	-2.92	118.52	124.18
28	M	303	DD6	C14-C13-C11	-2.92	121.00	125.53
28	G	504	DD6	C9-C10-C11	-2.91	123.19	127.28
30	b	715	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
30	L	316	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
30	a	709	CLA	C3B-C4B-NB	-2.91	107.93	110.53
28	K	301	DD6	C3-C2-C1	-2.91	123.19	127.28
28	B	306	DD6	C9-C10-C11	-2.91	123.20	127.28
31	N	308	KC1	C4B-CHC-C1C	-2.91	119.84	126.02
30	F	313	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
37	l	302	BCR	C38-C26-C27	2.91	119.79	113.60
29	h	201	UIX	C34-C30-C26	-2.91	123.20	127.28
30	j	104	CLA	C3B-C4B-NB	-2.91	107.94	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	D	312	CLA	C3B-C4B-NB	-2.91	107.94	110.53
30	B	315	CLA	CAA-C2A-C3A	-2.91	109.57	116.23
30	A	308	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
30	O	316	CLA	CAA-C2A-C3A	-2.91	109.57	116.23
30	a	705	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
31	A	306	KC1	C2D-C1D-ND	-2.90	107.32	110.33
31	N	306	KC1	C2D-C1D-ND	-2.90	107.32	110.33
30	b	707	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
30	a	708	CLA	C3B-C4B-NB	-2.90	107.94	110.53
30	b	705	CLA	C3B-C4B-NB	-2.90	107.94	110.53
30	J	316	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
31	H	310	KC1	C2D-C1D-ND	-2.90	107.32	110.33
28	I	303	DD6	C37-C36-C31	-2.90	118.74	124.16
29	K	302	UIX	C7-C10-C11	-2.90	121.03	125.53
30	F	307	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
30	A	320	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
37	l	302	BCR	C16-C15-C14	-2.89	117.60	123.52
30	b	718	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
30	b	710	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
30	H	307	CLA	C3B-C4B-NB	-2.89	107.95	110.53
30	b	724	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
28	B	306	DD6	O1-C15-C14	-2.89	108.61	116.88
37	b	702	BCR	C34-C9-C8	2.88	122.49	118.09
34	N	302	PID	C29-C24-C25	2.88	122.56	119.70
28	G	505	DD6	C21-C20-C19	2.88	117.48	114.24
37	l	302	BCR	C3-C4-C5	-2.88	108.92	114.06
32	I	317	DGD	O1G-C1A-C2A	2.88	119.90	111.15
28	K	303	DD6	C4-C5-C6	-2.88	123.24	127.28
30	b	709	CLA	C3B-C4B-NB	-2.88	107.96	110.53
30	H	304	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
30	I	307	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
28	I	301	DD6	C25-C26-C27	-2.88	118.56	126.61
31	M	314	KC1	C2D-C1D-ND	-2.88	107.34	110.33
28	M	303	DD6	C21-C20-C15	-2.88	117.57	122.30
34	F	304	PID	C8-C9-C10	2.88	129.23	123.60
30	B	301	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
31	P	211	KC1	C2D-C1D-ND	-2.87	107.35	110.33
30	A	317	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
30	b	725	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
30	l	313	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
30	a	715	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
30	P	209	CLA	O2D-CGD-O1D	-2.87	118.26	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	l	308	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
37	l	307	BCR	C15-C16-C17	-2.87	117.65	123.52
30	K	308	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
31	J	313	KC1	C2D-C1D-ND	-2.87	107.35	110.33
30	M	308	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
30	a	719	CLA	C3B-C4B-NB	-2.87	107.97	110.53
30	b	723	CLA	C3B-C4B-NB	-2.87	107.97	110.53
28	G	508	DD6	O1-C15-C14	-2.87	108.66	116.88
28	P	204	DD6	C37-C36-C31	-2.87	118.80	124.16
30	f	301	CLA	C3B-C4B-NB	-2.87	107.97	110.53
30	b	706	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
30	H	305	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
28	G	504	DD6	C24-C1-C2	2.86	123.51	119.01
30	a	716	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
30	a	728	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
30	L	310	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
31	P	216	KC1	CHB-C1B-C2B	-2.86	119.54	125.49
37	b	730	BCR	C27-C26-C25	-2.86	118.84	122.70
34	O	307	PID	C18-C19-C20	2.86	129.37	123.52
28	b	731	DD6	C26-C25-C24	-2.86	114.92	123.20
31	O	315	KC1	C2D-C1D-ND	-2.86	107.36	110.33
28	F	301	DD6	C37-C36-C35	2.86	119.67	114.42
30	b	711	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
30	L	314	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
33	b	734	LMG	O6-C1-O1	-2.85	103.30	110.04
30	P	210	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
30	M	317	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
30	N	305	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
28	H	303	DD6	O1-C20-C21	-2.85	111.86	115.05
31	K	314	KC1	CHC-C4B-C3B	-2.85	120.40	125.21
37	l	302	BCR	C10-C11-C12	-2.85	114.94	123.20
30	B	311	CLA	C3B-C4B-NB	-2.85	107.98	110.53
30	m	202	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
30	N	304	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
30	b	717	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
30	A	315	CLA	CAA-C2A-C3A	-2.85	109.69	116.23
31	P	211	KC1	CHC-C4B-C3B	-2.85	120.40	125.21
30	B	312	CLA	C3B-C4B-NB	-2.85	107.99	110.53
31	A	314	KC1	CHB-C1B-C2B	-2.85	119.56	125.49
30	F	308	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
30	N	307	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
28	D	303	DD6	C9-C10-C11	-2.85	123.29	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	I	321	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
30	K	311	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
30	a	718	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
30	a	718	CLA	C3B-C4B-NB	-2.85	107.99	110.53
30	a	738	CLA	C3B-C4B-NB	-2.85	107.99	110.53
30	f	303	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
30	b	712	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
28	J	303	DD6	C37-C36-C31	-2.84	118.84	124.16
30	K	313	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
37	l	306	BCR	C28-C27-C26	-2.84	108.99	114.06
28	M	305	DD6	C21-C20-C15	-2.84	117.62	122.30
30	a	722	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
30	B	307	CLA	C3B-C4B-NB	-2.84	107.99	110.53
31	L	315	KC1	C2D-C1D-ND	-2.84	107.38	110.33
30	l	304	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
31	H	306	KC1	CHC-C4B-C3B	-2.84	120.42	125.21
30	K	310	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
30	K	315	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
30	M	318	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
34	D	305	PID	CM5-C21-C20	-2.84	118.22	122.82
30	G	509	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
31	O	315	KC1	O1D-CGD-CBD	-2.84	118.92	124.52
31	I	314	KC1	C2D-C1D-ND	-2.84	107.38	110.33
31	F	309	KC1	C2D-C1D-ND	-2.84	107.38	110.33
29	G	503	UIX	C14-C13-C11	-2.84	123.30	127.28
30	A	320	CLA	C3B-C4B-NB	-2.84	108.00	110.53
30	O	308	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
30	M	316	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
37	a	734	BCR	C24-C23-C22	-2.83	122.04	126.23
28	J	302	DD6	C37-C36-C31	-2.83	118.86	124.16
34	j	105	PID	C7-C8-C9	2.83	129.62	126.06
30	B	317	CLA	C3B-C4B-NB	-2.83	108.00	110.53
30	N	304	CLA	C3B-C4B-NB	-2.83	108.01	110.53
30	A	319	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
30	l	305	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
28	D	303	DD6	C12-C11-C13	2.83	122.41	118.09
37	j	102	BCR	C11-C10-C9	-2.83	123.31	127.28
30	P	217	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
31	P	216	KC1	C2D-C1D-ND	-2.83	107.40	110.33
30	B	313	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
29	G	503	UIX	C34-C37-C39	-2.82	117.74	123.52
30	j	104	CLA	O2D-CGD-O1D	-2.82	118.35	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	F	314	KC1	C2D-C1D-ND	-2.82	107.40	110.33
37	b	730	BCR	C15-C16-C17	-2.82	117.74	123.52
30	A	313	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
30	a	708	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
28	I	301	DD6	O1-C15-C14	-2.82	108.79	116.88
31	N	311	KC1	CHC-C4B-C3B	-2.82	120.45	125.21
31	I	314	KC1	CHC-C4B-C3B	-2.82	120.45	125.21
30	M	311	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
28	b	731	DD6	O1-C15-C14	-2.82	108.80	116.88
30	I	307	CLA	C3B-C4B-NB	-2.82	108.01	110.53
30	L	312	CLA	C3B-C4B-NB	-2.82	108.01	110.53
31	N	306	KC1	O1D-CGD-CBD	-2.82	118.96	124.52
30	M	309	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
38	b	729	PQN	C11-C3-C2	-2.82	120.06	124.89
28	G	508	DD6	C14-C13-C11	-2.82	121.16	125.53
30	M	317	CLA	C3B-C4B-NB	-2.81	108.02	110.53
30	M	312	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
30	a	709	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
37	j	102	BCR	C7-C8-C9	-2.81	122.08	126.23
31	G	515	KC1	C2D-C1D-ND	-2.81	107.41	110.33
30	O	308	CLA	C3B-C4B-NB	-2.81	108.02	110.53
28	M	303	DD6	C25-C24-C1	-2.81	118.65	126.36
28	I	305	DD6	C24-C1-C2	2.81	123.43	119.01
31	D	315	KC1	CHB-C1B-C2B	-2.81	119.64	125.49
37	b	702	BCR	C15-C14-C13	-2.81	123.34	127.28
37	j	102	BCR	C28-C27-C26	-2.81	109.05	114.06
30	b	703	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
30	G	512	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
28	F	301	DD6	C28-C27-C26	-2.81	118.73	124.18
29	I	304	UIX	C37-C34-C30	-2.81	117.77	123.52
30	M	312	CLA	C3B-C4B-NB	-2.81	108.02	110.53
30	D	313	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
28	J	302	DD6	C37-C36-C35	2.81	119.58	114.42
30	K	306	CLA	C3B-C4B-NB	-2.81	108.03	110.53
30	b	705	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
31	H	306	KC1	C2D-C1D-ND	-2.81	107.42	110.33
30	A	319	CLA	C3B-C4B-NB	-2.80	108.03	110.53
31	N	306	KC1	CHC-C4B-C3B	-2.80	120.48	125.21
30	A	312	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
30	b	727	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
28	K	304	DD6	C37-C36-C35	2.80	119.57	114.42
30	H	305	CLA	C1-C2-C3	-2.80	121.61	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	L	318	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
34	F	305	PID	CM4-C14-C15	-2.80	118.28	122.82
30	a	725	CLA	C3B-C4B-NB	-2.80	108.03	110.53
29	I	304	UIX	C18-O2-C27	-2.80	112.90	117.85
30	K	307	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
37	m	201	BCR	C16-C17-C18	-2.80	123.35	127.28
30	H	309	CLA	C3B-C4B-NB	-2.80	108.03	110.53
30	F	315	CLA	CAA-C2A-C3A	-2.80	109.81	116.23
29	K	302	UIX	C14-C23-C26	-2.80	118.69	126.36
30	I	312	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
31	P	211	KC1	O2D-CGD-O1D	-2.80	118.40	123.85
30	b	720	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
30	J	312	CLA	C3B-C4B-NB	-2.80	108.03	110.53
37	a	736	BCR	C38-C26-C25	-2.80	121.43	124.48
30	a	701	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
29	A	304	UIX	C21-C15-C20	-2.80	107.97	110.47
28	K	305	DD6	O1-C15-C14	-2.80	108.86	116.88
37	j	102	BCR	C16-C15-C14	-2.80	117.80	123.52
28	J	304	DD6	O1-C20-C21	2.80	118.17	115.05
28	G	505	DD6	C25-C24-C1	-2.80	118.70	126.36
28	L	306	DD6	C37-C36-C35	2.80	119.56	114.42
30	A	316	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
30	B	317	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
30	J	309	CLA	C1-C2-C3	-2.79	121.62	126.20
30	a	735	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
30	a	727	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
30	O	313	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
33	D	317	LMG	O6-C1-O1	-2.79	103.44	110.04
31	P	213	KC1	C2D-C1D-ND	-2.79	107.43	110.33
28	M	304	DD6	C3-C4-C5	-2.79	117.80	123.52
28	G	505	DD6	C37-C36-C31	-2.79	118.94	124.16
30	I	311	CLA	C3B-C4B-NB	-2.79	108.04	110.53
30	B	308	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
31	M	314	KC1	CHB-C1B-C2B	-2.79	119.68	125.49
31	N	311	KC1	C2D-C1D-ND	-2.79	107.43	110.33
37	j	102	BCR	C8-C7-C6	-2.79	119.55	127.00
30	P	214	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
30	l	313	CLA	CHB-C4A-NA	2.79	128.42	124.40
31	A	314	KC1	CHC-C4B-C3B	-2.79	120.51	125.21
30	l	312	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
30	a	701	CLA	C3B-C4B-NB	-2.79	108.04	110.53
30	D	308	CLA	C3B-C4B-NB	-2.79	108.04	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	712	CLA	C3B-C4B-NB	-2.78	108.04	110.53
30	l	309	CLA	C3B-C4B-NB	-2.78	108.05	110.53
31	O	312	KC1	C2D-C1D-ND	-2.78	107.44	110.33
28	K	305	DD6	C21-C20-C15	-2.78	117.72	122.30
30	P	209	CLA	C3B-C4B-NB	-2.78	108.05	110.53
30	a	730	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
30	J	311	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
31	I	314	KC1	CHB-C1B-C2B	-2.78	119.70	125.49
30	G	516	CLA	C3B-C4B-NB	-2.78	108.05	110.53
29	O	306	UIX	C22-C15-C20	-2.78	107.98	110.47
30	l	311	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
30	B	316	CLA	C3B-C4B-NB	-2.78	108.05	110.53
37	m	201	BCR	C28-C27-C26	-2.78	109.10	114.06
29	O	306	UIX	C16-C20-C15	2.78	122.45	119.70
31	B	314	KC1	C2D-C1D-ND	-2.78	107.45	110.33
28	B	302	DD6	C25-C24-C1	-2.78	118.75	126.36
31	B	314	KC1	O1D-CGD-CBD	-2.78	119.04	124.52
30	J	306	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
29	B	305	UIX	C16-C20-C15	2.77	122.45	119.70
31	A	314	KC1	C2D-C1D-ND	-2.77	107.45	110.33
33	I	320	LMG	O6-C1-O1	-2.77	103.49	110.04
37	b	702	BCR	C20-C19-C18	-2.77	118.76	126.36
28	K	301	DD6	C37-C36-C31	-2.77	118.98	124.16
34	j	105	PID	C18-C19-C20	2.77	129.19	123.52
30	I	313	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
30	f	301	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
30	a	731	CLA	C3B-C4B-NB	-2.77	108.06	110.53
30	G	520	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
30	I	321	CLA	CHB-C4A-NA	2.77	128.39	124.40
37	a	736	BCR	C3-C4-C5	-2.77	109.12	114.06
31	B	314	KC1	CHC-C4B-C3B	-2.76	120.55	125.21
30	N	310	CLA	CHB-C4A-NA	2.76	128.39	124.40
30	K	310	CLA	C3B-C4B-NB	-2.76	108.06	110.53
30	h	202	CLA	C3B-C4B-NB	-2.76	108.06	110.53
30	a	706	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
28	A	303	DD6	C9-C10-C11	-2.76	123.40	127.28
28	B	303	DD6	C15-C14-C13	-2.76	120.15	125.99
28	G	505	DD6	C-C1-C2	-2.76	118.34	122.82
30	A	313	CLA	C3B-C4B-NB	-2.76	108.06	110.53
37	i	201	BCR	C1-C6-C5	-2.76	118.86	122.64
30	b	726	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
30	D	314	CLA	CHB-C4A-NA	2.76	128.38	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	311	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
30	B	310	CLA	C3B-C4B-NB	-2.76	108.07	110.53
31	O	315	KC1	CHC-C4B-C3B	-2.76	120.56	125.21
28	L	304	DD6	C37-C36-C31	-2.76	119.00	124.16
30	F	310	CLA	C3B-C4B-NB	-2.76	108.07	110.53
33	b	733	LMG	O6-C1-O1	-2.76	103.53	110.04
30	a	711	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
30	b	728	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
30	b	711	CLA	C3B-C4B-NB	-2.76	108.07	110.53
30	j	106	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
34	D	302	PID	CM2-C5-C4	-2.75	104.13	108.97
28	G	504	DD6	C15-C14-C13	-2.75	120.17	125.99
30	J	309	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
37	a	734	BCR	C38-C26-C25	-2.75	121.48	124.48
30	h	202	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
34	M	301	PID	C29-C24-C25	2.75	122.43	119.70
30	D	312	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
30	a	705	CLA	C3B-C4B-NB	-2.75	108.08	110.53
30	A	309	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
28	K	305	DD6	C14-C13-C11	-2.75	121.26	125.53
28	b	731	DD6	C14-C13-C11	-2.75	121.26	125.53
30	a	730	CLA	C3B-C4B-NB	-2.75	108.08	110.53
30	D	316	CLA	C3B-C4B-NB	-2.75	108.08	110.53
28	L	303	DD6	C37-C36-C35	2.75	119.47	114.42
28	O	303	DD6	C4-C3-C2	-2.75	117.90	123.52
30	J	315	CLA	C3B-C4B-NB	-2.74	108.08	110.53
31	B	314	KC1	CHB-C1B-C2B	-2.74	119.78	125.49
30	a	704	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
31	O	312	KC1	O1D-CGD-CBD	-2.74	119.11	124.52
30	D	311	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
28	F	301	DD6	C25-C24-C1	-2.74	118.85	126.36
30	b	721	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
30	D	311	CLA	C3B-C4B-NB	-2.74	108.08	110.53
32	G	521	DGD	C3E-C4E-C5E	2.74	115.20	110.23
30	D	316	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
30	N	309	CLA	C3B-C4B-NB	-2.74	108.09	110.53
30	B	316	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
37	l	306	BCR	C23-C24-C25	-2.74	119.69	127.00
30	L	318	CLA	CHB-C4A-NA	2.73	128.35	124.40
33	I	318	LMG	C1-C2-C3	-2.73	104.26	110.01
37	b	732	BCR	C11-C10-C9	-2.73	123.45	127.28
29	K	302	UIX	C37-C39-C40	-2.73	123.45	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	G	506	PID	C18-C19-C20	2.73	129.11	123.52
37	a	736	BCR	C33-C5-C6	-2.73	121.50	124.48
31	L	315	KC1	CHB-C1B-C2B	-2.73	119.81	125.49
37	l	302	BCR	C8-C7-C6	-2.73	119.71	127.00
28	F	301	DD6	O1-C20-C21	-2.73	112.00	115.05
30	D	308	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
31	D	310	KC1	CHB-C1B-C2B	-2.73	119.82	125.49
31	O	310	KC1	CHB-C1B-C2B	-2.72	119.82	125.49
30	A	317	CLA	CAA-C2A-C3A	-2.72	109.98	116.23
30	L	311	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
28	F	303	DD6	C9-C8-C6	-2.72	118.89	126.36
37	b	732	BCR	C7-C8-C9	-2.72	122.20	126.23
30	B	312	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
34	D	301	PID	CM5-C21-C20	-2.72	118.40	122.82
30	F	311	CLA	C3B-C4B-NB	-2.72	108.10	110.53
34	F	305	PID	C26-C25-C24	2.72	111.86	109.21
30	b	708	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
28	B	302	DD6	C24-C1-C2	2.72	123.29	119.01
30	K	312	CLA	C3B-C4B-NB	-2.72	108.10	110.53
30	M	311	CLA	C3B-C4B-NB	-2.72	108.10	110.53
30	a	724	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
30	A	315	CLA	C3B-C4B-NB	-2.72	108.10	110.53
30	K	309	CLA	C3B-C4B-NB	-2.72	108.11	110.53
30	b	727	CLA	C3B-C4B-NB	-2.72	108.11	110.53
30	A	316	CLA	C3B-C4B-NB	-2.71	108.11	110.53
31	K	314	KC1	C2D-C1D-ND	-2.71	107.51	110.33
33	K	317	LMG	O6-C1-O1	-2.71	103.63	110.04
30	l	309	CLA	CAA-C2A-C3A	-2.71	110.01	116.23
31	F	314	KC1	CHB-C1B-C2B	-2.71	119.84	125.49
30	f	302	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
37	l	307	BCR	C2-C1-C6	2.71	114.38	110.44
28	L	302	DD6	C21-C20-C15	-2.71	117.84	122.30
30	N	310	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
37	l	302	BCR	C7-C8-C9	-2.71	122.22	126.23
33	B	318	LMG	O6-C1-O1	-2.71	103.64	110.04
30	a	731	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
28	L	304	DD6	C10-C9-C8	-2.71	115.35	123.20
30	b	708	CLA	C3B-C4B-NB	-2.71	108.11	110.53
28	B	302	DD6	C32-C33-C34	-2.71	107.66	113.59
28	M	304	DD6	C32-C33-C34	-2.71	107.66	113.59
30	b	709	CLA	O2A-CGA-O1A	-2.71	116.86	123.63
37	j	102	BCR	C38-C26-C25	-2.71	121.53	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	504	DD6	C14-C13-C11	-2.70	121.33	125.53
30	A	310	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
37	b	732	BCR	C16-C15-C14	-2.70	117.99	123.52
31	M	314	KC1	CHC-C4B-C3B	-2.70	120.65	125.21
30	G	511	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
30	B	317	CLA	CHB-C4A-NA	2.70	128.30	124.40
30	I	321	CLA	CAC-C3C-C4C	2.70	128.30	124.79
30	I	319	CLA	C3B-C4B-NB	-2.70	108.12	110.53
28	I	303	DD6	C25-C24-C1	-2.70	118.96	126.36
31	O	315	KC1	CHB-C1B-C2B	-2.70	119.87	125.49
30	b	715	CLA	C3B-C4B-NB	-2.70	108.12	110.53
31	L	315	KC1	CHC-C4B-C3B	-2.70	120.66	125.21
29	B	305	UIX	C35-C36-C38	-2.70	115.38	123.20
30	P	215	CLA	O2D-CGD-CBD	2.70	115.94	111.23
29	K	302	UIX	C3-C5-C4	-2.70	105.75	110.79
30	l	311	CLA	CHB-C4A-NA	2.70	128.29	124.40
30	J	312	CLA	O2D-CGD-CBD	2.70	115.94	111.23
30	b	704	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
31	D	315	KC1	C2D-C1D-ND	-2.69	107.53	110.33
38	b	729	PQN	C2M-C2-C3	-2.69	120.02	124.45
37	b	702	BCR	C27-C26-C25	-2.69	119.06	122.70
30	b	713	CLA	C3B-C4B-NB	-2.69	108.13	110.53
30	a	721	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
28	D	303	DD6	C37-C36-C31	-2.69	119.13	124.16
28	h	203	DD6	C21-C20-C15	-2.69	117.87	122.30
30	l	304	CLA	CHB-C4A-NA	2.69	128.28	124.40
30	F	310	CLA	CHB-C4A-NA	2.69	128.28	124.40
28	J	303	DD6	C25-C24-C1	-2.69	118.98	126.36
30	a	707	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
31	A	306	KC1	CHC-C4B-C3B	-2.69	120.67	125.21
30	B	315	CLA	C3B-C4B-NB	-2.69	108.13	110.53
30	J	314	CLA	C3B-C4B-NB	-2.69	108.13	110.53
31	H	310	KC1	CHB-C1B-C2B	-2.69	119.90	125.49
30	M	310	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
30	a	710	CLA	C3B-C4B-NB	-2.69	108.13	110.53
30	O	309	CLA	C3B-C4B-NB	-2.69	108.13	110.53
30	a	710	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
30	b	728	CLA	C3B-C4B-NB	-2.69	108.13	110.53
30	L	310	CLA	C3B-C4B-NB	-2.69	108.13	110.53
30	K	312	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
30	O	309	CLA	C1-C2-C3	-2.69	121.80	126.20
28	A	303	DD6	C21-C20-C15	-2.69	117.88	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	F	306	PID	CM5-C21-C20	-2.69	118.47	122.82
31	L	307	KC1	CHB-C1B-C2B	-2.68	119.91	125.49
30	a	707	CLA	C3B-C4B-NB	-2.68	108.14	110.53
30	M	308	CLA	C3B-C4B-NB	-2.68	108.14	110.53
37	j	102	BCR	C20-C19-C18	-2.68	119.01	126.36
31	H	306	KC1	CHB-C1B-C2B	-2.68	119.91	125.49
34	D	301	PID	CM2-C5-C4	-2.68	104.25	108.97
30	I	306	CLA	C3B-C4B-NB	-2.68	108.14	110.53
28	M	302	DD6	C3-C4-C5	-2.68	118.03	123.52
31	N	308	KC1	CHB-C4A-C3A	-2.68	120.80	125.03
28	D	303	DD6	C4-C5-C6	-2.68	123.52	127.28
37	m	201	BCR	C21-C20-C19	-2.68	115.44	123.20
31	I	314	KC1	O1D-CGD-CBD	-2.68	119.24	124.52
31	O	310	KC1	C2D-C1D-ND	-2.68	107.55	110.33
30	G	517	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
30	O	311	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
31	F	314	KC1	CHC-C4B-C3B	-2.68	120.70	125.21
30	b	703	CLA	C1-C2-C3	-2.68	121.81	126.20
34	P	203	PID	CM5-C21-C20	-2.68	118.48	122.82
30	a	713	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
30	I	312	CLA	C3B-C4B-NB	-2.68	108.14	110.53
28	L	305	DD6	C21-C20-C15	-2.67	117.90	122.30
30	a	719	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
30	G	518	CLA	C3B-C4B-NB	-2.67	108.14	110.53
30	L	308	CLA	C3B-C4B-NB	-2.67	108.14	110.53
31	F	309	KC1	CHB-C1B-C2B	-2.67	119.93	125.49
30	a	703	CLA	C1-C2-C3	-2.67	121.82	126.20
31	H	310	KC1	CHC-C4B-C3B	-2.67	120.70	125.21
30	b	716	CLA	C3B-C4B-NB	-2.67	108.14	110.53
30	H	312	CLA	C3B-C4B-NB	-2.67	108.14	110.53
28	M	305	DD6	C14-C13-C11	-2.67	121.38	125.53
30	J	307	CLA	CHB-C4A-NA	2.67	128.26	124.40
30	J	312	CLA	CHB-C4A-NA	2.67	128.25	124.40
37	b	732	BCR	C23-C24-C25	-2.67	119.86	127.00
30	J	314	CLA	CAA-C2A-C3A	-2.67	110.11	116.23
30	M	317	CLA	CHB-C4A-NA	2.67	128.25	124.40
28	L	305	DD6	O1-C15-C14	-2.67	109.23	116.88
30	b	705	CLA	C1-C2-C3	-2.67	121.83	126.20
31	N	306	KC1	CHB-C1B-C2B	-2.67	119.94	125.49
28	h	203	DD6	C37-C36-C35	2.66	119.32	114.42
31	O	310	KC1	CHC-C4B-C3B	-2.66	120.72	125.21
28	L	306	DD6	C15-C14-C13	-2.66	120.36	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	P	205	PID	C16-C15-C14	-2.66	123.54	127.28
30	P	215	CLA	CHB-C4A-NA	2.66	128.24	124.40
30	M	315	CLA	CAA-C2A-C3A	-2.66	110.12	116.23
30	L	317	CLA	C3B-C4B-NB	-2.66	108.15	110.53
30	P	215	CLA	C3B-C4B-NB	-2.66	108.15	110.53
28	B	304	DD6	C10-C9-C8	-2.66	115.49	123.20
31	K	314	KC1	CHB-C1B-C2B	-2.66	119.95	125.49
30	K	316	CLA	C3B-C4B-NB	-2.66	108.16	110.53
30	P	217	CLA	C3B-C4B-NB	-2.66	108.16	110.53
28	I	302	DD6	O1-C20-C19	-2.66	111.00	113.49
30	O	316	CLA	C3B-C4B-NB	-2.66	108.16	110.53
31	G	515	KC1	CHB-C1B-C2B	-2.66	119.96	125.49
30	N	305	CLA	C3B-C4B-NB	-2.66	108.16	110.53
37	b	732	BCR	C20-C21-C22	-2.66	123.55	127.28
30	b	723	CLA	CHB-C4A-NA	2.66	128.23	124.40
30	G	519	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
30	M	309	CLA	C3B-C4B-NB	-2.65	108.16	110.53
30	a	720	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
34	P	208	PID	CM5-C21-C20	-2.65	118.52	122.82
31	L	315	KC1	O1D-CGD-CBD	-2.65	119.29	124.52
28	M	302	DD6	C37-C36-C31	-2.65	119.20	124.16
30	a	715	CLA	C3B-C4B-NB	-2.65	108.16	110.53
30	b	726	CLA	C3B-C4B-NB	-2.65	108.16	110.53
30	B	308	CLA	C3B-C4B-NB	-2.65	108.16	110.53
32	j	103	DGD	C2G-O2G-C1B	-2.65	111.45	117.80
28	G	505	DD6	C21-C20-C15	-2.65	117.94	122.30
29	J	305	UIX	O-C-C7	-2.65	109.29	116.88
29	h	201	UIX	C18-O2-C27	-2.65	113.17	117.85
30	I	315	CLA	C3B-C4B-NB	-2.65	108.17	110.53
30	G	514	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
30	J	309	CLA	C3B-C4B-NB	-2.65	108.17	110.53
37	i	201	BCR	C4-C5-C6	-2.65	119.13	122.70
31	F	309	KC1	C2A-C3A-C4A	2.65	108.40	106.41
37	i	201	BCR	C3-C4-C5	-2.65	109.34	114.06
30	b	713	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
33	j	101	LMG	O6-C1-O1	-2.64	103.80	110.04
29	B	305	UIX	C37-C34-C30	-2.64	118.11	123.52
30	a	716	CLA	CHB-C4A-NA	2.64	128.22	124.40
31	O	312	KC1	O2D-CGD-O1D	-2.64	118.70	123.85
28	I	305	DD6	C21-C20-C15	-2.64	117.95	122.30
30	H	312	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
30	L	311	CLA	C3B-C4B-NB	-2.64	108.17	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	P	212	CLA	C3B-C4B-NB	-2.64	108.17	110.53
37	b	730	BCR	C33-C5-C4	2.64	119.23	113.60
30	H	308	CLA	C3B-C4B-NB	-2.64	108.17	110.53
31	H	306	KC1	O1D-CGD-CBD	-2.64	119.31	124.52
30	I	321	CLA	C3B-C4B-NB	-2.64	108.17	110.53
30	b	725	CLA	C3B-C4B-NB	-2.64	108.17	110.53
30	a	726	CLA	CHB-C4A-NA	2.64	128.21	124.40
32	G	521	DGD	O1G-C1A-C2A	2.64	119.88	111.83
30	H	305	CLA	C3B-C4B-NB	-2.64	108.17	110.53
28	M	303	DD6	C9-C8-C6	-2.64	119.13	126.36
29	J	305	UIX	C35-C36-C38	-2.64	115.56	123.20
31	P	213	KC1	C4B-CHC-C1C	-2.64	120.42	126.02
30	L	313	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
30	O	311	CLA	C3B-C4B-NB	-2.64	108.18	110.53
30	G	516	CLA	CAA-C2A-C3A	-2.64	110.19	116.23
30	P	212	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
30	G	514	CLA	CHB-C4A-NA	2.63	128.20	124.40
28	A	302	DD6	C28-C27-C26	-2.63	119.07	124.18
30	b	701	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
30	b	707	CLA	C1-C2-C3	-2.63	121.89	126.20
28	K	301	DD6	C26-C25-C24	-2.63	115.58	123.20
30	A	307	CLA	C3B-C4B-NB	-2.63	108.19	110.53
29	K	302	UIX	C22-C15-C20	-2.62	108.12	110.47
30	J	316	CLA	C3B-C4B-NB	-2.62	108.19	110.53
31	P	216	KC1	CHC-C4B-C3B	-2.62	120.79	125.21
31	M	307	KC1	C1D-CHD-C4C	-2.62	120.08	126.25
30	A	311	CLA	C3B-C4B-NB	-2.62	108.19	110.53
30	b	701	CLA	C3B-C4B-NB	-2.62	108.19	110.53
34	O	305	PID	C6-C7-C8	2.62	131.53	125.99
30	L	311	CLA	CHB-C4A-NA	2.62	128.18	124.40
31	N	308	KC1	CHC-C4B-C3B	-2.62	120.79	125.21
31	F	309	KC1	C4B-CHC-C1C	-2.62	120.45	126.02
28	J	304	DD6	C37-C36-C35	2.62	119.23	114.42
30	a	728	CLA	C3B-C4B-NB	-2.62	108.19	110.53
30	L	318	CLA	C3B-C4B-NB	-2.62	108.19	110.53
32	L	301	DGD	C2G-O2G-C1B	-2.62	111.53	117.80
29	h	201	UIX	C22-C15-C20	-2.61	108.13	110.47
31	N	311	KC1	CHB-C1B-C2B	-2.61	120.05	125.49
30	f	303	CLA	C3B-C4B-NB	-2.61	108.20	110.53
30	b	703	CLA	C3B-C4B-NB	-2.61	108.20	110.53
31	D	315	KC1	C1D-CHD-C4C	-2.61	120.10	126.25
30	a	701	CLA	CHB-C4A-NA	2.61	128.17	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	707	CLA	CHB-C4A-NA	2.61	128.17	124.40
30	I	308	CLA	C3B-C4B-NB	-2.61	108.20	110.53
30	l	313	CLA	C3B-C4B-NB	-2.61	108.20	110.53
38	a	732	PQN	C11-C3-C2	-2.61	120.41	124.89
30	b	715	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
28	J	302	DD6	C32-C33-C34	-2.61	107.87	113.59
37	b	732	BCR	C15-C16-C17	-2.61	118.18	123.52
28	K	305	DD6	C25-C26-C27	-2.61	119.31	126.61
30	a	721	CLA	C1-C2-C3	-2.61	121.92	126.20
30	m	202	CLA	CMB-C2B-C1B	-2.61	121.45	125.42
30	G	510	CLA	CHB-C4A-NA	2.61	128.16	124.40
30	L	314	CLA	C3B-C4B-NB	-2.61	108.20	110.53
30	a	718	CLA	CHB-C4A-NA	2.61	128.16	124.40
30	a	729	CLA	C3B-C4B-NB	-2.61	108.20	110.53
37	a	734	BCR	C23-C24-C25	-2.61	120.03	127.00
31	L	307	KC1	C2D-C1D-ND	-2.61	107.62	110.33
31	H	306	KC1	C1D-CHD-C4C	-2.61	120.12	126.25
30	A	310	CLA	O2A-CGA-O1A	-2.61	117.11	123.63
37	l	302	BCR	C27-C26-C25	-2.61	119.18	122.70
34	P	202	PID	CM5-C21-C20	-2.61	118.59	122.82
28	M	304	DD6	C21-C20-C15	-2.61	118.01	122.30
30	D	316	CLA	CAA-C2A-C3A	-2.61	110.26	116.23
30	a	721	CLA	CHB-C4A-NA	2.60	128.16	124.40
30	I	316	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
31	A	306	KC1	CHB-C1B-C2B	-2.60	120.07	125.49
28	L	303	DD6	C14-C13-C11	-2.60	121.49	125.53
30	B	312	CLA	CHB-C4A-NA	2.60	128.16	124.40
31	J	313	KC1	C4B-CHC-C1C	-2.60	120.49	126.02
28	M	303	DD6	C24-C1-C2	2.60	123.10	119.01
31	A	314	KC1	C1D-CHD-C4C	-2.60	120.13	126.25
28	A	302	DD6	C3-C4-C5	-2.60	118.19	123.52
28	M	305	DD6	C3-C4-C5	-2.60	118.19	123.52
30	O	314	CLA	CHB-C4A-NA	2.60	128.16	124.40
30	G	513	CLA	CHB-C4A-NA	2.60	128.15	124.40
31	F	309	KC1	C1D-CHD-C4C	-2.60	120.13	126.25
37	m	201	BCR	C33-C5-C4	2.60	119.14	113.60
30	N	310	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	A	314	KC1	O1D-CGD-CBD	-2.60	119.39	124.52
30	M	315	CLA	CHB-C4A-NA	2.60	128.15	124.40
30	A	313	CLA	C1-C2-C3	-2.60	121.94	126.20
28	L	303	DD6	C3-C4-C5	-2.60	118.21	123.52
28	G	502	DD6	O1-C20-C21	-2.60	112.15	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D	315	KC1	C2A-C3A-C4A	2.60	108.36	106.41
30	a	711	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	J	313	KC1	CHB-C1B-C2B	-2.59	120.09	125.49
30	N	305	CLA	CHB-C4A-NA	2.59	128.14	124.40
28	B	306	DD6	C21-C20-C15	-2.59	118.04	122.30
30	b	714	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
34	O	301	PID	CM5-C21-C20	-2.59	118.62	122.82
30	G	519	CLA	CHB-C4A-NA	2.59	128.14	124.40
30	F	313	CLA	C3B-C4B-NB	-2.59	108.22	110.53
28	M	305	DD6	C25-C26-C27	-2.59	119.37	126.61
34	G	506	PID	CM5-C21-C20	-2.59	118.62	122.82
31	P	211	KC1	C1D-CHD-C4C	-2.59	120.16	126.25
31	G	515	KC1	CHC-C4B-C3B	-2.59	120.85	125.21
31	M	307	KC1	CHC-C4B-C3B	-2.59	120.85	125.21
30	F	315	CLA	C3B-C4B-NB	-2.59	108.22	110.53
37	b	730	BCR	C2-C1-C6	2.59	114.20	110.44
28	J	304	DD6	C25-C26-C27	-2.59	119.38	126.61
28	L	306	DD6	C37-C36-C31	-2.59	119.33	124.16
31	D	310	KC1	C4B-CHC-C1C	-2.59	120.52	126.02
28	A	305	DD6	C25-C26-C27	-2.58	119.38	126.61
31	P	211	KC1	CHB-C1B-C2B	-2.58	120.12	125.49
34	G	507	PID	CM5-C21-C20	-2.58	118.63	122.82
30	a	705	CLA	CHB-C4A-NA	2.58	128.12	124.40
30	l	308	CLA	C3B-C4B-NB	-2.58	108.23	110.53
30	J	309	CLA	CHB-C4A-NA	2.58	128.12	124.40
30	I	316	CLA	CHB-C4A-NA	2.58	128.12	124.40
29	P	207	UIX	C18-O2-C27	-2.58	113.29	117.85
30	L	308	CLA	C1-C2-C3	-2.58	122.59	126.76
31	O	310	KC1	O1D-CGD-CBD	-2.58	119.43	124.52
30	M	310	CLA	CHB-C4A-NA	2.58	128.12	124.40
31	J	313	KC1	CHC-C4B-C3B	-2.58	120.86	125.21
37	a	734	BCR	C33-C5-C4	2.58	119.09	113.60
30	b	709	CLA	C1-C2-C3	-2.58	121.97	126.20
30	M	310	CLA	C3B-C4B-NB	-2.58	108.23	110.53
31	L	307	KC1	C1D-CHD-C4C	-2.58	120.19	126.25
31	M	314	KC1	C1D-CHD-C4C	-2.58	120.19	126.25
31	I	314	KC1	C1D-CHD-C4C	-2.58	120.19	126.25
30	A	311	CLA	CHB-C4A-NA	2.58	128.12	124.40
30	b	719	CLA	C3B-C4B-NB	-2.58	108.23	110.53
31	O	315	KC1	C1D-CHD-C4C	-2.57	120.19	126.25
30	F	311	CLA	CHB-C4A-NA	2.57	128.11	124.40
31	L	307	KC1	O2A-CGA-O1A	-2.57	117.46	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	713	CLA	C3B-C4B-NB	-2.57	108.23	110.53
32	I	317	DGD	C2G-O2G-C1B	-2.57	111.64	117.80
28	M	306	DD6	C19-C18-C17	-2.57	105.98	110.79
31	B	314	KC1	O2D-CGD-O1D	-2.57	118.84	123.85
30	K	308	CLA	C3B-C4B-NB	-2.57	108.24	110.53
31	D	310	KC1	C1D-CHD-C4C	-2.57	120.21	126.25
30	L	312	CLA	CHB-C4A-NA	2.57	128.11	124.40
30	G	517	CLA	C3B-C4B-NB	-2.57	108.24	110.53
31	H	310	KC1	C1D-CHD-C4C	-2.57	120.21	126.25
29	O	306	UIX	C18-O2-C27	-2.57	113.31	117.85
30	I	306	CLA	CHB-C4A-NA	2.57	128.10	124.40
34	D	306	PID	CM5-C21-C20	-2.56	118.66	122.82
31	G	515	KC1	O1D-CGD-CBD	-2.56	119.46	124.52
29	G	503	UIX	C37-C39-C40	-2.56	123.68	127.28
28	M	304	DD6	C37-C36-C31	-2.56	119.37	124.16
30	I	319	CLA	CHB-C4A-NA	2.56	128.10	124.40
30	G	510	CLA	C3B-C4B-NB	-2.56	108.24	110.53
30	l	310	CLA	CMB-C2B-C3B	2.56	129.80	124.68
30	b	714	CLA	CHB-C4A-NA	2.56	128.10	124.40
28	K	303	DD6	C21-C20-C15	-2.56	118.08	122.30
30	B	308	CLA	CHB-C4A-NA	2.56	128.10	124.40
31	N	306	KC1	C1D-CHD-C4C	-2.56	120.22	126.25
30	a	715	CLA	CHB-C4A-NA	2.56	128.10	124.40
30	a	730	CLA	CHB-C4A-NA	2.56	128.10	124.40
30	b	701	CLA	CHB-C4A-NA	2.56	128.10	124.40
31	N	311	KC1	C1D-CHD-C4C	-2.56	120.23	126.25
30	D	311	CLA	CHB-C4A-NA	2.56	128.09	124.40
28	L	303	DD6	O1-C15-C14	-2.56	109.54	116.88
32	G	521	DGD	C6E-C5E-C4E	2.56	119.30	113.02
28	N	303	DD6	C14-C13-C11	-2.56	121.56	125.53
32	y	201	DGD	C2G-O2G-C1B	-2.56	111.67	117.80
31	B	314	KC1	C1D-CHD-C4C	-2.56	120.23	126.25
30	K	312	CLA	CHB-C4A-NA	2.56	128.09	124.40
30	J	306	CLA	CHB-C4A-NA	2.56	128.09	124.40
31	F	314	KC1	C1D-CHD-C4C	-2.56	120.24	126.25
34	P	203	PID	CM4-C14-C13	2.56	124.69	119.05
28	B	302	DD6	C8-C6-C5	-2.56	118.81	124.72
34	N	301	PID	CM5-C21-C20	-2.55	118.68	122.82
31	K	314	KC1	C1D-CHD-C4C	-2.55	120.24	126.25
28	M	306	DD6	C21-C20-C15	-2.55	118.10	122.30
30	A	310	CLA	C3B-C4B-NB	-2.55	108.25	110.53
29	B	305	UIX	O2-C27-O4	-2.55	118.07	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	306	DD6	C25-C26-C27	-2.55	119.48	126.61
30	J	307	CLA	C3B-C4B-NB	-2.55	108.25	110.53
31	N	308	KC1	C1D-CHD-C4C	-2.55	120.25	126.25
33	I	318	LMG	O7-C10-O9	-2.55	117.74	123.70
29	I	304	UIX	O2-C27-O4	-2.55	118.07	122.99
28	D	303	DD6	C4-C3-C2	-2.55	118.30	123.52
30	b	716	CLA	CHB-C4A-NA	2.55	128.08	124.40
31	O	310	KC1	C1D-CHD-C4C	-2.55	120.25	126.25
28	K	305	DD6	C9-C10-C11	-2.55	123.71	127.28
28	B	306	DD6	C10-C9-C8	-2.54	115.83	123.20
31	D	315	KC1	O1D-CGD-CBD	-2.54	119.50	124.52
31	M	307	KC1	CHB-C1B-C2B	-2.54	120.20	125.49
28	F	303	DD6	C4-C3-C2	-2.54	118.32	123.52
30	G	518	CLA	CHB-C4A-NA	2.54	128.06	124.40
29	A	304	UIX	C13-C14-C23	-2.54	115.84	123.20
30	j	104	CLA	C1-C2-C3	-2.54	122.04	126.20
30	A	309	CLA	C3B-C4B-NB	-2.54	108.26	110.53
30	l	312	CLA	C3B-C4B-NB	-2.54	108.26	110.53
30	M	315	CLA	C3B-C4B-NB	-2.54	108.26	110.53
30	h	202	CLA	CHB-C4A-NA	2.54	128.06	124.40
30	I	308	CLA	C1-C2-C3	-2.54	122.04	126.20
30	H	307	CLA	CHB-C4A-NA	2.54	128.06	124.40
28	K	304	DD6	O1-C20-C21	-2.54	112.21	115.05
30	a	731	CLA	C1-C2-C3	-2.54	122.04	126.20
38	b	729	PQN	C14-C13-C15	2.54	119.63	115.23
30	G	514	CLA	C3B-C4B-NB	-2.54	108.27	110.53
29	A	304	UIX	C22-C15-C20	-2.54	108.20	110.47
28	h	203	DD6	O1-C15-C14	-2.54	109.61	116.88
28	H	303	DD6	O1-C20-C19	-2.53	111.12	113.49
30	b	714	CLA	C3B-C4B-NB	-2.53	108.27	110.53
28	B	303	DD6	C9-C10-C11	-2.53	123.72	127.28
28	G	504	DD6	O1-C20-C15	-2.53	56.92	58.93
31	O	310	KC1	O2D-CGD-O1D	-2.53	118.92	123.85
30	l	308	CLA	CAA-C2A-C3A	-2.53	110.43	116.23
30	G	517	CLA	CHB-C4A-NA	2.53	128.05	124.40
34	P	208	PID	CM2-C5-C4	-2.53	104.53	108.97
30	A	313	CLA	CHB-C4A-NA	2.53	128.04	124.40
30	K	306	CLA	CHB-C4A-NA	2.52	128.04	124.40
30	a	706	CLA	CHB-C4A-NA	2.52	128.04	124.40
29	O	306	UIX	C36-C38-C40	-2.52	119.44	126.36
30	J	301	CLA	CHB-C4A-NA	2.52	128.04	124.40
30	I	316	CLA	C1-C2-C3	-2.52	122.06	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	I	310	CLA	CHB-C4A-NA	2.52	128.04	124.40
30	I	313	CLA	CHB-C4A-NA	2.52	128.04	124.40
31	G	515	KC1	C2A-C3A-C4A	2.52	108.31	106.41
37	f	304	BCR	C29-C30-C25	2.52	114.10	110.44
30	A	310	CLA	CHB-C4A-NA	2.52	128.04	124.40
30	B	313	CLA	CHB-C4A-NA	2.52	128.04	124.40
34	D	304	PID	CM5-C21-C20	-2.52	118.73	122.82
31	O	312	KC1	C1D-CHD-C4C	-2.52	120.32	126.25
30	F	311	CLA	O2D-CGD-CBD	2.52	115.63	111.23
31	H	306	KC1	C2A-C3A-C4A	2.52	108.30	106.41
31	O	310	KC1	C2A-C3A-C4A	2.52	108.30	106.41
31	O	312	KC1	C4B-CHC-C1C	-2.52	120.67	126.02
37	a	734	BCR	C29-C30-C25	2.52	114.10	110.44
30	B	313	CLA	C3B-C4B-NB	-2.52	108.28	110.53
28	M	304	DD6	C10-C9-C8	-2.52	115.90	123.20
31	H	310	KC1	C4B-CHC-C1C	-2.52	120.67	126.02
30	a	710	CLA	C1-C2-C3	-2.52	122.07	126.20
28	G	505	DD6	C32-C33-C34	-2.52	108.07	113.59
30	B	309	CLA	CHB-C4A-NA	2.52	128.03	124.40
34	M	301	PID	C19-C20-C21	2.52	130.81	127.28
28	I	302	DD6	C37-C36-C31	-2.51	119.46	124.16
37	l	307	BCR	C21-C20-C19	-2.51	115.91	123.20
28	L	306	DD6	O1-C20-C21	-2.51	112.24	115.05
28	A	302	DD6	C37-C36-C31	-2.51	119.46	124.16
30	P	210	CLA	CHB-C4A-NA	2.51	128.03	124.40
31	P	216	KC1	C1D-CHD-C4C	-2.51	120.34	126.25
28	L	305	DD6	C37-C36-C31	-2.51	119.46	124.16
29	A	304	UIX	O2-C27-O4	-2.51	118.14	122.99
34	j	105	PID	C8-C9-C10	2.51	128.52	123.60
30	F	315	CLA	CHB-C4A-NA	2.51	128.03	124.40
30	K	313	CLA	CHB-C4A-NA	2.51	128.02	124.40
30	A	315	CLA	CHB-C4A-NA	2.51	128.02	124.40
30	b	727	CLA	CHB-C4A-NA	2.51	128.02	124.40
31	P	213	KC1	O1D-CGD-CBD	-2.51	119.57	124.52
34	P	206	PID	O1-C6-C7	-2.51	109.69	116.88
31	M	307	KC1	C4B-CHC-C1C	-2.51	120.69	126.02
30	G	511	CLA	C3B-C4B-NB	-2.51	108.29	110.53
30	b	718	CLA	CHB-C4A-NA	2.51	128.02	124.40
31	J	313	KC1	C1D-CHD-C4C	-2.51	120.35	126.25
30	b	704	CLA	CAC-C3C-C4C	2.51	128.05	124.79
30	b	709	CLA	CHB-C4A-NA	2.51	128.02	124.40
34	O	302	PID	CM5-C21-C20	-2.51	118.76	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	301	CLA	CHB-C4A-NA	2.50	128.01	124.40
37	a	736	BCR	C24-C23-C22	-2.50	122.53	126.23
30	l	309	CLA	CHB-C4A-NA	2.50	128.01	124.40
30	L	316	CLA	CHB-C4A-NA	2.50	128.01	124.40
34	O	305	PID	CM5-C21-C20	-2.50	118.76	122.82
30	a	714	CLA	C3B-C4B-NB	-2.50	108.30	110.53
30	b	718	CLA	C3B-C4B-NB	-2.50	108.30	110.53
28	M	303	DD6	C37-C36-C35	2.50	119.02	114.42
37	m	201	BCR	C38-C26-C27	2.50	118.93	113.60
37	l	307	BCR	C28-C27-C26	-2.50	109.60	114.06
31	A	306	KC1	C1D-CHD-C4C	-2.50	120.37	126.25
30	L	317	CLA	CHB-C4A-NA	2.50	128.01	124.40
28	N	303	DD6	C4-C3-C2	-2.50	118.41	123.52
30	b	712	CLA	CHB-C4A-NA	2.50	128.01	124.40
31	L	315	KC1	O2D-CGD-O1D	-2.50	118.98	123.85
30	G	519	CLA	C3B-C4B-NB	-2.50	108.30	110.53
31	O	312	KC1	CHB-C1B-C2B	-2.50	120.29	125.49
30	H	309	CLA	CHB-C4A-NA	2.50	128.00	124.40
37	j	102	BCR	C10-C11-C12	-2.50	115.97	123.20
30	N	304	CLA	CHB-C4A-NA	2.50	128.00	124.40
31	F	309	KC1	O1D-CGD-CBD	-2.50	119.60	124.52
30	A	316	CLA	CHB-C4A-NA	2.50	128.00	124.40
30	a	711	CLA	CHB-C4A-NA	2.50	128.00	124.40
30	F	308	CLA	CHB-C4A-NA	2.50	128.00	124.40
30	O	311	CLA	CHB-C4A-NA	2.49	128.00	124.40
30	D	314	CLA	CAA-C2A-C3A	-2.49	106.26	113.00
28	N	303	DD6	C21-C20-C15	-2.49	118.20	122.30
30	A	317	CLA	CHB-C4A-NA	2.49	128.00	124.40
28	M	302	DD6	C9-C10-C11	-2.49	123.78	127.28
30	M	308	CLA	CHB-C4A-NA	2.49	128.00	124.40
34	N	302	PID	CM4-C14-C13	2.49	124.55	119.05
30	B	315	CLA	CHB-C4A-NA	2.49	128.00	124.40
37	f	304	BCR	C11-C12-C13	-2.49	119.53	126.36
30	K	309	CLA	C1-C2-C3	-2.49	122.73	126.76
30	G	520	CLA	C3B-C4B-NB	-2.49	108.31	110.53
30	P	212	CLA	CHB-C4A-NA	2.49	127.99	124.40
31	F	314	KC1	C4B-CHC-C1C	-2.49	120.73	126.02
31	O	315	KC1	O2D-CGD-O1D	-2.49	119.00	123.85
30	G	509	CLA	CHB-C4A-NA	2.49	127.99	124.40
30	a	731	CLA	CHB-C4A-NA	2.49	127.99	124.40
30	a	738	CLA	CHB-C4A-NA	2.49	127.99	124.40
30	b	704	CLA	CHB-C4A-NA	2.49	127.99	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	M	305	DD6	C37-C36-C31	-2.49	119.51	124.16
28	G	502	DD6	C37-C36-C31	-2.49	119.51	124.16
30	J	315	CLA	CHB-C4A-NA	2.49	127.99	124.40
32	j	103	DGD	O1G-C1A-C2A	2.49	119.42	111.83
30	F	308	CLA	C3B-C4B-NB	-2.49	108.31	110.53
28	K	301	DD6	C10-C9-C8	-2.49	115.99	123.20
33	b	733	LMG	C1-C2-C3	-2.49	104.78	110.01
30	a	720	CLA	C3B-C4B-NB	-2.49	108.31	110.53
34	P	206	PID	C15-C14-C13	2.49	123.19	116.80
30	b	712	CLA	CMB-C2B-C3B	2.49	130.14	123.53
30	D	309	CLA	C3B-C4B-NB	-2.48	108.31	110.53
30	J	306	CLA	C3B-C4B-NB	-2.48	108.31	110.53
28	M	304	DD6	O1-C20-C21	-2.48	112.27	115.05
28	J	304	DD6	C28-C27-C26	-2.48	119.36	124.18
34	P	206	PID	C7-C8-C9	-2.48	122.93	126.06
30	K	309	CLA	CHB-C4A-NA	2.48	127.98	124.40
30	b	705	CLA	CHB-C4A-NA	2.48	127.98	124.40
34	D	302	PID	CM5-C21-C20	-2.48	118.79	122.82
30	a	720	CLA	CHB-C4A-NA	2.48	127.98	124.40
31	K	314	KC1	C4B-CHC-C1C	-2.48	120.74	126.02
28	I	302	DD6	C3-C4-C5	-2.48	118.44	123.52
30	K	311	CLA	C3B-C4B-NB	-2.48	108.31	110.53
31	A	306	KC1	C4B-CHC-C1C	-2.48	120.75	126.02
30	b	710	CLA	C3B-C4B-NB	-2.48	108.32	110.53
30	I	309	CLA	CHB-C4A-NA	2.48	127.98	124.40
30	J	316	CLA	CHB-C4A-NA	2.48	127.98	124.40
30	M	313	CLA	CHB-C4A-NA	2.48	127.98	124.40
37	a	734	BCR	C15-C16-C17	-2.48	118.45	123.52
30	A	309	CLA	CHB-C4A-NA	2.48	127.98	124.40
30	G	511	CLA	CHB-C4A-NA	2.48	127.98	124.40
30	I	321	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
28	M	302	DD6	C10-C9-C8	-2.48	116.02	123.20
30	F	307	CLA	CHB-C4A-NA	2.48	127.97	124.40
30	I	313	CLA	C3B-C4B-NB	-2.48	108.32	110.53
30	L	313	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
30	G	509	CLA	C3B-C4B-NB	-2.47	108.32	110.53
30	b	719	CLA	CHB-C4A-NA	2.47	127.97	124.40
28	G	505	DD6	O1-C20-C19	2.47	115.81	113.49
30	a	708	CLA	CHB-C4A-NA	2.47	127.97	124.40
28	O	303	DD6	C37-C36-C31	-2.47	119.54	124.16
28	N	303	DD6	C37-C36-C35	2.47	118.97	114.42
30	b	728	CLA	CHB-C4A-NA	2.47	127.97	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	P	213	KC1	CHB-C1B-C2B	-2.47	120.35	125.49
31	G	515	KC1	C4B-CHC-C1C	-2.47	120.77	126.02
30	K	313	CLA	C3B-C4B-NB	-2.47	108.33	110.53
28	A	301	DD6	O1-C20-C21	-2.47	112.29	115.05
30	O	308	CLA	CHB-C4A-NA	2.47	127.96	124.40
28	L	306	DD6	C21-C20-C15	-2.47	118.24	122.30
30	A	307	CLA	CHB-C4A-NA	2.47	127.96	124.40
30	A	308	CLA	CHB-C4A-NA	2.47	127.96	124.40
30	a	714	CLA	CHB-C4A-NA	2.47	127.96	124.40
30	D	309	CLA	CHB-C4A-NA	2.47	127.96	124.40
30	G	513	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
28	M	304	DD6	C9-C10-C11	-2.47	123.82	127.28
30	K	308	CLA	CHB-C4A-NA	2.47	127.96	124.40
31	M	307	KC1	O2A-CGA-O1A	-2.47	117.68	122.70
31	I	314	KC1	C4B-CHC-C1C	-2.46	120.78	126.02
30	l	305	CLA	C3B-C4B-NB	-2.46	108.33	110.53
30	O	309	CLA	CHB-C4A-NA	2.46	127.96	124.40
28	b	731	DD6	C10-C9-C8	-2.46	116.06	123.20
30	G	516	CLA	CHB-C4A-NA	2.46	127.95	124.40
30	J	311	CLA	CHB-C4A-NA	2.46	127.95	124.40
37	i	201	BCR	C28-C27-C26	-2.46	109.66	114.06
28	L	302	DD6	O1-C20-C19	-2.46	111.18	113.49
30	b	709	CLA	O2D-CGD-CBD	2.46	115.53	111.23
30	H	312	CLA	CHB-C4A-NA	2.46	127.95	124.40
29	G	503	UIX	C13-C14-C23	-2.46	116.07	123.20
28	h	203	DD6	C3-C4-C5	-2.46	118.49	123.52
30	F	307	CLA	C3B-C4B-NB	-2.46	108.33	110.53
31	P	211	KC1	C4B-CHC-C1C	-2.46	120.80	126.02
30	D	312	CLA	CHB-C4A-NA	2.46	127.95	124.40
28	I	303	DD6	C12-C11-C10	-2.46	118.83	122.82
30	M	316	CLA	CHB-C4A-NA	2.46	127.94	124.40
29	A	304	UIX	C34-C37-C39	-2.46	118.50	123.52
31	L	307	KC1	O2D-CGD-O1D	-2.46	119.07	123.85
30	b	708	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	a	706	CLA	C3B-C4B-NB	-2.45	108.34	110.53
30	b	721	CLA	C3B-C4B-NB	-2.45	108.34	110.53
28	A	303	DD6	C37-C36-C31	-2.45	119.57	124.16
31	N	311	KC1	C4B-CHC-C1C	-2.45	120.80	126.02
28	K	318	DD6	C37-C36-C31	-2.45	119.57	124.16
34	O	302	PID	C17-C16-C15	2.45	128.54	123.52
30	j	104	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	a	709	CLA	CHB-C4A-NA	2.45	127.94	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	h	201	UIX	O2-C27-O4	-2.45	118.26	122.99
30	a	724	CLA	C3B-C4B-NB	-2.45	108.34	110.53
30	B	307	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	J	311	CLA	C3B-C4B-NB	-2.45	108.34	110.53
30	f	303	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	J	308	CLA	CHB-C4A-NA	2.45	127.94	124.40
31	N	308	KC1	CGD-CBD-CAD	-2.45	102.92	110.85
28	K	304	DD6	C32-C33-C34	-2.45	108.22	113.59
37	l	306	BCR	C35-C13-C12	2.45	121.83	118.09
28	I	301	DD6	C28-C27-C26	-2.45	119.43	124.18
28	A	301	DD6	C37-C36-C31	-2.45	119.58	124.16
28	I	303	DD6	C19-C18-C17	-2.45	106.21	110.79
30	b	715	CLA	CHB-C4A-NA	2.45	127.93	124.40
31	F	314	KC1	O1D-CGD-CBD	-2.45	119.69	124.52
28	O	303	DD6	C14-C13-C11	-2.45	121.73	125.53
31	N	311	KC1	O1D-CGD-CBD	-2.45	119.69	124.52
30	L	314	CLA	CHB-C4A-NA	2.45	127.93	124.40
30	M	311	CLA	CHB-C4A-NA	2.45	127.93	124.40
30	a	727	CLA	CHB-C4A-NA	2.45	127.93	124.40
28	L	305	DD6	C37-C36-C35	2.45	118.92	114.42
28	P	204	DD6	C21-C20-C15	-2.44	118.28	122.30
31	A	314	KC1	C4B-CHC-C1C	-2.44	120.83	126.02
28	I	305	DD6	C37-C36-C31	-2.44	119.59	124.16
32	G	521	DGD	C1D-O6D-C5D	-2.44	108.95	113.72
29	h	201	UIX	C12-C11-C10	2.44	121.82	118.09
30	H	305	CLA	CHB-C4A-NA	2.44	127.92	124.40
28	M	303	DD6	C12-C11-C10	-2.44	118.86	122.82
34	H	302	PID	CM5-C21-C20	-2.44	118.86	122.82
30	D	316	CLA	CHB-C4A-NA	2.44	127.92	124.40
30	H	308	CLA	CHB-C4A-NA	2.44	127.92	124.40
28	G	504	DD6	C28-C27-C26	-2.44	119.44	124.18
28	H	303	DD6	C37-C36-C31	-2.44	119.60	124.16
28	I	305	DD6	C-C1-C2	-2.44	118.86	122.82
30	K	315	CLA	C3B-C4B-NB	-2.44	108.35	110.53
30	b	707	CLA	C3B-C4B-NB	-2.44	108.35	110.53
30	J	314	CLA	CHB-C4A-NA	2.44	127.92	124.40
37	a	736	BCR	C33-C5-C4	2.44	118.79	113.60
31	P	213	KC1	CAC-C3C-C4C	2.44	127.96	124.79
37	l	306	BCR	C10-C11-C12	-2.44	116.14	123.20
30	f	302	CLA	C3B-C4B-NB	-2.43	108.36	110.53
29	O	306	UIX	C12-C11-C13	-2.43	118.87	122.82
30	L	309	CLA	CHB-C4A-NA	2.43	127.91	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	728	CLA	CHB-C4A-NA	2.43	127.91	124.40
28	G	504	DD6	C25-C24-C1	-2.43	119.69	126.36
28	A	305	DD6	C21-C20-C15	-2.43	118.30	122.30
28	G	502	DD6	C37-C36-C35	2.43	118.89	114.42
31	O	315	KC1	C4B-CHC-C1C	-2.43	120.85	126.02
30	b	722	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
31	L	307	KC1	C4B-CHC-C1C	-2.43	120.85	126.02
28	L	302	DD6	C37-C36-C31	-2.43	119.62	124.16
31	F	314	KC1	O2D-CGD-O1D	-2.43	119.12	123.85
37	b	732	BCR	C38-C26-C25	-2.43	121.83	124.48
30	a	723	CLA	C3B-C4B-NB	-2.43	108.36	110.53
30	b	724	CLA	CHB-C4A-NA	2.43	127.90	124.40
30	a	735	CLA	C1-C2-C3	-2.43	122.22	126.20
30	B	309	CLA	C3B-C4B-NB	-2.43	108.36	110.53
30	a	712	CLA	CHB-C4A-NA	2.43	127.90	124.40
30	b	728	CLA	C1-C2-C3	-2.43	122.22	126.20
29	h	201	UIX	C35-C36-C38	-2.43	116.17	123.20
30	l	303	CLA	CHB-C4A-NA	2.43	127.90	124.40
31	L	315	KC1	C4B-CHC-C1C	-2.43	120.86	126.02
30	a	707	CLA	CHB-C4A-NA	2.43	127.90	124.40
34	O	307	PID	CM5-C21-C20	-2.43	118.89	122.82
30	I	307	CLA	CHB-C4A-NA	2.42	127.90	124.40
30	K	310	CLA	CHB-C4A-NA	2.42	127.90	124.40
31	N	306	KC1	C4B-CHC-C1C	-2.42	120.87	126.02
28	G	504	DD6	O1-C15-C14	-2.42	109.94	116.88
34	O	302	PID	CM4-C14-C13	2.42	124.39	119.05
37	a	734	BCR	C21-C20-C19	-2.42	116.19	123.20
30	H	311	CLA	CAA-C2A-C3A	-2.42	110.68	116.23
37	l	302	BCR	C37-C22-C21	-2.42	118.90	122.82
30	b	711	CLA	CHB-C4A-NA	2.42	127.89	124.40
28	N	303	DD6	C25-C26-C27	-2.42	119.85	126.61
30	K	311	CLA	CHB-C4A-NA	2.42	127.89	124.40
30	L	310	CLA	CHB-C4A-NA	2.42	127.89	124.40
28	L	306	DD6	C28-C27-C26	-2.42	119.49	124.18
28	A	302	DD6	C25-C26-C27	-2.42	119.86	126.61
29	P	207	UIX	C22-C15-C20	-2.41	108.31	110.47
29	P	207	UIX	C16-C20-C15	2.41	122.09	119.70
31	I	314	KC1	O2D-CGD-O1D	-2.41	119.15	123.85
29	I	304	UIX	C41-C40-C38	2.41	121.77	118.09
28	A	302	DD6	O1-C20-C21	-2.41	112.35	115.05
37	m	201	BCR	C36-C18-C19	2.41	121.77	118.09
30	b	726	CLA	CHB-C4A-NA	2.41	127.88	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	303	DD6	C10-C9-C8	-2.41	116.22	123.20
31	M	307	KC1	C2A-C3A-C4A	2.41	108.22	106.41
28	G	508	DD6	C37-C36-C35	2.41	118.85	114.42
31	D	310	KC1	O1D-CGD-CBD	-2.41	119.77	124.52
31	L	315	KC1	C2A-C3A-C4A	2.41	108.22	106.41
28	h	203	DD6	C10-C9-C8	-2.41	116.22	123.20
34	D	305	PID	C18-C17-C16	2.41	130.29	124.72
34	j	105	PID	CM5-C21-C20	-2.41	118.91	122.82
28	K	301	DD6	C4-C3-C2	-2.41	118.59	123.52
30	K	316	CLA	CHB-C4A-NA	2.41	127.87	124.40
30	K	307	CLA	CHB-C4A-NA	2.41	127.87	124.40
37	b	730	BCR	C36-C18-C19	2.41	121.76	118.09
29	P	207	UIX	O2-C27-O4	-2.41	118.35	122.99
37	a	736	BCR	C21-C20-C19	-2.41	116.23	123.20
30	J	312	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
30	A	320	CLA	CHB-C4A-NA	2.41	127.87	124.40
30	b	712	CLA	CAB-C3B-C2B	2.40	129.92	123.53
30	l	303	CLA	C3B-C4B-NB	-2.40	108.38	110.53
30	I	308	CLA	CHB-C4A-NA	2.40	127.87	124.40
28	F	303	DD6	C21-C20-C15	-2.40	118.35	122.30
30	a	725	CLA	CHB-C4A-NA	2.40	127.87	124.40
34	D	305	PID	CM4-C14-C13	2.40	124.35	119.05
28	B	303	DD6	C3-C4-C5	-2.40	118.61	123.52
30	l	308	CLA	CHB-C4A-NA	2.40	127.86	124.40
30	N	309	CLA	CHB-C4A-NA	2.40	127.86	124.40
34	P	206	PID	C6-C7-C8	2.40	131.06	125.99
31	L	315	KC1	C1D-CHD-C4C	-2.40	120.61	126.25
30	I	321	CLA	C1-C2-C3	-2.40	122.27	126.20
30	a	710	CLA	CHB-C4A-NA	2.40	127.86	124.40
28	B	306	DD6	O1-C20-C21	-2.39	112.37	115.05
30	a	703	CLA	CHB-C4A-NA	2.39	127.86	124.40
34	H	302	PID	C8-C9-C10	2.39	128.29	123.60
28	B	306	DD6	C25-C24-C1	-2.39	119.80	126.36
31	N	306	KC1	O2D-CGD-O1D	-2.39	119.19	123.85
30	O	316	CLA	CHB-C4A-NA	2.39	127.85	124.40
30	a	713	CLA	C1-C2-C3	-2.39	122.28	126.20
30	K	315	CLA	CHB-C4A-NA	2.39	127.85	124.40
30	a	717	CLA	C3B-C4B-NB	-2.39	108.40	110.53
31	P	216	KC1	C4B-CHC-C1C	-2.39	120.94	126.02
34	P	206	PID	CM5-C21-C20	-2.39	118.95	122.82
30	a	722	CLA	CHB-C4A-NA	2.39	127.85	124.40
30	b	713	CLA	CHB-C4A-NA	2.39	127.84	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	301	CLA	C3B-C4B-NB	-2.39	108.40	110.53
34	D	302	PID	CM4-C14-C13	2.39	124.32	119.05
30	m	202	CLA	CHB-C4A-NA	2.39	127.84	124.40
37	b	702	BCR	C35-C13-C12	2.39	121.73	118.09
31	G	515	KC1	CAC-C3C-C4C	2.39	127.89	124.79
30	H	304	CLA	CHB-C4A-NA	2.39	127.84	124.40
28	J	304	DD6	C-C1-C2	-2.39	118.95	122.82
29	O	306	UIX	C10-C11-C13	2.38	122.76	119.01
34	O	304	PID	C7-C8-C9	2.38	129.06	126.06
28	b	731	DD6	C37-C36-C31	-2.38	119.70	124.16
28	B	306	DD6	C37-C36-C35	2.38	118.80	114.42
30	G	512	CLA	CHB-C4A-NA	2.38	127.84	124.40
29	O	306	UIX	O2-C27-O4	-2.38	118.39	122.99
28	I	302	DD6	C7-C6-C5	-2.38	118.96	122.82
30	M	312	CLA	CHB-C4A-NA	2.38	127.84	124.40
28	G	505	DD6	C25-C26-C27	-2.38	119.95	126.61
30	a	725	CLA	C1-C2-C3	-2.38	122.30	126.20
30	a	728	CLA	C1-C2-C3	-2.38	122.30	126.20
28	K	305	DD6	C37-C36-C31	-2.38	119.71	124.16
28	B	306	DD6	C28-C27-C26	-2.38	119.56	124.18
28	L	303	DD6	O1-C20-C19	-2.38	111.26	113.49
30	I	315	CLA	CHB-C4A-NA	2.38	127.83	124.40
31	O	310	KC1	C4B-CHC-C1C	-2.38	120.97	126.02
30	J	309	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
28	M	303	DD6	C13-C11-C10	2.38	122.75	119.01
30	M	315	CLA	O2D-CGD-CBD	2.38	115.39	111.23
37	a	736	BCR	C23-C24-C25	-2.38	120.65	127.00
30	L	309	CLA	O2D-CGD-CBD	2.38	115.38	111.23
30	A	308	CLA	C3B-C4B-NB	-2.37	108.41	110.53
33	B	318	LMG	O7-C10-O9	-2.37	118.15	123.70
28	B	302	DD6	C8-C9-C10	-2.37	118.66	123.52
31	H	306	KC1	C4B-CHC-C1C	-2.37	120.97	126.02
28	J	304	DD6	C12-C11-C10	-2.37	118.97	122.82
30	a	717	CLA	C1-C2-C3	-2.37	122.31	126.20
30	O	313	CLA	CHB-C4A-NA	2.37	127.82	124.40
30	l	305	CLA	CHB-C4A-NA	2.37	127.82	124.40
34	D	305	PID	O1-C6-C7	-2.37	110.09	116.88
28	J	302	DD6	C25-C26-C27	-2.37	119.98	126.61
30	I	311	CLA	CHB-C4A-NA	2.37	127.81	124.40
30	I	316	CLA	C3B-C4B-NB	-2.36	108.42	110.53
30	M	318	CLA	CHB-C4A-NA	2.36	127.81	124.40
30	H	311	CLA	C3B-C4B-NB	-2.36	108.42	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	508	DD6	C37-C36-C31	-2.36	119.74	124.16
28	G	505	DD6	C19-C18-C17	-2.36	106.37	110.79
30	G	520	CLA	CHB-C4A-NA	2.36	127.81	124.40
30	a	717	CLA	CHB-C4A-NA	2.36	127.81	124.40
30	b	706	CLA	CHB-C4A-NA	2.36	127.81	124.40
31	B	314	KC1	C4B-CHC-C1C	-2.36	121.00	126.02
28	M	303	DD6	C21-C20-C19	2.36	116.89	114.24
31	O	312	KC1	C1A-C2A-C3A	-2.36	105.11	107.28
30	b	703	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
31	K	314	KC1	C2A-C3A-C4A	2.36	108.18	106.41
30	K	307	CLA	C3B-C4B-NB	-2.36	108.42	110.53
28	B	303	DD6	C21-C20-C15	-2.36	118.42	122.30
30	a	723	CLA	CHB-C4A-NA	2.36	127.80	124.40
30	b	720	CLA	CHB-C4A-NA	2.36	127.80	124.40
31	O	312	KC1	C2A-C3A-C4A	2.36	108.18	106.41
28	G	504	DD6	C-C1-C2	-2.36	119.00	122.82
30	A	312	CLA	CHB-C4A-NA	2.36	127.80	124.40
30	f	302	CLA	CHB-C4A-NA	2.35	127.80	124.40
30	J	311	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
28	M	305	DD6	C37-C36-C35	2.35	118.75	114.42
30	b	725	CLA	CHB-C4A-NA	2.35	127.79	124.40
30	P	217	CLA	CHB-C4A-NA	2.35	127.79	124.40
28	I	301	DD6	C14-C13-C11	-2.35	121.89	125.53
31	P	216	KC1	O1D-CGD-CBD	-2.35	119.89	124.52
28	h	203	DD6	C14-C13-C11	-2.35	121.89	125.53
30	D	313	CLA	CHB-C4A-NA	2.35	127.79	124.40
33	b	733	LMG	C38-C37-C36	-2.35	102.50	114.37
31	M	314	KC1	C4B-CHC-C1C	-2.35	121.03	126.02
30	I	316	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
30	F	310	CLA	O2D-CGD-CBD	2.35	115.33	111.23
28	F	303	DD6	C41-C32-C31	-2.34	106.32	110.52
28	G	504	DD6	C25-C26-C27	-2.34	120.05	126.61
28	M	305	DD6	C10-C9-C8	-2.34	116.41	123.20
28	M	305	DD6	O1-C15-C14	-2.34	110.16	116.88
30	M	309	CLA	CHB-C4A-NA	2.34	127.78	124.40
30	b	723	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
37	l	306	BCR	C21-C20-C19	-2.34	116.41	123.20
28	M	303	DD6	C37-C36-C31	-2.34	119.78	124.16
31	M	314	KC1	O1D-CGD-CBD	-2.34	119.90	124.52
33	I	320	LMG	O1-C7-C8	-2.34	105.12	110.82
30	a	702	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
30	B	316	CLA	CHB-C4A-NA	2.34	127.78	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	732	BCR	C34-C9-C8	2.34	121.66	118.09
34	O	305	PID	C15-C14-C13	2.34	122.81	116.80
30	G	513	CLA	C3B-C4B-NB	-2.34	108.44	110.53
30	b	708	CLA	C1-C2-C3	-2.34	122.37	126.20
30	N	307	CLA	C3B-C4B-NB	-2.34	108.44	110.53
30	I	311	CLA	O2D-CGD-CBD	2.34	115.31	111.23
30	I	313	CLA	O2A-CGA-O1A	-2.34	117.79	123.63
38	a	732	PQN	C2M-C2-C3	-2.34	120.61	124.45
30	j	106	CLA	C1-C2-C3	-2.33	122.37	126.20
31	A	306	KC1	O1D-CGD-CBD	-2.33	119.92	124.52
28	N	303	DD6	C37-C36-C31	-2.33	119.80	124.16
29	A	304	UIX	C-C7-C10	-2.33	121.06	125.99
31	J	313	KC1	O1D-CGD-CBD	-2.33	119.92	124.52
28	I	302	DD6	C4-C5-C6	-2.33	124.01	127.28
28	A	301	DD6	C37-C36-C35	2.33	118.71	114.42
29	I	304	UIX	C34-C30-C26	-2.33	124.01	127.28
30	G	510	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
30	N	305	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
30	b	707	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
28	A	301	DD6	C3-C4-C5	-2.33	118.75	123.52
30	j	106	CLA	CHB-C4A-NA	2.33	127.76	124.40
30	l	304	CLA	C3B-C4B-NB	-2.33	108.45	110.53
28	A	302	DD6	C9-C8-C6	-2.33	119.98	126.36
34	O	304	PID	O1-C6-C7	-2.33	110.21	116.88
30	K	313	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
28	K	301	DD6	C37-C36-C35	2.33	118.70	114.42
28	h	203	DD6	C37-C36-C31	-2.32	119.81	124.16
37	b	730	BCR	C30-C25-C26	-2.32	119.46	122.64
30	a	717	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
28	F	301	DD6	O1-C15-C14	-2.32	110.22	116.88
30	b	706	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
30	I	315	CLA	O2D-CGD-CBD	2.32	115.29	111.23
30	G	514	CLA	C1-C2-C3	-2.32	122.39	126.20
33	I	320	LMG	O7-C10-O9	-2.32	118.28	123.70
30	G	512	CLA	C3B-C4B-NB	-2.32	108.46	110.53
28	G	505	DD6	C28-C27-C26	-2.32	119.68	124.18
28	J	303	DD6	C37-C36-C35	2.32	118.68	114.42
28	L	306	DD6	C9-C8-C6	-2.32	120.01	126.36
29	P	207	UIX	C12-C11-C13	-2.32	119.06	122.82
34	H	301	PID	CM5-C21-C20	-2.32	119.06	122.82
28	P	204	DD6	C9-C8-C6	-2.31	120.02	126.36
30	a	735	CLA	C3B-C4B-NB	-2.31	108.46	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	K	304	DD6	C37-C36-C31	-2.31	119.83	124.16
30	L	313	CLA	CHB-C4A-NA	2.31	127.74	124.40
33	B	318	LMG	C38-C37-C36	-2.31	102.68	114.37
28	K	305	DD6	C28-C27-C26	-2.31	119.69	124.18
30	L	308	CLA	CHB-C4A-NA	2.31	127.74	124.40
30	m	202	CLA	CMB-C2B-C3B	2.31	131.98	126.55
30	a	724	CLA	CHB-C4A-NA	2.31	127.73	124.40
34	O	305	PID	O4-C12-C11	-2.31	106.07	107.39
37	b	730	BCR	C38-C26-C27	2.31	118.52	113.60
30	L	309	CLA	C3B-C4B-NB	-2.31	108.47	110.53
29	K	302	UIX	O2-C27-O4	-2.31	118.53	122.99
30	l	312	CLA	CHB-C4A-NA	2.31	127.73	124.40
31	P	211	KC1	C2A-C3A-C4A	2.31	108.14	106.41
28	M	302	DD6	C37-C36-C35	2.31	118.66	114.42
28	B	302	DD6	C4-C3-C2	-2.31	118.80	123.52
31	H	306	KC1	O2D-CGD-O1D	-2.31	119.36	123.85
31	P	213	KC1	C1D-CHD-C4C	-2.30	120.83	126.25
30	j	106	CLA	C3B-C4B-NB	-2.30	108.47	110.53
28	N	303	DD6	C9-C8-C6	-2.30	120.05	126.36
30	L	309	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
33	K	317	LMG	O1-C1-C2	-2.30	104.78	108.27
37	b	732	BCR	C37-C22-C23	2.30	121.60	118.09
28	K	303	DD6	C37-C36-C31	-2.30	119.86	124.16
28	I	303	DD6	C28-C27-C26	-2.30	119.71	124.18
30	D	308	CLA	CHB-C4A-NA	2.30	127.72	124.40
30	P	210	CLA	C3B-C4B-NB	-2.30	108.48	110.53
34	N	302	PID	C8-C9-C10	2.30	128.10	123.60
28	B	306	DD6	O1-C20-C19	-2.30	111.34	113.49
28	A	303	DD6	C26-C25-C24	-2.30	116.54	123.20
30	I	312	CLA	CHB-C4A-NA	2.30	127.72	124.40
30	a	705	CLA	CAA-CBA-CGA	-2.30	106.68	113.21
28	O	303	DD6	C9-C8-C6	-2.30	120.06	126.36
37	l	307	BCR	C8-C7-C6	-2.30	120.86	127.00
34	N	301	PID	C15-C14-C13	2.30	122.70	116.80
30	a	730	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
30	B	310	CLA	O2D-CGD-CBD	2.30	115.24	111.23
30	a	711	CLA	CMB-C2B-C1B	-2.29	121.92	125.42
30	F	312	CLA	O2D-CGD-O1D	-2.29	119.38	123.85
28	J	303	DD6	C-C1-C2	-2.29	119.10	122.82
30	b	727	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
31	G	515	KC1	C1D-CHD-C4C	-2.29	120.85	126.25
34	M	301	PID	C7-C8-C9	-2.29	123.17	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	319	CLA	CHB-C4A-NA	2.29	127.71	124.40
29	O	306	UIX	C3-C5-C4	-2.29	106.50	110.79
37	b	730	BCR	C24-C23-C22	-2.29	122.84	126.23
28	A	301	DD6	O1-C15-C14	-2.29	110.31	116.88
30	L	308	CLA	CAC-C3C-C4C	2.29	127.77	124.79
28	B	303	DD6	C26-C25-C24	-2.29	116.57	123.20
38	a	732	PQN	C12-C11-C3	-2.29	106.44	112.08
29	A	304	UIX	C7-C10-C11	-2.29	121.98	125.53
30	b	706	CLA	C3B-C4B-NB	-2.29	108.49	110.53
33	D	317	LMG	O1-C7-C8	-2.29	105.26	110.82
30	a	729	CLA	C1-C2-C3	-2.29	122.45	126.20
28	B	304	DD6	C3-C4-C5	-2.29	118.84	123.52
28	K	318	DD6	C9-C8-C6	-2.29	120.10	126.36
31	M	314	KC1	C2A-C3A-C4A	2.29	108.13	106.41
29	J	305	UIX	C18-O2-C27	-2.28	113.81	117.85
34	O	304	PID	CM5-C21-C20	-2.28	119.12	122.82
32	y	201	DGD	O1G-C1A-C2A	2.28	118.80	111.83
30	H	311	CLA	CHB-C4A-NA	2.28	127.69	124.40
28	B	304	DD6	C37-C36-C35	2.28	118.62	114.42
30	B	310	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
29	G	503	UIX	C12-C11-C10	2.28	121.57	118.09
30	b	717	CLA	CHB-C4A-NA	2.28	127.69	124.40
28	b	731	DD6	C21-C20-C15	-2.28	118.55	122.30
29	G	503	UIX	O2-C27-O4	-2.28	118.59	122.99
28	F	301	DD6	C4-C3-C2	-2.28	118.85	123.52
30	P	210	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
28	A	303	DD6	C4-C3-C2	-2.28	118.86	123.52
33	P	201	LMG	O7-C10-O9	-2.28	118.38	123.70
30	a	729	CLA	CHB-C4A-NA	2.28	127.69	124.40
30	P	209	CLA	CHB-C4A-NA	2.28	127.69	124.40
30	L	314	CLA	C1-C2-C3	-2.28	122.47	126.20
34	j	105	PID	O1-C6-C7	-2.28	110.36	116.88
28	L	305	DD6	C28-C27-C26	-2.28	119.76	124.18
31	D	315	KC1	CAB-C3B-C4B	2.28	130.25	124.82
37	b	730	BCR	C37-C22-C23	2.27	121.56	118.09
37	b	732	BCR	C35-C13-C12	2.27	121.56	118.09
34	D	302	PID	C17-C16-C15	2.27	128.17	123.52
28	I	305	DD6	C9-C10-C11	-2.27	124.09	127.28
28	J	303	DD6	C9-C8-C6	-2.27	120.13	126.36
30	A	317	CLA	CMA-C3A-C2A	-2.27	111.02	116.23
34	D	307	PID	CM5-C21-C20	-2.27	119.14	122.82
28	B	302	DD6	O1-C20-C19	2.27	115.62	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	K	318	DD6	C37-C36-C35	2.27	118.59	114.42
28	O	303	DD6	C25-C26-C27	-2.27	120.27	126.61
28	K	318	DD6	C3-C4-C5	-2.27	118.88	123.52
30	M	308	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
30	a	719	CLA	CHB-C4A-NA	2.27	127.67	124.40
37	l	302	BCR	C11-C10-C9	-2.26	124.10	127.28
30	J	311	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
28	K	304	DD6	C21-C20-C15	-2.26	118.58	122.30
30	F	312	CLA	CHB-C4A-NA	2.26	127.66	124.40
37	i	201	BCR	C33-C5-C4	2.26	118.41	113.60
30	B	310	CLA	CHB-C4A-NA	2.26	127.66	124.40
28	M	302	DD6	C28-C27-C26	-2.26	119.80	124.18
29	J	305	UIX	C29-C26-C30	-2.26	119.16	122.82
29	P	207	UIX	C10-C11-C13	2.26	122.56	119.01
30	a	730	CLA	C1-C2-C3	-2.26	122.50	126.20
37	f	304	BCR	C8-C7-C6	-2.26	120.97	127.00
37	a	736	BCR	C4-C5-C6	-2.25	119.66	122.70
30	I	310	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
37	l	302	BCR	C33-C5-C4	2.25	118.40	113.60
28	G	502	DD6	C25-C24-C1	-2.25	120.19	126.36
30	b	701	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
31	D	315	KC1	CHC-C4B-C3B	-2.25	121.41	125.21
28	L	302	DD6	C32-C33-C34	-2.25	108.66	113.59
34	N	302	PID	C6-C7-C8	-2.25	121.23	125.99
37	b	730	BCR	C20-C21-C22	-2.25	124.13	127.28
30	b	716	CLA	C1-C2-C3	-2.25	123.13	126.76
30	B	311	CLA	CHB-C4A-NA	2.25	127.64	124.40
29	h	201	UIX	C21-C15-C20	-2.25	108.46	110.47
30	G	518	CLA	O2D-CGD-CBD	2.25	115.16	111.23
33	b	733	LMG	O1-C7-C8	-2.25	105.36	110.82
34	D	305	PID	C8-C9-C10	2.25	128.00	123.60
30	b	710	CLA	CHB-C4A-NA	2.24	127.64	124.40
29	P	207	UIX	C3-C5-C4	-2.24	106.59	110.79
30	D	314	CLA	O2D-CGD-CBD	2.24	115.15	111.23
28	B	303	DD6	C37-C36-C35	2.24	118.54	114.42
31	P	211	KC1	O2A-CGA-O1A	-2.24	118.14	122.70
30	B	301	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
31	J	313	KC1	C2A-C3A-C4A	2.24	108.09	106.41
37	l	307	BCR	C10-C11-C12	-2.24	116.71	123.20
37	l	302	BCR	C34-C9-C8	2.24	121.50	118.09
30	G	520	CLA	CMB-C2B-C1B	-2.24	122.02	125.42
31	A	314	KC1	O2A-CGA-O1A	-2.24	118.15	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	302	DD6	C25-C24-C1	-2.23	120.23	126.36
28	F	303	DD6	C25-C26-C27	-2.23	120.36	126.61
28	K	305	DD6	C37-C36-C35	2.23	118.53	114.42
30	H	309	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
34	P	205	PID	CM5-C21-C20	-2.23	119.20	122.82
29	A	304	UIX	C19-C18-C17	-2.23	105.88	109.89
28	K	301	DD6	C-C1-C24	2.23	121.50	118.09
28	I	303	DD6	C37-C36-C35	2.23	118.52	114.42
30	l	310	CLA	C4D-ND-C1D	-2.23	106.20	108.87
33	j	101	LMG	O7-C10-O9	-2.23	118.49	123.70
28	B	306	DD6	C37-C36-C31	-2.23	119.99	124.16
31	N	311	KC1	C2A-C3A-C4A	2.23	108.08	106.41
31	N	311	KC1	O2D-CGD-O1D	-2.23	119.51	123.85
28	N	303	DD6	O1-C20-C21	-2.23	112.56	115.05
31	D	310	KC1	C2A-C3A-C4A	2.23	108.08	106.41
28	M	303	DD6	C19-C18-C17	-2.23	106.62	110.79
28	I	301	DD6	C21-C20-C15	-2.23	118.64	122.30
30	a	726	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
28	B	302	DD6	C37-C36-C35	2.23	118.52	114.42
34	H	302	PID	O1-C6-C7	-2.23	110.50	116.88
30	a	713	CLA	CHB-C4A-NA	2.23	127.61	124.40
31	O	315	KC1	C2A-C3A-C4A	2.23	108.08	106.41
30	a	728	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
37	b	732	BCR	C36-C18-C19	2.23	121.49	118.09
30	a	738	CLA	O2D-CGD-CBD	2.22	115.12	111.23
34	G	506	PID	CM4-C14-C13	2.22	123.96	119.05
30	f	302	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
37	i	201	BCR	C38-C26-C27	2.22	118.33	113.60
28	M	306	DD6	O1-C20-C15	-2.22	57.17	58.93
30	O	313	CLA	C3B-C4B-NB	-2.22	108.55	110.53
28	J	302	DD6	C21-C20-C15	-2.22	118.65	122.30
28	L	305	DD6	C25-C26-C27	-2.22	120.40	126.61
31	N	306	KC1	C2A-C3A-C4A	2.22	108.08	106.41
31	L	315	KC1	CAC-C3C-C4C	2.22	127.68	124.79
28	K	304	DD6	C25-C24-C1	-2.22	120.28	126.36
33	j	101	LMG	O3-C3-C2	-2.22	105.15	110.38
37	l	307	BCR	C33-C5-C6	-2.22	122.06	124.48
30	A	309	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
30	O	309	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
28	L	304	DD6	C28-C27-C26	-2.21	119.88	124.18
30	f	301	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
30	a	705	CLA	O2A-CGA-O1A	-2.21	118.09	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	G	514	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
30	a	726	CLA	O2D-CGD-CBD	2.21	115.10	111.23
28	M	303	DD6	C32-C33-C34	-2.21	108.74	113.59
30	a	713	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
30	a	722	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
30	L	314	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
28	J	303	DD6	C21-C20-C19	2.21	116.72	114.24
28	A	305	DD6	C10-C9-C8	-2.21	116.80	123.20
31	K	314	KC1	O1D-CGD-CBD	-2.21	120.16	124.52
30	L	310	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
28	A	305	DD6	C28-C27-C26	-2.20	119.90	124.18
30	a	710	CLA	CAA-CBA-CGA	-2.20	106.95	113.21
31	I	314	KC1	O2A-CGA-O1A	-2.20	118.21	122.70
31	F	309	KC1	O2D-CGD-O1D	-2.20	119.56	123.85
30	I	308	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
31	H	310	KC1	O1D-CGD-CBD	-2.20	120.17	124.52
28	G	508	DD6	C21-C20-C15	-2.20	118.68	122.30
28	A	305	DD6	C15-C14-C13	-2.20	121.34	125.99
28	I	301	DD6	C9-C8-C6	-2.20	120.33	126.36
28	N	303	DD6	C25-C24-C1	-2.20	120.33	126.36
28	G	504	DD6	C4-C3-C2	-2.20	119.02	123.52
34	G	507	PID	CM4-C14-C13	2.20	123.90	119.05
31	D	310	KC1	O2D-CGD-O1D	-2.20	119.57	123.85
30	b	722	CLA	CHB-C4A-NA	2.20	127.57	124.40
37	b	730	BCR	C23-C24-C25	-2.20	121.13	127.00
30	l	313	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
30	B	309	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
28	I	301	DD6	C25-C24-C1	-2.19	120.35	126.36
34	D	304	PID	O1-C6-C7	-2.19	110.59	116.88
30	b	718	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
34	F	304	PID	C19-C20-C21	2.19	130.35	127.28
33	j	101	LMG	O2-C2-C1	-2.19	104.85	110.08
37	a	736	BCR	C16-C15-C14	-2.19	119.03	123.52
28	D	303	DD6	C-C1-C24	2.19	121.43	118.09
31	P	213	KC1	O2D-CGD-O1D	-2.19	119.59	123.85
34	j	105	PID	O4-C12-C13	2.19	127.56	122.89
33	B	318	LMG	O2-C2-C1	-2.19	104.86	110.08
28	K	303	DD6	C3-C4-C5	-2.19	119.04	123.52
34	H	301	PID	C16-C15-C14	-2.19	124.21	127.28
30	K	313	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
30	a	724	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
34	P	205	PID	C15-C14-C13	2.19	122.42	116.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	D	313	CLA	C3B-C4B-NB	-2.19	108.58	110.53
30	a	712	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
30	I	313	CLA	C1-C2-C3	-2.18	122.62	126.20
30	J	301	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
28	L	306	DD6	C4-C3-C2	-2.18	119.05	123.52
33	b	734	LMG	O3-C3-C2	-2.18	105.23	110.38
28	L	302	DD6	O1-C15-C14	-2.18	110.63	116.88
28	K	304	DD6	C14-C13-C11	-2.18	122.15	125.53
37	b	730	BCR	C11-C12-C13	-2.18	120.39	126.36
34	D	301	PID	C15-C14-C13	2.18	122.41	116.80
30	K	316	CLA	O2D-CGD-CBD	2.18	115.04	111.23
34	F	304	PID	CM5-C21-C20	-2.18	119.29	122.82
30	b	710	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
28	L	302	DD6	C37-C36-C35	2.18	118.42	114.42
31	O	310	KC1	O2A-CGA-O1A	-2.18	118.27	122.70
33	I	320	LMG	O2-C2-C1	-2.18	104.89	110.08
30	I	306	CLA	O2D-CGD-CBD	2.17	115.03	111.23
30	H	307	CLA	C1-C2-C3	-2.17	122.63	126.20
30	O	314	CLA	C3B-C4B-NB	-2.17	108.59	110.53
30	P	214	CLA	CHB-C4A-NA	2.17	127.53	124.40
28	G	502	DD6	C4-C3-C2	-2.17	119.07	123.52
31	H	310	KC1	O2D-CGD-O1D	-2.17	119.62	123.85
30	a	703	CLA	CAA-CBA-CGA	-2.17	107.05	113.21
30	M	308	CLA	C1-C2-C3	-2.17	122.64	126.20
30	b	725	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
30	b	703	CLA	CHB-C4A-NA	2.17	127.53	124.40
31	L	307	KC1	O1D-CGD-CBD	-2.17	120.24	124.52
33	K	317	LMG	O1-C7-C8	-2.17	105.54	110.82
30	b	705	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
33	K	317	LMG	O2-C2-C1	-2.17	104.91	110.08
30	b	720	CLA	C3B-C4B-NB	-2.17	108.60	110.53
37	f	304	BCR	C23-C24-C25	-2.17	121.21	127.00
30	G	513	CLA	CMB-C2B-C1B	-2.16	122.12	125.42
28	G	505	DD6	C37-C36-C35	2.16	118.40	114.42
28	M	303	DD6	C25-C26-C27	-2.16	120.56	126.61
31	P	216	KC1	C2A-C3A-C4A	2.16	108.04	106.41
30	A	312	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
37	l	302	BCR	C23-C22-C21	2.16	122.41	119.01
31	I	314	KC1	C2A-C3A-C4A	2.16	108.03	106.41
34	H	301	PID	C15-C14-C13	2.16	122.36	116.80
30	G	513	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
28	I	302	DD6	C9-C8-C6	2.16	132.29	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	I	320	LMG	O3-C3-C2	-2.16	105.28	110.38
30	H	304	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
31	L	307	KC1	C2A-C3A-C4A	2.16	108.03	106.41
28	L	305	DD6	O1-C20-C21	-2.16	112.64	115.05
29	K	302	UIX	C41-C40-C38	2.16	121.39	118.09
28	I	303	DD6	O1-C20-C15	-2.16	57.22	58.93
30	G	512	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
30	l	303	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
28	B	306	DD6	C3-C4-C5	-2.16	119.11	123.52
33	I	320	LMG	O1-C1-C2	-2.16	105.00	108.27
28	D	303	DD6	C7-C6-C8	2.15	121.38	118.09
28	M	306	DD6	C7-C6-C5	-2.15	119.33	122.82
30	K	311	CLA	C1-C2-C3	-2.15	122.67	126.20
30	G	511	CLA	C1-C2-C3	-2.15	122.67	126.20
28	I	303	DD6	C25-C26-C27	-2.15	120.60	126.61
30	a	726	CLA	C1-C2-C3	-2.15	122.68	126.20
33	D	317	LMG	O2-C2-C1	-2.15	104.95	110.08
28	b	731	DD6	C-C1-C24	2.15	121.37	118.09
28	L	302	DD6	O1-C20-C21	-2.15	112.65	115.05
31	A	314	KC1	O2D-CGD-O1D	-2.15	119.67	123.85
33	b	733	LMG	O7-C10-O9	-2.15	118.69	123.70
30	I	309	CLA	C1-C2-C3	-2.15	122.68	126.20
30	K	309	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
28	M	306	DD6	C12-C11-C10	-2.15	119.34	122.82
30	a	705	CLA	C1-C2-C3	-2.15	122.68	126.20
30	M	312	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
28	K	303	DD6	C28-C27-C26	-2.14	120.02	124.18
28	H	303	DD6	C28-C27-C26	-2.14	120.02	124.18
30	a	702	CLA	CHB-C4A-NA	2.14	127.49	124.40
34	P	202	PID	CM3-C5-C4	-2.14	105.20	108.97
37	l	302	BCR	C35-C13-C12	2.14	121.36	118.09
33	D	317	LMG	O1-C1-C2	-2.14	105.02	108.27
30	I	311	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
30	I	312	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
30	I	310	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
30	K	315	CLA	CMA-C3A-C2A	-2.14	111.32	116.23
28	L	302	DD6	C25-C26-C27	-2.14	120.62	126.61
34	j	105	PID	CM4-C14-C13	2.14	123.77	119.05
30	a	716	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
28	A	301	DD6	C9-C8-C6	-2.14	120.50	126.36
28	M	302	DD6	C26-C25-C24	-2.14	117.00	123.20
28	M	305	DD6	C25-C24-C1	-2.14	120.50	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	J	304	DD6	C15-C14-C13	-2.14	121.47	125.99
28	P	204	DD6	C25-C26-C27	-2.14	120.64	126.61
37	i	201	BCR	C35-C13-C12	2.14	121.35	118.09
29	J	305	UIX	C3-C5-C4	-2.14	106.79	110.79
31	P	213	KC1	C2A-C3A-C4A	2.14	108.02	106.41
28	P	204	DD6	O1-C20-C21	-2.14	112.66	115.05
37	i	201	BCR	C20-C19-C18	-2.14	120.51	126.36
30	b	720	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
28	I	301	DD6	C3-C4-C5	-2.13	119.15	123.52
31	G	515	KC1	O2D-CGD-O1D	-2.13	119.69	123.85
28	K	305	DD6	C3-C4-C5	-2.13	119.16	123.52
33	I	318	LMG	O3-C3-C2	-2.13	105.35	110.38
30	L	317	CLA	O2D-CGD-CBD	2.13	114.96	111.23
29	J	305	UIX	O2-C27-O4	-2.13	118.88	122.99
28	L	303	DD6	C25-C24-C1	-2.13	120.52	126.36
30	K	306	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
30	J	310	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
30	H	305	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
33	b	734	LMG	O2-C2-C1	-2.13	105.00	110.08
30	F	313	CLA	C2A-C1A-CHA	2.13	127.56	123.87
30	h	202	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
28	A	305	DD6	C25-C24-C1	-2.13	120.53	126.36
30	a	722	CLA	C3B-C4B-NB	-2.13	108.63	110.53
32	I	317	DGD	O6D-C5D-C6D	2.13	110.91	106.69
28	M	306	DD6	C28-C27-C26	-2.13	120.06	124.18
30	A	312	CLA	C3B-C4B-NB	-2.13	108.63	110.53
37	b	702	BCR	C33-C5-C4	2.12	118.12	113.60
30	I	310	CLA	C3B-C4B-NB	-2.12	108.64	110.53
30	a	720	CLA	C1-C2-C3	-2.12	122.72	126.20
31	A	314	KC1	C2A-C3A-C4A	2.12	108.00	106.41
37	i	201	BCR	C21-C20-C19	-2.12	117.06	123.20
30	J	308	CLA	O2D-CGD-CBD	2.12	114.94	111.23
31	A	306	KC1	C2A-C3A-C4A	2.12	108.00	106.41
29	B	305	UIX	C22-C15-C20	-2.12	108.58	110.47
28	K	303	DD6	C25-C26-C27	-2.12	120.69	126.61
30	a	731	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
32	l	301	DGD	O1G-C1A-C2A	2.12	118.30	111.83
28	G	504	DD6	C10-C9-C8	-2.12	117.07	123.20
30	N	304	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
32	G	501	DGD	C2G-O2G-C1B	-2.12	112.73	117.80
30	G	510	CLA	CMB-C2B-C1B	-2.12	122.20	125.42
37	l	306	BCR	C15-C16-C17	-2.12	119.19	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	j	102	BCR	C33-C5-C4	2.11	118.11	113.60
30	M	309	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
30	m	202	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
30	A	313	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
28	K	305	DD6	C25-C24-C1	-2.11	120.57	126.36
28	F	303	DD6	O1-C20-C21	-2.11	112.69	115.05
28	K	305	DD6	C10-C9-C8	-2.11	117.08	123.20
30	b	725	CLA	C1-C2-C3	-2.11	122.74	126.20
29	P	207	UIX	C29-C26-C30	-2.11	119.40	122.82
37	a	734	BCR	C16-C15-C14	-2.11	119.20	123.52
37	f	304	BCR	C3-C4-C5	-2.11	110.29	114.06
28	A	302	DD6	C12-C11-C10	-2.11	119.40	122.82
30	b	723	CLA	O2D-CGD-CBD	2.11	114.92	111.23
30	N	307	CLA	CHB-C4A-NA	2.11	127.44	124.40
30	B	311	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
28	L	304	DD6	C12-C11-C13	2.11	121.31	118.09
37	a	736	BCR	C37-C22-C23	2.11	121.31	118.09
30	O	308	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
33	D	317	LMG	O3-C3-C2	-2.11	105.41	110.38
28	L	304	DD6	C25-C26-C27	-2.11	120.72	126.61
30	I	308	CLA	O2D-CGD-CBD	2.11	114.91	111.23
30	K	312	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
33	K	317	LMG	O3-C3-C2	-2.11	105.41	110.38
29	G	503	UIX	C3-C5-C4	-2.11	106.85	110.79
30	b	723	CLA	C1-C2-C3	-2.11	123.36	126.76
37	l	307	BCR	C36-C18-C19	2.11	121.30	118.09
28	H	303	DD6	C21-C20-C15	-2.10	118.84	122.30
37	i	201	BCR	C34-C9-C8	2.10	121.30	118.09
30	a	724	CLA	O2D-CGD-CBD	2.10	114.91	111.23
30	M	317	CLA	O2D-CGD-CBD	2.10	114.91	111.23
30	I	319	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
28	b	731	DD6	C12-C11-C13	2.10	121.30	118.09
37	a	734	BCR	C37-C22-C23	2.10	121.30	118.09
28	B	306	DD6	C14-C13-C11	-2.10	122.27	125.53
34	F	302	PID	C17-C18-C19	2.10	129.57	124.72
30	G	513	CLA	C1-C2-C3	-2.10	122.76	126.20
30	b	708	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
37	a	736	BCR	C11-C12-C13	-2.10	120.61	126.36
29	I	304	UIX	C13-C14-C23	-2.10	117.12	123.20
28	M	305	DD6	O1-C20-C21	-2.10	112.70	115.05
28	M	302	DD6	C24-C1-C2	2.10	122.31	119.01
30	a	722	CLA	C1-C2-C3	-2.10	122.76	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	a	736	BCR	C15-C16-C17	-2.10	119.23	123.52
30	N	310	CLA	C2A-C1A-CHA	2.10	127.51	123.87
30	K	310	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
33	P	201	LMG	O3-C3-C2	-2.10	105.44	110.38
28	F	301	DD6	C34-C35-C36	-2.10	106.96	112.18
30	M	312	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
30	O	311	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
37	f	304	BCR	C38-C26-C27	2.10	118.06	113.60
30	I	313	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
30	P	212	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
30	a	720	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
31	B	314	KC1	C2A-C3A-C4A	2.09	107.98	106.41
34	G	506	PID	C7-C8-C9	-2.09	123.42	126.06
28	J	302	DD6	C28-C27-C26	-2.09	120.12	124.18
28	B	306	DD6	C7-C6-C8	2.09	121.28	118.09
28	K	318	DD6	O1-C15-C14	-2.09	110.89	116.88
37	l	307	BCR	C23-C24-C25	-2.09	121.42	127.00
33	B	318	LMG	O1-C7-C8	-2.09	105.74	110.82
28	B	302	DD6	C37-C36-C31	-2.09	120.26	124.16
30	B	307	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
30	F	315	CLA	O2D-CGD-CBD	2.09	114.88	111.23
34	H	302	PID	C6-C7-C8	-2.09	121.58	125.99
28	J	304	DD6	C37-C36-C31	-2.08	120.26	124.16
30	P	214	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
28	M	305	DD6	C28-C27-C26	-2.08	120.14	124.18
30	j	106	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
28	B	303	DD6	C12-C11-C13	2.08	121.27	118.09
30	G	520	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
28	N	303	DD6	C28-C27-C26	-2.08	120.14	124.18
30	I	315	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
28	D	303	DD6	C28-C27-C26	-2.08	120.14	124.18
30	a	708	CLA	C1-C2-C3	-2.08	122.79	126.20
34	P	205	PID	C7-C8-C9	-2.08	123.44	126.06
30	P	215	CLA	CED-O2D-CGD	2.08	120.63	115.92
30	L	311	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
30	b	722	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
28	L	306	DD6	O1-C15-C14	-2.08	110.92	116.88
30	b	704	CLA	O1D-CGD-CBD	2.08	128.62	124.52
28	B	304	DD6	C21-C20-C15	-2.08	118.88	122.30
29	h	201	UIX	C3-C5-C4	-2.08	106.91	110.79
31	A	306	KC1	O2D-CGD-O1D	-2.08	119.81	123.85
30	a	708	CLA	O2A-CGA-O1A	-2.08	118.43	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	J	304	DD6	C19-C18-C17	-2.08	106.91	110.79
30	B	301	CLA	CHB-C4A-NA	2.08	127.39	124.40
30	a	703	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
30	j	104	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
33	K	317	LMG	C1-C2-C3	-2.07	105.65	110.01
33	B	318	LMG	O3-C3-C2	-2.07	105.49	110.38
30	a	712	CLA	C1-C2-C3	-2.07	122.80	126.20
30	G	509	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
30	J	308	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
31	M	314	KC1	O2A-CGA-O1A	-2.07	118.48	122.70
30	M	310	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
28	A	303	DD6	C37-C36-C35	2.07	118.23	114.42
30	L	308	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
30	b	717	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
28	A	303	DD6	O1-C15-C14	-2.07	110.94	116.88
30	a	722	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
30	O	314	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
30	J	312	CLA	C1-C2-C3	-2.07	122.81	126.20
30	M	315	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
30	b	726	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
28	O	303	DD6	C37-C36-C35	2.07	118.22	114.42
37	a	734	BCR	C38-C26-C27	2.07	118.00	113.60
30	l	303	CLA	O2D-CGD-CBD	2.07	114.84	111.23
29	h	201	UIX	C36-C35-C32	-2.07	124.38	127.28
38	b	729	PQN	C16-C15-C13	-2.07	108.43	113.47
31	N	308	KC1	O2A-CGA-O1A	-2.07	118.49	122.70
28	K	301	DD6	C28-C27-C26	-2.07	120.17	124.18
30	a	725	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
30	b	717	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
31	D	315	KC1	C4B-CHC-C1C	-2.07	121.63	126.02
29	I	304	UIX	O-C-C7	-2.07	110.96	116.88
28	K	318	DD6	C12-C11-C10	-2.06	119.47	122.82
28	J	304	DD6	O1-C20-C19	-2.06	111.56	113.49
30	A	316	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
30	b	722	CLA	C3B-C4B-NB	-2.06	108.69	110.53
28	D	303	DD6	C32-C33-C34	-2.06	109.07	113.59
28	M	306	DD6	C37-C36-C31	-2.06	120.31	124.16
28	I	301	DD6	C4-C3-C2	-2.06	119.30	123.52
30	b	711	CLA	C1-C2-C3	-2.06	122.82	126.20
30	A	309	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
28	K	303	DD6	O1-C20-C21	-2.06	112.75	115.05
30	K	306	CLA	O2D-CGD-CBD	2.06	114.83	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	502	DD6	C9-C8-C6	-2.06	120.72	126.36
31	D	315	KC1	O2D-CGD-O1D	-2.06	119.85	123.85
30	a	710	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
30	J	314	CLA	CMA-C3A-C2A	-2.05	111.52	116.23
30	I	309	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
30	a	707	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
28	J	303	DD6	C3-C4-C5	-2.05	119.32	123.52
34	D	302	PID	C8-C9-C10	2.05	127.62	123.60
30	A	308	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
30	P	209	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
28	I	305	DD6	O1-C20-C15	-2.05	57.30	58.93
28	M	302	DD6	O1-C20-C15	-2.05	57.30	58.93
31	H	310	KC1	C2A-C3A-C4A	2.05	107.95	106.41
34	P	203	PID	C8-C9-C10	2.05	127.61	123.60
29	K	302	UIX	C19-C18-C17	-2.05	106.20	109.89
37	i	201	BCR	C16-C15-C14	-2.05	119.33	123.52
28	M	306	DD6	C7-C6-C8	2.05	121.22	118.09
34	P	206	PID	C28-C27-C26	2.05	113.57	109.89
28	I	302	DD6	C37-C36-C35	2.05	118.19	114.42
28	B	306	DD6	C4-C3-C2	-2.05	119.33	123.52
30	B	312	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
31	F	309	KC1	O2A-CGA-O1A	-2.05	118.53	122.70
34	G	507	PID	C28-C27-C26	2.05	113.56	109.89
28	H	303	DD6	C3-C4-C5	-2.05	119.33	123.52
30	b	712	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
31	F	314	KC1	C2A-C3A-C4A	2.05	107.95	106.41
28	I	302	DD6	C15-C14-C13	2.05	130.32	125.99
30	O	313	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
30	b	721	CLA	CHB-C4A-NA	2.05	127.35	124.40
30	K	308	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
30	b	713	CLA	C1-C2-C3	-2.04	122.85	126.20
37	j	102	BCR	C34-C9-C8	2.04	121.21	118.09
30	K	315	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
30	H	307	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
30	L	317	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
28	L	303	DD6	C25-C26-C27	-2.04	120.90	126.61
37	m	201	BCR	C24-C23-C22	-2.04	123.22	126.23
30	b	711	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
28	A	302	DD6	C37-C36-C35	2.04	118.17	114.42
30	A	308	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
28	L	304	DD6	C3-C4-C5	-2.04	119.34	123.52
28	M	304	DD6	C37-C36-C35	2.04	118.17	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	l	304	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
29	P	207	UIX	C41-C40-C39	-2.04	119.51	122.82
30	K	307	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
30	P	210	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
30	l	311	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
33	P	201	LMG	C6-C5-C4	-2.04	108.01	113.02
30	b	714	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
30	a	723	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
30	I	315	CLA	C1-C2-C3	-2.04	122.86	126.20
30	a	717	CLA	O2D-CGD-CBD	2.04	114.79	111.23
30	a	721	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
31	I	314	KC1	C1A-C2A-C3A	-2.03	105.41	107.28
28	A	303	DD6	C10-C9-C8	-2.03	117.31	123.20
30	K	308	CLA	C1-C2-C3	-2.03	122.86	126.20
28	I	301	DD6	C37-C36-C31	-2.03	120.36	124.16
29	A	304	UIX	C37-C34-C30	-2.03	119.36	123.52
29	J	305	UIX	C37-C39-C40	-2.03	124.43	127.28
30	B	309	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
30	I	306	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
33	b	733	LMG	O3-C3-C2	-2.03	105.59	110.38
34	D	305	PID	C17-C16-C15	2.03	127.67	123.52
30	b	706	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
31	D	315	KC1	O2A-CGA-O1A	-2.03	118.57	122.70
37	f	304	BCR	C21-C20-C19	-2.03	117.32	123.20
30	b	713	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
34	D	302	PID	O1-C6-C7	-2.03	111.07	116.88
29	G	503	UIX	C41-C40-C38	2.03	121.19	118.09
28	P	204	DD6	C28-C27-C26	-2.03	120.24	124.18
28	K	301	DD6	C21-C20-C15	-2.03	118.97	122.30
30	O	314	CLA	C2A-C1A-CHA	2.02	127.38	123.87
30	a	719	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
34	N	302	PID	O4-C12-C13	2.02	127.21	122.89
28	L	305	DD6	O1-C20-C19	-2.02	111.59	113.49
33	b	734	LMG	O7-C10-O9	-2.02	118.97	123.70
28	M	304	DD6	C7-C6-C8	2.02	121.18	118.09
30	I	319	CLA	O2D-CGD-CBD	2.02	114.77	111.23
33	b	733	LMG	O2-C2-C1	-2.02	105.25	110.08
28	A	305	DD6	C4-C3-C2	-2.02	119.38	123.52
29	G	503	UIX	C35-C36-C38	-2.02	117.34	123.20
31	L	307	KC1	CAA-CBA-CGA	-2.02	116.77	127.05
30	N	310	CLA	C3A-C2A-C1A	2.02	104.37	101.34
30	a	703	CLA	O2A-CGA-O1A	-2.02	118.57	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	303	DD6	C25-C26-C27	-2.02	120.96	126.61
30	a	724	CLA	C1-C2-C3	-2.02	122.89	126.20
30	b	718	CLA	C1-C2-C3	-2.02	122.89	126.20
28	L	302	DD6	C3-C4-C5	-2.02	119.39	123.52
37	a	736	BCR	C1-C6-C5	-2.02	119.88	122.64
28	G	508	DD6	C25-C24-C1	-2.02	120.83	126.36
28	J	304	DD6	C9-C8-C6	-2.02	120.83	126.36
30	a	709	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
31	M	314	KC1	O2D-CGD-O1D	-2.02	119.92	123.85
28	A	301	DD6	C25-C26-C27	-2.02	120.97	126.61
28	M	306	DD6	C3-C4-C5	-2.02	119.39	123.52
34	M	301	PID	CM5-C21-C20	-2.02	119.55	122.82
28	A	301	DD6	C26-C25-C24	-2.02	117.36	123.20
37	f	304	BCR	C15-C16-C17	-2.02	119.40	123.52
30	G	520	CLA	CMB-C2B-C3B	2.01	131.29	126.55
30	a	706	CLA	C1-C2-C3	-2.01	122.90	126.20
28	b	731	DD6	C3-C4-C5	-2.01	119.40	123.52
38	a	732	PQN	C11-C12-C13	-2.01	123.36	126.83
34	F	302	PID	CM1-C1-C6	-2.01	118.99	122.30
30	a	735	CLA	CAA-CBA-CGA	-2.01	107.50	113.21
32	G	501	DGD	O1G-C1A-O1A	-2.01	118.60	123.63
34	H	302	PID	CM4-C14-C13	2.01	123.49	119.05
28	J	302	DD6	C12-C11-C10	-2.01	119.56	122.82
28	F	303	DD6	C28-C27-C26	-2.01	120.28	124.18
30	D	308	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
30	P	215	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
28	I	305	DD6	C19-C18-C17	-2.01	107.03	110.79
30	I	319	CLA	O2A-CGA-O1A	-2.01	118.17	123.33
29	J	305	UIX	C-C7-C10	-2.01	121.75	125.99
30	a	709	CLA	C1-C2-C3	-2.01	122.91	126.20
30	M	315	CLA	CMA-C3A-C2A	-2.01	111.63	116.23
34	O	304	PID	CM4-C14-C13	2.01	123.48	119.05
30	a	711	CLA	O2A-CGA-O1A	-2.01	118.17	123.33
30	K	309	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
28	H	303	DD6	C14-C13-C11	-2.01	122.42	125.53
30	K	310	CLA	C1-C2-C3	-2.01	122.91	126.20
30	K	311	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
30	L	310	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
30	b	712	CLA	C3B-C4B-NB	-2.00	108.25	110.33
30	a	714	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
30	a	711	CLA	CMB-C2B-C3B	2.00	131.26	126.55
28	B	302	DD6	C-C1-C2	-2.00	119.57	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	309	CLA	CMB-C2B-C3B	2.00	131.26	126.55
30	a	722	CLA	CMB-C2B-C3B	2.00	131.26	126.55
30	a	726	CLA	CHB-C1B-NB	2.00	127.05	124.05
32	L	301	DGD	O6D-C5D-C6D	2.00	110.67	106.69
28	G	504	DD6	C37-C36-C31	-2.00	120.42	124.16
30	A	309	CLA	C1-C2-C3	-2.00	122.92	126.20
28	G	508	DD6	C10-C9-C8	-2.00	117.40	123.20
28	M	302	DD6	C25-C26-C27	-2.00	121.01	126.61
30	G	510	CLA	O2D-CGD-CBD	2.00	114.73	111.23
28	I	302	DD6	C21-C20-C15	-2.00	119.01	122.30
37	a	734	BCR	C10-C11-C12	-2.00	117.40	123.20
30	F	313	CLA	CHA-C1A-NA	-2.00	121.86	126.39
30	N	307	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
28	L	302	DD6	C9-C8-C6	-2.00	120.88	126.36
30	K	313	CLA	CMB-C2B-C3B	2.00	131.26	126.55
29	A	304	UIX	C41-C40-C38	2.00	121.14	118.09
37	j	102	BCR	C23-C24-C25	-2.00	121.65	127.00
28	F	301	DD6	C7-C6-C5	-2.00	119.58	122.82
37	l	302	BCR	C40-C30-C25	-2.00	107.11	110.24
28	L	305	DD6	C25-C24-C1	-2.00	120.88	126.36

All (198) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	I	306	CLA	ND
30	I	307	CLA	ND
30	I	308	CLA	ND
30	I	309	CLA	ND
30	I	310	CLA	ND
30	I	311	CLA	ND
30	I	312	CLA	ND
30	I	313	CLA	ND
30	I	315	CLA	ND
30	I	316	CLA	ND
30	I	319	CLA	ND
30	I	321	CLA	ND
30	K	306	CLA	ND
30	K	307	CLA	ND
30	K	308	CLA	ND
30	K	309	CLA	ND
30	K	310	CLA	ND
30	K	311	CLA	ND

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Mol	Chain	Res	Type	Atom
30	K	312	CLA	ND
30	K	313	CLA	ND
30	K	315	CLA	ND
30	K	316	CLA	ND
30	G	509	CLA	ND
30	G	510	CLA	ND
30	G	511	CLA	ND
30	G	512	CLA	ND
30	G	513	CLA	ND
30	G	514	CLA	ND
30	G	516	CLA	ND
30	G	517	CLA	ND
30	G	518	CLA	ND
30	G	519	CLA	ND
30	G	520	CLA	ND
30	A	307	CLA	ND
30	A	308	CLA	ND
30	A	309	CLA	ND
30	A	310	CLA	ND
30	A	311	CLA	ND
30	A	312	CLA	ND
30	A	313	CLA	ND
30	A	315	CLA	ND
30	A	316	CLA	ND
30	A	317	CLA	ND
30	A	319	CLA	ND
30	A	320	CLA	ND
30	f	301	CLA	ND
30	f	302	CLA	ND
30	f	303	CLA	ND
30	h	202	CLA	ND
30	j	104	CLA	ND
30	j	106	CLA	ND
30	l	303	CLA	ND
30	l	304	CLA	ND
30	l	305	CLA	ND
30	l	308	CLA	ND
30	l	309	CLA	ND
30	l	311	CLA	ND
30	l	312	CLA	ND
30	l	313	CLA	ND
30	m	202	CLA	ND

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Mol	Chain	Res	Type	Atom
30	a	701	CLA	ND
30	a	702	CLA	ND
30	a	703	CLA	ND
30	a	704	CLA	ND
30	a	705	CLA	ND
30	a	706	CLA	ND
30	a	707	CLA	ND
30	a	708	CLA	ND
30	a	709	CLA	ND
30	a	710	CLA	ND
30	a	711	CLA	ND
30	a	712	CLA	ND
30	a	713	CLA	ND
30	a	714	CLA	ND
30	a	715	CLA	ND
30	a	716	CLA	ND
30	a	717	CLA	ND
30	a	718	CLA	ND
30	a	719	CLA	ND
30	a	720	CLA	ND
30	a	721	CLA	ND
30	a	722	CLA	ND
30	a	723	CLA	ND
30	a	724	CLA	ND
30	a	725	CLA	ND
30	a	726	CLA	ND
30	a	727	CLA	ND
30	a	728	CLA	ND
30	a	729	CLA	ND
30	a	730	CLA	ND
30	a	731	CLA	ND
30	a	735	CLA	ND
30	a	738	CLA	ND
30	b	701	CLA	ND
30	b	703	CLA	ND
30	b	704	CLA	ND
30	b	705	CLA	ND
30	b	706	CLA	ND
30	b	707	CLA	ND
30	b	708	CLA	ND
30	b	709	CLA	ND
30	b	710	CLA	ND

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Mol	Chain	Res	Type	Atom
30	b	711	CLA	ND
30	b	712	CLA	ND
30	b	713	CLA	ND
30	b	714	CLA	ND
30	b	715	CLA	ND
30	b	716	CLA	ND
30	b	717	CLA	ND
30	b	718	CLA	ND
30	b	719	CLA	ND
30	b	720	CLA	ND
30	b	721	CLA	ND
30	b	722	CLA	ND
30	b	723	CLA	ND
30	b	724	CLA	ND
30	b	725	CLA	ND
30	b	726	CLA	ND
30	b	727	CLA	ND
30	b	728	CLA	ND
30	B	301	CLA	ND
30	B	307	CLA	ND
30	B	308	CLA	ND
30	B	309	CLA	ND
30	B	310	CLA	ND
30	B	311	CLA	ND
30	B	312	CLA	ND
30	B	313	CLA	ND
30	B	315	CLA	ND
30	B	316	CLA	ND
30	B	317	CLA	ND
30	D	308	CLA	ND
30	D	309	CLA	ND
30	D	311	CLA	ND
30	D	312	CLA	ND
30	D	313	CLA	ND
30	D	314	CLA	ND
30	D	316	CLA	ND
30	F	307	CLA	ND
30	F	308	CLA	ND
30	F	310	CLA	ND
30	F	311	CLA	ND
30	F	312	CLA	ND
30	F	313	CLA	ND

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Mol	Chain	Res	Type	Atom
30	F	315	CLA	ND
30	H	304	CLA	ND
30	H	305	CLA	ND
30	H	307	CLA	ND
30	H	308	CLA	ND
30	H	309	CLA	ND
30	H	312	CLA	ND
30	J	301	CLA	ND
30	J	306	CLA	ND
30	J	307	CLA	ND
30	J	308	CLA	ND
30	J	309	CLA	ND
30	J	310	CLA	ND
30	J	311	CLA	ND
30	J	312	CLA	ND
30	J	314	CLA	ND
30	J	315	CLA	ND
30	L	308	CLA	ND
30	L	309	CLA	ND
30	L	310	CLA	ND
30	L	311	CLA	ND
30	L	312	CLA	ND
30	L	313	CLA	ND
30	L	314	CLA	ND
30	L	316	CLA	ND
30	L	317	CLA	ND
30	L	318	CLA	ND
30	M	308	CLA	ND
30	M	309	CLA	ND
30	M	310	CLA	ND
30	M	311	CLA	ND
30	M	312	CLA	ND
30	M	313	CLA	ND
30	M	315	CLA	ND
30	M	316	CLA	ND
30	M	317	CLA	ND
30	M	318	CLA	ND
30	N	304	CLA	ND
30	N	305	CLA	ND
30	N	307	CLA	ND
30	N	309	CLA	ND
30	N	310	CLA	ND

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Mol	Chain	Res	Type	Atom
30	O	308	CLA	ND
30	O	309	CLA	ND
30	O	311	CLA	ND
30	O	313	CLA	ND
30	O	314	CLA	ND
30	O	316	CLA	ND
30	P	209	CLA	ND
30	P	210	CLA	ND
30	P	212	CLA	ND
30	P	214	CLA	ND
30	P	215	CLA	ND
30	P	217	CLA	ND

All (2247) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	K	301	DD6	C12-C11-C13-C14
28	G	502	DD6	C-C1-C24-C25
28	G	502	DD6	C2-C1-C24-C25
28	G	504	DD6	C10-C11-C13-C14
28	G	504	DD6	C12-C11-C13-C14
28	G	505	DD6	C5-C6-C8-C9
28	A	301	DD6	C13-C14-C15-C16
28	A	305	DD6	C13-C14-C15-O1
28	B	303	DD6	C13-C14-C15-O1
28	B	306	DD6	C13-C14-C15-O1
28	D	303	DD6	C13-C14-C15-O1
28	F	301	DD6	C10-C11-C13-C14
28	F	301	DD6	C12-C11-C13-C14
28	J	302	DD6	C10-C11-C13-C14
28	J	302	DD6	C12-C11-C13-C14
28	J	303	DD6	C10-C11-C13-C14
28	J	303	DD6	C12-C11-C13-C14
28	J	304	DD6	C10-C11-C13-C14
28	L	302	DD6	C13-C14-C15-O1
28	L	305	DD6	C13-C14-C15-O1
28	M	305	DD6	C13-C14-C15-O1
28	M	306	DD6	C10-C11-C13-C14
28	M	306	DD6	C12-C11-C13-C14
29	I	304	UIX	C2-C-C7-C10
29	K	302	UIX	O4-C27-O2-C18
29	K	302	UIX	C31-C27-O2-C18

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Mol	Chain	Res	Type	Atoms
29	G	503	UIX	C31-C27-O2-C18
29	h	201	UIX	O4-C27-O2-C18
29	J	305	UIX	O-C-C7-C10
29	J	305	UIX	C14-C23-C26-C29
29	J	305	UIX	C14-C23-C26-C30
29	O	306	UIX	C31-C27-O2-C18
29	P	207	UIX	C36-C38-C40-C39
30	I	306	CLA	CHA-CBD-CGD-O1D
30	I	306	CLA	CHA-CBD-CGD-O2D
30	I	307	CLA	CBA-CGA-O2A-C1
30	I	307	CLA	O1A-CGA-O2A-C1
30	I	310	CLA	CAD-CBD-CGD-O1D
30	I	310	CLA	CAD-CBD-CGD-O2D
30	I	311	CLA	C1A-C2A-CAA-CBA
30	I	311	CLA	C3A-C2A-CAA-CBA
30	I	311	CLA	CHA-CBD-CGD-O1D
30	I	311	CLA	CHA-CBD-CGD-O2D
30	I	312	CLA	C2-C3-C5-C6
30	I	312	CLA	C4-C3-C5-C6
30	I	313	CLA	CBD-CGD-O2D-CED
30	I	316	CLA	C1A-C2A-CAA-CBA
30	I	316	CLA	C3A-C2A-CAA-CBA
30	I	319	CLA	CHA-CBD-CGD-O1D
30	I	319	CLA	CHA-CBD-CGD-O2D
30	K	308	CLA	CBD-CGD-O2D-CED
30	K	311	CLA	C1A-C2A-CAA-CBA
30	K	311	CLA	C3A-C2A-CAA-CBA
30	K	311	CLA	C3-C5-C6-C7
30	K	315	CLA	CBD-CGD-O2D-CED
30	G	509	CLA	C2-C3-C5-C6
30	G	509	CLA	C4-C3-C5-C6
30	G	514	CLA	C4-C3-C5-C6
30	G	516	CLA	CAD-CBD-CGD-O1D
30	G	516	CLA	CAD-CBD-CGD-O2D
30	G	516	CLA	CBD-CGD-O2D-CED
30	G	517	CLA	CBA-CGA-O2A-C1
30	G	518	CLA	C1A-C2A-CAA-CBA
30	G	518	CLA	C3A-C2A-CAA-CBA
30	G	519	CLA	C1A-C2A-CAA-CBA
30	G	519	CLA	C3A-C2A-CAA-CBA
30	G	520	CLA	C1A-C2A-CAA-CBA
30	G	520	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	A	311	CLA	CBA-CGA-O2A-C1
30	A	315	CLA	CAD-CBD-CGD-O1D
30	A	315	CLA	CAD-CBD-CGD-O2D
30	A	319	CLA	C2B-C3B-CAB-CBB
30	A	319	CLA	C4B-C3B-CAB-CBB
30	A	319	CLA	CAD-CBD-CGD-O1D
30	A	319	CLA	CAD-CBD-CGD-O2D
30	A	320	CLA	CBA-CGA-O2A-C1
30	A	320	CLA	CHA-CBD-CGD-O1D
30	A	320	CLA	CHA-CBD-CGD-O2D
30	f	301	CLA	C1A-C2A-CAA-CBA
30	f	301	CLA	C3A-C2A-CAA-CBA
30	f	301	CLA	CBD-CGD-O2D-CED
30	f	302	CLA	CBA-CGA-O2A-C1
30	f	303	CLA	C1A-C2A-CAA-CBA
30	f	303	CLA	C3A-C2A-CAA-CBA
30	j	106	CLA	C1A-C2A-CAA-CBA
30	j	106	CLA	C3A-C2A-CAA-CBA
30	l	304	CLA	CHA-CBD-CGD-O1D
30	l	304	CLA	CHA-CBD-CGD-O2D
30	l	309	CLA	CAD-CBD-CGD-O1D
30	l	309	CLA	CAD-CBD-CGD-O2D
30	l	310	CLA	CBD-CGD-O2D-CED
30	l	311	CLA	C1A-C2A-CAA-CBA
30	l	312	CLA	C3A-C2A-CAA-CBA
30	l	312	CLA	CBD-CGD-O2D-CED
30	l	313	CLA	CHA-CBD-CGD-O1D
30	l	313	CLA	CHA-CBD-CGD-O2D
30	a	702	CLA	CBD-CGD-O2D-CED
30	a	705	CLA	C1A-C2A-CAA-CBA
30	a	705	CLA	C3A-C2A-CAA-CBA
30	a	706	CLA	CAD-CBD-CGD-O1D
30	a	706	CLA	CAD-CBD-CGD-O2D
30	a	707	CLA	C3A-C2A-CAA-CBA
30	a	707	CLA	CBD-CGD-O2D-CED
30	a	709	CLA	C1A-C2A-CAA-CBA
30	a	709	CLA	C3A-C2A-CAA-CBA
30	a	709	CLA	CHA-CBD-CGD-O1D
30	a	709	CLA	CHA-CBD-CGD-O2D
30	a	710	CLA	C2B-C3B-CAB-CBB
30	a	710	CLA	C4B-C3B-CAB-CBB
30	a	713	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	a	714	CLA	CHA-CBD-CGD-O1D
30	a	714	CLA	CHA-CBD-CGD-O2D
30	a	715	CLA	CBD-CGD-O2D-CED
30	a	716	CLA	C1A-C2A-CAA-CBA
30	a	716	CLA	C3A-C2A-CAA-CBA
30	a	717	CLA	C3A-C2A-CAA-CBA
30	a	717	CLA	C6-C7-C8-C9
30	a	718	CLA	C1A-C2A-CAA-CBA
30	a	718	CLA	CAD-CBD-CGD-O2D
30	a	719	CLA	C2B-C3B-CAB-CBB
30	a	719	CLA	C4B-C3B-CAB-CBB
30	a	720	CLA	C3A-C2A-CAA-CBA
30	a	721	CLA	CAD-CBD-CGD-O2D
30	a	721	CLA	CBD-CGD-O2D-CED
30	a	722	CLA	CBD-CGD-O2D-CED
30	a	724	CLA	CHA-CBD-CGD-O1D
30	a	724	CLA	CHA-CBD-CGD-O2D
30	a	726	CLA	CHA-CBD-CGD-O1D
30	a	726	CLA	CHA-CBD-CGD-O2D
30	a	727	CLA	CBA-CGA-O2A-C1
30	a	727	CLA	O1A-CGA-O2A-C1
30	a	727	CLA	CHA-CBD-CGD-O1D
30	a	727	CLA	CHA-CBD-CGD-O2D
30	a	728	CLA	C4-C3-C5-C6
30	a	731	CLA	C1A-C2A-CAA-CBA
30	a	731	CLA	C3A-C2A-CAA-CBA
30	a	731	CLA	CBD-CGD-O2D-CED
30	a	735	CLA	CAD-CBD-CGD-O1D
30	a	735	CLA	CAD-CBD-CGD-O2D
30	a	738	CLA	CHA-CBD-CGD-O1D
30	a	738	CLA	CHA-CBD-CGD-O2D
30	b	701	CLA	CBD-CGD-O2D-CED
30	b	703	CLA	C2B-C3B-CAB-CBB
30	b	703	CLA	C4B-C3B-CAB-CBB
30	b	703	CLA	CBD-CGD-O2D-CED
30	b	704	CLA	C1A-C2A-CAA-CBA
30	b	704	CLA	C3A-C2A-CAA-CBA
30	b	704	CLA	CBD-CGD-O2D-CED
30	b	704	CLA	C14-C13-C15-C16
30	b	707	CLA	CHA-CBD-CGD-O2D
30	b	709	CLA	CHA-CBD-CGD-O1D
30	b	709	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	b	710	CLA	C1A-C2A-CAA-CBA
30	b	710	CLA	C3A-C2A-CAA-CBA
30	b	711	CLA	CAD-CBD-CGD-O1D
30	b	711	CLA	CAD-CBD-CGD-O2D
30	b	711	CLA	CBD-CGD-O2D-CED
30	b	715	CLA	C1A-C2A-CAA-CBA
30	b	715	CLA	C3A-C2A-CAA-CBA
30	b	717	CLA	C1A-C2A-CAA-CBA
30	b	717	CLA	C3A-C2A-CAA-CBA
30	b	717	CLA	C14-C13-C15-C16
30	b	719	CLA	CAD-CBD-CGD-O1D
30	b	719	CLA	CAD-CBD-CGD-O2D
30	b	720	CLA	CBD-CGD-O2D-CED
30	b	723	CLA	C3A-C2A-CAA-CBA
30	b	723	CLA	CHA-CBD-CGD-O1D
30	b	723	CLA	CHA-CBD-CGD-O2D
30	b	724	CLA	C1A-C2A-CAA-CBA
30	b	725	CLA	C2-C3-C5-C6
30	b	725	CLA	C4-C3-C5-C6
30	B	308	CLA	C1A-C2A-CAA-CBA
30	B	311	CLA	CBD-CGD-O2D-CED
30	B	311	CLA	C14-C13-C15-C16
30	B	315	CLA	CAD-CBD-CGD-O1D
30	B	315	CLA	CAD-CBD-CGD-O2D
30	B	315	CLA	CBD-CGD-O2D-CED
30	B	317	CLA	C1A-C2A-CAA-CBA
30	D	312	CLA	CBA-CGA-O2A-C1
30	D	314	CLA	CBA-CGA-O2A-C1
30	D	314	CLA	CBD-CGD-O2D-CED
30	F	310	CLA	C1A-C2A-CAA-CBA
30	F	310	CLA	CHA-CBD-CGD-O1D
30	F	310	CLA	CHA-CBD-CGD-O2D
30	F	311	CLA	C4B-C3B-CAB-CBB
30	F	313	CLA	CBD-CGD-O2D-CED
30	F	315	CLA	CHA-CBD-CGD-O1D
30	F	315	CLA	CHA-CBD-CGD-O2D
30	H	307	CLA	CBD-CGD-O2D-CED
30	H	308	CLA	CBA-CGA-O2A-C1
30	H	309	CLA	C3A-C2A-CAA-CBA
30	H	309	CLA	CBD-CGD-O2D-CED
30	H	311	CLA	CAD-CBD-CGD-O1D
30	H	311	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	H	311	CLA	CBD-CGD-O2D-CED
30	H	312	CLA	C1A-C2A-CAA-CBA
30	H	312	CLA	C3A-C2A-CAA-CBA
30	H	312	CLA	CBD-CGD-O2D-CED
30	J	301	CLA	C4B-C3B-CAB-CBB
30	J	307	CLA	C1A-C2A-CAA-CBA
30	J	307	CLA	C3A-C2A-CAA-CBA
30	J	307	CLA	CAD-CBD-CGD-O2D
30	J	309	CLA	CHA-CBD-CGD-O1D
30	J	309	CLA	CHA-CBD-CGD-O2D
30	J	311	CLA	C1A-C2A-CAA-CBA
30	J	311	CLA	C3A-C2A-CAA-CBA
30	L	308	CLA	C1A-C2A-CAA-CBA
30	L	308	CLA	C3A-C2A-CAA-CBA
30	L	308	CLA	C2B-C3B-CAB-CBB
30	L	308	CLA	C4B-C3B-CAB-CBB
30	L	312	CLA	C3A-C2A-CAA-CBA
30	L	312	CLA	CBD-CGD-O2D-CED
30	L	313	CLA	C3A-C2A-CAA-CBA
30	L	317	CLA	C3-C5-C6-C7
30	L	318	CLA	C4B-C3B-CAB-CBB
30	L	318	CLA	CBD-CGD-O2D-CED
30	M	315	CLA	CHA-CBD-CGD-O1D
30	M	315	CLA	CHA-CBD-CGD-O2D
30	M	317	CLA	CBD-CGD-O2D-CED
30	M	317	CLA	O1D-CGD-O2D-CED
30	M	318	CLA	C1A-C2A-CAA-CBA
30	M	318	CLA	C3A-C2A-CAA-CBA
30	M	318	CLA	CAD-CBD-CGD-O1D
30	M	318	CLA	CAD-CBD-CGD-O2D
30	N	309	CLA	C1A-C2A-CAA-CBA
30	N	310	CLA	C1A-C2A-CAA-CBA
30	N	310	CLA	CBD-CGD-O2D-CED
30	O	314	CLA	CBD-CGD-O2D-CED
30	O	316	CLA	CAD-CBD-CGD-O1D
30	O	316	CLA	CAD-CBD-CGD-O2D
30	P	212	CLA	CHA-CBD-CGD-O1D
30	P	212	CLA	CHA-CBD-CGD-O2D
30	P	214	CLA	CBD-CGD-O2D-CED
30	P	215	CLA	CBD-CGD-O2D-CED
31	I	314	KC1	C2B-C3B-CAB-CBB
31	I	314	KC1	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	I	314	KC1	C2A-CAA-CBA-CGA
31	I	314	KC1	CHA-CBD-CGD-O1D
31	I	314	KC1	CHA-CBD-CGD-O2D
31	K	314	KC1	C2B-C3B-CAB-CBB
31	K	314	KC1	CHA-CBD-CGD-O1D
31	K	314	KC1	CHA-CBD-CGD-O2D
31	G	515	KC1	CHA-CBD-CGD-O1D
31	A	306	KC1	C2B-C3B-CAB-CBB
31	A	306	KC1	CHA-CBD-CGD-O1D
31	A	306	KC1	CHA-CBD-CGD-O2D
31	A	314	KC1	C2B-C3B-CAB-CBB
31	A	314	KC1	C4B-C3B-CAB-CBB
31	A	314	KC1	C2A-CAA-CBA-CGA
31	B	314	KC1	C2B-C3B-CAB-CBB
31	B	314	KC1	CBD-CGD-O2D-CED
31	D	310	KC1	C3A-C2A-CAA-CBA
31	D	310	KC1	C2B-C3B-CAB-CBB
31	D	310	KC1	C2A-CAA-CBA-CGA
31	D	310	KC1	CHA-CBD-CGD-O1D
31	D	310	KC1	CHA-CBD-CGD-O2D
31	D	315	KC1	C1A-C2A-CAA-CBA
31	F	309	KC1	C1A-C2A-CAA-CBA
31	F	309	KC1	C2B-C3B-CAB-CBB
31	F	309	KC1	CHA-CBD-CGD-O1D
31	F	309	KC1	CHA-CBD-CGD-O2D
31	F	314	KC1	C2B-C3B-CAB-CBB
31	H	306	KC1	C3A-C2A-CAA-CBA
31	H	306	KC1	C2B-C3B-CAB-CBB
31	H	310	KC1	C1A-C2A-CAA-CBA
31	H	310	KC1	C3A-C2A-CAA-CBA
31	H	310	KC1	C2B-C3B-CAB-CBB
31	H	310	KC1	CBD-CGD-O2D-CED
31	J	313	KC1	C2B-C3B-CAB-CBB
31	L	307	KC1	CHA-CBD-CGD-O1D
31	L	307	KC1	CHA-CBD-CGD-O2D
31	L	315	KC1	C1A-C2A-CAA-CBA
31	L	315	KC1	C3A-C2A-CAA-CBA
31	L	315	KC1	C2B-C3B-CAB-CBB
31	L	315	KC1	C2A-CAA-CBA-CGA
31	L	315	KC1	CBD-CGD-O2D-CED
31	M	307	KC1	C2B-C3B-CAB-CBB
31	M	307	KC1	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	M	314	KC1	C3A-C2A-CAA-CBA
31	M	314	KC1	C2B-C3B-CAB-CBB
31	M	314	KC1	CBD-CGD-O2D-CED
31	N	306	KC1	C3A-C2A-CAA-CBA
31	N	306	KC1	C2B-C3B-CAB-CBB
31	N	308	KC1	C2B-C3B-CAB-CBB
31	N	308	KC1	C2A-CAA-CBA-CGA
31	N	308	KC1	CHA-CBD-CGD-O1D
31	N	311	KC1	C3A-C2A-CAA-CBA
31	N	311	KC1	C2B-C3B-CAB-CBB
31	N	311	KC1	CBD-CGD-O2D-CED
31	O	310	KC1	C3A-C2A-CAA-CBA
31	O	312	KC1	C2B-C3B-CAB-CBB
31	O	312	KC1	C4B-C3B-CAB-CBB
31	O	312	KC1	C2A-CAA-CBA-CGA
31	O	312	KC1	CHA-CBD-CGD-O1D
31	O	312	KC1	CHA-CBD-CGD-O2D
31	O	315	KC1	CBD-CGD-O2D-CED
31	P	211	KC1	C1A-C2A-CAA-CBA
31	P	211	KC1	C2B-C3B-CAB-CBB
31	P	211	KC1	C2A-CAA-CBA-CGA
31	P	213	KC1	C2B-C3B-CAB-CBB
31	P	213	KC1	C4B-C3B-CAB-CBB
31	P	213	KC1	C2A-CAA-CBA-CGA
31	P	213	KC1	CHA-CBD-CGD-O2D
31	P	216	KC1	C3A-C2A-CAA-CBA
31	P	216	KC1	C2B-C3B-CAB-CBB
31	P	216	KC1	CBD-CGD-O2D-CED
32	G	521	DGD	O6E-C1E-O5D-C6D
32	j	103	DGD	C2B-C1B-O2G-C2G
33	I	318	LMG	O6-C1-O1-C7
33	K	317	LMG	O7-C8-C9-O8
33	K	317	LMG	C11-C10-O7-C8
33	j	101	LMG	O9-C10-O7-C8
33	j	101	LMG	C11-C10-O7-C8
33	b	734	LMG	C2-C1-O1-C7
33	b	734	LMG	O6-C1-O1-C7
33	b	734	LMG	O1-C7-C8-O7
33	b	734	LMG	C11-C10-O7-C8
33	B	318	LMG	O10-C28-O8-C9
33	P	201	LMG	C2-C1-O1-C7
33	P	201	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
33	P	201	LMG	C11-C10-O7-C8
34	G	506	PID	O1-C6-C7-C8
34	j	105	PID	C20-C21-C22-C23
34	j	105	PID	CM5-C21-C22-C23
34	j	105	PID	O7-C30-O6-C27
34	D	301	PID	O1-C6-C7-C8
34	D	301	PID	O4-C12-C13-C14
34	D	306	PID	O1-C6-C7-C8
34	D	307	PID	O1-C6-C7-C8
34	F	304	PID	O7-C30-O6-C27
34	F	305	PID	O7-C30-O6-C27
34	H	301	PID	O1-C6-C7-C8
34	N	301	PID	O4-C12-C13-C14
34	N	301	PID	C12-C13-C14-CM4
34	N	301	PID	O7-C30-O6-C27
34	N	302	PID	O7-C30-O6-C27
34	O	301	PID	O1-C6-C7-C8
34	O	301	PID	O7-C30-O6-C27
34	O	304	PID	O7-C30-O6-C27
34	O	305	PID	C1-C6-C7-C8
34	O	305	PID	C19-C20-C21-C22
34	O	305	PID	C19-C20-C21-CM5
34	O	305	PID	C31-C30-O6-C27
34	O	305	PID	O7-C30-O6-C27
34	O	307	PID	O1-C6-C7-C8
34	P	202	PID	O1-C6-C7-C8
34	P	203	PID	O7-C30-O6-C27
34	P	205	PID	O4-C12-C13-C14
34	P	208	PID	O7-C30-O6-C27
35	A	318	SQD	C46-C45-O47-C7
35	A	318	SQD	C8-C7-O47-C45
37	i	201	BCR	C5-C6-C7-C8
37	i	201	BCR	C7-C8-C9-C10
37	i	201	BCR	C21-C22-C23-C24
37	i	201	BCR	C37-C22-C23-C24
37	i	201	BCR	C23-C24-C25-C26
37	i	201	BCR	C23-C24-C25-C30
37	j	102	BCR	C7-C8-C9-C10
37	m	201	BCR	C7-C8-C9-C10
37	m	201	BCR	C7-C8-C9-C34
37	a	734	BCR	C7-C8-C9-C10
37	a	736	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
37	b	730	BCR	C21-C22-C23-C24
37	b	730	BCR	C37-C22-C23-C24
30	a	722	CLA	O1D-CGD-O2D-CED
30	a	731	CLA	O1D-CGD-O2D-CED
30	H	309	CLA	O1D-CGD-O2D-CED
30	H	311	CLA	O1D-CGD-O2D-CED
31	I	314	KC1	O1D-CGD-O2D-CED
31	H	310	KC1	O1D-CGD-O2D-CED
31	L	315	KC1	O1D-CGD-O2D-CED
31	M	314	KC1	O1D-CGD-O2D-CED
31	N	311	KC1	O1D-CGD-O2D-CED
31	O	315	KC1	O1D-CGD-O2D-CED
31	P	216	KC1	O1D-CGD-O2D-CED
29	I	304	UIX	C31-C27-O2-C18
29	h	201	UIX	C31-C27-O2-C18
29	P	207	UIX	C31-C27-O2-C18
34	F	304	PID	C31-C30-O6-C27
34	F	305	PID	C31-C30-O6-C27
34	N	301	PID	C31-C30-O6-C27
34	N	302	PID	C31-C30-O6-C27
34	P	203	PID	C31-C30-O6-C27
34	P	208	PID	C31-C30-O6-C27
30	K	312	CLA	O1D-CGD-O2D-CED
30	a	712	CLA	O1D-CGD-O2D-CED
30	a	715	CLA	O1D-CGD-O2D-CED
30	B	311	CLA	O1D-CGD-O2D-CED
30	F	312	CLA	O1D-CGD-O2D-CED
30	L	312	CLA	O1D-CGD-O2D-CED
30	N	310	CLA	O1D-CGD-O2D-CED
31	B	314	KC1	O1D-CGD-O2D-CED
29	G	503	UIX	O4-C27-O2-C18
34	H	302	PID	C31-C30-O6-C27
34	H	302	PID	O7-C30-O6-C27
30	I	309	CLA	CBD-CGD-O2D-CED
30	I	316	CLA	CBD-CGD-O2D-CED
30	K	312	CLA	CBD-CGD-O2D-CED
30	A	313	CLA	CBD-CGD-O2D-CED
30	A	319	CLA	CBD-CGD-O2D-CED
30	j	106	CLA	CBD-CGD-O2D-CED
30	a	704	CLA	CBD-CGD-O2D-CED
30	a	712	CLA	CBD-CGD-O2D-CED
30	a	714	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	a	730	CLA	CBD-CGD-O2D-CED
30	B	317	CLA	CBD-CGD-O2D-CED
30	D	313	CLA	CBD-CGD-O2D-CED
30	F	310	CLA	CBD-CGD-O2D-CED
30	F	312	CLA	CBD-CGD-O2D-CED
30	L	316	CLA	CBD-CGD-O2D-CED
30	M	315	CLA	CBD-CGD-O2D-CED
30	M	316	CLA	CBD-CGD-O2D-CED
30	M	318	CLA	CBD-CGD-O2D-CED
30	N	307	CLA	CBD-CGD-O2D-CED
30	O	313	CLA	CBD-CGD-O2D-CED
30	O	316	CLA	CBD-CGD-O2D-CED
30	P	212	CLA	CBD-CGD-O2D-CED
30	P	217	CLA	CBD-CGD-O2D-CED
31	I	314	KC1	CBD-CGD-O2D-CED
31	P	211	KC1	CBD-CGD-O2D-CED
30	b	701	CLA	O1A-CGA-O2A-C1
30	H	304	CLA	O1A-CGA-O2A-C1
30	J	307	CLA	O1A-CGA-O2A-C1
30	J	311	CLA	O1A-CGA-O2A-C1
30	N	310	CLA	O1A-CGA-O2A-C1
30	O	308	CLA	O1A-CGA-O2A-C1
30	O	314	CLA	O1A-CGA-O2A-C1
30	A	311	CLA	O1A-CGA-O2A-C1
30	A	320	CLA	O1A-CGA-O2A-C1
30	D	312	CLA	O1A-CGA-O2A-C1
30	D	314	CLA	O1A-CGA-O2A-C1
30	H	308	CLA	O1A-CGA-O2A-C1
30	D	314	CLA	O1D-CGD-O2D-CED
30	P	215	CLA	O1D-CGD-O2D-CED
29	J	305	UIX	C31-C27-O2-C18
34	j	105	PID	C31-C30-O6-C27
34	O	301	PID	C31-C30-O6-C27
34	O	304	PID	C31-C30-O6-C27
29	J	305	UIX	C19-C18-O2-C27
34	D	302	PID	C26-C27-O6-C30
34	P	205	PID	C26-C27-O6-C30
30	l	310	CLA	CBA-CGA-O2A-C1
30	D	309	CLA	CBA-CGA-O2A-C1
30	F	311	CLA	CBA-CGA-O2A-C1
30	I	309	CLA	O1D-CGD-O2D-CED
30	a	702	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	D	313	CLA	O1D-CGD-O2D-CED
30	F	313	CLA	O1D-CGD-O2D-CED
30	M	318	CLA	O1D-CGD-O2D-CED
30	N	307	CLA	O1D-CGD-O2D-CED
30	O	314	CLA	O1D-CGD-O2D-CED
30	O	316	CLA	O1D-CGD-O2D-CED
30	b	701	CLA	CBA-CGA-O2A-C1
30	H	304	CLA	CBA-CGA-O2A-C1
30	J	307	CLA	CBA-CGA-O2A-C1
30	J	311	CLA	CBA-CGA-O2A-C1
30	O	308	CLA	CBA-CGA-O2A-C1
30	O	314	CLA	CBA-CGA-O2A-C1
32	G	521	DGD	C2A-C1A-O1G-C1G
33	K	317	LMG	C29-C28-O8-C9
33	j	101	LMG	C29-C28-O8-C9
29	O	306	UIX	O4-C27-O2-C18
34	P	202	PID	O7-C30-O6-C27
30	I	308	CLA	O1A-CGA-O2A-C1
30	I	315	CLA	O1A-CGA-O2A-C1
30	K	308	CLA	O1A-CGA-O2A-C1
30	G	513	CLA	O1A-CGA-O2A-C1
30	a	706	CLA	O1A-CGA-O2A-C1
30	a	721	CLA	O1A-CGA-O2A-C1
30	b	707	CLA	O1A-CGA-O2A-C1
30	b	717	CLA	O1A-CGA-O2A-C1
30	B	311	CLA	O1A-CGA-O2A-C1
30	H	309	CLA	O1A-CGA-O2A-C1
30	L	313	CLA	O1A-CGA-O2A-C1
32	G	521	DGD	O1A-C1A-O1G-C1G
33	I	318	LMG	O10-C28-O8-C9
33	K	317	LMG	O10-C28-O8-C9
33	j	101	LMG	O10-C28-O8-C9
33	b	733	LMG	O10-C28-O8-C9
30	G	517	CLA	O1A-CGA-O2A-C1
30	f	302	CLA	O1A-CGA-O2A-C1
30	F	311	CLA	O1A-CGA-O2A-C1
30	I	316	CLA	O1D-CGD-O2D-CED
30	K	308	CLA	O1D-CGD-O2D-CED
30	H	312	CLA	O1D-CGD-O2D-CED
30	P	214	CLA	O1D-CGD-O2D-CED
34	P	202	PID	C31-C30-O6-C27
31	K	314	KC1	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	B	314	KC1	CAA-CBA-CGA-O1A
31	D	310	KC1	CAA-CBA-CGA-O2A
30	I	313	CLA	O1D-CGD-O2D-CED
30	f	301	CLA	O1D-CGD-O2D-CED
30	l	312	CLA	O1D-CGD-O2D-CED
30	a	707	CLA	O1D-CGD-O2D-CED
30	b	701	CLA	O1D-CGD-O2D-CED
30	b	703	CLA	O1D-CGD-O2D-CED
30	b	711	CLA	O1D-CGD-O2D-CED
30	B	315	CLA	O1D-CGD-O2D-CED
30	H	307	CLA	O1D-CGD-O2D-CED
29	P	207	UIX	O4-C27-O2-C18
32	j	103	DGD	O1B-C1B-O2G-C2G
33	I	318	LMG	O9-C10-O7-C8
33	I	320	LMG	O9-C10-O7-C8
33	K	317	LMG	O9-C10-O7-C8
33	b	734	LMG	O9-C10-O7-C8
33	B	318	LMG	O9-C10-O7-C8
35	A	318	SQD	O49-C7-O47-C45
29	I	304	UIX	O4-C27-O2-C18
34	G	506	PID	C31-C30-O6-C27
34	G	506	PID	O7-C30-O6-C27
30	G	518	CLA	CBA-CGA-O2A-C1
30	F	307	CLA	CBA-CGA-O2A-C1
30	J	310	CLA	CBA-CGA-O2A-C1
30	a	718	CLA	O1A-CGA-O2A-C1
30	F	310	CLA	O1A-CGA-O2A-C1
30	I	311	CLA	C3-C5-C6-C7
30	I	312	CLA	C3-C5-C6-C7
30	I	316	CLA	C3-C5-C6-C7
30	K	313	CLA	C3-C5-C6-C7
30	G	514	CLA	C3-C5-C6-C7
30	G	519	CLA	C3-C5-C6-C7
30	j	104	CLA	C3-C5-C6-C7
30	l	305	CLA	C3-C5-C6-C7
30	a	702	CLA	C3-C5-C6-C7
30	a	705	CLA	C3-C5-C6-C7
30	a	706	CLA	C3-C5-C6-C7
30	b	701	CLA	C3-C5-C6-C7
30	b	707	CLA	C3-C5-C6-C7
30	b	717	CLA	C3-C5-C6-C7
30	B	310	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	J	307	CLA	C3-C5-C6-C7
30	L	309	CLA	C3-C5-C6-C7
30	K	315	CLA	O1D-CGD-O2D-CED
30	I	315	CLA	CBA-CGA-O2A-C1
30	K	308	CLA	CBA-CGA-O2A-C1
30	G	513	CLA	CBA-CGA-O2A-C1
30	a	706	CLA	CBA-CGA-O2A-C1
30	a	728	CLA	CBA-CGA-O2A-C1
30	b	720	CLA	CBA-CGA-O2A-C1
30	B	310	CLA	CBA-CGA-O2A-C1
30	H	309	CLA	CBA-CGA-O2A-C1
30	L	314	CLA	CBA-CGA-O2A-C1
30	L	317	CLA	CBA-CGA-O2A-C1
30	N	310	CLA	CBA-CGA-O2A-C1
33	b	733	LMG	C29-C28-O8-C9
30	I	319	CLA	CBD-CGD-O2D-CED
30	I	321	CLA	CBD-CGD-O2D-CED
30	A	315	CLA	CBD-CGD-O2D-CED
30	l	308	CLA	CBD-CGD-O2D-CED
30	m	202	CLA	CBD-CGD-O2D-CED
30	a	711	CLA	CBD-CGD-O2D-CED
30	a	725	CLA	CBD-CGD-O2D-CED
30	a	726	CLA	CBD-CGD-O2D-CED
30	b	707	CLA	CBD-CGD-O2D-CED
30	b	713	CLA	CBD-CGD-O2D-CED
30	H	304	CLA	CBD-CGD-O2D-CED
30	H	308	CLA	CBD-CGD-O2D-CED
30	J	306	CLA	CBD-CGD-O2D-CED
30	J	307	CLA	CBD-CGD-O2D-CED
30	J	308	CLA	CBD-CGD-O2D-CED
30	J	315	CLA	CBD-CGD-O2D-CED
30	L	313	CLA	CBD-CGD-O2D-CED
30	M	308	CLA	CBD-CGD-O2D-CED
30	M	309	CLA	CBD-CGD-O2D-CED
30	M	310	CLA	CBD-CGD-O2D-CED
30	P	209	CLA	CBD-CGD-O2D-CED
33	I	318	LMG	C11-C10-O7-C8
33	I	320	LMG	C11-C10-O7-C8
33	B	318	LMG	C11-C10-O7-C8
30	l	310	CLA	O1D-CGD-O2D-CED
30	a	721	CLA	O1D-CGD-O2D-CED
30	b	704	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	b	720	CLA	O1D-CGD-O2D-CED
30	F	310	CLA	O1D-CGD-O2D-CED
30	L	318	CLA	O1D-CGD-O2D-CED
30	M	315	CLA	O1D-CGD-O2D-CED
34	D	305	PID	O7-C30-O6-C27
30	N	304	CLA	O1A-CGA-O2A-C1
30	P	215	CLA	O1A-CGA-O2A-C1
30	D	309	CLA	O1A-CGA-O2A-C1
30	F	313	CLA	O1A-CGA-O2A-C1
30	G	516	CLA	O1D-CGD-O2D-CED
30	a	713	CLA	O1D-CGD-O2D-CED
34	D	305	PID	C31-C30-O6-C27
31	F	309	KC1	CAA-CBA-CGA-O2A
30	I	308	CLA	C4-C3-C5-C6
30	I	313	CLA	C4-C3-C5-C6
30	K	308	CLA	C4-C3-C5-C6
30	K	313	CLA	C4-C3-C5-C6
30	A	313	CLA	C4-C3-C5-C6
30	j	106	CLA	C4-C3-C5-C6
30	a	706	CLA	C4-C3-C5-C6
30	a	713	CLA	C4-C3-C5-C6
30	a	724	CLA	C4-C3-C5-C6
30	a	731	CLA	C4-C3-C5-C6
30	a	735	CLA	C4-C3-C5-C6
30	b	701	CLA	C4-C3-C5-C6
30	b	715	CLA	C4-C3-C5-C6
30	J	307	CLA	C4-C3-C5-C6
30	M	308	CLA	C4-C3-C5-C6
38	a	732	PQN	C14-C13-C15-C16
30	I	313	CLA	C2-C3-C5-C6
30	K	308	CLA	C2-C3-C5-C6
30	K	313	CLA	C2-C3-C5-C6
30	G	514	CLA	C2-C3-C5-C6
30	j	106	CLA	C2-C3-C5-C6
30	a	706	CLA	C2-C3-C5-C6
30	a	728	CLA	C2-C3-C5-C6
30	a	731	CLA	C2-C3-C5-C6
30	b	701	CLA	C2-C3-C5-C6
30	b	715	CLA	C2-C3-C5-C6
30	J	307	CLA	C2-C3-C5-C6
30	M	308	CLA	C2-C3-C5-C6
38	a	732	PQN	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	a	718	CLA	CBA-CGA-O2A-C1
30	F	310	CLA	CBA-CGA-O2A-C1
30	F	313	CLA	CBA-CGA-O2A-C1
30	O	313	CLA	O1D-CGD-O2D-CED
30	a	711	CLA	C2A-CAA-CBA-CGA
30	b	714	CLA	C2A-CAA-CBA-CGA
30	J	308	CLA	C2A-CAA-CBA-CGA
30	M	316	CLA	C3-C5-C6-C7
30	M	318	CLA	C2A-CAA-CBA-CGA
30	A	308	CLA	C3-C5-C6-C7
30	A	312	CLA	C3-C5-C6-C7
30	h	202	CLA	C3-C5-C6-C7
30	I	308	CLA	CBA-CGA-O2A-C1
30	G	514	CLA	CBA-CGA-O2A-C1
30	a	721	CLA	CBA-CGA-O2A-C1
30	b	707	CLA	CBA-CGA-O2A-C1
30	b	717	CLA	CBA-CGA-O2A-C1
30	B	311	CLA	CBA-CGA-O2A-C1
30	L	313	CLA	CBA-CGA-O2A-C1
30	N	304	CLA	CBA-CGA-O2A-C1
30	P	215	CLA	CBA-CGA-O2A-C1
33	I	318	LMG	C29-C28-O8-C9
33	B	318	LMG	C29-C28-O8-C9
30	G	518	CLA	O1A-CGA-O2A-C1
30	J	310	CLA	O1A-CGA-O2A-C1
29	J	305	UIX	O4-C27-O2-C18
28	I	301	DD6	C24-C25-C26-C27
28	G	502	DD6	C24-C25-C26-C27
28	M	302	DD6	C1-C2-C3-C4
34	F	305	PID	C14-C15-C16-C17
34	F	305	PID	C18-C19-C20-C21
34	O	305	PID	C14-C15-C16-C17
30	G	514	CLA	O1A-CGA-O2A-C1
30	l	313	CLA	O1A-CGA-O2A-C1
30	a	728	CLA	O1A-CGA-O2A-C1
30	b	720	CLA	O1A-CGA-O2A-C1
30	L	317	CLA	O1A-CGA-O2A-C1
30	l	310	CLA	O1A-CGA-O2A-C1
30	F	307	CLA	O1A-CGA-O2A-C1
30	j	106	CLA	O1D-CGD-O2D-CED
30	B	317	CLA	O1D-CGD-O2D-CED
31	P	213	KC1	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	P	213	KC1	CAA-CBA-CGA-O2A
30	G	511	CLA	C3-C5-C6-C7
30	A	309	CLA	C3-C5-C6-C7
30	A	312	CLA	CBD-CGD-O2D-CED
30	b	715	CLA	CBD-CGD-O2D-CED
30	J	311	CLA	CBD-CGD-O2D-CED
30	M	311	CLA	CBD-CGD-O2D-CED
31	O	312	KC1	CBD-CGD-O2D-CED
30	A	319	CLA	O1D-CGD-O2D-CED
30	a	714	CLA	O1D-CGD-O2D-CED
30	a	730	CLA	O1D-CGD-O2D-CED
30	P	212	CLA	O1D-CGD-O2D-CED
30	J	301	CLA	CBA-CGA-O2A-C1
34	P	206	PID	C31-C30-O6-C27
30	B	310	CLA	O1A-CGA-O2A-C1
30	L	314	CLA	O1A-CGA-O2A-C1
33	B	318	LMG	C4-C5-C6-O5
30	A	313	CLA	O1D-CGD-O2D-CED
30	M	316	CLA	O1D-CGD-O2D-CED
29	B	305	UIX	O4-C27-O2-C18
29	B	305	UIX	C31-C27-O2-C18
34	F	302	PID	C31-C30-O6-C27
34	F	302	PID	O7-C30-O6-C27
34	H	301	PID	C31-C30-O6-C27
34	H	301	PID	O7-C30-O6-C27
34	O	302	PID	C31-C30-O6-C27
34	O	302	PID	O7-C30-O6-C27
34	P	206	PID	O7-C30-O6-C27
30	G	512	CLA	CBD-CGD-O2D-CED
30	L	314	CLA	CBD-CGD-O2D-CED
31	M	307	KC1	CBD-CGD-O2D-CED
30	K	316	CLA	CBA-CGA-O2A-C1
30	H	312	CLA	CBA-CGA-O2A-C1
33	K	317	LMG	O6-C5-C6-O5
30	b	703	CLA	C3-C5-C6-C7
30	a	723	CLA	CBD-CGD-O2D-CED
30	B	312	CLA	CBD-CGD-O2D-CED
30	a	704	CLA	O1D-CGD-O2D-CED
30	L	316	CLA	O1D-CGD-O2D-CED
30	P	217	CLA	O1D-CGD-O2D-CED
30	l	313	CLA	CBA-CGA-O2A-C1
31	D	315	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	J	313	KC1	CAA-CBA-CGA-O2A
31	O	310	KC1	CAA-CBA-CGA-O2A
30	G	510	CLA	C4-C3-C5-C6
30	l	305	CLA	C4-C3-C5-C6
30	l	311	CLA	C4-C3-C5-C6
30	L	309	CLA	C4-C3-C5-C6
30	L	317	CLA	C4-C3-C5-C6
30	M	316	CLA	C4-C3-C5-C6
30	P	210	CLA	C4-C3-C5-C6
30	G	510	CLA	C2-C3-C5-C6
30	a	713	CLA	C2-C3-C5-C6
30	a	724	CLA	C2-C3-C5-C6
30	a	735	CLA	C2-C3-C5-C6
30	P	210	CLA	C2-C3-C5-C6
30	J	301	CLA	O1A-CGA-O2A-C1
33	P	201	LMG	O6-C5-C6-O5
30	b	704	CLA	C2C-C3C-CAC-CBC
30	a	721	CLA	C2A-CAA-CBA-CGA
30	O	314	CLA	C2A-CAA-CBA-CGA
32	G	501	DGD	O6E-C1E-O5D-C6D
33	D	317	LMG	O6-C1-O1-C7
30	a	708	CLA	CBA-CGA-O2A-C1
30	a	709	CLA	CBA-CGA-O2A-C1
30	b	723	CLA	CBA-CGA-O2A-C1
30	B	309	CLA	CBA-CGA-O2A-C1
30	M	308	CLA	CBA-CGA-O2A-C1
30	I	306	CLA	CBD-CGD-O2D-CED
30	I	311	CLA	CBD-CGD-O2D-CED
30	A	308	CLA	CBD-CGD-O2D-CED
30	A	320	CLA	CBD-CGD-O2D-CED
30	f	303	CLA	CBD-CGD-O2D-CED
30	l	313	CLA	CBD-CGD-O2D-CED
30	a	705	CLA	CBD-CGD-O2D-CED
30	a	709	CLA	CBD-CGD-O2D-CED
30	b	712	CLA	CBD-CGD-O2D-CED
30	b	727	CLA	CBD-CGD-O2D-CED
30	J	301	CLA	CBD-CGD-O2D-CED
30	J	314	CLA	CBD-CGD-O2D-CED
30	L	317	CLA	CBD-CGD-O2D-CED
31	D	310	KC1	CBD-CGD-O2D-CED
31	B	314	KC1	CAA-CBA-CGA-O2A
31	F	309	KC1	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
33	B	318	LMG	O6-C5-C6-O5
30	G	519	CLA	CBD-CGD-O2D-CED
30	a	710	CLA	CBD-CGD-O2D-CED
30	B	316	CLA	CBD-CGD-O2D-CED
30	J	309	CLA	CBD-CGD-O2D-CED
30	a	708	CLA	O1A-CGA-O2A-C1
30	b	723	CLA	O1A-CGA-O2A-C1
30	M	308	CLA	O1A-CGA-O2A-C1
30	I	321	CLA	CBA-CGA-O2A-C1
30	G	519	CLA	CBA-CGA-O2A-C1
30	A	313	CLA	CBA-CGA-O2A-C1
30	l	311	CLA	CBA-CGA-O2A-C1
30	a	707	CLA	CBA-CGA-O2A-C1
30	a	712	CLA	CBA-CGA-O2A-C1
30	M	312	CLA	CBA-CGA-O2A-C1
31	N	306	KC1	CBD-CGD-O2D-CED
31	A	314	KC1	CAA-CBA-CGA-O2A
31	N	308	KC1	CAA-CBA-CGA-O2A
31	P	216	KC1	CAA-CBA-CGA-O2A
30	b	703	CLA	C4-C3-C5-C6
30	I	308	CLA	C2-C3-C5-C6
30	A	313	CLA	C2-C3-C5-C6
30	b	703	CLA	C2-C3-C5-C6
30	L	309	CLA	C2-C3-C5-C6
30	M	316	CLA	C2-C3-C5-C6
30	b	728	CLA	C3-C5-C6-C7
30	M	308	CLA	C3-C5-C6-C7
30	I	312	CLA	C14-C13-C15-C16
30	l	303	CLA	C11-C12-C13-C14
30	l	304	CLA	C11-C10-C8-C9
30	l	305	CLA	C11-C12-C13-C14
30	a	707	CLA	C11-C10-C8-C9
30	a	720	CLA	C11-C12-C13-C14
30	a	721	CLA	C14-C13-C15-C16
30	a	722	CLA	C6-C7-C8-C9
30	a	724	CLA	C6-C7-C8-C9
30	a	731	CLA	C11-C12-C13-C14
30	b	704	CLA	C6-C7-C8-C9
30	b	708	CLA	C6-C7-C8-C9
30	B	311	CLA	C6-C7-C8-C9
30	b	707	CLA	O1D-CGD-O2D-CED
30	H	308	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	M	309	CLA	O1D-CGD-O2D-CED
32	G	521	DGD	C2E-C1E-O5D-C6D
30	K	316	CLA	O1A-CGA-O2A-C1
30	H	312	CLA	O1A-CGA-O2A-C1
30	b	719	CLA	CBA-CGA-O2A-C1
30	M	317	CLA	CBA-CGA-O2A-C1
30	J	308	CLA	O1D-CGD-O2D-CED
30	a	735	CLA	CBD-CGD-O2D-CED
30	I	319	CLA	O1D-CGD-O2D-CED
30	b	713	CLA	O1D-CGD-O2D-CED
30	J	307	CLA	O1D-CGD-O2D-CED
28	G	504	DD6	C7-C6-C8-C9
28	G	505	DD6	C7-C6-C8-C9
28	D	303	DD6	C12-C11-C13-C14
28	L	302	DD6	C12-C11-C13-C14
29	P	207	UIX	C36-C38-C40-C41
37	i	201	BCR	C7-C8-C9-C34
37	j	102	BCR	C7-C8-C9-C34
37	l	306	BCR	C37-C22-C23-C24
37	a	734	BCR	C7-C8-C9-C34
37	a	736	BCR	C7-C8-C9-C34
37	b	702	BCR	C37-C22-C23-C24
37	b	730	BCR	C7-C8-C9-C34
28	K	301	DD6	C10-C11-C13-C14
28	B	302	DD6	C10-C11-C13-C14
28	D	303	DD6	C10-C11-C13-C14
28	L	302	DD6	C10-C11-C13-C14
37	l	306	BCR	C21-C22-C23-C24
37	b	702	BCR	C21-C22-C23-C24
37	b	730	BCR	C7-C8-C9-C10
30	G	520	CLA	C2A-CAA-CBA-CGA
32	y	201	DGD	C1B-C2B-C3B-C4B
30	G	519	CLA	O1A-CGA-O2A-C1
30	A	313	CLA	O1A-CGA-O2A-C1
30	a	707	CLA	O1A-CGA-O2A-C1
30	M	312	CLA	O1A-CGA-O2A-C1
30	G	514	CLA	CBD-CGD-O2D-CED
31	K	314	KC1	CAA-CBA-CGA-O2A
31	L	307	KC1	CAA-CBA-CGA-O2A
31	M	307	KC1	CAA-CBA-CGA-O2A
31	O	315	KC1	CAA-CBA-CGA-O1A
31	P	211	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	P	216	KC1	CAA-CBA-CGA-O1A
32	y	201	DGD	O2G-C2G-C3G-O3G
33	P	201	LMG	C4-C5-C6-O5
30	a	721	CLA	C10-C11-C12-C13
30	b	717	CLA	C5-C6-C7-C8
30	A	315	CLA	O1D-CGD-O2D-CED
30	J	306	CLA	O1D-CGD-O2D-CED
30	J	315	CLA	O1D-CGD-O2D-CED
30	L	313	CLA	O1D-CGD-O2D-CED
30	O	308	CLA	CBD-CGD-O2D-CED
34	O	305	PID	C17-C18-C19-C20
30	a	730	CLA	C5-C6-C7-C8
30	l	308	CLA	O1D-CGD-O2D-CED
30	a	725	CLA	O1D-CGD-O2D-CED
30	M	308	CLA	O1D-CGD-O2D-CED
30	l	311	CLA	O1A-CGA-O2A-C1
30	b	713	CLA	C10-C11-C12-C13
30	B	313	CLA	CBD-CGD-O2D-CED
30	F	315	CLA	CBD-CGD-O2D-CED
30	O	311	CLA	CBD-CGD-O2D-CED
30	b	717	CLA	C6-C7-C8-C10
30	H	304	CLA	O1D-CGD-O2D-CED
31	D	310	KC1	CAA-CBA-CGA-O1A
31	N	308	KC1	CAA-CBA-CGA-O1A
30	a	706	CLA	C5-C6-C7-C8
30	B	313	CLA	C10-C11-C12-C13
28	I	305	DD6	C11-C10-C9-C8
28	M	302	DD6	C24-C25-C26-C27
28	M	306	DD6	C24-C25-C26-C27
29	P	207	UIX	C32-C35-C36-C38
34	O	305	PID	C18-C19-C20-C21
30	I	321	CLA	C2C-C3C-CAC-CBC
30	a	711	CLA	O1D-CGD-O2D-CED
30	a	726	CLA	O1D-CGD-O2D-CED
30	P	209	CLA	O1D-CGD-O2D-CED
30	I	313	CLA	C5-C6-C7-C8
33	I	318	LMG	C10-C11-C12-C13
30	J	310	CLA	CBD-CGD-O2D-CED
30	I	312	CLA	C13-C15-C16-C17
30	j	106	CLA	C5-C6-C7-C8
30	l	303	CLA	C8-C10-C11-C12
30	b	722	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	B	313	CLA	C8-C10-C11-C12
30	J	307	CLA	C8-C10-C11-C12
30	K	308	CLA	C2A-CAA-CBA-CGA
30	G	513	CLA	C2A-CAA-CBA-CGA
30	A	319	CLA	C2A-CAA-CBA-CGA
30	a	709	CLA	C2A-CAA-CBA-CGA
30	a	719	CLA	C2A-CAA-CBA-CGA
30	b	719	CLA	C2A-CAA-CBA-CGA
30	b	724	CLA	C2A-CAA-CBA-CGA
30	H	312	CLA	C2A-CAA-CBA-CGA
30	M	310	CLA	C2A-CAA-CBA-CGA
30	N	305	CLA	C2A-CAA-CBA-CGA
30	I	309	CLA	C5-C6-C7-C8
30	I	312	CLA	C15-C16-C17-C18
30	m	202	CLA	C5-C6-C7-C8
30	a	713	CLA	C10-C11-C12-C13
30	a	724	CLA	C15-C16-C17-C18
30	b	713	CLA	C8-C10-C11-C12
30	J	307	CLA	C13-C15-C16-C17
30	J	309	CLA	C5-C6-C7-C8
33	I	318	LMG	C28-C29-C30-C31
33	j	101	LMG	C28-C29-C30-C31
30	m	202	CLA	O1D-CGD-O2D-CED
30	I	321	CLA	O1A-CGA-O2A-C1
30	a	712	CLA	O1A-CGA-O2A-C1
33	j	101	LMG	O6-C1-O1-C7
30	I	321	CLA	O1D-CGD-O2D-CED
30	M	310	CLA	O1D-CGD-O2D-CED
30	a	707	CLA	C5-C6-C7-C8
30	a	723	CLA	C13-C15-C16-C17
30	a	726	CLA	C15-C16-C17-C18
30	b	707	CLA	C10-C11-C12-C13
30	B	310	CLA	C5-C6-C7-C8
30	P	210	CLA	C15-C16-C17-C18
30	K	313	CLA	CBA-CGA-O2A-C1
31	F	314	KC1	CBD-CGD-O2D-CED
30	a	709	CLA	O1A-CGA-O2A-C1
30	B	309	CLA	O1A-CGA-O2A-C1
30	H	305	CLA	C15-C16-C17-C18
30	b	715	CLA	O1D-CGD-O2D-CED
30	J	311	CLA	O1D-CGD-O2D-CED
30	M	311	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	G	510	CLA	C5-C6-C7-C8
30	l	313	CLA	C5-C6-C7-C8
30	a	709	CLA	C5-C6-C7-C8
30	a	735	CLA	C13-C15-C16-C17
30	b	705	CLA	C13-C15-C16-C17
30	B	309	CLA	C13-C15-C16-C17
31	O	310	KC1	CBD-CGD-O2D-CED
30	L	317	CLA	C2-C3-C5-C6
30	A	312	CLA	O1D-CGD-O2D-CED
32	G	521	DGD	C4A-C5A-C6A-C7A
30	I	312	CLA	C10-C11-C12-C13
30	l	305	CLA	C5-C6-C7-C8
30	b	705	CLA	C10-C11-C12-C13
30	b	722	CLA	C5-C6-C7-C8
30	A	309	CLA	CBD-CGD-O2D-CED
30	a	706	CLA	CBD-CGD-O2D-CED
31	K	314	KC1	C2A-CAA-CBA-CGA
31	B	314	KC1	C2A-CAA-CBA-CGA
31	F	314	KC1	C2A-CAA-CBA-CGA
31	J	313	KC1	C2A-CAA-CBA-CGA
30	A	313	CLA	C3-C5-C6-C7
32	G	501	DGD	O6D-C5D-C6D-O5D
29	J	305	UIX	C11-C13-C14-C23
32	G	521	DGD	O1B-C1B-O2G-C2G
30	a	722	CLA	C2A-CAA-CBA-CGA
30	b	727	CLA	C2A-CAA-CBA-CGA
30	L	312	CLA	C2A-CAA-CBA-CGA
30	I	306	CLA	CBA-CGA-O2A-C1
30	b	716	CLA	CBA-CGA-O2A-C1
30	B	313	CLA	CBA-CGA-O2A-C1
30	L	309	CLA	CBA-CGA-O2A-C1
30	I	311	CLA	C5-C6-C7-C8
30	h	202	CLA	C5-C6-C7-C8
30	l	311	CLA	C8-C10-C11-C12
30	a	705	CLA	C5-C6-C7-C8
30	a	723	CLA	C5-C6-C7-C8
30	b	707	CLA	C15-C16-C17-C18
30	B	311	CLA	C13-C15-C16-C17
30	I	313	CLA	C3-C5-C6-C7
30	L	314	CLA	O1D-CGD-O2D-CED
30	I	308	CLA	C8-C10-C11-C12
30	l	311	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	B	311	CLA	C10-C11-C12-C13
33	j	101	LMG	O6-C5-C6-O5
30	I	312	CLA	C5-C6-C7-C8
30	I	316	CLA	C5-C6-C7-C8
30	a	723	CLA	C15-C16-C17-C18
31	I	314	KC1	CAA-CBA-CGA-O2A
30	l	305	CLA	C2-C3-C5-C6
30	l	311	CLA	C2-C3-C5-C6
30	G	512	CLA	O1D-CGD-O2D-CED
38	b	729	PQN	C20-C21-C22-C23
30	b	709	CLA	C3-C5-C6-C7
30	b	720	CLA	C3-C5-C6-C7
30	L	313	CLA	C3-C5-C6-C7
30	L	314	CLA	C3-C5-C6-C7
32	G	521	DGD	C2B-C1B-O2G-C2G
30	a	723	CLA	O1D-CGD-O2D-CED
33	P	201	LMG	O9-C10-O7-C8
30	K	312	CLA	O2A-C1-C2-C3
32	G	521	DGD	C2D-C1D-O3G-C3G
33	I	318	LMG	C2-C1-O1-C7
33	j	101	LMG	C2-C1-O1-C7
35	A	318	SQD	C2-C1-O6-C44
32	G	521	DGD	C1A-C2A-C3A-C4A
30	m	202	CLA	C11-C12-C13-C15
30	B	309	CLA	C15-C16-C17-C18
34	D	307	PID	C19-C20-C21-CM5
34	F	305	PID	C19-C20-C21-CM5
31	M	307	KC1	CAA-CBA-CGA-O1A
31	O	312	KC1	CAA-CBA-CGA-O2A
30	a	716	CLA	CBD-CGD-O2D-CED
30	a	707	CLA	C8-C10-C11-C12
28	K	305	DD6	C12-C11-C13-C14
28	K	318	DD6	C12-C11-C13-C14
28	A	301	DD6	C12-C11-C13-C14
28	b	731	DD6	C12-C11-C13-C14
28	B	302	DD6	C12-C11-C13-C14
28	J	304	DD6	C12-C11-C13-C14
28	M	303	DD6	C12-C11-C13-C14
29	J	305	UIX	C7-C10-C11-C12
28	K	318	DD6	C10-C11-C13-C14
28	A	301	DD6	C10-C11-C13-C14
28	M	303	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
29	J	305	UIX	C7-C10-C11-C13
30	f	303	CLA	C2A-CAA-CBA-CGA
30	j	106	CLA	C2A-CAA-CBA-CGA
30	a	717	CLA	C2A-CAA-CBA-CGA
30	B	309	CLA	C2A-CAA-CBA-CGA
30	B	317	CLA	C2A-CAA-CBA-CGA
30	F	311	CLA	C2A-CAA-CBA-CGA
30	J	315	CLA	C2A-CAA-CBA-CGA
30	N	310	CLA	C2A-CAA-CBA-CGA
30	P	215	CLA	C2A-CAA-CBA-CGA
34	F	305	PID	C16-C17-C18-C19
33	B	318	LMG	C7-C8-O7-C10
30	G	512	CLA	C11-C12-C13-C14
30	h	202	CLA	C6-C7-C8-C9
30	B	311	CLA	C16-C17-C18-C20
30	B	312	CLA	O1D-CGD-O2D-CED
38	a	732	PQN	C13-C15-C16-C17
30	G	513	CLA	C5-C6-C7-C8
34	D	306	PID	C19-C20-C21-C22
34	D	307	PID	C19-C20-C21-C22
34	F	305	PID	C19-C20-C21-C22
32	y	201	DGD	O6D-C1D-O3G-C3G
32	G	521	DGD	O6D-C1D-O3G-C3G
35	A	318	SQD	O5-C1-O6-C44
31	P	211	KC1	CAA-CBA-CGA-O1A
30	D	309	CLA	CBD-CGD-O2D-CED
31	N	308	KC1	CBD-CGD-O2D-CED
30	I	309	CLA	C3-C5-C6-C7
30	I	316	CLA	C6-C7-C8-C9
30	G	512	CLA	C11-C12-C13-C15
30	j	104	CLA	C6-C7-C8-C10
30	b	708	CLA	C16-C17-C18-C20
30	b	715	CLA	C11-C12-C13-C15
30	b	717	CLA	C16-C17-C18-C20
30	B	311	CLA	C16-C17-C18-C19
30	J	307	CLA	C16-C17-C18-C19
38	a	732	PQN	C26-C27-C28-C29
30	L	309	CLA	O1A-CGA-O2A-C1
30	I	311	CLA	O1D-CGD-O2D-CED
34	D	307	PID	C17-C18-C19-C20
34	O	305	PID	C15-C16-C17-C18
33	D	317	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	A	314	KC1	CAA-CBA-CGA-O1A
30	K	313	CLA	O1A-CGA-O2A-C1
30	B	301	CLA	CBA-CGA-O2A-C1
33	I	318	LMG	C29-C30-C31-C32
28	I	302	DD6	C27-C29-C30-C31
28	J	302	DD6	C27-C29-C30-C31
33	D	317	LMG	C32-C33-C34-C35
32	G	501	DGD	C4D-C5D-C6D-O5D
30	f	301	CLA	C4B-C3B-CAB-CBB
30	l	313	CLA	C4B-C3B-CAB-CBB
30	a	708	CLA	C4B-C3B-CAB-CBB
30	B	317	CLA	C4B-C3B-CAB-CBB
30	F	308	CLA	C4B-C3B-CAB-CBB
30	J	310	CLA	C4B-C3B-CAB-CBB
30	N	309	CLA	C4B-C3B-CAB-CBB
30	h	202	CLA	C6-C7-C8-C10
30	j	104	CLA	C6-C7-C8-C9
30	l	311	CLA	C16-C17-C18-C20
30	b	717	CLA	C16-C17-C18-C19
30	B	301	CLA	C11-C12-C13-C14
30	J	307	CLA	C16-C17-C18-C20
30	L	313	CLA	C6-C7-C8-C10
38	a	732	PQN	C26-C27-C28-C30
30	I	308	CLA	C2A-CAA-CBA-CGA
30	I	319	CLA	C2A-CAA-CBA-CGA
30	D	312	CLA	C2A-CAA-CBA-CGA
30	L	308	CLA	C2A-CAA-CBA-CGA
32	l	301	DGD	C2B-C3B-C4B-C5B
30	A	312	CLA	C5-C6-C7-C8
30	a	735	CLA	C15-C16-C17-C18
33	K	317	LMG	C4-C5-C6-O5
30	b	707	CLA	C11-C10-C8-C7
33	K	317	LMG	C32-C33-C34-C35
30	I	313	CLA	CBA-CGA-O2A-C1
30	L	308	CLA	C2C-C3C-CAC-CBC
30	j	104	CLA	C5-C6-C7-C8
30	a	702	CLA	C8-C10-C11-C12
33	K	317	LMG	C34-C35-C36-C37
31	D	315	KC1	CAA-CBA-CGA-O1A
31	J	313	KC1	CAA-CBA-CGA-O1A
31	L	307	KC1	CAA-CBA-CGA-O1A
31	N	306	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	f	302	CLA	C3A-C2A-CAA-CBA
30	a	718	CLA	C3A-C2A-CAA-CBA
30	a	719	CLA	C3A-C2A-CAA-CBA
30	a	725	CLA	C3A-C2A-CAA-CBA
30	a	727	CLA	C3A-C2A-CAA-CBA
30	a	735	CLA	C3A-C2A-CAA-CBA
30	B	308	CLA	C3A-C2A-CAA-CBA
30	D	314	CLA	C3A-C2A-CAA-CBA
30	F	310	CLA	C3A-C2A-CAA-CBA
30	J	308	CLA	C3A-C2A-CAA-CBA
30	L	317	CLA	C3A-C2A-CAA-CBA
30	N	310	CLA	C3A-C2A-CAA-CBA
30	O	314	CLA	C3A-C2A-CAA-CBA
30	P	215	CLA	C3A-C2A-CAA-CBA
30	a	709	CLA	O1D-CGD-O2D-CED
30	J	301	CLA	O1D-CGD-O2D-CED
30	L	317	CLA	O1D-CGD-O2D-CED
38	a	732	PQN	C18-C20-C21-C22
30	a	705	CLA	O1D-CGD-O2D-CED
32	I	317	DGD	C1B-C2B-C3B-C4B
30	l	311	CLA	C16-C17-C18-C19
30	b	715	CLA	C11-C12-C13-C14
30	B	301	CLA	C11-C12-C13-C15
30	L	313	CLA	C6-C7-C8-C9
32	G	521	DGD	O6D-C5D-C6D-O5D
30	I	306	CLA	O1A-CGA-O2A-C1
30	b	716	CLA	O1A-CGA-O2A-C1
30	B	313	CLA	O1A-CGA-O2A-C1
30	J	314	CLA	O1D-CGD-O2D-CED
30	b	717	CLA	CBD-CGD-O2D-CED
33	b	733	LMG	C36-C37-C38-C39
30	b	727	CLA	O1D-CGD-O2D-CED
30	b	704	CLA	C4C-C3C-CAC-CBC
30	b	703	CLA	CBA-CGA-O2A-C1
30	b	724	CLA	C3-C5-C6-C7
33	b	733	LMG	C33-C34-C35-C36
30	M	317	CLA	O1A-CGA-O2A-C1
33	B	318	LMG	C31-C32-C33-C34
33	K	317	LMG	C31-C32-C33-C34
32	G	521	DGD	C4D-C5D-C6D-O5D
30	A	308	CLA	O1D-CGD-O2D-CED
30	A	320	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	b	712	CLA	O1D-CGD-O2D-CED
33	D	317	LMG	C33-C34-C35-C36
30	I	316	CLA	C6-C7-C8-C10
30	a	728	CLA	C6-C7-C8-C9
30	b	708	CLA	C16-C17-C18-C19
30	f	301	CLA	C2B-C3B-CAB-CBB
30	a	708	CLA	C2B-C3B-CAB-CBB
30	B	317	CLA	C2B-C3B-CAB-CBB
30	F	311	CLA	C2B-C3B-CAB-CBB
30	J	301	CLA	C2B-C3B-CAB-CBB
30	J	310	CLA	C2B-C3B-CAB-CBB
30	L	318	CLA	C2B-C3B-CAB-CBB
37	i	201	BCR	C1-C6-C7-C8
37	b	730	BCR	C1-C6-C7-C8
37	b	730	BCR	C5-C6-C7-C8
33	b	733	LMG	C37-C38-C39-C40
30	B	301	CLA	CBD-CGD-O2D-CED
30	G	519	CLA	O1D-CGD-O2D-CED
30	G	510	CLA	CBA-CGA-O2A-C1
30	h	202	CLA	CBA-CGA-O2A-C1
30	a	705	CLA	CBA-CGA-O2A-C1
30	a	704	CLA	C15-C16-C17-C18
30	J	312	CLA	C3-C5-C6-C7
30	I	306	CLA	O1D-CGD-O2D-CED
30	f	303	CLA	O1D-CGD-O2D-CED
30	l	313	CLA	O1D-CGD-O2D-CED
30	f	302	CLA	C2A-CAA-CBA-CGA
30	b	701	CLA	C2A-CAA-CBA-CGA
30	B	308	CLA	C2A-CAA-CBA-CGA
30	J	316	CLA	C2A-CAA-CBA-CGA
30	M	311	CLA	C2A-CAA-CBA-CGA
30	l	303	CLA	C10-C11-C12-C13
30	I	313	CLA	O1A-CGA-O2A-C1
30	B	301	CLA	O1A-CGA-O2A-C1
30	b	722	CLA	C4-C3-C5-C6
33	b	733	LMG	C32-C33-C34-C35
33	j	101	LMG	C33-C34-C35-C36
33	K	317	LMG	C28-C29-C30-C31
33	D	317	LMG	C10-C11-C12-C13
30	K	311	CLA	CBA-CGA-O2A-C1
30	a	735	CLA	CBA-CGA-O2A-C1
32	l	301	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
30	K	308	CLA	C3-C5-C6-C7
30	b	725	CLA	C3-C5-C6-C7
30	a	723	CLA	C11-C12-C13-C14
30	b	717	CLA	C11-C12-C13-C14
30	b	719	CLA	O1A-CGA-O2A-C1
33	I	320	LMG	O6-C1-O1-C7
33	D	317	LMG	O6-C5-C6-O5
30	J	309	CLA	O1D-CGD-O2D-CED
33	D	317	LMG	C30-C31-C32-C33
30	f	301	CLA	CBA-CGA-O2A-C1
32	G	501	DGD	C2B-C1B-O2G-C2G
39	a	733	LHG	C8-C7-O7-C5
30	l	311	CLA	C10-C11-C12-C13
30	b	712	CLA	C5-C6-C7-C8
39	a	733	LHG	C26-C27-C28-C29
30	a	712	CLA	C10-C11-C12-C13
30	B	311	CLA	C5-C6-C7-C8
28	I	301	DD6	C12-C11-C13-C14
28	I	305	DD6	C7-C6-C8-C9
28	G	502	DD6	C12-C11-C13-C14
30	a	729	CLA	C3-C5-C6-C7
28	I	301	DD6	C10-C11-C13-C14
28	I	305	DD6	C5-C6-C8-C9
30	A	311	CLA	C2A-CAA-CBA-CGA
30	M	316	CLA	C2A-CAA-CBA-CGA
30	I	313	CLA	C6-C7-C8-C9
30	I	313	CLA	C6-C7-C8-C10
30	m	202	CLA	C11-C12-C13-C14
30	a	728	CLA	C6-C7-C8-C10
30	a	735	CLA	C16-C17-C18-C20
31	G	515	KC1	C2B-C3B-CAB-CBB
31	L	307	KC1	C2B-C3B-CAB-CBB
31	O	310	KC1	C2B-C3B-CAB-CBB
33	B	318	LMG	C32-C33-C34-C35
31	G	515	KC1	C2C-C3C-CAC-CBC
30	b	722	CLA	CBD-CGD-O2D-CED
30	a	705	CLA	O1A-CGA-O2A-C1
30	b	701	CLA	C10-C11-C12-C13
30	b	704	CLA	C13-C15-C16-C17
32	L	301	DGD	O6E-C5E-C6E-O5E
38	a	732	PQN	C15-C16-C17-C18
31	K	314	KC1	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	A	306	KC1	C4B-C3B-CAB-CBB
31	F	309	KC1	C4B-C3B-CAB-CBB
31	L	307	KC1	C4B-C3B-CAB-CBB
31	L	315	KC1	C4B-C3B-CAB-CBB
31	M	307	KC1	C4B-C3B-CAB-CBB
31	N	308	KC1	C4B-C3B-CAB-CBB
31	P	211	KC1	C4B-C3B-CAB-CBB
31	P	216	KC1	C4B-C3B-CAB-CBB
30	A	310	CLA	C16-C17-C18-C20
31	M	314	KC1	CAA-CBA-CGA-O2A
31	O	310	KC1	CAA-CBA-CGA-O1A
30	b	703	CLA	O1A-CGA-O2A-C1
30	a	710	CLA	O1D-CGD-O2D-CED
30	B	316	CLA	O1D-CGD-O2D-CED
33	I	318	LMG	C30-C31-C32-C33
33	K	317	LMG	C30-C31-C32-C33
33	B	318	LMG	C33-C34-C35-C36
33	I	318	LMG	C14-C15-C16-C17
30	l	304	CLA	C8-C10-C11-C12
30	a	731	CLA	C8-C10-C11-C12
33	I	320	LMG	C16-C17-C18-C19
30	I	316	CLA	C2A-CAA-CBA-CGA
30	G	510	CLA	C2A-CAA-CBA-CGA
30	G	514	CLA	C2A-CAA-CBA-CGA
30	m	202	CLA	C2A-CAA-CBA-CGA
30	b	708	CLA	C2A-CAA-CBA-CGA
30	b	718	CLA	C2A-CAA-CBA-CGA
30	b	723	CLA	C2A-CAA-CBA-CGA
30	D	309	CLA	C2A-CAA-CBA-CGA
30	J	312	CLA	C2A-CAA-CBA-CGA
33	K	317	LMG	C12-C13-C14-C15
30	b	711	CLA	C5-C6-C7-C8
38	b	729	PQN	C23-C25-C26-C27
30	b	712	CLA	C6-C7-C8-C9
30	b	712	CLA	C6-C7-C8-C10
30	K	311	CLA	O1A-CGA-O2A-C1
30	G	510	CLA	O1A-CGA-O2A-C1
30	h	202	CLA	O1A-CGA-O2A-C1
30	I	315	CLA	C1A-C2A-CAA-CBA
30	A	319	CLA	C1A-C2A-CAA-CBA
30	f	302	CLA	C1A-C2A-CAA-CBA
30	l	312	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	a	707	CLA	C1A-C2A-CAA-CBA
30	a	711	CLA	C1A-C2A-CAA-CBA
30	a	712	CLA	C1A-C2A-CAA-CBA
30	a	715	CLA	C1A-C2A-CAA-CBA
30	a	717	CLA	C1A-C2A-CAA-CBA
30	a	719	CLA	C1A-C2A-CAA-CBA
30	a	720	CLA	C1A-C2A-CAA-CBA
30	a	725	CLA	C1A-C2A-CAA-CBA
30	a	727	CLA	C1A-C2A-CAA-CBA
30	a	735	CLA	C1A-C2A-CAA-CBA
30	b	706	CLA	C1A-C2A-CAA-CBA
30	b	720	CLA	C1A-C2A-CAA-CBA
30	b	721	CLA	C1A-C2A-CAA-CBA
30	b	723	CLA	C1A-C2A-CAA-CBA
30	D	314	CLA	C1A-C2A-CAA-CBA
30	F	308	CLA	C1A-C2A-CAA-CBA
30	H	309	CLA	C1A-C2A-CAA-CBA
30	J	301	CLA	C1A-C2A-CAA-CBA
30	J	308	CLA	C1A-C2A-CAA-CBA
30	L	312	CLA	C1A-C2A-CAA-CBA
30	L	313	CLA	C1A-C2A-CAA-CBA
30	L	317	CLA	C1A-C2A-CAA-CBA
30	M	313	CLA	C1A-C2A-CAA-CBA
30	N	305	CLA	C1A-C2A-CAA-CBA
30	O	314	CLA	C1A-C2A-CAA-CBA
30	P	215	CLA	C1A-C2A-CAA-CBA
32	I	317	DGD	O6E-C5E-C6E-O5E
29	J	305	UIX	C17-C18-O2-C27
32	l	301	DGD	O1A-C1A-O1G-C1G
33	D	317	LMG	C13-C14-C15-C16
30	l	304	CLA	C3-C5-C6-C7
30	I	312	CLA	C12-C13-C15-C16
30	G	510	CLA	C11-C12-C13-C15
30	G	519	CLA	C6-C7-C8-C10
30	G	519	CLA	C11-C10-C8-C7
30	l	313	CLA	C6-C7-C8-C10
30	a	702	CLA	C12-C13-C15-C16
30	a	709	CLA	C12-C13-C15-C16
30	a	717	CLA	C11-C10-C8-C7
30	b	703	CLA	C11-C10-C8-C7
30	b	709	CLA	C11-C10-C8-C7
30	B	301	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
30	B	309	CLA	C6-C7-C8-C10
30	B	309	CLA	C11-C12-C13-C15
30	B	311	CLA	C11-C12-C13-C15
30	B	311	CLA	C12-C13-C15-C16
30	B	313	CLA	C11-C10-C8-C7
30	J	307	CLA	C11-C10-C8-C7
30	N	305	CLA	C11-C12-C13-C15
30	P	210	CLA	C11-C12-C13-C15
30	l	303	CLA	C16-C17-C18-C20
30	A	310	CLA	C8-C10-C11-C12
30	f	301	CLA	O1A-CGA-O2A-C1
30	a	735	CLA	O1A-CGA-O2A-C1
30	I	310	CLA	CBD-CGD-O2D-CED
31	A	306	KC1	CAA-CBA-CGA-O2A
30	G	512	CLA	C5-C6-C7-C8
30	a	731	CLA	C15-C16-C17-C18
30	b	701	CLA	C5-C6-C7-C8
30	b	707	CLA	C5-C6-C7-C8
30	b	709	CLA	C2-C3-C5-C6
30	a	721	CLA	C8-C10-C11-C12
30	b	704	CLA	C10-C11-C12-C13
30	b	717	CLA	C13-C15-C16-C17
30	I	307	CLA	C2A-CAA-CBA-CGA
30	I	313	CLA	C2A-CAA-CBA-CGA
30	I	315	CLA	C2A-CAA-CBA-CGA
30	A	310	CLA	C2A-CAA-CBA-CGA
30	H	307	CLA	C2A-CAA-CBA-CGA
30	J	301	CLA	C2A-CAA-CBA-CGA
30	G	510	CLA	C11-C12-C13-C14
30	G	512	CLA	C11-C10-C8-C9
30	A	310	CLA	C14-C13-C15-C16
30	a	709	CLA	C14-C13-C15-C16
30	B	309	CLA	C11-C12-C13-C14
30	N	305	CLA	C11-C12-C13-C14
30	P	210	CLA	C11-C12-C13-C14
33	b	734	LMG	O6-C5-C6-O5
37	l	306	BCR	C13-C14-C15-C16
30	b	705	CLA	CBA-CGA-O2A-C1
30	L	308	CLA	CBA-CGA-O2A-C1
32	G	501	DGD	O1B-C1B-O2G-C2G
30	I	310	CLA	O2A-C1-C2-C3
32	G	501	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
33	K	317	LMG	C7-C8-C9-O8
33	b	734	LMG	O1-C7-C8-C9
30	a	735	CLA	C3-C5-C6-C7
30	G	514	CLA	O1D-CGD-O2D-CED
33	D	317	LMG	C14-C15-C16-C17
30	D	311	CLA	CBA-CGA-O2A-C1
30	a	735	CLA	O1D-CGD-O2D-CED
30	A	312	CLA	CBA-CGA-O2A-C1
30	b	704	CLA	CBA-CGA-O2A-C1
33	b	734	LMG	C29-C28-O8-C9
30	a	721	CLA	C16-C17-C18-C19
30	b	711	CLA	C6-C7-C8-C9
33	b	733	LMG	C15-C16-C17-C18
30	O	308	CLA	O1D-CGD-O2D-CED
30	l	310	CLA	CHA-CBD-CGD-O1D
30	l	310	CLA	CHA-CBD-CGD-O2D
34	D	306	PID	C19-C20-C21-CM5
34	O	305	PID	CM4-C14-C15-C16
30	a	729	CLA	C5-C6-C7-C8
33	D	317	LMG	C18-C19-C20-C21
28	G	505	DD6	C12-C11-C13-C14
28	L	305	DD6	C12-C11-C13-C14
30	A	310	CLA	C16-C17-C18-C19
30	l	303	CLA	C16-C17-C18-C19
28	I	303	DD6	C10-C11-C13-C14
28	G	505	DD6	C10-C11-C13-C14
30	a	723	CLA	C2A-CAA-CBA-CGA
30	f	303	CLA	CBA-CGA-O2A-C1
33	b	733	LMG	C14-C15-C16-C17
30	l	311	CLA	C13-C15-C16-C17
30	b	704	CLA	C15-C16-C17-C18
32	G	521	DGD	C1B-C2B-C3B-C4B
30	O	311	CLA	O1D-CGD-O2D-CED
30	I	312	CLA	CBA-CGA-O2A-C1
31	O	315	KC1	CAA-CBA-CGA-O2A
30	l	313	CLA	C15-C16-C17-C18
30	a	731	CLA	C5-C6-C7-C8
33	K	317	LMG	C29-C30-C31-C32
29	P	207	UIX	C11-C13-C14-C23
30	a	721	CLA	C16-C17-C18-C20
30	J	306	CLA	CBA-CGA-O2A-C1
30	L	308	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
34	O	305	PID	C13-C14-C15-C16
30	a	713	CLA	C8-C10-C11-C12
32	l	301	DGD	C3B-C4B-C5B-C6B
30	B	309	CLA	C4-C3-C5-C6
30	F	315	CLA	O1D-CGD-O2D-CED
32	G	521	DGD	O2G-C2G-C3G-O3G
30	K	308	CLA	C6-C7-C8-C9
33	I	318	LMG	C15-C16-C17-C18
33	I	320	LMG	C32-C33-C34-C35
30	P	210	CLA	C3-C5-C6-C7
30	M	310	CLA	O2A-C1-C2-C3
30	P	210	CLA	CBD-CGD-O2D-CED
30	B	313	CLA	O1D-CGD-O2D-CED
30	K	306	CLA	CBA-CGA-O2A-C1
30	a	724	CLA	CBA-CGA-O2A-C1
30	a	726	CLA	CBA-CGA-O2A-C1
30	b	712	CLA	CBA-CGA-O2A-C1
30	P	209	CLA	CBA-CGA-O2A-C1
30	l	303	CLA	CBD-CGD-O2D-CED
30	K	310	CLA	C5-C6-C7-C8
30	J	310	CLA	O1D-CGD-O2D-CED
30	a	723	CLA	C10-C11-C12-C13
30	A	309	CLA	O1D-CGD-O2D-CED
30	I	311	CLA	C6-C7-C8-C10
30	f	301	CLA	C6-C7-C8-C10
30	A	311	CLA	CBD-CGD-O2D-CED
30	H	305	CLA	C4-C3-C5-C6
30	a	707	CLA	C2-C3-C5-C6
30	b	728	CLA	CBA-CGA-O2A-C1
28	K	301	DD6	C27-C29-C30-C31
28	K	305	DD6	C27-C29-C30-C31
28	K	318	DD6	C27-C29-C30-C31
28	G	502	DD6	C27-C29-C30-C31
28	G	508	DD6	C27-C29-C30-C31
28	A	303	DD6	C27-C29-C30-C31
28	h	203	DD6	C27-C29-C30-C31
28	B	303	DD6	C27-C29-C30-C31
28	D	303	DD6	C27-C29-C30-C31
28	F	303	DD6	C27-C29-C30-C31
30	b	711	CLA	C3-C5-C6-C7
30	I	312	CLA	C11-C12-C13-C14
30	G	519	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	l	313	CLA	C6-C7-C8-C9
30	m	202	CLA	C6-C7-C8-C9
30	a	707	CLA	C11-C12-C13-C14
30	a	717	CLA	C11-C10-C8-C9
30	b	703	CLA	C11-C10-C8-C9
30	b	705	CLA	C14-C13-C15-C16
30	b	709	CLA	C11-C10-C8-C9
30	B	309	CLA	C6-C7-C8-C9
38	a	732	PQN	C21-C22-C23-C24
39	a	733	LHG	C2-C3-O3-P
30	K	307	CLA	C4B-C3B-CAB-CBB
30	G	516	CLA	C4B-C3B-CAB-CBB
30	h	202	CLA	C4B-C3B-CAB-CBB
30	a	718	CLA	C4B-C3B-CAB-CBB
30	a	725	CLA	C4B-C3B-CAB-CBB
30	a	726	CLA	C4B-C3B-CAB-CBB
30	b	726	CLA	C4B-C3B-CAB-CBB
30	B	311	CLA	C4B-C3B-CAB-CBB
30	B	312	CLA	C4B-C3B-CAB-CBB
30	H	311	CLA	C4B-C3B-CAB-CBB
30	J	308	CLA	C4B-C3B-CAB-CBB
30	L	316	CLA	C4B-C3B-CAB-CBB
30	M	317	CLA	C4B-C3B-CAB-CBB
30	O	308	CLA	C4B-C3B-CAB-CBB
30	L	318	CLA	CAA-CBA-CGA-O2A
30	a	724	CLA	C5-C6-C7-C8
33	I	320	LMG	C17-C18-C19-C20
30	I	310	CLA	C2A-CAA-CBA-CGA
30	G	512	CLA	C11-C10-C8-C7
30	A	310	CLA	C12-C13-C15-C16
30	m	202	CLA	C6-C7-C8-C10
30	a	709	CLA	C11-C10-C8-C7
30	a	713	CLA	C11-C10-C8-C7
30	a	717	CLA	C6-C7-C8-C10
30	a	725	CLA	C11-C10-C8-C7
30	b	704	CLA	C12-C13-C15-C16
30	J	309	CLA	C6-C7-C8-C10
30	a	720	CLA	C10-C11-C12-C13
30	b	704	CLA	O1A-CGA-O2A-C1
33	b	733	LMG	C38-C39-C40-C41
30	A	312	CLA	O1A-CGA-O2A-C1
30	b	705	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	I	310	CLA	C3A-C2A-CAA-CBA
30	b	706	CLA	C3A-C2A-CAA-CBA
30	b	709	CLA	C4-C3-C5-C6
30	b	724	CLA	C3A-C2A-CAA-CBA
30	B	317	CLA	C3A-C2A-CAA-CBA
28	I	305	DD6	C1-C2-C3-C4
28	I	305	DD6	C3-C4-C5-C6
28	I	303	DD6	C12-C11-C13-C14
37	j	102	BCR	C36-C18-C19-C20
30	b	714	CLA	CAA-CBA-CGA-O2A
30	I	312	CLA	O1A-CGA-O2A-C1
31	O	312	KC1	CAA-CBA-CGA-O1A
28	G	504	DD6	C5-C6-C8-C9
28	L	305	DD6	C10-C11-C13-C14
30	b	706	CLA	O2A-C1-C2-C3
32	y	201	DGD	C1G-C2G-C3G-O3G
33	I	318	LMG	C7-C8-C9-O8
33	B	318	LMG	C7-C8-C9-O8
33	D	317	LMG	C7-C8-C9-O8
30	a	726	CLA	C3-C5-C6-C7
30	I	311	CLA	C6-C7-C8-C9
30	a	735	CLA	C16-C17-C18-C19
33	I	318	LMG	C12-C13-C14-C15
30	a	707	CLA	C4-C3-C5-C6
30	a	716	CLA	O1D-CGD-O2D-CED
30	D	309	CLA	O1D-CGD-O2D-CED
30	f	301	CLA	C6-C7-C8-C9
33	j	101	LMG	C31-C32-C33-C34
30	a	718	CLA	C2B-C3B-CAB-CBB
30	b	726	CLA	C2B-C3B-CAB-CBB
30	O	308	CLA	C2B-C3B-CAB-CBB
30	B	316	CLA	CBA-CGA-O2A-C1
30	a	721	CLA	C5-C6-C7-C8
32	G	521	DGD	O1G-C1G-C2G-O2G
32	j	103	DGD	O1G-C1G-C2G-O2G
32	l	301	DGD	O2G-C2G-C3G-O3G
33	I	318	LMG	O1-C7-C8-O7
33	I	318	LMG	O7-C8-C9-O8
33	j	101	LMG	O7-C8-C9-O8
33	b	734	LMG	O7-C8-C9-O8
33	I	320	LMG	C31-C32-C33-C34
31	P	211	KC1	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	G	515	KC1	CAA-CBA-CGA-O2A
33	b	733	LMG	C28-C29-C30-C31
30	B	311	CLA	C4-C3-C5-C6
30	B	311	CLA	C2-C3-C5-C6
33	I	318	LMG	C32-C33-C34-C35
30	K	311	CLA	C2-C1-O2A-CGA
30	a	706	CLA	O1D-CGD-O2D-CED
30	a	709	CLA	C11-C10-C8-C9
30	a	713	CLA	C11-C10-C8-C9
30	a	725	CLA	C11-C10-C8-C9
30	b	704	CLA	C11-C12-C13-C14
30	b	728	CLA	C6-C7-C8-C9
30	B	313	CLA	C11-C10-C8-C9
30	J	301	CLA	C11-C10-C8-C9
30	b	708	CLA	C5-C6-C7-C8
30	l	313	CLA	C2C-C3C-CAC-CBC
34	D	306	PID	C15-C16-C17-C18
33	b	734	LMG	C11-C12-C13-C14
30	B	310	CLA	C6-C7-C8-C9
30	a	704	CLA	C5-C6-C7-C8
30	b	717	CLA	O1D-CGD-O2D-CED
30	a	713	CLA	C3-C5-C6-C7
30	b	722	CLA	C2-C3-C5-C6
30	a	724	CLA	C13-C15-C16-C17
34	D	306	PID	CM4-C14-C15-C16
30	B	301	CLA	O1D-CGD-O2D-CED
30	b	711	CLA	C6-C7-C8-C10
28	L	306	DD6	C12-C11-C13-C14
29	K	302	UIX	C7-C10-C11-C12
30	A	310	CLA	C11-C10-C8-C7
30	l	305	CLA	C11-C12-C13-C15
30	l	313	CLA	C11-C12-C13-C15
30	b	704	CLA	C6-C7-C8-C10
30	b	705	CLA	C11-C12-C13-C15
30	b	707	CLA	C6-C7-C8-C10
30	b	728	CLA	C6-C7-C8-C10
30	B	309	CLA	C12-C13-C15-C16
30	H	305	CLA	C11-C12-C13-C15
30	J	301	CLA	C11-C10-C8-C7
33	I	318	LMG	C31-C32-C33-C34
30	b	719	CLA	CBD-CGD-O2D-CED
28	K	305	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
28	b	731	DD6	C10-C11-C13-C14
28	L	306	DD6	C10-C11-C13-C14
29	K	302	UIX	C7-C10-C11-C13
37	j	102	BCR	C17-C18-C19-C20
37	m	201	BCR	C11-C12-C13-C14
30	a	717	CLA	CBA-CGA-O2A-C1
30	a	720	CLA	CBA-CGA-O2A-C1
30	b	712	CLA	O1A-CGA-O2A-C1
31	L	315	KC1	C2C-C3C-CAC-CBC
30	l	310	CLA	C2A-CAA-CBA-CGA
30	b	712	CLA	C2A-CAA-CBA-CGA
30	B	310	CLA	C6-C7-C8-C10
30	I	307	CLA	CBD-CGD-O2D-CED
30	K	306	CLA	O1A-CGA-O2A-C1
30	b	728	CLA	O1A-CGA-O2A-C1
32	G	521	DGD	C1G-C2G-O2G-C1B
33	P	201	LMG	C28-C29-C30-C31
30	a	724	CLA	O1A-CGA-O2A-C1
30	P	209	CLA	O1A-CGA-O2A-C1
30	G	519	CLA	C10-C11-C12-C13
30	a	726	CLA	O1A-CGA-O2A-C1
30	a	702	CLA	C15-C16-C17-C18
30	b	722	CLA	O1D-CGD-O2D-CED
34	D	306	PID	C13-C14-C15-C16
32	G	521	DGD	O1G-C1G-C2G-C3G
32	l	301	DGD	C1G-C2G-C3G-O3G
33	I	318	LMG	O1-C7-C8-C9
33	b	734	LMG	C7-C8-C9-O8
31	G	515	KC1	C4B-C3B-CAB-CBB
31	B	314	KC1	C4B-C3B-CAB-CBB
31	D	310	KC1	C4B-C3B-CAB-CBB
31	F	314	KC1	C4B-C3B-CAB-CBB
31	H	306	KC1	C4B-C3B-CAB-CBB
31	H	310	KC1	C4B-C3B-CAB-CBB
31	J	313	KC1	C4B-C3B-CAB-CBB
31	M	314	KC1	C4B-C3B-CAB-CBB
31	N	306	KC1	C4B-C3B-CAB-CBB
31	N	311	KC1	C4B-C3B-CAB-CBB
31	O	310	KC1	C4B-C3B-CAB-CBB
30	K	310	CLA	C2A-CAA-CBA-CGA
29	O	306	UIX	C25-C28-C32-C33
30	a	722	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	a	703	CLA	C3-C5-C6-C7
32	G	501	DGD	O2G-C2G-C3G-O3G
33	B	318	LMG	O7-C8-C9-O8
30	G	510	CLA	C14-C13-C15-C16
30	A	310	CLA	C11-C10-C8-C9
30	b	727	CLA	C11-C12-C13-C14
30	H	305	CLA	C11-C12-C13-C14
30	J	308	CLA	CAA-CBA-CGA-O2A
33	I	320	LMG	C14-C15-C16-C17
34	N	301	PID	C12-C13-C14-C15
34	O	305	PID	C12-C13-C14-C15
33	I	318	LMG	C11-C12-C13-C14
30	N	305	CLA	C3-C5-C6-C7
28	D	303	DD6	C11-C10-C9-C8
30	M	312	CLA	O2A-C1-C2-C3
30	a	709	CLA	C8-C10-C11-C12
39	a	733	LHG	C24-C25-C26-C27
30	K	311	CLA	C4-C3-C5-C6
38	b	729	PQN	C14-C13-C15-C16
30	a	704	CLA	C2A-CAA-CBA-CGA
30	b	705	CLA	C2A-CAA-CBA-CGA
30	L	309	CLA	C2A-CAA-CBA-CGA
33	b	733	LMG	C35-C36-C37-C38
30	A	313	CLA	C6-C7-C8-C9
30	N	305	CLA	C16-C17-C18-C20
30	I	321	CLA	C4C-C3C-CAC-CBC
31	P	213	KC1	C2C-C3C-CAC-CBC
30	b	720	CLA	C5-C6-C7-C8
28	K	304	DD6	C27-C29-C30-C31
28	H	303	DD6	C27-C29-C30-C31
28	L	306	DD6	C27-C29-C30-C31
30	J	301	CLA	C8-C10-C11-C12
28	A	302	DD6	C7-C6-C8-C9
30	I	306	CLA	C4B-C3B-CAB-CBB
30	I	307	CLA	C4B-C3B-CAB-CBB
30	I	312	CLA	C4B-C3B-CAB-CBB
30	K	306	CLA	C4B-C3B-CAB-CBB
30	K	311	CLA	C4B-C3B-CAB-CBB
30	G	518	CLA	C4B-C3B-CAB-CBB
30	l	303	CLA	C4B-C3B-CAB-CBB
30	a	707	CLA	C4B-C3B-CAB-CBB
30	a	713	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	a	716	CLA	C4B-C3B-CAB-CBB
30	a	724	CLA	C1A-C2A-CAA-CBA
30	a	738	CLA	C4B-C3B-CAB-CBB
30	b	718	CLA	C4B-C3B-CAB-CBB
30	b	719	CLA	C4B-C3B-CAB-CBB
30	b	724	CLA	C4B-C3B-CAB-CBB
30	b	728	CLA	C4B-C3B-CAB-CBB
30	B	316	CLA	C4B-C3B-CAB-CBB
30	D	308	CLA	C4B-C3B-CAB-CBB
30	D	312	CLA	C4B-C3B-CAB-CBB
30	D	314	CLA	C4B-C3B-CAB-CBB
30	H	304	CLA	C4B-C3B-CAB-CBB
30	H	305	CLA	C1A-C2A-CAA-CBA
30	H	309	CLA	C4B-C3B-CAB-CBB
30	L	312	CLA	C4B-C3B-CAB-CBB
30	M	318	CLA	C4B-C3B-CAB-CBB
30	N	304	CLA	C4B-C3B-CAB-CBB
30	N	310	CLA	C4B-C3B-CAB-CBB
30	P	209	CLA	C4B-C3B-CAB-CBB
39	a	733	LHG	C24-C23-O8-C6
30	b	707	CLA	C4-C3-C5-C6
28	G	502	DD6	C10-C11-C13-C14
30	a	721	CLA	C13-C15-C16-C17
30	a	717	CLA	O1A-CGA-O2A-C1
30	a	720	CLA	O1A-CGA-O2A-C1
30	a	725	CLA	C5-C6-C7-C8
39	a	733	LHG	O9-C7-O7-C5
30	a	708	CLA	C2-C3-C5-C6
30	O	311	CLA	C2-C3-C5-C6
30	P	212	CLA	C2-C3-C5-C6
30	I	310	CLA	O1D-CGD-O2D-CED
30	A	310	CLA	C6-C7-C8-C10
30	A	310	CLA	C11-C12-C13-C15
30	l	303	CLA	C11-C12-C13-C15
30	a	722	CLA	C11-C10-C8-C7
30	a	724	CLA	C6-C7-C8-C10
30	b	708	CLA	C11-C10-C8-C7
30	B	301	CLA	C6-C7-C8-C10
30	B	311	CLA	C6-C7-C8-C10
30	N	305	CLA	C12-C13-C15-C16
30	b	709	CLA	C11-C12-C13-C14
30	b	725	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	l	312	CLA	CBA-CGA-O2A-C1
30	a	706	CLA	C3A-C2A-CAA-CBA
30	F	312	CLA	C2C-C3C-CAC-CBC
31	M	314	KC1	C2C-C3C-CAC-CBC
34	D	306	PID	C17-C18-C19-C20
33	P	201	LMG	C10-C11-C12-C13
30	A	311	CLA	O1D-CGD-O2D-CED
30	A	310	CLA	C11-C12-C13-C14
30	l	304	CLA	C6-C7-C8-C9
30	l	311	CLA	C14-C13-C15-C16
30	l	313	CLA	C11-C12-C13-C14
30	b	705	CLA	C11-C12-C13-C14
30	b	707	CLA	C6-C7-C8-C9
30	b	715	CLA	C6-C7-C8-C9
30	B	309	CLA	C14-C13-C15-C16
30	J	309	CLA	C6-C7-C8-C9
30	B	309	CLA	C10-C11-C12-C13
30	K	313	CLA	C6-C7-C8-C10
30	l	303	CLA	O1D-CGD-O2D-CED
30	P	210	CLA	O1D-CGD-O2D-CED
33	b	733	LMG	C31-C32-C33-C34
29	O	306	UIX	C25-C28-C32-C35
30	G	520	CLA	C1-C2-C3-C4
31	K	314	KC1	C1A-C2A-CAA-CBA
31	A	306	KC1	C1A-C2A-CAA-CBA
31	N	306	KC1	C1A-C2A-CAA-CBA
31	N	308	KC1	C1A-C2A-CAA-CBA
31	P	211	KC1	C3A-C2A-CAA-CBA
31	P	216	KC1	C1A-C2A-CAA-CBA
30	b	712	CLA	C3-C5-C6-C7
33	D	317	LMG	O7-C8-C9-O8
30	A	313	CLA	C6-C7-C8-C10
32	G	521	DGD	C1G-C2G-C3G-O3G
32	j	103	DGD	O1G-C1G-C2G-C3G
30	l	313	CLA	C13-C15-C16-C17
30	A	319	CLA	CAA-CBA-CGA-O2A
30	b	703	CLA	CAA-CBA-CGA-O2A
30	K	311	CLA	C2-C3-C5-C6
30	K	310	CLA	CAD-CBD-CGD-O2D
30	G	512	CLA	CAD-CBD-CGD-O2D
30	a	729	CLA	CAD-CBD-CGD-O2D
30	F	311	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	H	312	CLA	CAD-CBD-CGD-O2D
30	P	217	CLA	CAD-CBD-CGD-O2D
34	D	306	PID	O4-C12-C13-C14
34	H	301	PID	O4-C12-C13-C14
34	O	301	PID	O4-C12-C13-C14
34	O	307	PID	O4-C12-C13-C14
33	D	317	LMG	C28-C29-C30-C31
30	b	704	CLA	C16-C17-C18-C20
30	O	313	CLA	C2A-CAA-CBA-CGA
30	b	725	CLA	O1A-CGA-O2A-C1
29	P	207	UIX	C34-C37-C39-C40
30	K	310	CLA	CAD-CBD-CGD-O1D
30	G	512	CLA	CAD-CBD-CGD-O1D
30	j	104	CLA	CHA-CBD-CGD-O1D
30	j	104	CLA	CHA-CBD-CGD-O2D
30	a	707	CLA	CHA-CBD-CGD-O1D
30	a	707	CLA	CHA-CBD-CGD-O2D
30	a	718	CLA	CAD-CBD-CGD-O1D
30	a	719	CLA	CHA-CBD-CGD-O1D
30	a	719	CLA	CHA-CBD-CGD-O2D
30	a	720	CLA	CHA-CBD-CGD-O1D
30	a	721	CLA	CAD-CBD-CGD-O1D
30	a	729	CLA	CAD-CBD-CGD-O1D
30	b	707	CLA	CHA-CBD-CGD-O1D
30	b	717	CLA	CHA-CBD-CGD-O1D
30	B	307	CLA	CHA-CBD-CGD-O2D
30	F	311	CLA	CAD-CBD-CGD-O1D
30	H	312	CLA	CAD-CBD-CGD-O1D
30	J	307	CLA	CAD-CBD-CGD-O1D
30	L	311	CLA	CHA-CBD-CGD-O1D
30	L	311	CLA	CHA-CBD-CGD-O2D
30	M	310	CLA	CHA-CBD-CGD-O1D
30	M	310	CLA	CHA-CBD-CGD-O2D
30	P	217	CLA	CAD-CBD-CGD-O1D
31	P	213	KC1	CHA-CBD-CGD-O1D
39	a	733	LHG	C3-O3-P-O5
39	a	733	LHG	C4-O6-P-O5
30	a	726	CLA	C13-C15-C16-C17
30	K	307	CLA	C2B-C3B-CAB-CBB
30	K	311	CLA	C2B-C3B-CAB-CBB
30	G	516	CLA	C2B-C3B-CAB-CBB
30	l	313	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	B	312	CLA	C2B-C3B-CAB-CBB
30	D	312	CLA	C2B-C3B-CAB-CBB
30	D	314	CLA	C2B-C3B-CAB-CBB
30	F	308	CLA	C2B-C3B-CAB-CBB
30	J	308	CLA	C2B-C3B-CAB-CBB
30	L	312	CLA	C2B-C3B-CAB-CBB
30	L	316	CLA	C2B-C3B-CAB-CBB
30	N	304	CLA	C2B-C3B-CAB-CBB
30	N	309	CLA	C2B-C3B-CAB-CBB
38	b	729	PQN	C12-C13-C15-C16
31	F	309	KC1	C2A-CAA-CBA-CGA
37	m	201	BCR	C11-C12-C13-C35
30	a	703	CLA	C6-C7-C8-C9
30	P	210	CLA	C10-C11-C12-C13
30	N	305	CLA	C16-C17-C18-C19
33	I	318	LMG	C9-C8-O7-C10
30	D	311	CLA	O1A-CGA-O2A-C1
28	I	302	DD6	C6-C8-C9-C10
30	l	303	CLA	C15-C16-C17-C18
30	b	724	CLA	C5-C6-C7-C8
33	b	733	LMG	C34-C35-C36-C37
30	l	304	CLA	C11-C12-C13-C14
30	M	310	CLA	CBA-CGA-O2A-C1
30	M	310	CLA	O1A-CGA-O2A-C1
34	O	305	PID	C16-C17-C18-C19
30	G	513	CLA	C14-C13-C15-C16
30	l	313	CLA	C14-C13-C15-C16
30	a	723	CLA	C14-C13-C15-C16
30	a	726	CLA	C14-C13-C15-C16
30	G	513	CLA	C12-C13-C15-C16
30	l	304	CLA	C11-C10-C8-C7
30	l	313	CLA	C12-C13-C15-C16
30	B	309	CLA	C11-C10-C8-C7
34	D	304	PID	C19-C20-C21-C22
39	a	733	LHG	C23-C24-C25-C26
30	M	316	CLA	O1A-CGA-O2A-C1
30	b	719	CLA	O1D-CGD-O2D-CED
30	b	710	CLA	CBA-CGA-O2A-C1
30	M	316	CLA	CBA-CGA-O2A-C1
33	D	317	LMG	C29-C28-O8-C9
30	A	316	CLA	CAA-CBA-CGA-O2A
30	a	702	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	M	317	CLA	CAA-CBA-CGA-O2A
30	f	303	CLA	O1A-CGA-O2A-C1
30	b	710	CLA	O1A-CGA-O2A-C1
30	B	309	CLA	C2-C3-C5-C6
28	F	303	DD6	C11-C10-C9-C8
33	b	733	LMG	C11-C10-O7-C8
31	M	314	KC1	C4C-C3C-CAC-CBC
33	B	318	LMG	C36-C37-C38-C39
30	b	707	CLA	C2-C1-O2A-CGA
30	a	717	CLA	C4-C3-C5-C6
33	B	318	LMG	C34-C35-C36-C37
30	f	303	CLA	CAA-CBA-CGA-O2A
30	G	513	CLA	C8-C10-C11-C12
33	b	733	LMG	C29-C30-C31-C32
30	K	313	CLA	C6-C7-C8-C9
33	b	733	LMG	C8-C7-O1-C1
32	y	201	DGD	C9B-CAB-CBB-CCB
30	G	512	CLA	C2A-CAA-CBA-CGA
30	L	318	CLA	C2A-CAA-CBA-CGA
30	P	212	CLA	C2A-CAA-CBA-CGA
30	J	307	CLA	C10-C11-C12-C13
28	B	306	DD6	C27-C29-C30-C31
30	b	707	CLA	C16-C17-C18-C20
30	J	306	CLA	O1A-CGA-O2A-C1
30	a	722	CLA	C11-C10-C8-C9
30	B	301	CLA	C6-C7-C8-C9
30	b	728	CLA	C5-C6-C7-C8
30	I	315	CLA	C4B-C3B-CAB-CBB
30	a	721	CLA	C4B-C3B-CAB-CBB
30	J	306	CLA	C4B-C3B-CAB-CBB
39	a	733	LHG	C32-C33-C34-C35
28	G	504	DD6	C24-C25-C26-C27
28	M	302	DD6	C3-C4-C5-C6
30	b	708	CLA	C6-C7-C8-C10
30	b	713	CLA	C11-C10-C8-C7
30	l	305	CLA	C10-C11-C12-C13
33	b	733	LMG	C30-C31-C32-C33
30	I	307	CLA	O1D-CGD-O2D-CED
34	O	305	PID	C28-C27-O6-C30
30	l	304	CLA	C11-C12-C13-C15
30	b	716	CLA	C3A-C2A-CAA-CBA
30	b	719	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	B	307	CLA	C3A-C2A-CAA-CBA
30	F	313	CLA	C3A-C2A-CAA-CBA
30	H	305	CLA	C16-C17-C18-C20
28	I	302	DD6	C9-C10-C11-C12
34	D	304	PID	C19-C20-C21-CM5
37	f	304	BCR	C35-C13-C14-C15
37	l	302	BCR	C20-C21-C22-C37
30	L	308	CLA	C4C-C3C-CAC-CBC
30	O	311	CLA	C4-C3-C5-C6
30	P	212	CLA	C4-C3-C5-C6
30	B	316	CLA	O1A-CGA-O2A-C1
33	b	734	LMG	C14-C15-C16-C17
30	a	721	CLA	C11-C12-C13-C14
30	b	704	CLA	C11-C10-C8-C9
30	b	724	CLA	C11-C10-C8-C9
30	b	724	CLA	C11-C12-C13-C14
30	b	727	CLA	C6-C7-C8-C9
30	N	305	CLA	C14-C13-C15-C16
39	a	733	LHG	C29-C30-C31-C32
33	I	320	LMG	C7-C8-O7-C10
39	a	733	LHG	C4-C5-O7-C7
39	a	733	LHG	C6-C5-O7-C7
32	G	501	DGD	C3A-C4A-C5A-C6A
34	O	305	PID	C26-C27-O6-C30
30	D	308	CLA	CBA-CGA-O2A-C1
33	I	320	LMG	C2-C1-O1-C7
30	G	518	CLA	C2A-CAA-CBA-CGA
30	L	311	CLA	C2A-CAA-CBA-CGA
30	D	308	CLA	O1A-CGA-O2A-C1
28	I	302	DD6	C9-C10-C11-C13
30	I	308	CLA	C1A-C2A-CAA-CBA
30	I	310	CLA	C1A-C2A-CAA-CBA
30	a	706	CLA	C1A-C2A-CAA-CBA
30	b	716	CLA	C1A-C2A-CAA-CBA
30	B	313	CLA	C1A-C2A-CAA-CBA
37	f	304	BCR	C12-C13-C14-C15
37	l	302	BCR	C20-C21-C22-C23
30	I	308	CLA	C10-C11-C12-C13
30	I	306	CLA	C2B-C3B-CAB-CBB
30	I	307	CLA	C2B-C3B-CAB-CBB
30	I	312	CLA	C2B-C3B-CAB-CBB
30	I	315	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	K	306	CLA	C2B-C3B-CAB-CBB
30	K	312	CLA	C2B-C3B-CAB-CBB
30	G	518	CLA	C2B-C3B-CAB-CBB
30	h	202	CLA	C2B-C3B-CAB-CBB
30	l	303	CLA	C2B-C3B-CAB-CBB
30	a	707	CLA	C2B-C3B-CAB-CBB
30	a	712	CLA	C2B-C3B-CAB-CBB
30	a	713	CLA	C2B-C3B-CAB-CBB
30	a	716	CLA	C2B-C3B-CAB-CBB
30	a	721	CLA	C2B-C3B-CAB-CBB
30	a	725	CLA	C2B-C3B-CAB-CBB
30	a	726	CLA	C2B-C3B-CAB-CBB
30	a	738	CLA	C2B-C3B-CAB-CBB
30	b	718	CLA	C2B-C3B-CAB-CBB
30	b	723	CLA	C2B-C3B-CAB-CBB
30	b	724	CLA	C2B-C3B-CAB-CBB
30	b	728	CLA	C2B-C3B-CAB-CBB
30	B	311	CLA	C2B-C3B-CAB-CBB
30	B	316	CLA	C2B-C3B-CAB-CBB
30	D	308	CLA	C2B-C3B-CAB-CBB
30	H	304	CLA	C2B-C3B-CAB-CBB
30	H	309	CLA	C2B-C3B-CAB-CBB
30	J	306	CLA	C2B-C3B-CAB-CBB
30	M	312	CLA	C2B-C3B-CAB-CBB
30	M	317	CLA	C2B-C3B-CAB-CBB
30	M	318	CLA	C2B-C3B-CAB-CBB
30	N	310	CLA	C2B-C3B-CAB-CBB
30	P	209	CLA	C2B-C3B-CAB-CBB
37	j	102	BCR	C23-C24-C25-C30
37	l	306	BCR	C1-C6-C7-C8
37	l	306	BCR	C23-C24-C25-C30
30	a	723	CLA	C3-C5-C6-C7
30	I	315	CLA	C4C-C3C-CAC-CBC
30	L	318	CLA	CAA-CBA-CGA-O1A
28	P	204	DD6	C11-C10-C9-C8
30	a	704	CLA	C11-C10-C8-C7
30	a	735	CLA	C12-C13-C15-C16
30	b	704	CLA	C11-C10-C8-C7
30	b	717	CLA	C12-C13-C15-C16
30	b	724	CLA	C11-C12-C13-C15
30	b	727	CLA	C16-C17-C18-C20
30	a	728	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	D	311	CLA	C2A-CAA-CBA-CGA
30	O	314	CLA	C2-C1-O2A-CGA
32	j	103	DGD	C2A-C3A-C4A-C5A
30	b	707	CLA	C16-C17-C18-C19
34	O	307	PID	C28-C27-O6-C30
30	a	729	CLA	C11-C10-C8-C7
29	G	503	UIX	C36-C38-C40-C41
30	L	311	CLA	C4-C3-C5-C6
30	b	715	CLA	CBA-CGA-O2A-C1
30	H	305	CLA	C2-C3-C5-C6
39	a	733	LHG	O2-C2-C3-O3
31	N	311	KC1	C2A-CAA-CBA-CGA
30	l	303	CLA	C14-C13-C15-C16
30	b	701	CLA	C11-C12-C13-C14
30	b	724	CLA	C14-C13-C15-C16
30	B	311	CLA	C11-C10-C8-C9
28	K	301	DD6	C24-C25-C26-C27
29	J	305	UIX	C26-C30-C34-C37
30	A	310	CLA	C13-C15-C16-C17
30	B	307	CLA	O2A-C1-C2-C3
30	B	316	CLA	C2C-C3C-CAC-CBC
32	G	501	DGD	O1G-C1G-C2G-C3G
30	A	308	CLA	C2A-CAA-CBA-CGA
30	b	725	CLA	C2A-CAA-CBA-CGA
30	L	314	CLA	C2A-CAA-CBA-CGA
28	b	731	DD6	C27-C29-C30-C31
28	B	302	DD6	C27-C29-C30-C31
28	L	302	DD6	C27-C29-C30-C31
28	M	306	DD6	C27-C29-C30-C31
30	b	720	CLA	C4-C3-C5-C6
30	L	313	CLA	C4-C3-C5-C6
30	l	305	CLA	CAA-CBA-CGA-O2A
30	l	308	CLA	C4B-C3B-CAB-CBB
30	l	309	CLA	C4B-C3B-CAB-CBB
30	a	702	CLA	C4B-C3B-CAB-CBB
30	a	712	CLA	C4B-C3B-CAB-CBB
30	b	723	CLA	C4B-C3B-CAB-CBB
30	F	307	CLA	C4B-C3B-CAB-CBB
30	M	312	CLA	C4B-C3B-CAB-CBB
30	I	316	CLA	O1A-CGA-O2A-C1
30	b	715	CLA	O1A-CGA-O2A-C1
39	a	733	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
33	j	101	LMG	C4-C5-C6-O5
30	A	316	CLA	O1A-CGA-O2A-C1
30	B	308	CLA	CAA-CBA-CGA-O2A
30	a	703	CLA	C6-C7-C8-C10
30	b	714	CLA	CAA-CBA-CGA-O1A
30	l	312	CLA	O1A-CGA-O2A-C1
34	D	304	PID	CM4-C14-C15-C16
30	a	729	CLA	CAA-CBA-CGA-O2A
30	a	725	CLA	O1A-CGA-O2A-C1
30	a	710	CLA	C6-C7-C8-C10
30	a	728	CLA	C5-C6-C7-C8
30	a	725	CLA	CBA-CGA-O2A-C1
30	l	303	CLA	C13-C15-C16-C17
30	B	309	CLA	C5-C6-C7-C8
33	b	733	LMG	C17-C18-C19-C20
30	a	709	CLA	C6-C7-C8-C10
30	a	731	CLA	C11-C12-C13-C15
30	H	305	CLA	C16-C17-C18-C19
30	I	312	CLA	C6-C7-C8-C9
30	A	310	CLA	C6-C7-C8-C9
30	a	702	CLA	C11-C12-C13-C14
30	b	717	CLA	C6-C7-C8-C9
32	j	103	DGD	C2G-C3G-O3G-C1D
30	b	720	CLA	C2A-CAA-CBA-CGA
30	J	309	CLA	C2A-CAA-CBA-CGA
30	P	210	CLA	C2A-CAA-CBA-CGA
30	a	703	CLA	C2-C1-O2A-CGA
30	b	725	CLA	C2-C1-O2A-CGA
30	M	309	CLA	C2-C1-O2A-CGA
30	l	311	CLA	C3A-C2A-CAA-CBA
30	H	307	CLA	C3A-C2A-CAA-CBA
30	L	318	CLA	C3A-C2A-CAA-CBA
30	M	311	CLA	C3A-C2A-CAA-CBA
30	G	509	CLA	O1A-CGA-O2A-C1
30	b	707	CLA	C2-C3-C5-C6
30	a	715	CLA	CAA-CBA-CGA-O2A
33	I	320	LMG	C9-C8-O7-C10
30	a	711	CLA	CAA-CBA-CGA-O2A
30	a	727	CLA	O1D-CGD-O2D-CED
28	K	301	DD6	C13-C14-C15-O1
28	K	305	DD6	C13-C14-C15-O1
28	K	318	DD6	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
28	A	302	DD6	C13-C14-C15-O1
28	M	306	DD6	C13-C14-C15-O1
29	I	304	UIX	O-C-C7-C10
34	F	305	PID	O1-C6-C7-C8
34	M	301	PID	O1-C6-C7-C8
34	N	301	PID	O1-C6-C7-C8
34	O	305	PID	O1-C6-C7-C8
33	D	317	LMG	C16-C17-C18-C19
30	G	520	CLA	O2A-C1-C2-C3
33	K	317	LMG	C18-C19-C20-C21
30	A	316	CLA	CBA-CGA-O2A-C1
30	a	711	CLA	CAA-CBA-CGA-O1A
33	j	101	LMG	O1-C7-C8-C9
31	G	515	KC1	C4C-C3C-CAC-CBC
30	I	315	CLA	C2C-C3C-CAC-CBC
30	B	308	CLA	CAA-CBA-CGA-O1A
30	G	509	CLA	CBA-CGA-O2A-C1
30	a	710	CLA	C2A-CAA-CBA-CGA
29	P	207	UIX	C25-C28-C32-C33
30	l	305	CLA	C15-C16-C17-C18
33	D	317	LMG	C20-C21-C22-C23
30	a	715	CLA	CAA-CBA-CGA-O1A
30	l	313	CLA	C3-C5-C6-C7
30	a	730	CLA	C3-C5-C6-C7
30	a	729	CLA	C6-C7-C8-C9
30	b	708	CLA	C11-C10-C8-C9
30	b	727	CLA	C14-C13-C15-C16
30	B	311	CLA	C11-C12-C13-C14
30	b	725	CLA	C16-C17-C18-C20
30	b	713	CLA	CAA-CBA-CGA-O2A
28	A	302	DD6	C5-C6-C8-C9
30	m	202	CLA	CAA-CBA-CGA-O2A
30	B	310	CLA	CAA-CBA-CGA-O2A
30	I	308	CLA	C11-C12-C13-C15
30	a	731	CLA	C16-C17-C18-C19
30	G	517	CLA	C2A-CAA-CBA-CGA
30	J	312	CLA	CBD-CGD-O2D-CED
30	a	702	CLA	C11-C12-C13-C15
30	a	707	CLA	C11-C10-C8-C7
30	a	721	CLA	C12-C13-C15-C16
30	b	701	CLA	C11-C12-C13-C15
30	b	724	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	B	311	CLA	C11-C10-C8-C7
32	j	103	DGD	O6D-C5D-C6D-O5D
30	a	701	CLA	C2B-C3B-CAB-CBB
30	a	702	CLA	C2B-C3B-CAB-CBB
30	a	715	CLA	C2B-C3B-CAB-CBB
30	H	311	CLA	C2B-C3B-CAB-CBB
30	J	309	CLA	C2B-C3B-CAB-CBB
30	M	308	CLA	C2B-C3B-CAB-CBB
30	P	210	CLA	C2B-C3B-CAB-CBB
37	l	306	BCR	C5-C6-C7-C8
37	l	306	BCR	C23-C24-C25-C26
30	f	301	CLA	C2-C1-O2A-CGA
32	l	301	DGD	C3A-C4A-C5A-C6A
28	I	302	DD6	C11-C13-C14-C15
28	D	303	DD6	C11-C13-C14-C15
34	F	304	PID	C6-C7-C8-C9
30	b	724	CLA	CAA-CBA-CGA-O2A
30	L	317	CLA	CAA-CBA-CGA-O2A
30	l	305	CLA	O1A-CGA-O2A-C1
33	K	317	LMG	C19-C20-C21-C22
30	I	319	CLA	CAA-CBA-CGA-O2A
30	I	309	CLA	O1A-CGA-O2A-C1
30	I	308	CLA	CAA-CBA-CGA-O2A
30	G	511	CLA	CAA-CBA-CGA-O2A
30	A	310	CLA	CAA-CBA-CGA-O2A
33	I	320	LMG	O8-C28-C29-C30
30	l	310	CLA	CAA-CBA-CGA-O2A
30	a	706	CLA	CAA-CBA-CGA-O2A
30	a	717	CLA	CAA-CBA-CGA-O2A
30	a	723	CLA	CAA-CBA-CGA-O2A
33	D	317	LMG	C36-C37-C38-C39
30	l	313	CLA	C4-C3-C5-C6
30	L	309	CLA	C5-C6-C7-C8
33	j	101	LMG	C10-C11-C12-C13
30	I	316	CLA	CAA-CBA-CGA-O2A
30	a	717	CLA	C2-C3-C5-C6
34	O	304	PID	CM4-C14-C15-C16
30	b	722	CLA	C2A-CAA-CBA-CGA
30	D	309	CLA	CAA-CBA-CGA-O2A
30	l	305	CLA	CBA-CGA-O2A-C1
30	I	306	CLA	O2A-C1-C2-C3
34	D	302	PID	C28-C27-O6-C30

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Mol	Chain	Res	Type	Atoms
30	a	723	CLA	C11-C10-C8-C9
30	a	735	CLA	C14-C13-C15-C16
30	B	309	CLA	C11-C10-C8-C9
30	J	307	CLA	C11-C10-C8-C9
30	O	309	CLA	C13-C15-C16-C17
37	m	201	BCR	C37-C22-C23-C24
30	K	312	CLA	C4B-C3B-CAB-CBB
30	K	316	CLA	C4B-C3B-CAB-CBB
30	A	307	CLA	C4B-C3B-CAB-CBB
30	A	316	CLA	C4B-C3B-CAB-CBB
30	a	701	CLA	C4B-C3B-CAB-CBB
30	a	715	CLA	C4B-C3B-CAB-CBB
30	a	727	CLA	C4B-C3B-CAB-CBB
30	b	705	CLA	C4B-C3B-CAB-CBB
30	b	711	CLA	C4B-C3B-CAB-CBB
30	b	728	CLA	C1A-C2A-CAA-CBA
30	B	309	CLA	C1A-C2A-CAA-CBA
30	J	309	CLA	C4B-C3B-CAB-CBB
30	J	316	CLA	C4B-C3B-CAB-CBB
30	M	308	CLA	C4B-C3B-CAB-CBB
30	P	210	CLA	C1A-C2A-CAA-CBA
30	J	310	CLA	CAA-CBA-CGA-O2A
30	M	316	CLA	CAA-CBA-CGA-O2A
29	G	503	UIX	C36-C38-C40-C39
30	a	706	CLA	C10-C11-C12-C13
30	K	309	CLA	CAA-CBA-CGA-O2A
30	G	514	CLA	CAA-CBA-CGA-O2A
30	b	708	CLA	CAA-CBA-CGA-O2A
30	b	711	CLA	CAA-CBA-CGA-O2A
30	A	313	CLA	C2A-CAA-CBA-CGA
30	a	735	CLA	C2A-CAA-CBA-CGA
32	y	201	DGD	C2A-C3A-C4A-C5A
30	G	511	CLA	C6-C7-C8-C10
30	N	307	CLA	C2-C3-C5-C6
30	b	713	CLA	C13-C15-C16-C17
30	J	312	CLA	O1D-CGD-O2D-CED
32	G	501	DGD	C2A-C3A-C4A-C5A
30	I	308	CLA	C2-C1-O2A-CGA
30	I	321	CLA	C2-C1-O2A-CGA
30	G	514	CLA	C2-C1-O2A-CGA
30	A	309	CLA	C2-C1-O2A-CGA
30	L	313	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
30	a	722	CLA	C6-C7-C8-C10
30	a	725	CLA	C6-C7-C8-C10
30	b	717	CLA	C11-C12-C13-C15
30	I	309	CLA	CBA-CGA-O2A-C1
30	b	701	CLA	C8-C10-C11-C12
30	a	726	CLA	C5-C6-C7-C8
30	I	316	CLA	CBA-CGA-O2A-C1
30	A	310	CLA	CAA-CBA-CGA-O1A
30	I	321	CLA	C2A-CAA-CBA-CGA
30	l	305	CLA	C2A-CAA-CBA-CGA
30	J	307	CLA	C2A-CAA-CBA-CGA
30	M	313	CLA	C2A-CAA-CBA-CGA
30	b	705	CLA	C5-C6-C7-C8
30	B	316	CLA	C4C-C3C-CAC-CBC
30	b	724	CLA	C16-C17-C18-C20
30	B	309	CLA	C16-C17-C18-C19
30	P	212	CLA	CAA-CBA-CGA-O2A
32	I	317	DGD	O6D-C5D-C6D-O5D
30	G	519	CLA	C4-C3-C5-C6
30	J	301	CLA	C3A-C2A-CAA-CBA
30	N	309	CLA	C3A-C2A-CAA-CBA
30	J	312	CLA	CAA-CBA-CGA-O2A
30	I	319	CLA	CAA-CBA-CGA-O1A
39	a	733	LHG	C31-C32-C33-C34
30	m	202	CLA	CAA-CBA-CGA-O1A
30	a	717	CLA	CAA-CBA-CGA-O1A
32	j	103	DGD	C1A-C2A-C3A-C4A
30	a	706	CLA	CAA-CBA-CGA-O1A
30	B	310	CLA	CAA-CBA-CGA-O1A
30	l	303	CLA	C2A-CAA-CBA-CGA
30	M	317	CLA	C2A-CAA-CBA-CGA
30	J	311	CLA	C2-C1-O2A-CGA
30	G	510	CLA	C6-C7-C8-C9
30	a	724	CLA	C14-C13-C15-C16
30	a	725	CLA	C6-C7-C8-C9
30	B	301	CLA	C11-C10-C8-C9
32	y	201	DGD	C2B-C3B-C4B-C5B
30	K	308	CLA	CAA-CBA-CGA-O2A
30	b	724	CLA	CAA-CBA-CGA-O1A
30	J	308	CLA	CAA-CBA-CGA-O1A
30	J	310	CLA	CAA-CBA-CGA-O1A
31	F	314	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	j	106	CLA	O1A-CGA-O2A-C1
30	I	308	CLA	CAA-CBA-CGA-O1A
30	I	316	CLA	CAA-CBA-CGA-O1A
30	b	713	CLA	CAA-CBA-CGA-O1A
30	M	316	CLA	CAA-CBA-CGA-O1A
30	b	706	CLA	CAA-CBA-CGA-O2A
31	I	314	KC1	C1A-C2A-CAA-CBA
31	K	314	KC1	C3A-C2A-CAA-CBA
31	A	306	KC1	C3A-C2A-CAA-CBA
31	D	310	KC1	C1A-C2A-CAA-CBA
31	D	315	KC1	C3A-C2A-CAA-CBA
31	F	309	KC1	C3A-C2A-CAA-CBA
31	H	306	KC1	C1A-C2A-CAA-CBA
31	J	313	KC1	C1A-C2A-CAA-CBA
31	J	313	KC1	C3A-C2A-CAA-CBA
31	M	314	KC1	C1A-C2A-CAA-CBA
31	N	311	KC1	C1A-C2A-CAA-CBA
31	O	310	KC1	C1A-C2A-CAA-CBA
31	O	312	KC1	C3A-C2A-CAA-CBA
31	O	315	KC1	C1A-C2A-CAA-CBA
31	O	315	KC1	C3A-C2A-CAA-CBA
30	G	519	CLA	C11-C12-C13-C14
30	a	727	CLA	CBD-CGD-O2D-CED
30	D	312	CLA	CBD-CGD-O2D-CED
37	l	302	BCR	C17-C18-C19-C20
33	K	317	LMG	C8-C7-O1-C1
33	P	201	LMG	C8-C7-O1-C1
30	G	511	CLA	CAA-CBA-CGA-O1A
30	a	723	CLA	CAA-CBA-CGA-O1A
30	l	311	CLA	C2A-CAA-CBA-CGA
30	a	703	CLA	C2A-CAA-CBA-CGA
30	M	309	CLA	C2A-CAA-CBA-CGA
30	l	310	CLA	CAA-CBA-CGA-O1A
30	D	309	CLA	CAA-CBA-CGA-O1A
33	B	318	LMG	O9-C10-C11-C12
30	b	715	CLA	C8-C10-C11-C12
30	a	731	CLA	CAA-CBA-CGA-O2A
30	N	310	CLA	C2-C1-O2A-CGA
30	J	312	CLA	CAA-CBA-CGA-O1A
33	I	320	LMG	O9-C10-C11-C12
30	K	311	CLA	CAD-CBD-CGD-O2D
30	G	517	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	f	302	CLA	CAD-CBD-CGD-O2D
30	l	310	CLA	CAD-CBD-CGD-O2D
30	B	316	CLA	CAD-CBD-CGD-O2D
30	H	307	CLA	CAD-CBD-CGD-O2D
30	J	316	CLA	CAD-CBD-CGD-O2D
30	P	214	CLA	CAD-CBD-CGD-O2D
34	D	302	PID	O4-C12-C13-C14
34	P	206	PID	O4-C12-C13-C14
30	G	512	CLA	CAA-CBA-CGA-O2A
30	A	309	CLA	CAA-CBA-CGA-O2A
30	G	514	CLA	CAA-CBA-CGA-O1A
30	b	708	CLA	CAA-CBA-CGA-O1A
30	L	317	CLA	CAA-CBA-CGA-O1A
30	a	729	CLA	CBD-CGD-O2D-CED
32	l	301	DGD	O6D-C5D-C6D-O5D
33	K	317	LMG	C16-C17-C18-C19
30	j	106	CLA	C2-C1-O2A-CGA
30	M	308	CLA	C2-C1-O2A-CGA
33	I	320	LMG	O10-C28-C29-C30
34	O	307	PID	C26-C27-O6-C30
30	b	711	CLA	CAA-CBA-CGA-O1A
30	K	310	CLA	CAA-CBA-CGA-O2A
30	h	202	CLA	CAA-CBA-CGA-O2A
30	a	718	CLA	CAA-CBA-CGA-O2A
30	L	311	CLA	CAA-CBA-CGA-O2A
30	M	309	CLA	CAA-CBA-CGA-O2A
30	P	210	CLA	CAA-CBA-CGA-O2A
29	K	302	UIX	C19-C18-O2-C27
34	P	205	PID	C28-C27-O6-C30
30	b	725	CLA	C16-C17-C18-C19
30	P	212	CLA	CAA-CBA-CGA-O1A
30	D	312	CLA	O1D-CGD-O2D-CED
30	a	703	CLA	CAA-CBA-CGA-O2A
30	b	705	CLA	CAA-CBA-CGA-O2A
30	j	106	CLA	CBA-CGA-O2A-C1
30	K	309	CLA	CAA-CBA-CGA-O1A
29	G	503	UIX	C17-C18-O2-C27

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	G	507	PID	C24-C25-C26-C27-C28-C29

264 monomers are involved in 671 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	b	721	CLA	2	0
30	b	723	CLA	3	0
30	P	209	CLA	2	0
30	P	210	CLA	4	0
30	P	214	CLA	3	0
33	j	101	LMG	4	0
30	B	317	CLA	2	0
30	M	309	CLA	8	0
29	J	305	UIX	1	0
28	I	301	DD6	1	0
30	D	309	CLA	2	0
34	O	304	PID	1	0
30	a	716	CLA	3	0
28	F	301	DD6	1	0
30	J	310	CLA	3	0
28	A	305	DD6	1	0
30	m	202	CLA	2	0
30	j	106	CLA	3	0
28	B	302	DD6	1	0
30	K	308	CLA	3	0
30	G	518	CLA	1	0
30	a	711	CLA	3	0
30	b	708	CLA	2	0
30	A	311	CLA	1	0
30	A	309	CLA	2	0
30	G	513	CLA	4	0
31	D	310	KC1	1	0
30	b	714	CLA	1	0
34	D	305	PID	3	0
30	l	308	CLA	1	0
33	D	317	LMG	5	0
34	D	304	PID	2	0
30	D	308	CLA	1	0
30	b	727	CLA	6	0
37	m	201	BCR	4	0
30	B	313	CLA	4	0
34	F	302	PID	2	0
33	b	733	LMG	2	0
34	O	307	PID	5	0
30	l	311	CLA	4	0
30	B	311	CLA	2	0
30	A	315	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	a	720	CLA	2	0
30	J	312	CLA	2	0
30	H	312	CLA	1	0
30	F	311	CLA	1	0
28	M	303	DD6	2	0
34	P	206	PID	4	0
30	b	722	CLA	4	0
34	P	203	PID	5	0
30	L	312	CLA	1	0
30	H	304	CLA	3	0
30	M	318	CLA	1	0
30	N	305	CLA	2	0
34	F	304	PID	6	0
30	D	314	CLA	10	0
30	a	735	CLA	5	0
31	M	307	KC1	1	0
38	a	732	PQN	5	0
30	a	708	CLA	2	0
34	H	302	PID	5	0
30	G	517	CLA	6	0
33	B	318	LMG	1	0
34	G	506	PID	2	0
30	F	308	CLA	1	0
28	L	304	DD6	1	0
34	N	301	PID	1	0
30	a	725	CLA	5	0
30	N	309	CLA	4	0
30	J	309	CLA	3	0
30	a	738	CLA	1	0
30	H	311	CLA	2	0
30	H	305	CLA	4	0
30	J	308	CLA	3	0
28	I	305	DD6	1	0
35	A	318	SQD	8	0
30	a	729	CLA	3	0
30	O	311	CLA	1	0
34	O	301	PID	1	0
30	a	704	CLA	5	0
30	b	706	CLA	3	0
34	M	301	PID	1	0
34	P	208	PID	2	0
30	a	709	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	320	CLA	3	0
30	a	728	CLA	3	0
30	a	705	CLA	2	0
37	l	307	BCR	3	0
30	J	316	CLA	4	0
30	l	305	CLA	3	0
30	F	310	CLA	5	0
30	b	716	CLA	4	0
30	f	301	CLA	5	0
30	b	726	CLA	1	0
30	L	313	CLA	7	0
28	G	505	DD6	1	0
37	a	734	BCR	3	0
30	P	215	CLA	6	0
30	O	308	CLA	1	0
30	K	307	CLA	1	0
30	B	315	CLA	2	0
30	H	307	CLA	1	0
30	A	316	CLA	1	0
30	K	312	CLA	2	0
34	P	205	PID	2	0
30	a	731	CLA	6	0
29	I	304	UIX	2	0
38	b	729	PQN	4	0
30	G	520	CLA	3	0
34	G	507	PID	5	0
33	I	320	LMG	2	0
31	O	315	KC1	3	0
37	l	302	BCR	3	0
30	I	310	CLA	4	0
30	b	710	CLA	6	0
34	F	306	PID	2	0
30	a	717	CLA	4	0
30	G	510	CLA	4	0
30	j	104	CLA	5	0
30	L	309	CLA	1	0
30	b	715	CLA	5	0
31	O	312	KC1	1	0
28	J	304	DD6	3	0
28	A	303	DD6	1	0
37	b	702	BCR	6	0
32	j	103	DGD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	b	701	CLA	7	0
30	I	308	CLA	4	0
30	b	718	CLA	4	0
30	b	707	CLA	5	0
28	H	303	DD6	1	0
30	I	321	CLA	3	0
30	N	307	CLA	1	0
34	N	302	PID	3	0
31	F	309	KC1	2	0
30	O	316	CLA	2	0
30	M	315	CLA	2	0
30	b	712	CLA	4	0
30	B	309	CLA	4	0
30	I	315	CLA	1	0
30	a	719	CLA	4	0
30	F	315	CLA	1	0
30	L	317	CLA	5	0
30	J	306	CLA	1	0
30	a	706	CLA	7	0
30	K	316	CLA	1	0
30	a	724	CLA	3	0
30	P	217	CLA	3	0
30	l	304	CLA	3	0
31	N	308	KC1	1	0
30	b	728	CLA	3	0
30	M	308	CLA	2	0
30	l	313	CLA	6	0
30	a	721	CLA	6	0
36	c	202	SF4	1	0
30	I	312	CLA	2	0
30	I	313	CLA	3	0
30	a	727	CLA	1	0
34	H	301	PID	3	0
30	B	316	CLA	1	0
30	F	312	CLA	5	0
30	l	310	CLA	1	0
30	D	311	CLA	2	0
30	I	307	CLA	2	0
30	F	313	CLA	8	0
30	M	316	CLA	1	0
30	l	312	CLA	3	0
30	O	314	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	f	303	CLA	1	0
39	a	733	LHG	3	0
30	H	309	CLA	2	0
30	a	710	CLA	4	0
30	b	713	CLA	6	0
30	B	307	CLA	1	0
31	P	213	KC1	1	0
29	K	302	UIX	1	0
37	b	732	BCR	4	0
30	A	313	CLA	4	0
30	a	703	CLA	5	0
30	a	723	CLA	7	0
30	M	310	CLA	2	0
30	b	709	CLA	7	0
30	J	301	CLA	5	0
30	a	726	CLA	6	0
30	b	720	CLA	8	0
28	G	508	DD6	1	0
30	b	703	CLA	6	0
28	G	504	DD6	3	0
30	G	509	CLA	1	0
34	F	305	PID	3	0
30	b	704	CLA	14	0
30	J	311	CLA	2	0
30	b	717	CLA	6	0
30	l	303	CLA	5	0
33	b	734	LMG	3	0
30	A	319	CLA	2	0
34	D	306	PID	1	0
30	K	306	CLA	1	0
28	L	305	DD6	1	0
30	a	722	CLA	5	0
31	H	310	KC1	1	0
29	A	304	UIX	1	0
30	a	707	CLA	7	0
30	D	312	CLA	2	0
30	G	514	CLA	3	0
36	c	201	SF4	1	0
30	H	308	CLA	2	0
37	b	730	BCR	5	0
30	a	702	CLA	5	0
30	J	307	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	O	313	CLA	2	0
30	G	511	CLA	2	0
37	f	304	BCR	4	0
34	O	305	PID	14	0
30	K	313	CLA	5	0
30	A	312	CLA	3	0
32	L	301	DGD	2	0
30	A	310	CLA	4	0
30	f	302	CLA	4	0
30	a	718	CLA	1	0
30	L	308	CLA	2	0
30	G	519	CLA	1	0
30	K	311	CLA	2	0
37	j	102	BCR	5	0
37	l	306	BCR	4	0
30	K	310	CLA	1	0
30	b	725	CLA	4	0
30	M	317	CLA	2	0
30	A	317	CLA	2	0
28	J	303	DD6	2	0
30	O	309	CLA	3	0
30	I	316	CLA	3	0
30	a	714	CLA	3	0
34	D	302	PID	2	0
30	D	313	CLA	1	0
30	a	712	CLA	1	0
30	A	308	CLA	3	0
34	O	302	PID	2	0
30	M	312	CLA	1	0
34	P	202	PID	5	0
30	B	310	CLA	1	0
37	a	736	BCR	2	0
30	I	311	CLA	5	0
30	B	308	CLA	1	0
34	D	301	PID	4	0
30	a	713	CLA	3	0
34	j	105	PID	4	0
30	b	705	CLA	4	0
30	M	313	CLA	3	0
36	a	737	SF4	1	0
30	L	314	CLA	4	0
32	G	501	DGD	2	0

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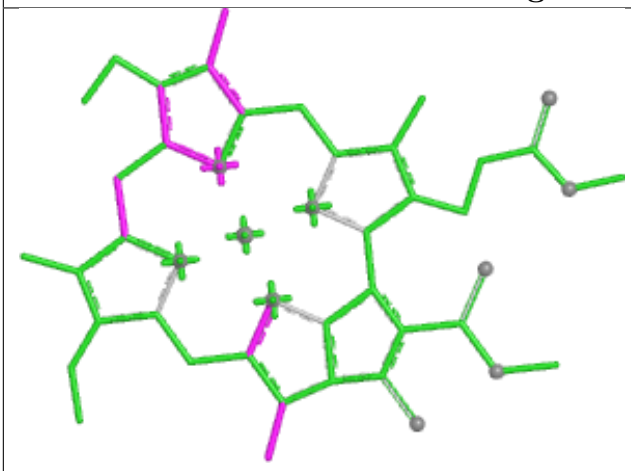
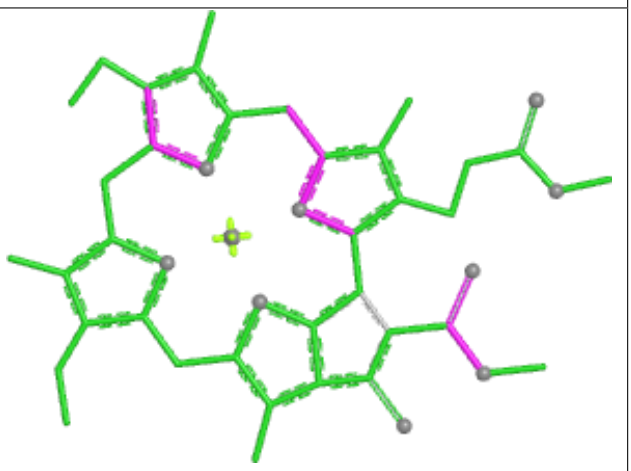
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	F	307	CLA	1	0
30	I	319	CLA	2	0
30	I	306	CLA	2	0
30	I	309	CLA	1	0
37	i	201	BCR	7	0
30	B	301	CLA	3	0
30	N	310	CLA	3	0
30	b	724	CLA	4	0
30	L	316	CLA	1	0
30	a	730	CLA	6	0
30	K	309	CLA	2	0
32	y	201	DGD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

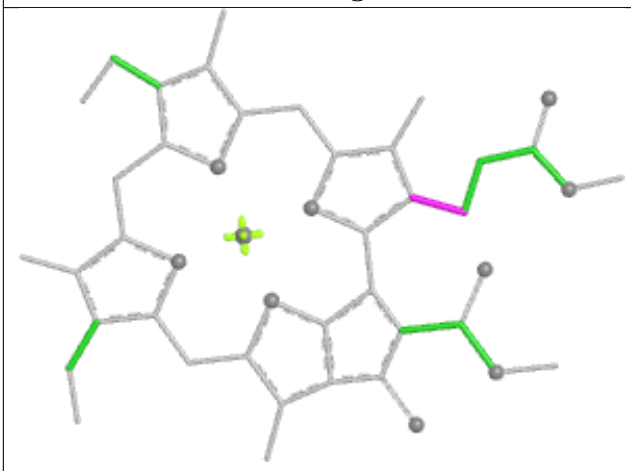
Ligand CLA b 721



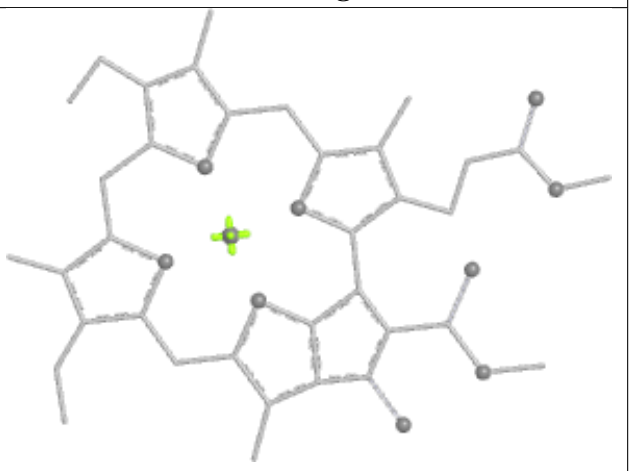
Bond lengths



Bond angles

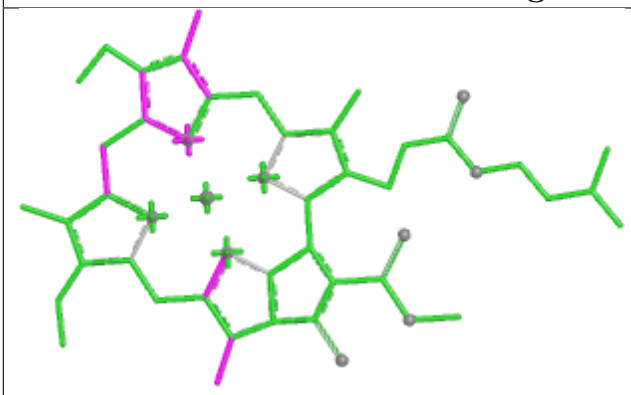


Torsions



Rings

Ligand CLA b 723



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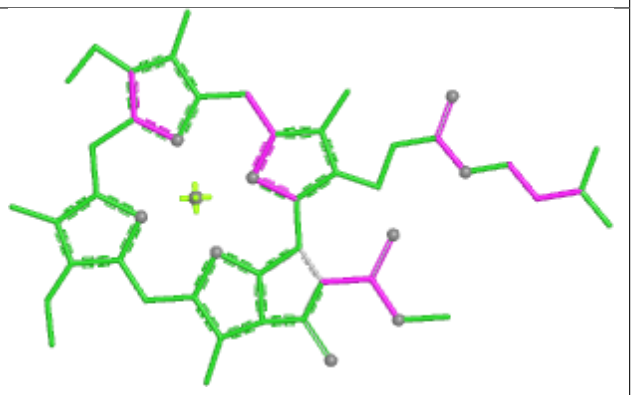
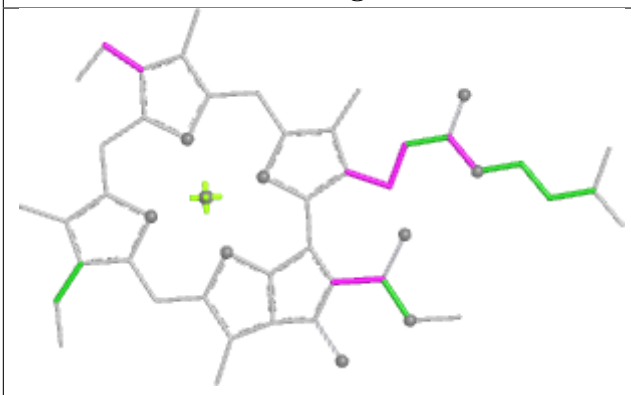
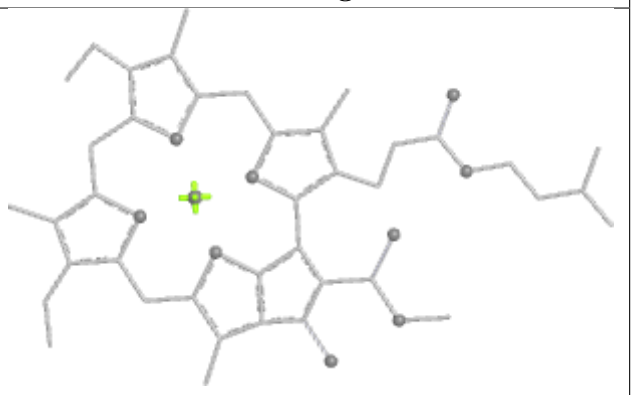


Bond angles

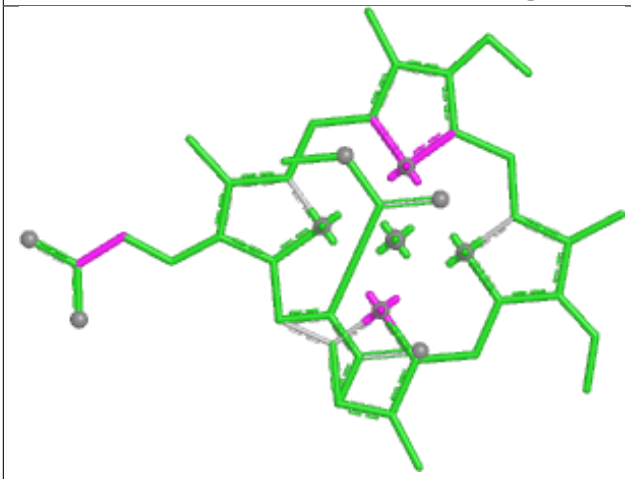


Torsions

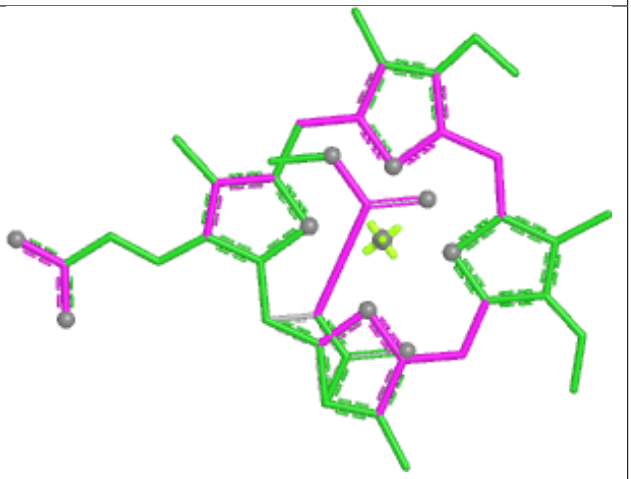


Rings

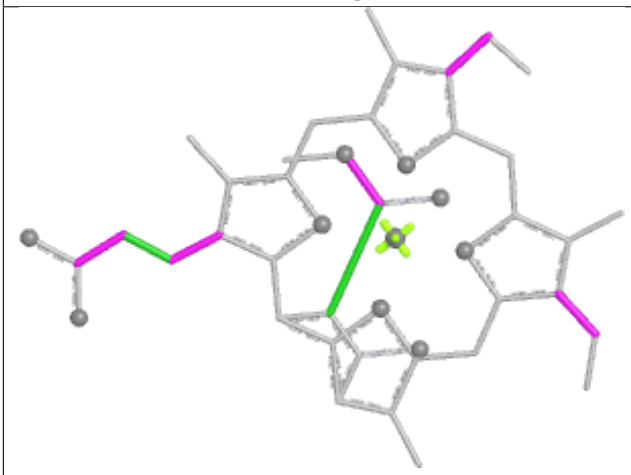
Ligand KC1 M 314



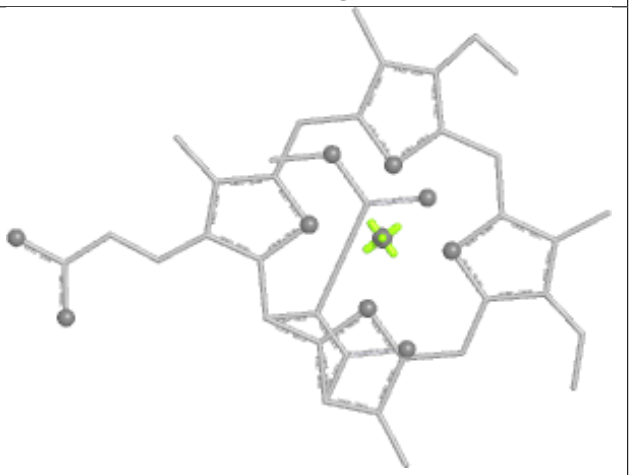
Bond lengths



Bond angles

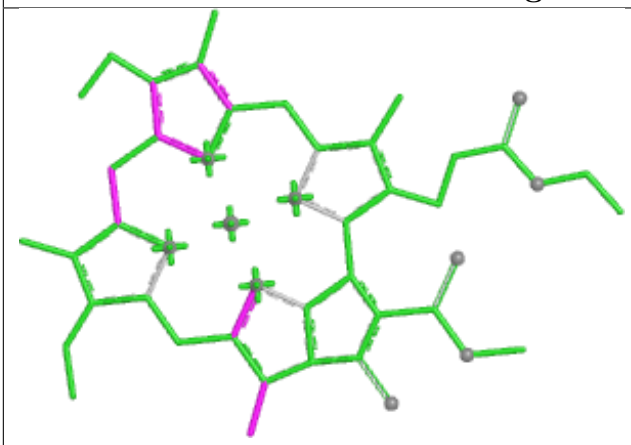


Torsions



Rings

Ligand CLA P 209



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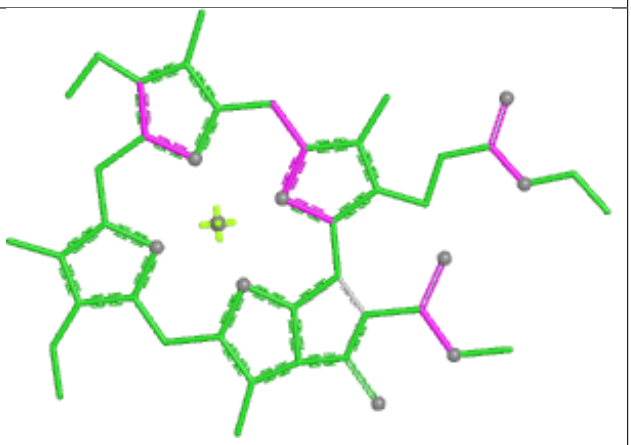
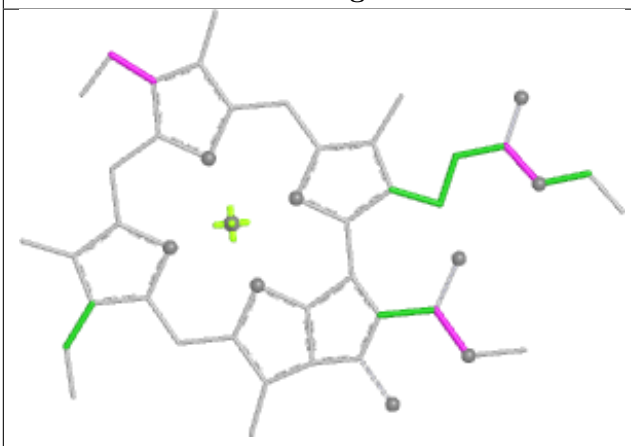
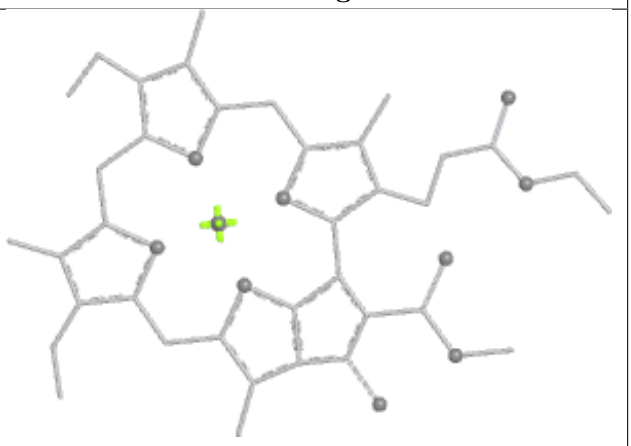


Bond angles



Torsions



Rings

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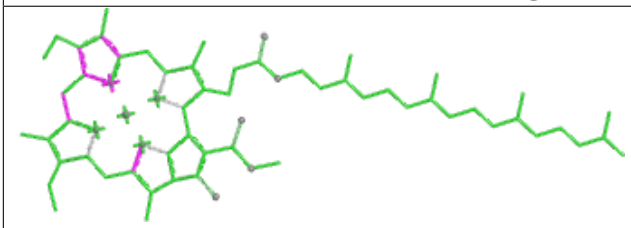

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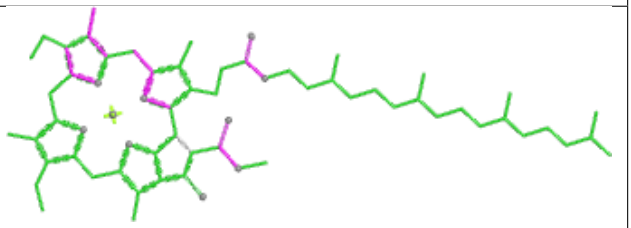
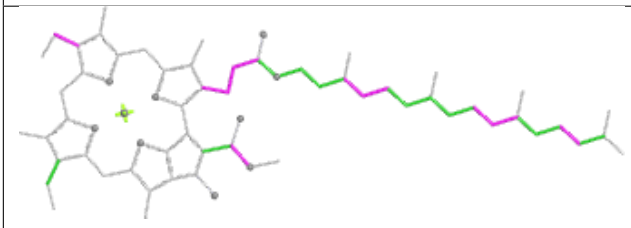


Bond angles



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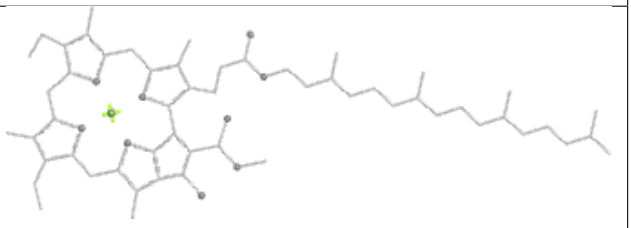
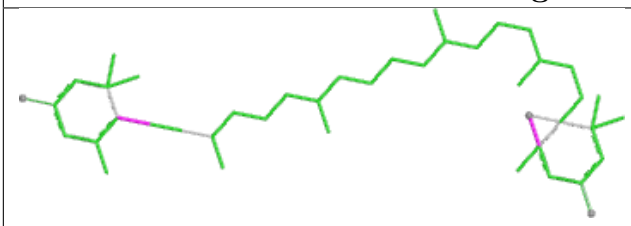


Rings

Ligand DD6 I 302



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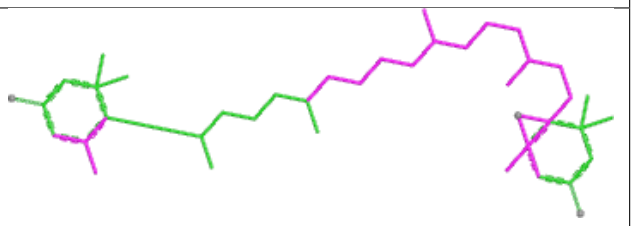

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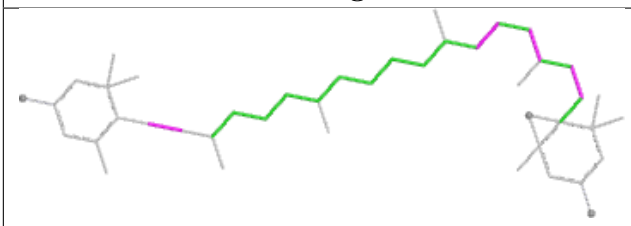

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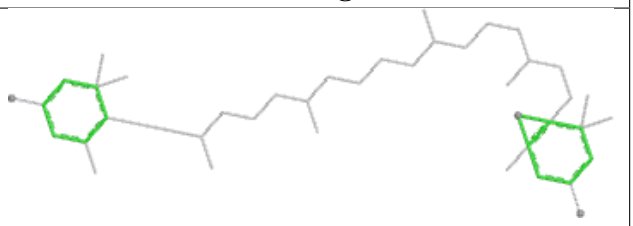
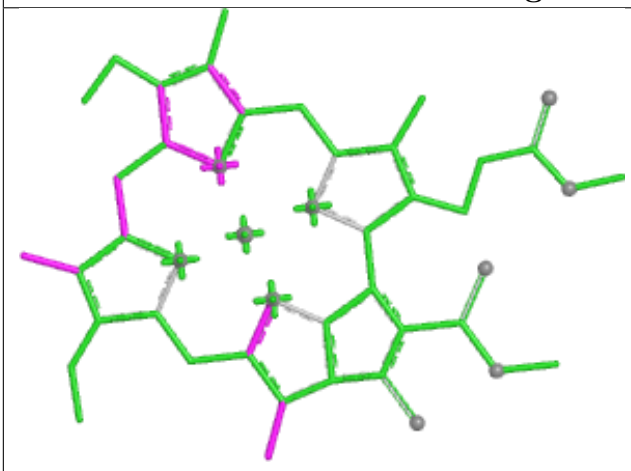


Rings

Ligand CLA P 214



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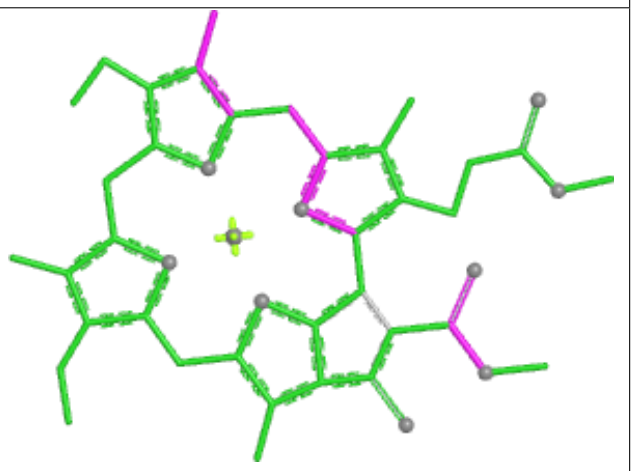

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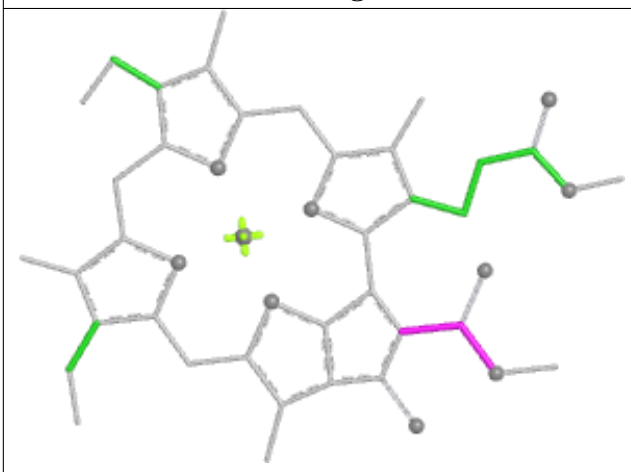

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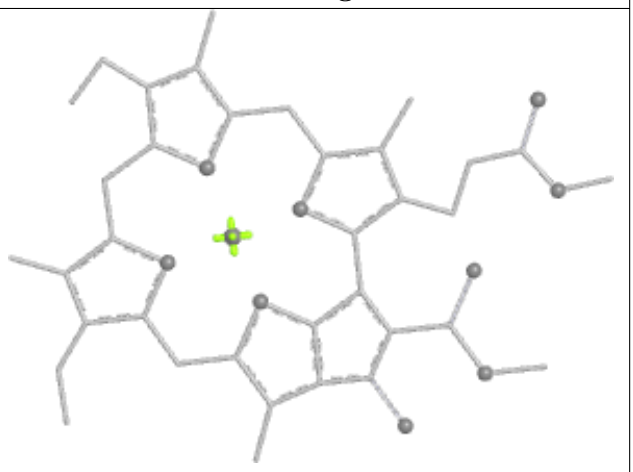
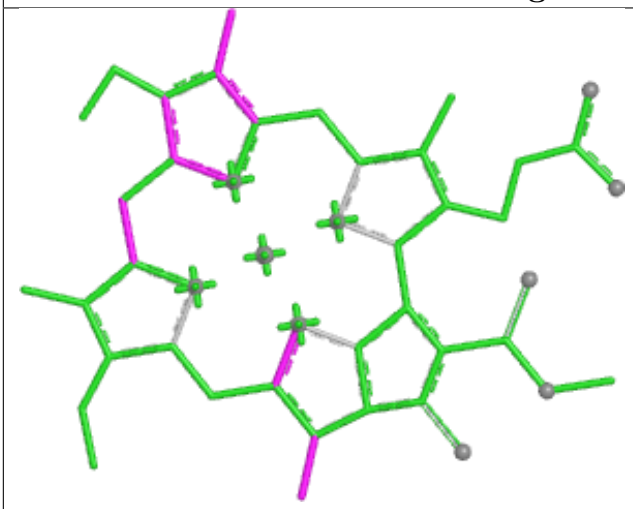


Rings

Ligand CLA a 701



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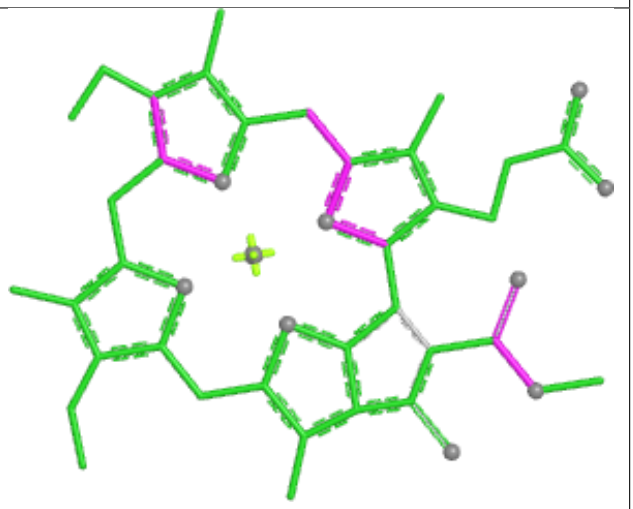
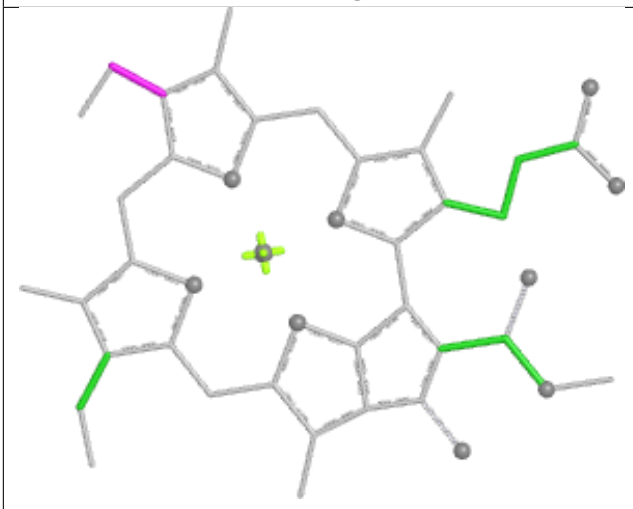


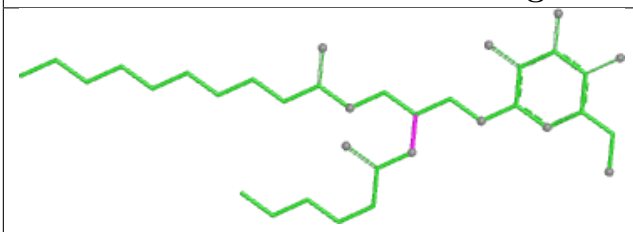
Bond angles



Torsions

Rings

Ligand LMG j 101



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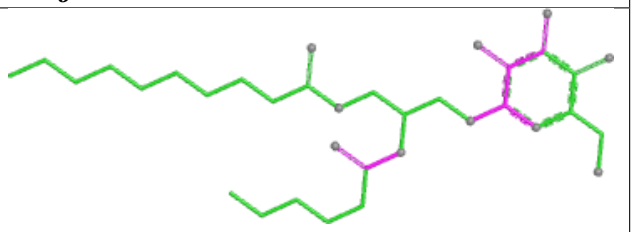

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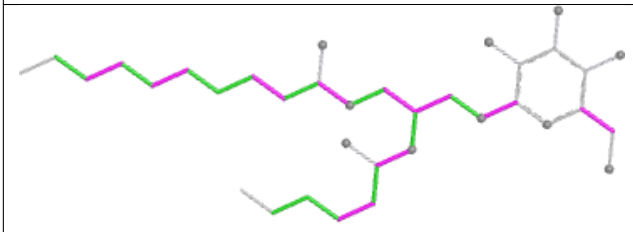
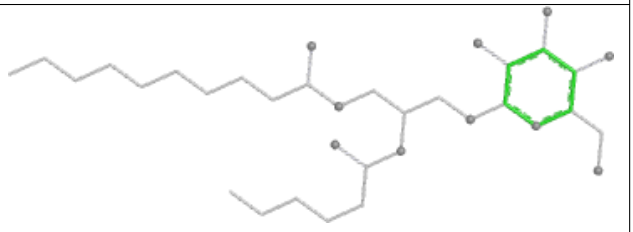
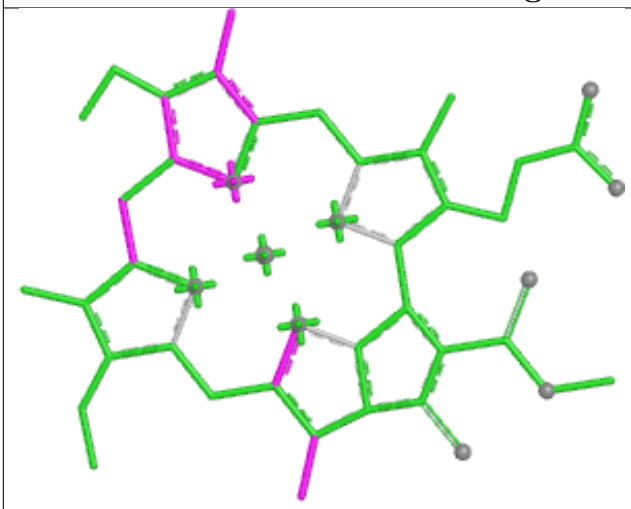


Torsions



Rings

Ligand CLA B 317



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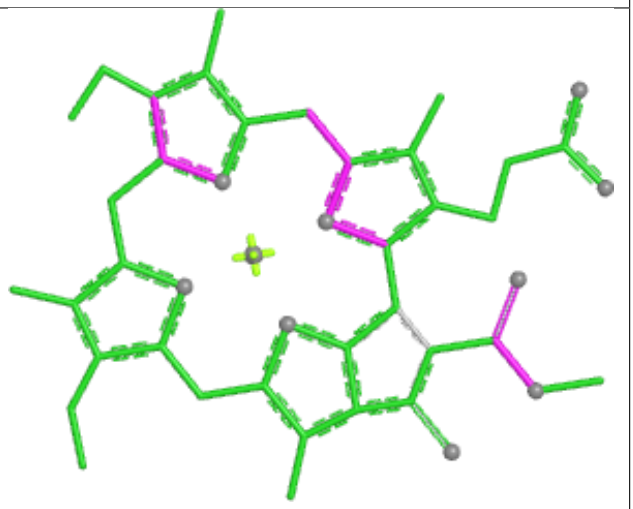
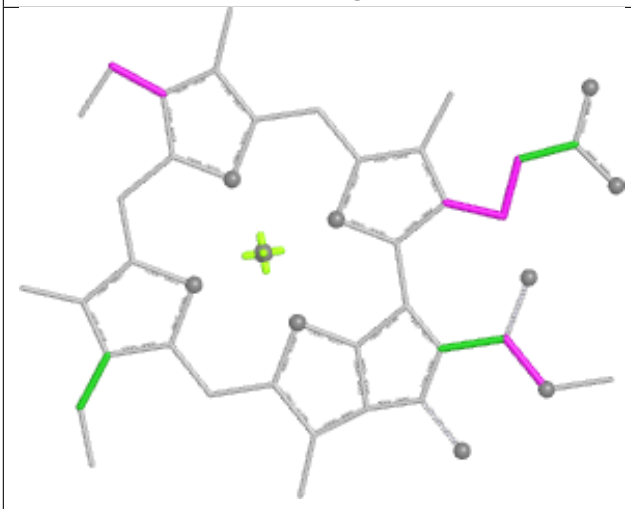


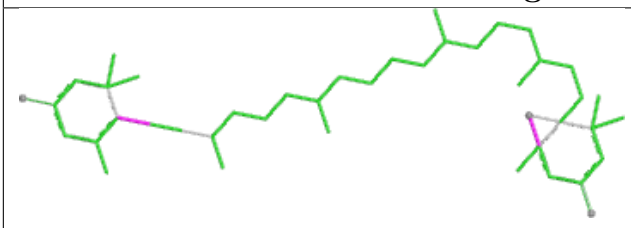
Bond angles



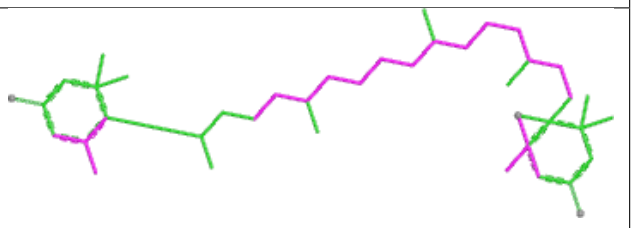
Torsions

Rings

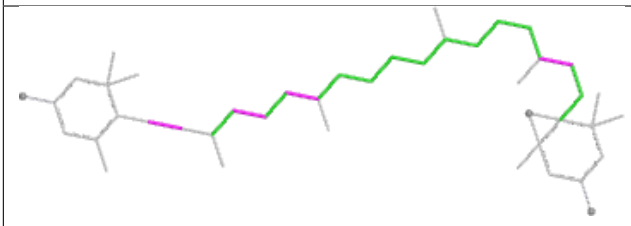
Ligand DD6 G 502



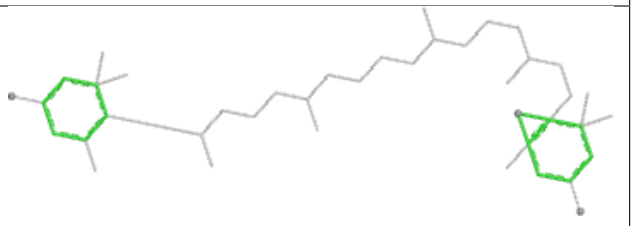
Bond lengths



Bond angles

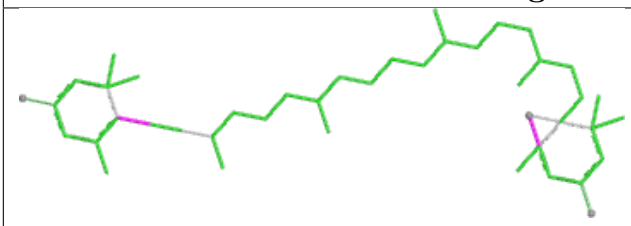


Torsions

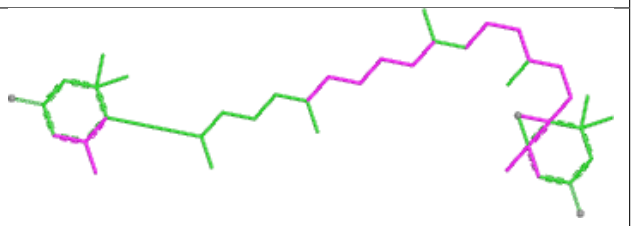


Rings

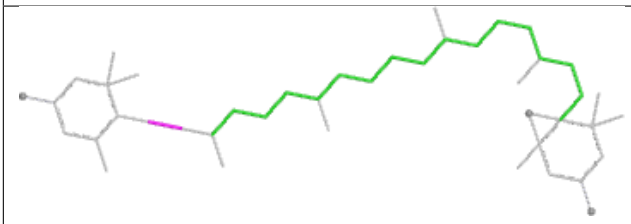
Ligand DD6 h 203



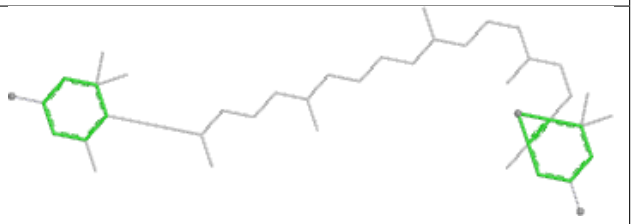
Bond lengths



Bond angles

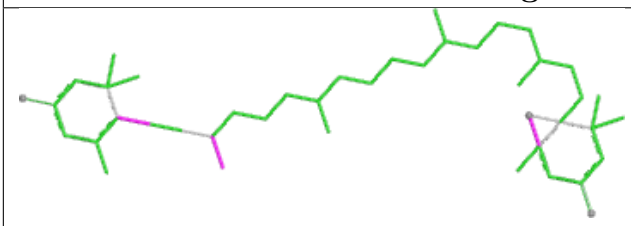


Torsions



Rings

Ligand DD6 M 305



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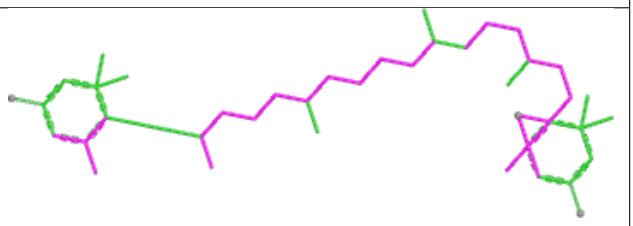
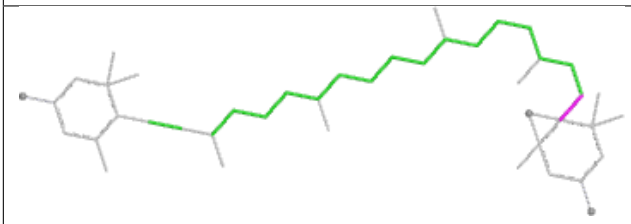


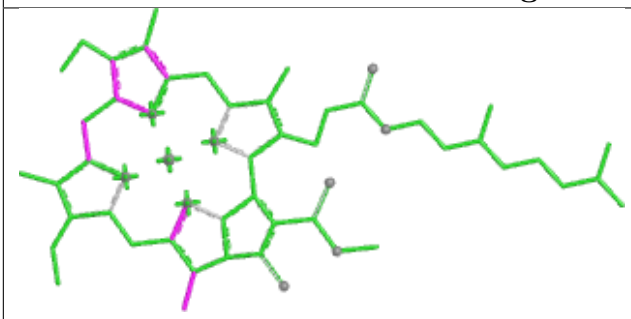
Bond angles



Torsions

Rings

Ligand CLA M 309



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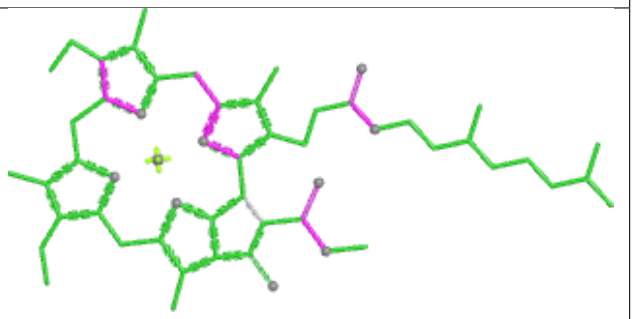

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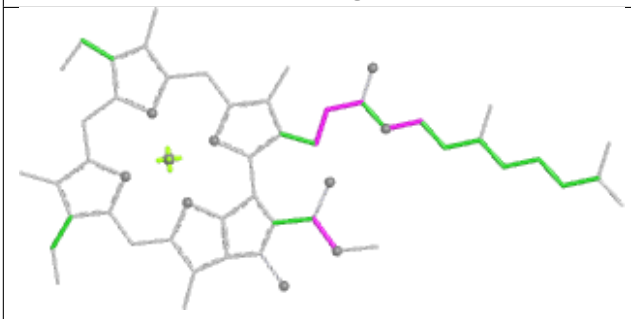

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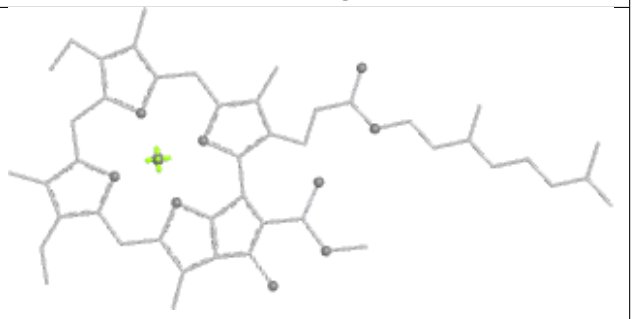
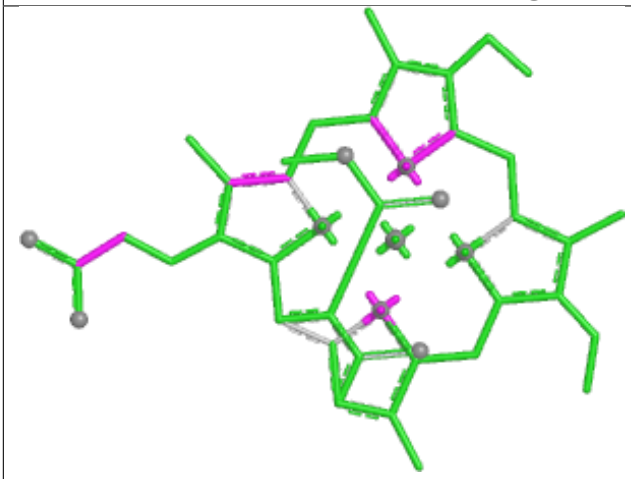


Rings

Ligand KC1 D 315



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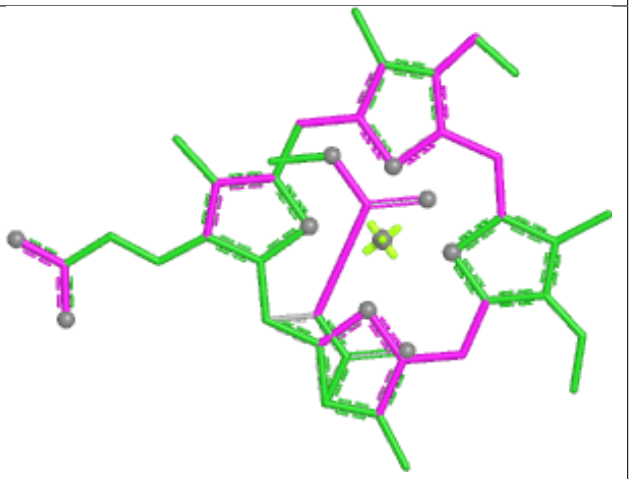

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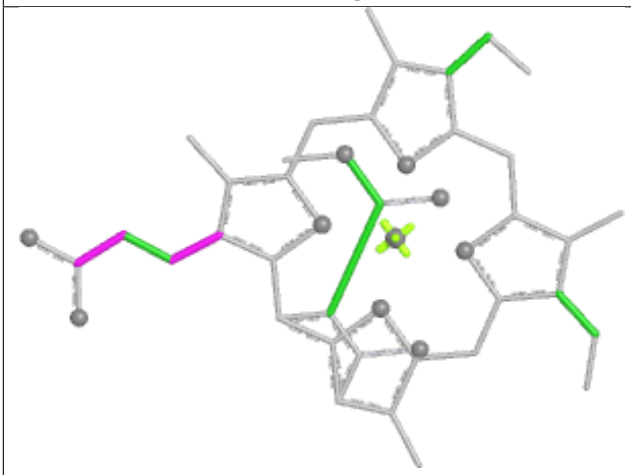

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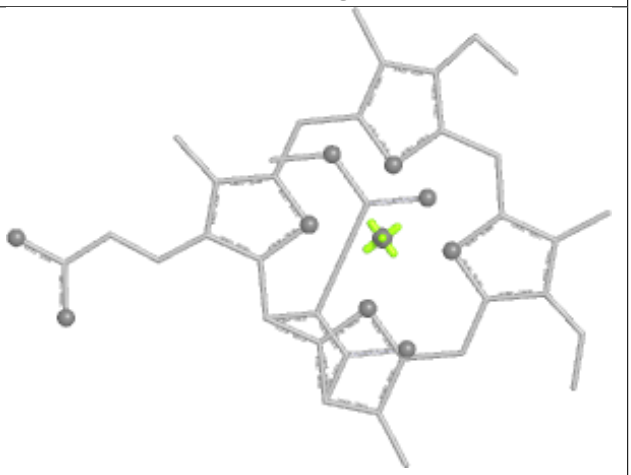
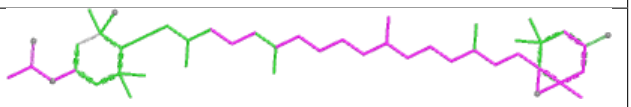


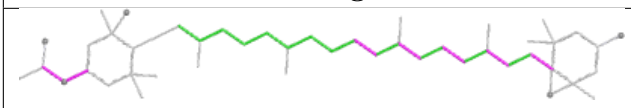
Rings

Ligand UIX J 305

Bond lengths



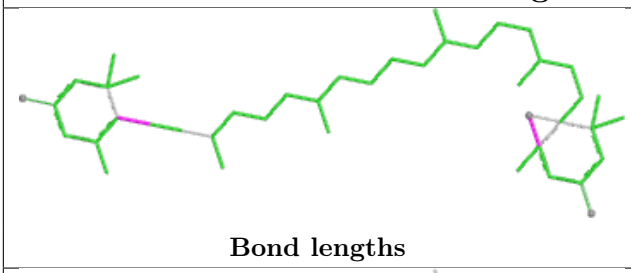
Bond angles



Torsions

Rings

Ligand DD6 I 301



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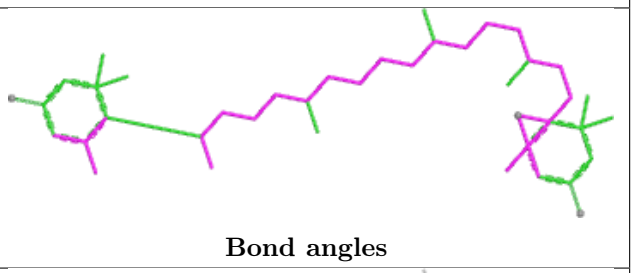

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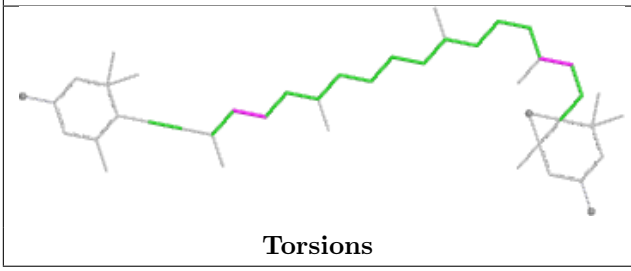

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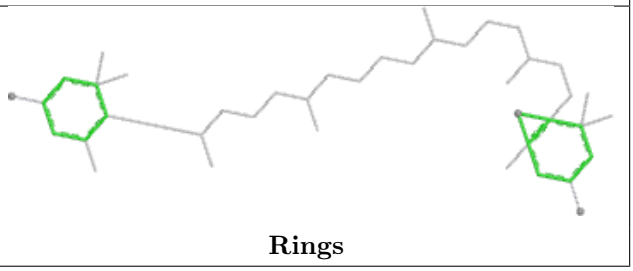
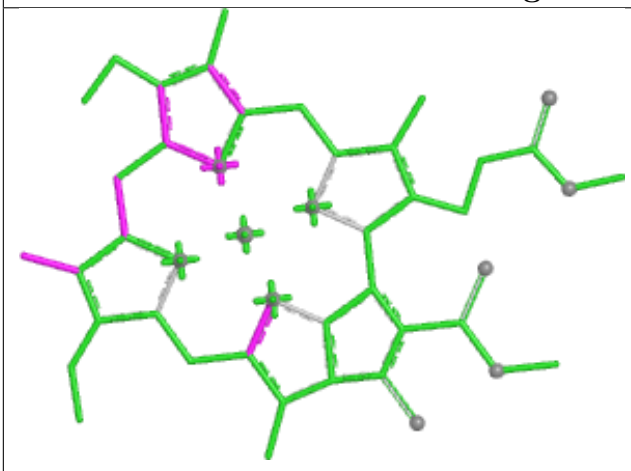


Rings

Ligand CLA D 309



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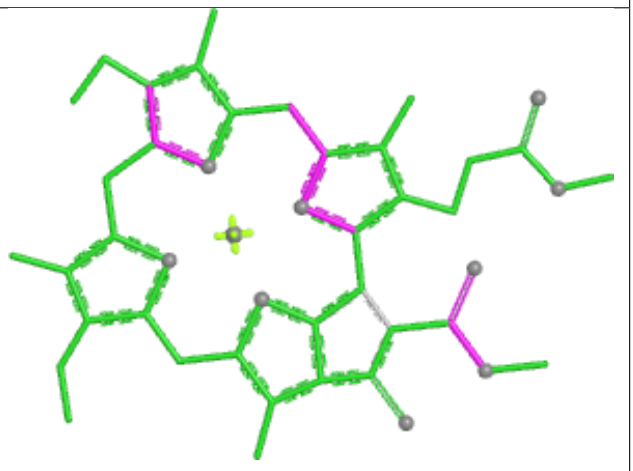

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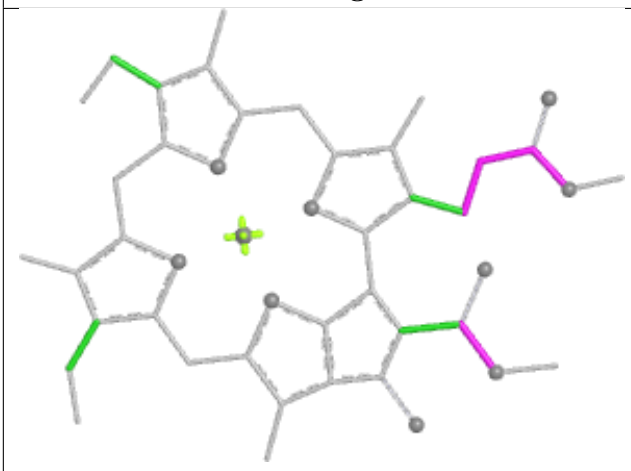

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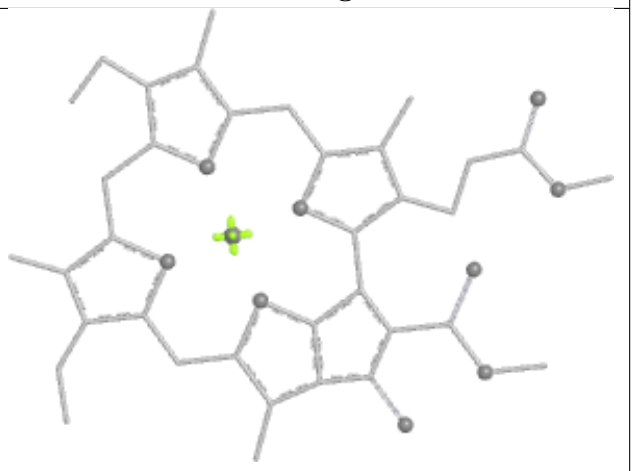
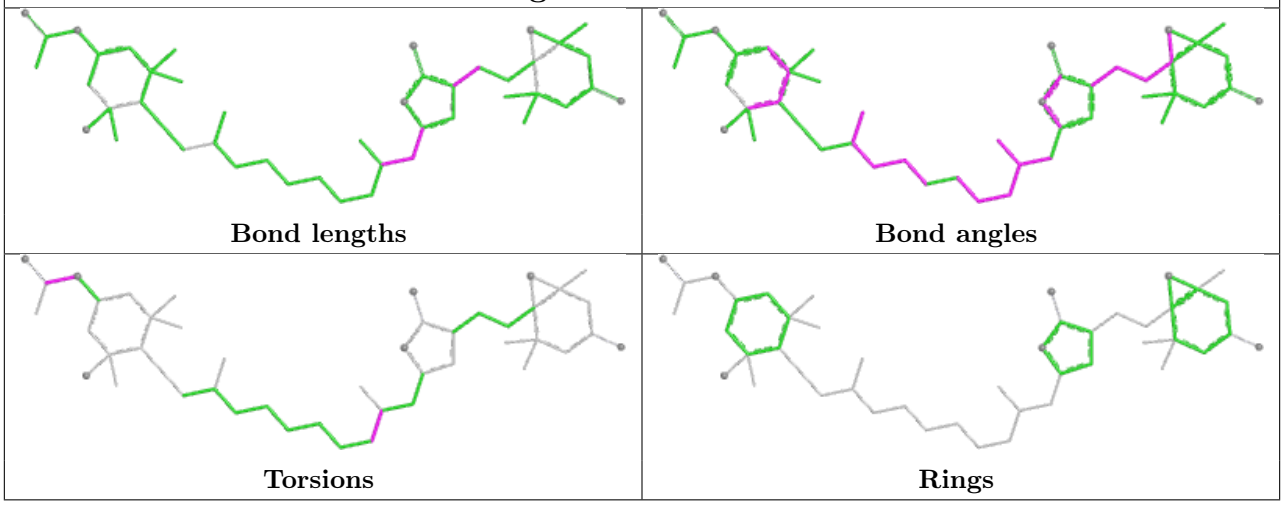
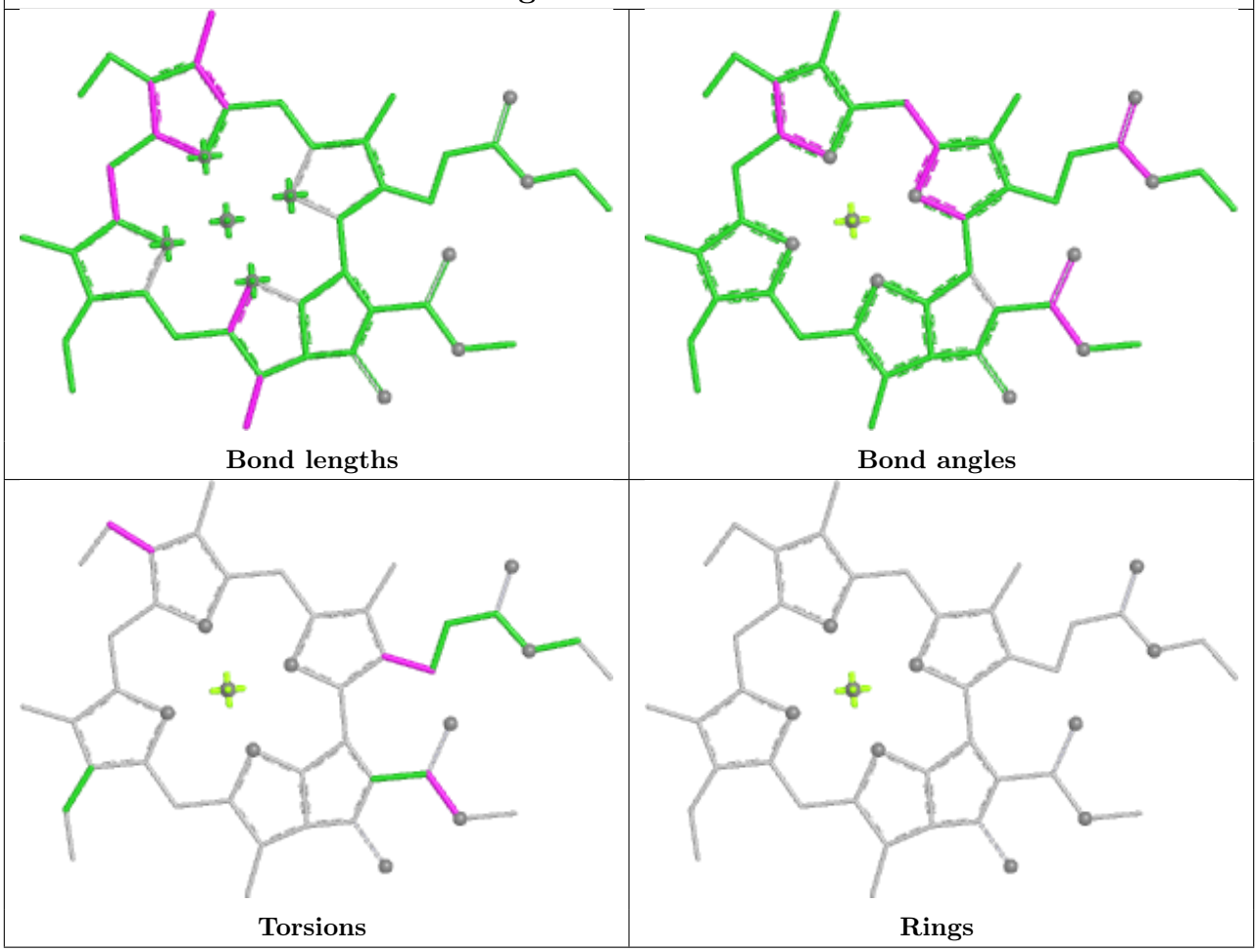


Rings

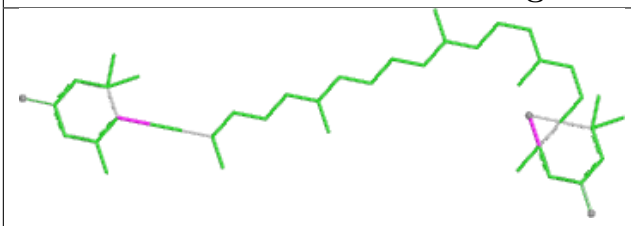
Ligand PID O 304



Ligand CLA a 716



Ligand DD6 F 301



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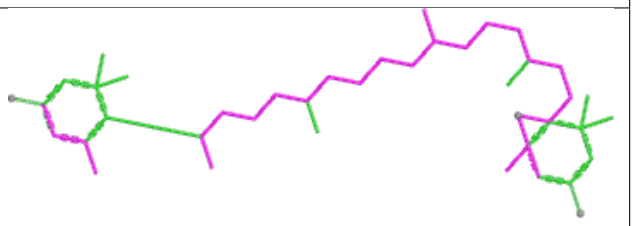
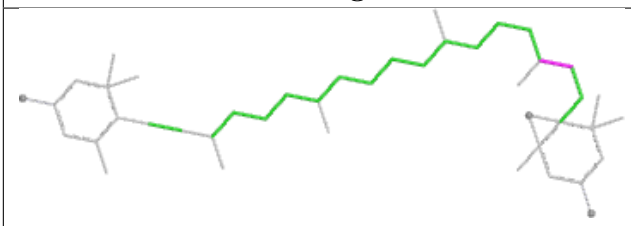


Bond angles



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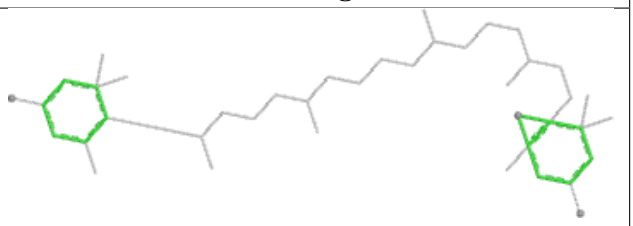
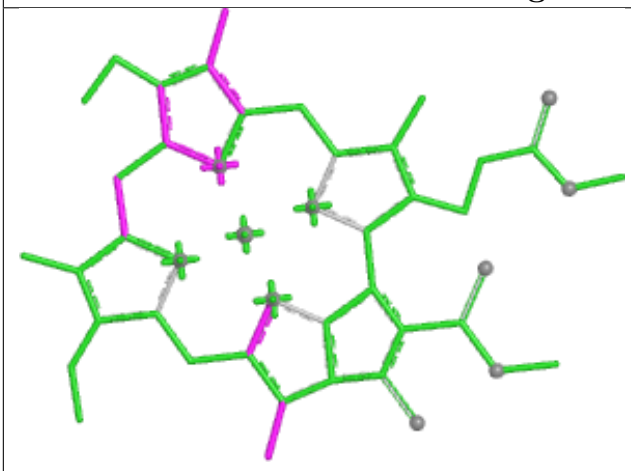


Rings

Ligand CLA J 310



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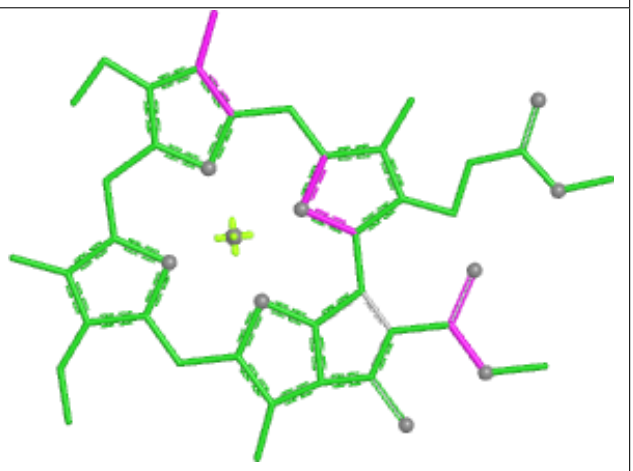

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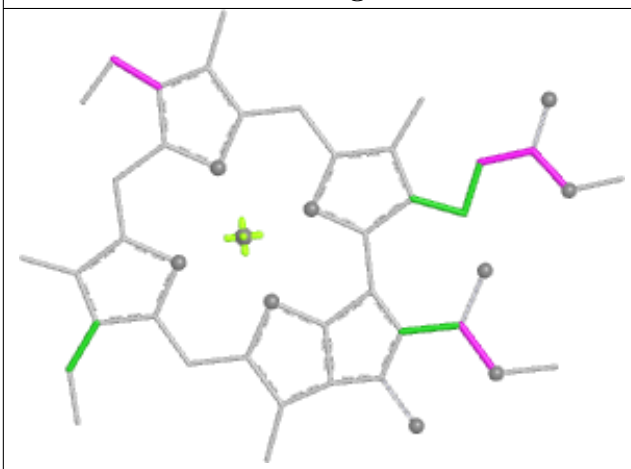

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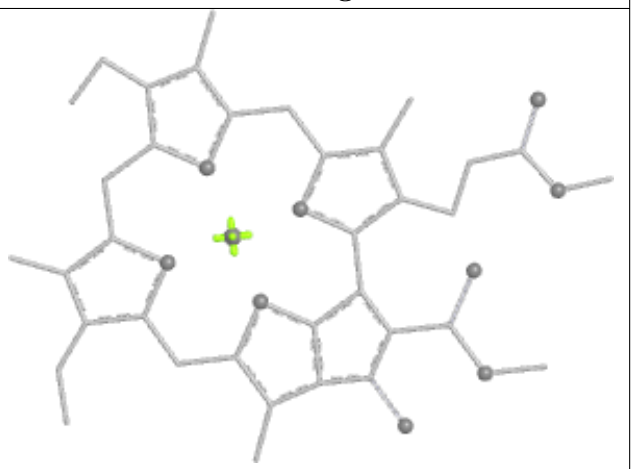
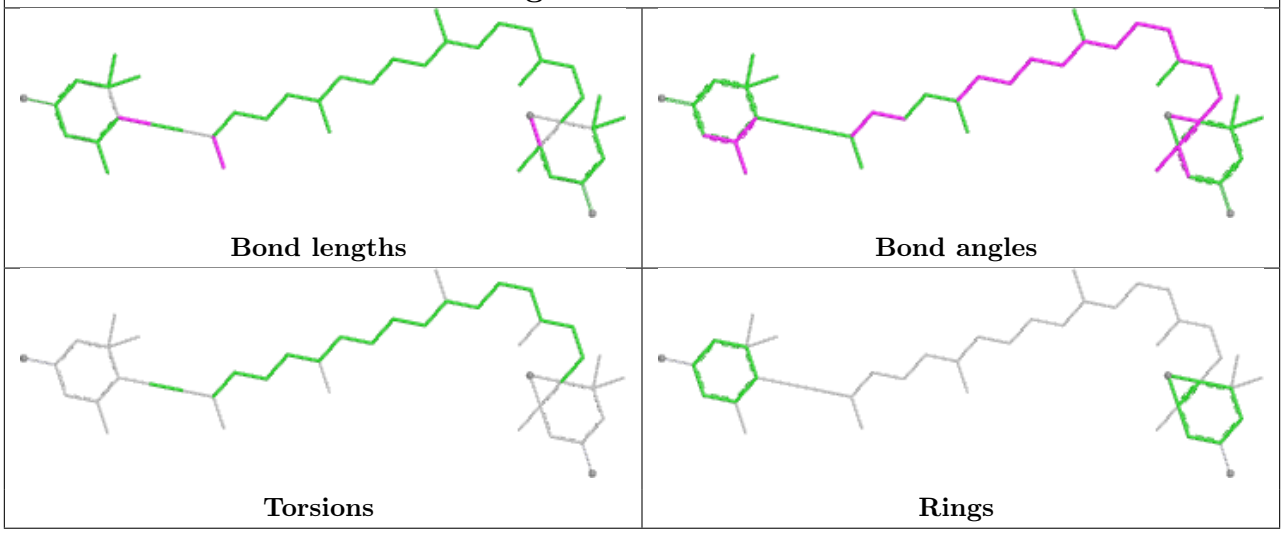
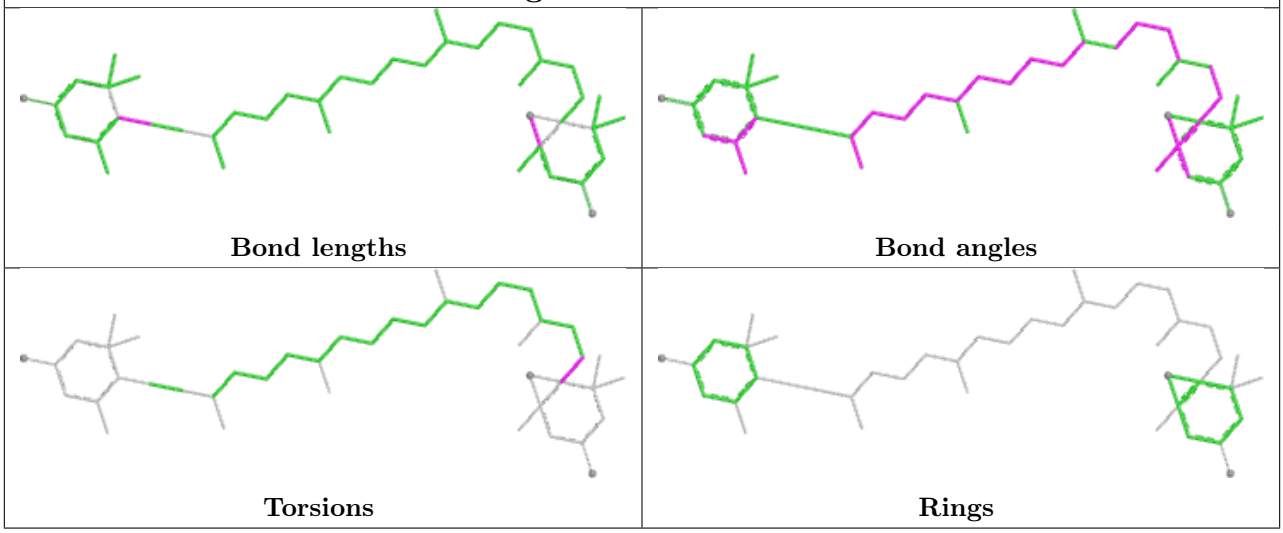


Rings

Ligand DD6 O 303



Ligand DD6 A 305



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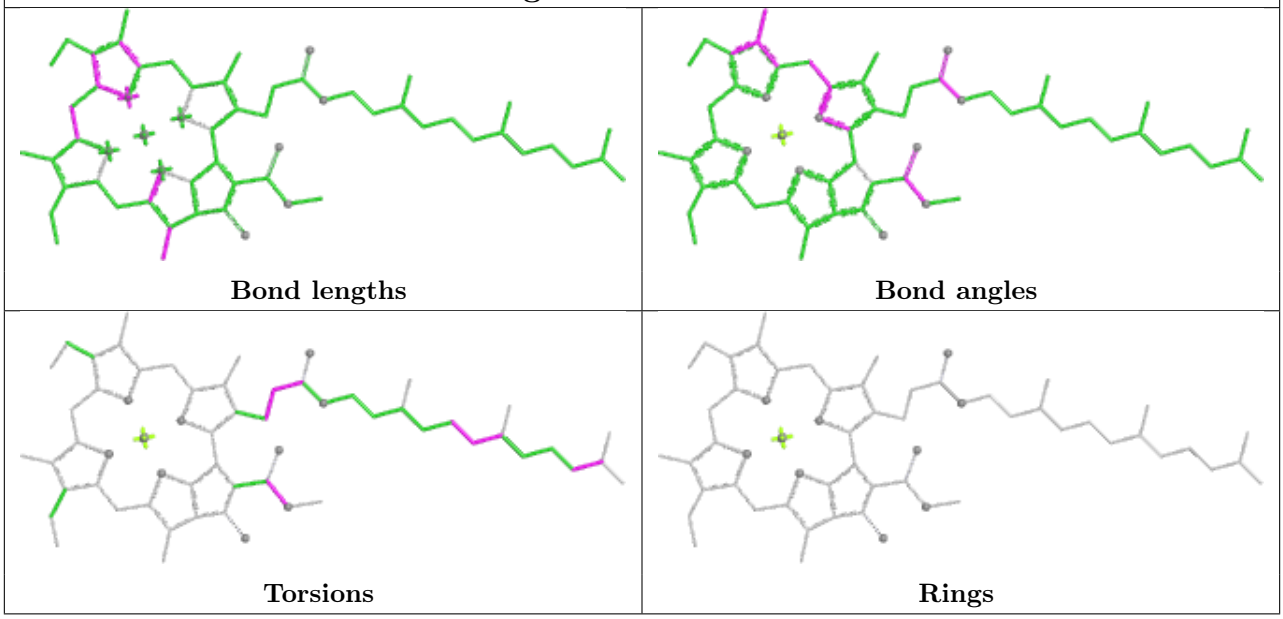
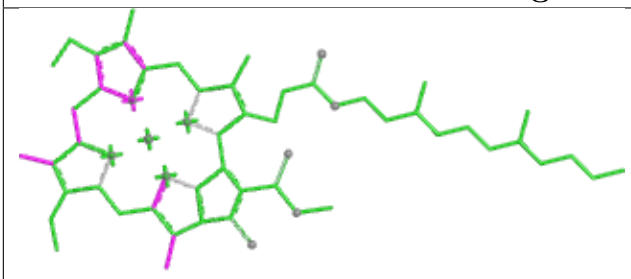
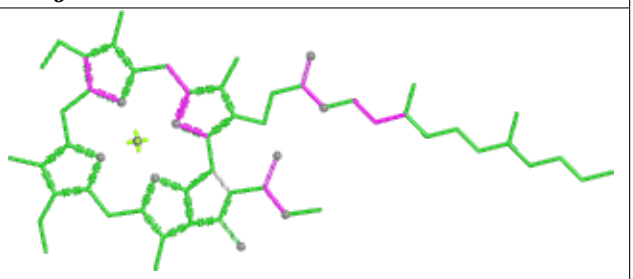


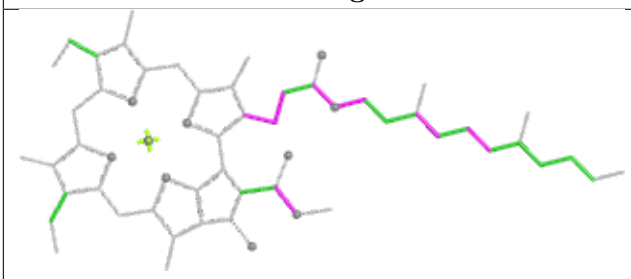
Ligand CLA j 106



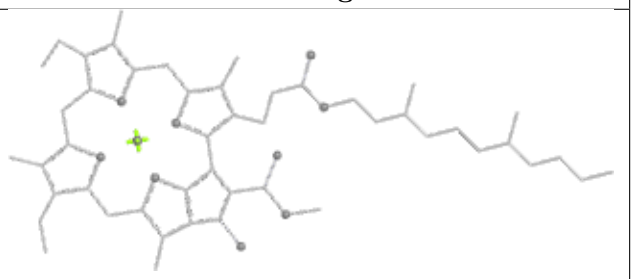
Bond lengths



Bond angles

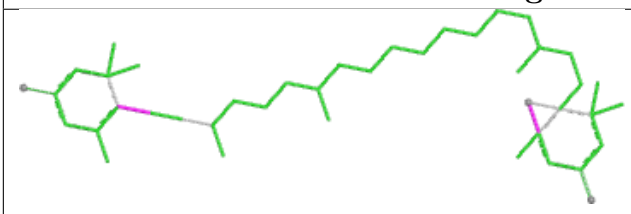


Torsions



Rings

Ligand DD6 B 302



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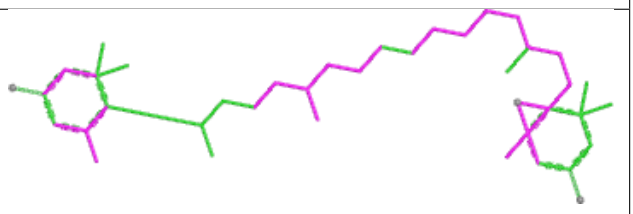

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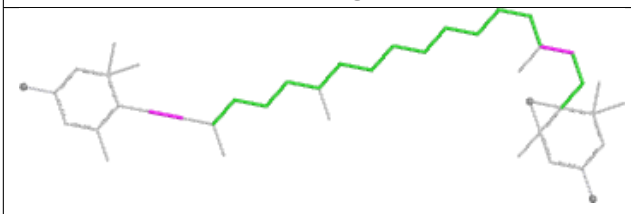

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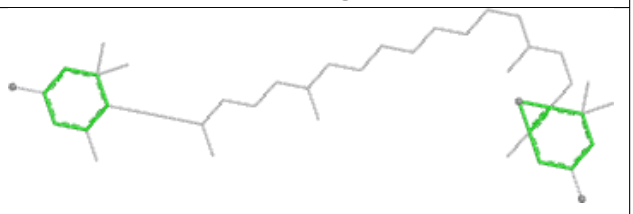
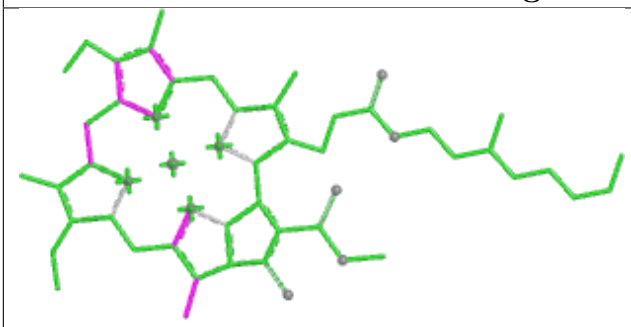


Rings

Ligand CLA K 308



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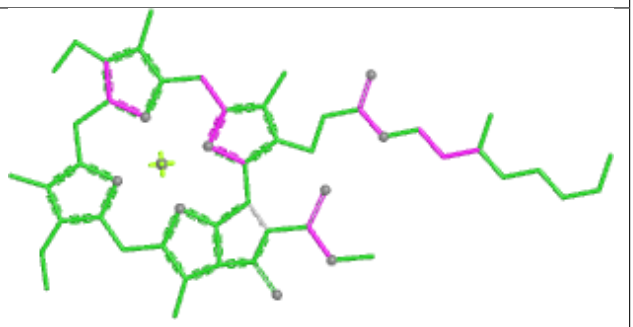
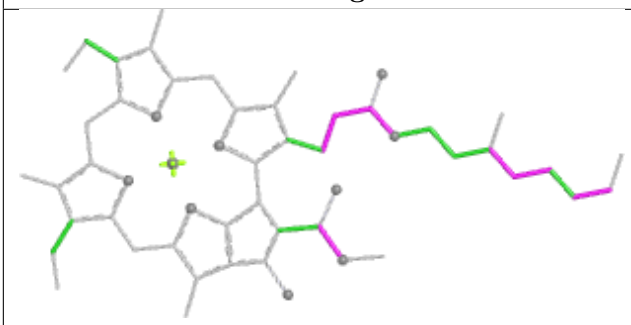


Bond angles



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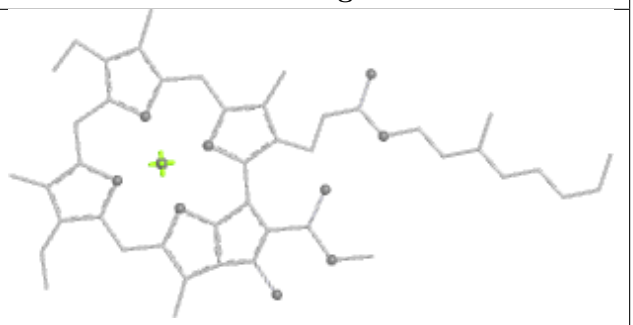
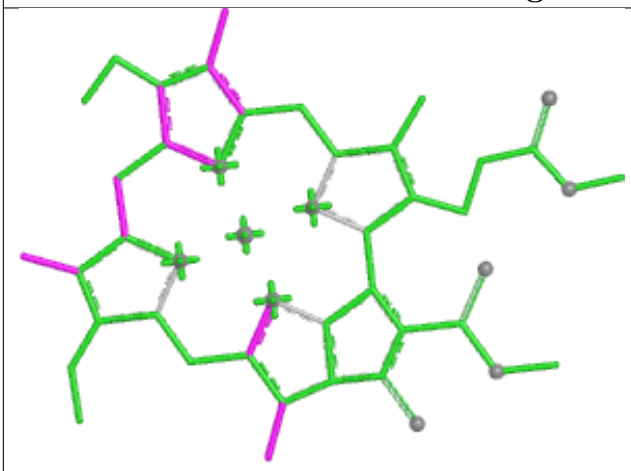


Rings

Ligand CLA L 318



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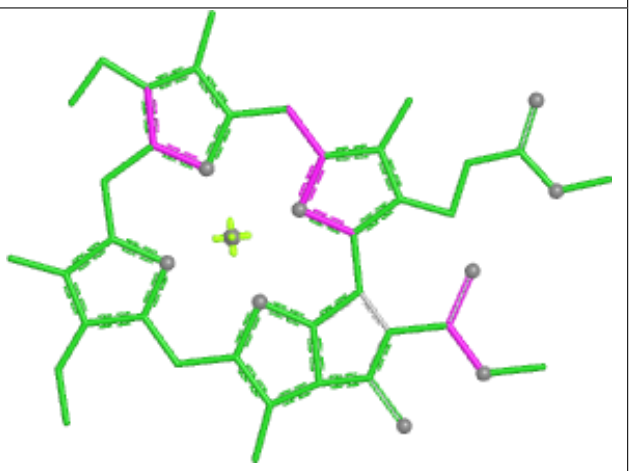
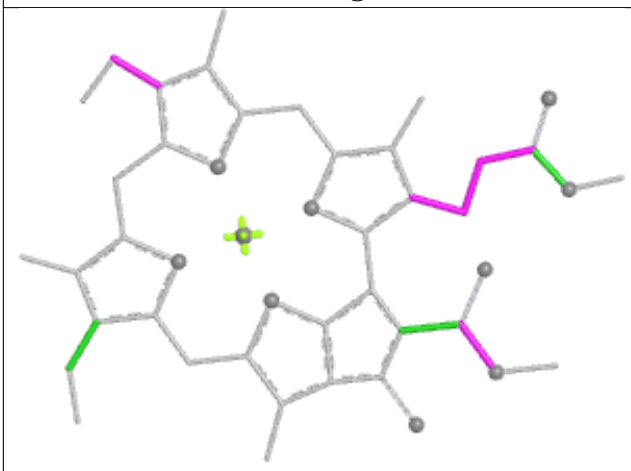


Bond angles



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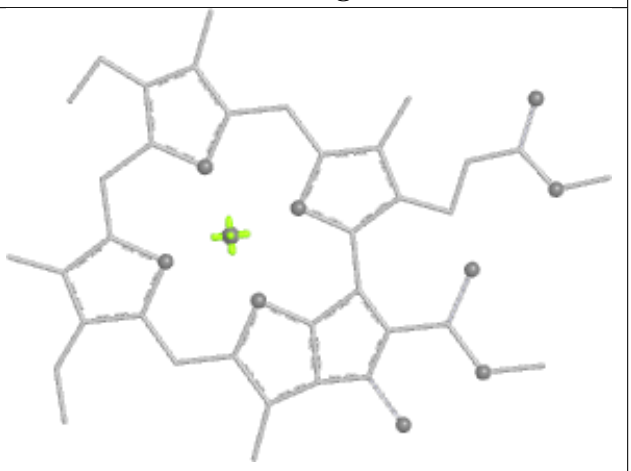
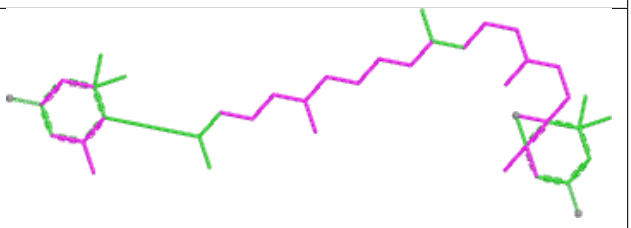


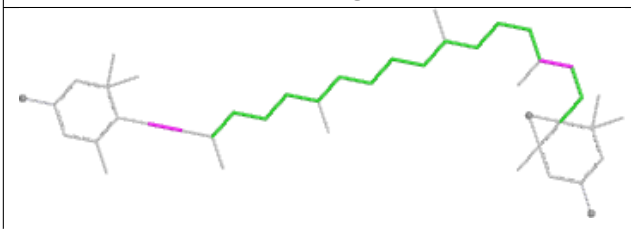
Rings

Ligand DD6 b 731

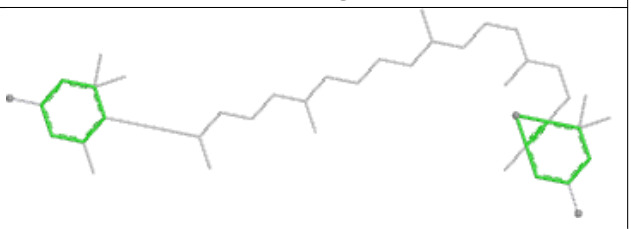
Bond lengths



Bond angles

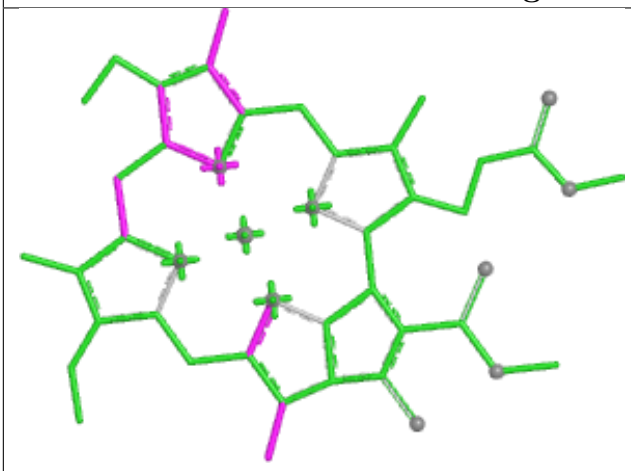


Torsions

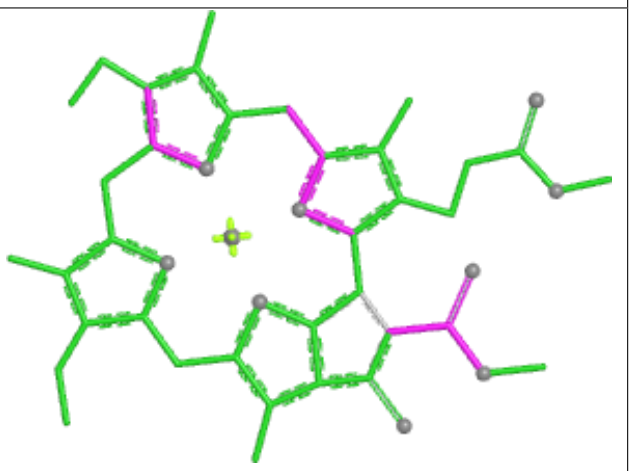


Rings

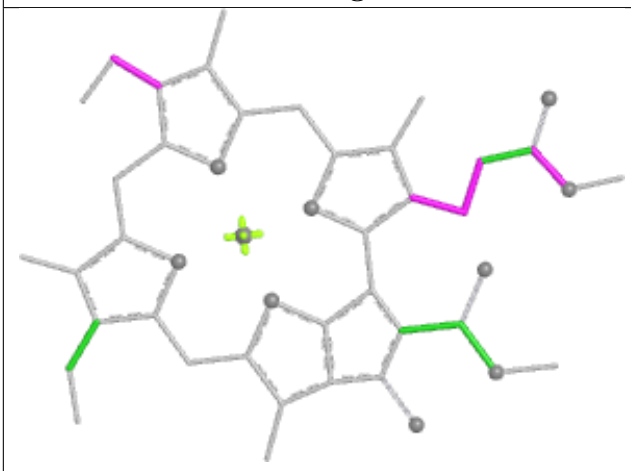
Ligand CLA G 518



Bond lengths



Bond angles



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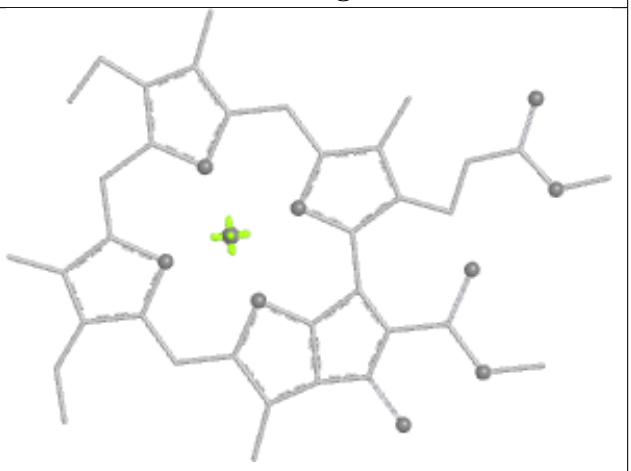
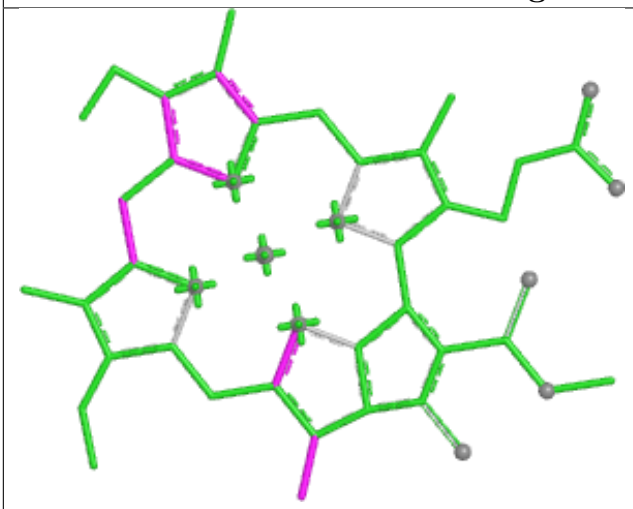
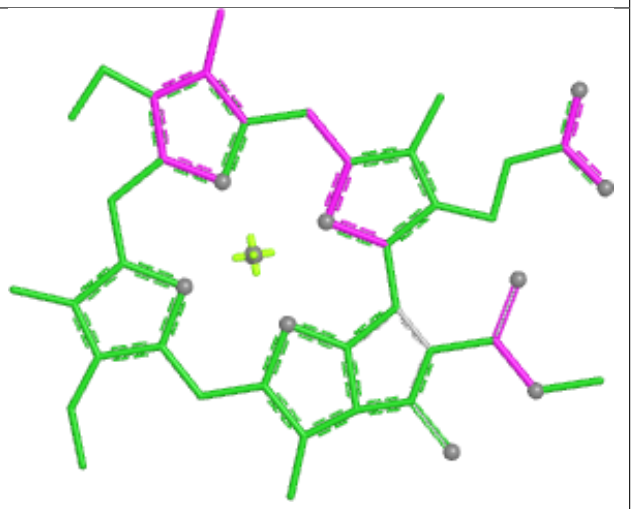


Rings

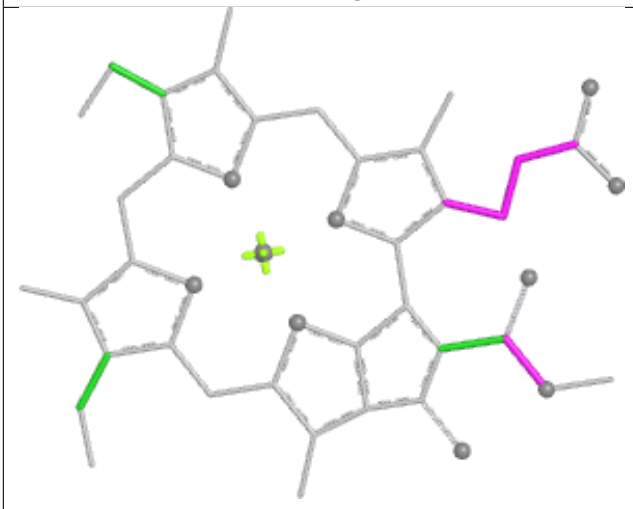
Ligand CLA a 711



Bond lengths



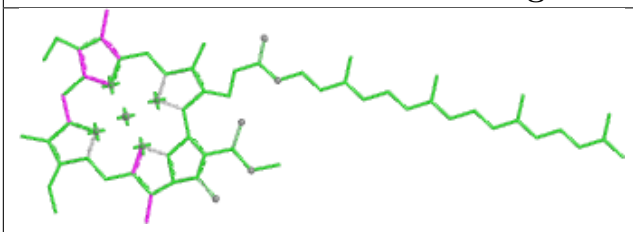
Bond angles



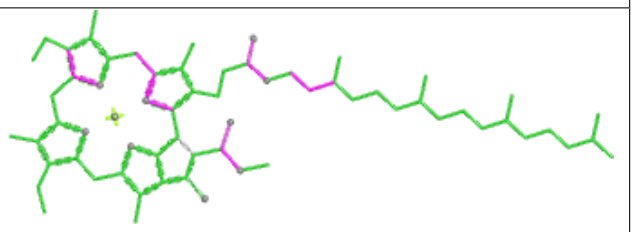
Torsions

Rings

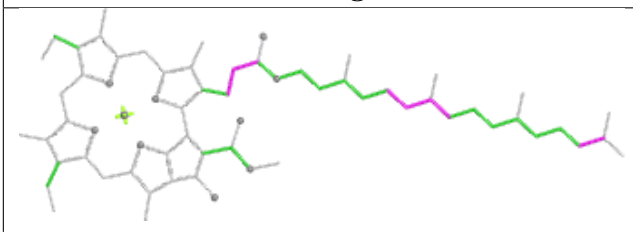
Ligand CLA b 708



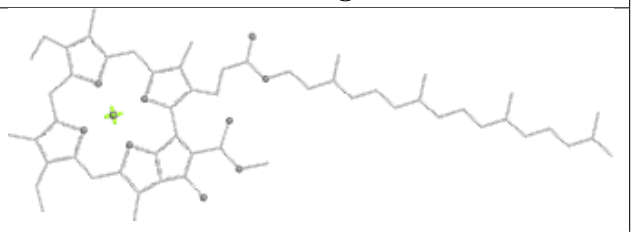
Bond lengths



Bond angles

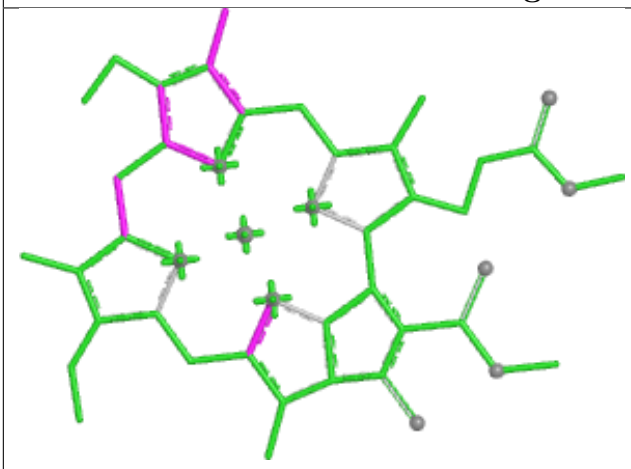


Torsions

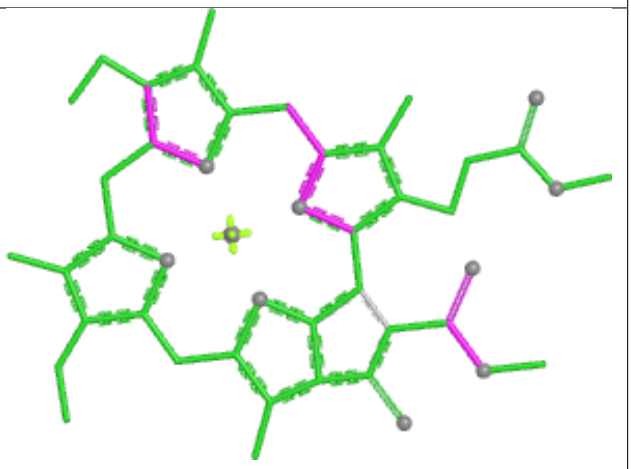


Rings

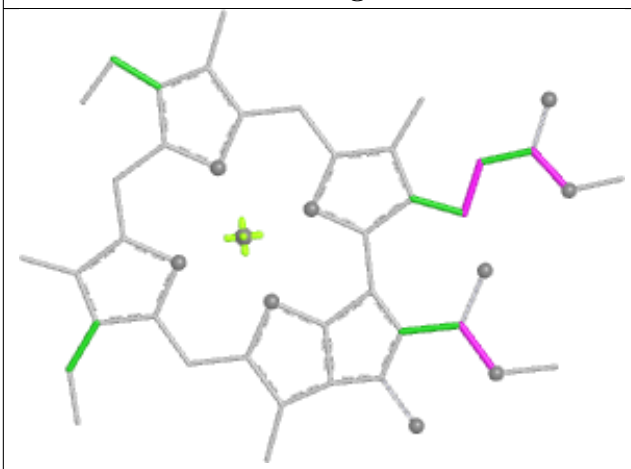
Ligand CLA A 311



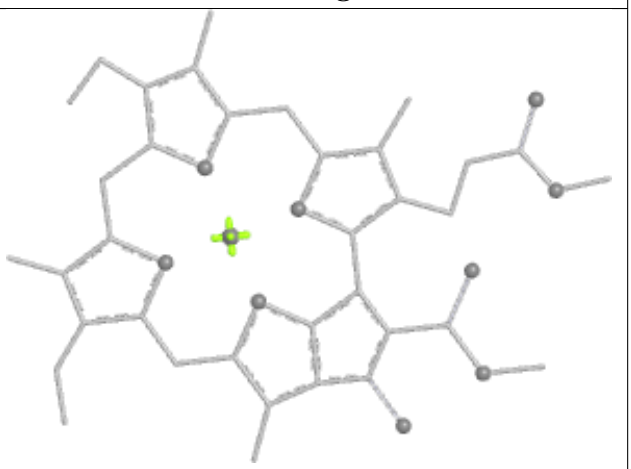
Bond lengths



Bond angles

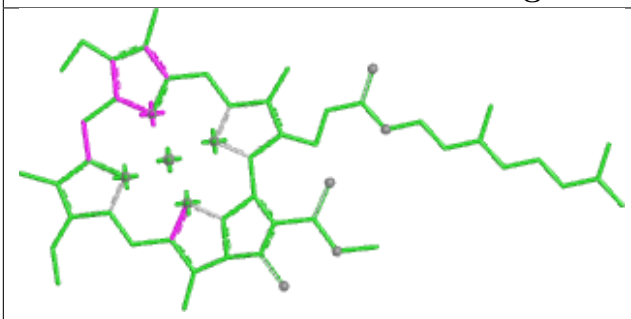


Torsions

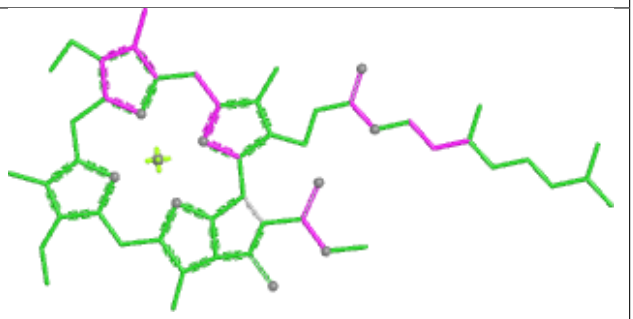


Rings

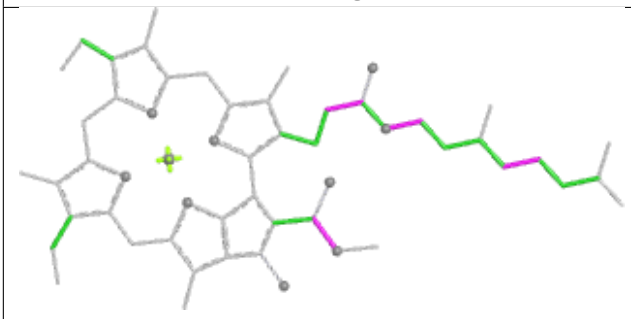
Ligand CLA A 309



Bond lengths



Bond angles



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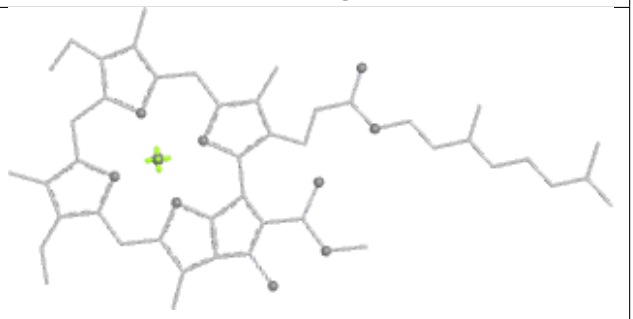
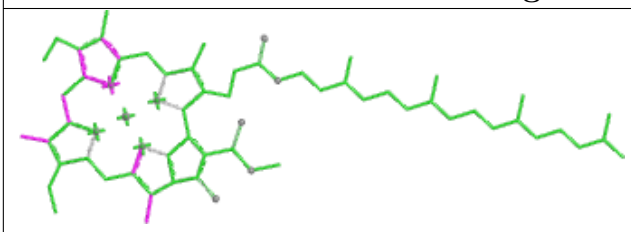
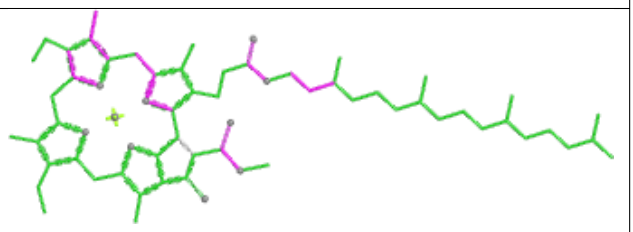


Rings

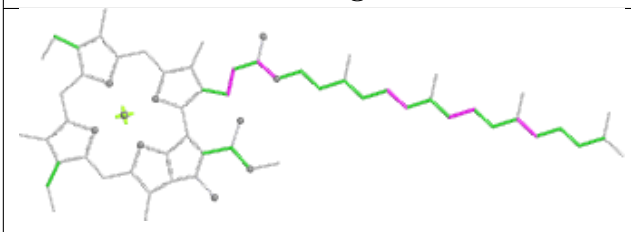
Ligand CLA G 513



Bond lengths



Bond angles



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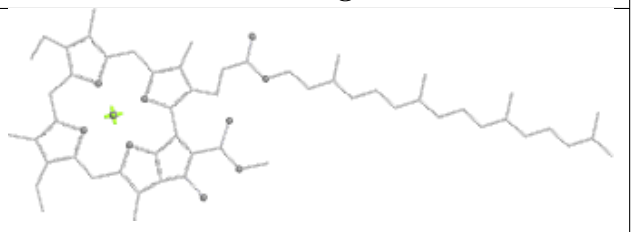
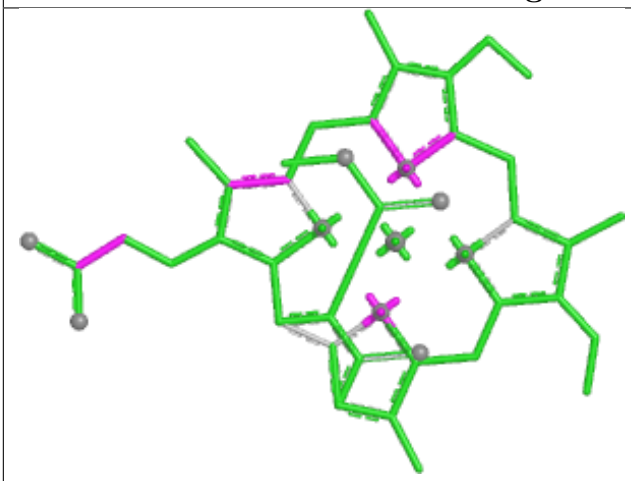
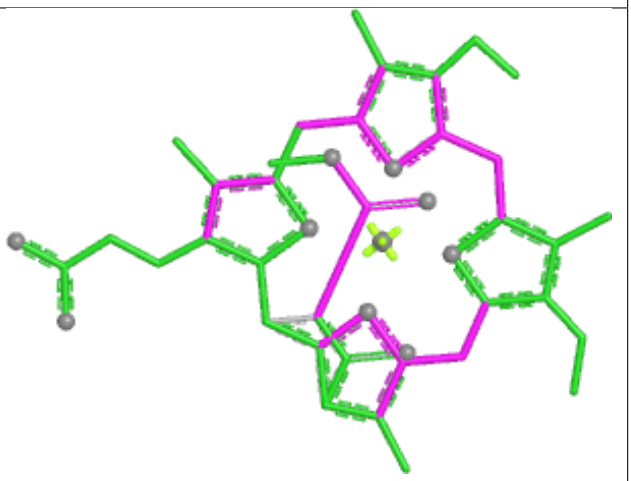


Rings

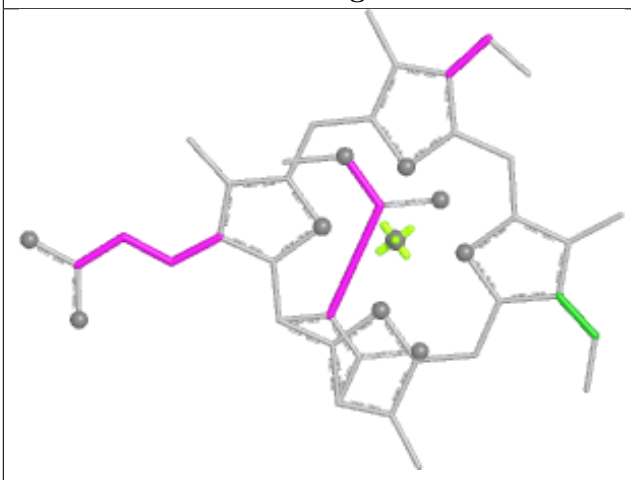
Ligand KC1 D 310



Bond lengths



Bond angles



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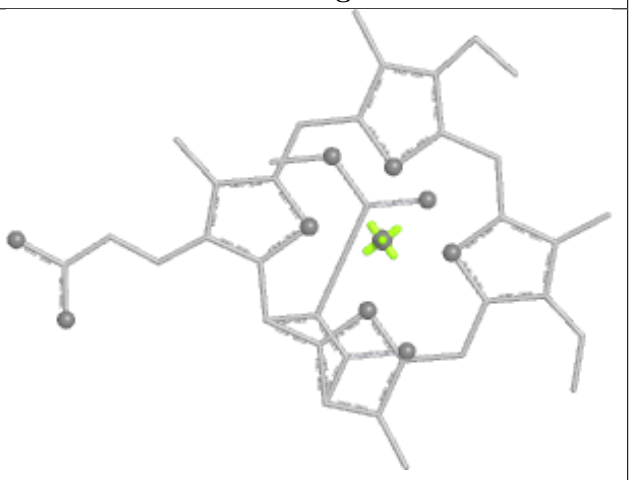
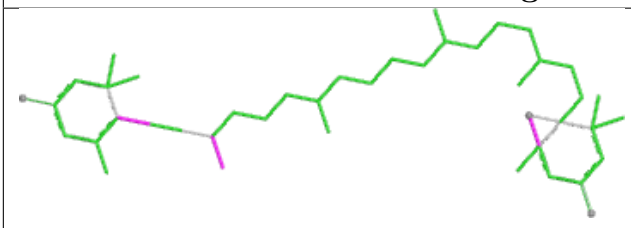


Rings

Ligand DD6 M 304



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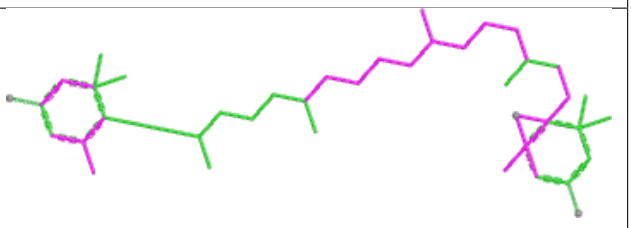
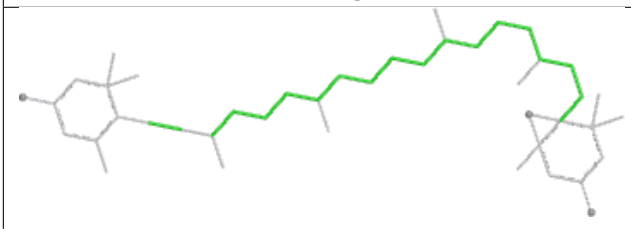


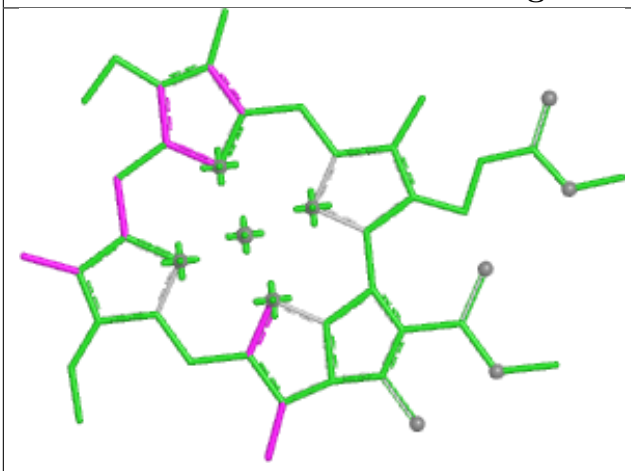
Bond angles



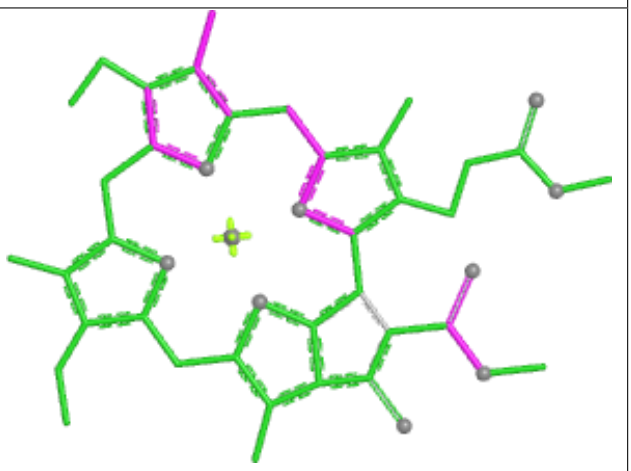
Torsions

Rings

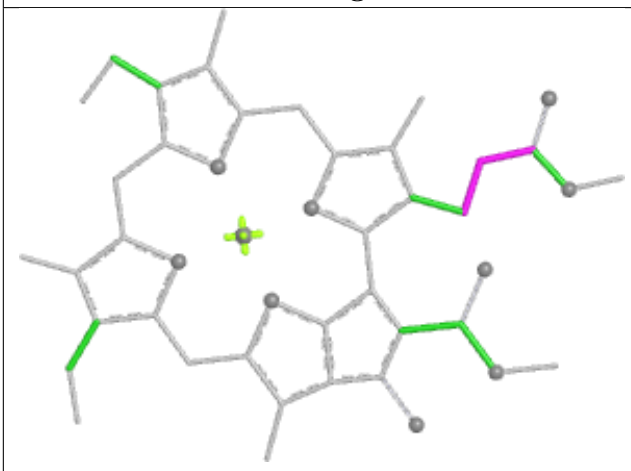
Ligand CLA b 714



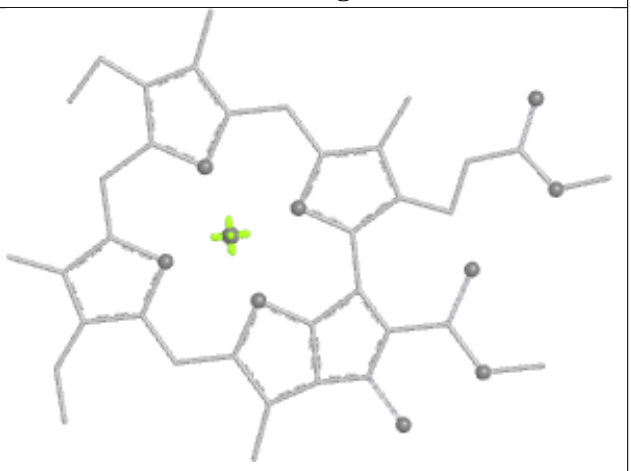
Bond lengths



Bond angles

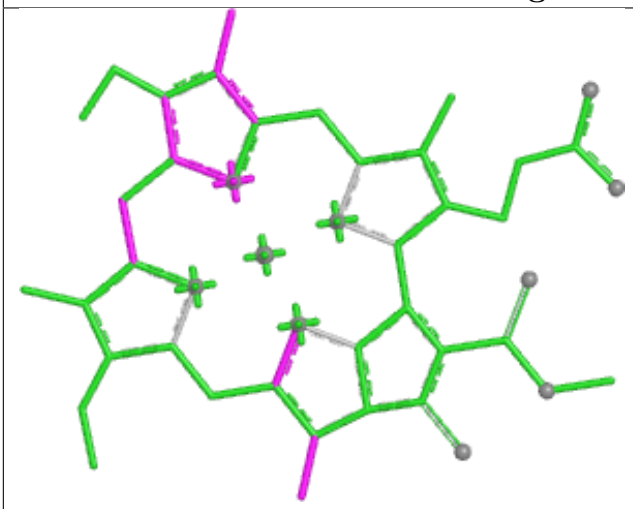


Torsions



Rings

Ligand CLA a 715



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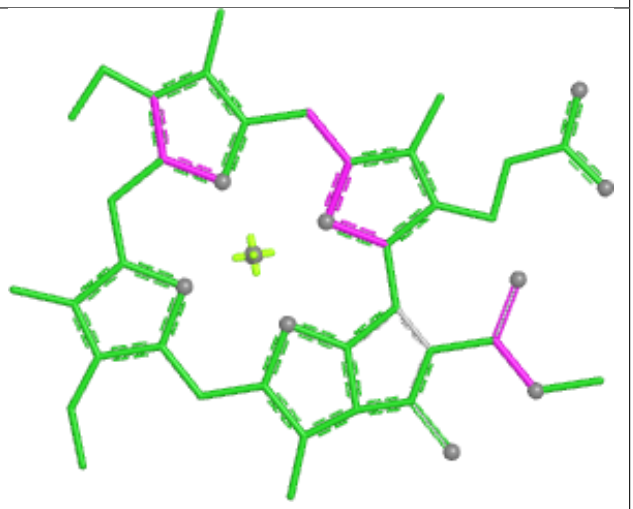
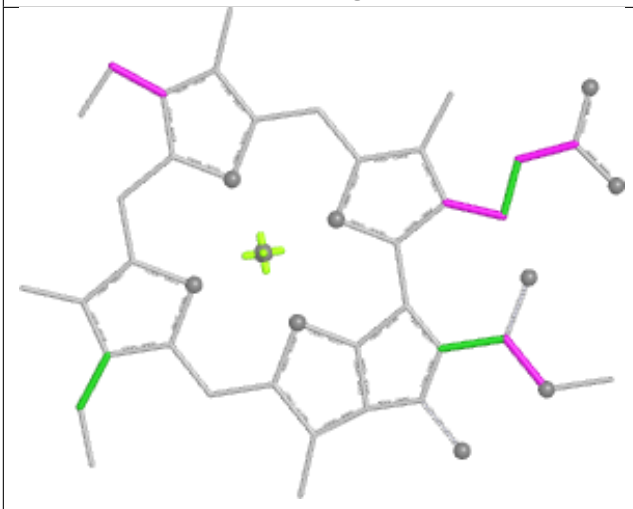


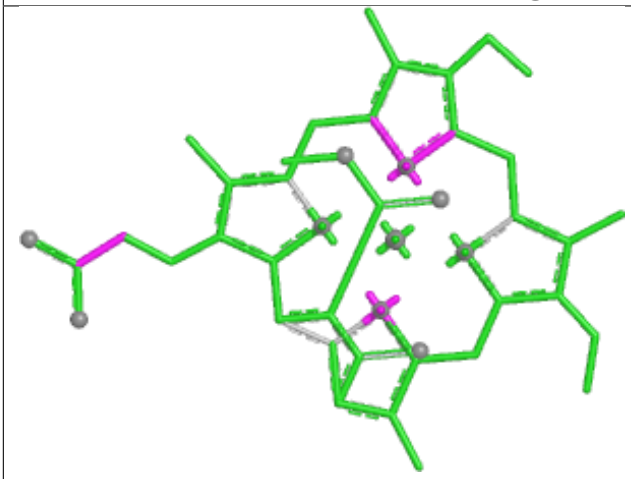
Bond angles



Torsions

Rings

Ligand KC1 P 211



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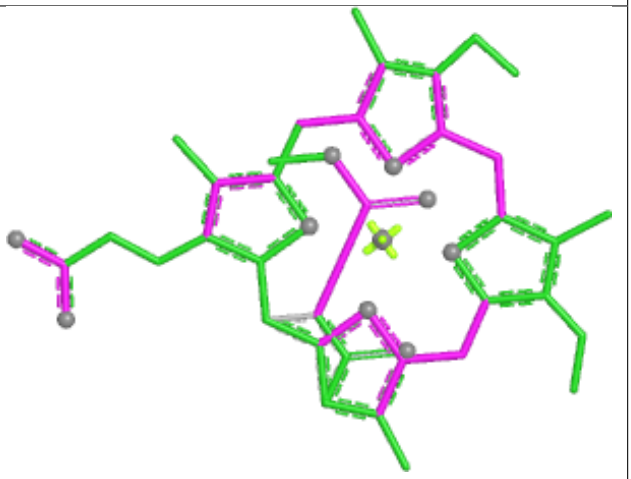
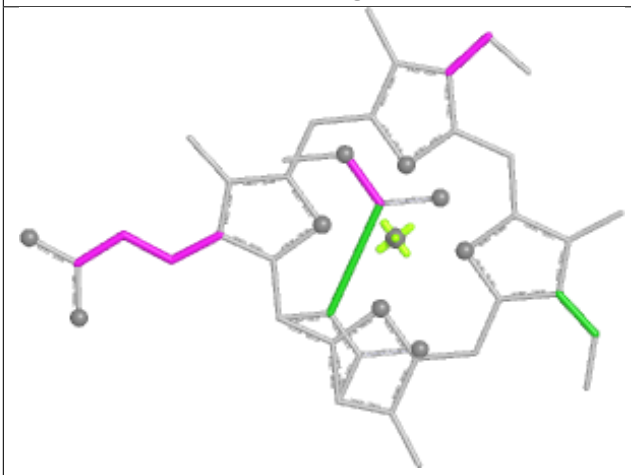


Bond angles



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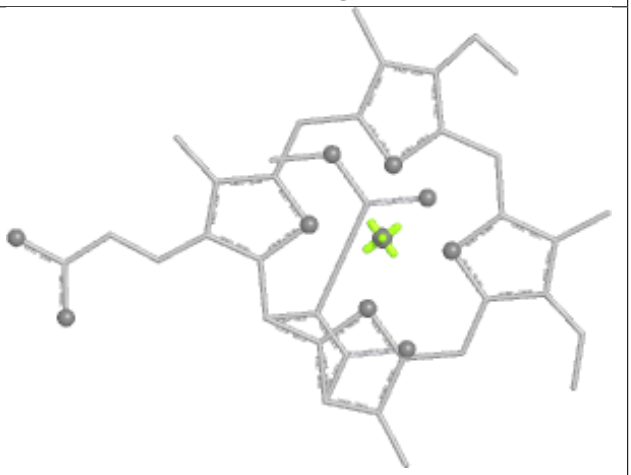
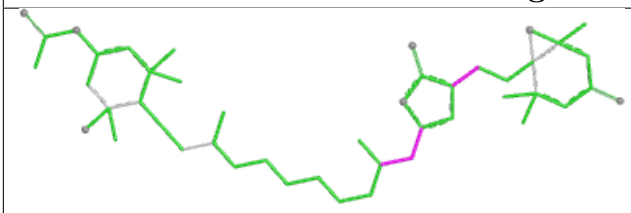


Rings

Ligand PID D 305



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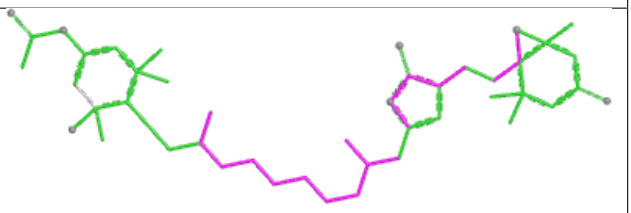
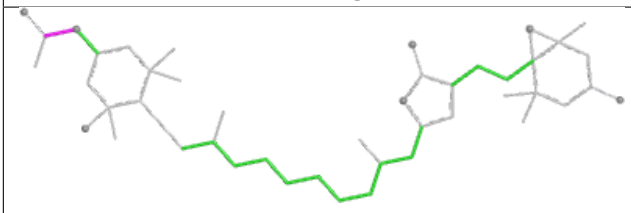
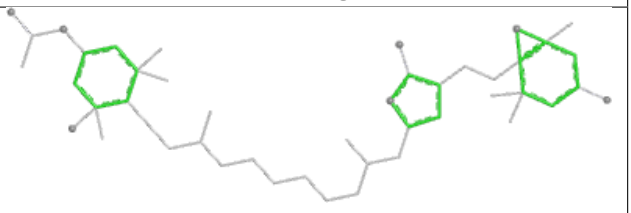


Bond angles

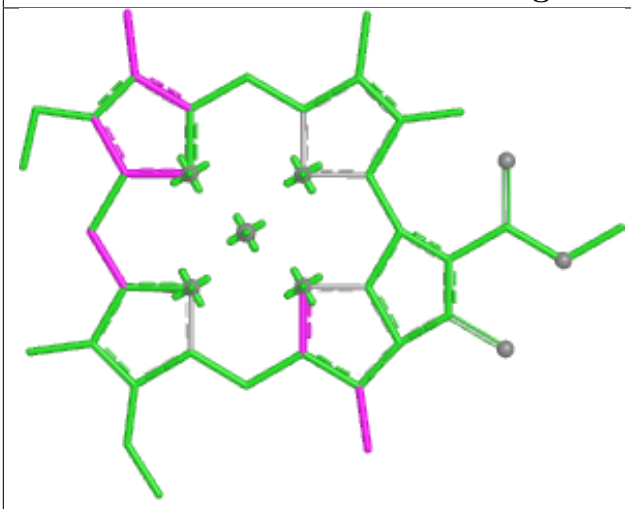


Torsions

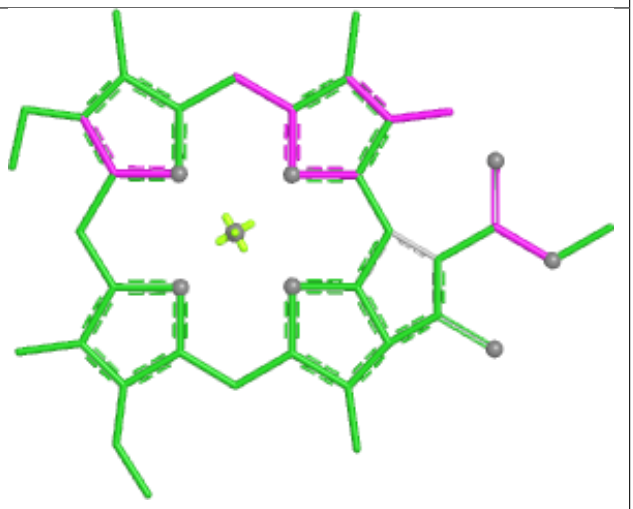


Rings

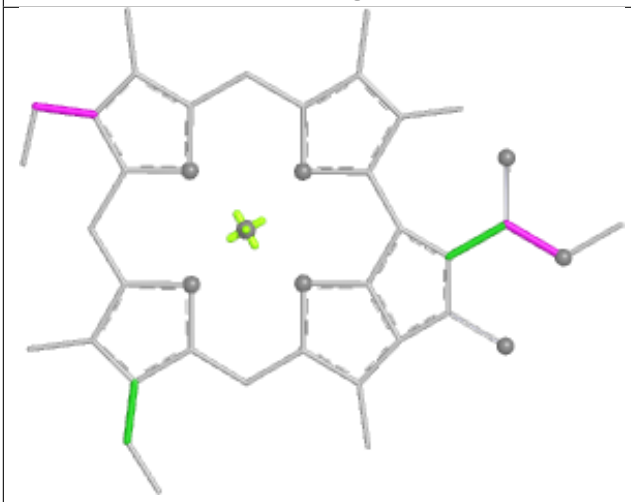
Ligand CLA l 308



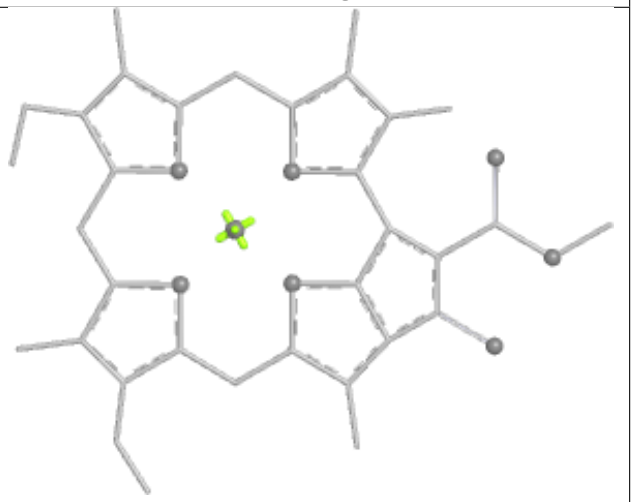
Bond lengths



Bond angles

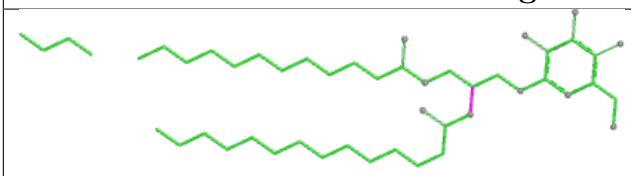


Torsions

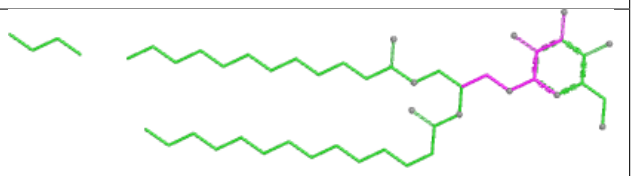


Rings

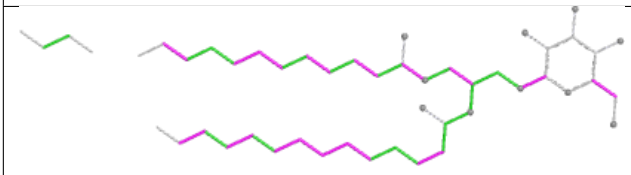
Ligand LMG D 317



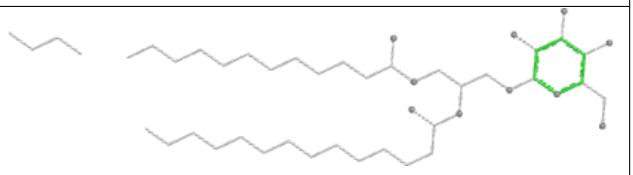
Bond lengths



Bond angles

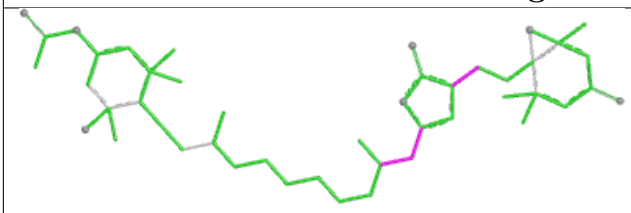


Torsions

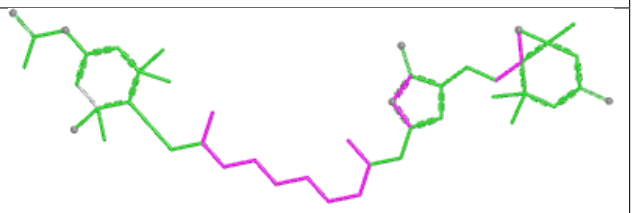


Rings

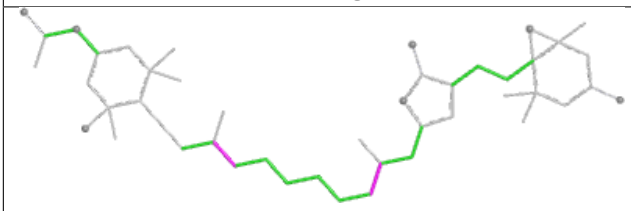
Ligand PID D 304



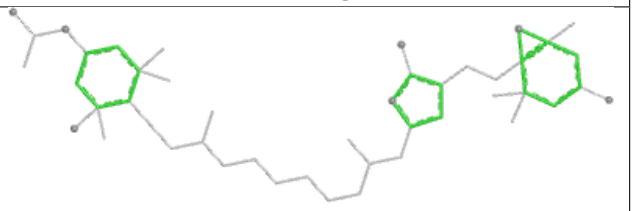
Bond lengths



Bond angles

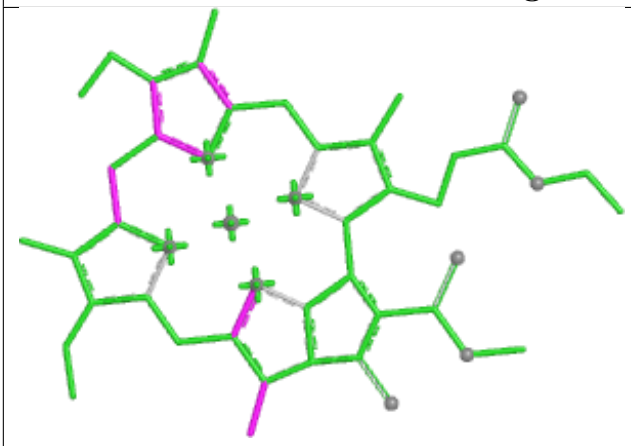


Torsions



Rings

Ligand CLA D 308



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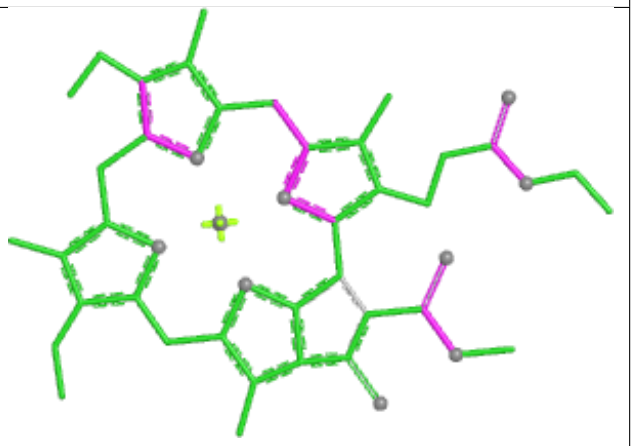
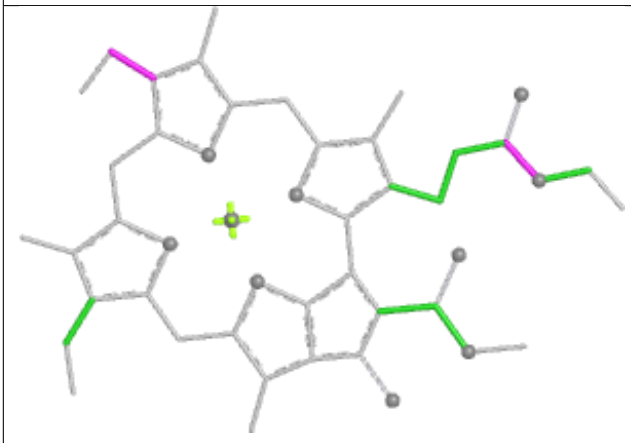


Bond angles



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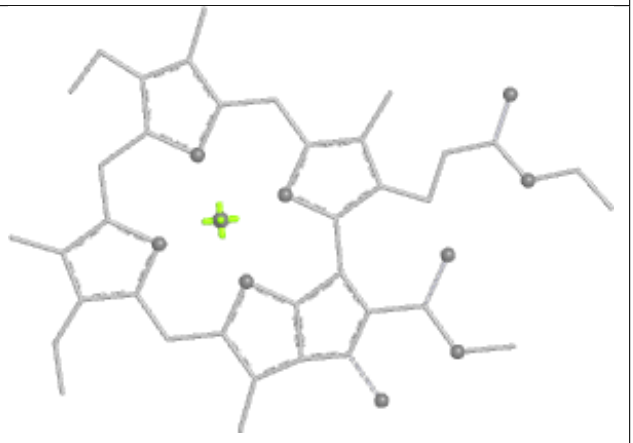
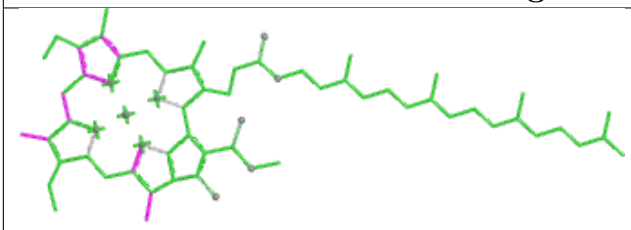


Rings

Ligand CLA b 727



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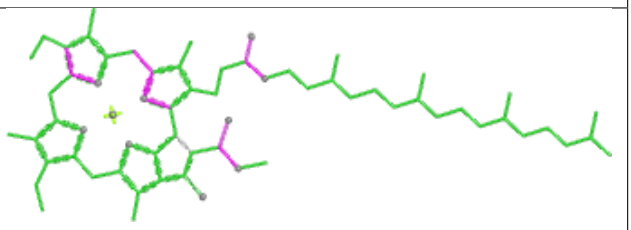
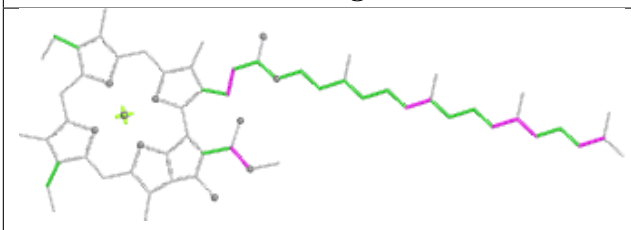


Bond angles



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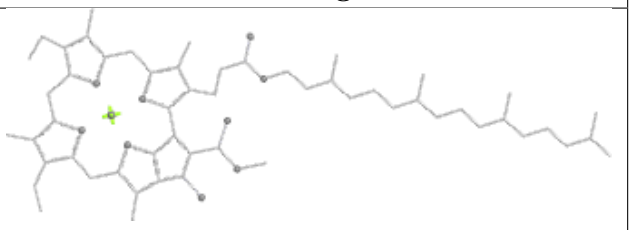
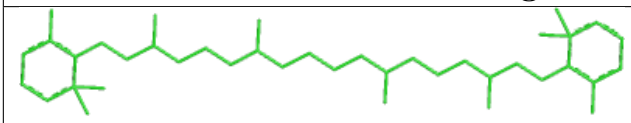


Rings

Ligand BCR m 201



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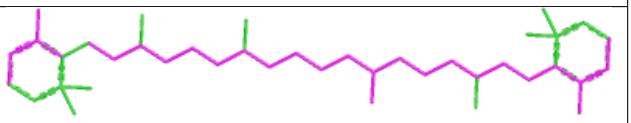
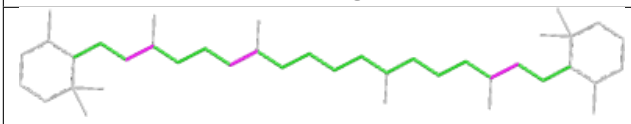


Bond angles



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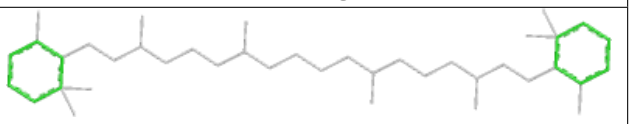
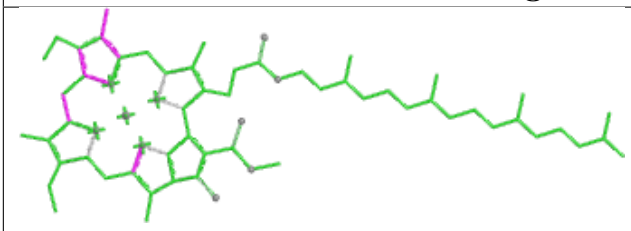


Rings

Ligand CLA B 313



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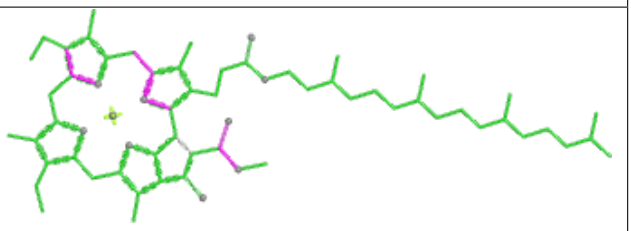
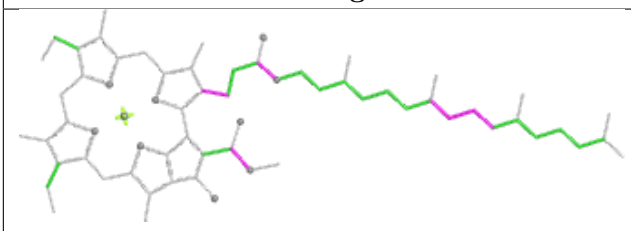


Bond angles



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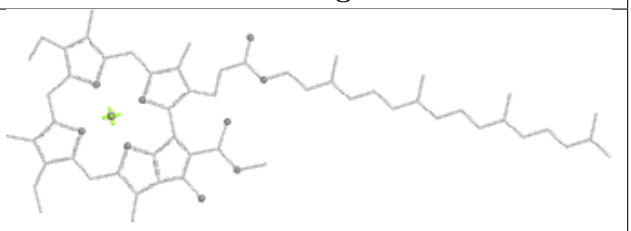
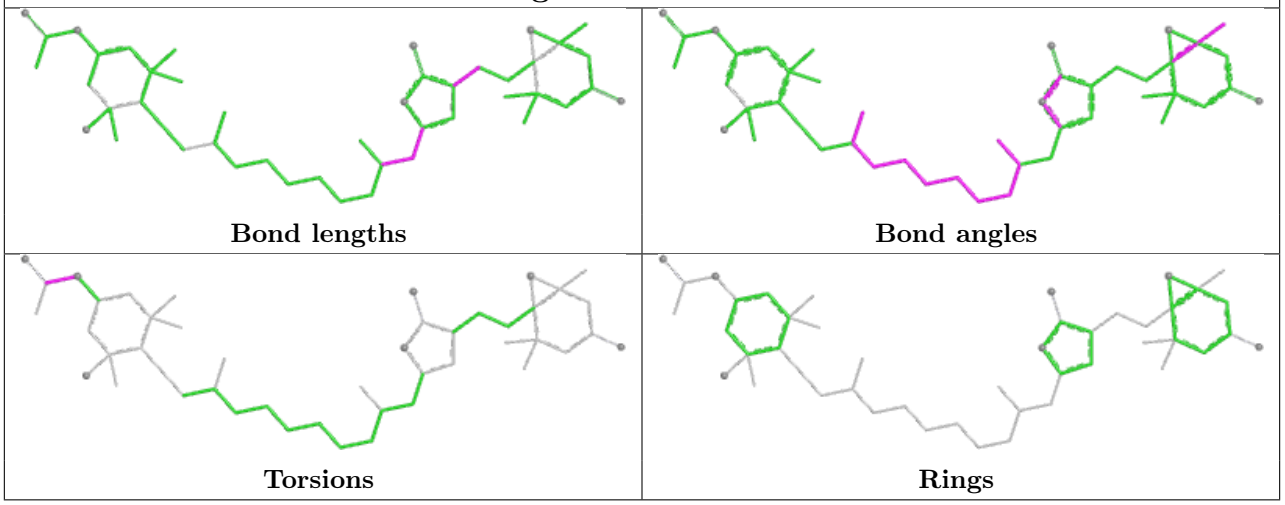
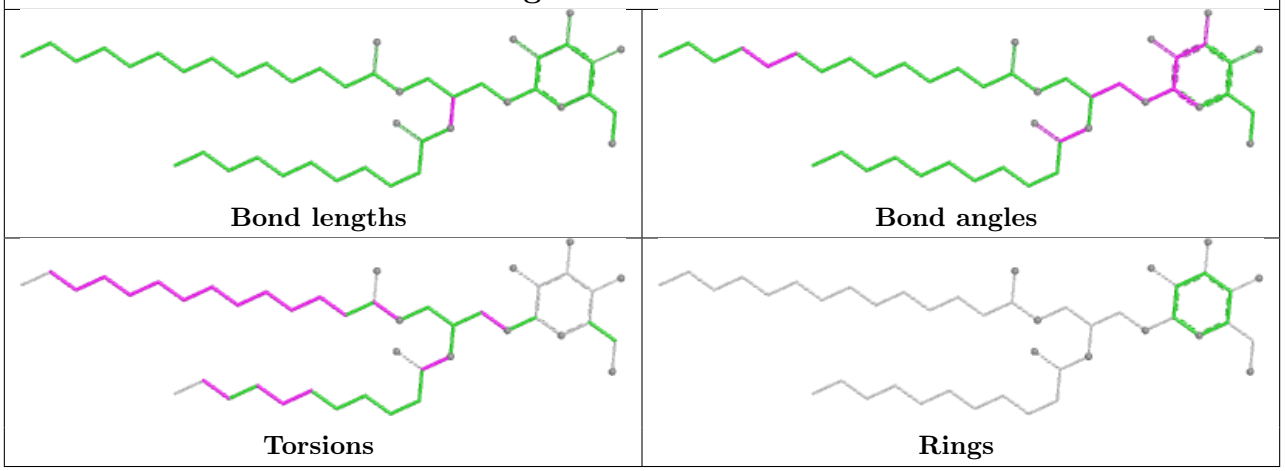


Rings

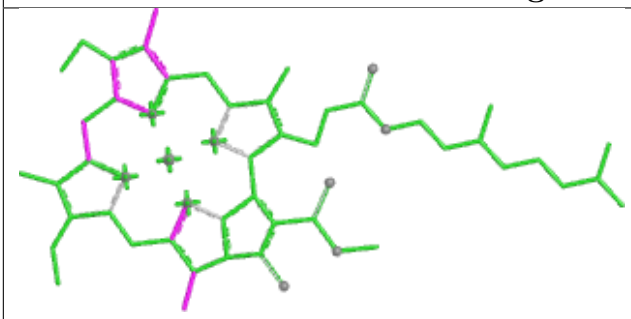
Ligand PID F 302



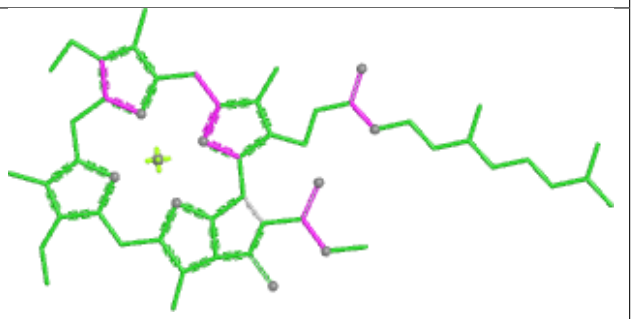
Ligand LMG b 733



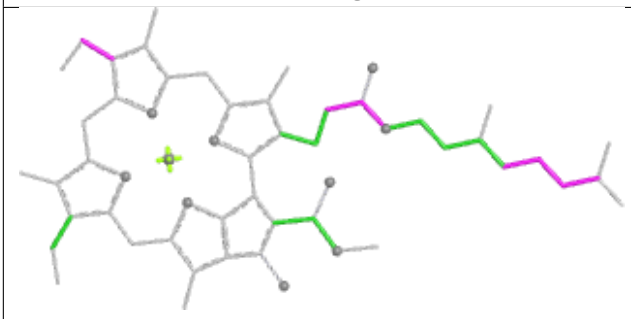
Ligand CLA h 202



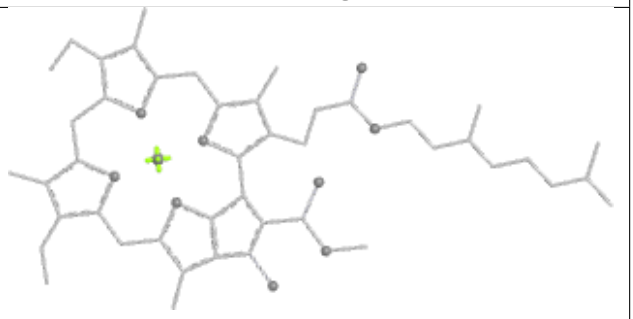
Bond lengths



Bond angles

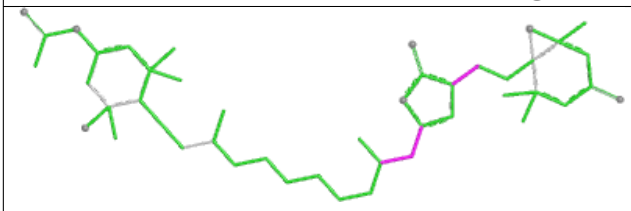


Torsions



Rings

Ligand PID O 307



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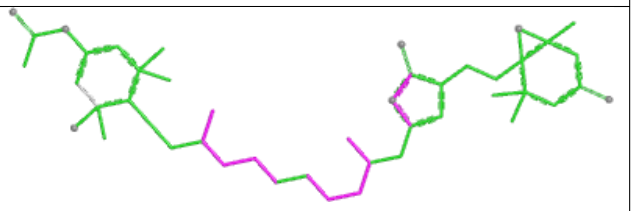
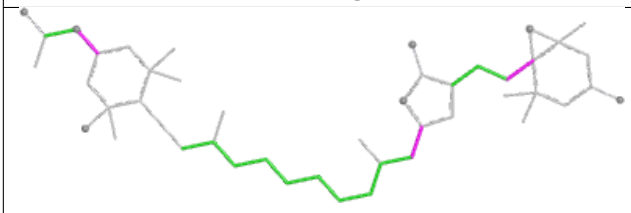


Bond angles



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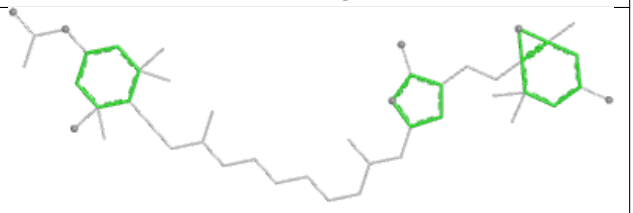
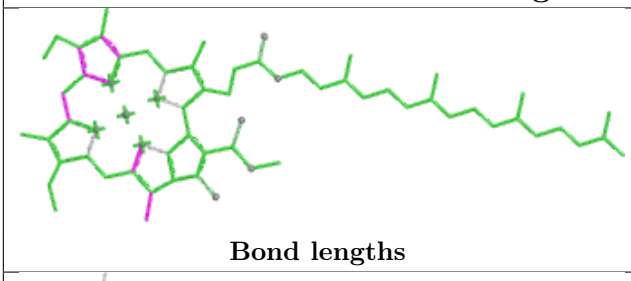


Rings

Ligand CLA l 311



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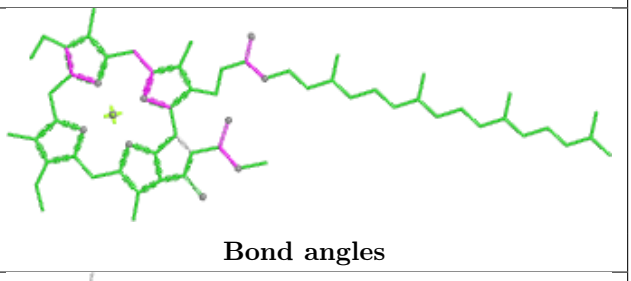
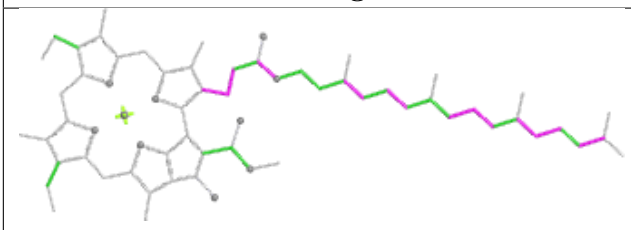
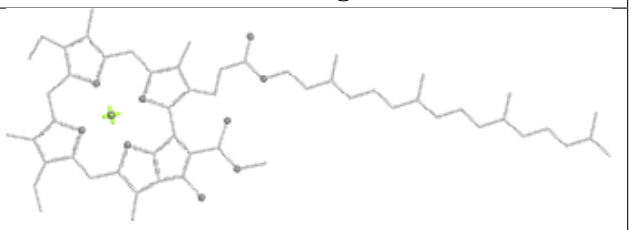


Bond angles

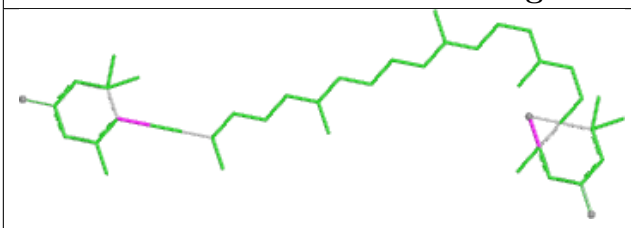


Torsions

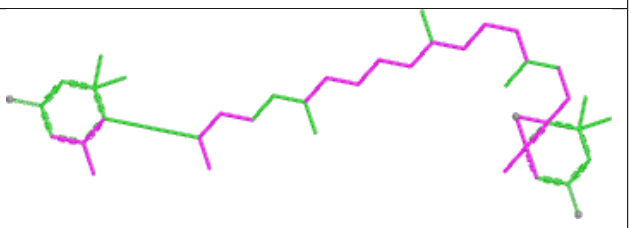


Rings

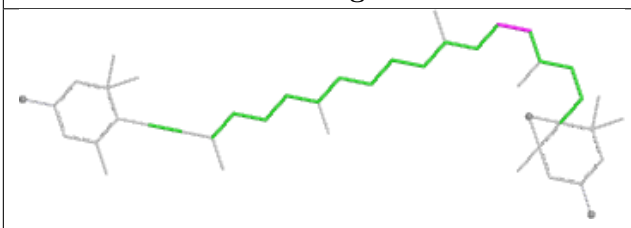
Ligand DD6 P 204



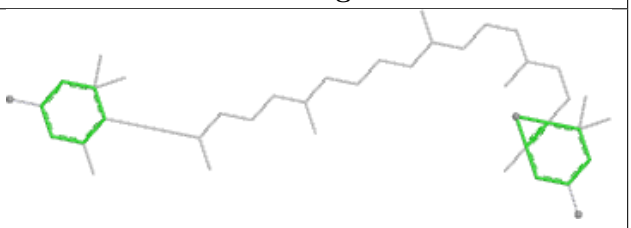
Bond lengths



Bond angles

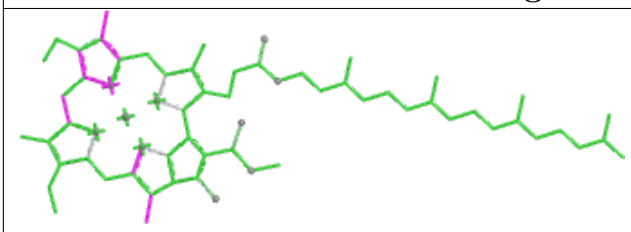


Torsions



Rings

Ligand CLA B 311



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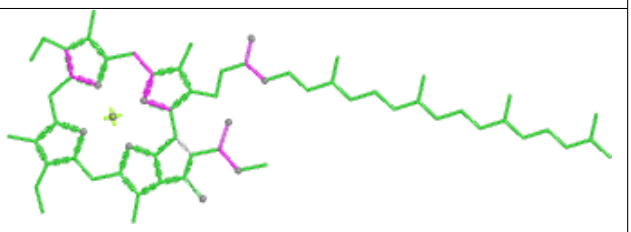
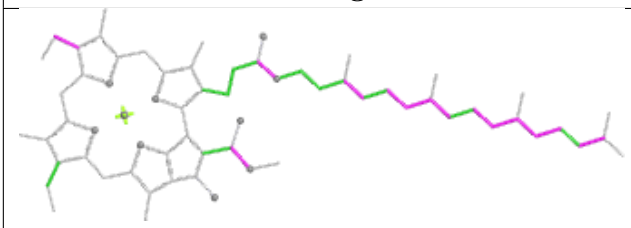


Bond angles



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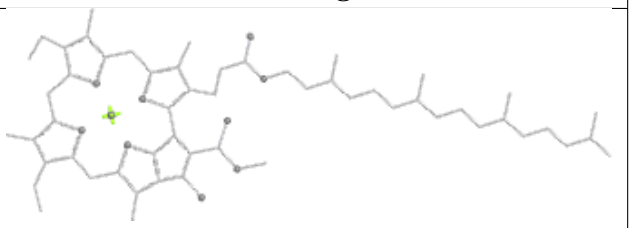
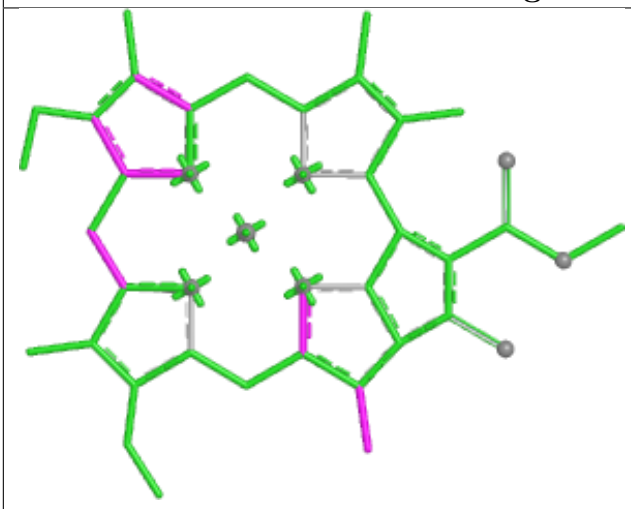


Rings

Ligand CLA A 315



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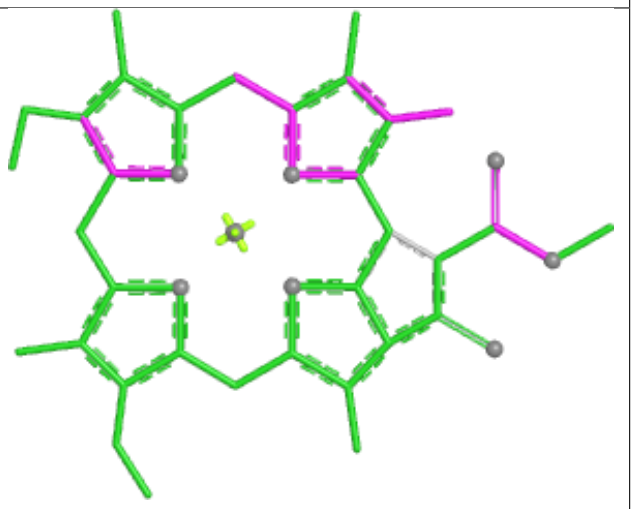
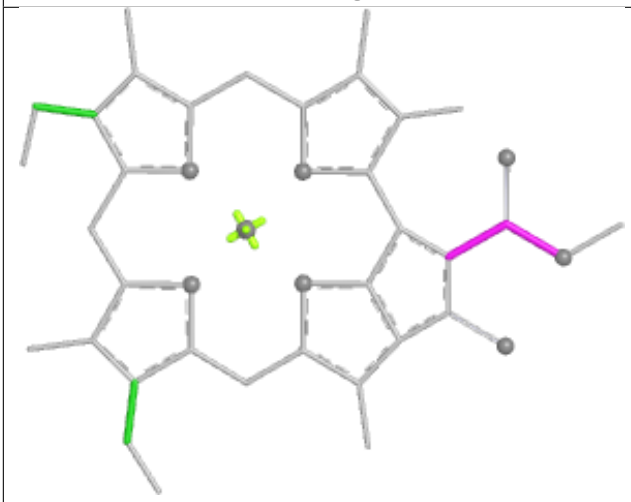


Bond angles



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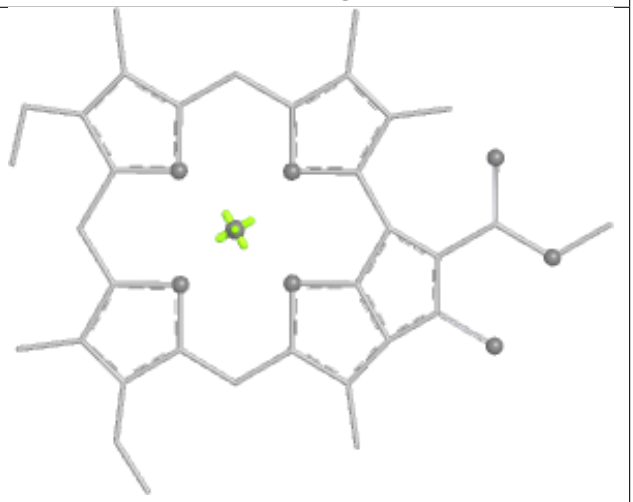
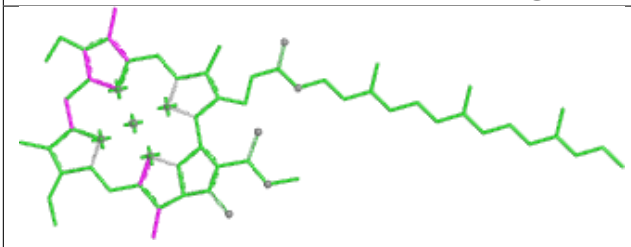


Rings

Ligand CLA a 720



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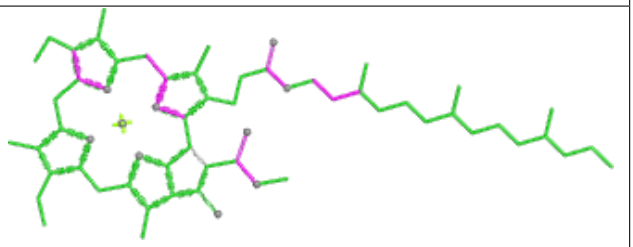
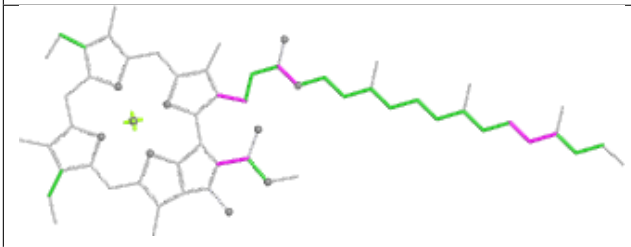
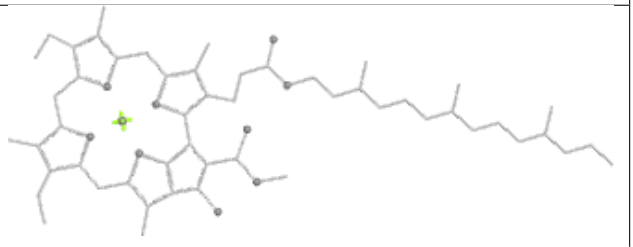


Bond angles

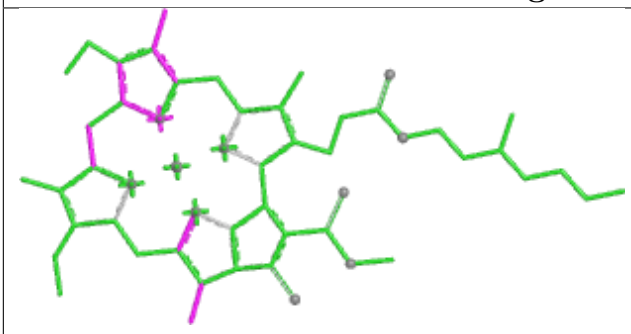


Torsions

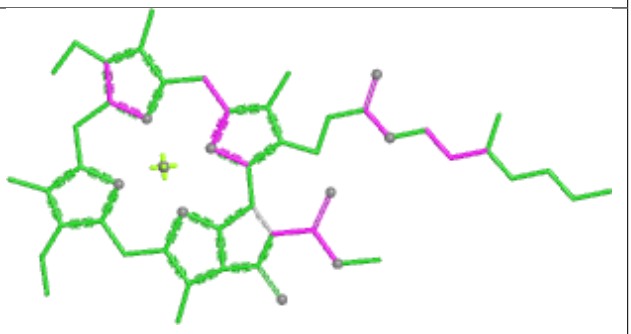


Rings

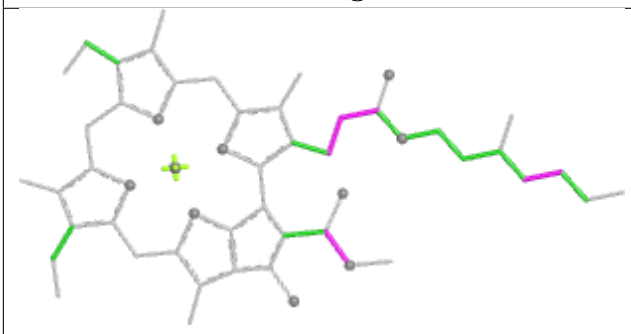
Ligand CLA J 312



Bond lengths



Bond angles



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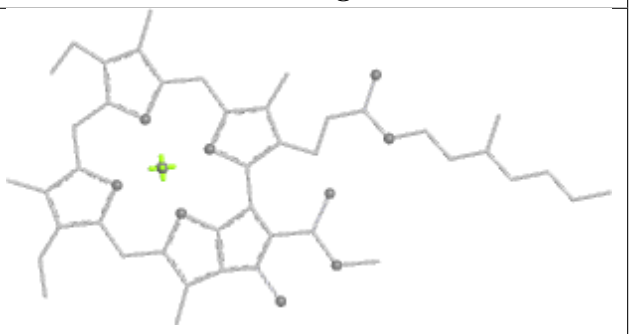
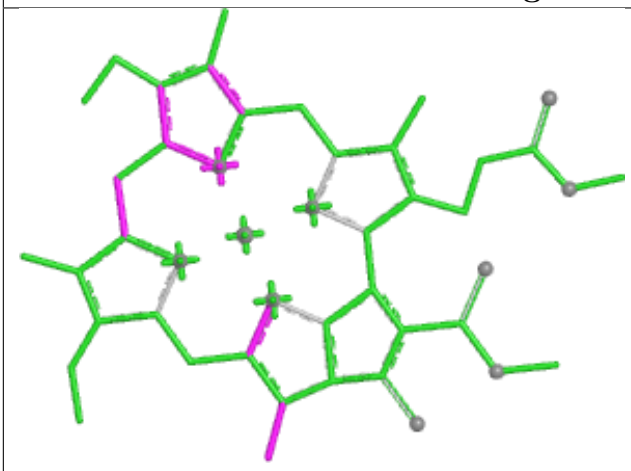
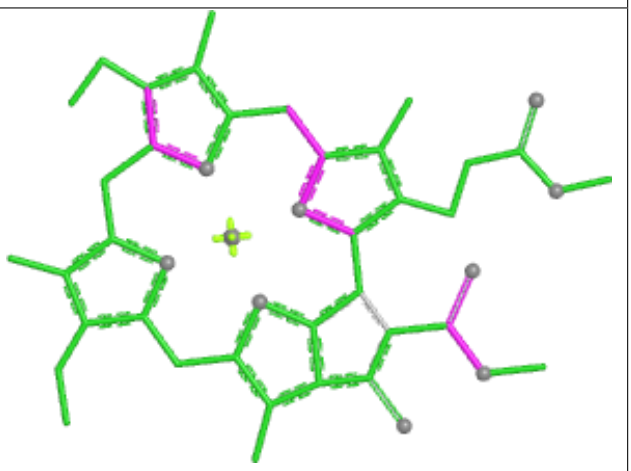


Rings

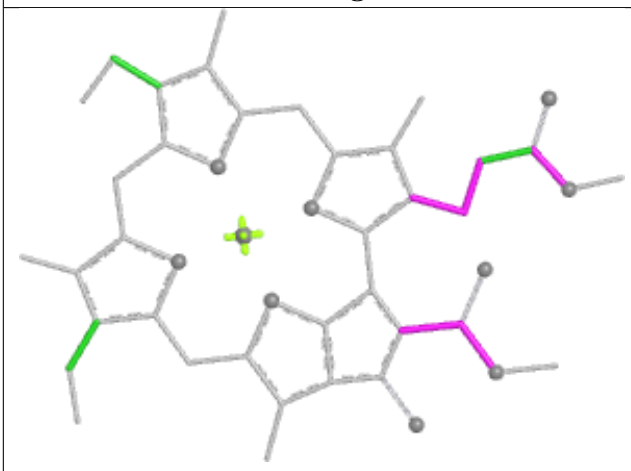
Ligand CLA H 312



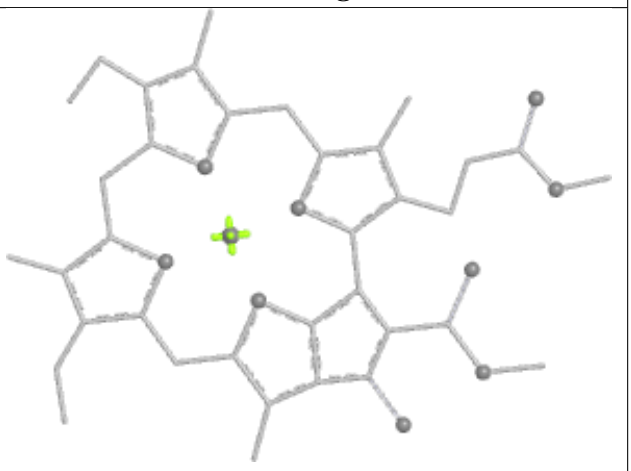
Bond lengths



Bond angles

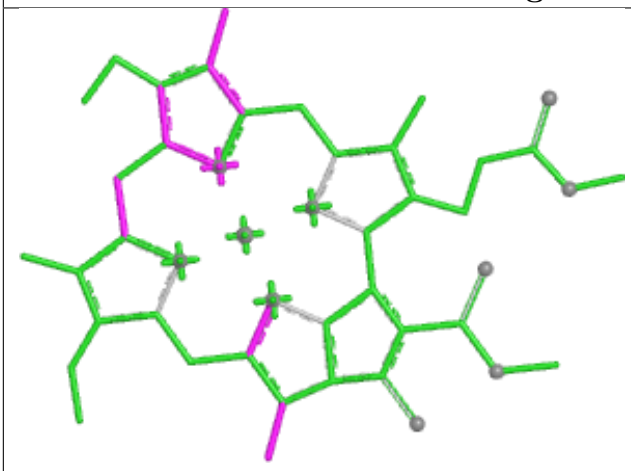


Torsions



Rings

Ligand CLA F 311



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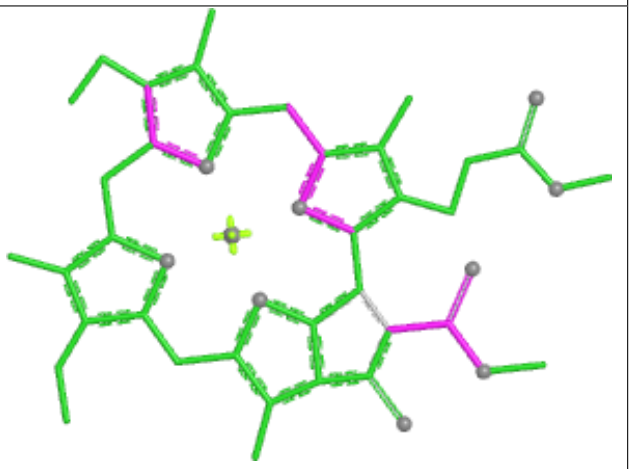
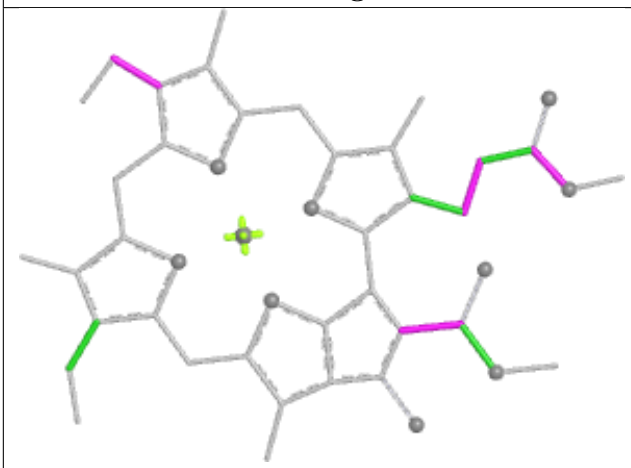


Bond angles



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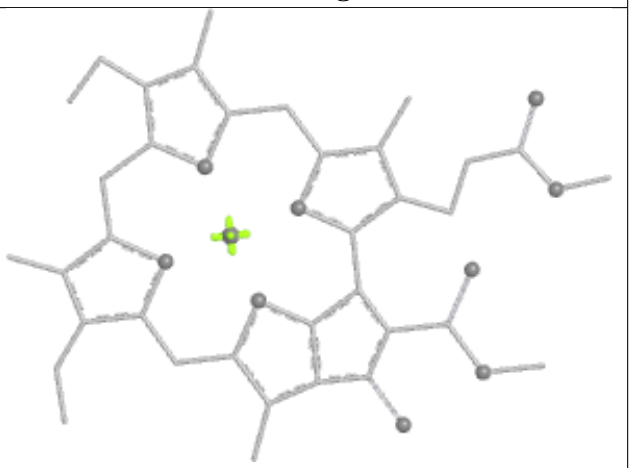
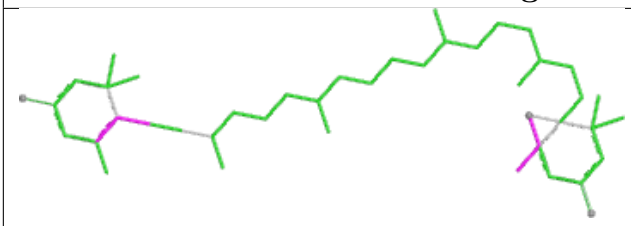


Rings

Ligand DD6 M 303



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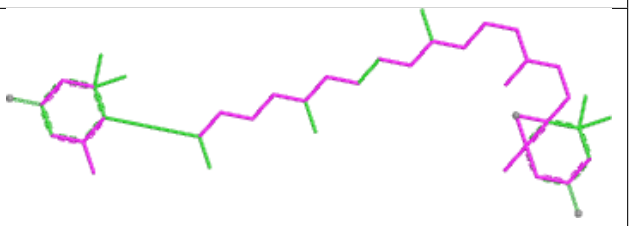
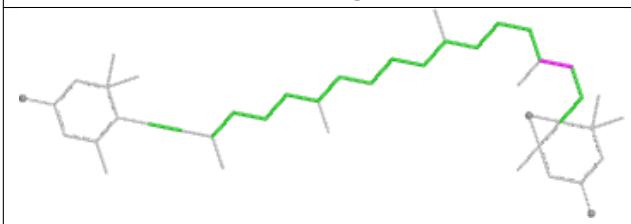
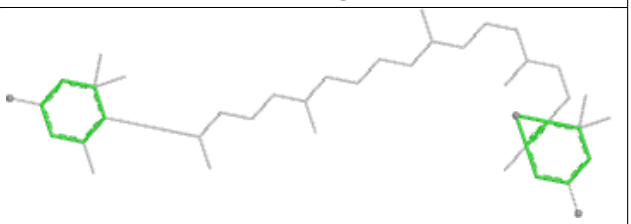


Bond angles

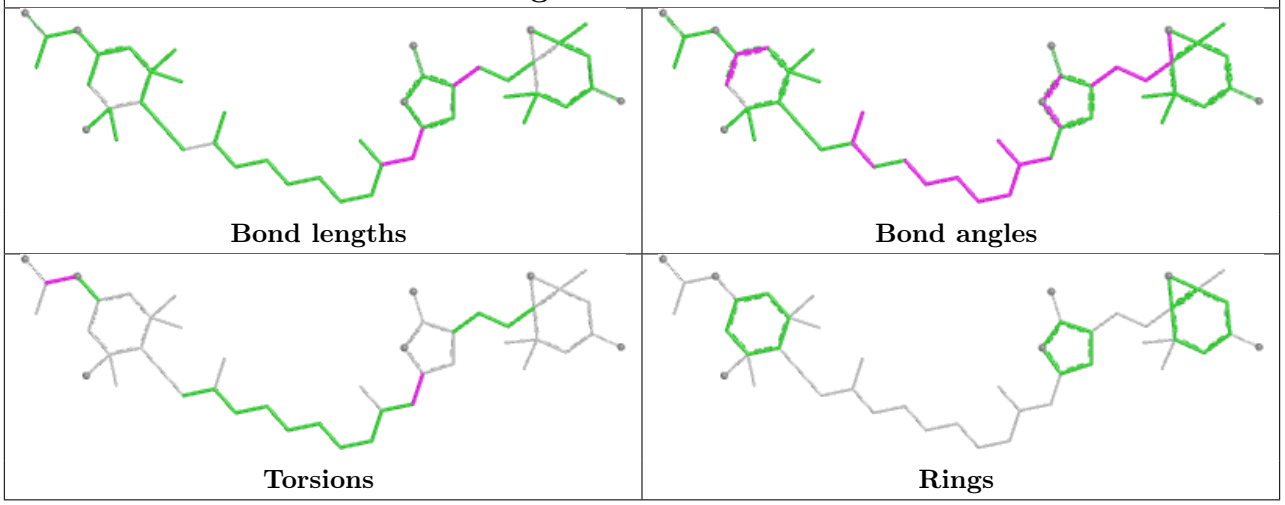


Torsions

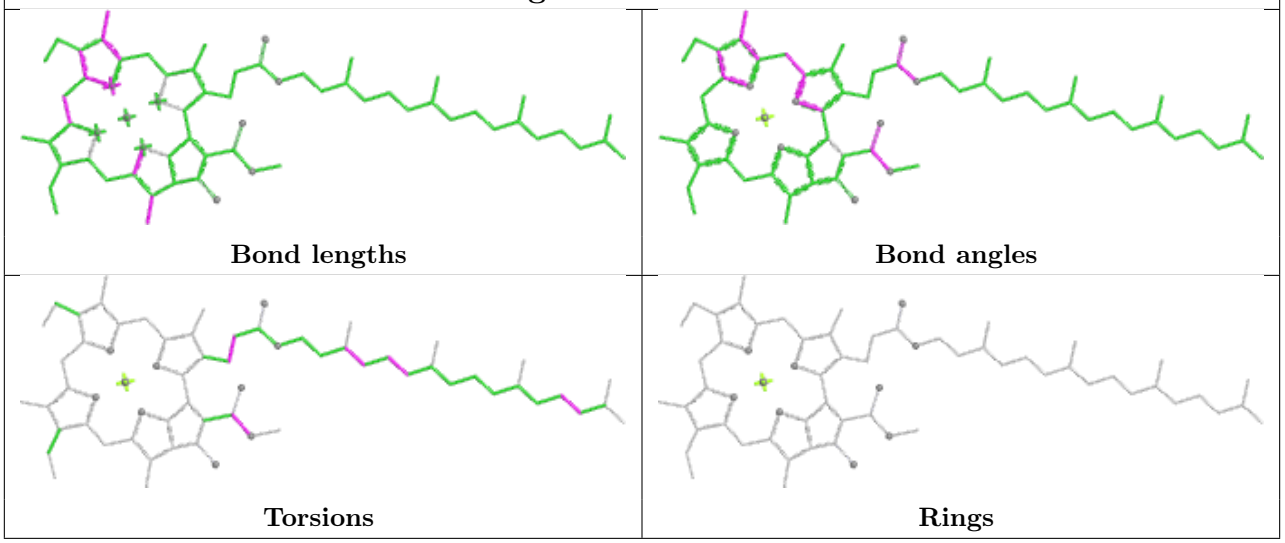


Rings

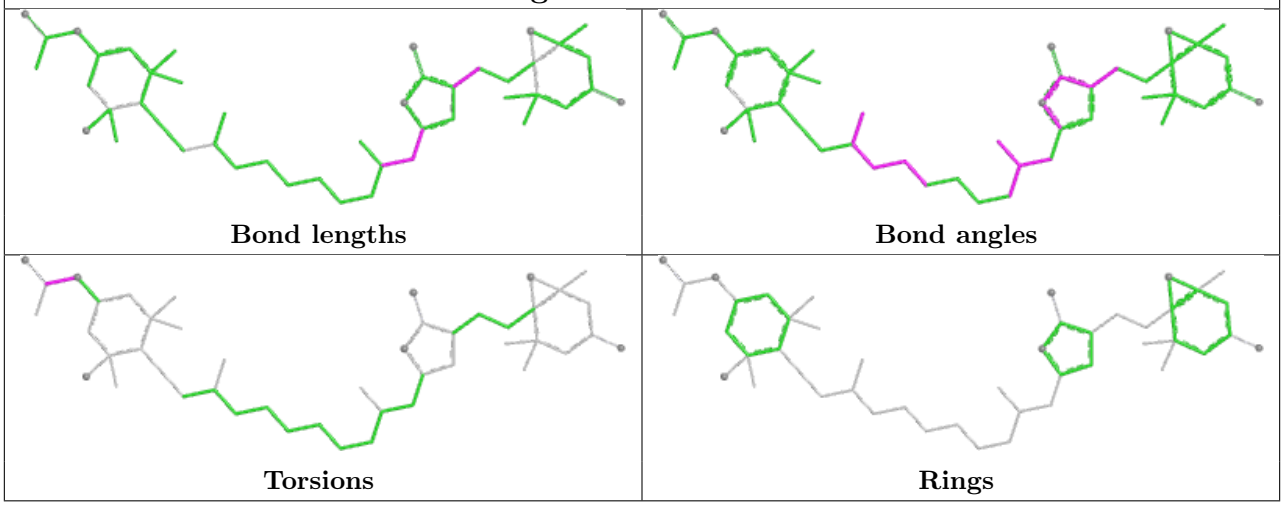
Ligand PID P 206



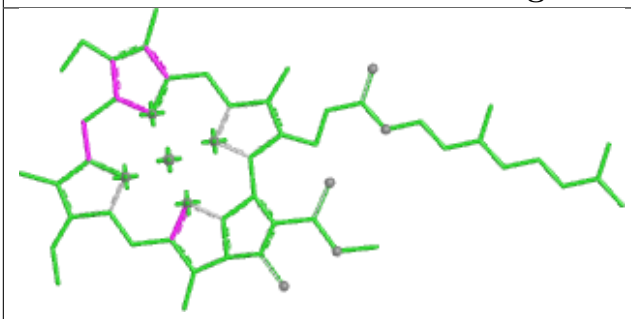
Ligand CLA b 722



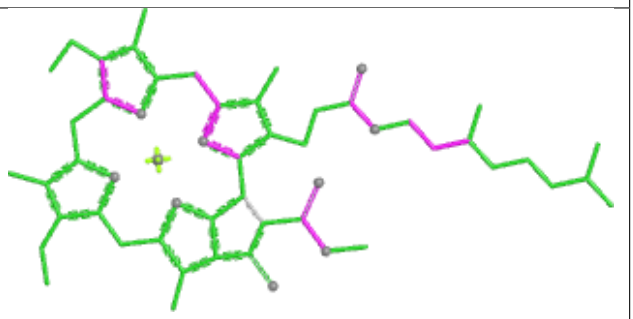
Ligand PID P 203



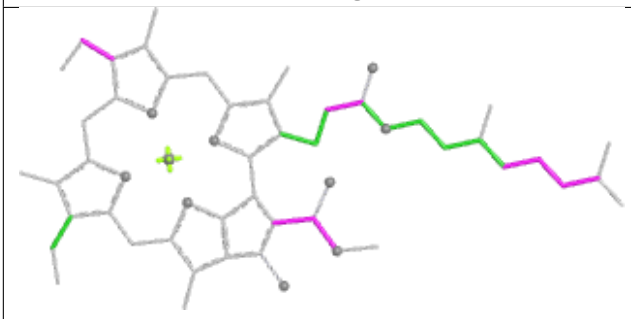
Ligand CLA b 711



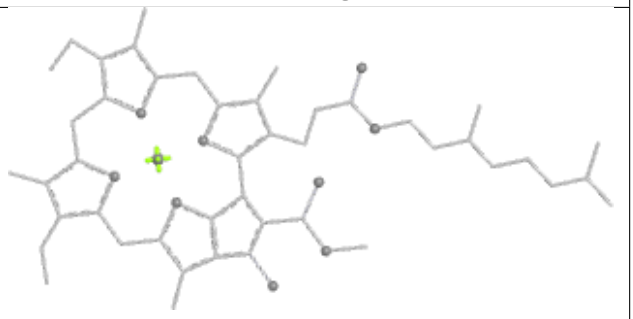
Bond lengths



Bond angles

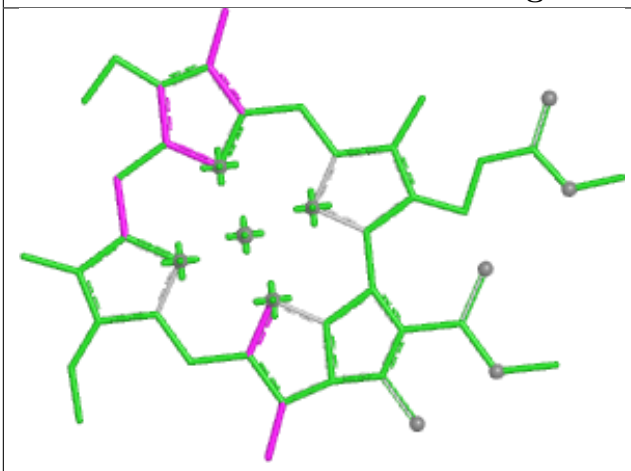


Torsions

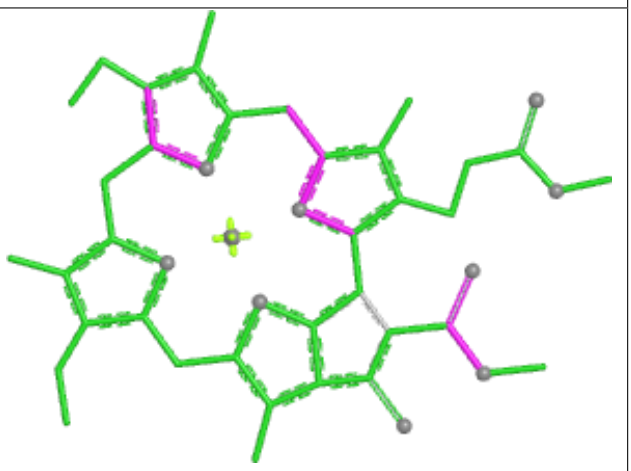


Rings

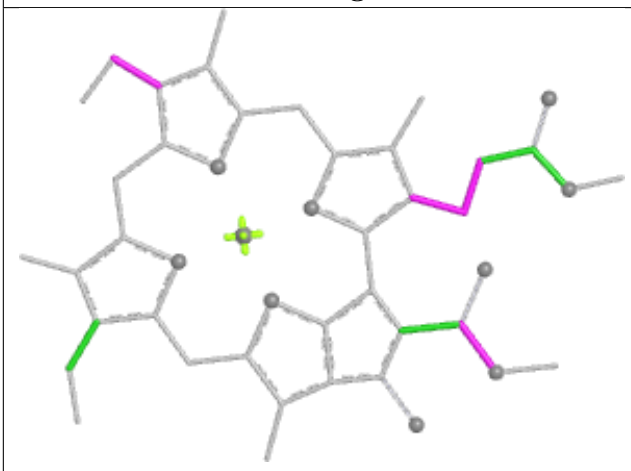
Ligand CLA L 312



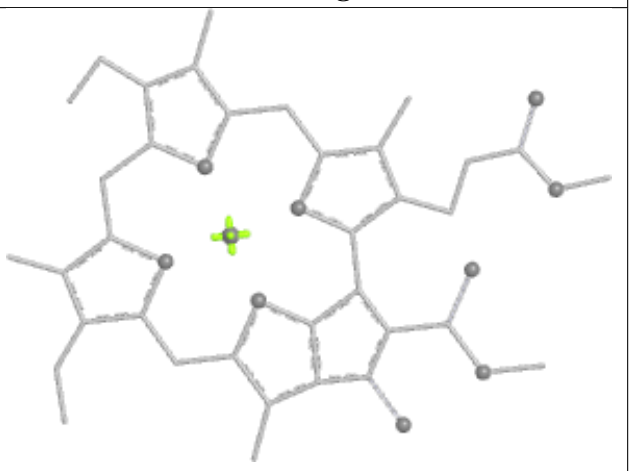
Bond lengths



Bond angles

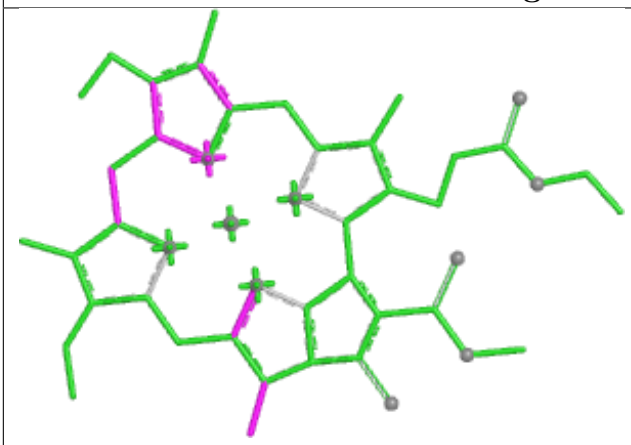


Torsions

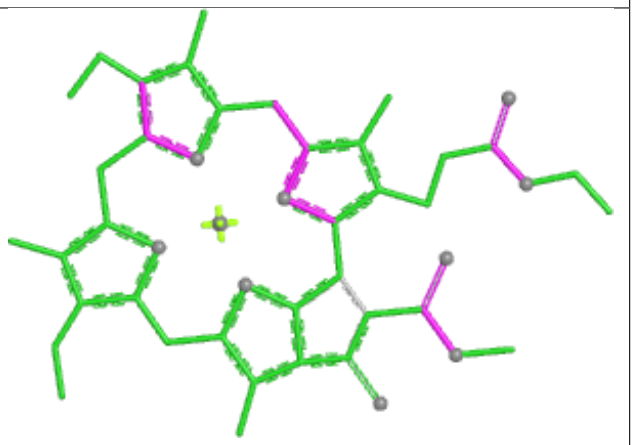


Rings

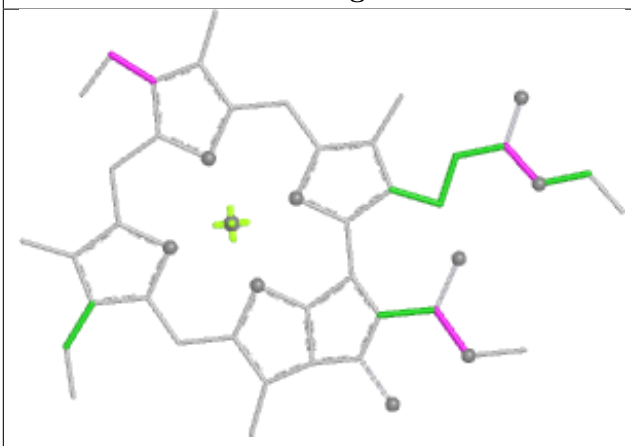
Ligand CLA H 304



Bond lengths



Bond angles



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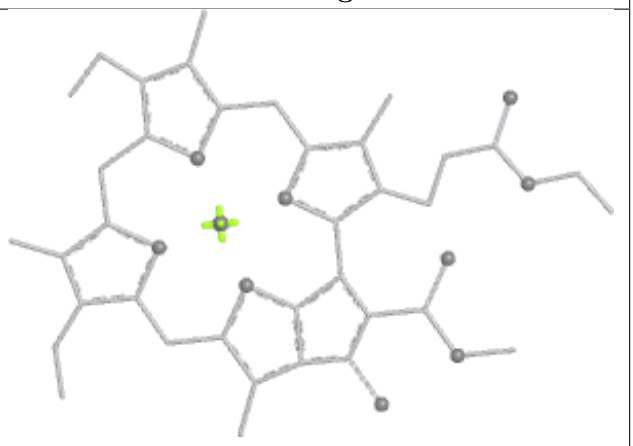
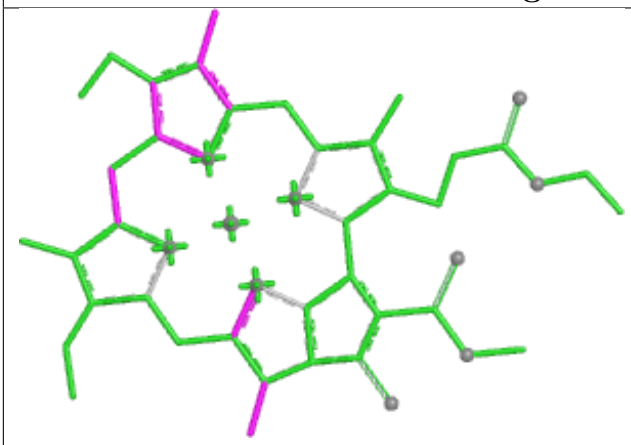
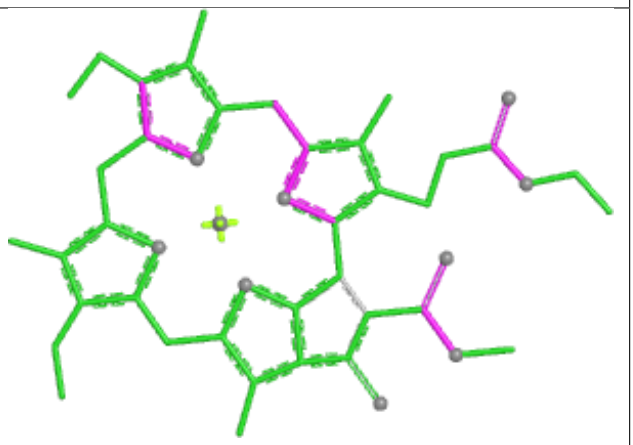


Rings

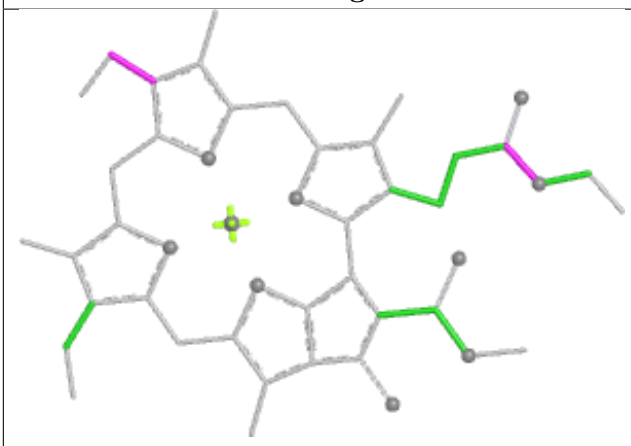
Ligand CLA N 304



Bond lengths



Bond angles



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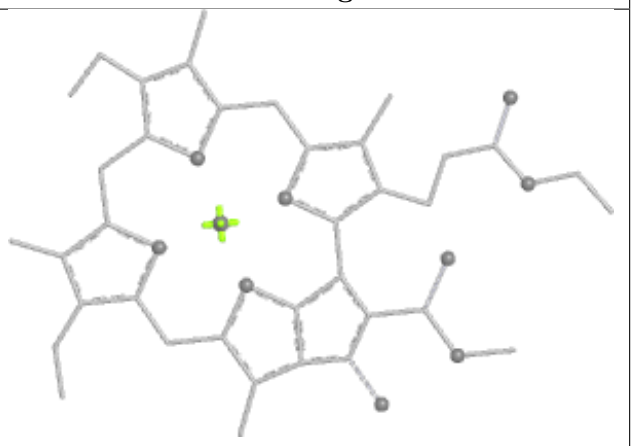
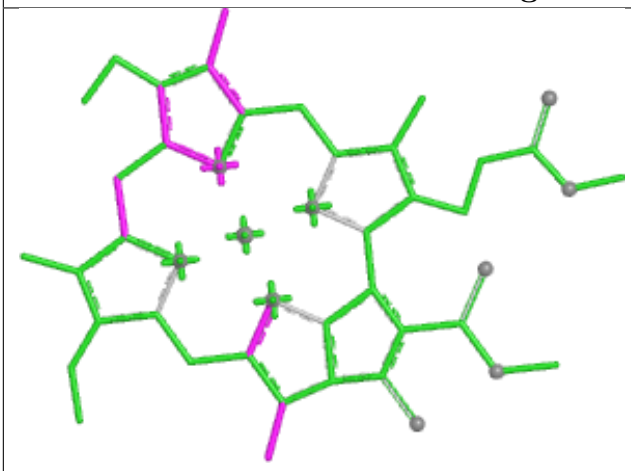
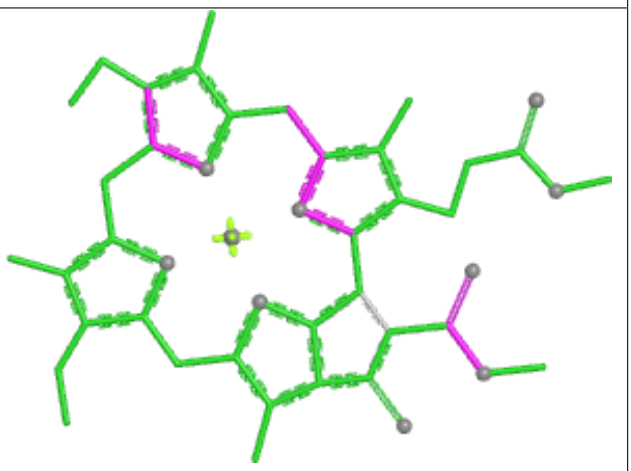


Rings

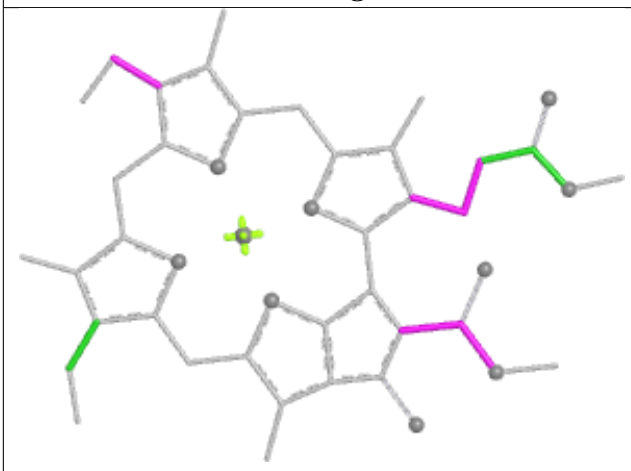
Ligand CLA M 318



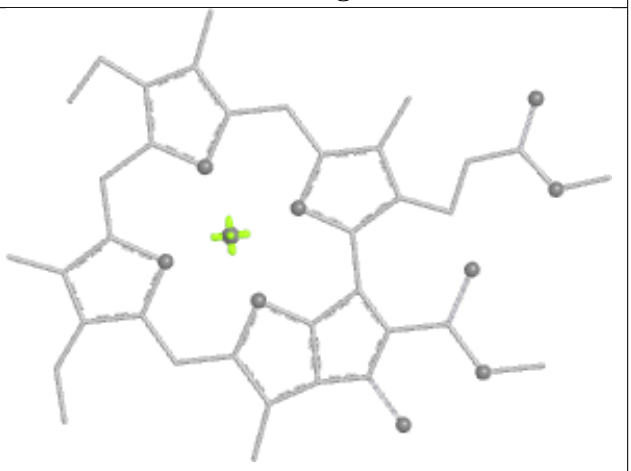
Bond lengths



Bond angles

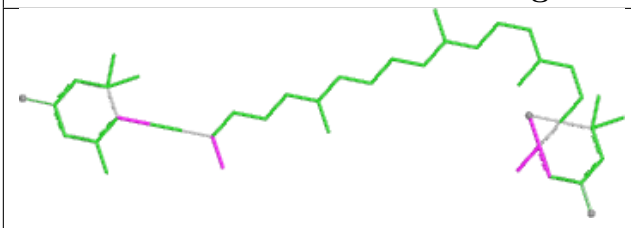


Torsions

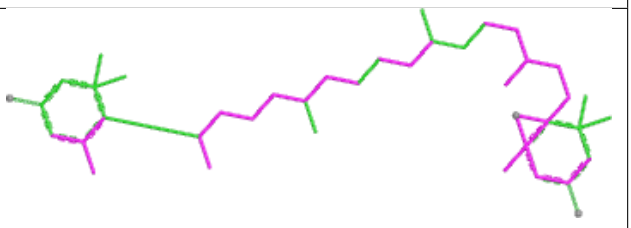


Rings

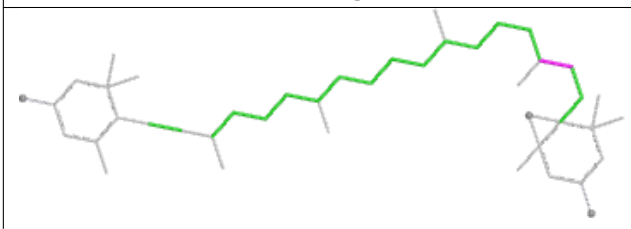
Ligand DD6 I 303



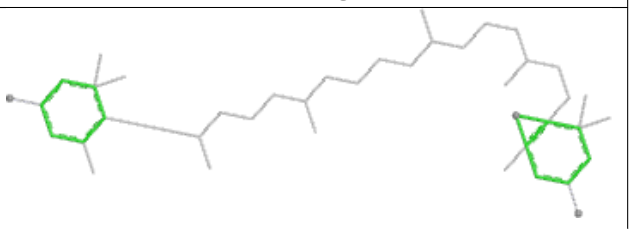
Bond lengths



Bond angles

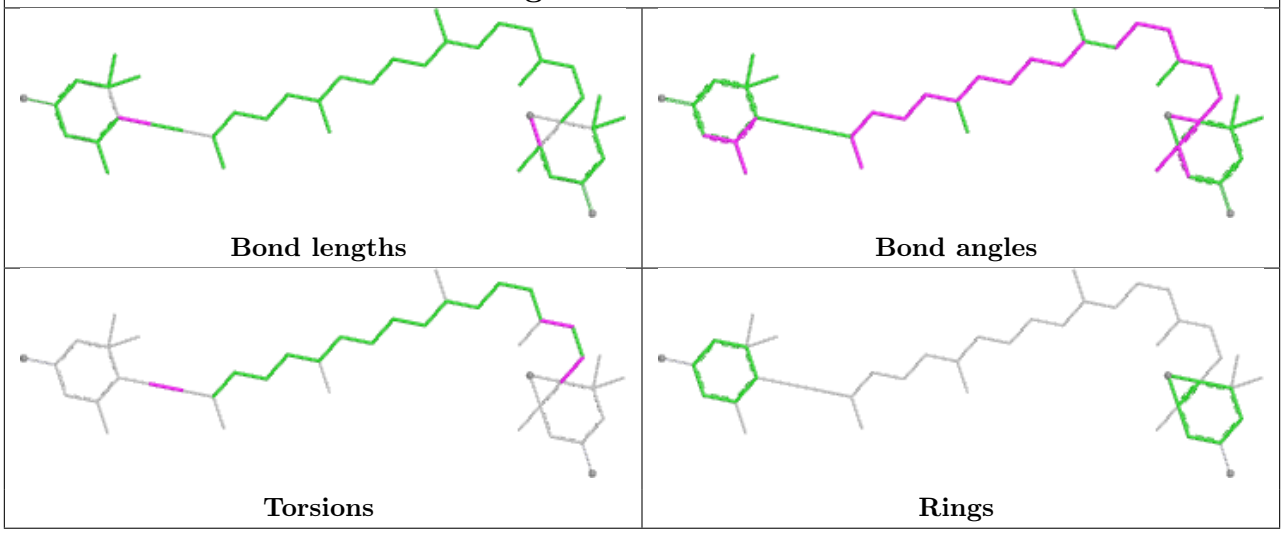


Torsions

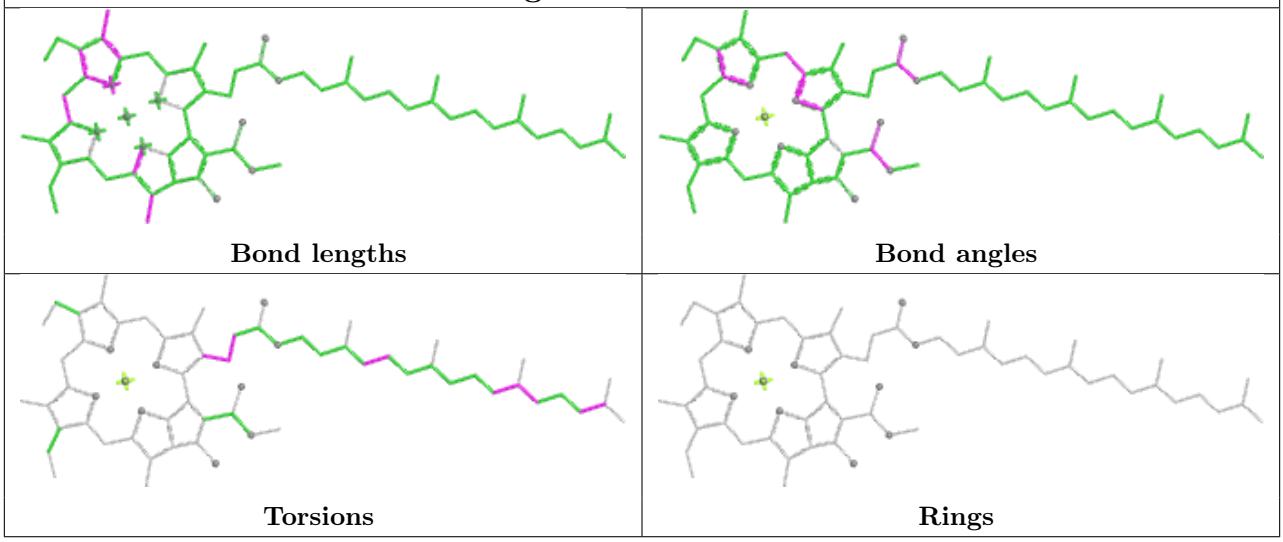


Rings

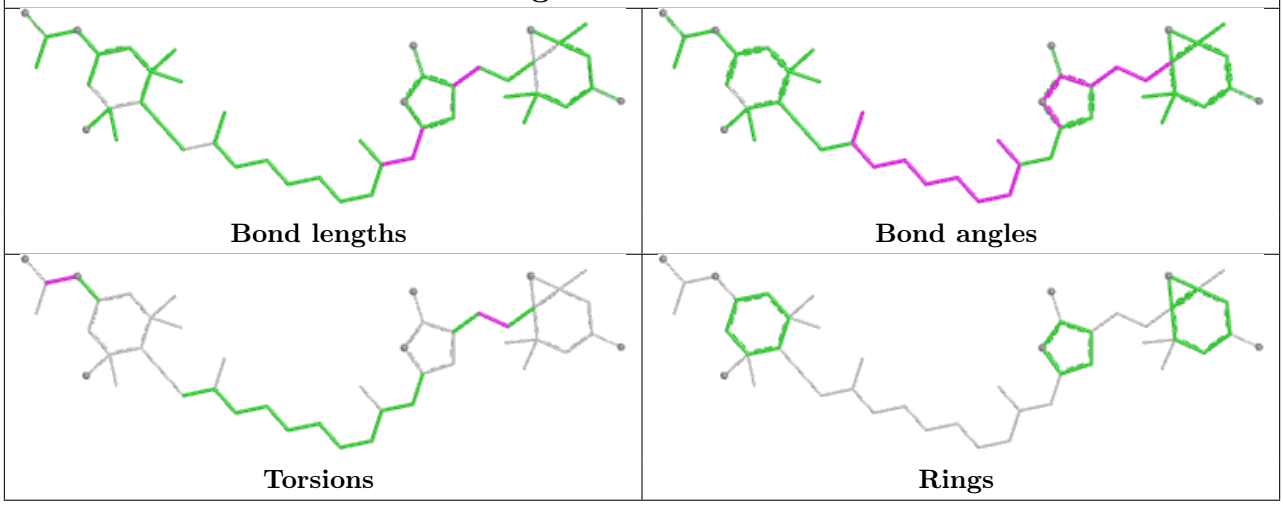
Ligand DD6 K 305



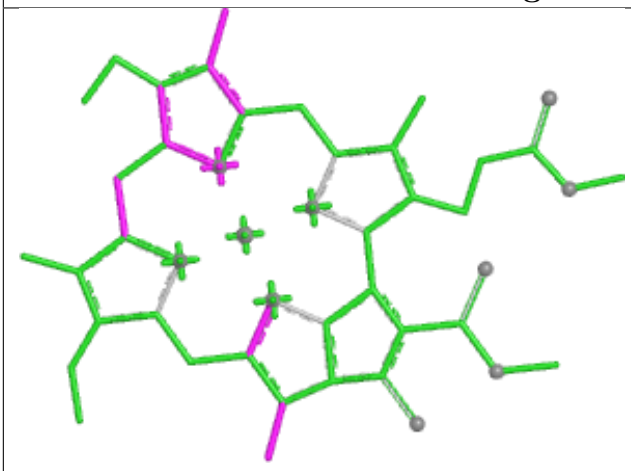
Ligand CLA N 305



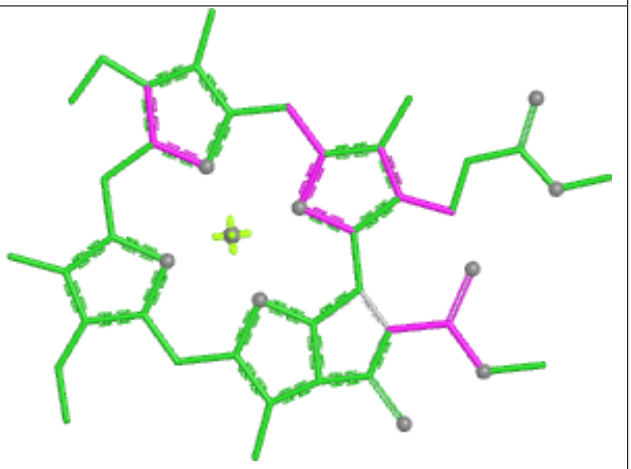
Ligand PID F 304



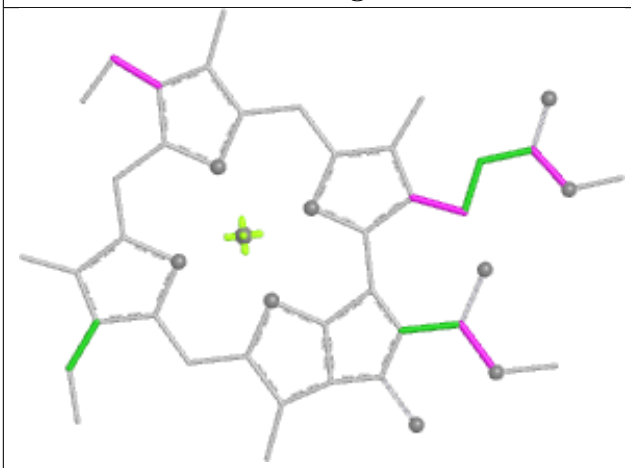
Ligand CLA D 314



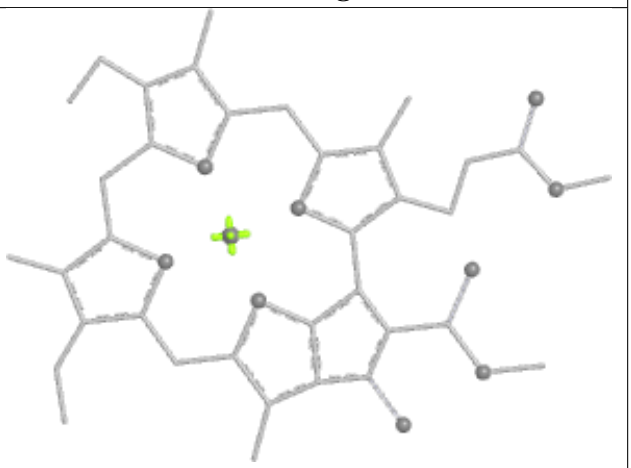
Bond lengths



Bond angles

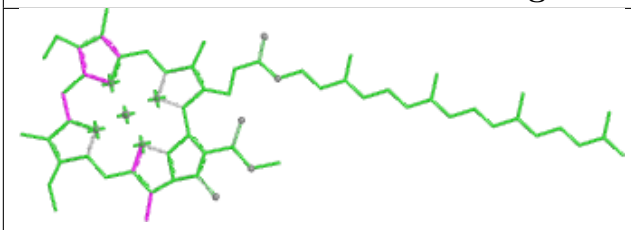


Torsions



Rings

Ligand CLA a 735



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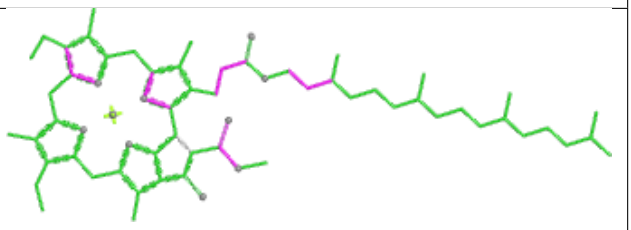
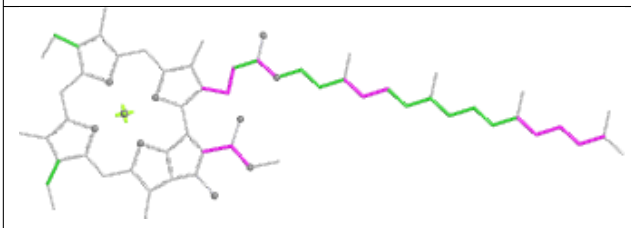
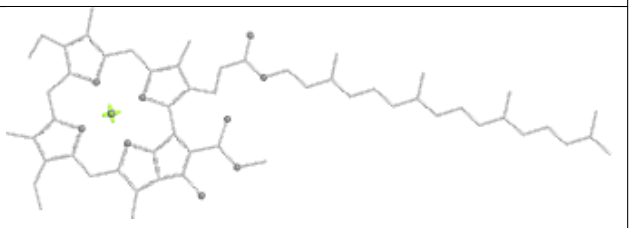


Bond angles

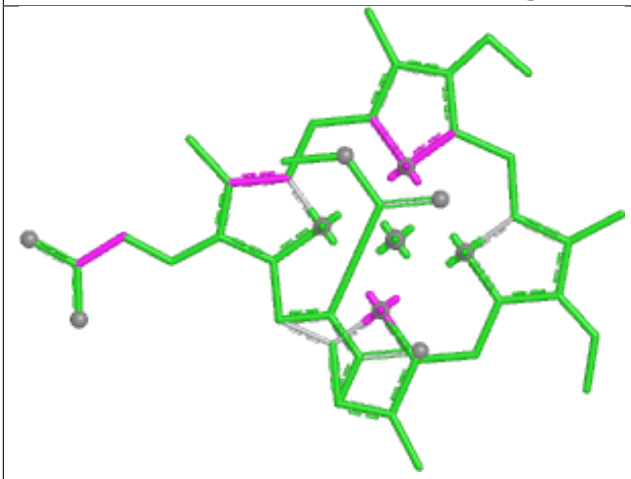


Torsions



Rings

Ligand KC1 M 307



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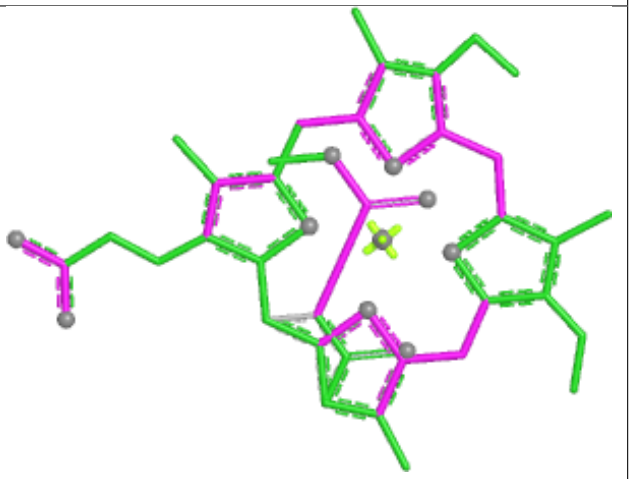
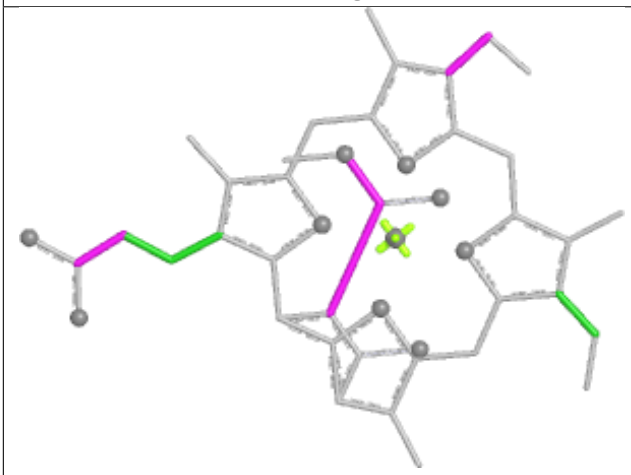


Bond angles



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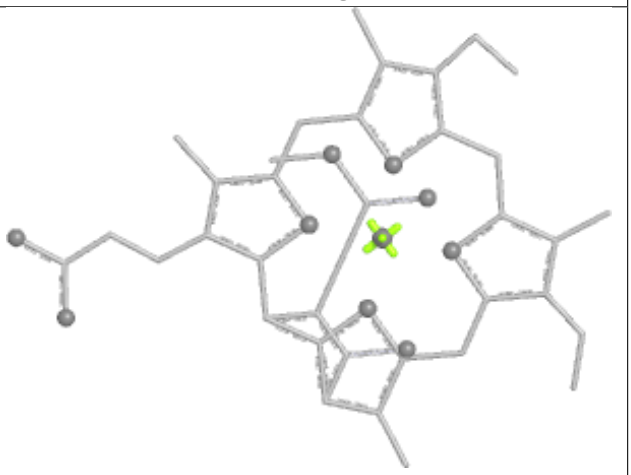
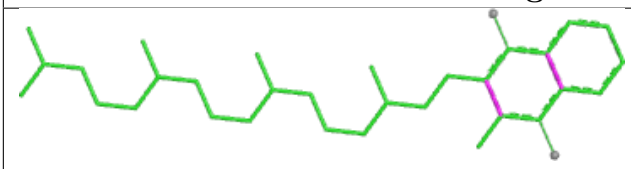
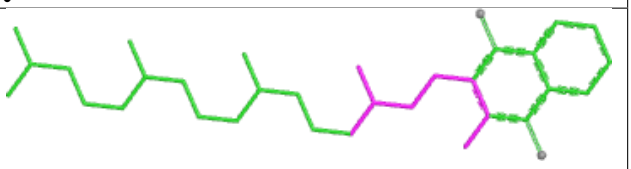


Rings

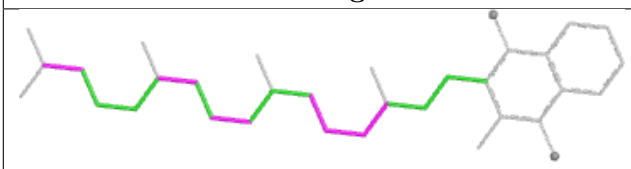
Ligand PQN a 732



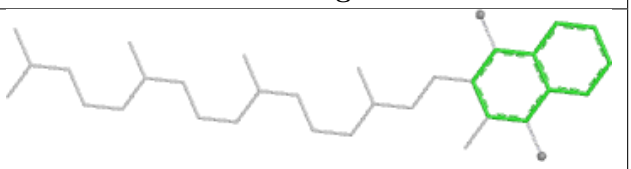
Bond lengths



Bond angles

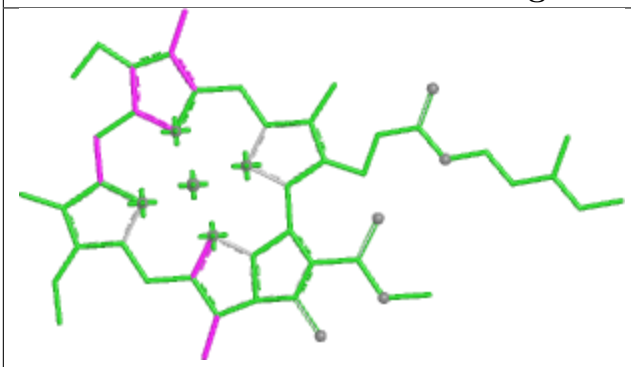


Torsions

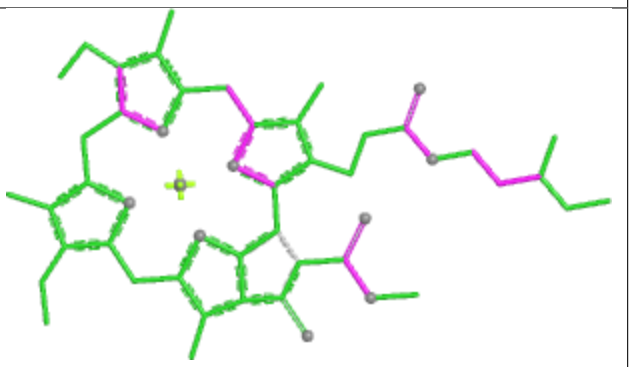


Rings

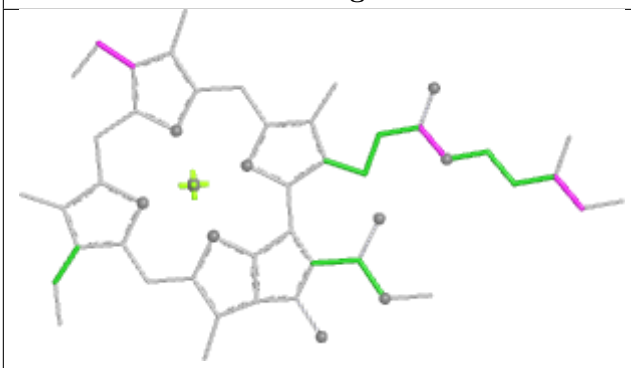
Ligand CLA a 708



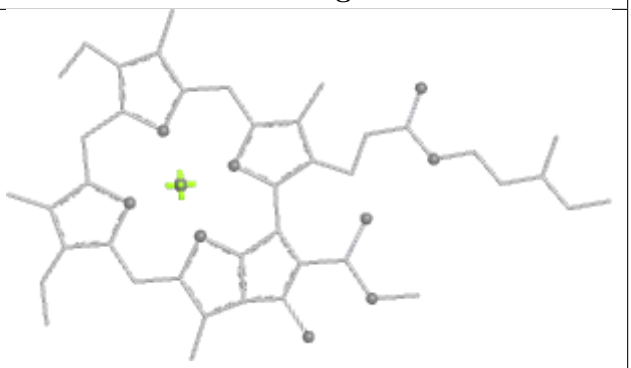
Bond lengths



Bond angles

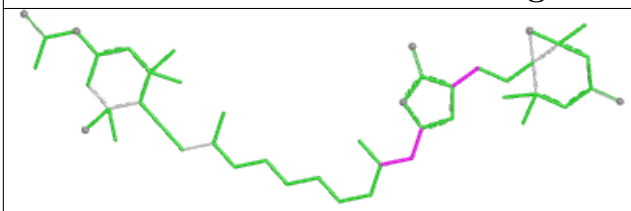


Torsions



Rings

Ligand PID H 302



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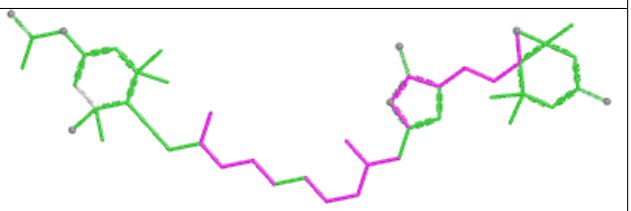
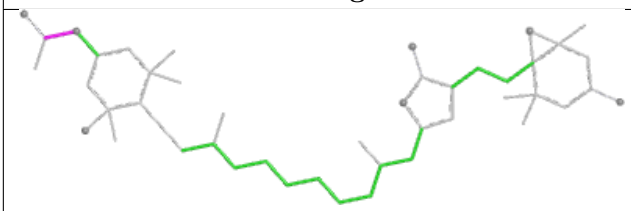
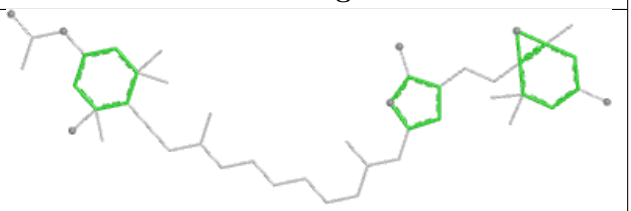


Bond angles

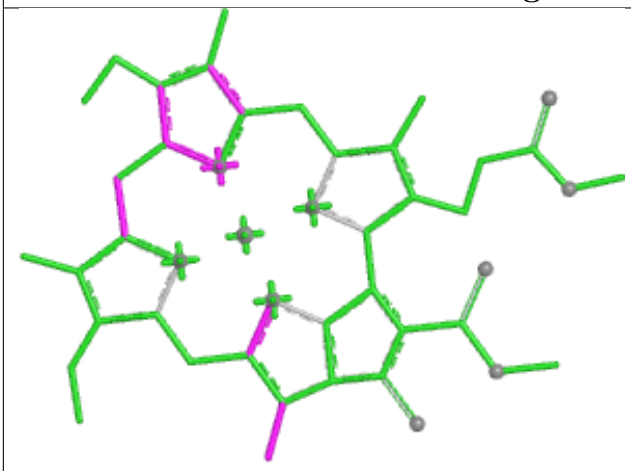


Torsions



Rings

Ligand CLA G 517



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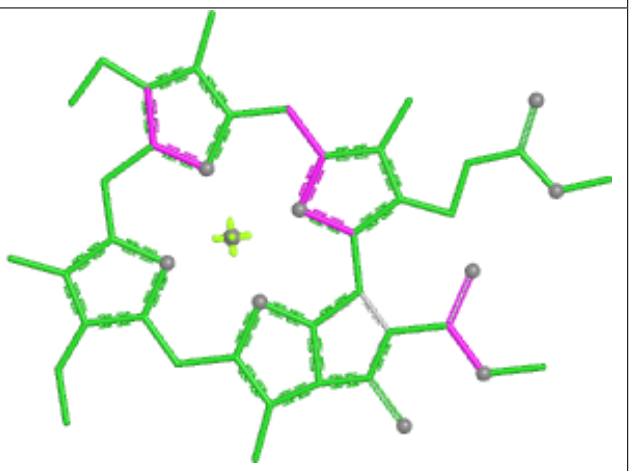
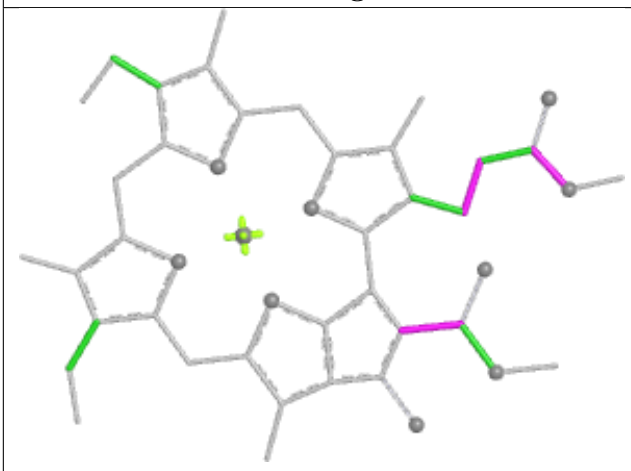
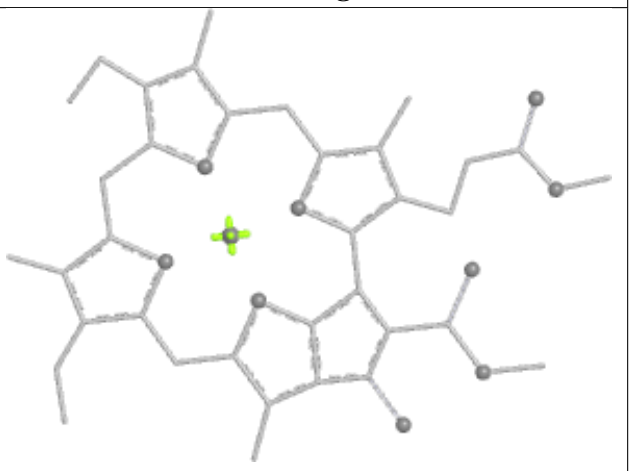


Bond angles

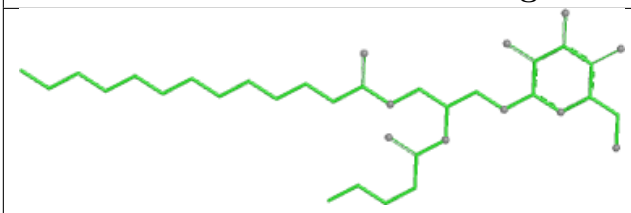


Torsions



Rings

Ligand LMG B 318



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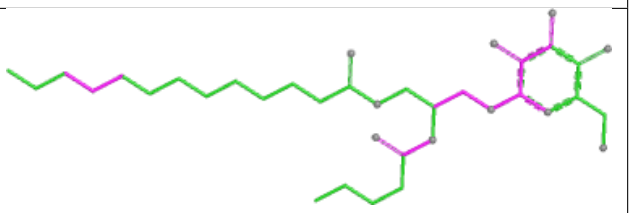
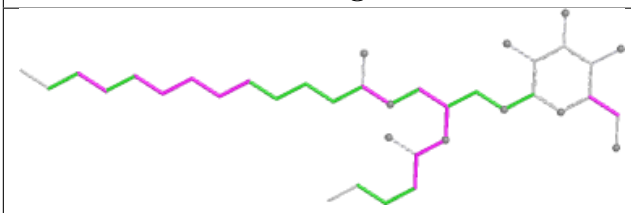
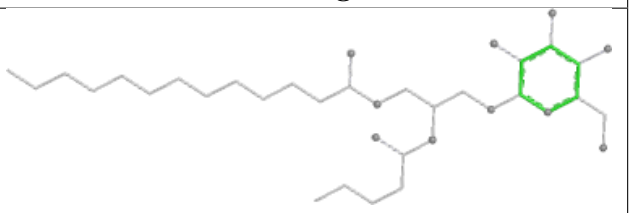


Bond angles

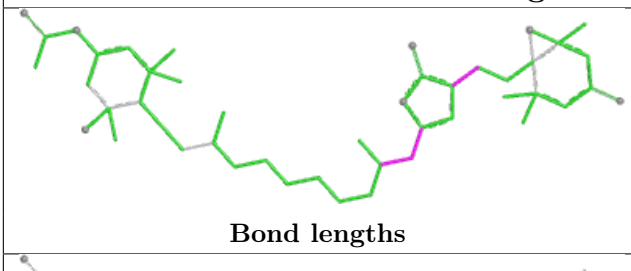


Torsions



Rings

Ligand PID G 506



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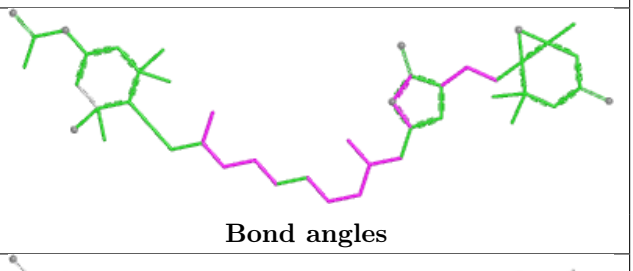
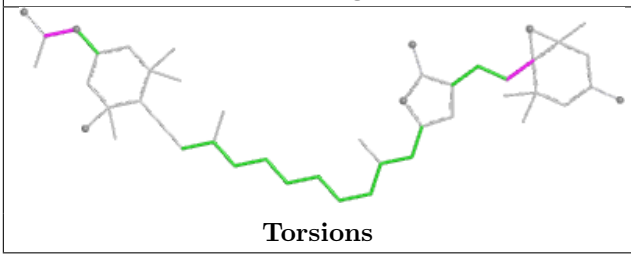
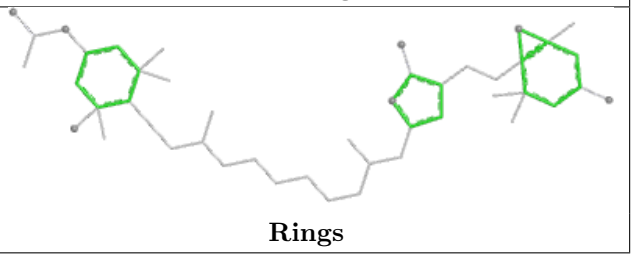


Bond angles

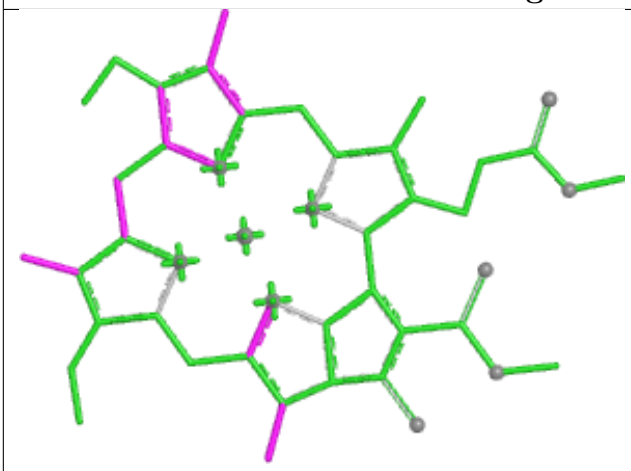


Torsions

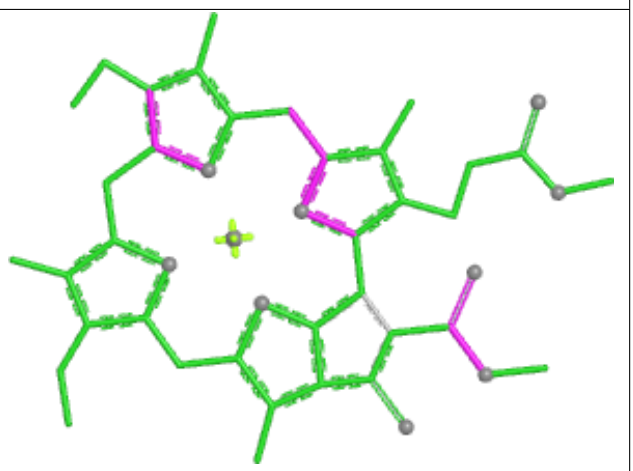


Rings

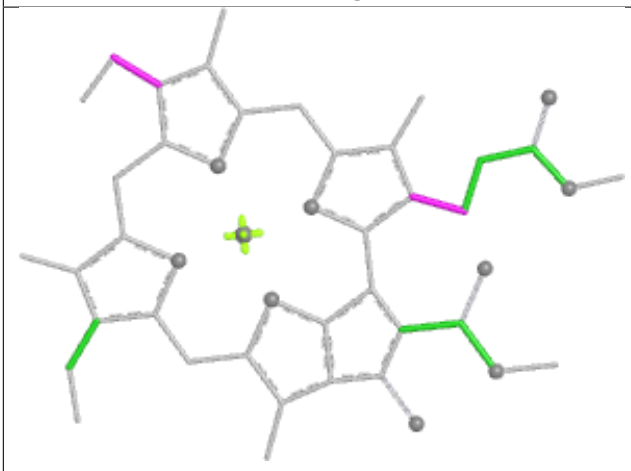
Ligand CLA F 308



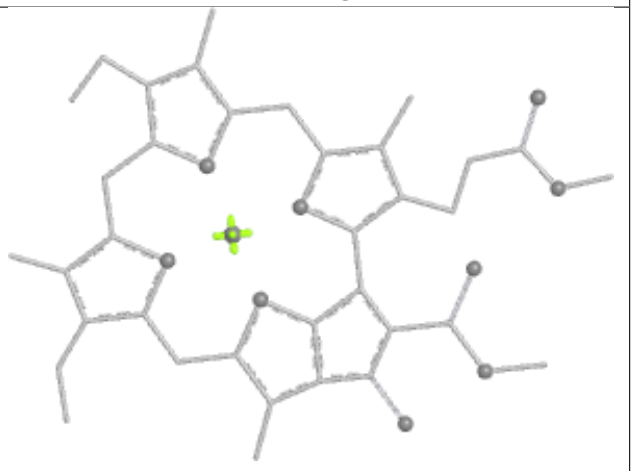
Bond lengths



Bond angles

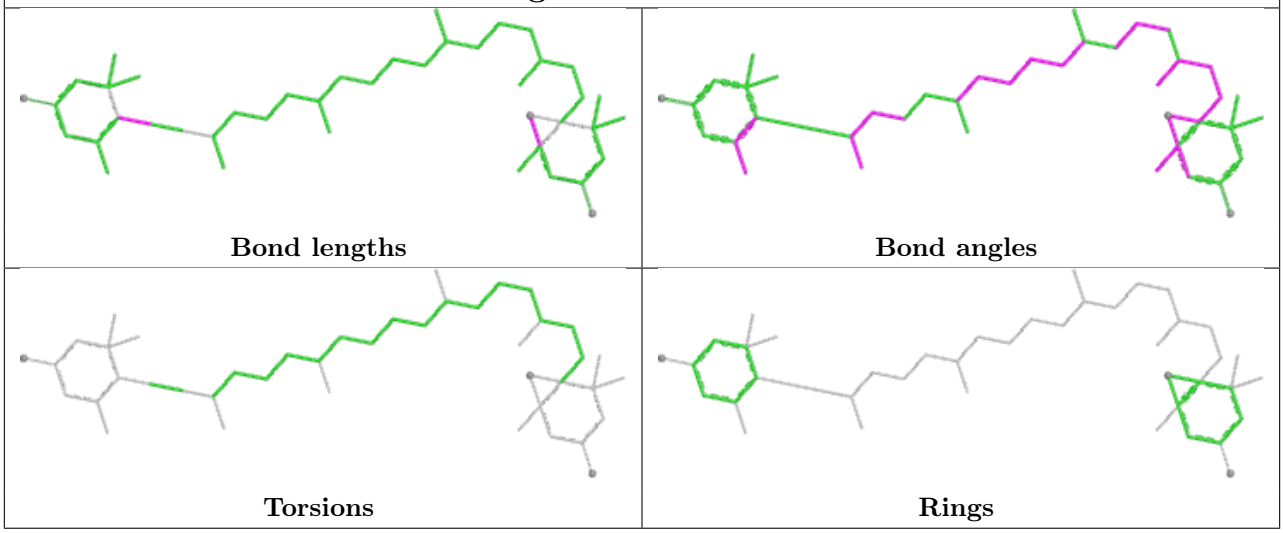


Torsions

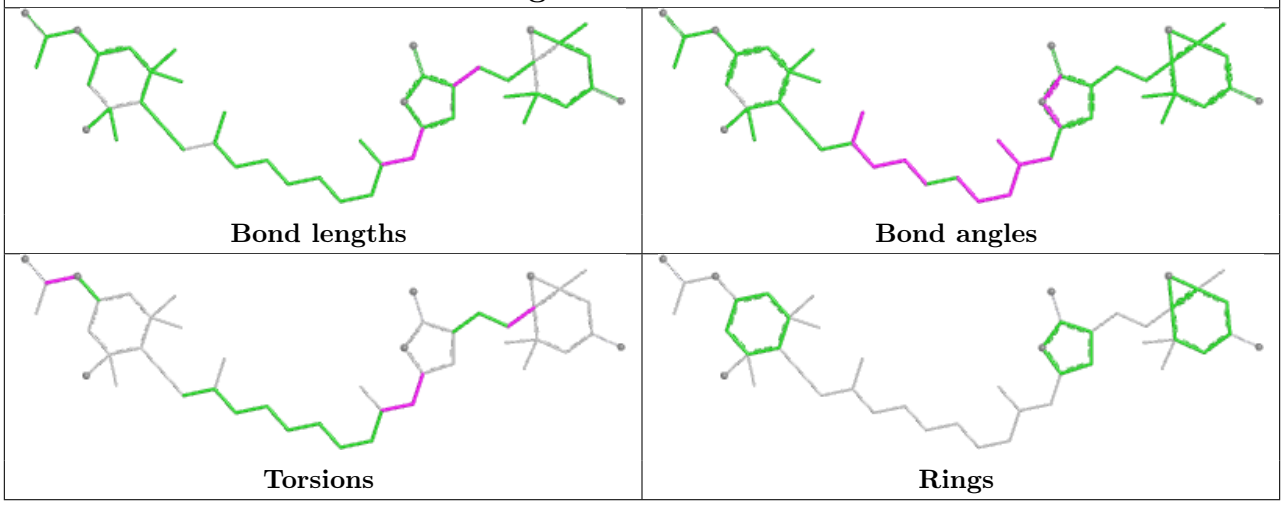


Rings

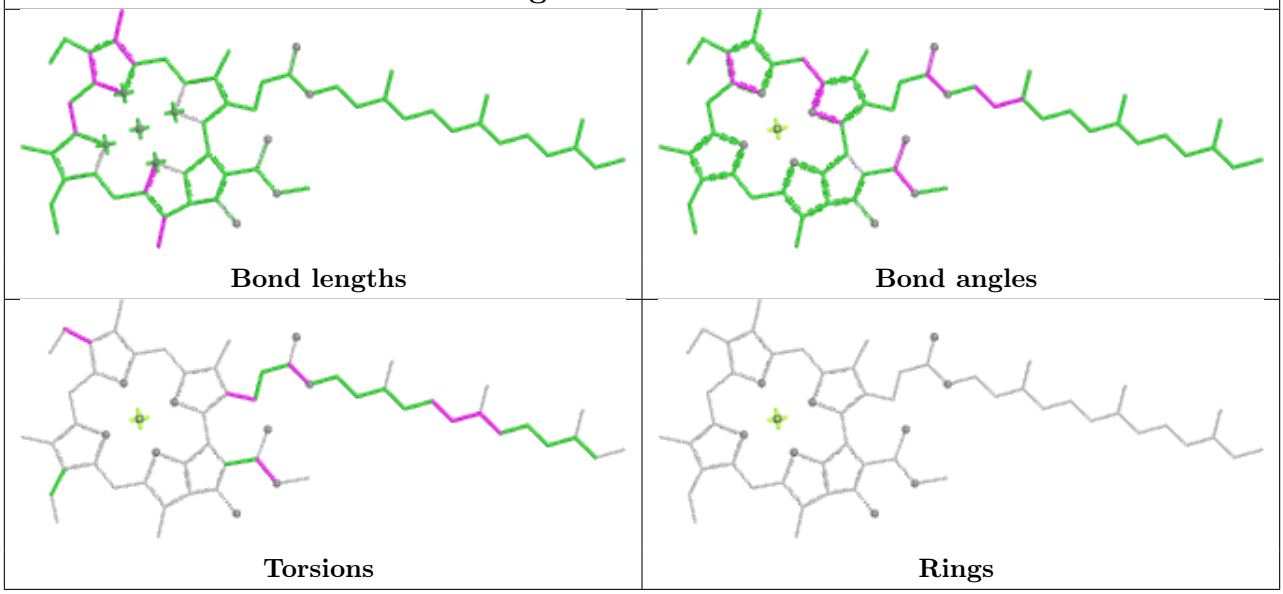
Ligand DD6 L 304



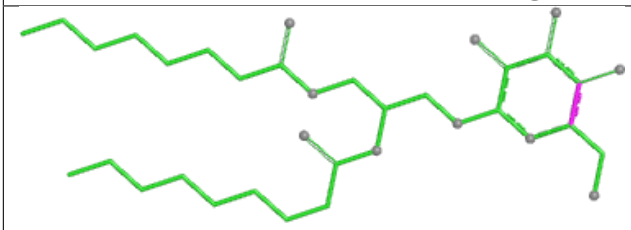
Ligand PID N 301



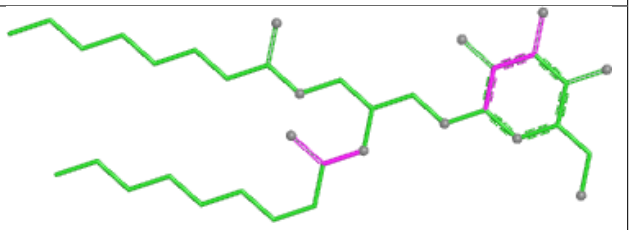
Ligand CLA a 725



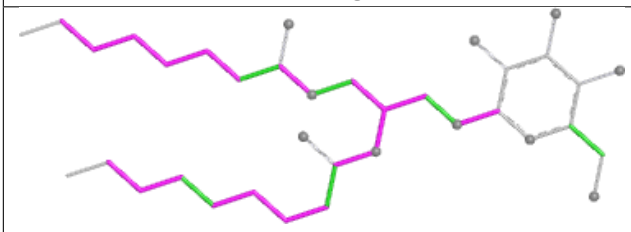
Ligand LMG I 318



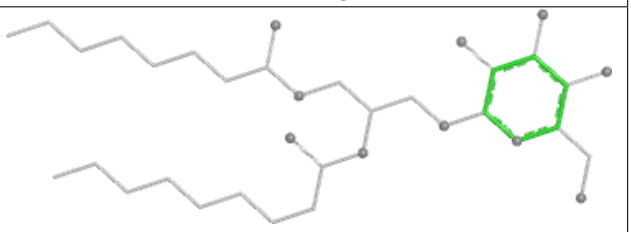
Bond lengths



Bond angles

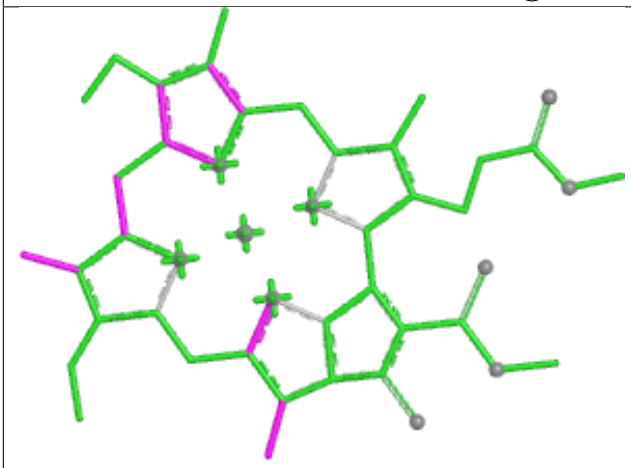


Torsions

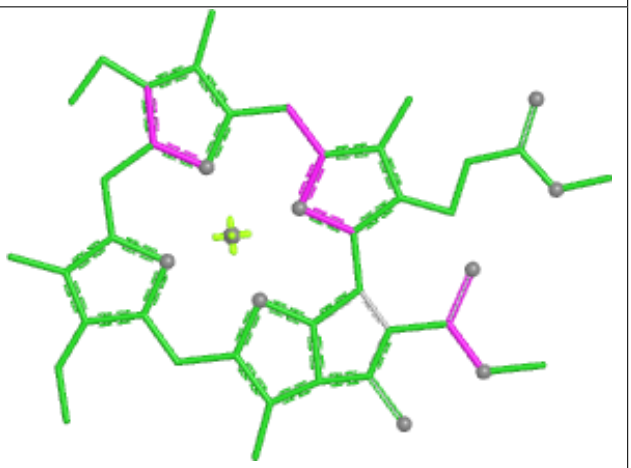


Rings

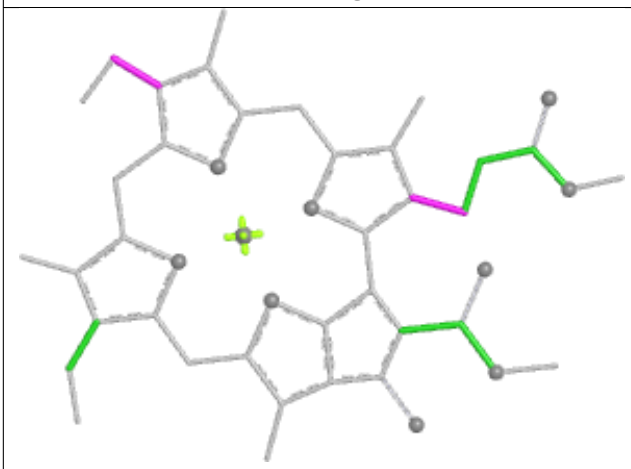
Ligand CLA N 309



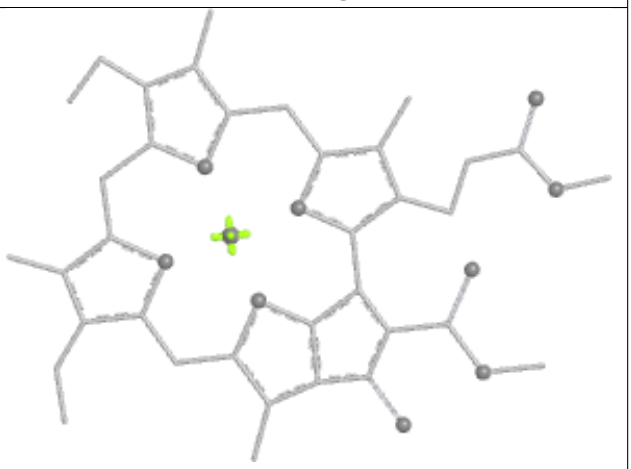
Bond lengths



Bond angles

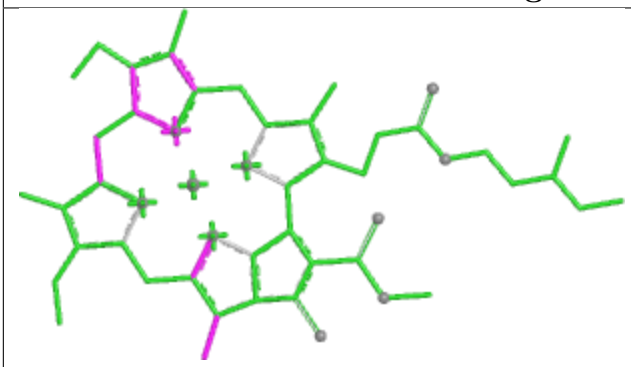


Torsions



Rings

Ligand CLA P 212



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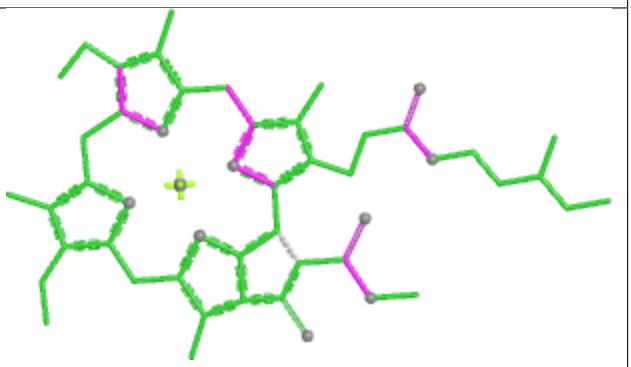
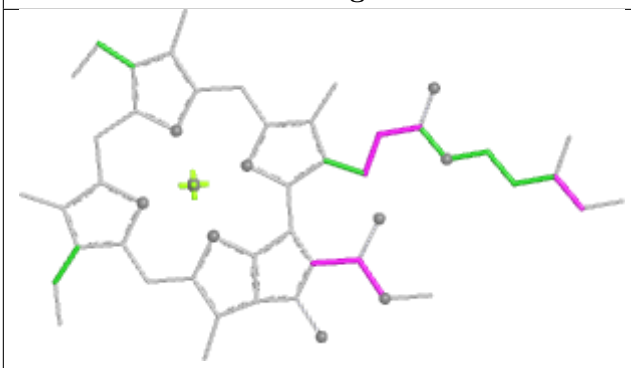


Bond angles



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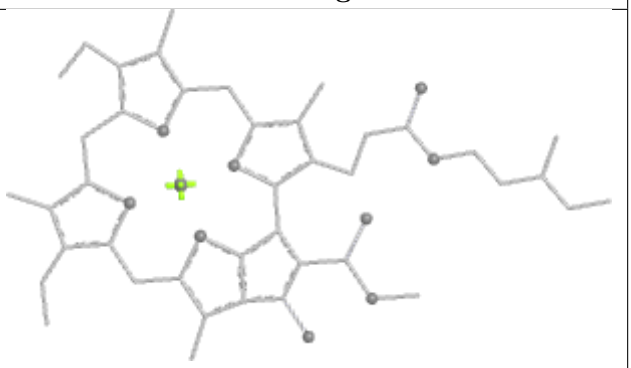
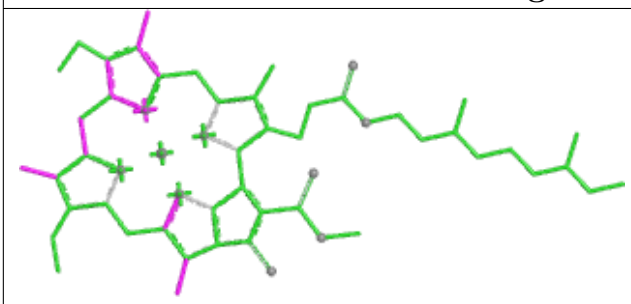


Rings

Ligand CLA J 309



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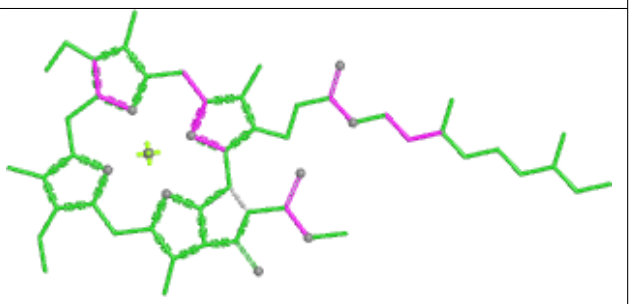
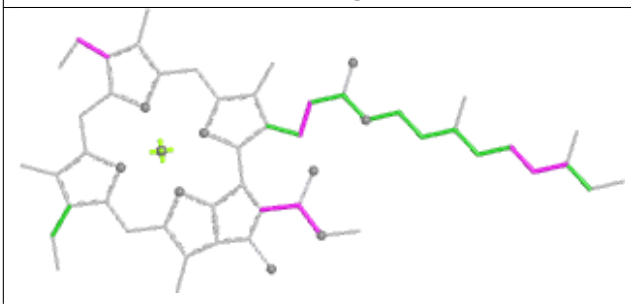


Bond angles



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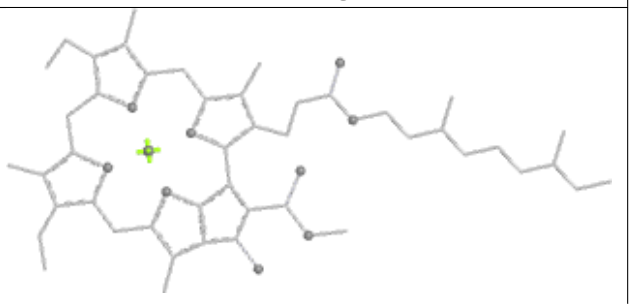
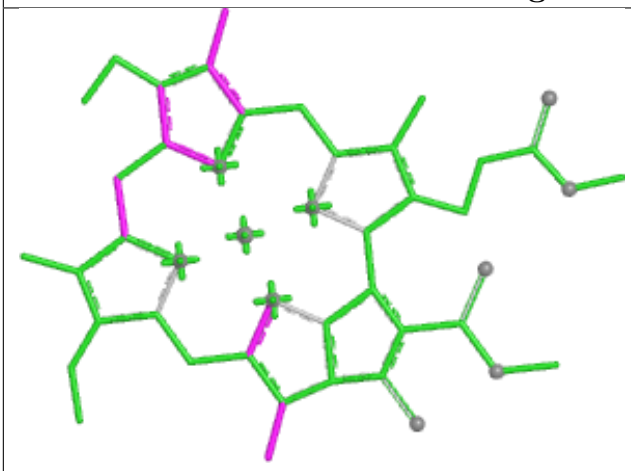


Rings

Ligand CLA a 738



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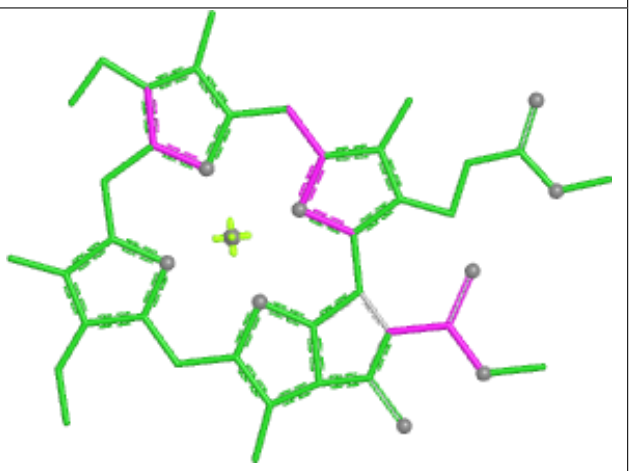
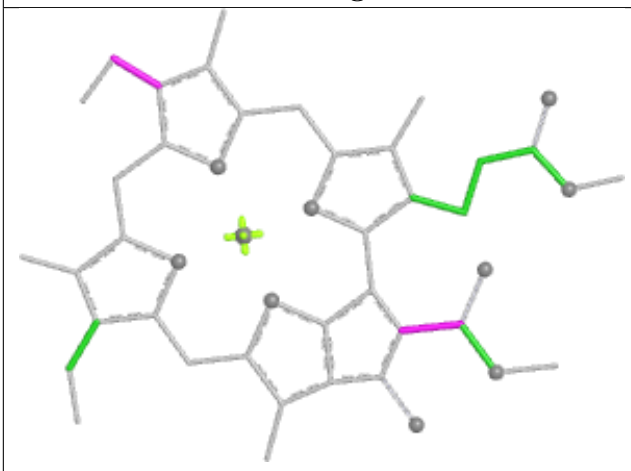


Bond angles



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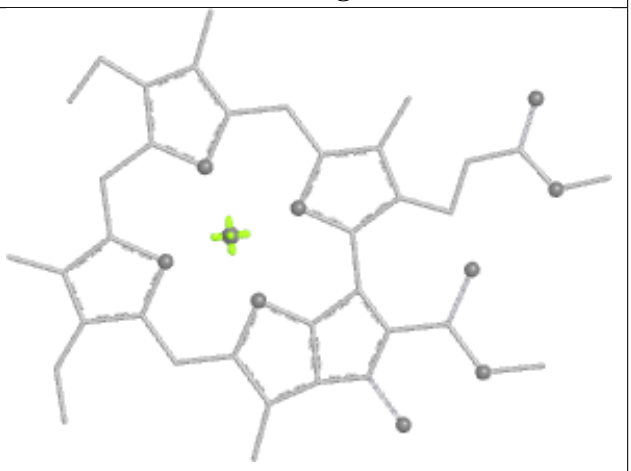
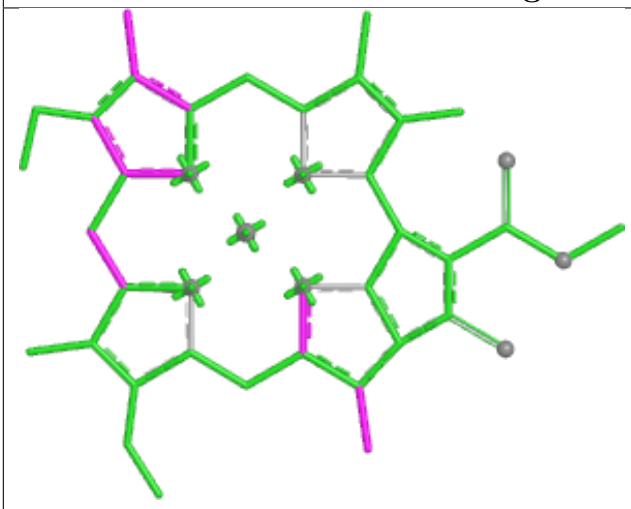


Rings

Ligand CLA H 311



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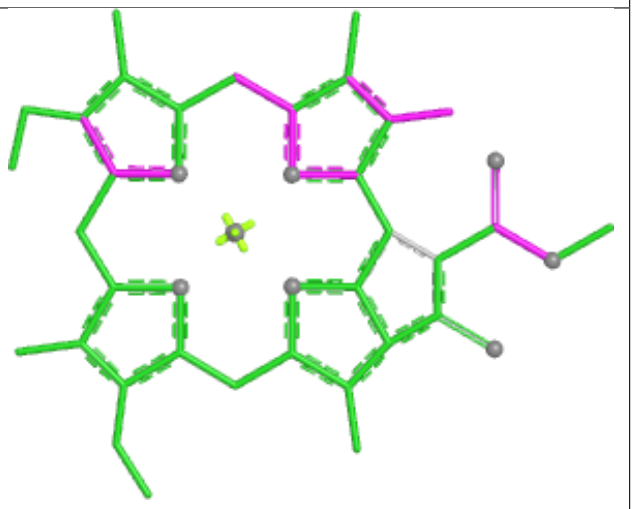
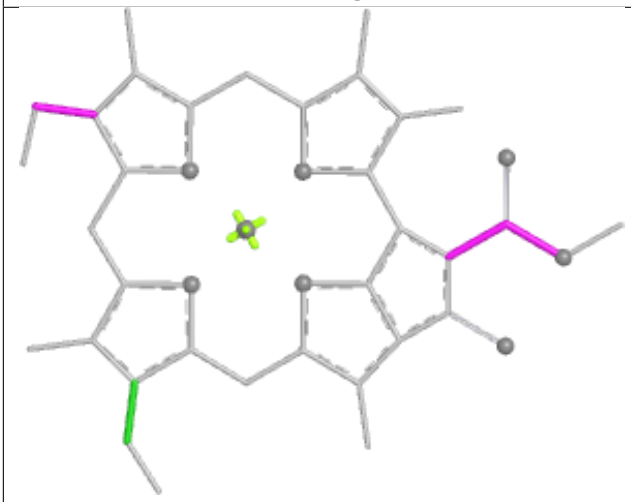


Bond angles



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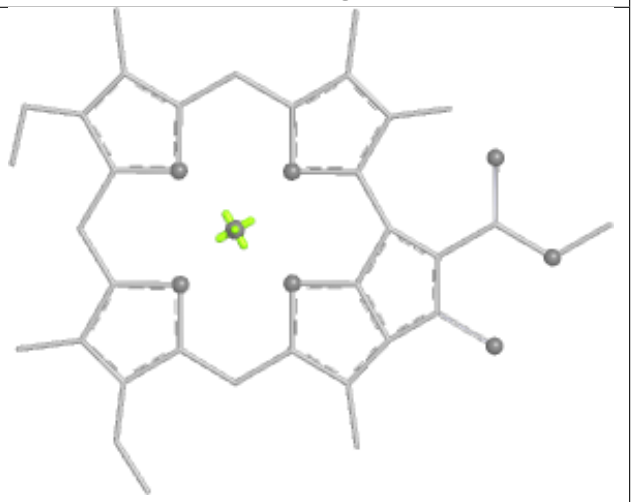
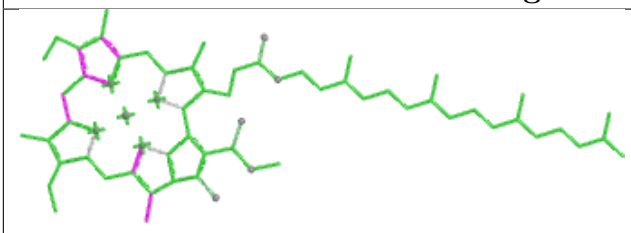
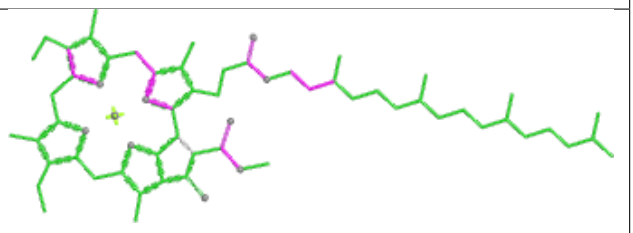


Rings

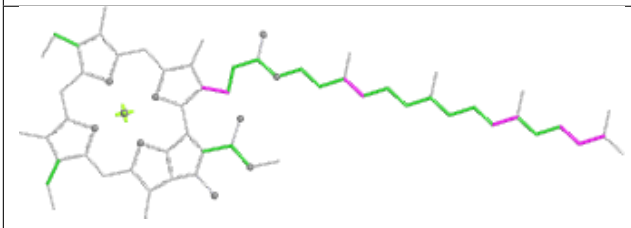
Ligand CLA H 305



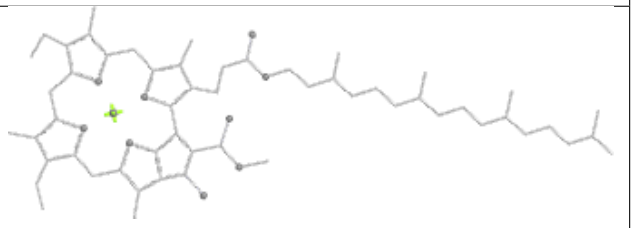
Bond lengths



Bond angles

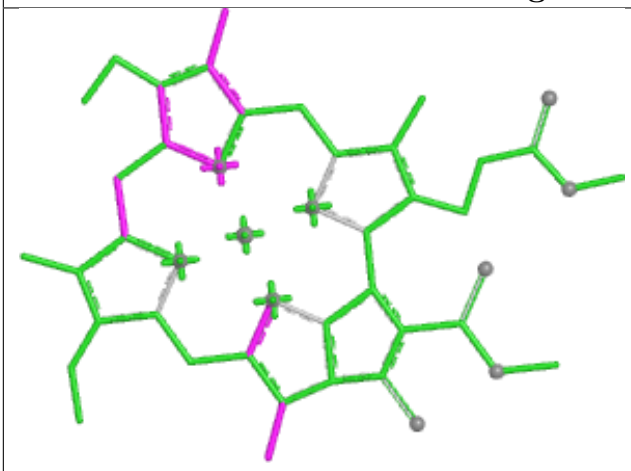


Torsions

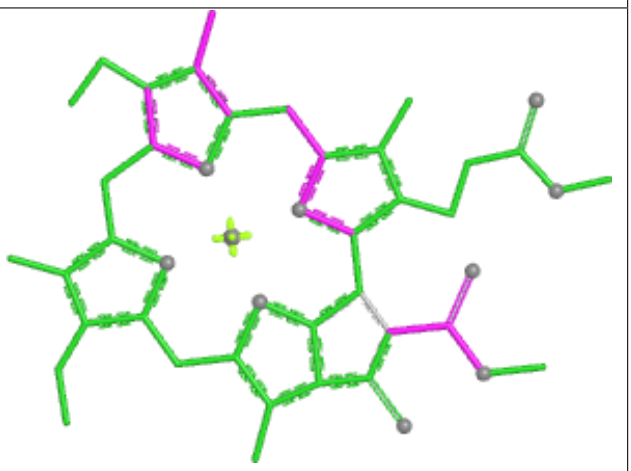


Rings

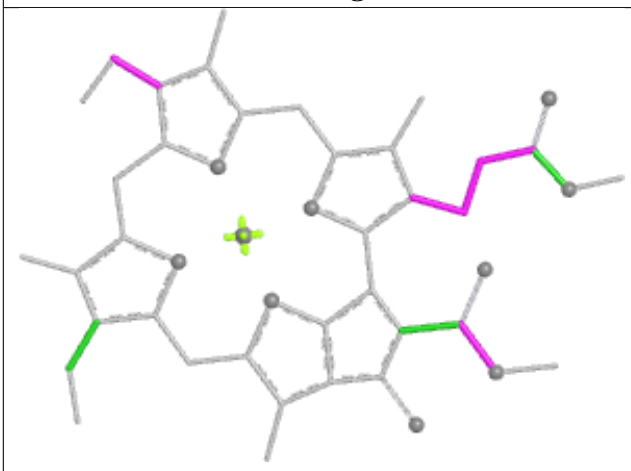
Ligand CLA J 308



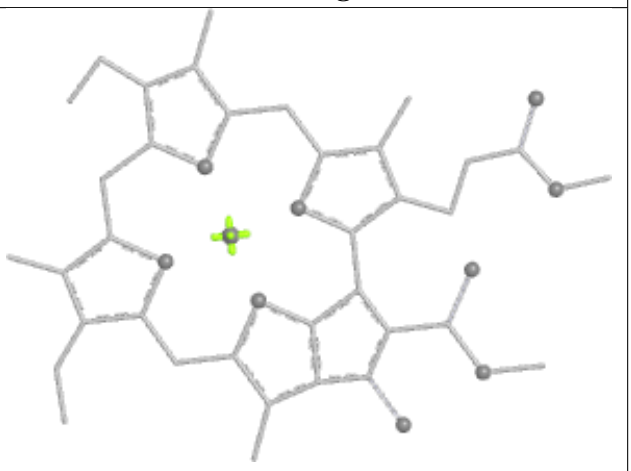
Bond lengths



Bond angles



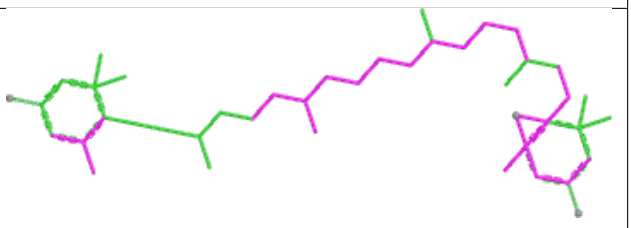
Torsions



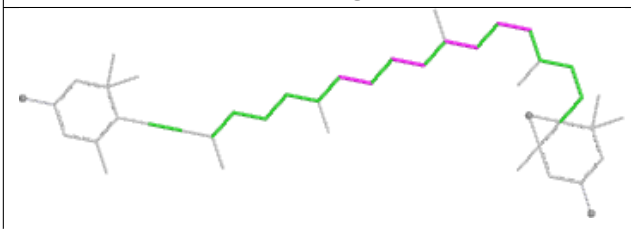
Rings

Ligand DD6 I 305

Bond lengths



Bond angles



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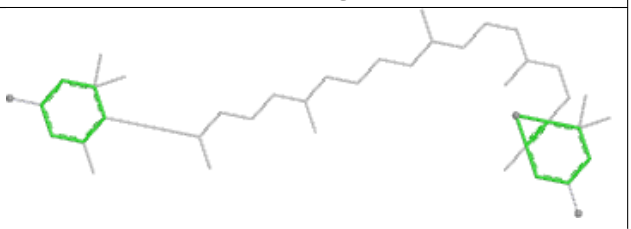
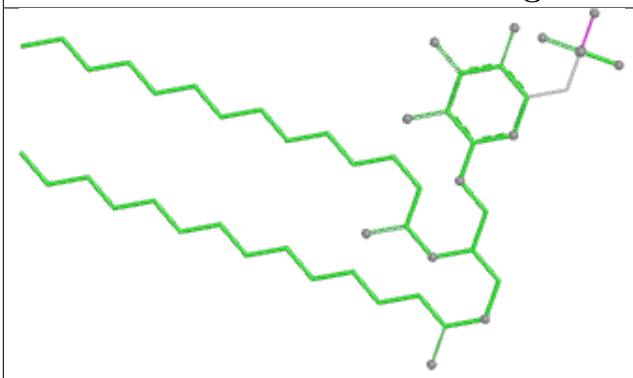


Rings

Ligand SQD A 318



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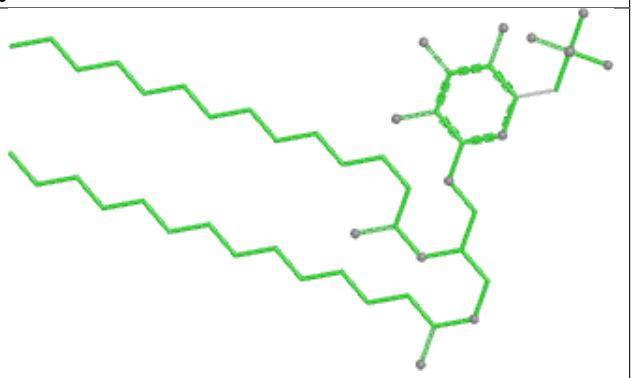
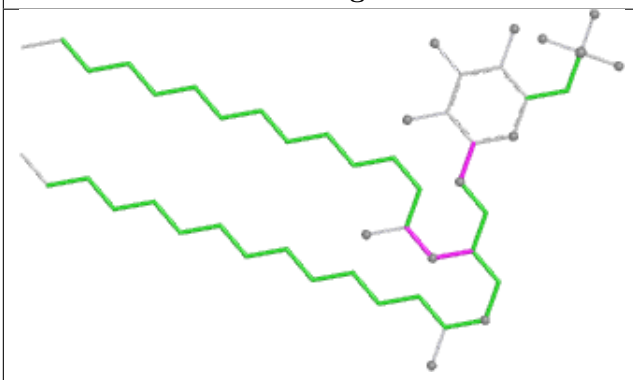
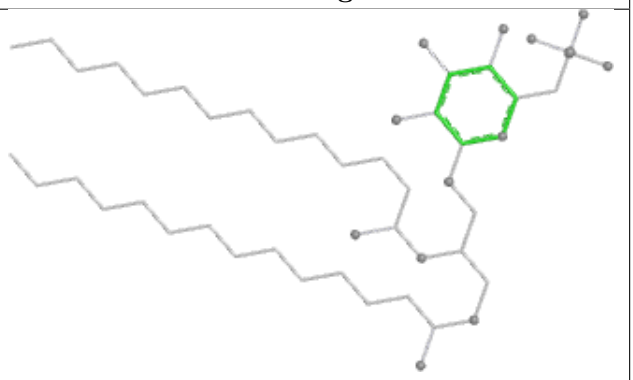


Bond angles

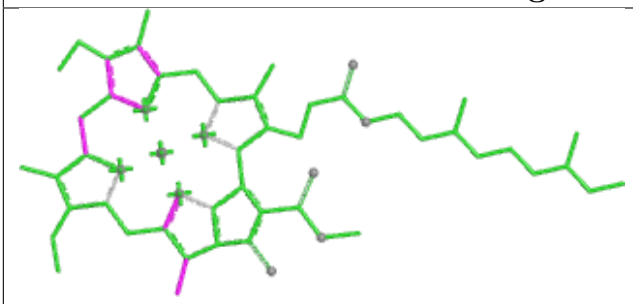


Torsions



Rings

Ligand CLA a 729



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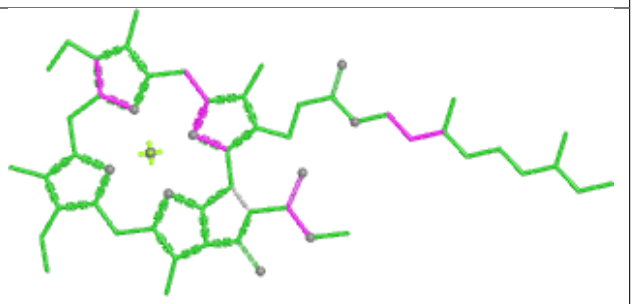
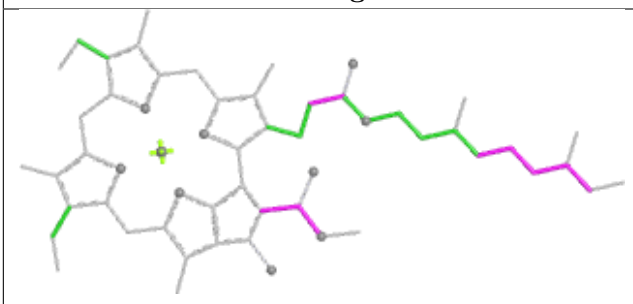
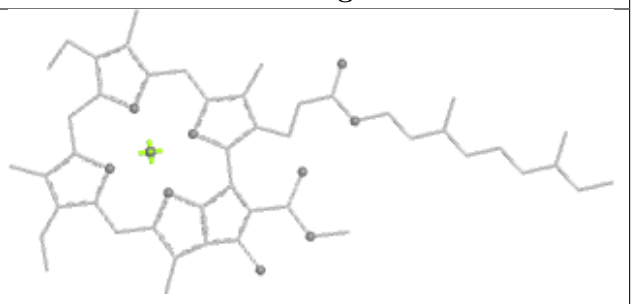


Bond angles

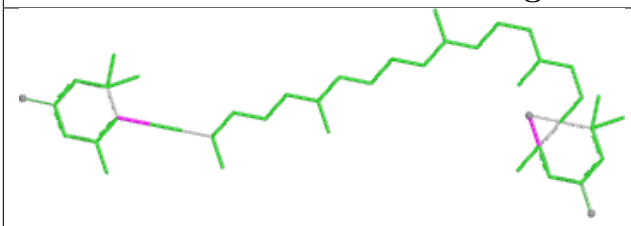


Torsions

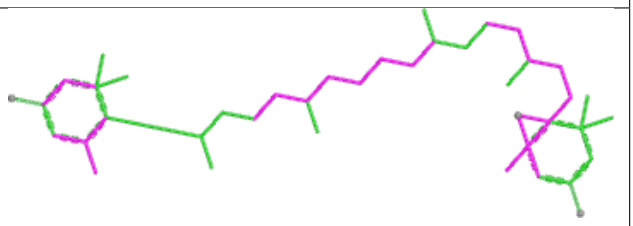


Rings

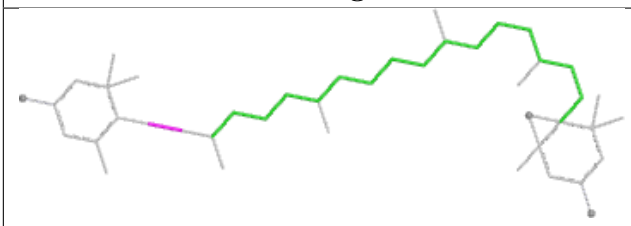
Ligand DD6 K 304



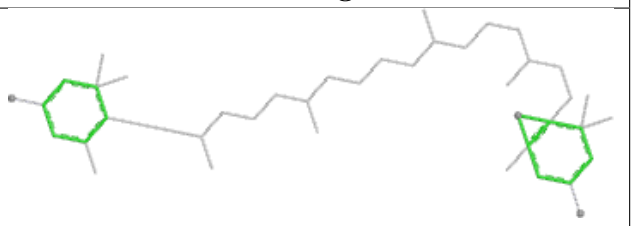
Bond lengths



Bond angles

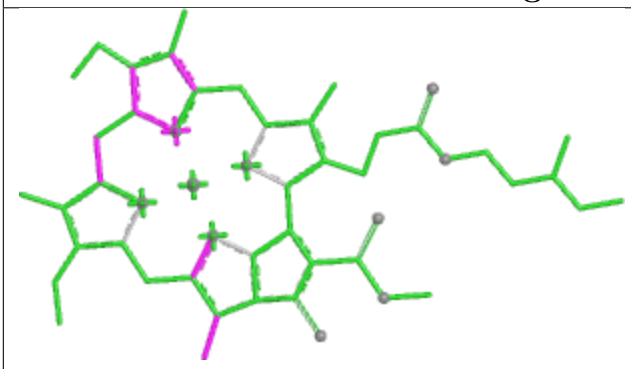


Torsions

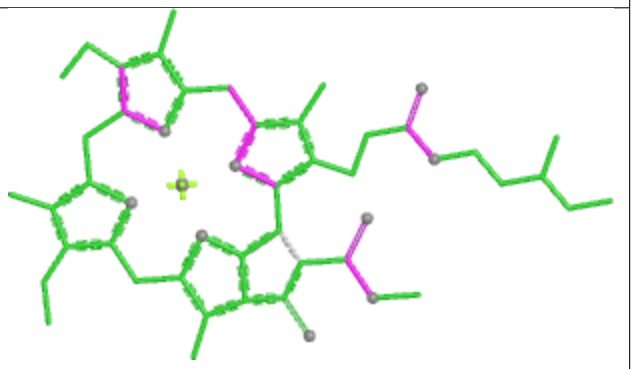


Rings

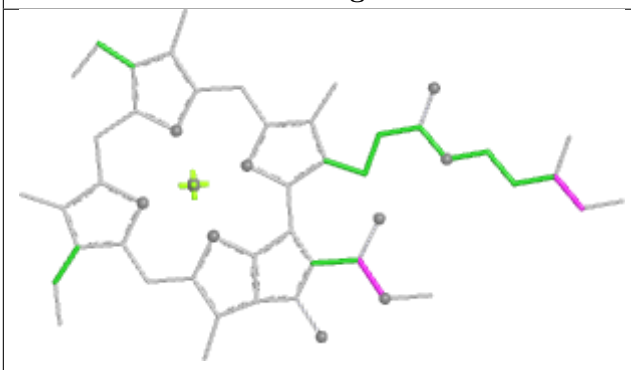
Ligand CLA O 311



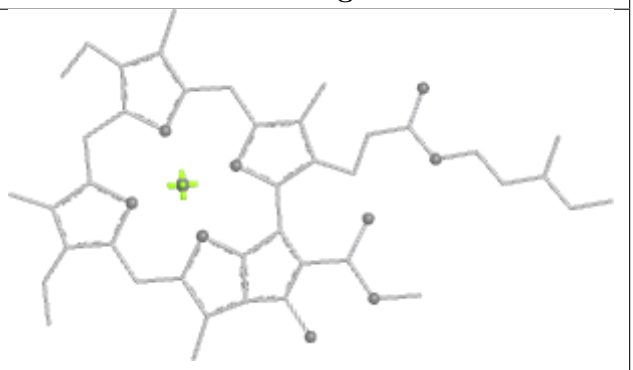
Bond lengths



Bond angles

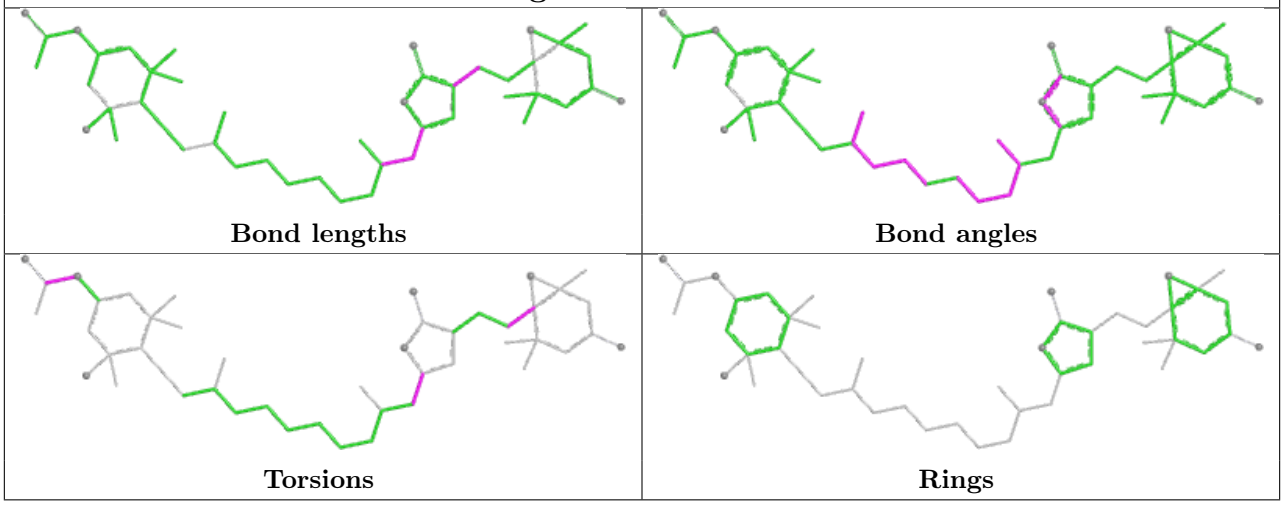


Torsions

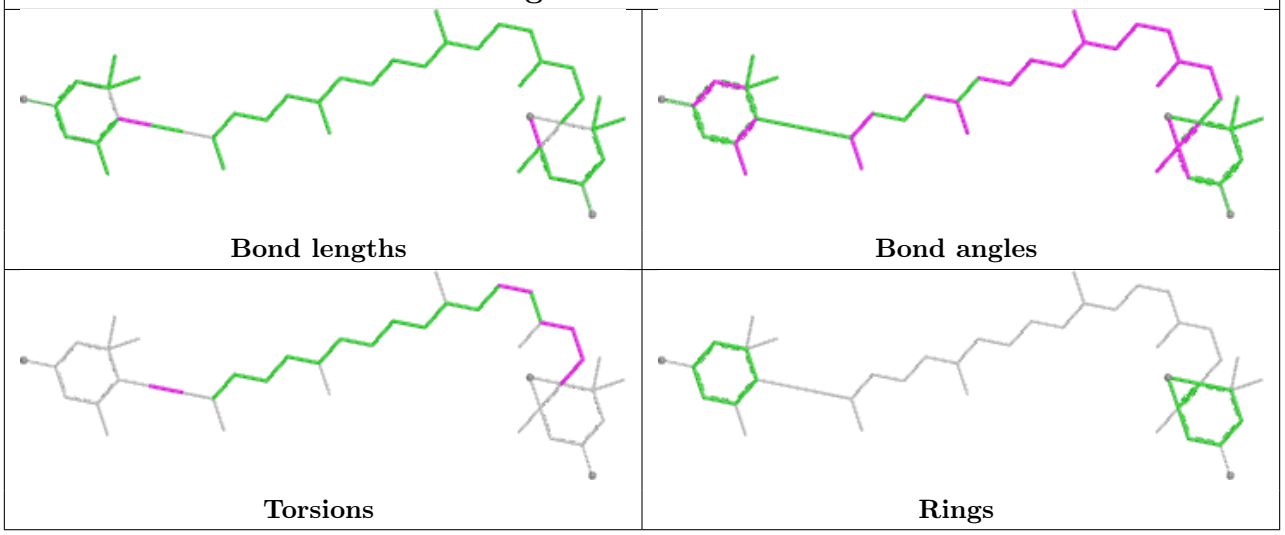


Rings

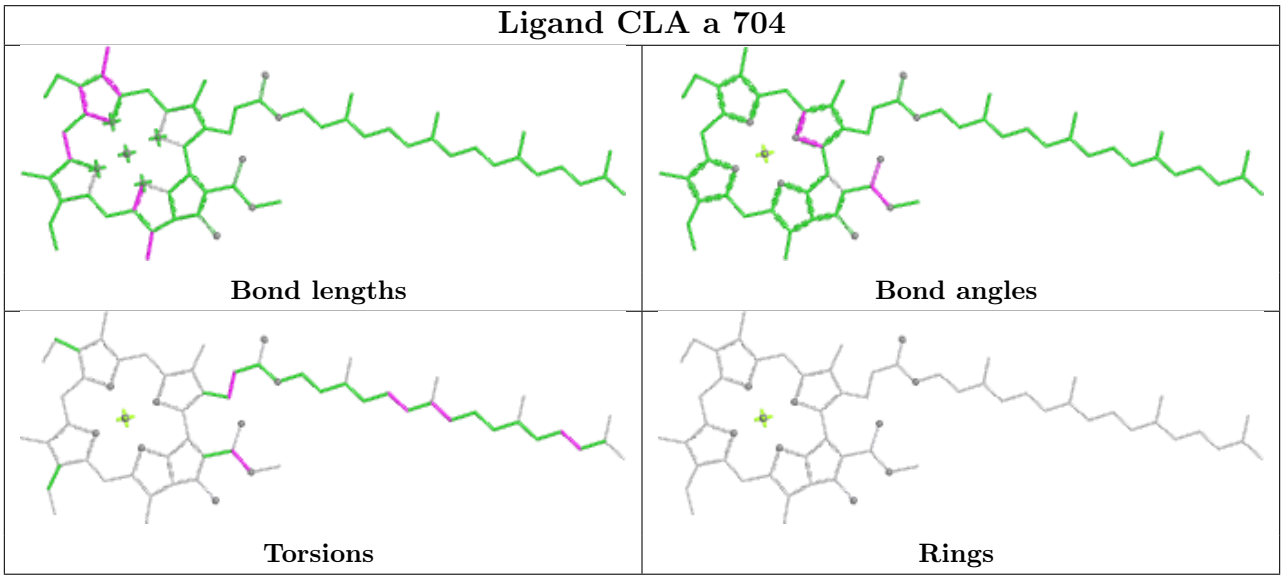
Ligand PID O 301



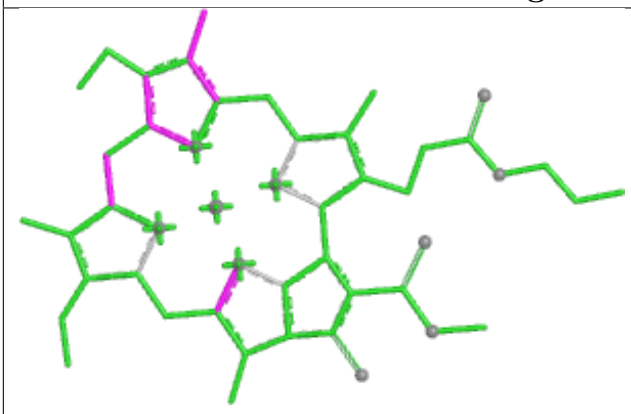
Ligand DD6 D 303



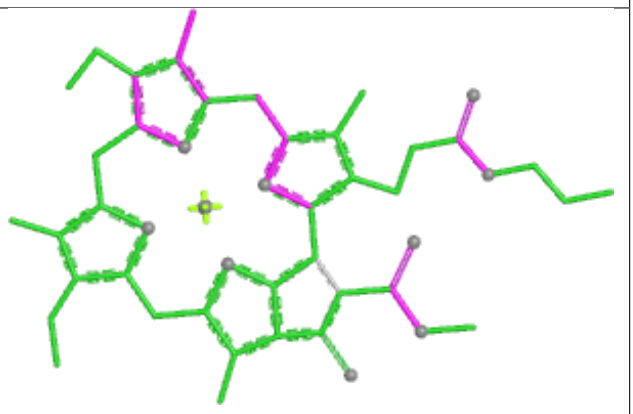
Ligand CLA a 704



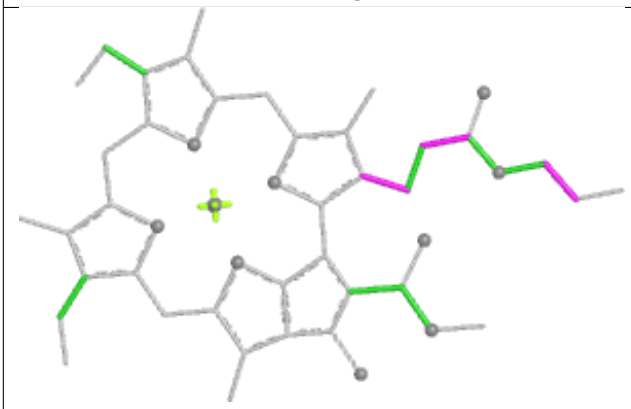
Ligand CLA b 706



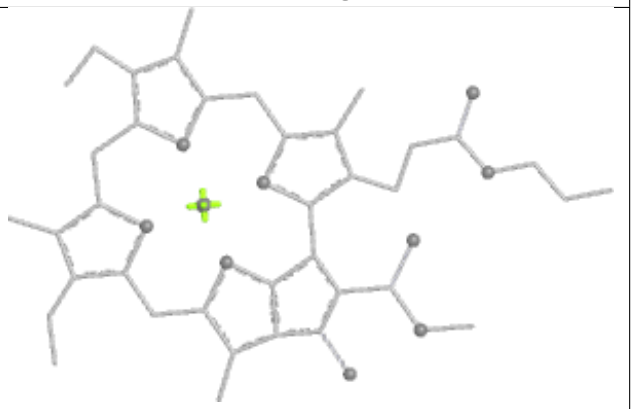
Bond lengths



Bond angles

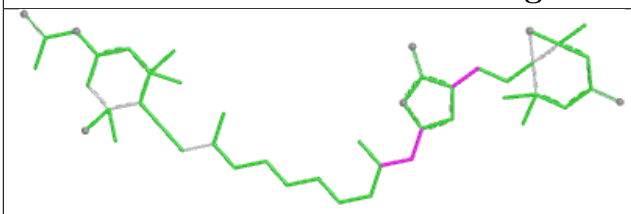


Torsions

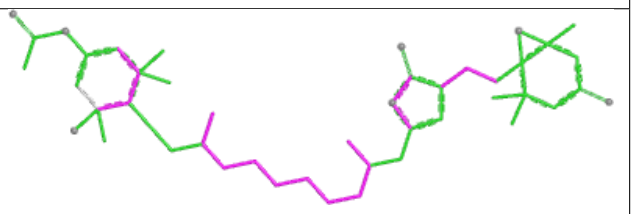


Rings

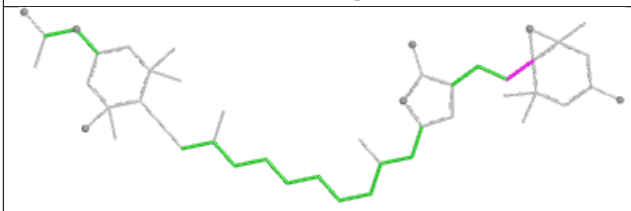
Ligand PID M 301



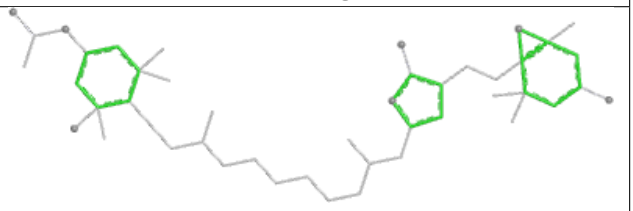
Bond lengths



Bond angles

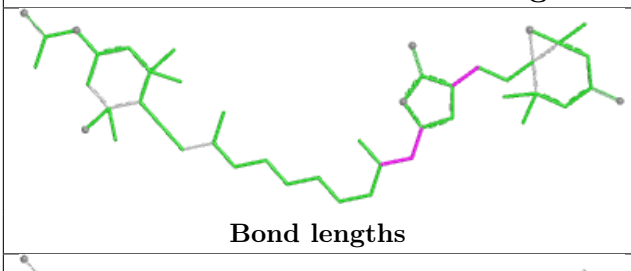


Torsions

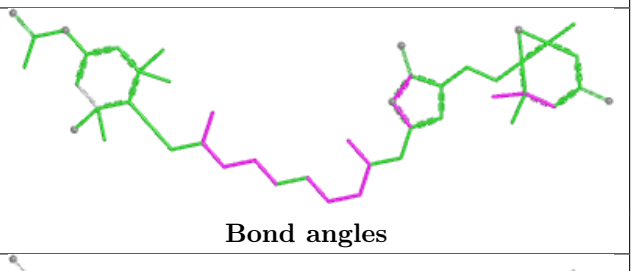


Rings

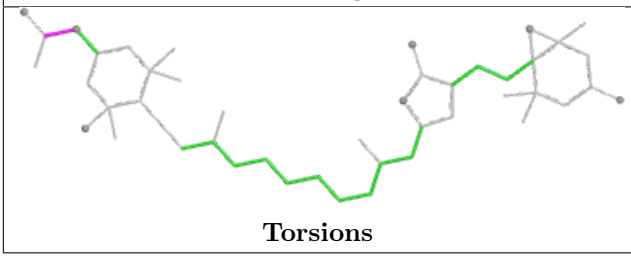
Ligand PID P 208



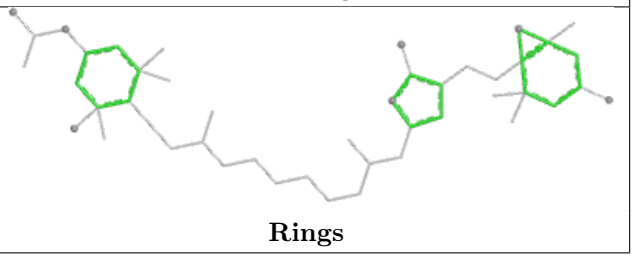
Bond lengths



Bond angles

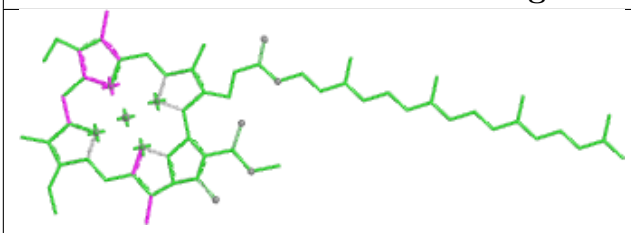


Torsions



Rings

Ligand CLA a 709



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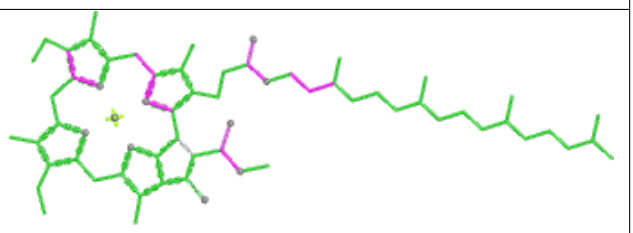
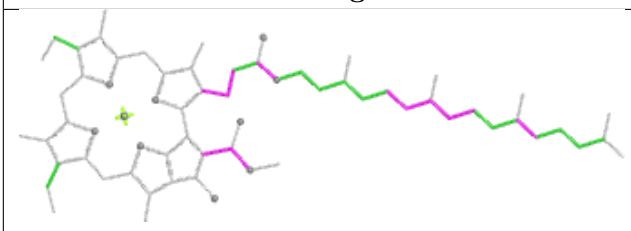


Bond angles



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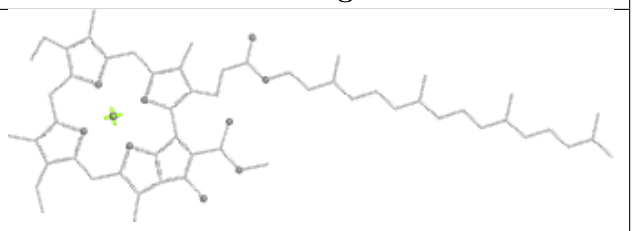
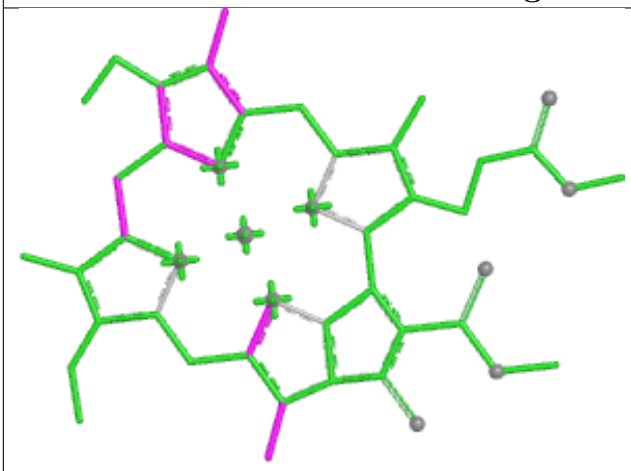


Rings

Ligand CLA A 320



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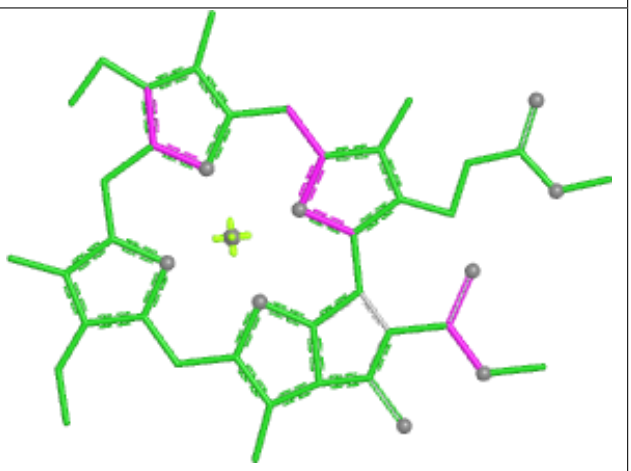
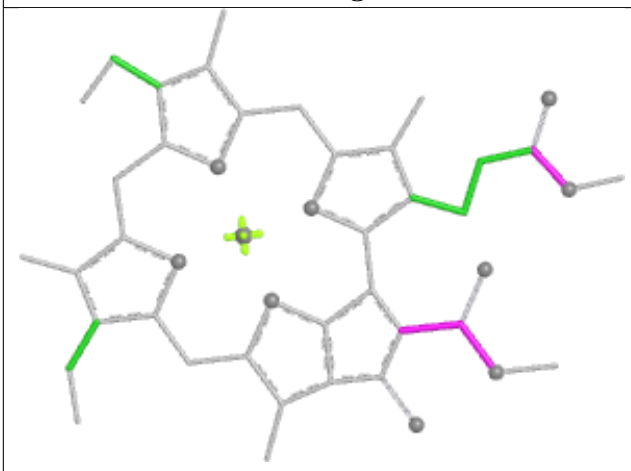
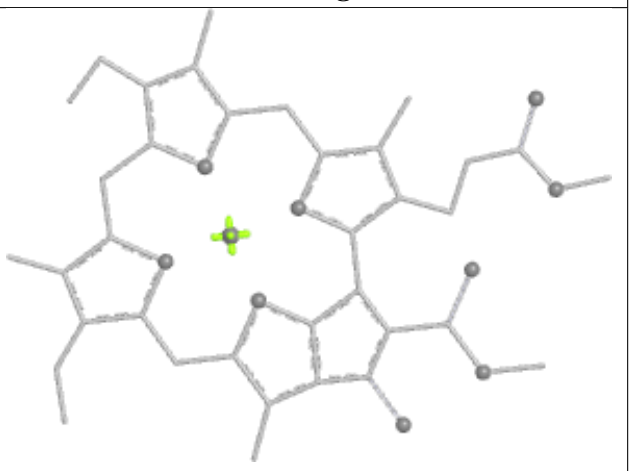


Bond angles

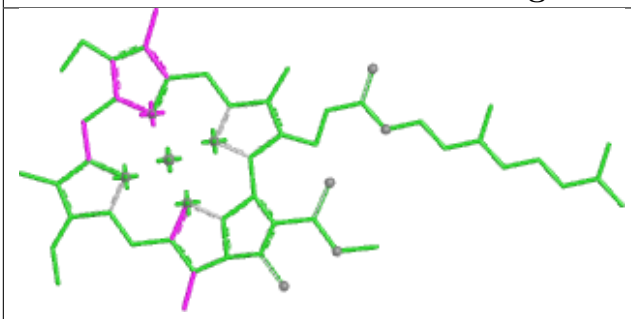


Torsions

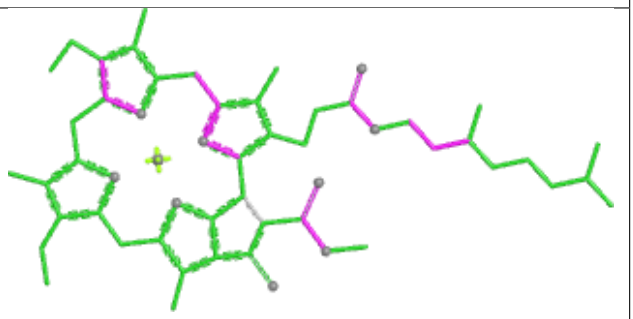


Rings

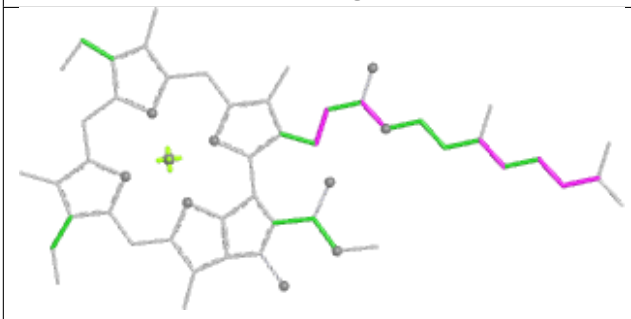
Ligand CLA a 728



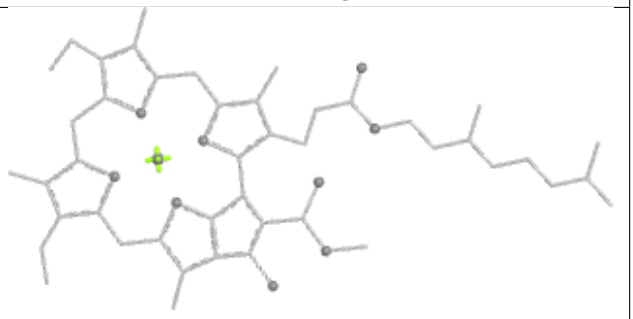
Bond lengths



Bond angles

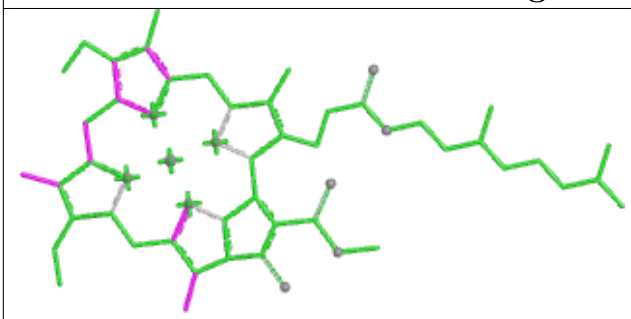


Torsions

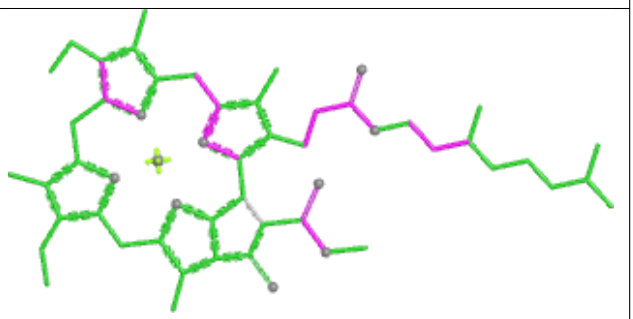


Rings

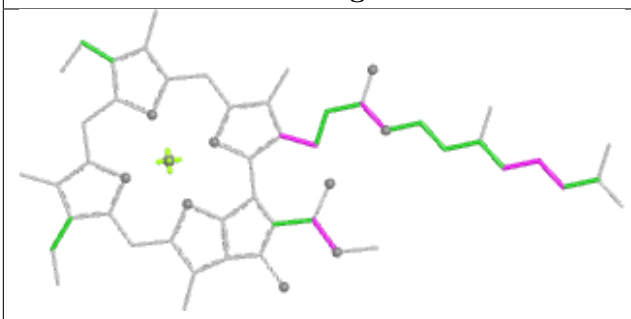
Ligand CLA a 705



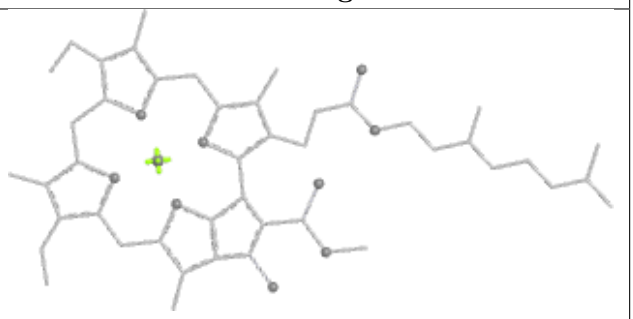
Bond lengths



Bond angles

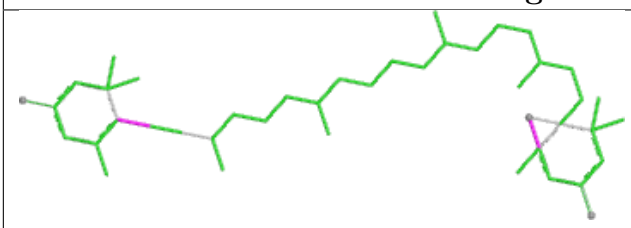


Torsions

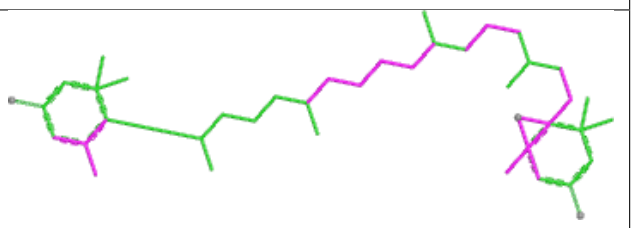


Rings

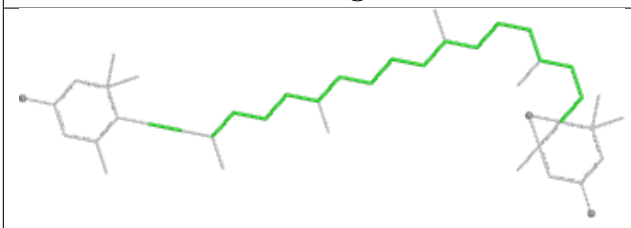
Ligand DD6 B 304



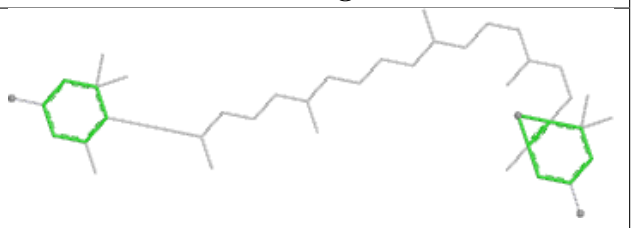
Bond lengths



Bond angles

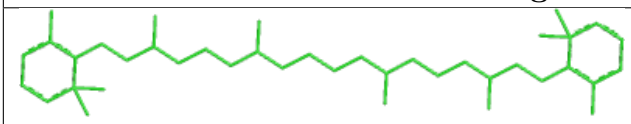


Torsions

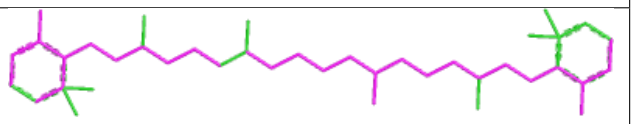


Rings

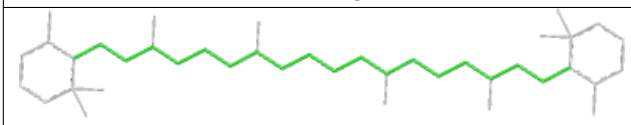
Ligand BCR l 307



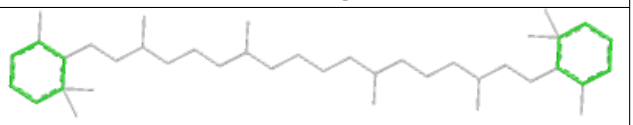
Bond lengths



Bond angles

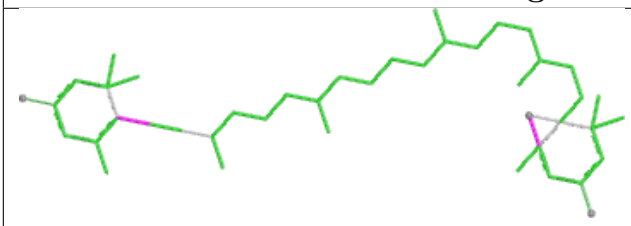


Torsions



Rings

Ligand DD6 L 303



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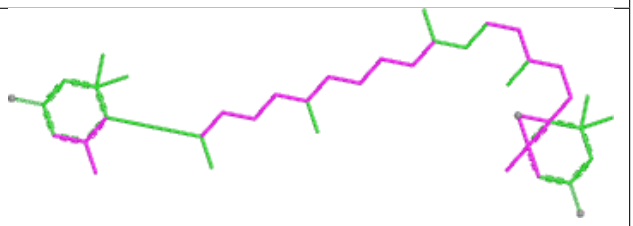
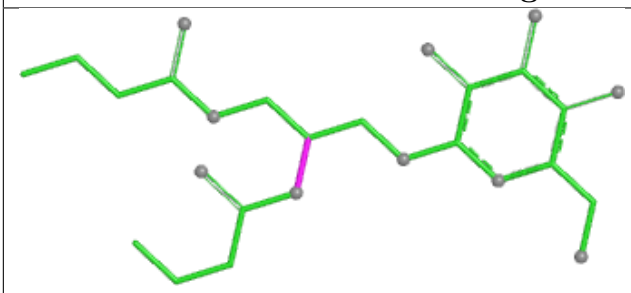


Bond angles

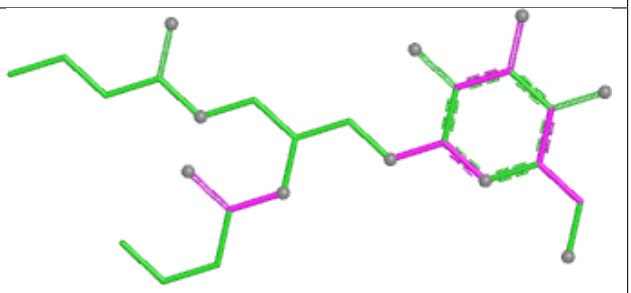
Torsions

Rings

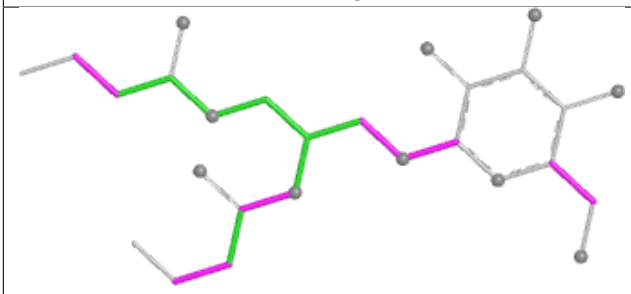
Ligand LMG P 201



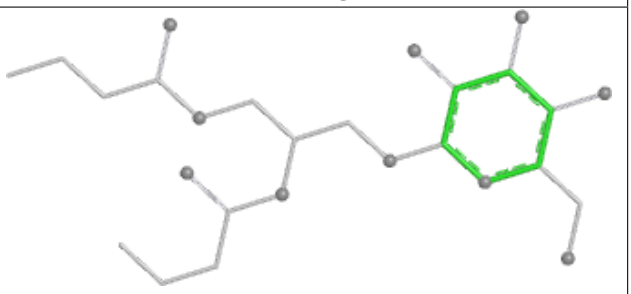
Bond lengths



Bond angles

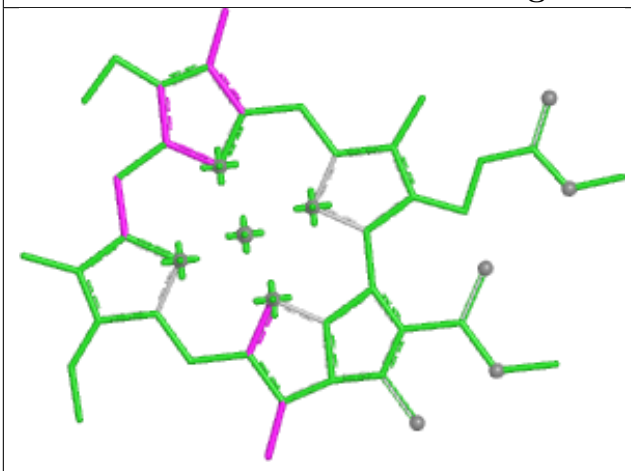


Torsions



Rings

Ligand CLA J 316



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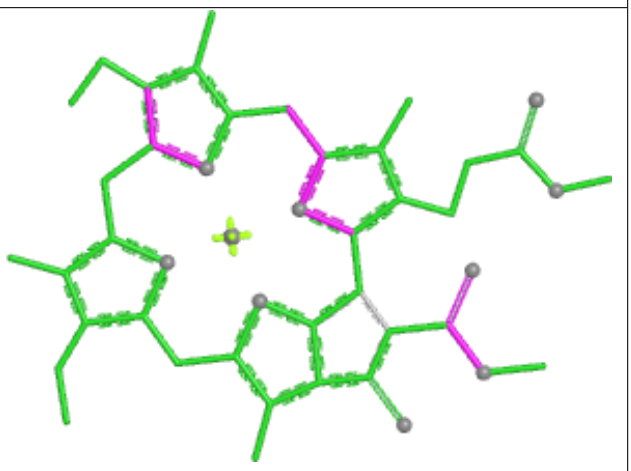
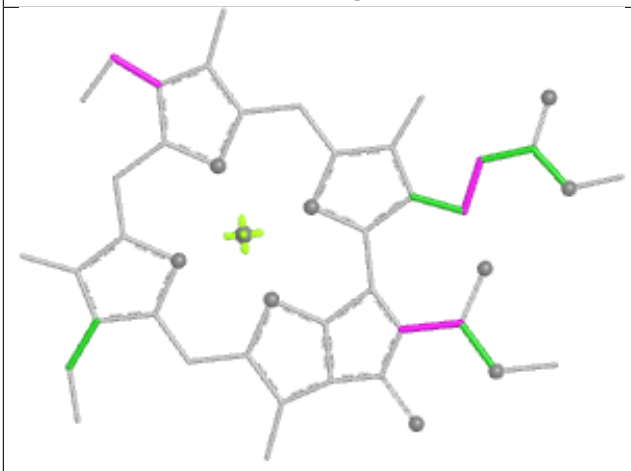


Bond angles



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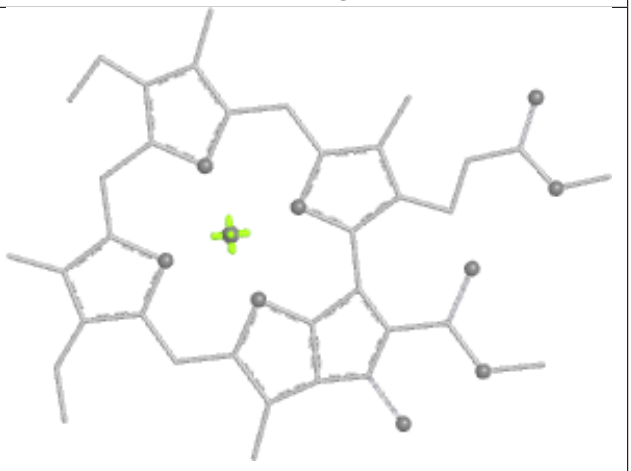
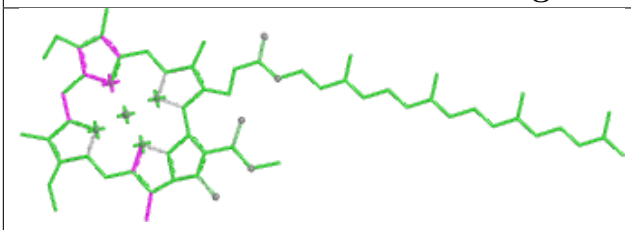
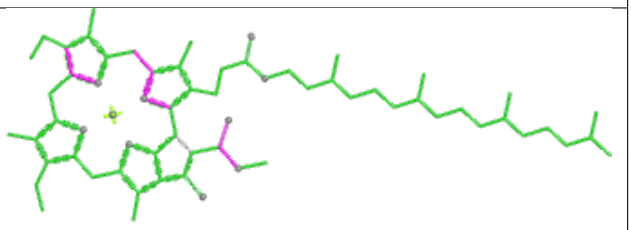


Rings

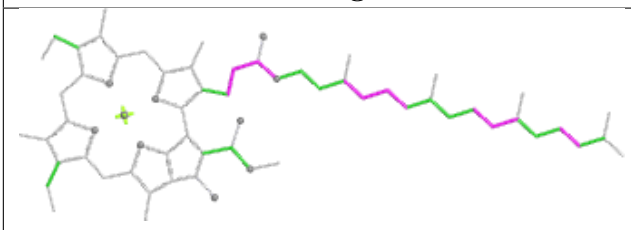
Ligand CLA l 305



Bond lengths



Bond angles



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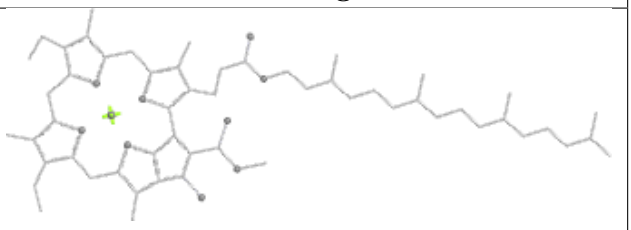
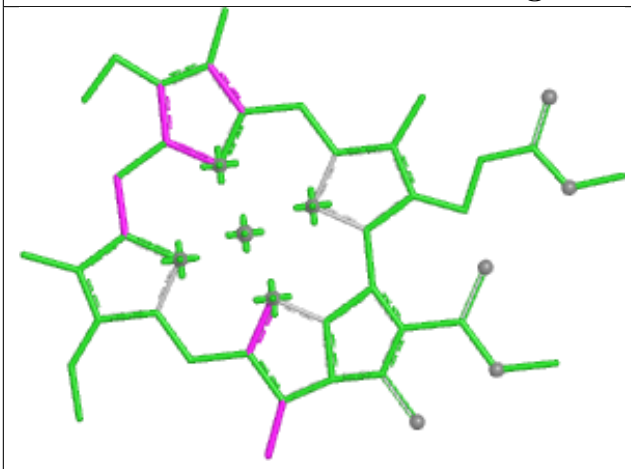


Rings

Ligand CLA F 310



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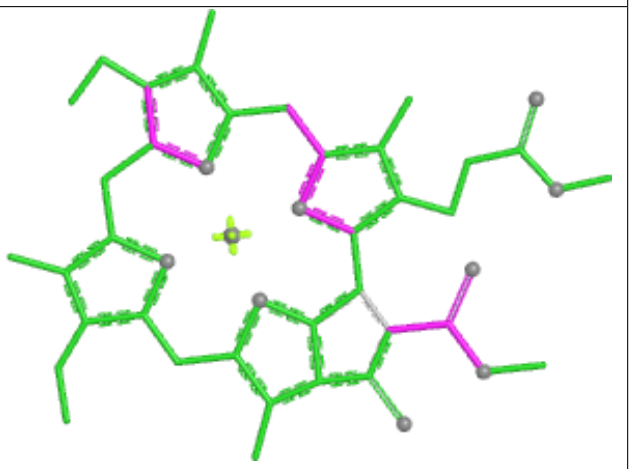
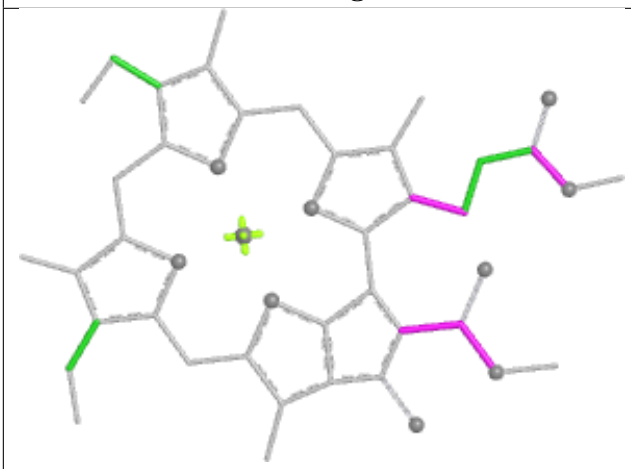
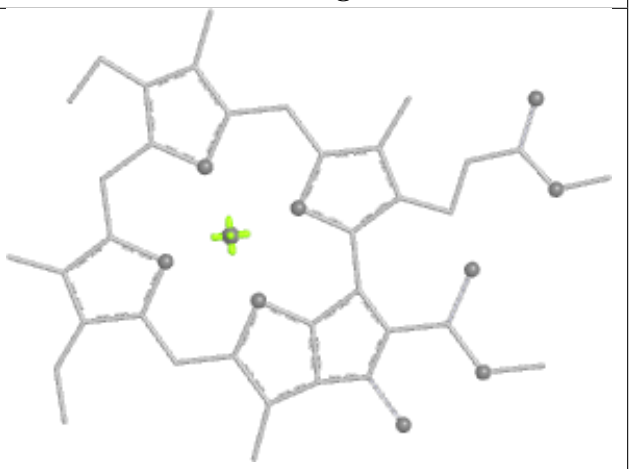


Bond angles

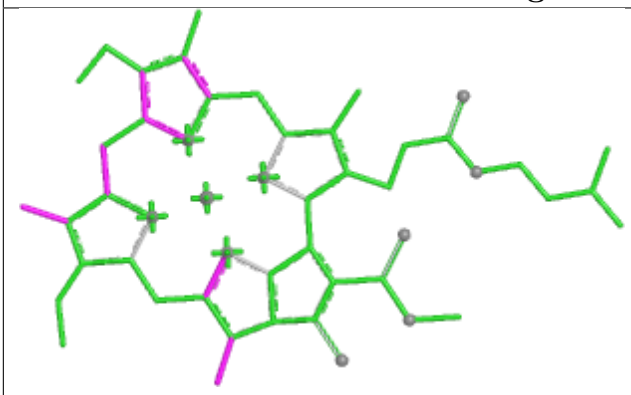


Torsions

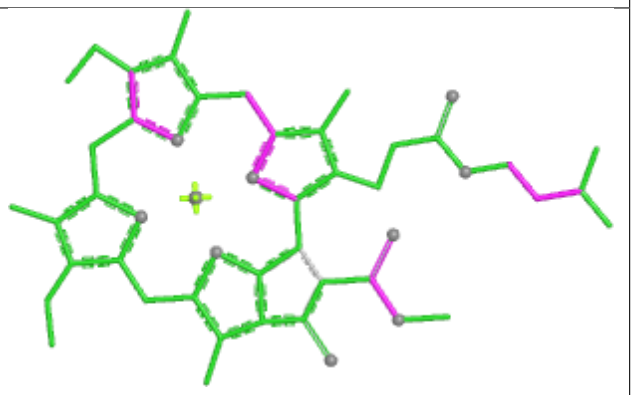


Rings

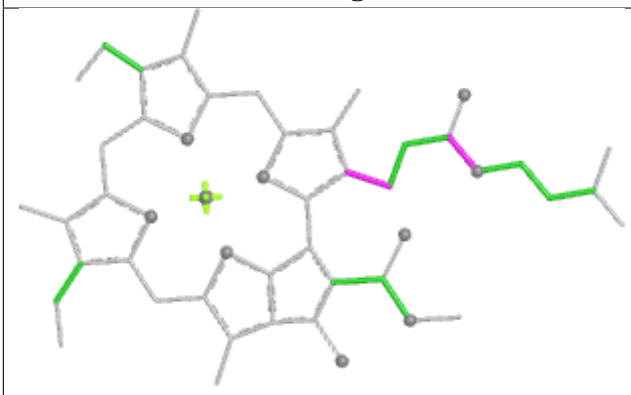
Ligand CLA b 716



Bond lengths



Bond angles



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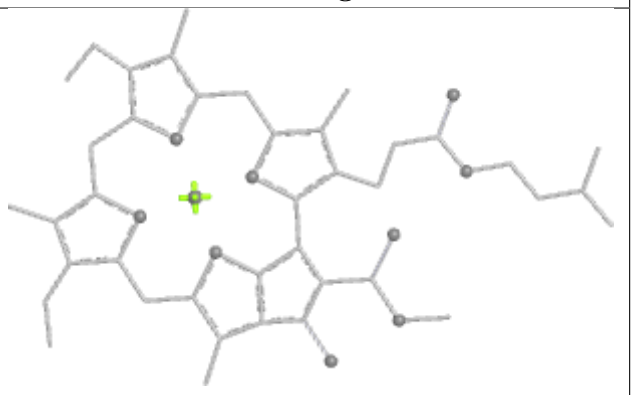
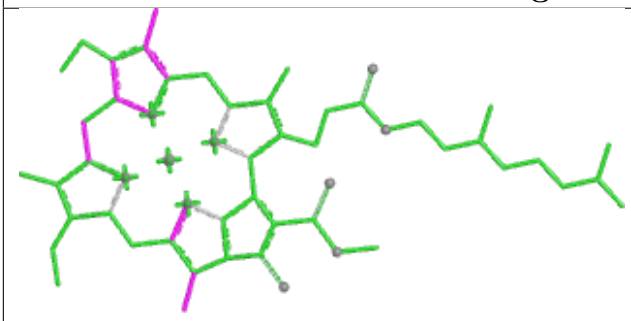


Rings

Ligand CLA f 301



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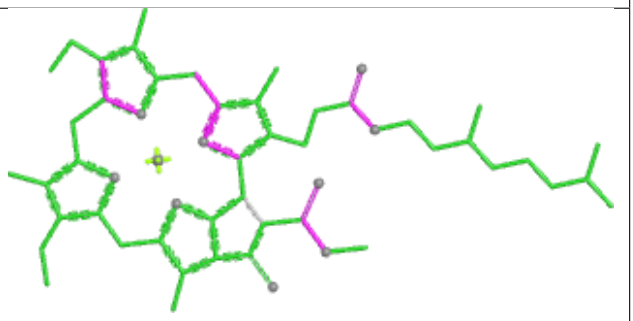
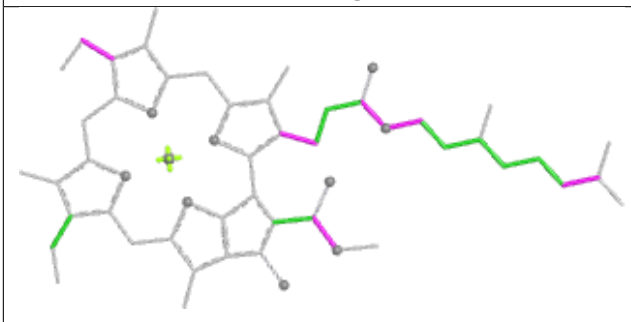


Bond angles



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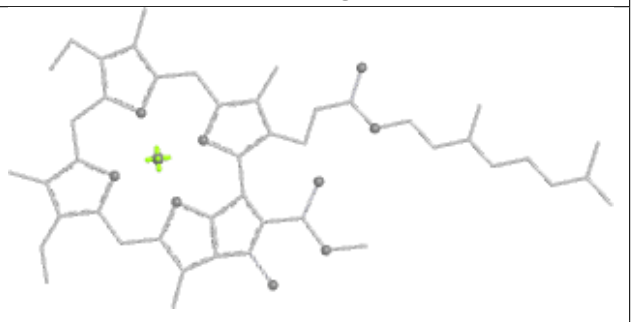
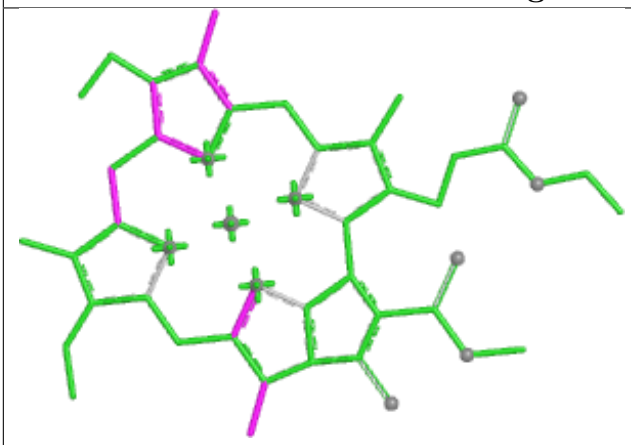
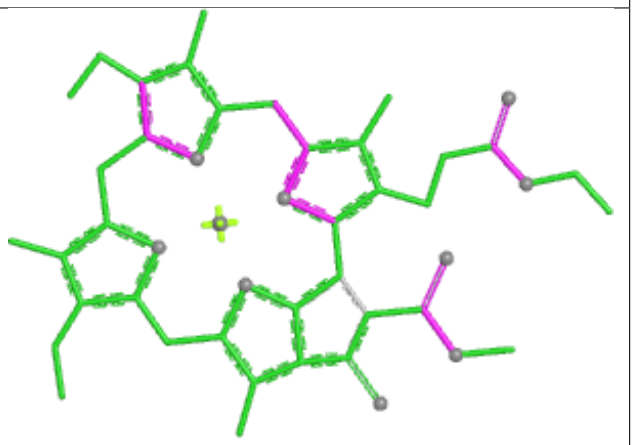


Rings

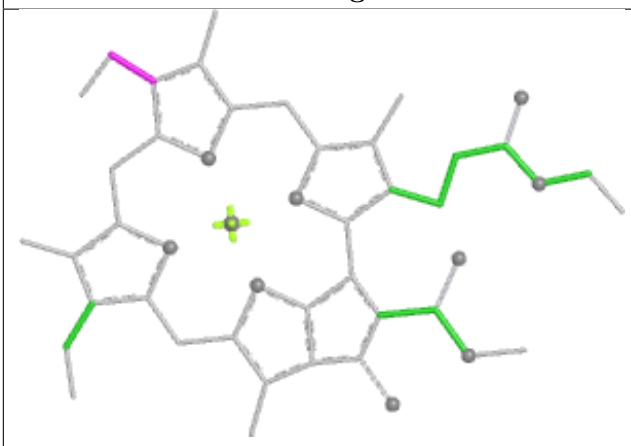
Ligand CLA b 726



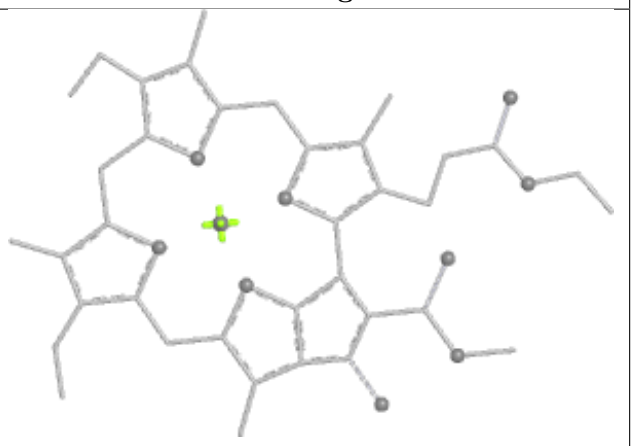
Bond lengths



Bond angles

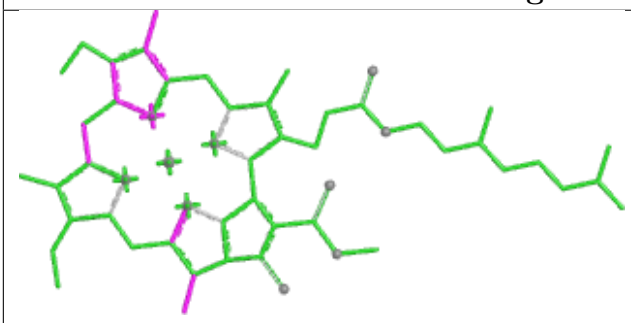


Torsions



Rings

Ligand CLA L 313



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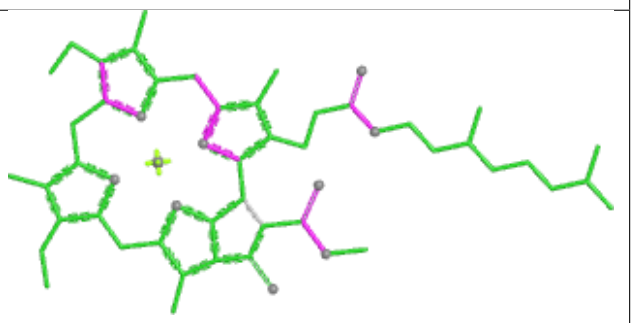
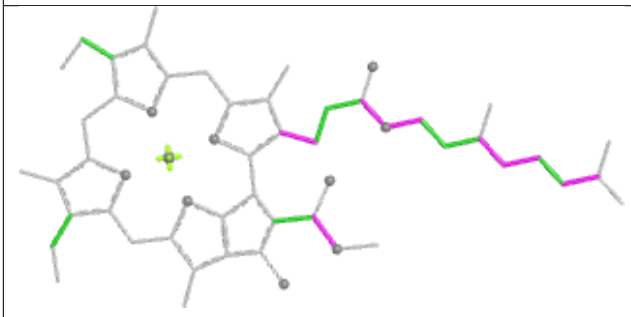
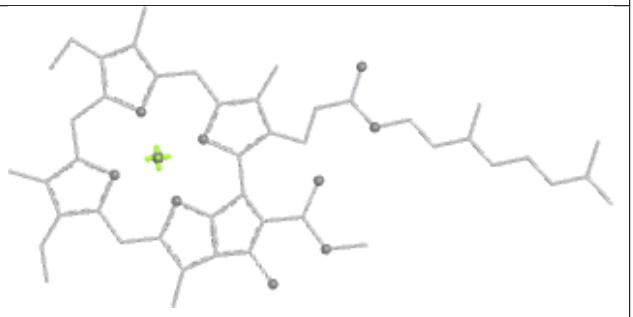


Bond angles

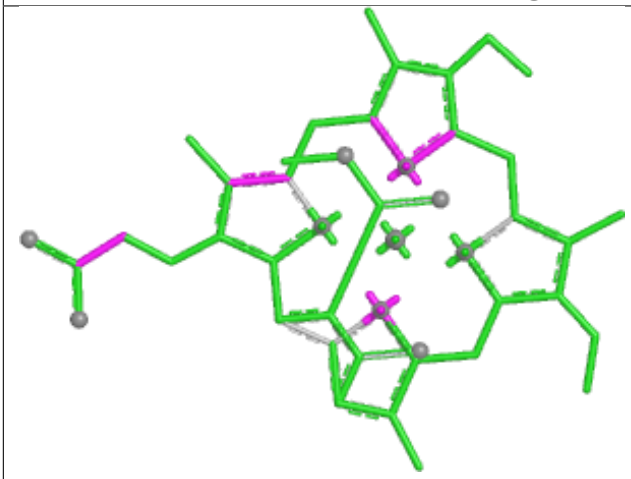


Torsions

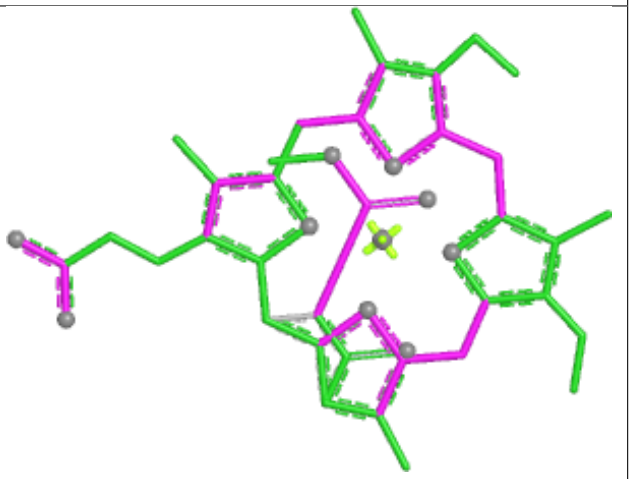


Rings

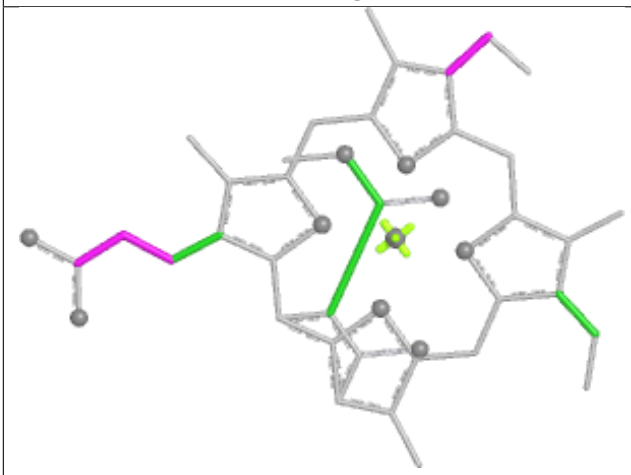
Ligand KC1 A 314



Bond lengths



Bond angles



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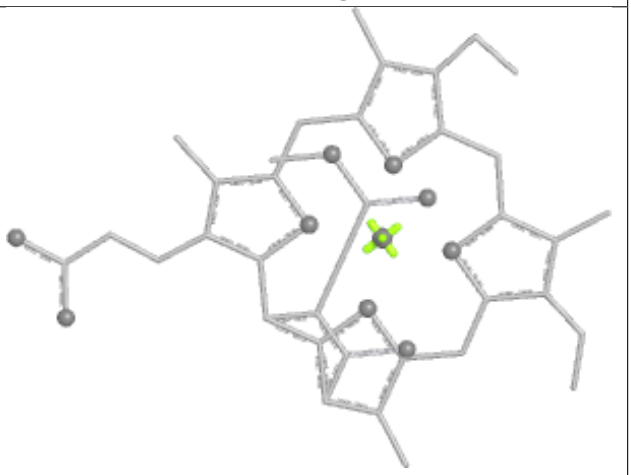
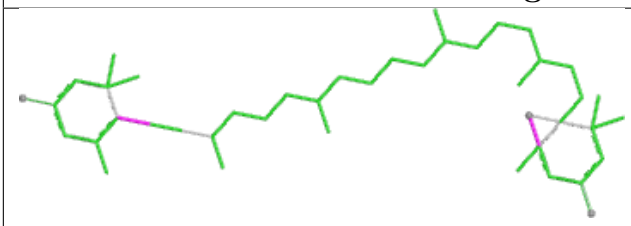
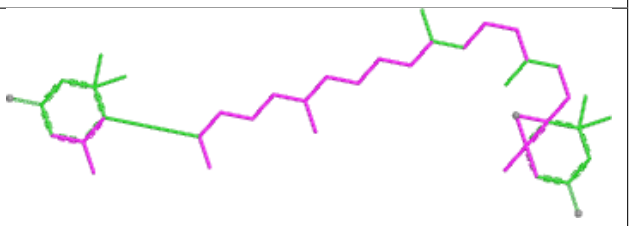


Rings

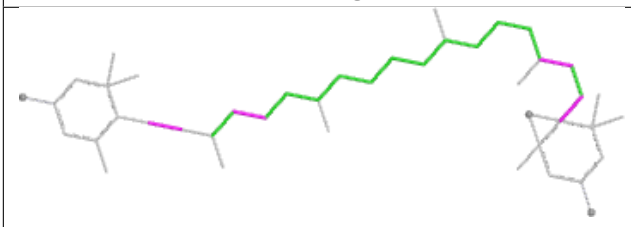
Ligand DD6 K 301



Bond lengths



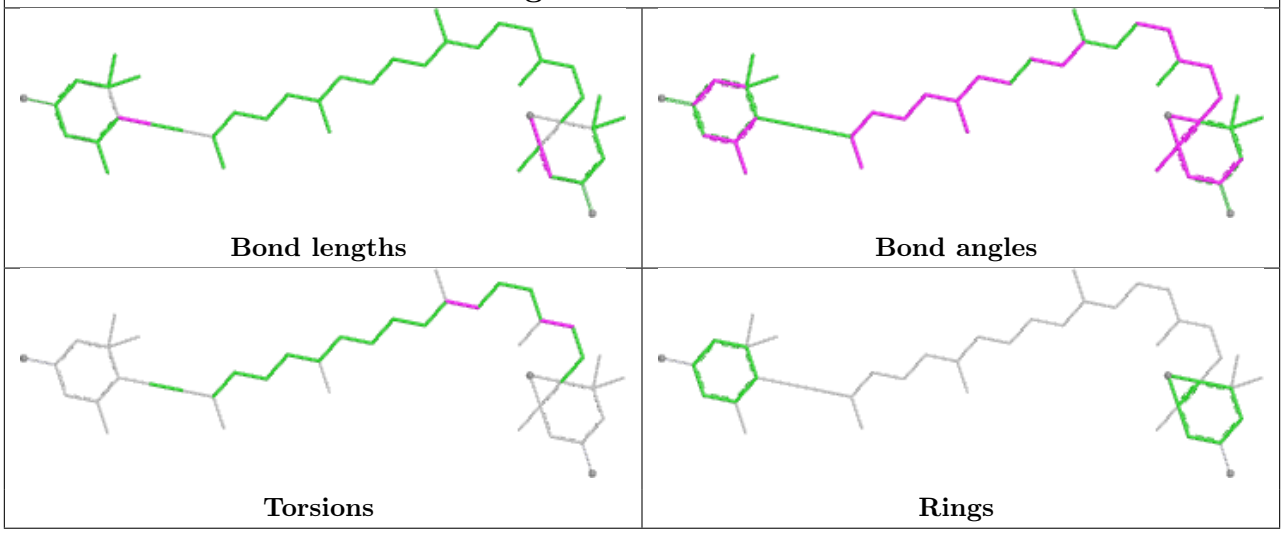
Bond angles



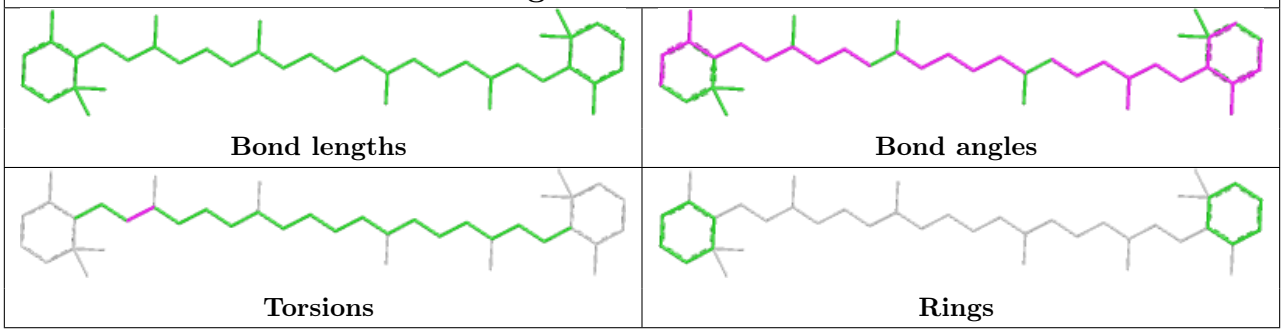
Torsions

Rings

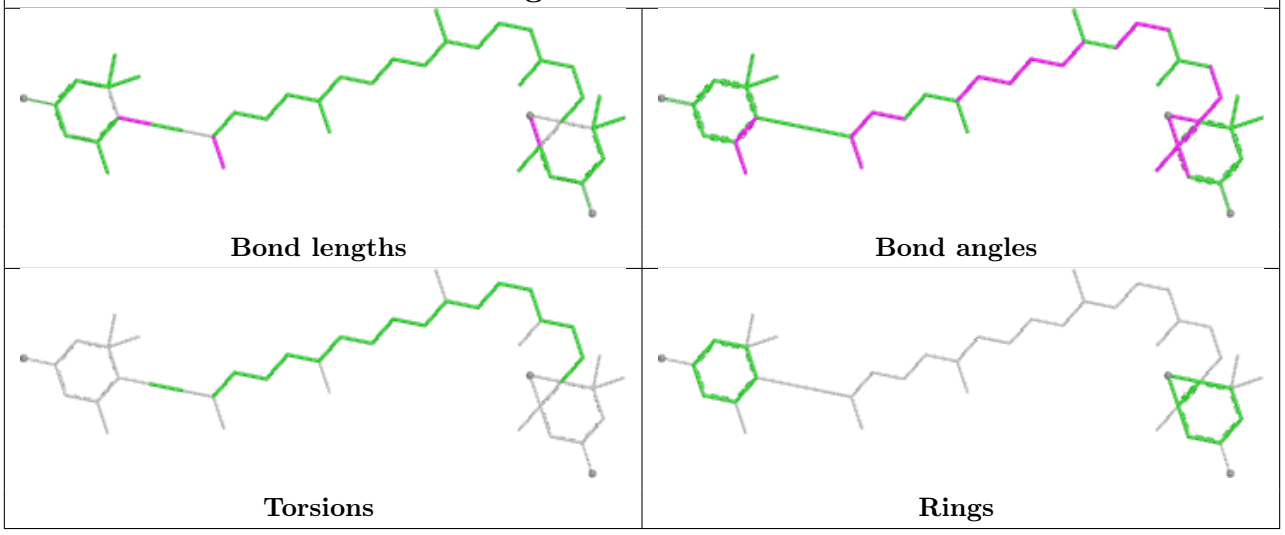
Ligand DD6 G 505



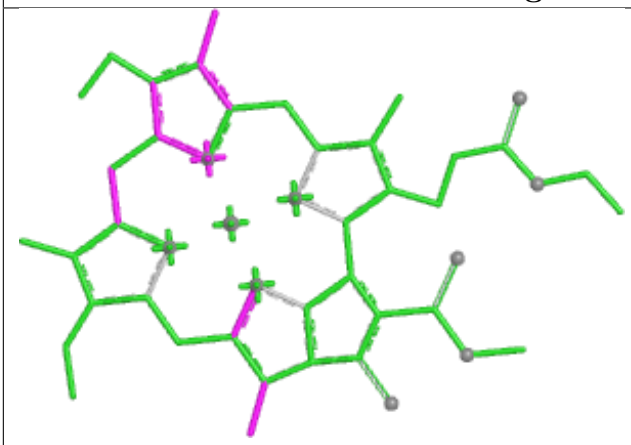
Ligand BCR a 734



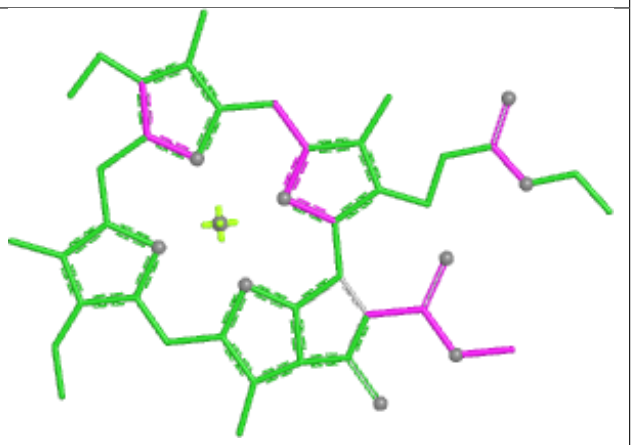
Ligand DD6 K 303



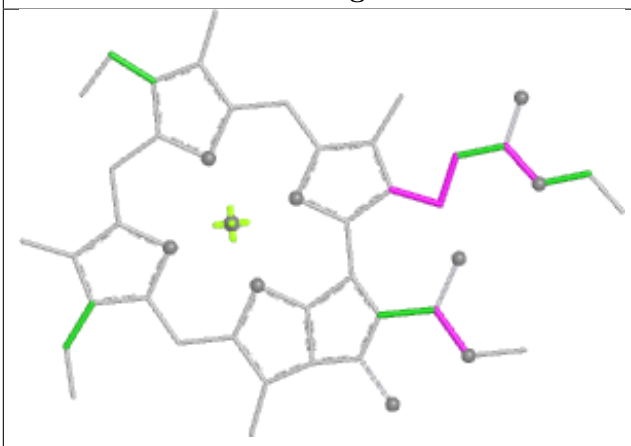
Ligand CLA P 215



Bond lengths



Bond angles



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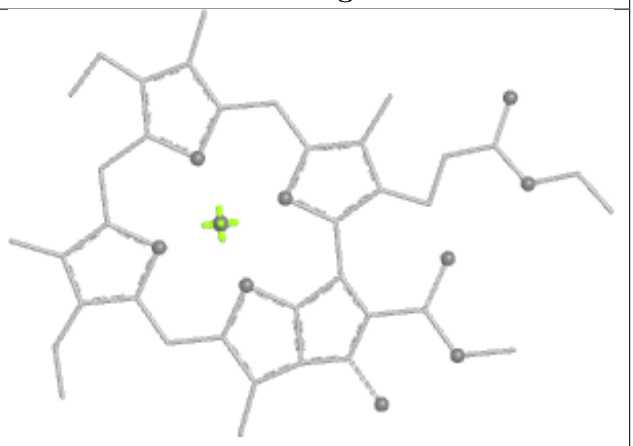
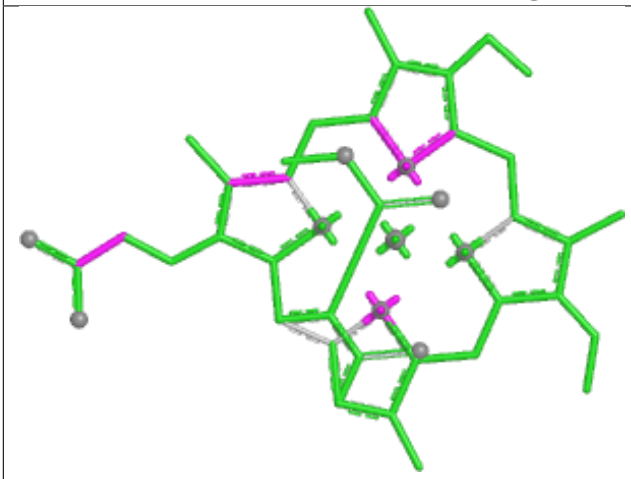
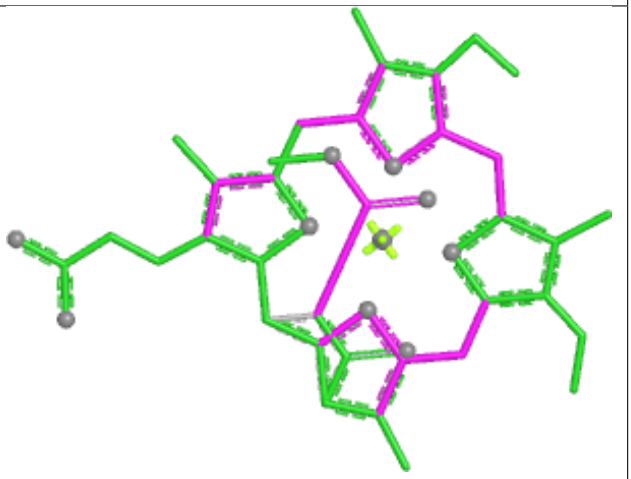


Rings

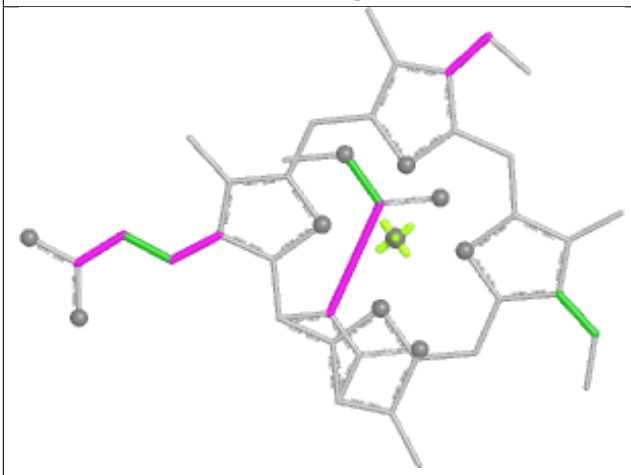
Ligand KC1 A 306



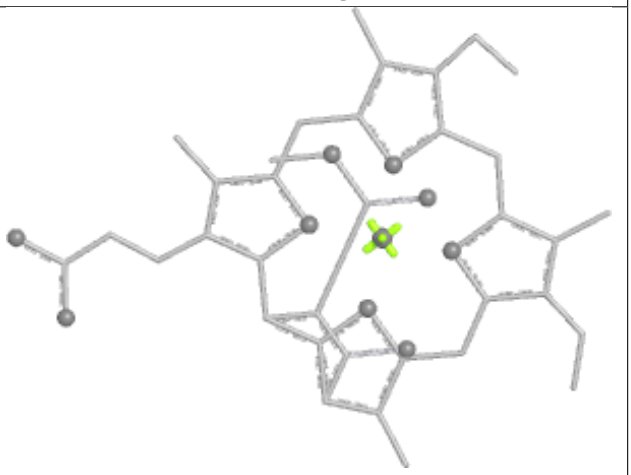
Bond lengths



Bond angles

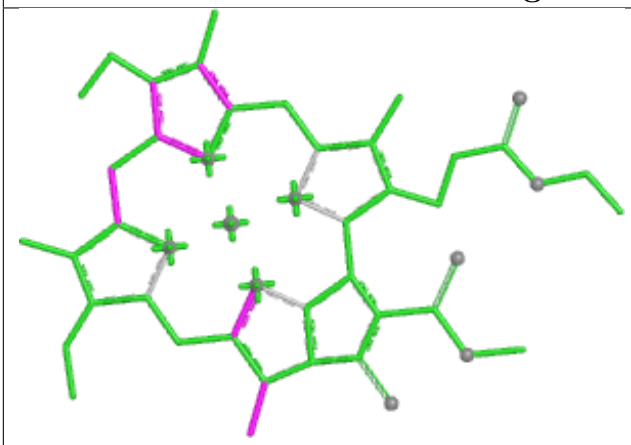


Torsions



Rings

Ligand CLA O 308



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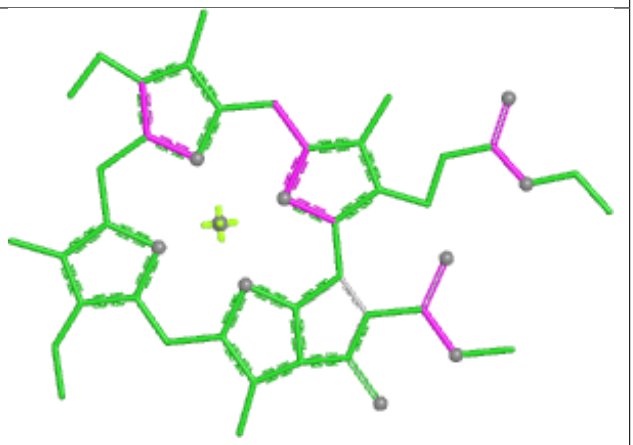

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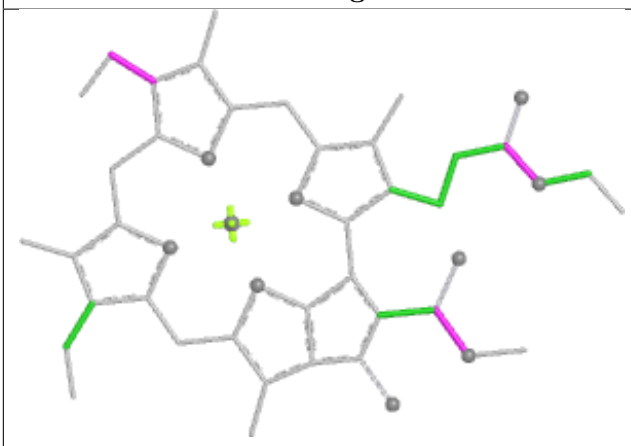

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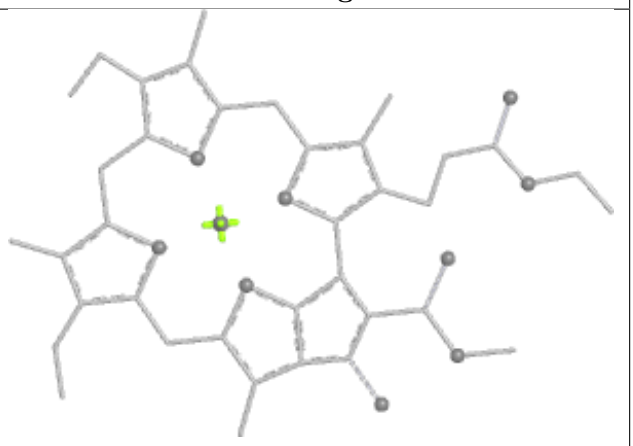
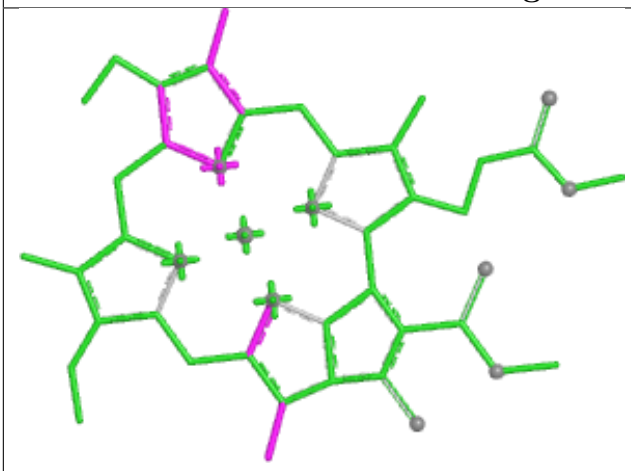


Rings

Ligand CLA K 307



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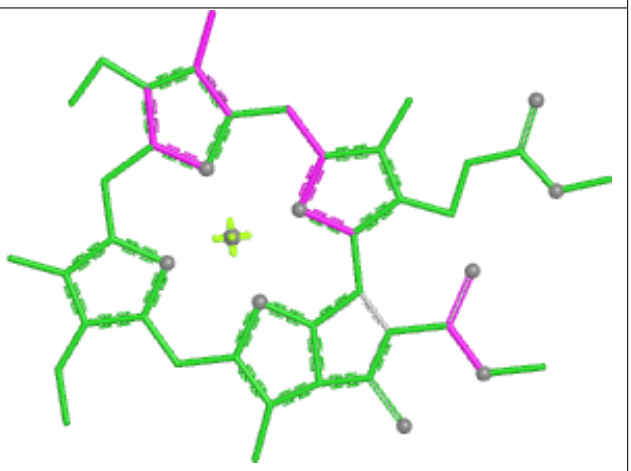

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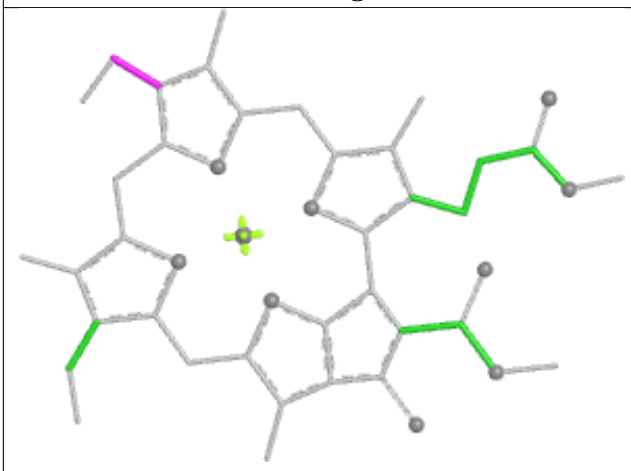

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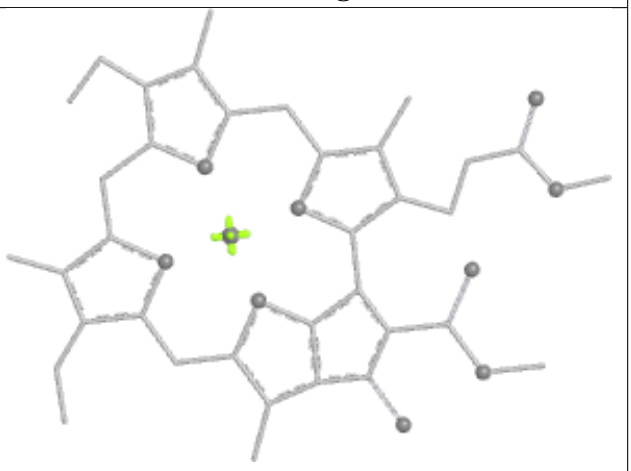
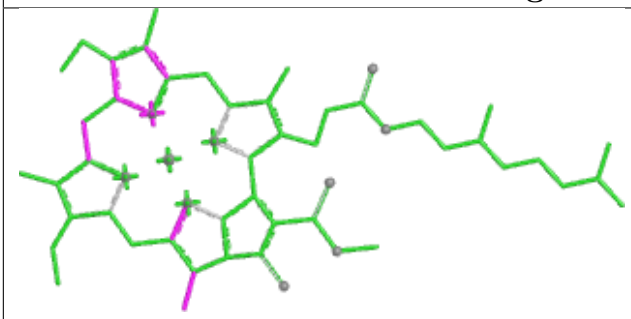


Rings

Ligand CLA L 310



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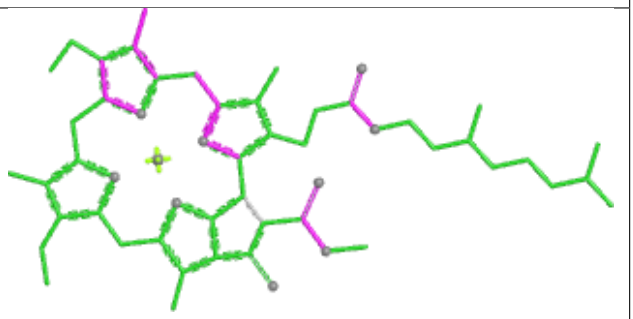
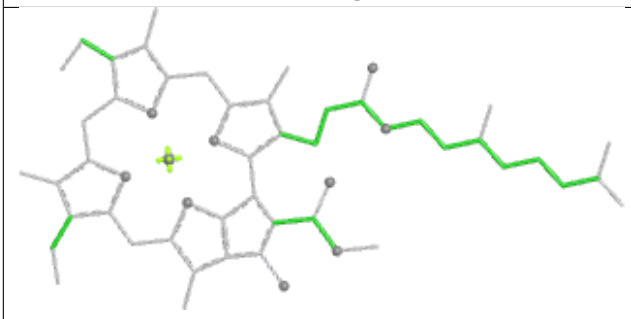


Bond angles



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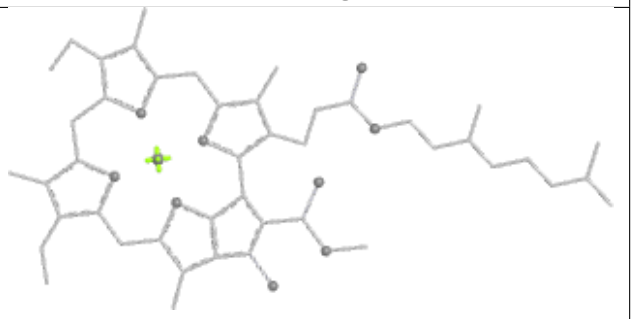
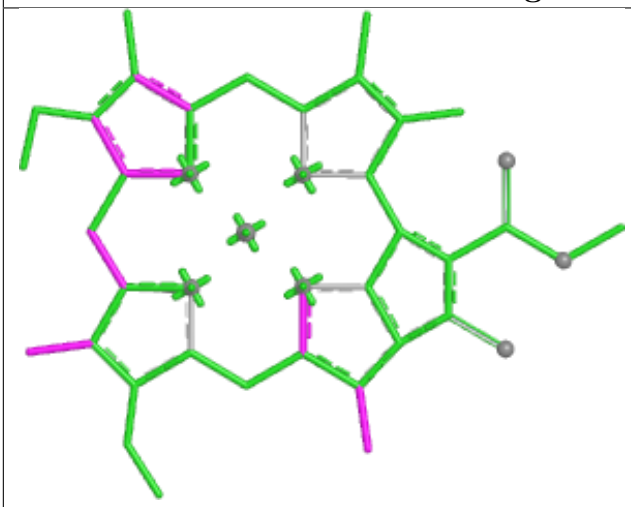


Rings

Ligand CLA B 315



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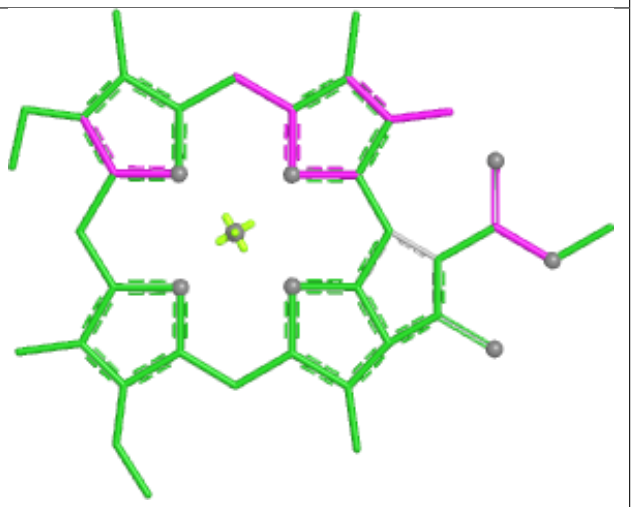
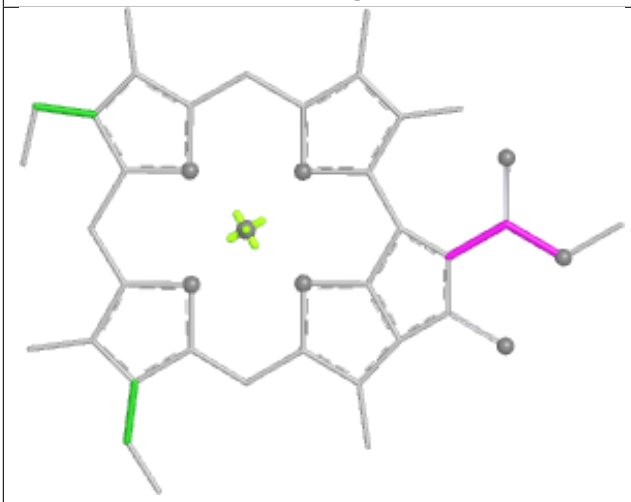


Bond angles



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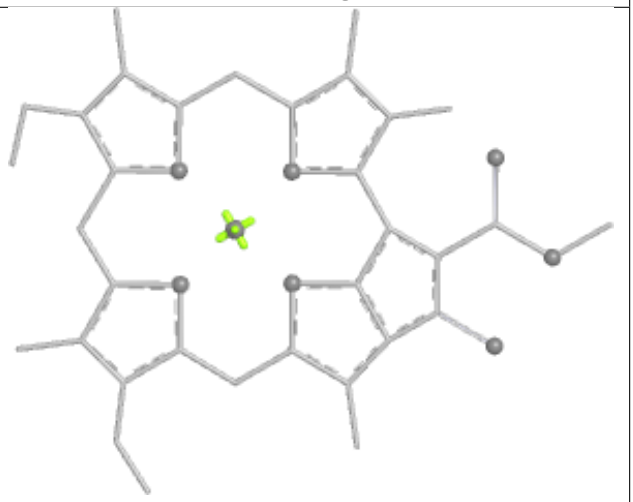
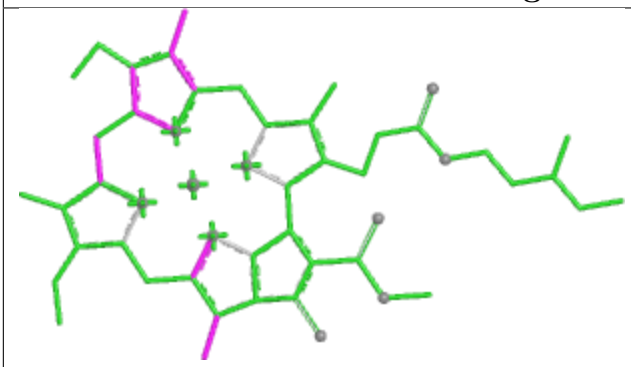


Rings

Ligand CLA H 307



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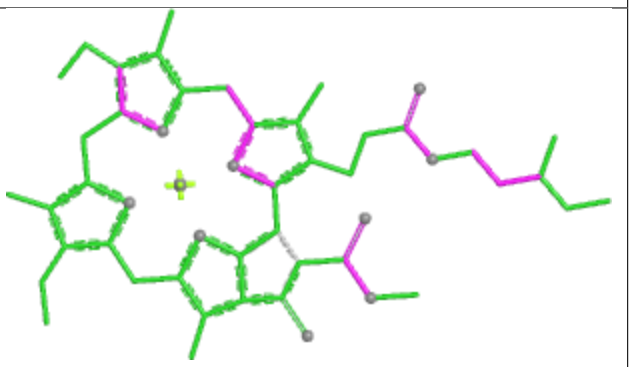
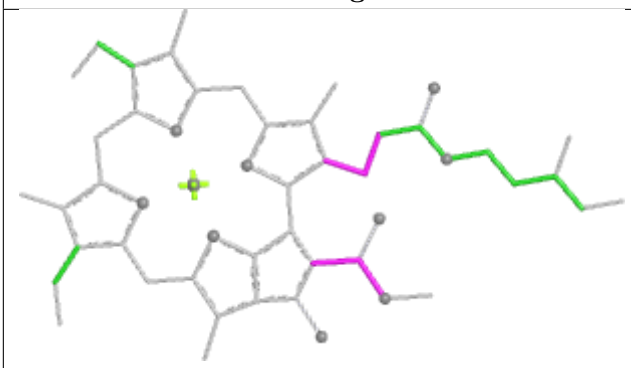


Bond angles



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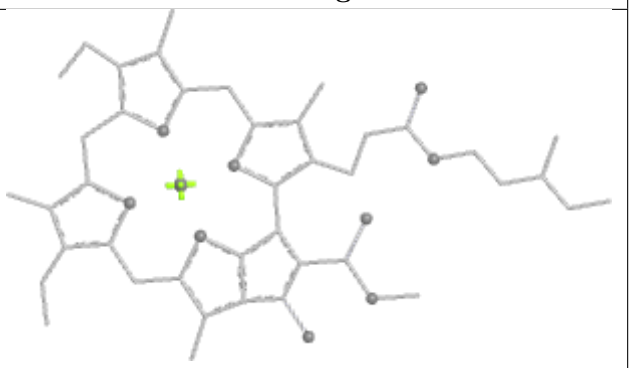
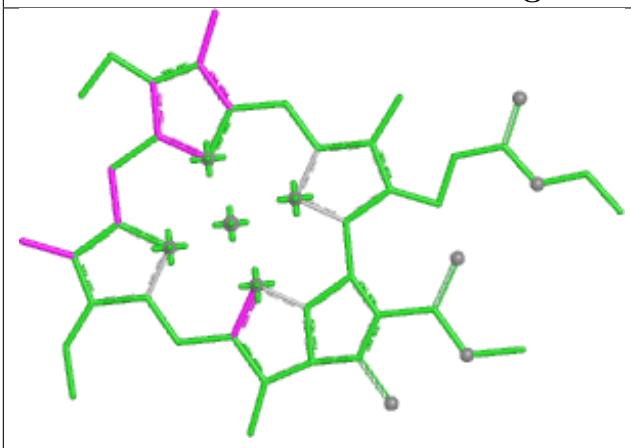


Rings

Ligand CLA A 316



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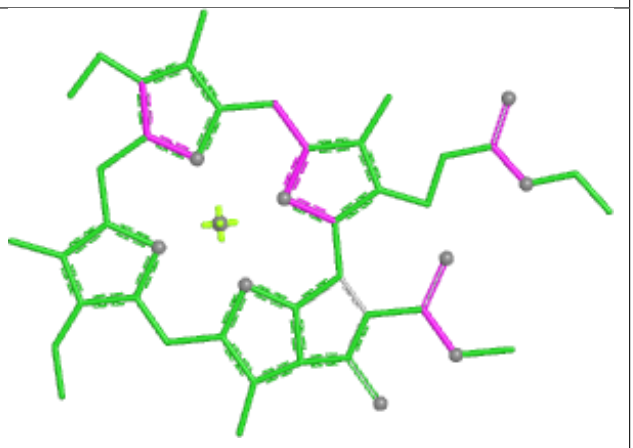
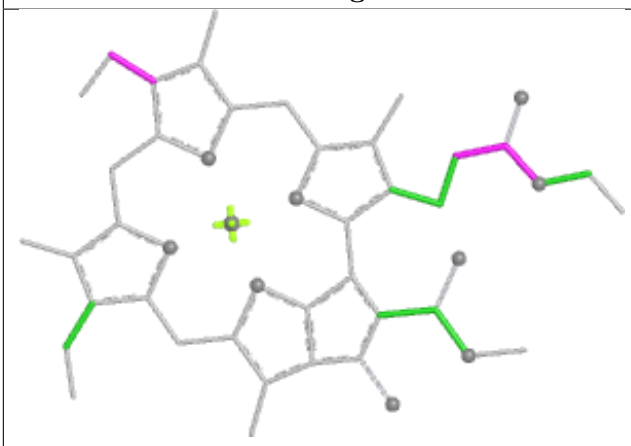


Bond angles



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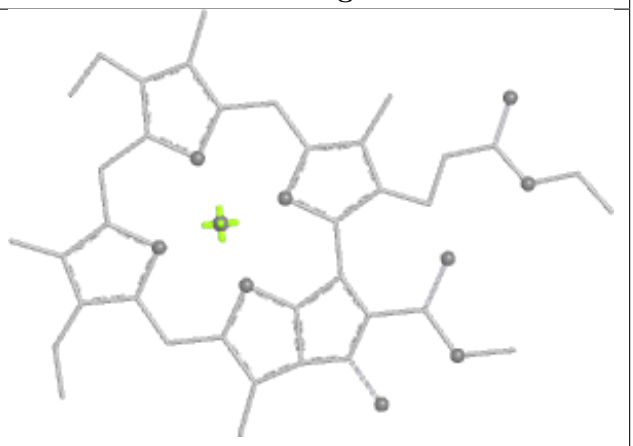
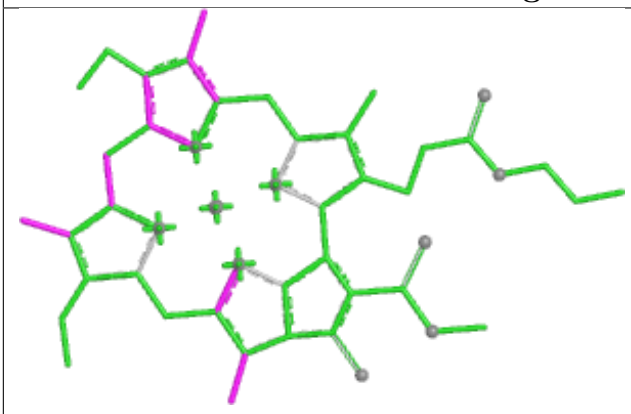


Rings

Ligand CLA K 312



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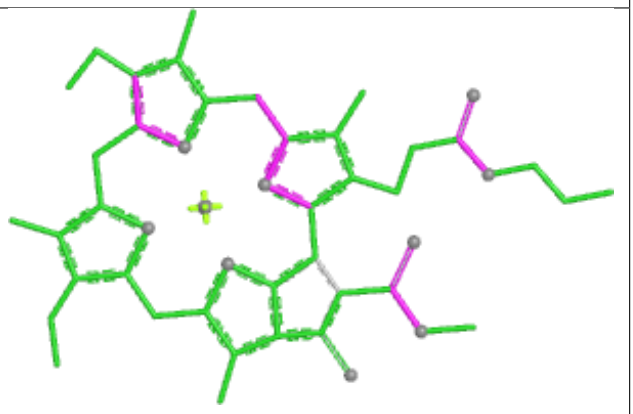
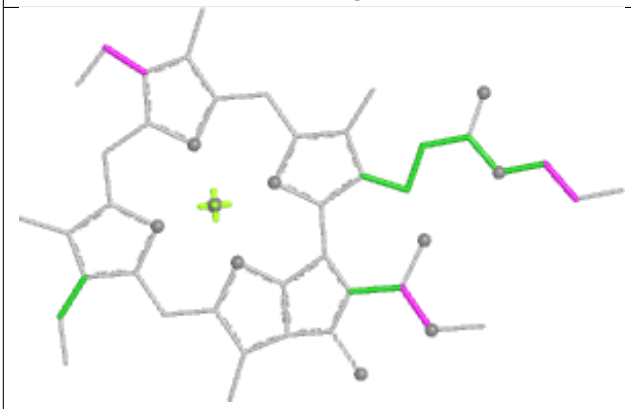


Bond angles



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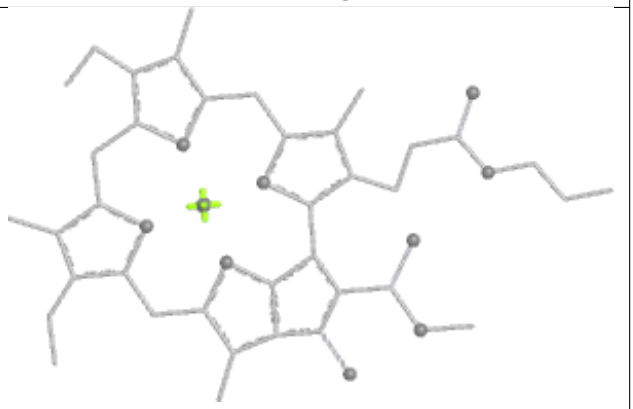
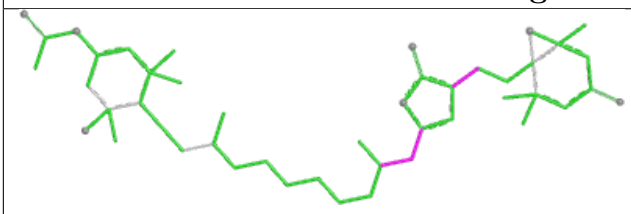
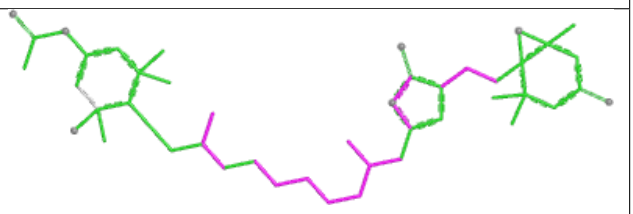


Rings

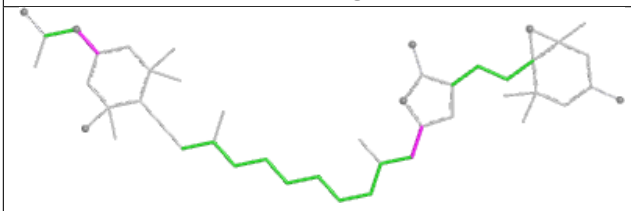
Ligand PID P 205



Bond lengths



Bond angles



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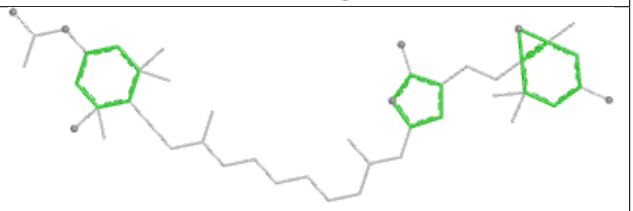
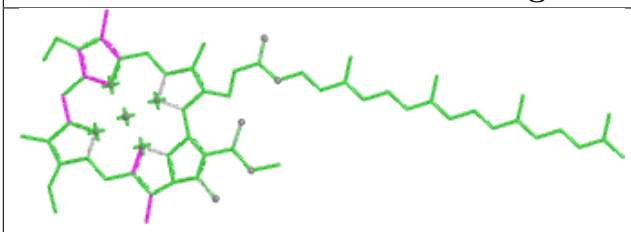
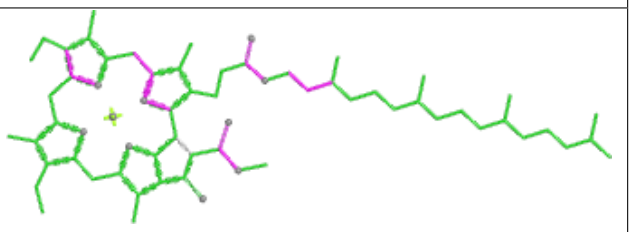


Rings

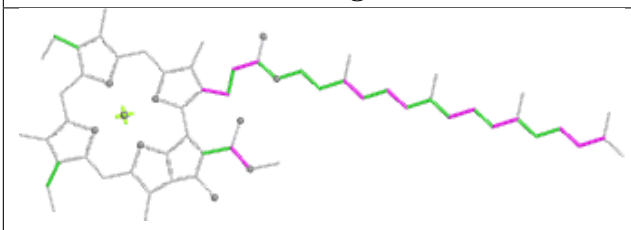
Ligand CLA a 731



Bond lengths



Bond angles



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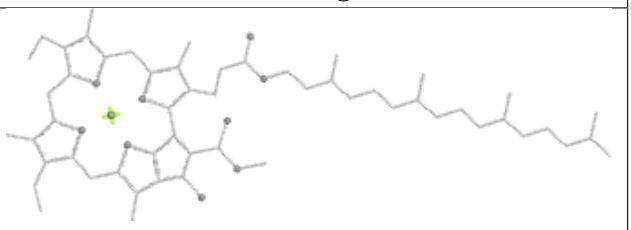
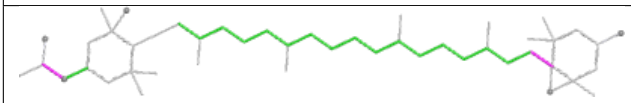


Rings

Ligand UIX I 304

Bond lengths

Bond angles



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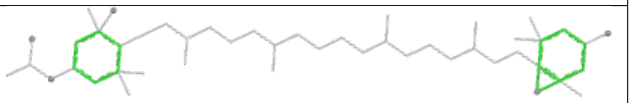
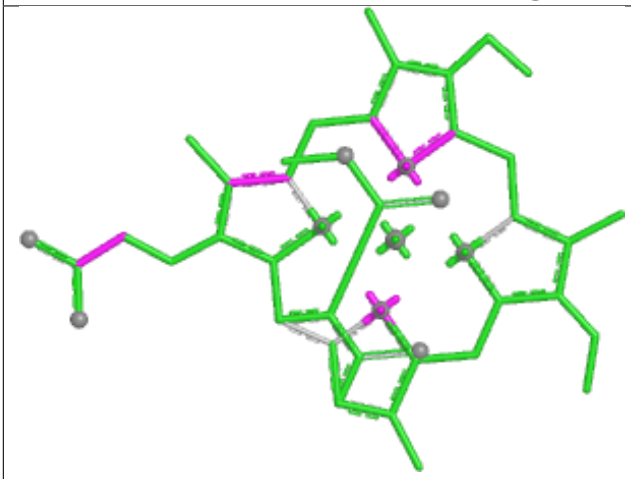


Rings

Ligand KC1 P 216



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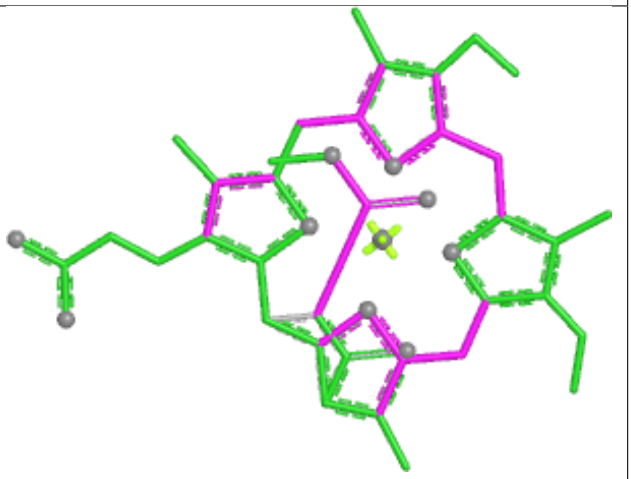
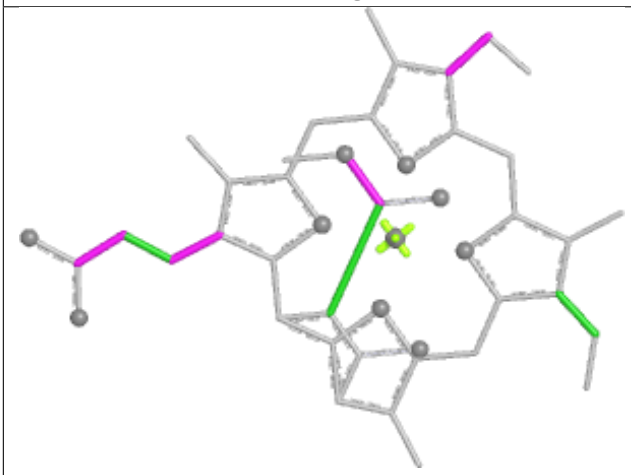


Bond angles



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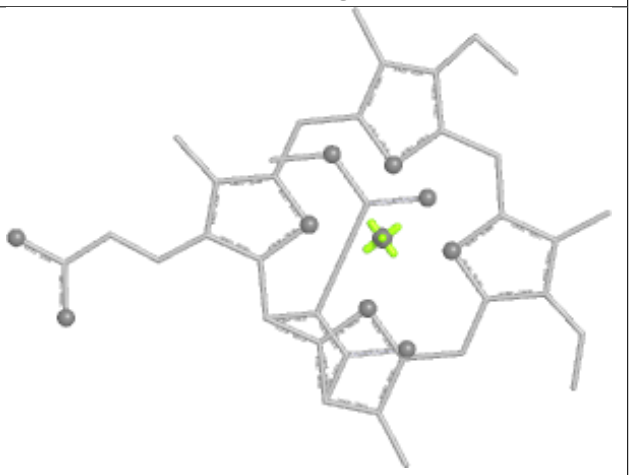
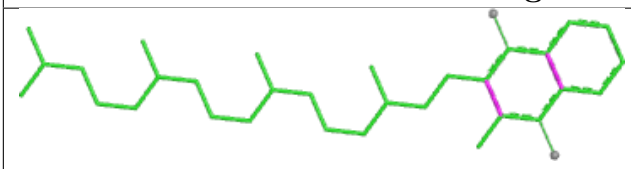


Rings

Ligand PQN b 729



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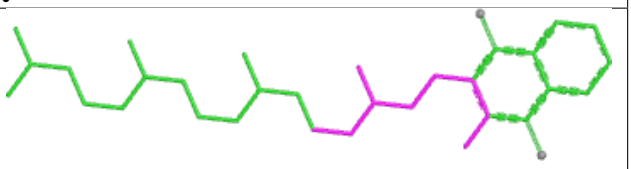
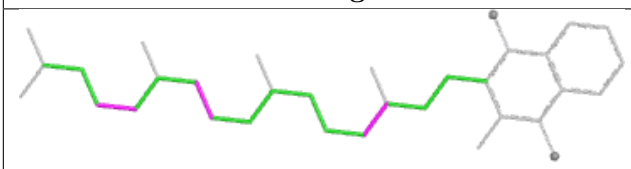


Bond angles



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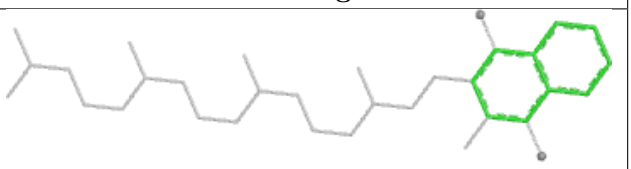
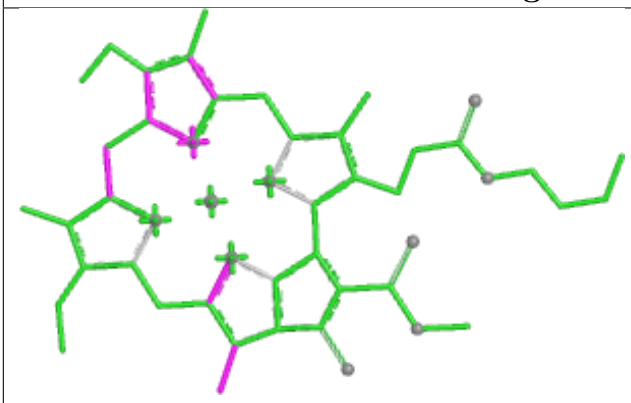
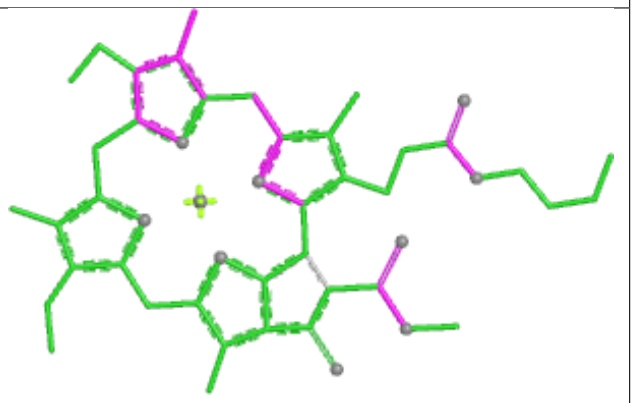


Rings

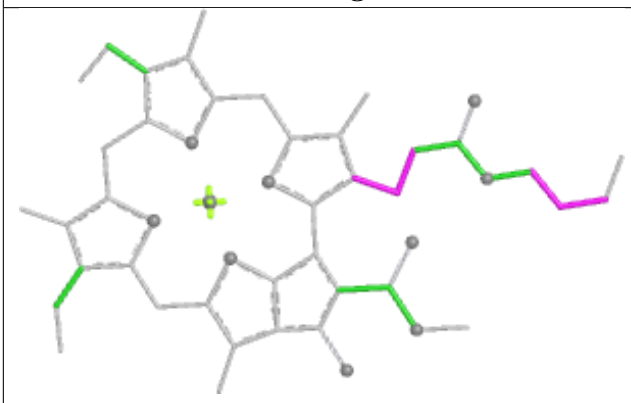
Ligand CLA G 520



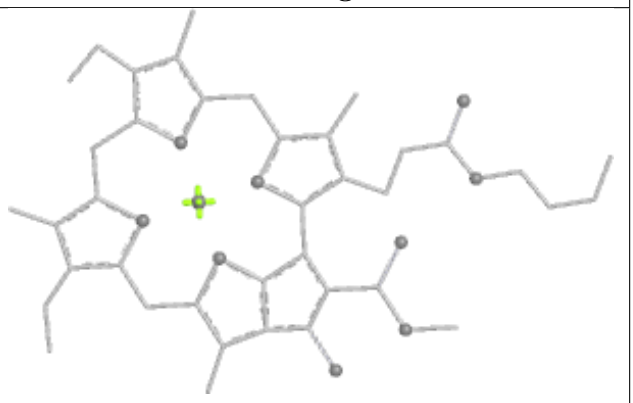
Bond lengths



Bond angles

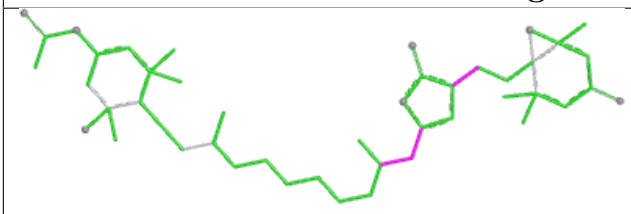


Torsions

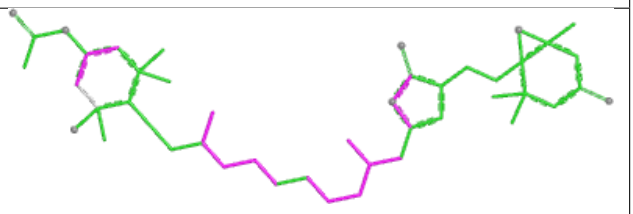


Rings

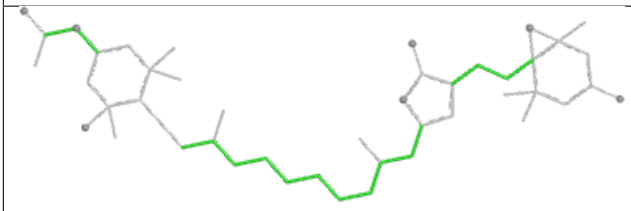
Ligand PID G 507



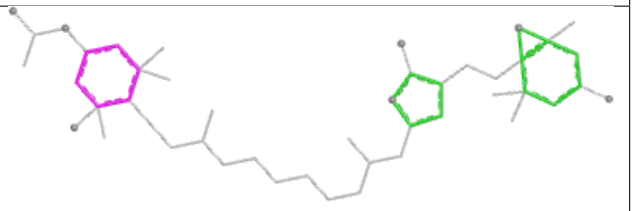
Bond lengths



Bond angles

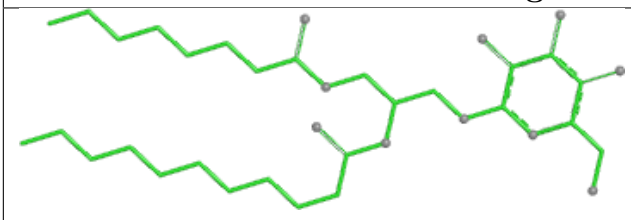


Torsions

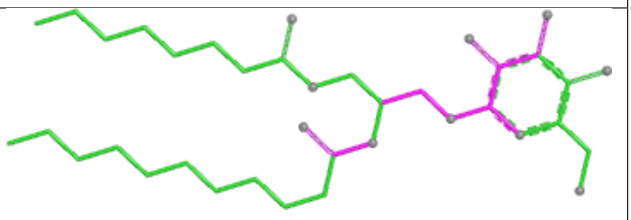


Rings

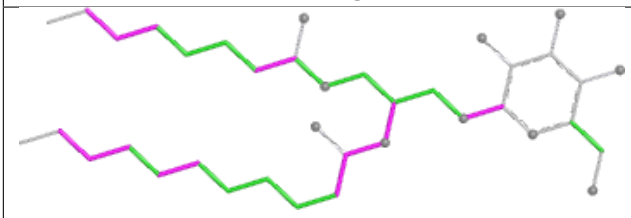
Ligand LMG I 320



Bond lengths



Bond angles



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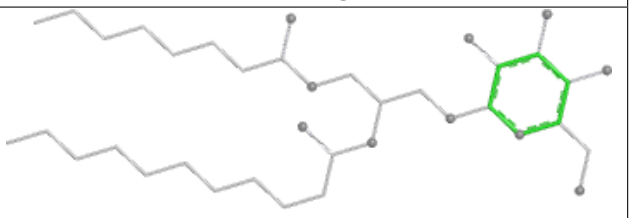
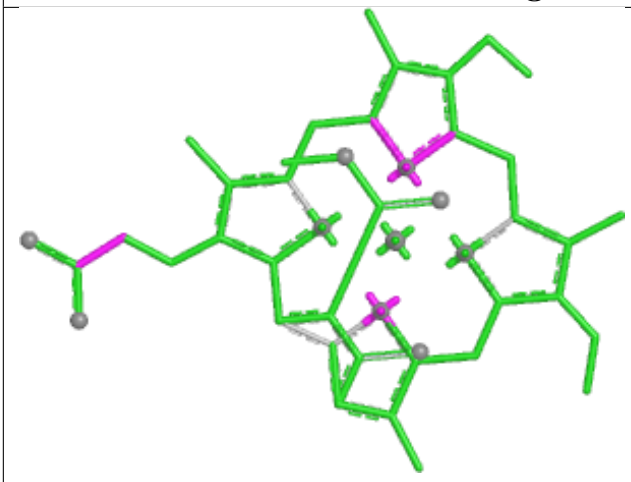


Rings

Ligand KC1 O 315



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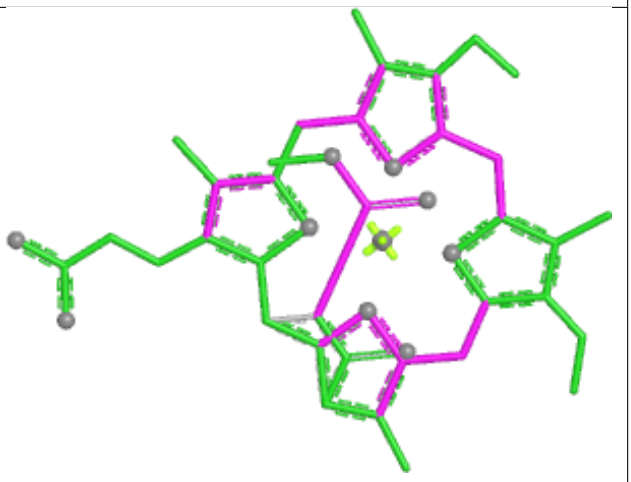
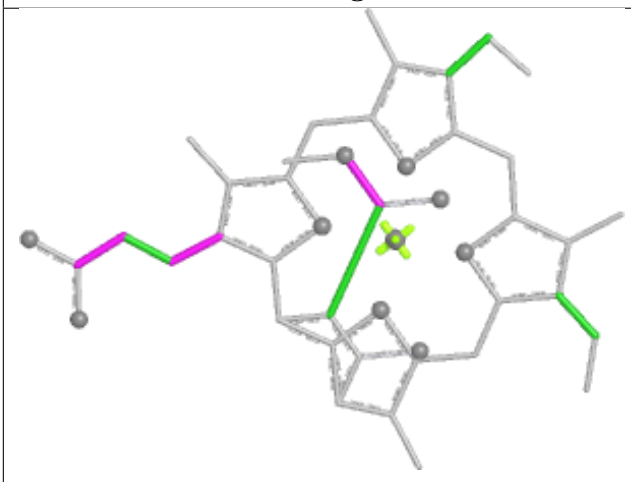
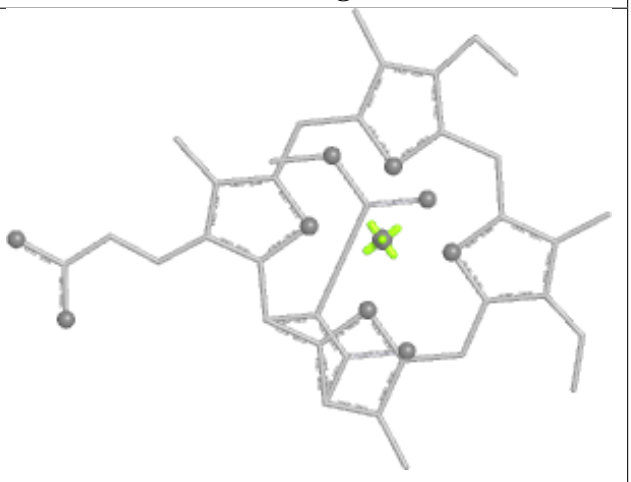


Bond angles

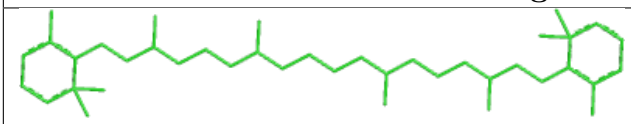


Torsions



Rings

Ligand BCR l 302



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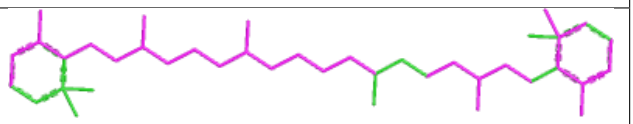
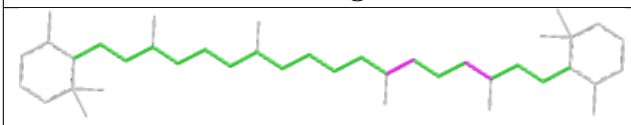


Bond angles



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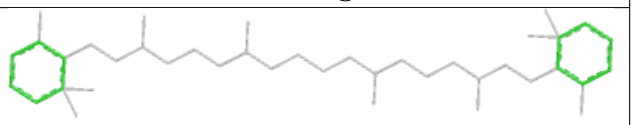
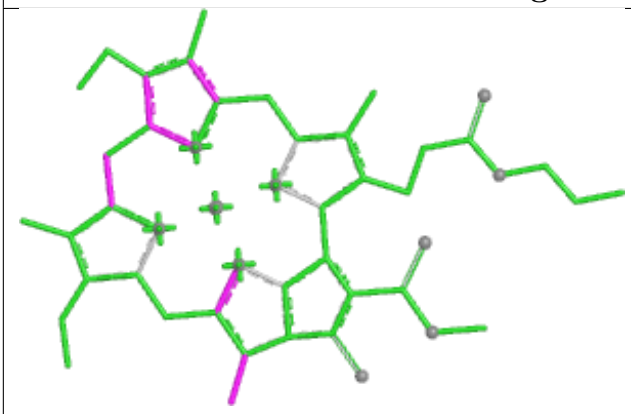


Rings

Ligand CLA I 310



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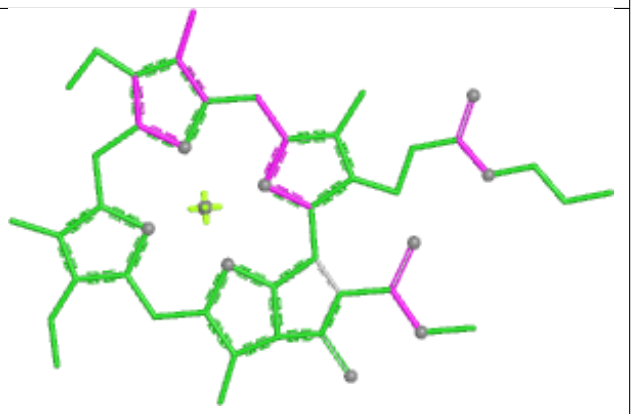
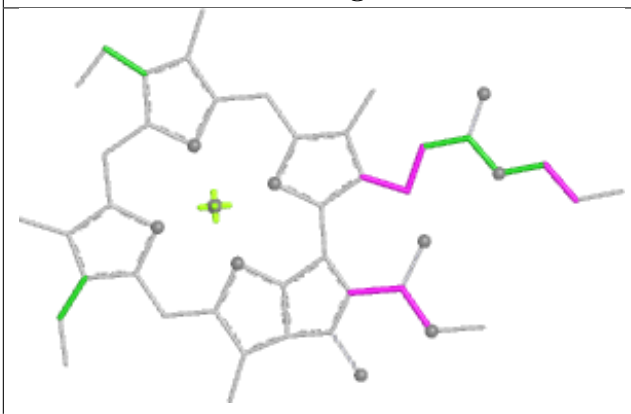


Bond angles



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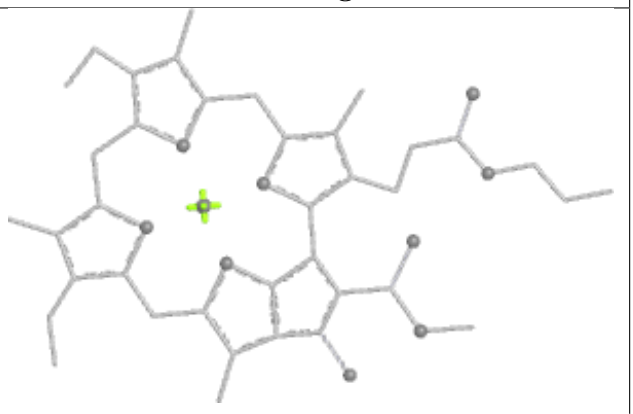
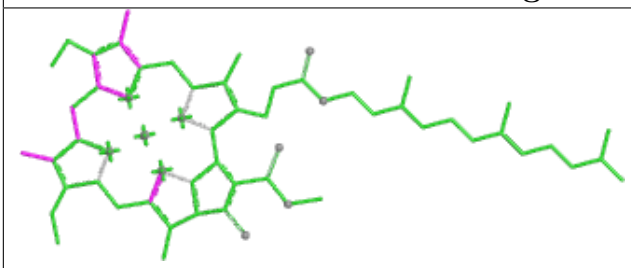
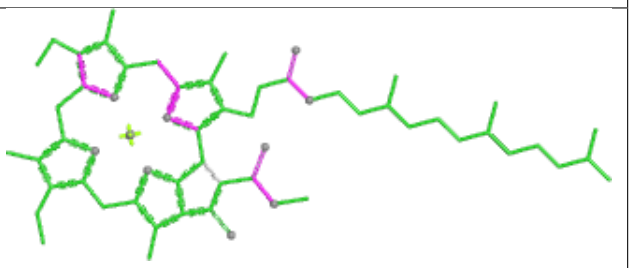
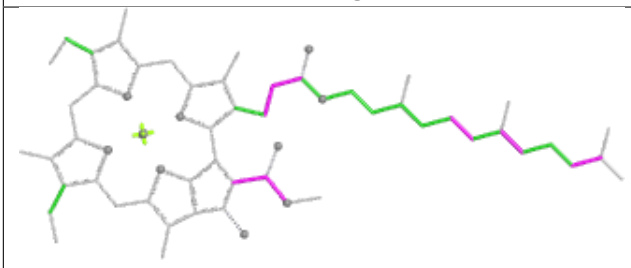
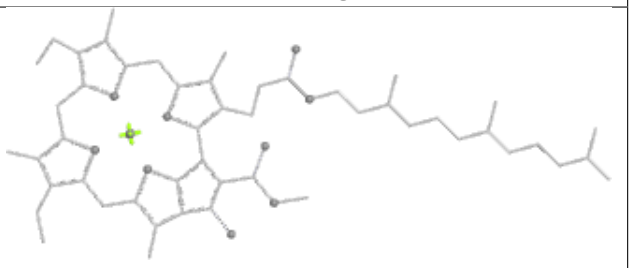
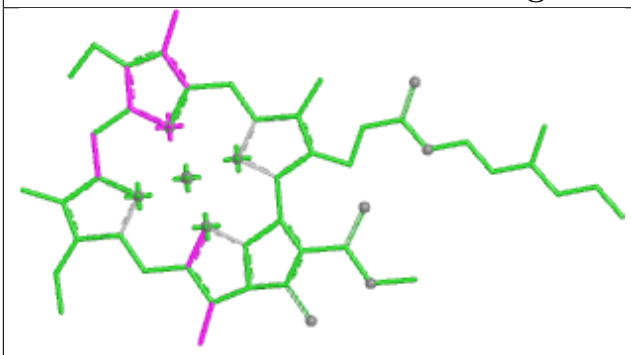
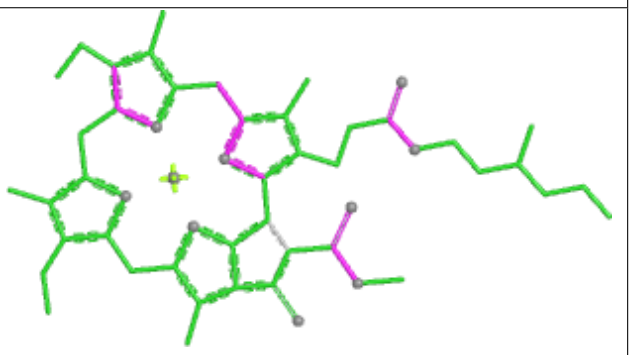
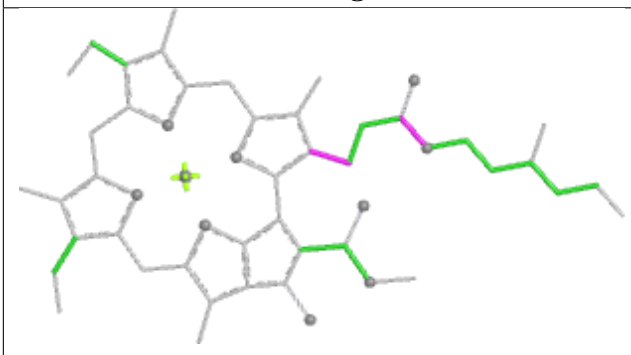
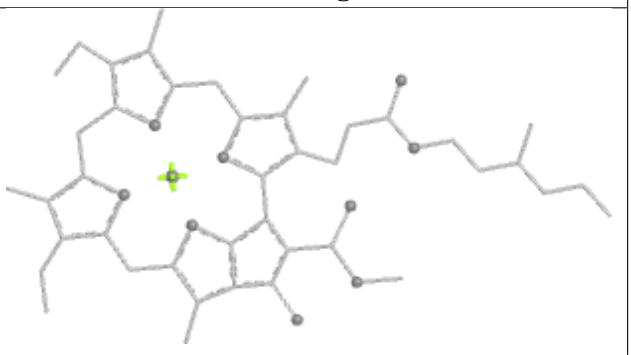
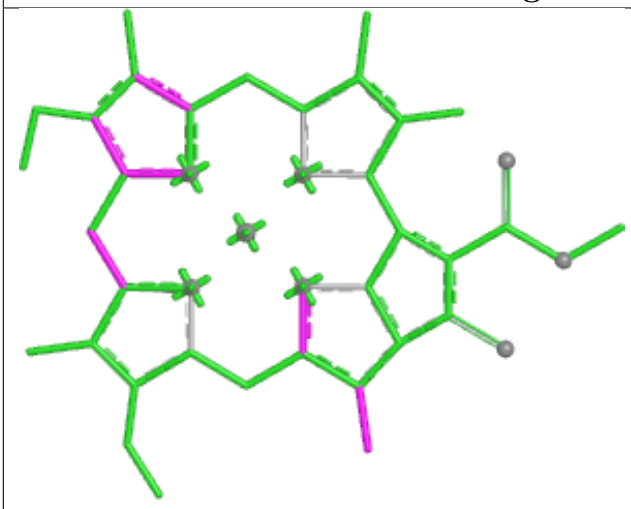


Rings

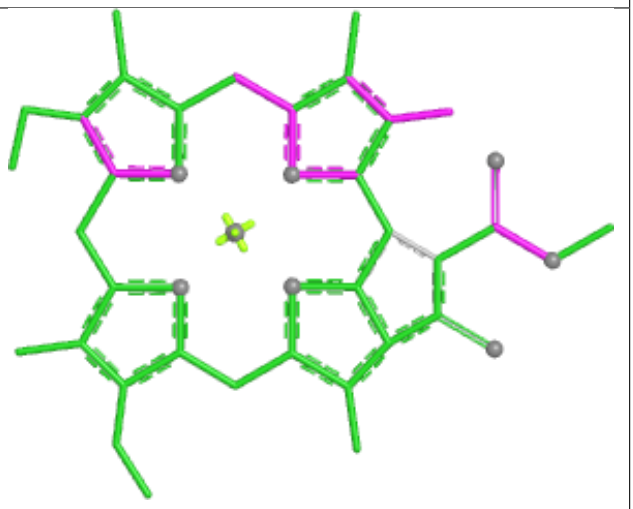
Ligand CLA G 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 710	
	
Bond lengths	Bond angles
	
Torsions	Rings

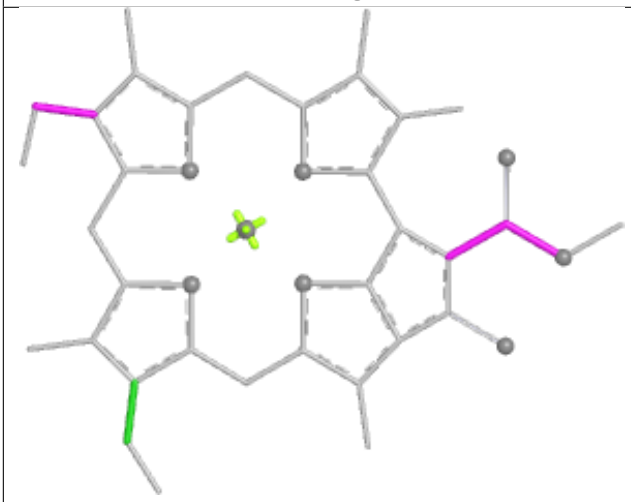
Ligand CLA G 516



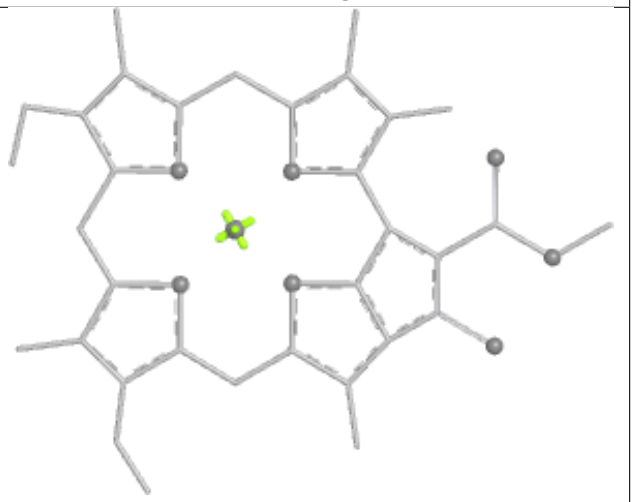
Bond lengths



Bond angles

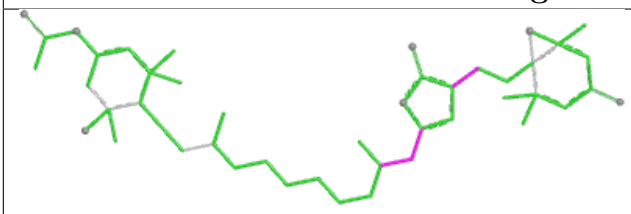


Torsions

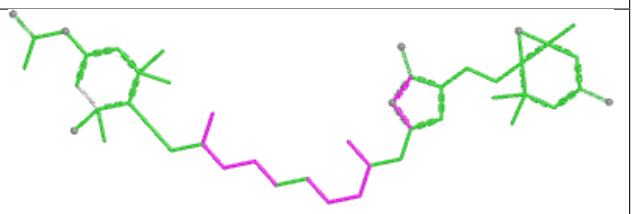


Rings

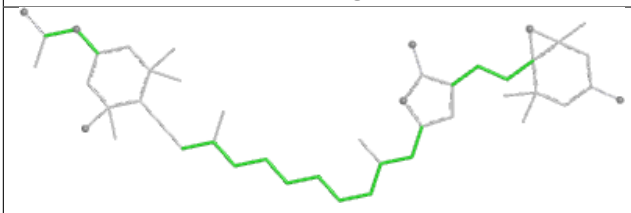
Ligand PID F 306



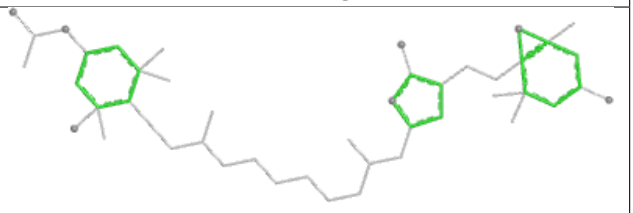
Bond lengths



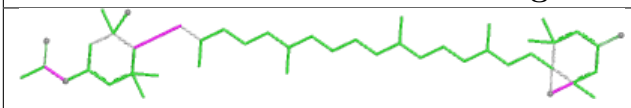
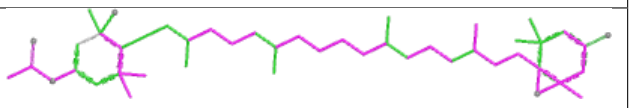
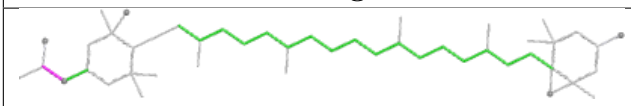
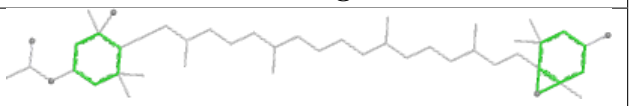
Bond angles

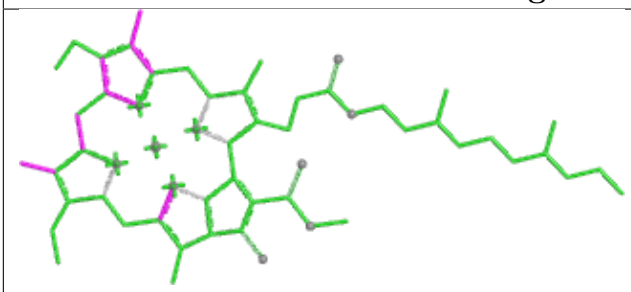
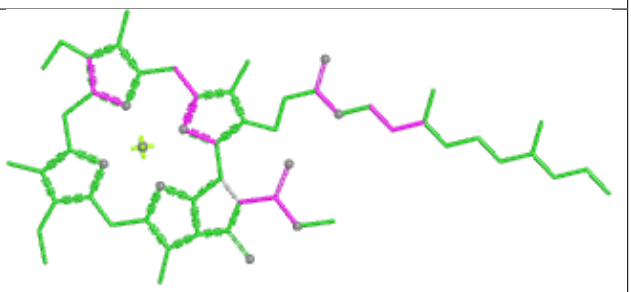
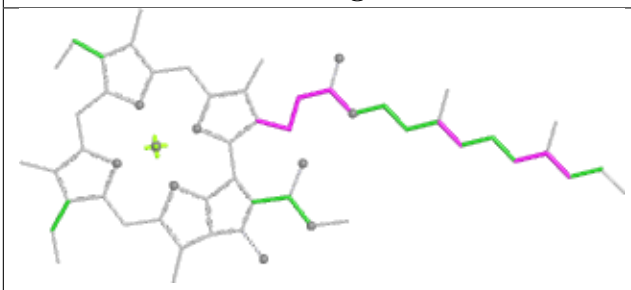
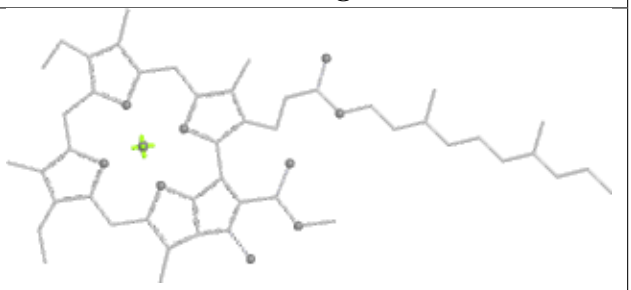


Torsions

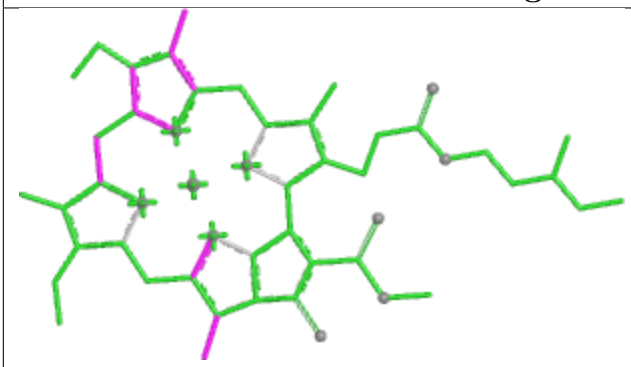


Rings

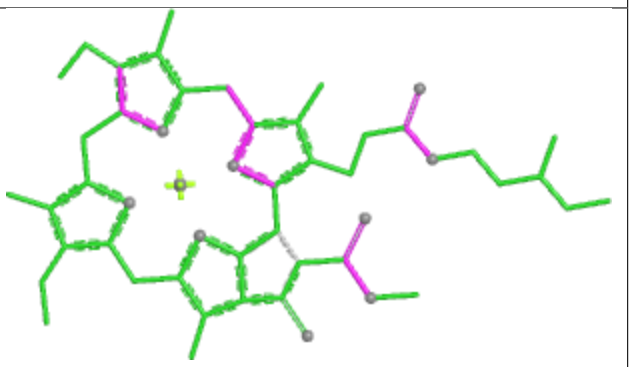
Ligand UIX h 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 717	
 Bond lengths	 Bond angles
 Torsions	 Rings

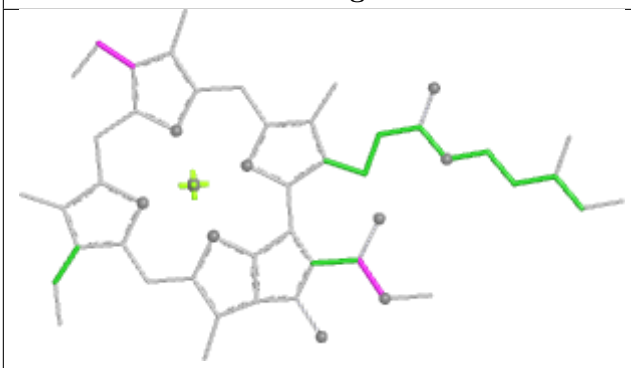
Ligand CLA B 312



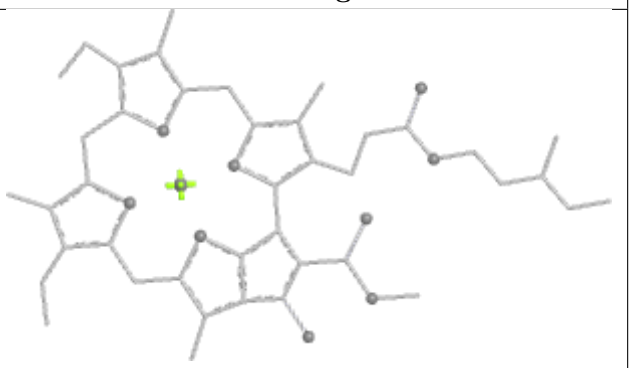
Bond lengths



Bond angles

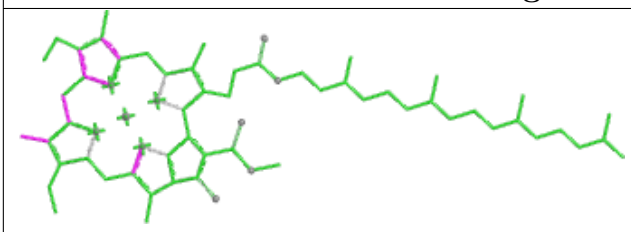


Torsions

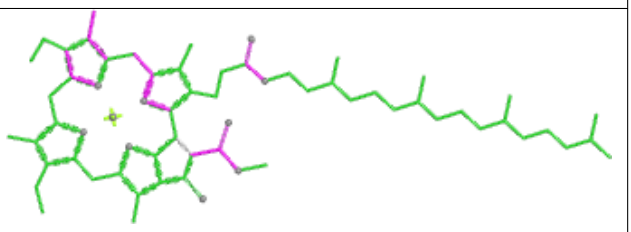


Rings

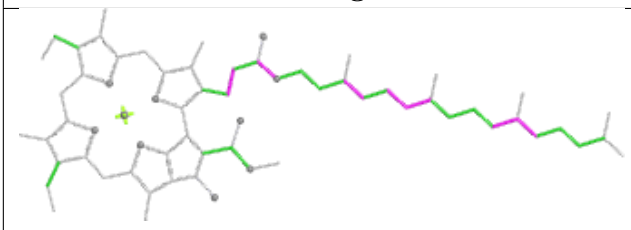
Ligand CLA G 510



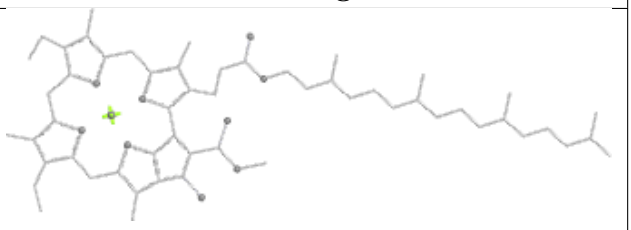
Bond lengths



Bond angles

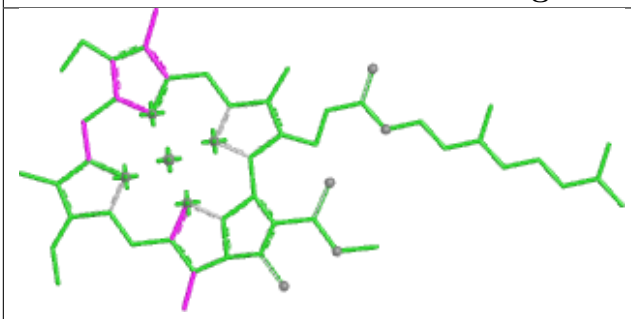


Torsions

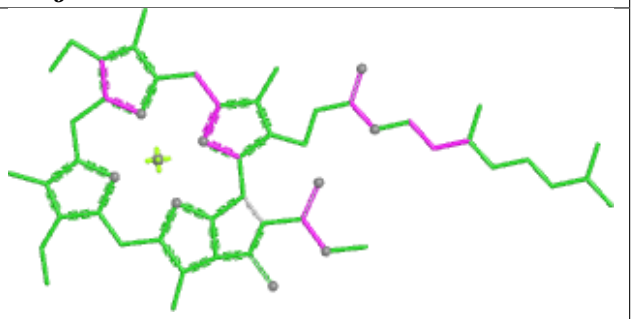


Rings

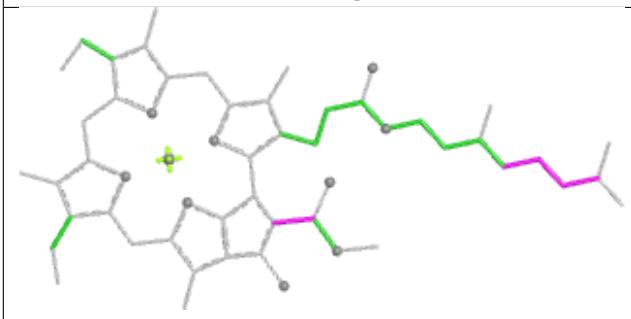
Ligand CLA j 104



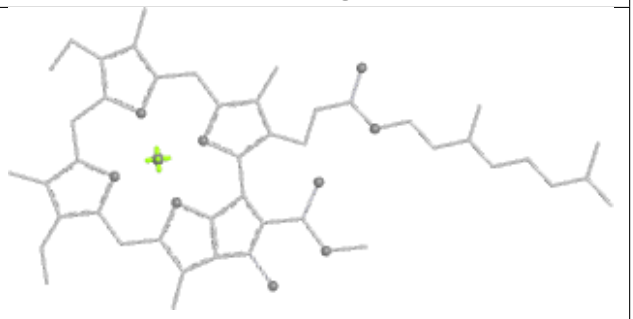
Bond lengths



Bond angles

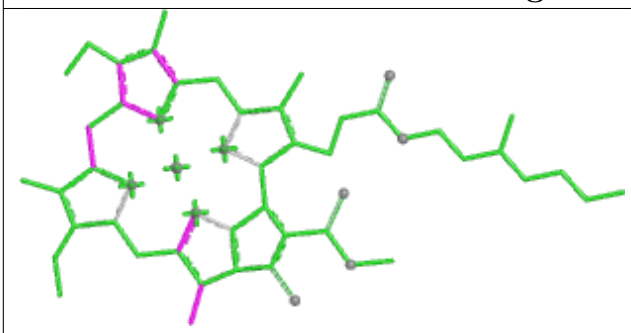


Torsions

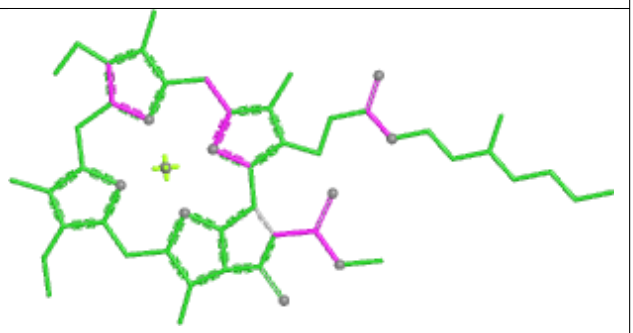


Rings

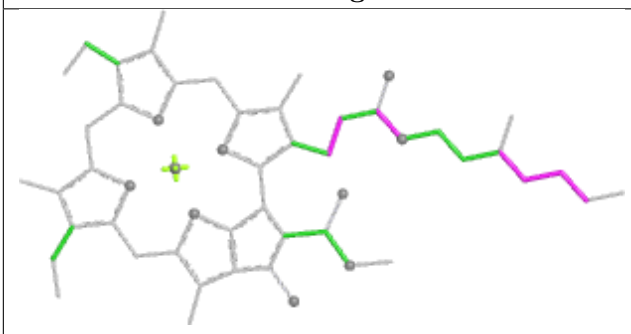
Ligand CLA L 309



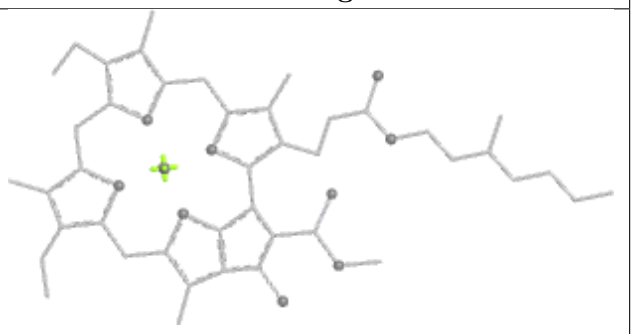
Bond lengths



Bond angles

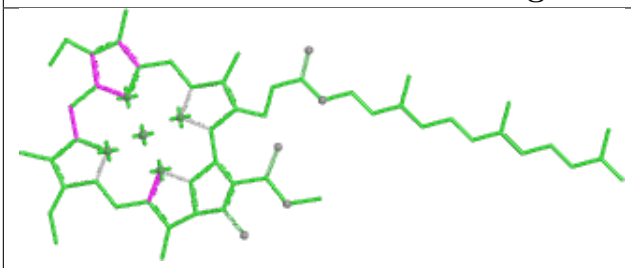


Torsions

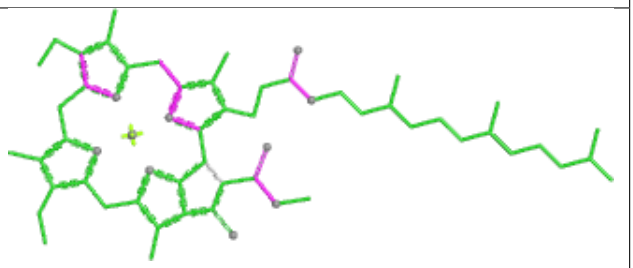


Rings

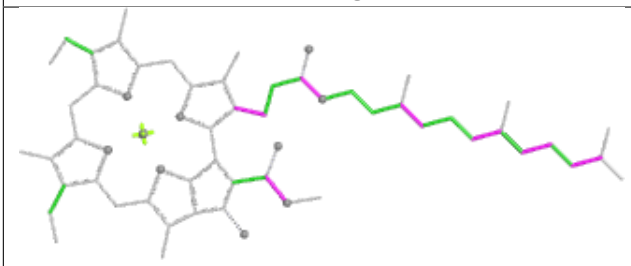
Ligand CLA b 715



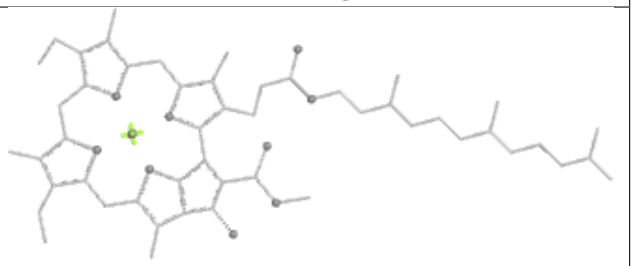
Bond lengths



Bond angles

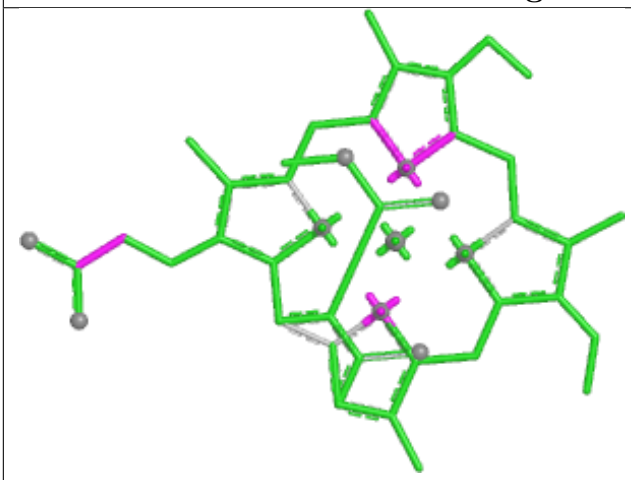


Torsions

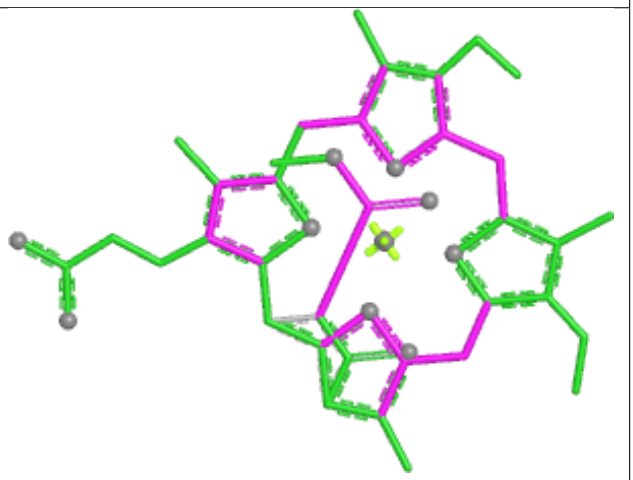


Rings

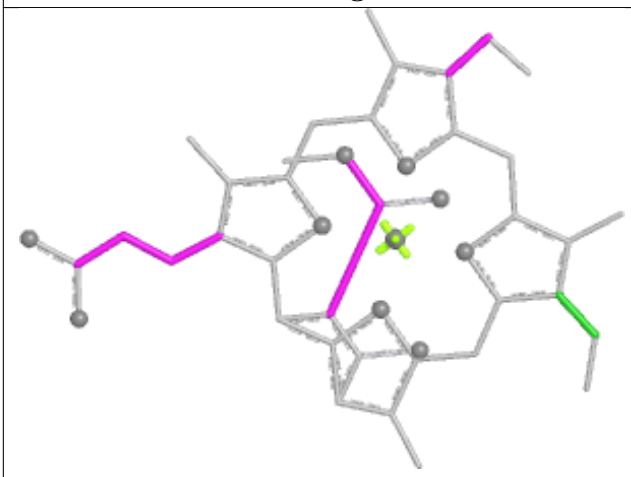
Ligand KC1 O 312



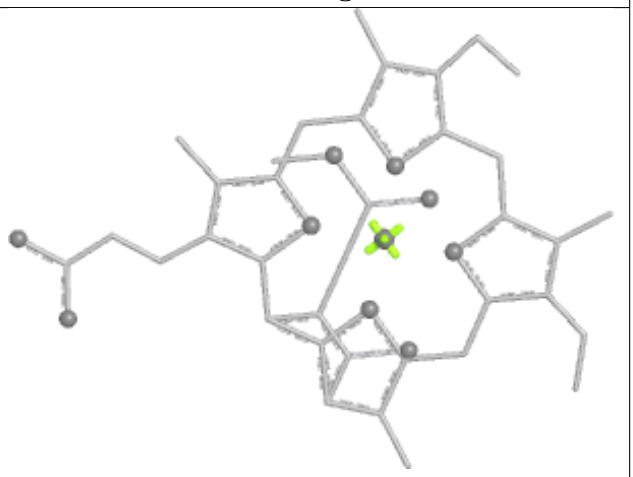
Bond lengths



Bond angles

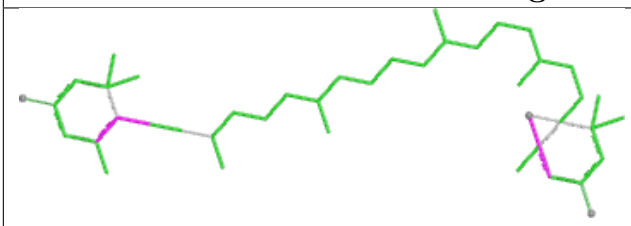


Torsions



Rings

Ligand DD6 J 304



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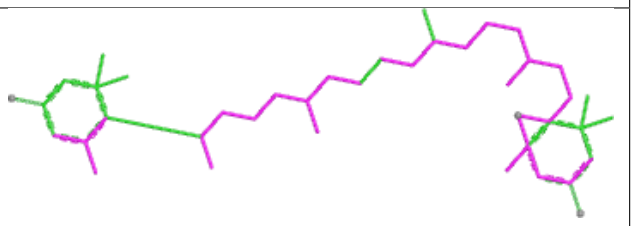
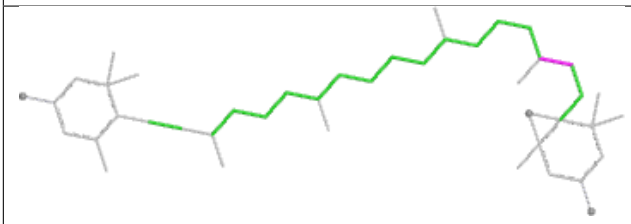


Bond angles



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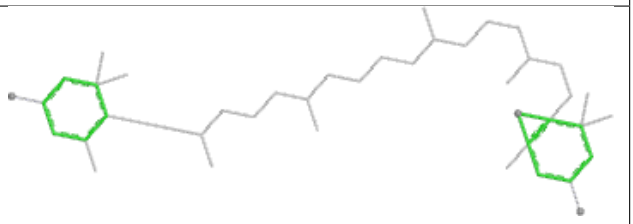
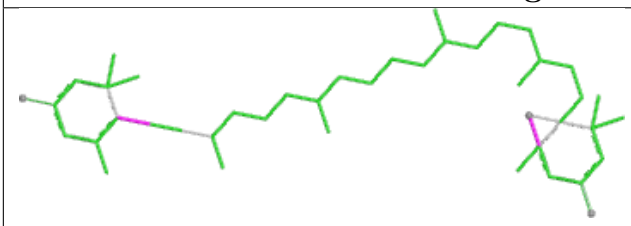


Rings

Ligand DD6 A 303



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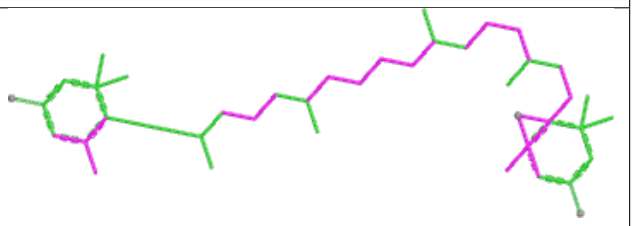
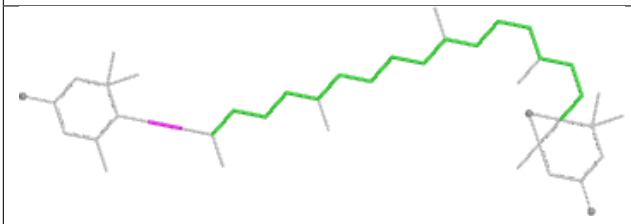


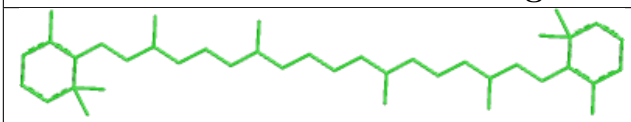
Bond angles



Torsions

Rings

Ligand BCR b 702



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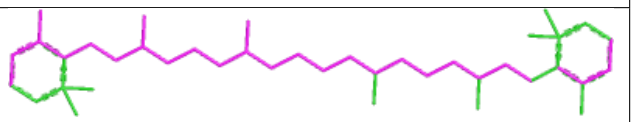
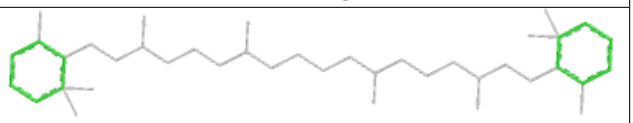


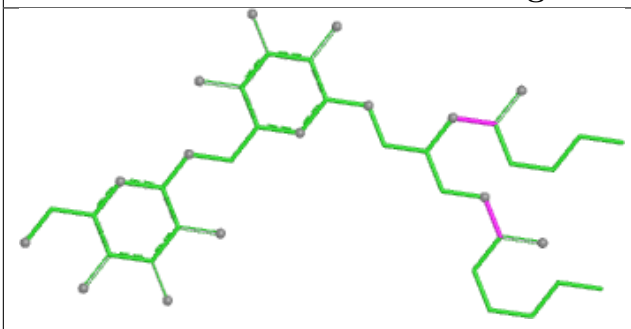
Bond angles

Torsions



Rings

Ligand DGD j 103



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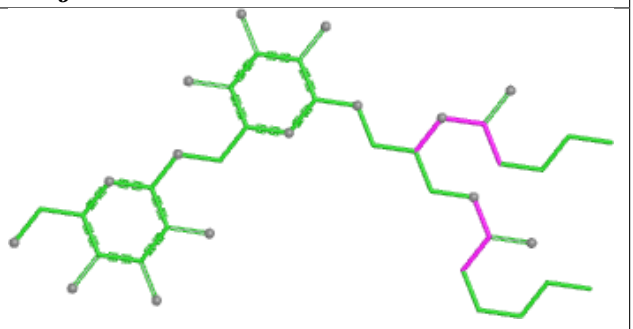
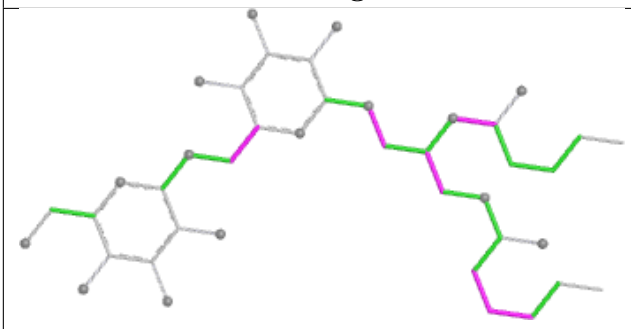


Bond angles



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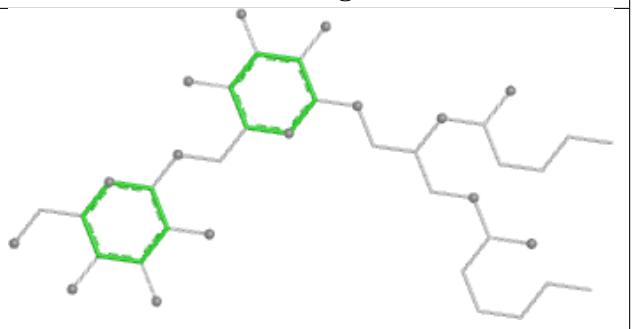
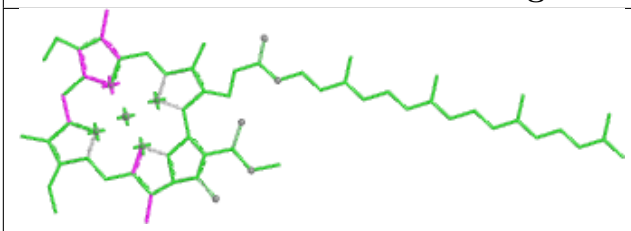
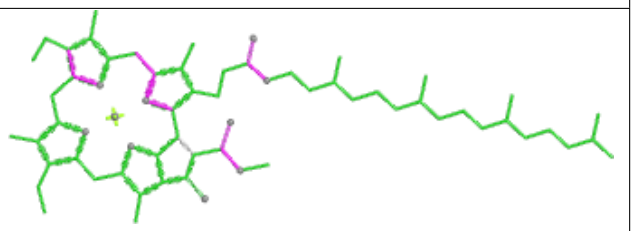


Rings

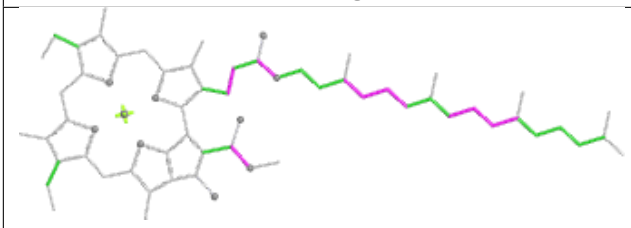
Ligand CLA b 701



Bond lengths



Bond angles



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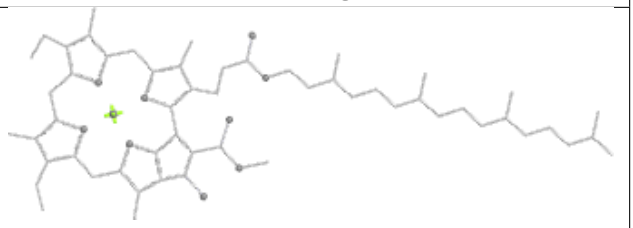
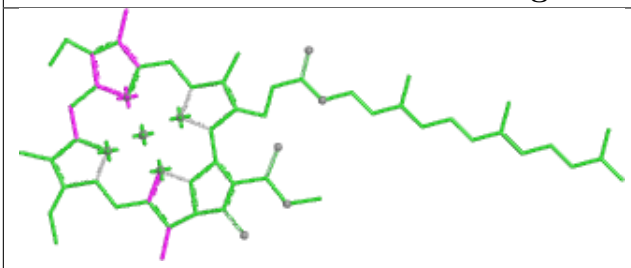


Rings

Ligand CLA I 308



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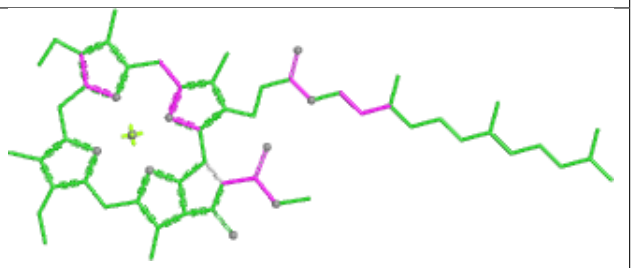
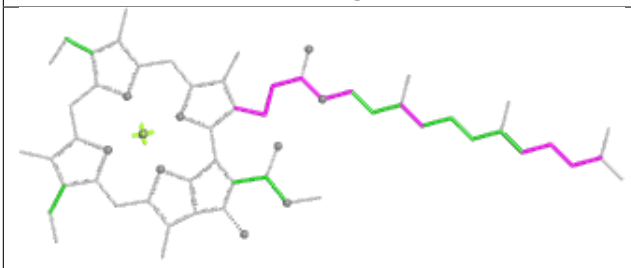


Bond angles



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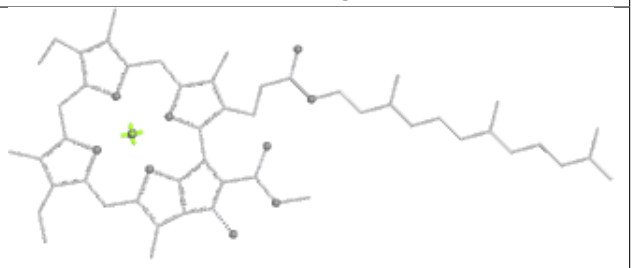
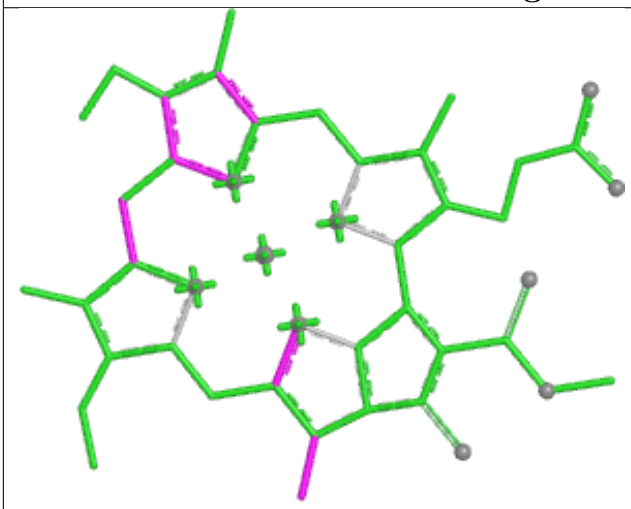
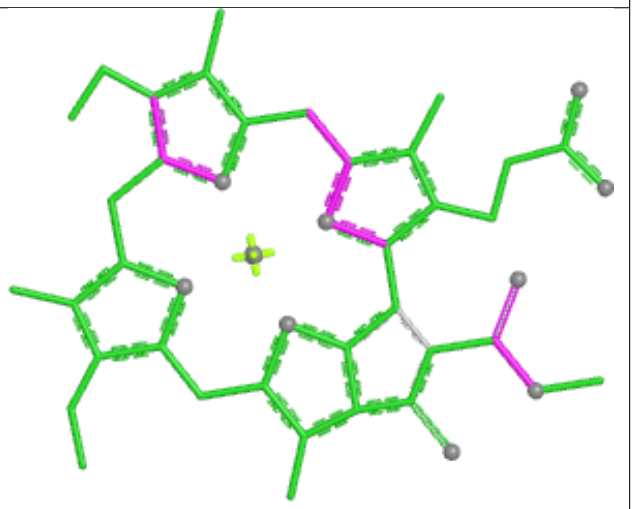


Rings

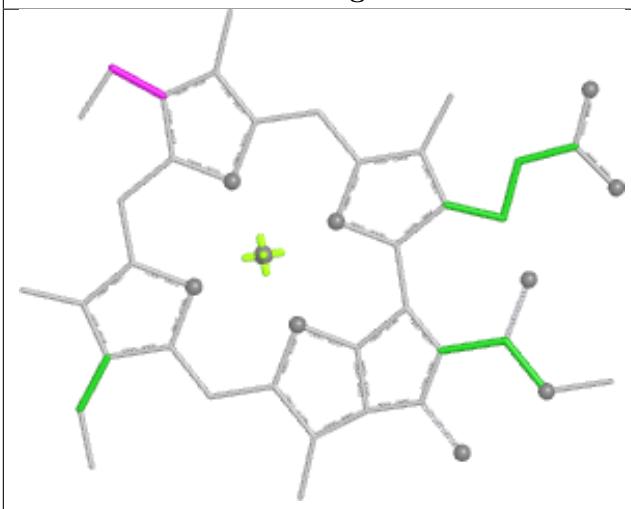
Ligand CLA A 307



Bond lengths



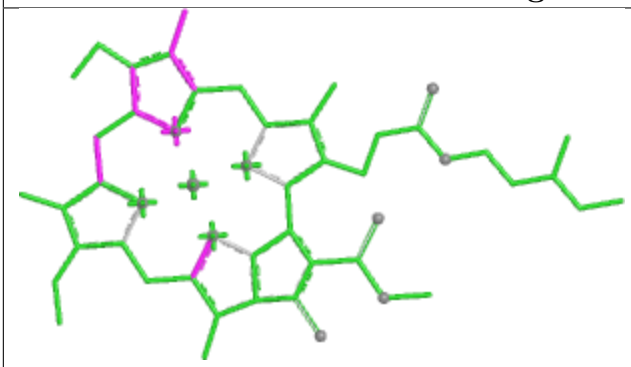
Bond angles



Torsions

Rings

Ligand CLA b 718



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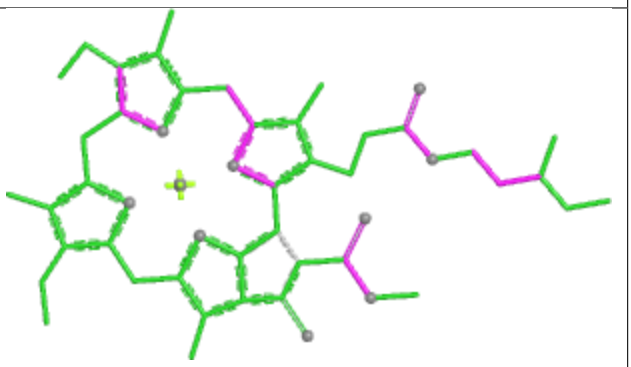
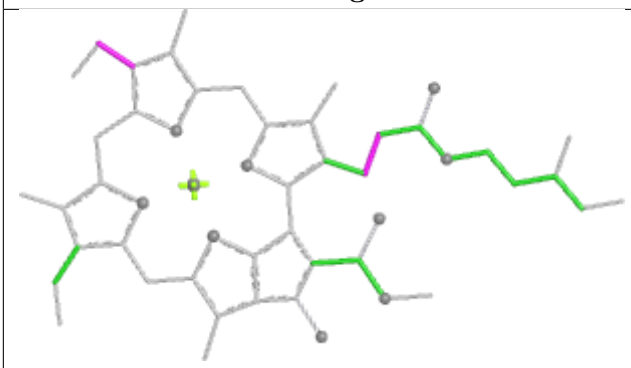


Bond angles



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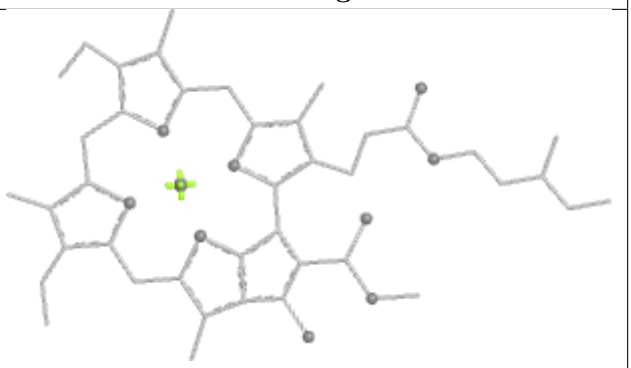
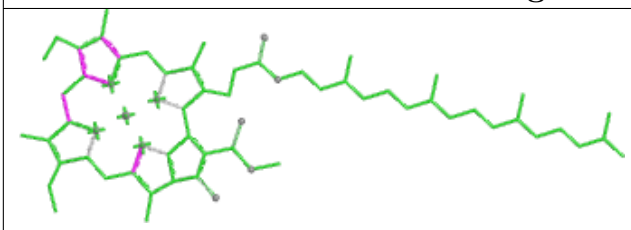


Rings

Ligand CLA b 707



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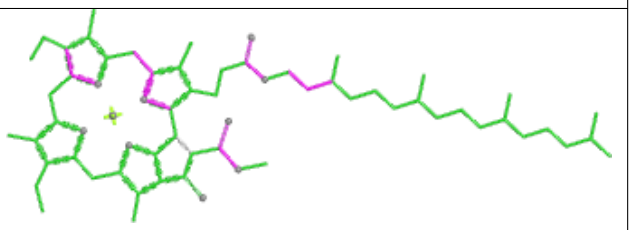
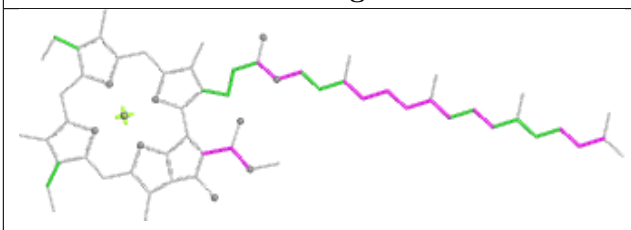


Bond angles



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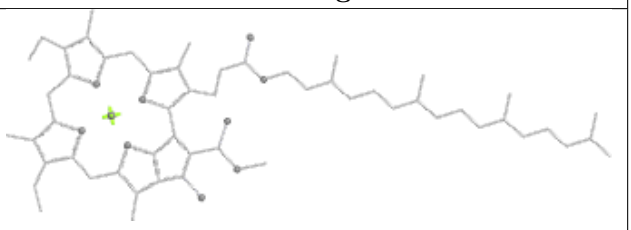
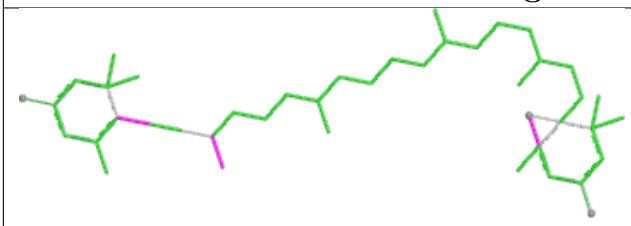


Rings

Ligand DD6 H 303



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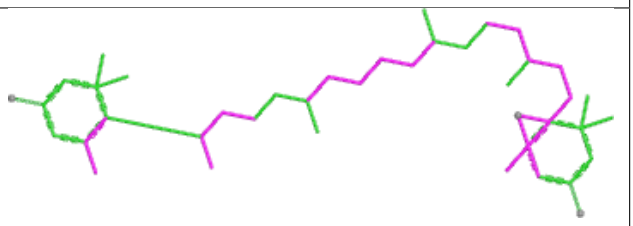
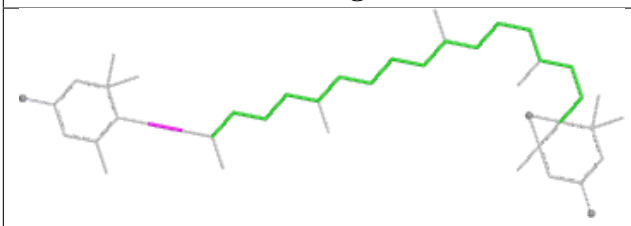


Bond angles



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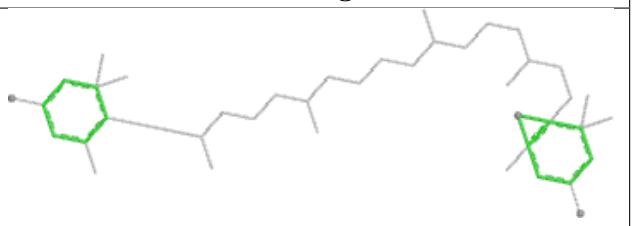
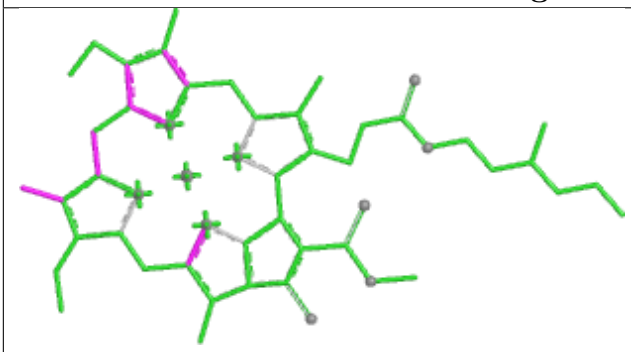


Rings

Ligand CLA I 321



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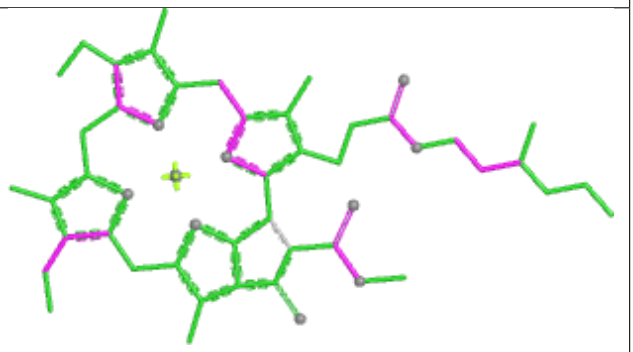
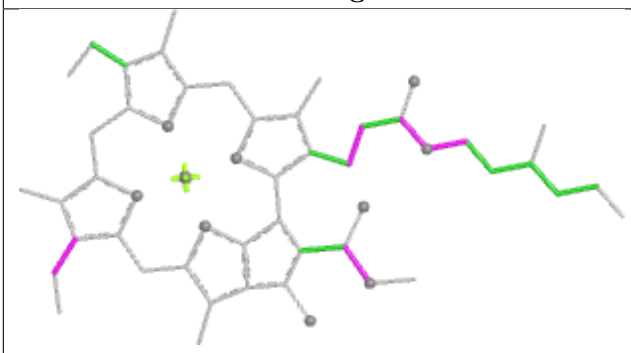


Bond angles



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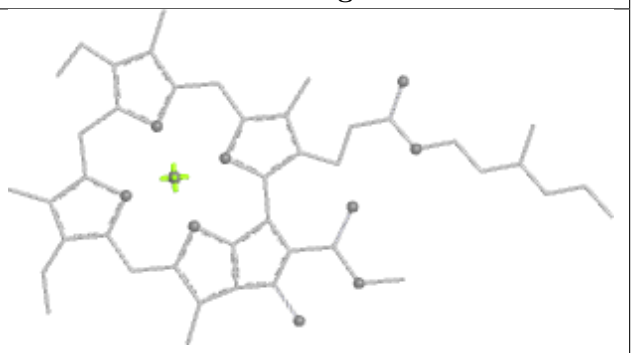
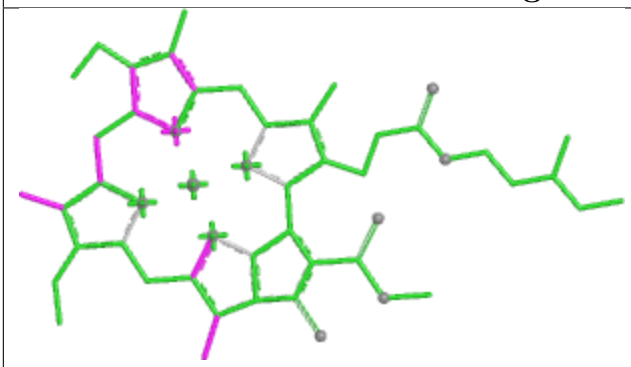
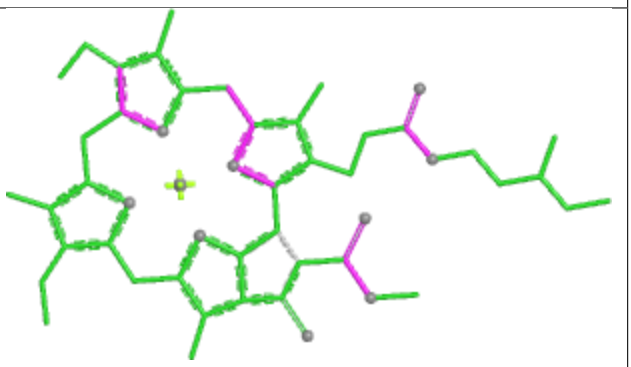


Rings

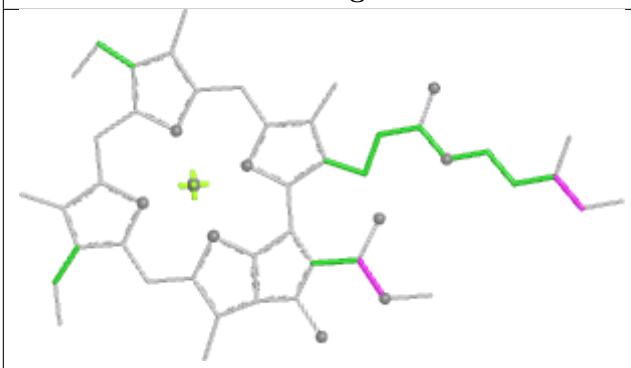
Ligand CLA N 307



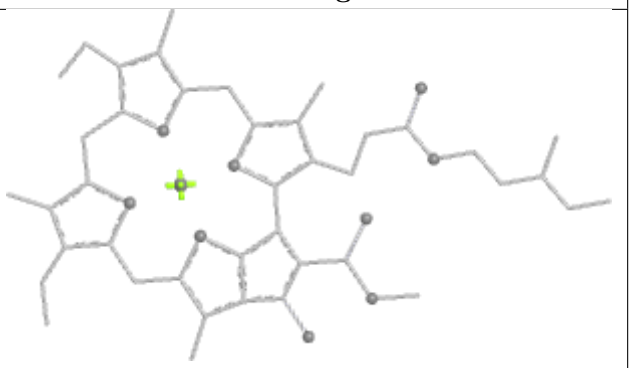
Bond lengths



Bond angles

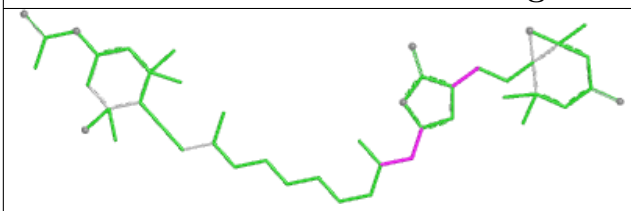


Torsions

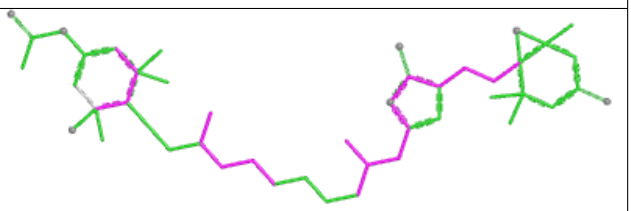


Rings

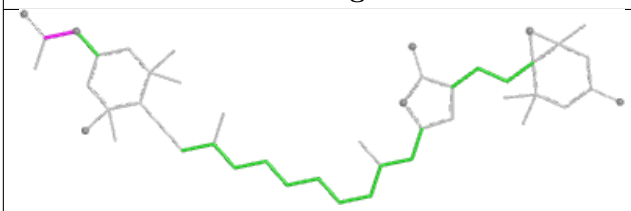
Ligand PID N 302



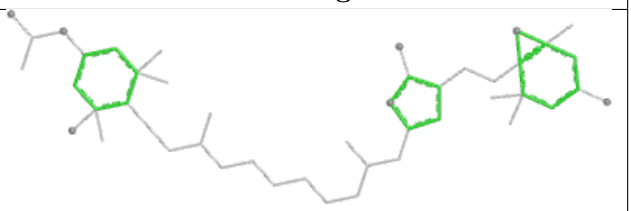
Bond lengths



Bond angles

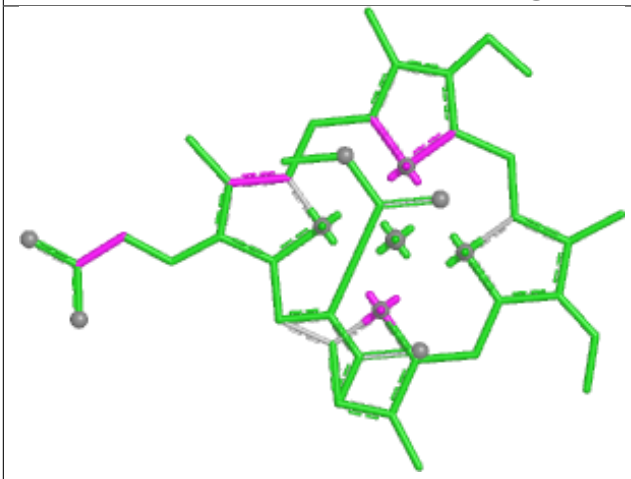


Torsions



Rings

Ligand KC1 F 309



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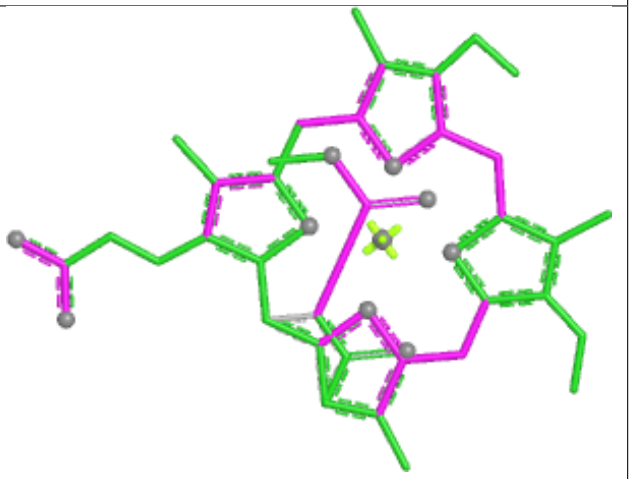
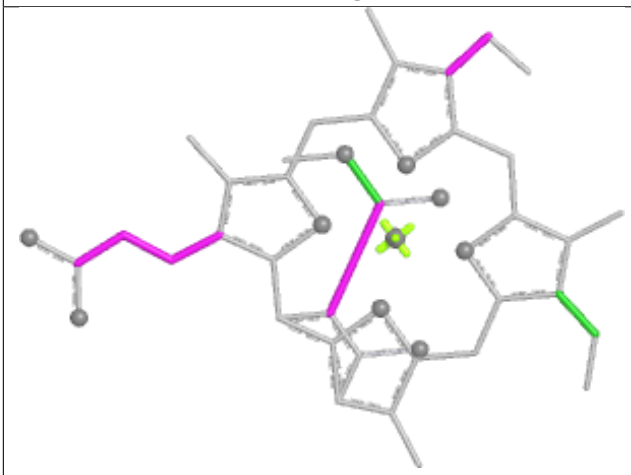


Bond angles



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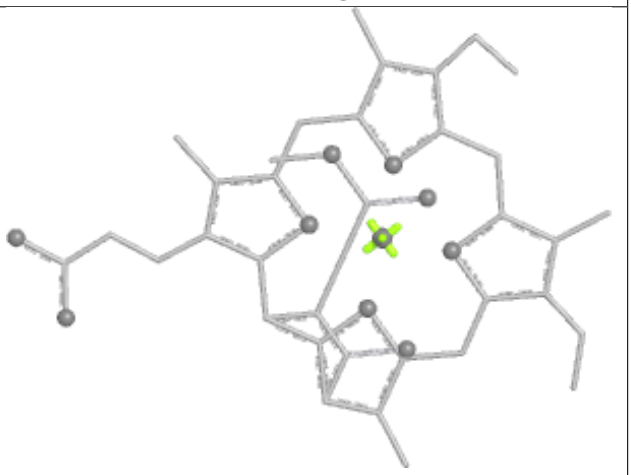


Rings

Ligand UIX O 306

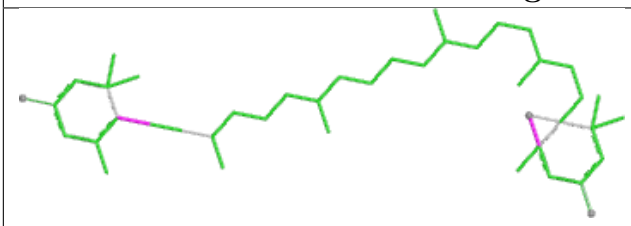
Bond lengths

Bond angles

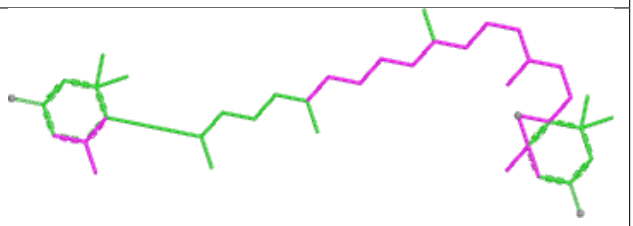
Torsions

Rings

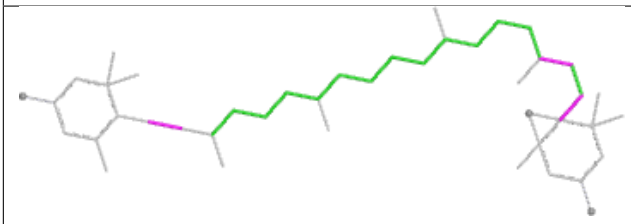
Ligand DD6 K 318



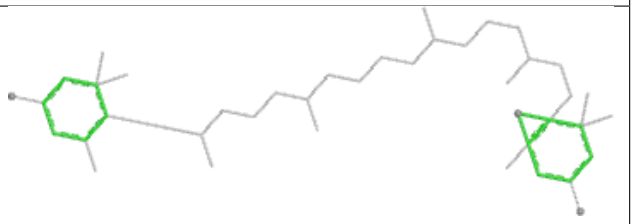
Bond lengths



Bond angles

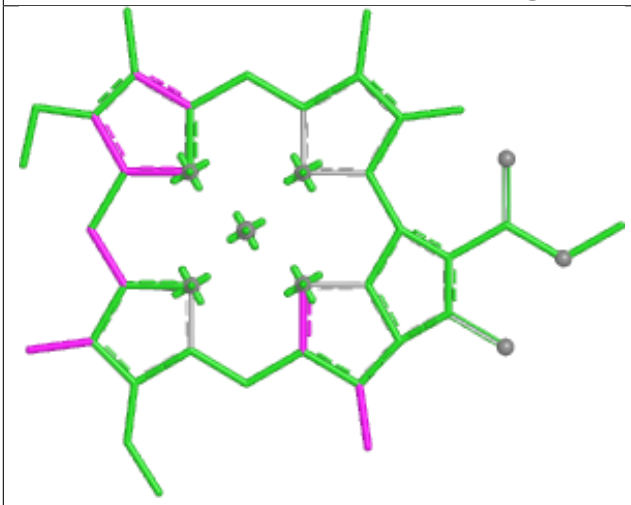


Torsions



Rings

Ligand CLA O 316



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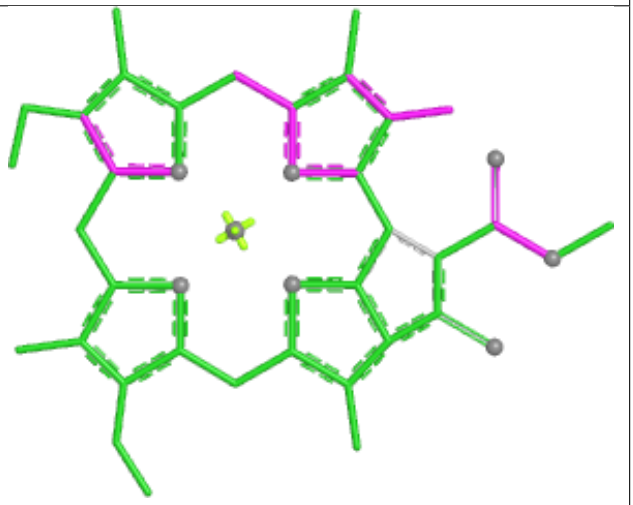
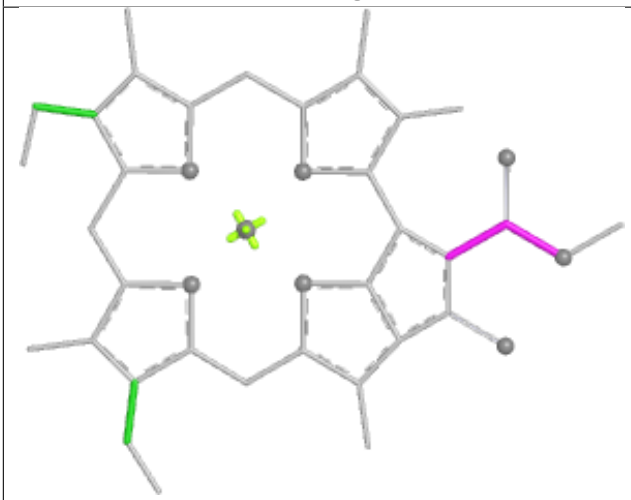


Bond angles



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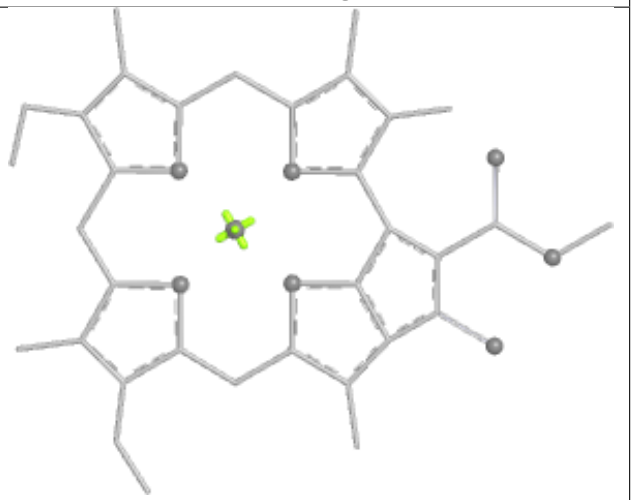
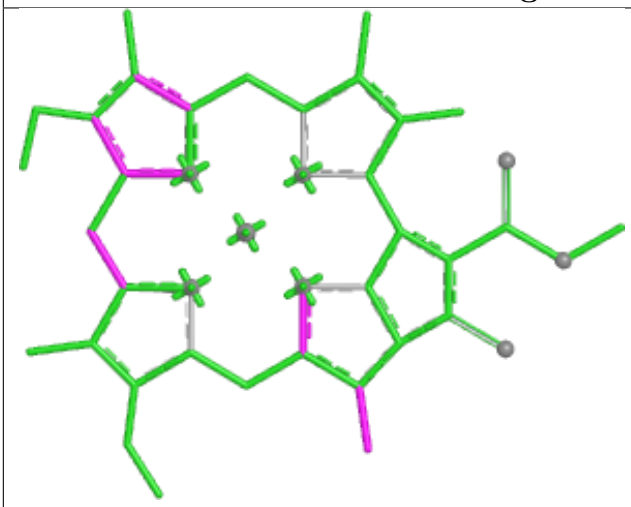


Rings

Ligand CLA M 315



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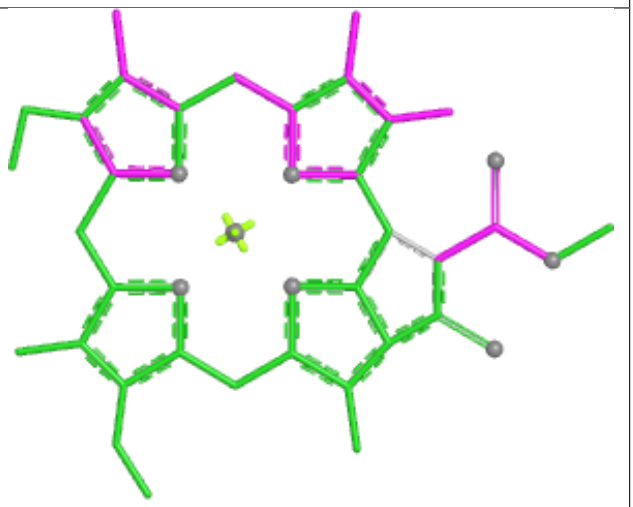
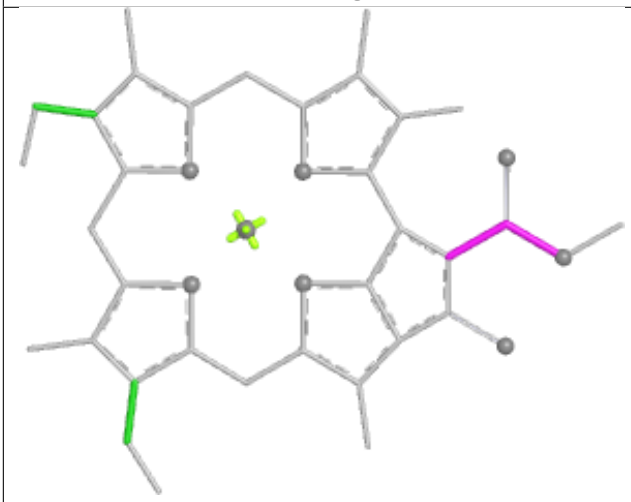
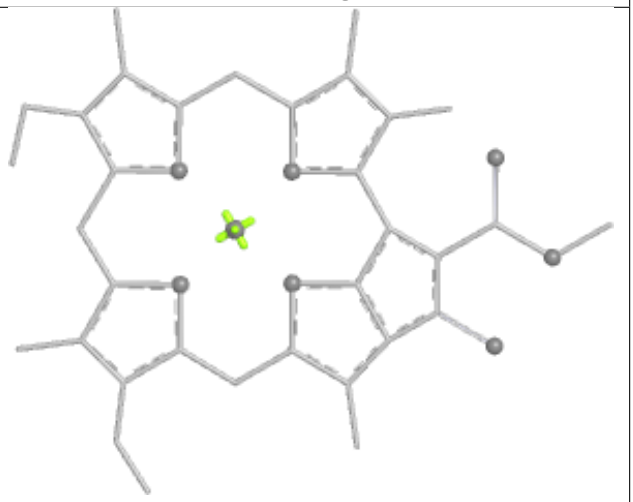


Bond angles

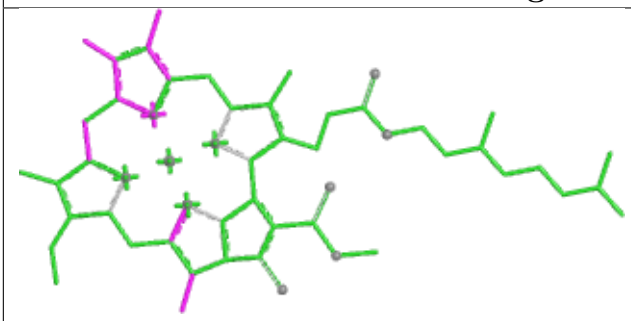


Torsions

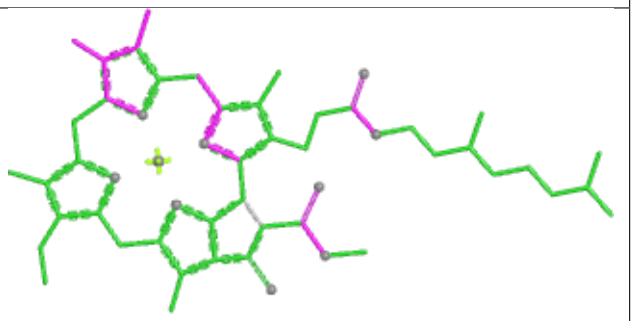


Rings

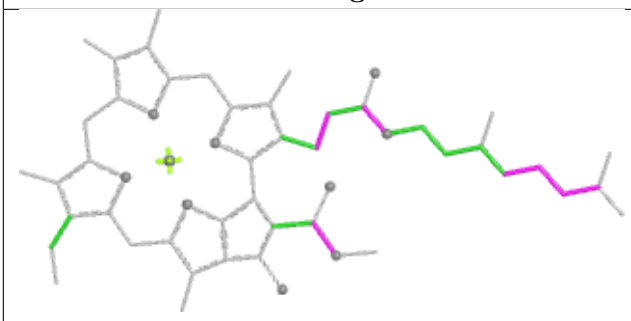
Ligand CLA b 712



Bond lengths



Bond angles



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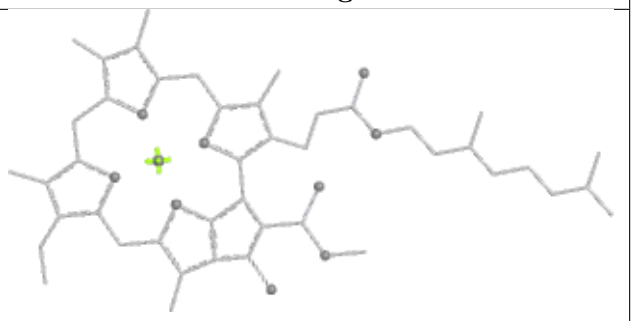
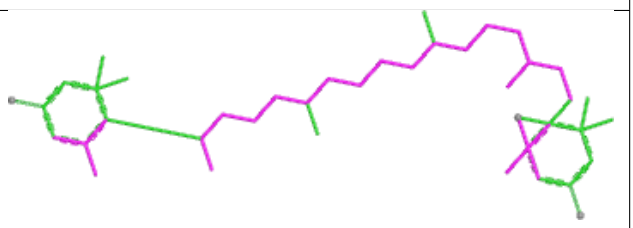


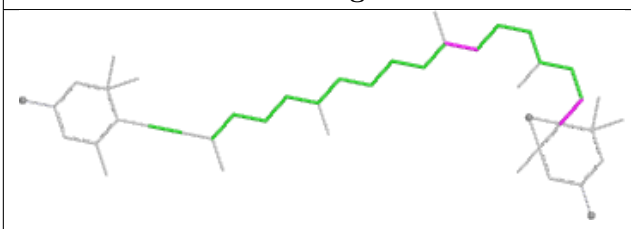
Rings

Ligand DD6 A 302

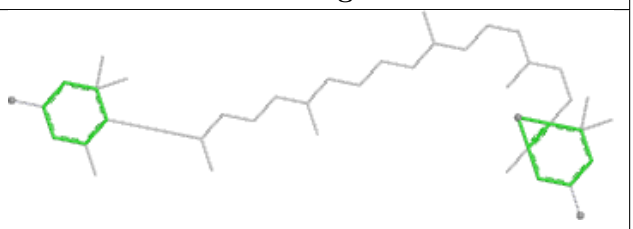
Bond lengths



Bond angles

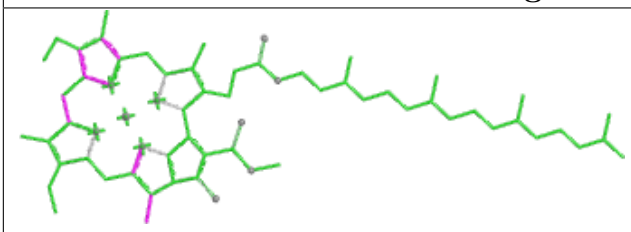


Torsions



Rings

Ligand CLA B 309



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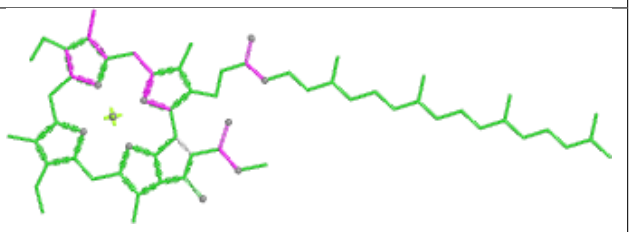

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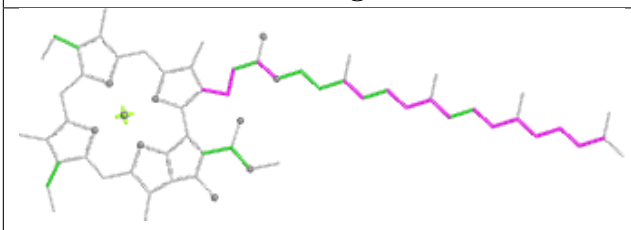

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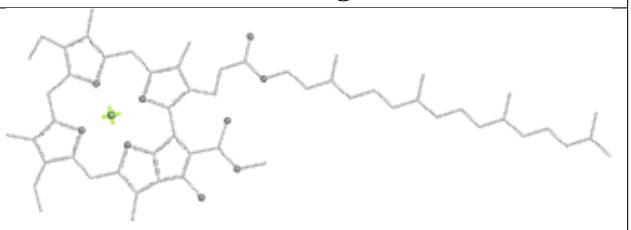
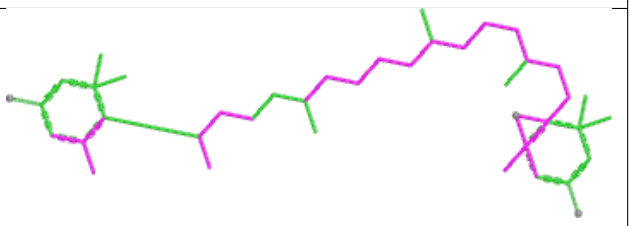


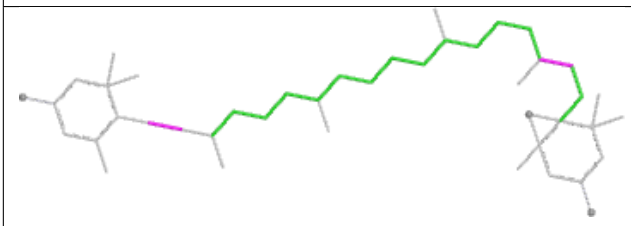
Rings

Ligand DD6 L 306

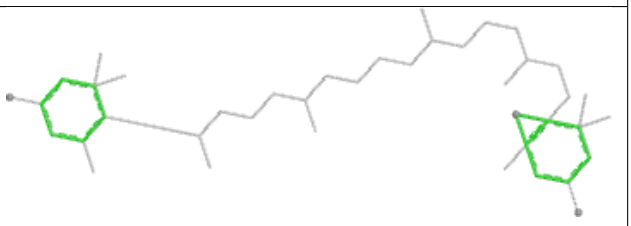
Bond lengths



Bond angles

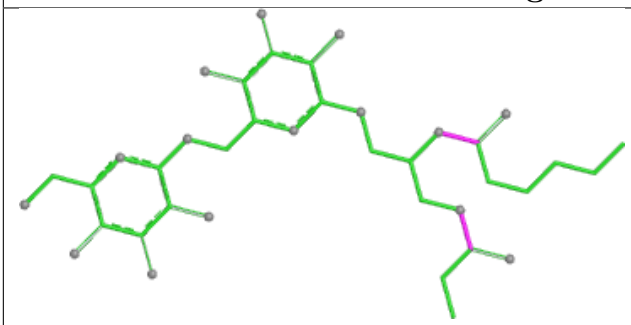


Torsions

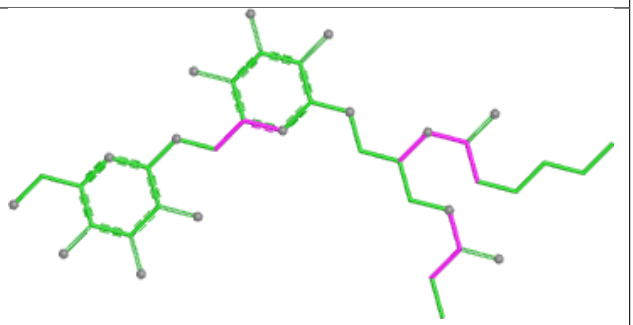


Rings

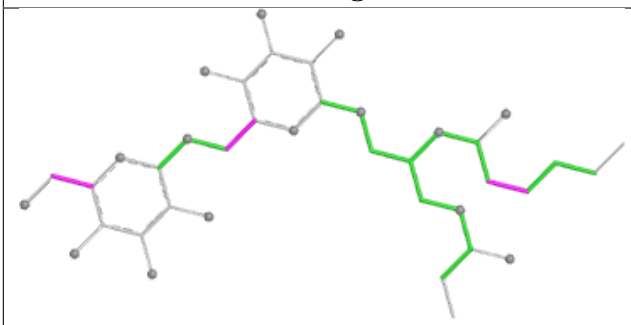
Ligand DGD I 317



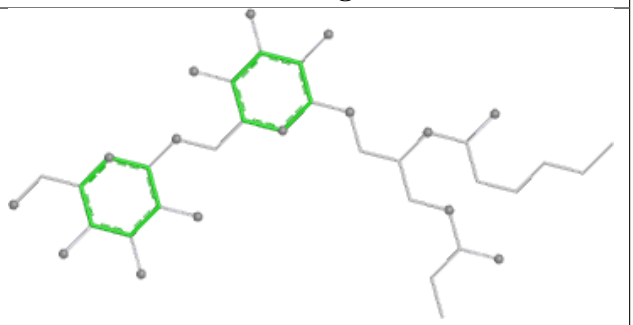
Bond lengths



Bond angles

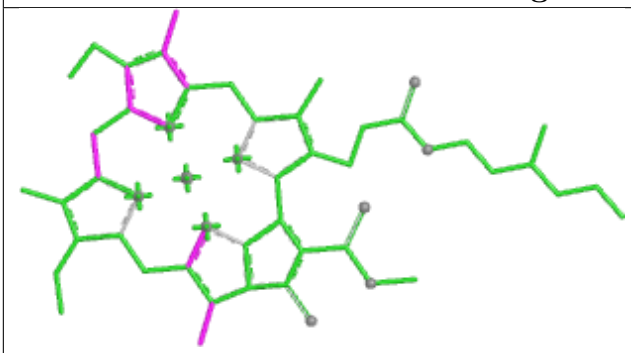


Torsions

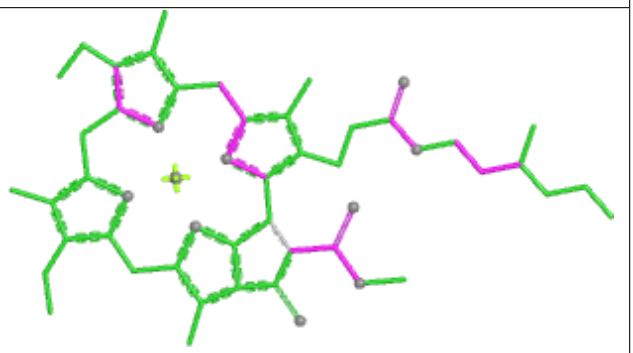


Rings

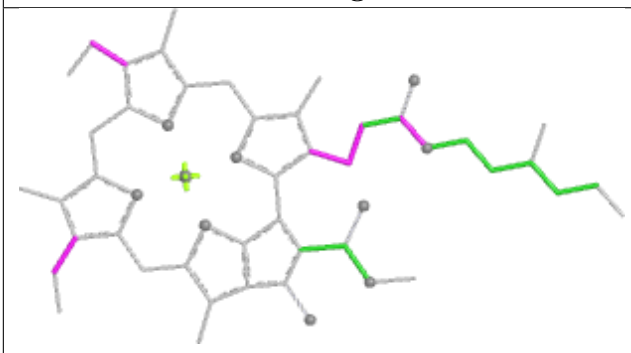
Ligand CLA I 315



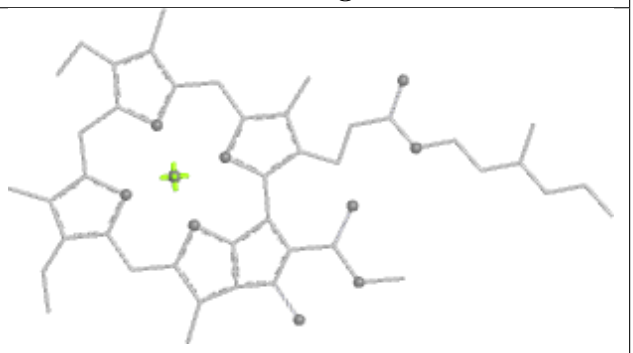
Bond lengths



Bond angles

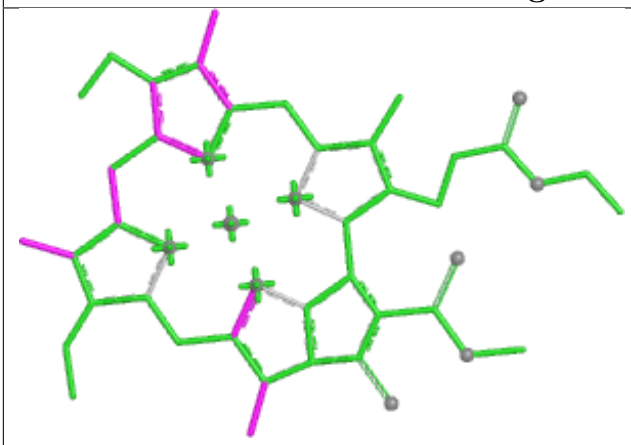


Torsions

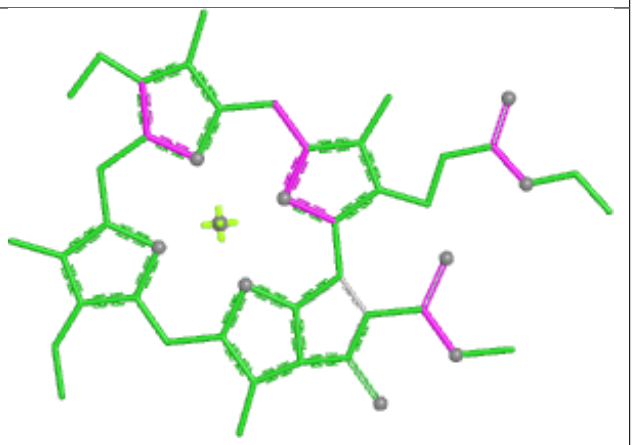


Rings

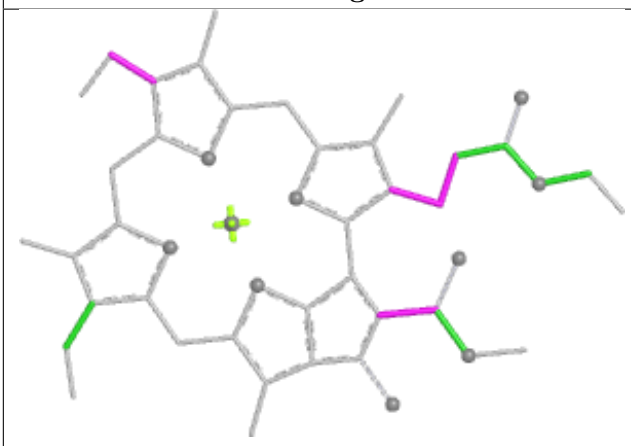
Ligand CLA a 719



Bond lengths



Bond angles



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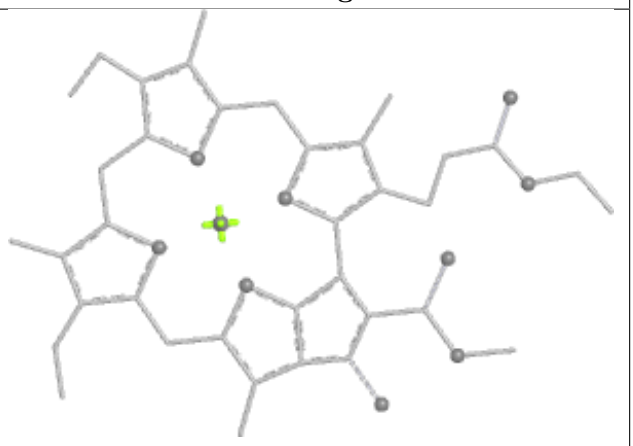
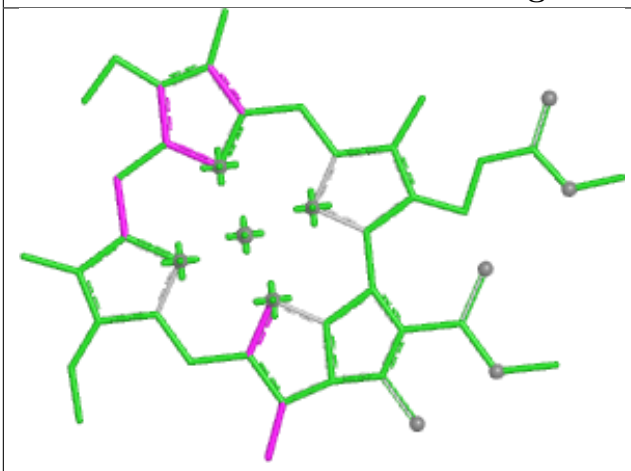


Rings

Ligand CLA J 315



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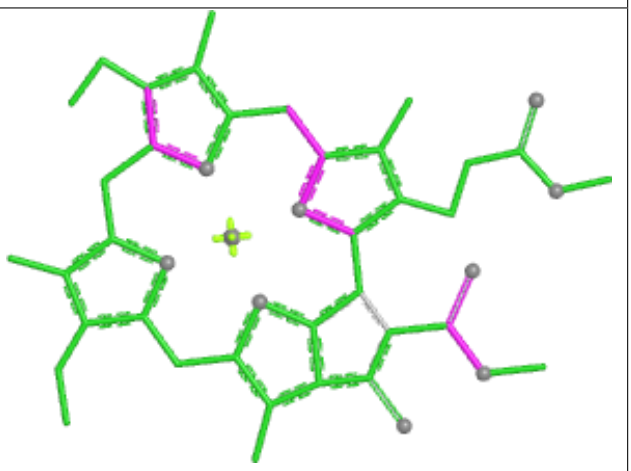
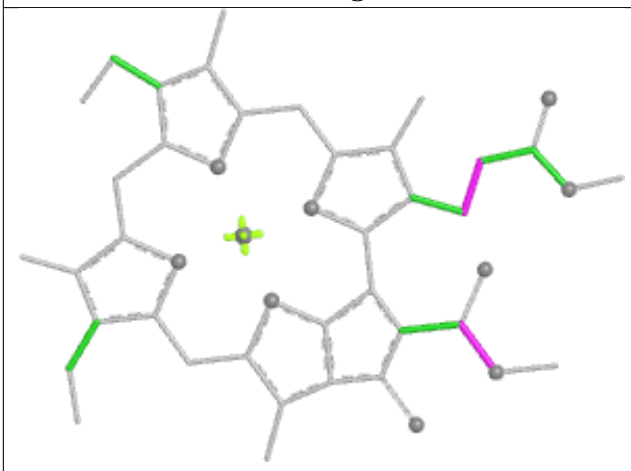
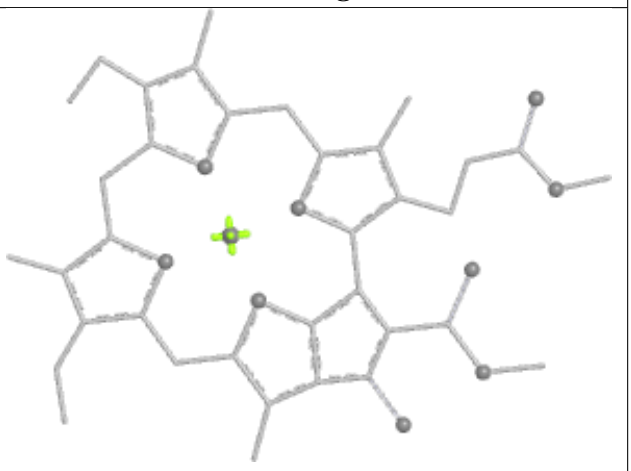


Bond angles

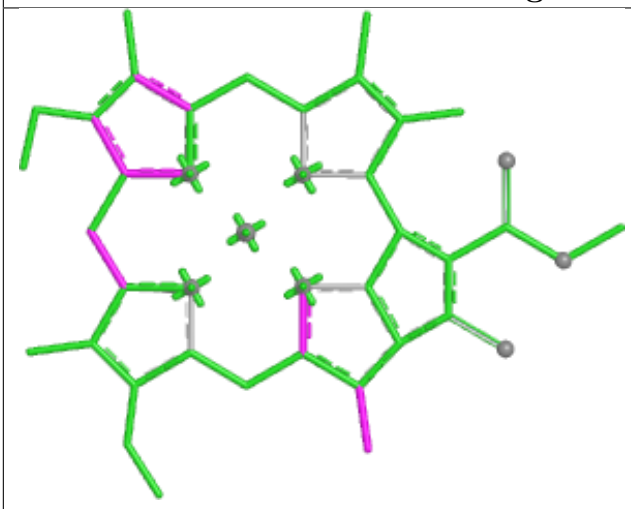


Torsions

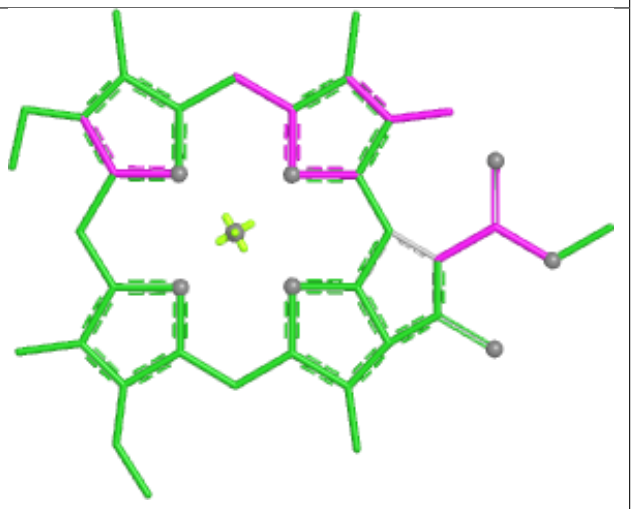


Rings

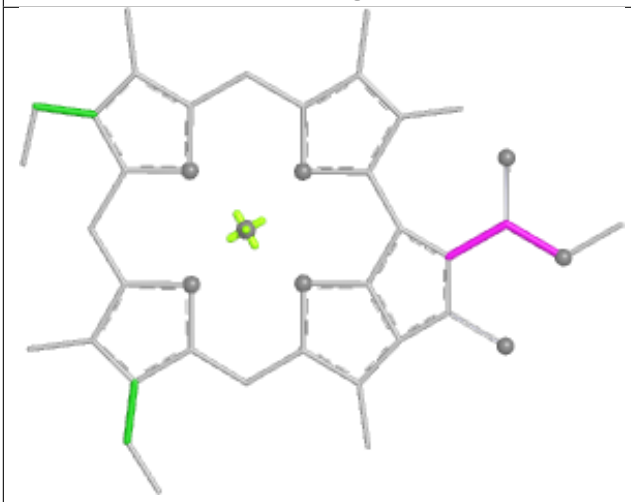
Ligand CLA F 315



Bond lengths



Bond angles



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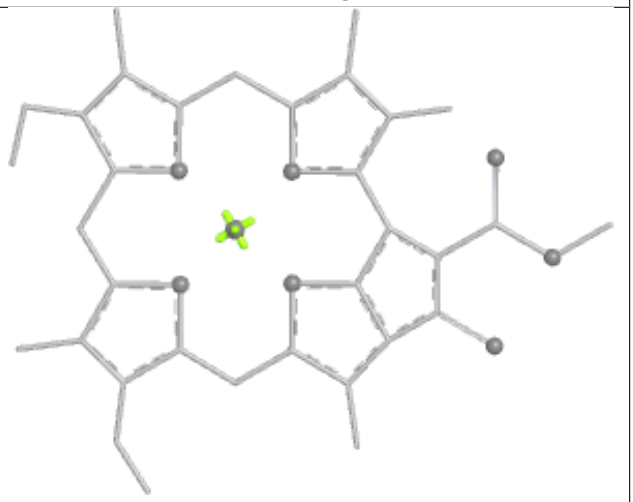
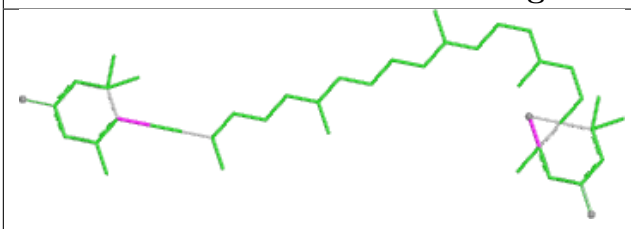
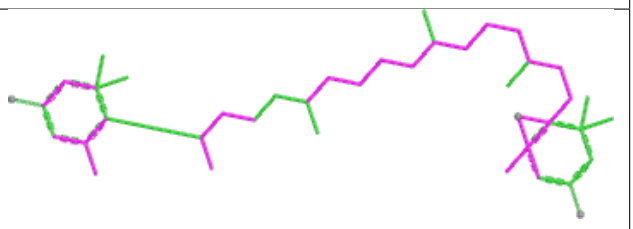


Rings

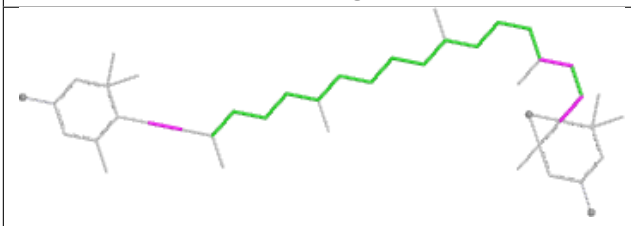
Ligand DD6 L 302



Bond lengths



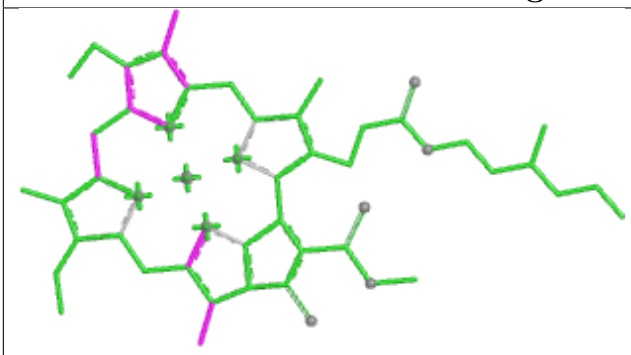
Bond angles



Torsions

Rings

Ligand CLA L 317



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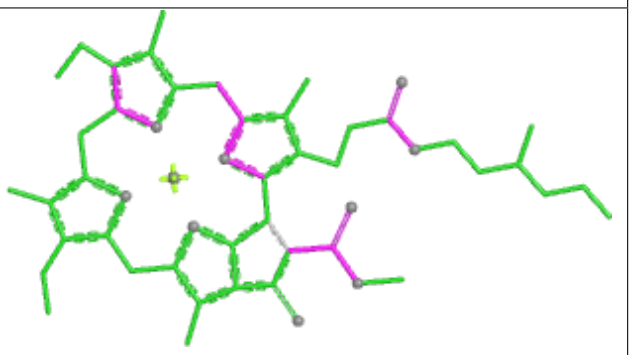

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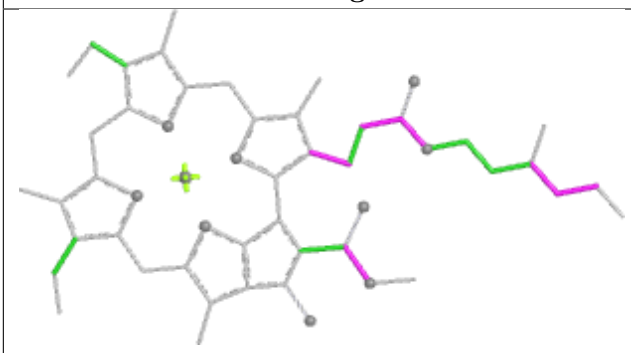
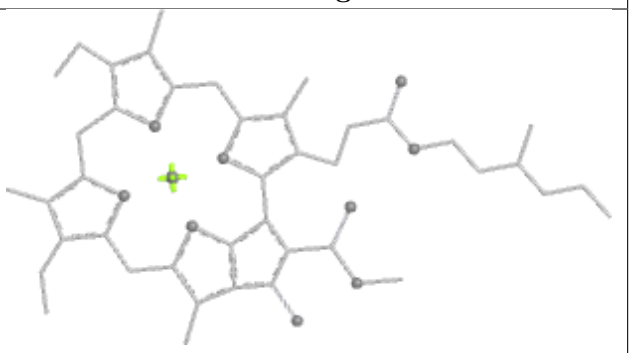
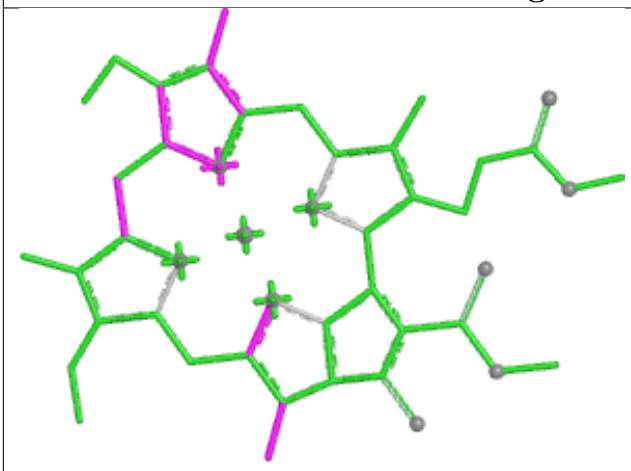


Torsions



Rings

Ligand CLA J 306



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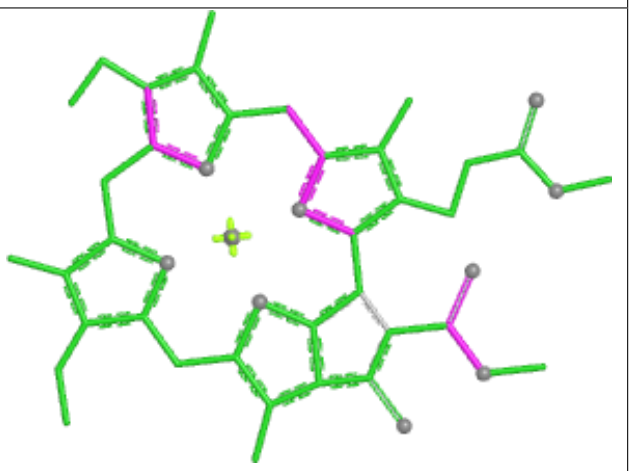
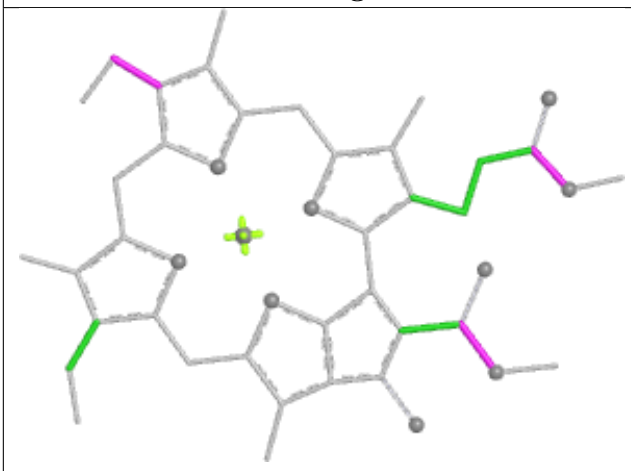


Bond angles



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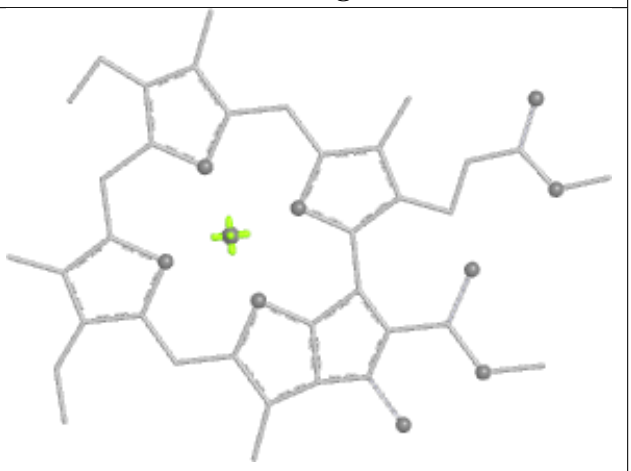
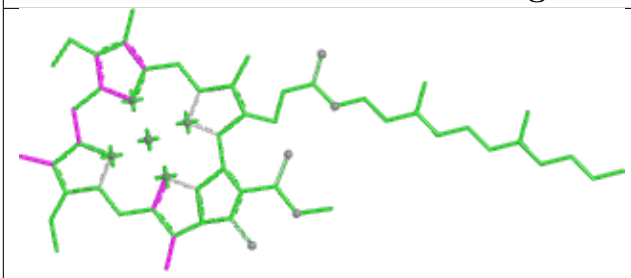


Rings

Ligand CLA a 706



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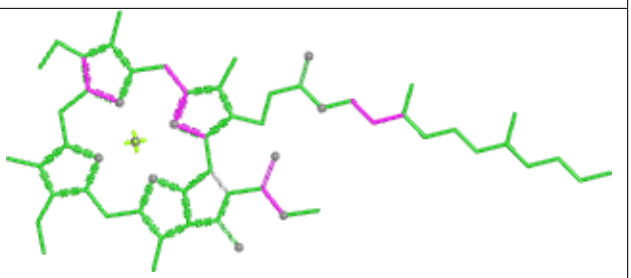
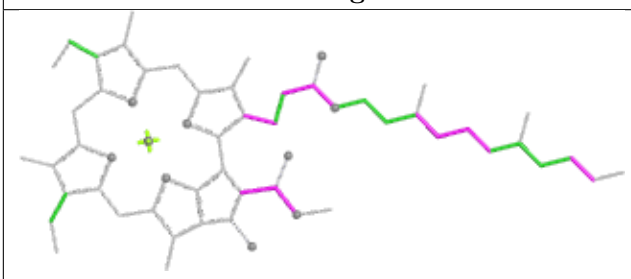


Bond angles



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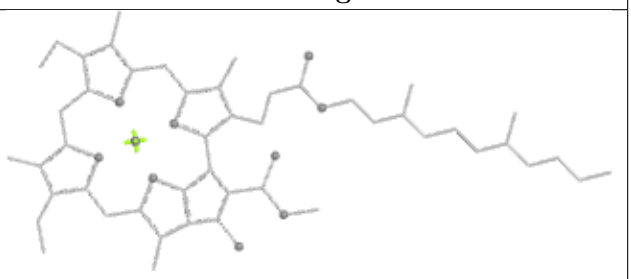
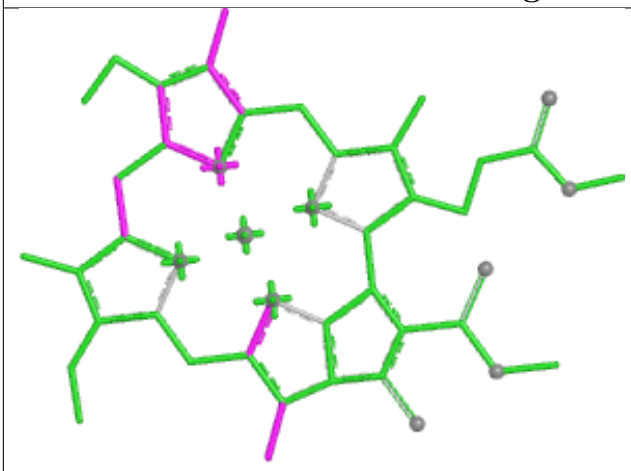


Rings

Ligand CLA K 316



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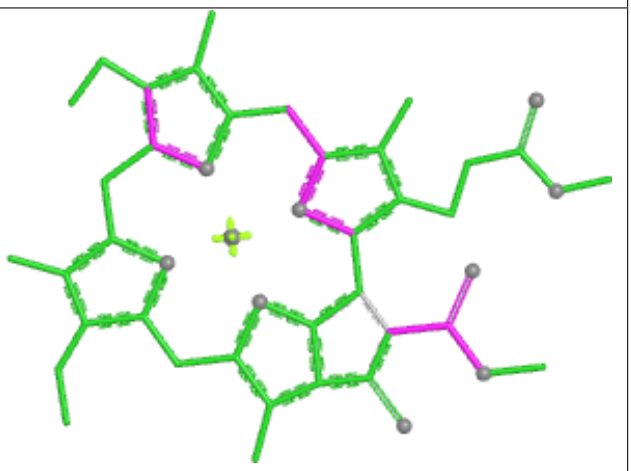
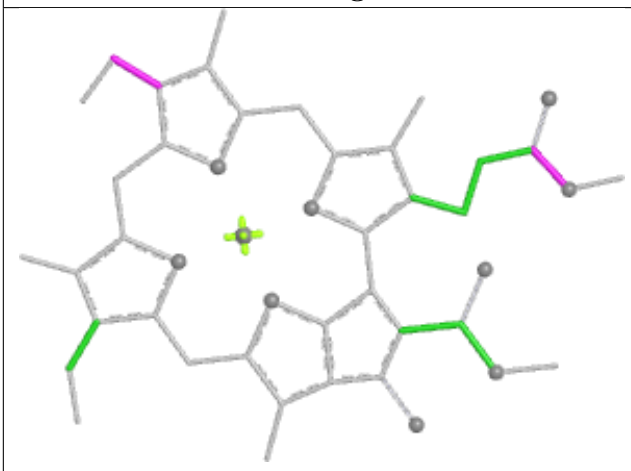


Bond angles



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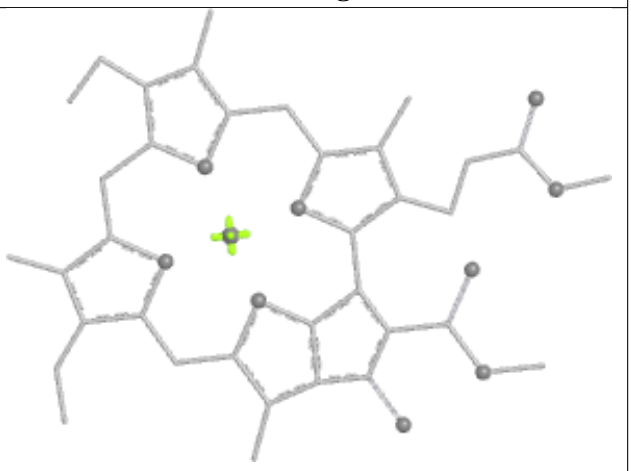
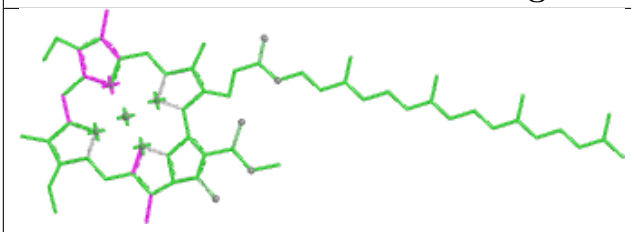


Rings

Ligand CLA a 724



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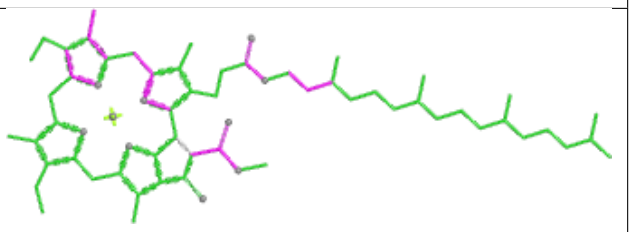
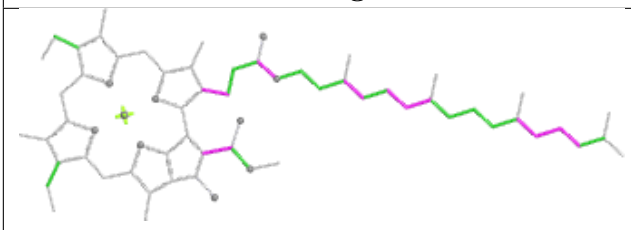


Bond angles



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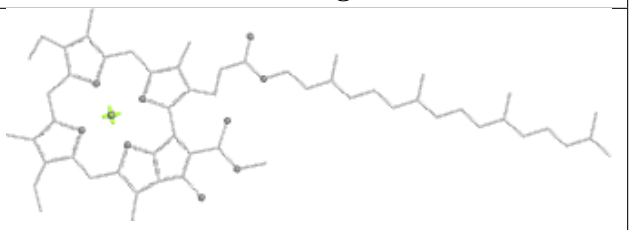
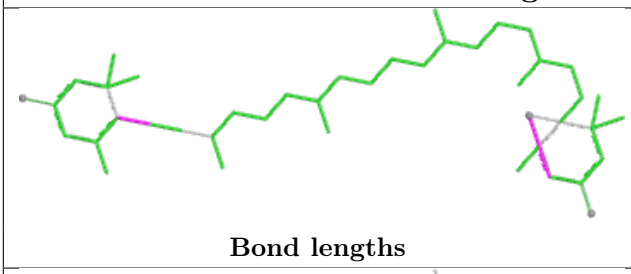


Rings

Ligand DD6 M 302



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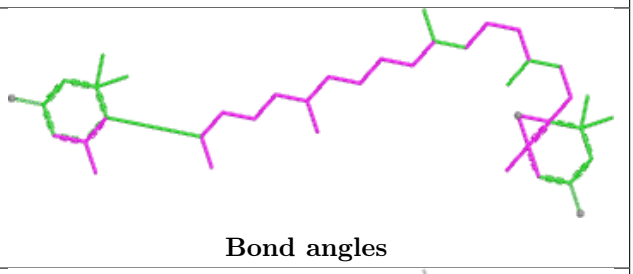
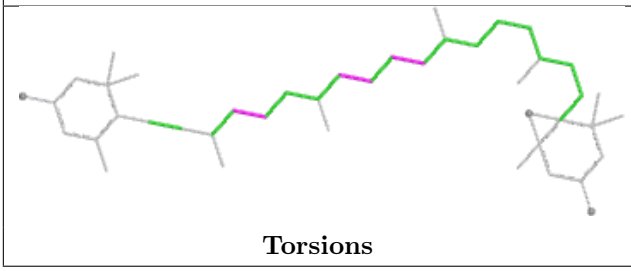


Bond angles



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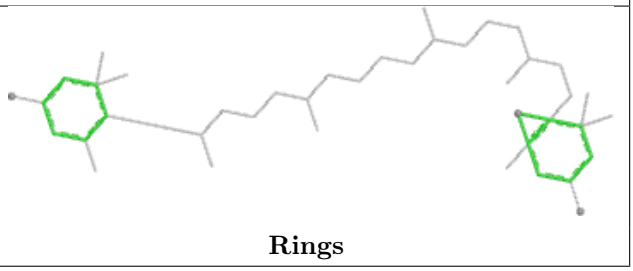
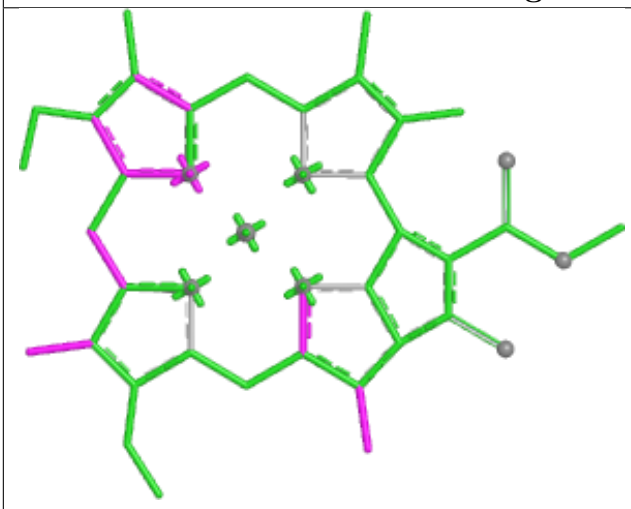


Rings

Ligand CLA P 217



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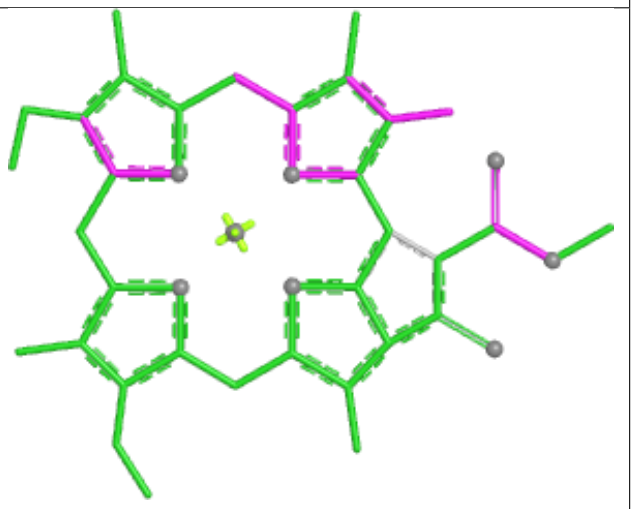

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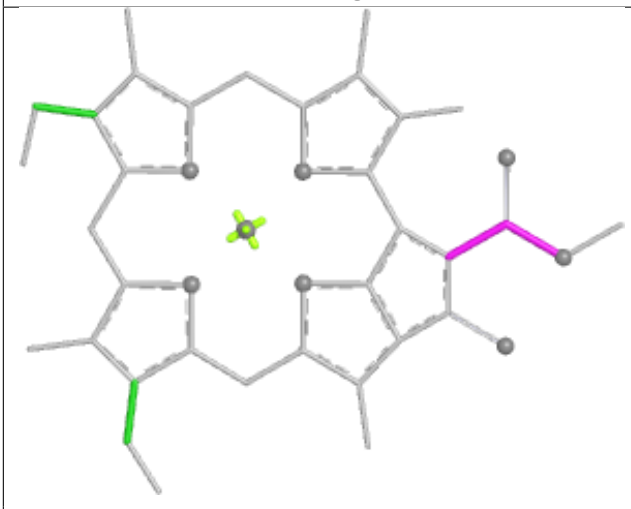

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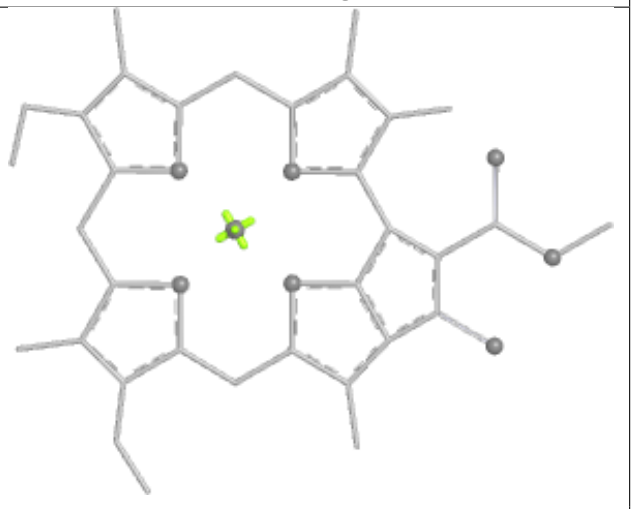
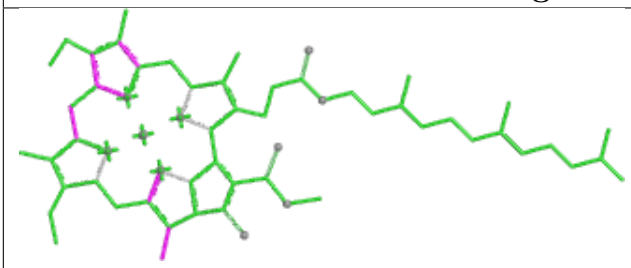


Rings

Ligand CLA l 304



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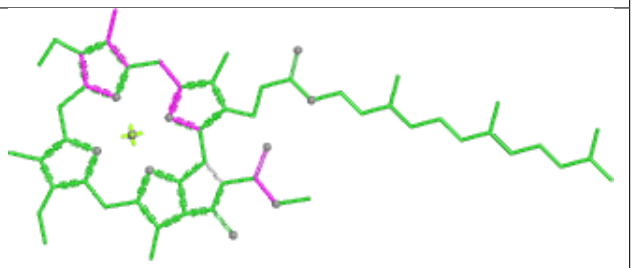

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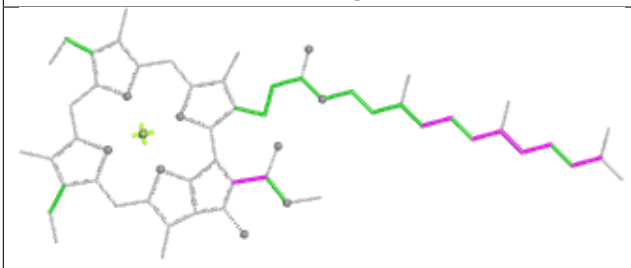

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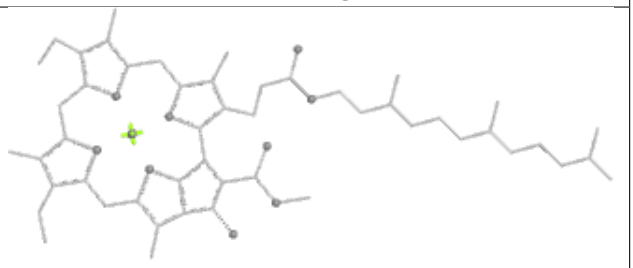
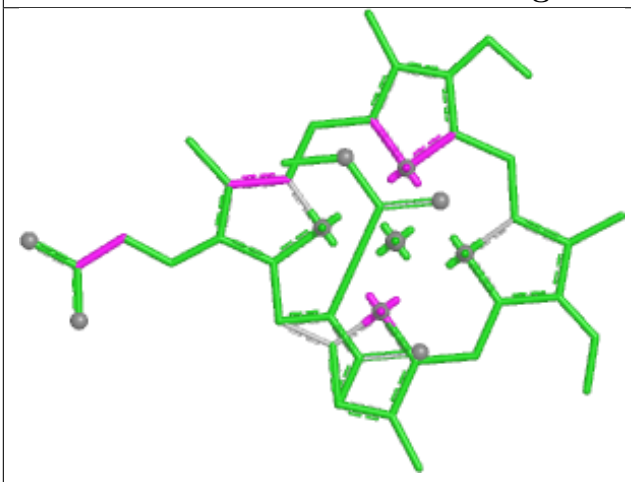


Rings

Ligand KC1 I 314



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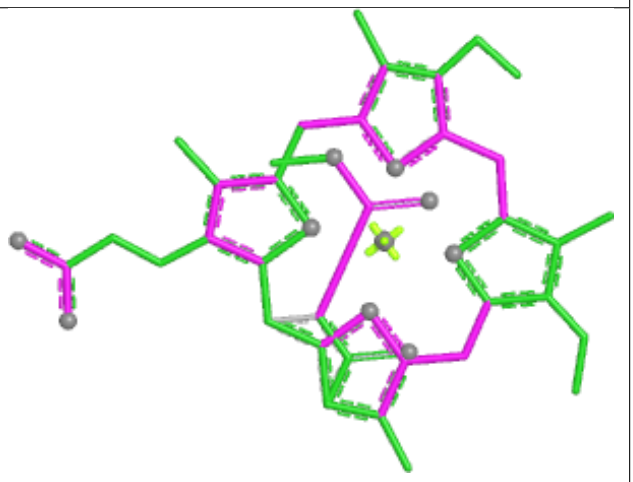
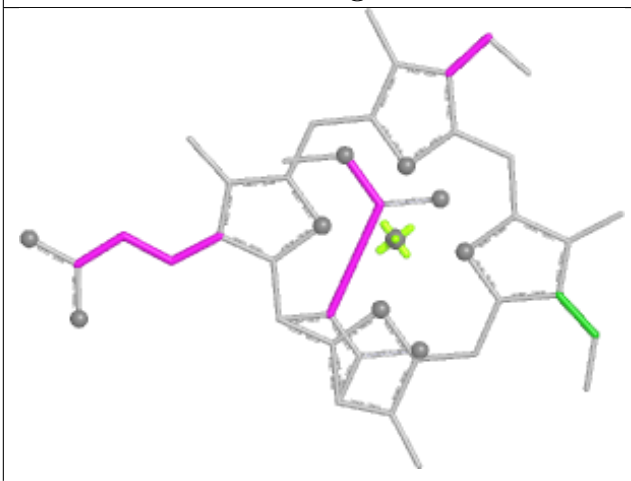


Bond angles



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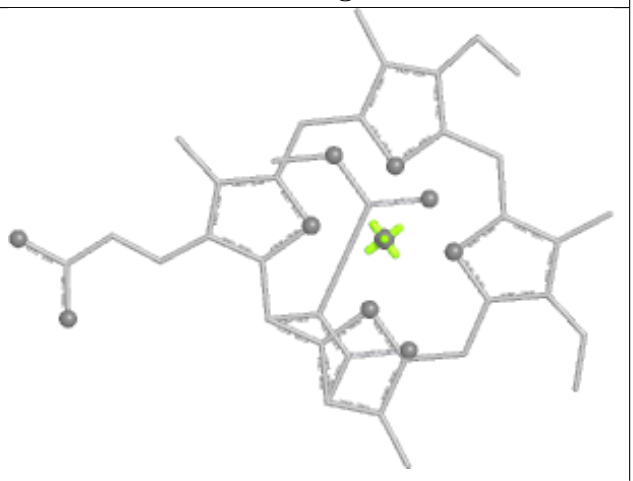
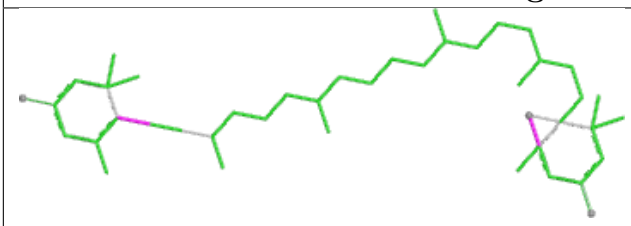


Rings

Ligand DD6 F 303



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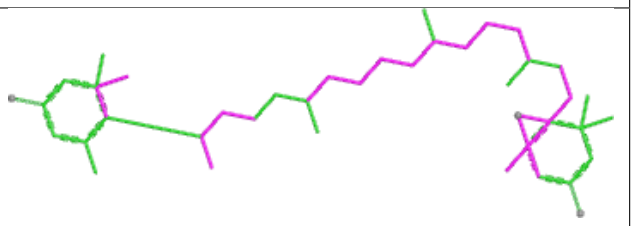
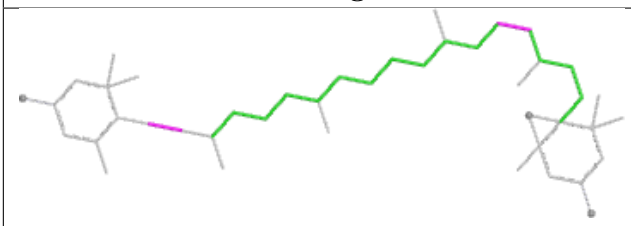


Bond angles



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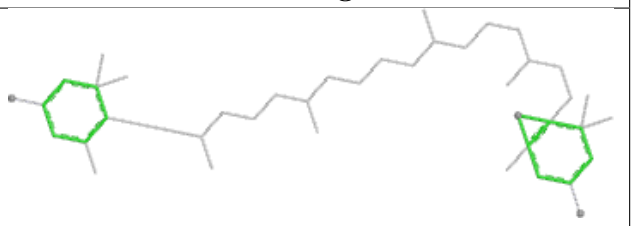
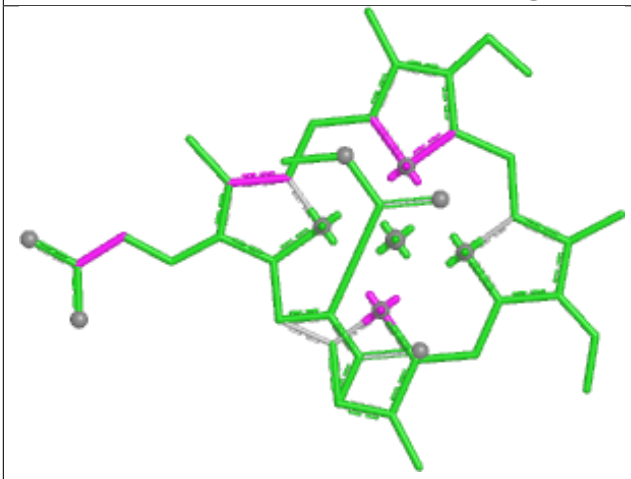


Rings

Ligand KC1 N 308



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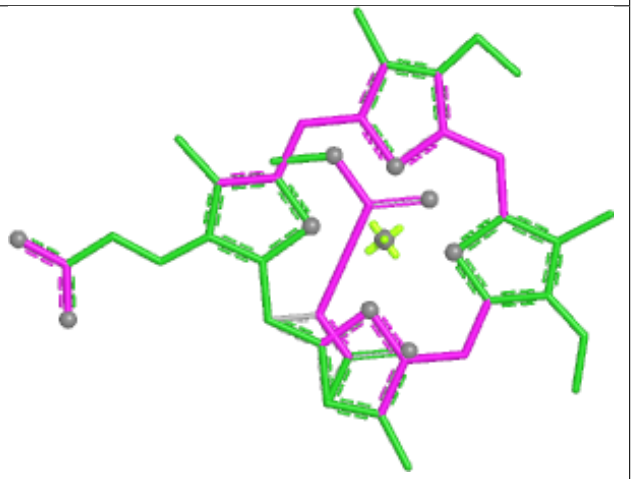
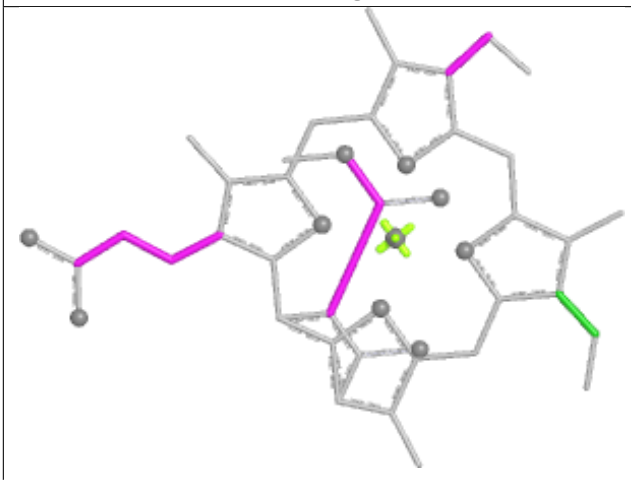
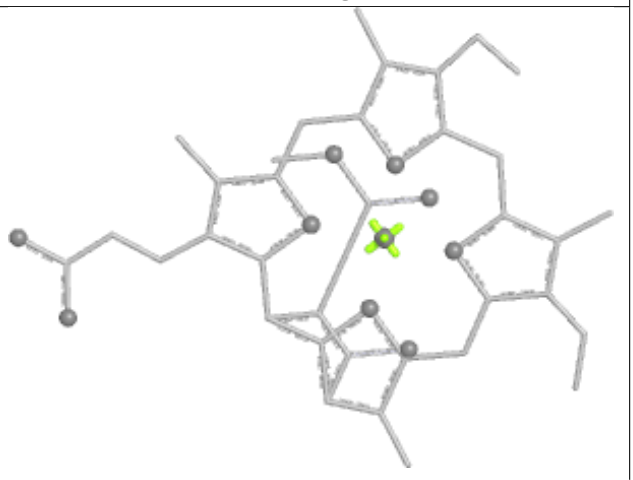


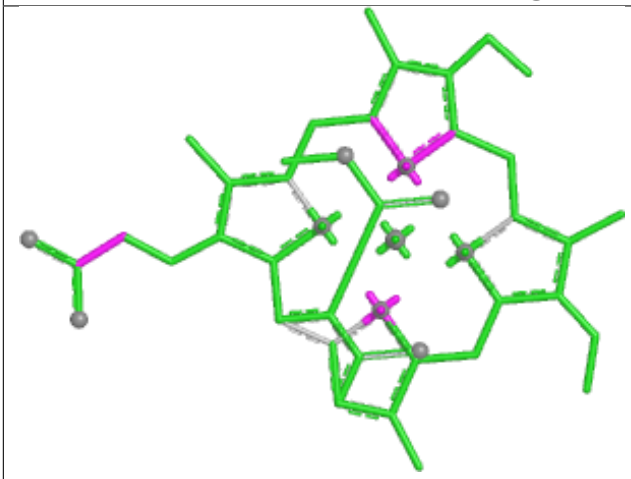
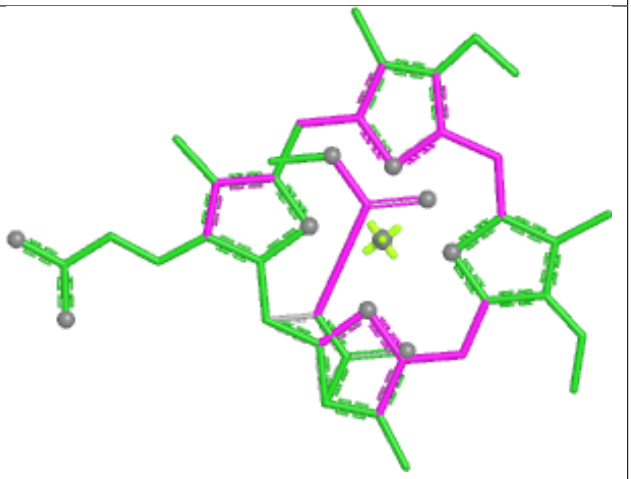
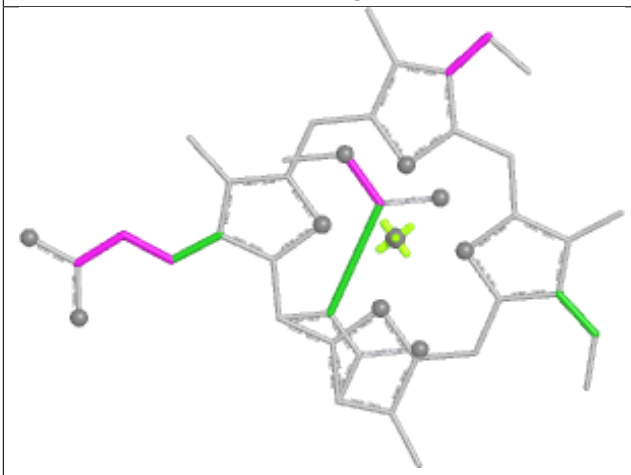
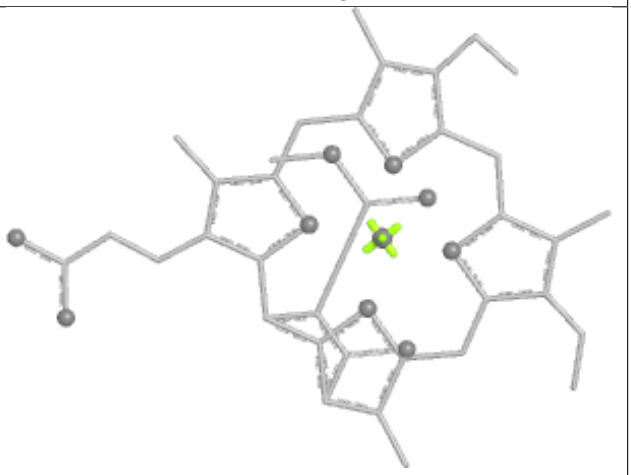
Bond angles

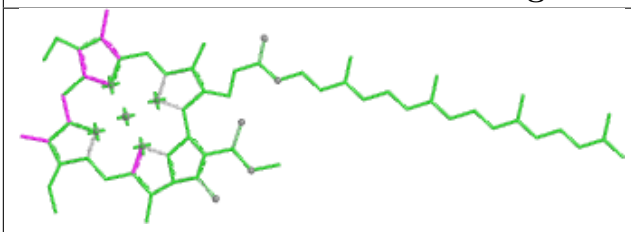
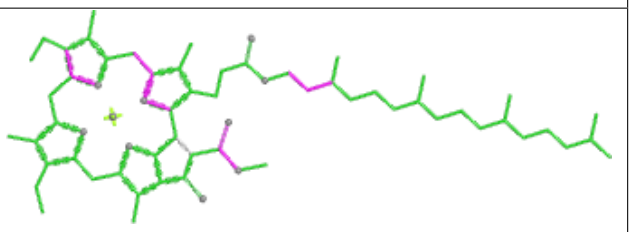
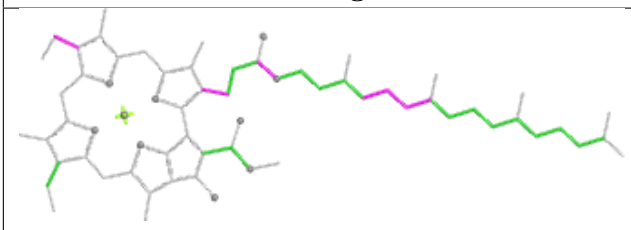
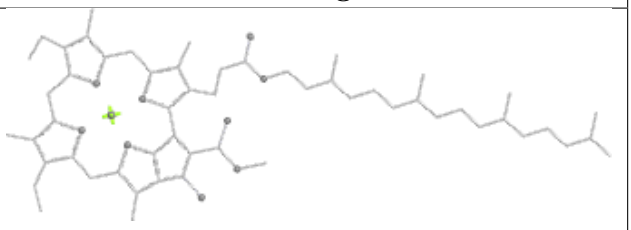


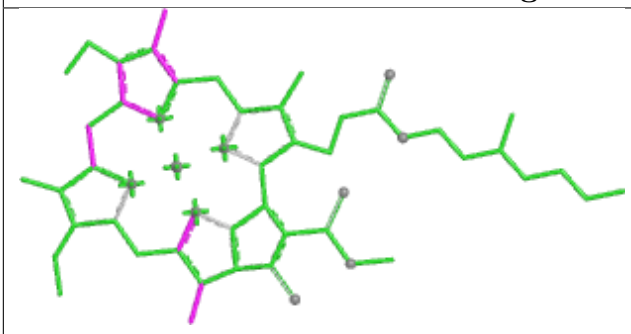
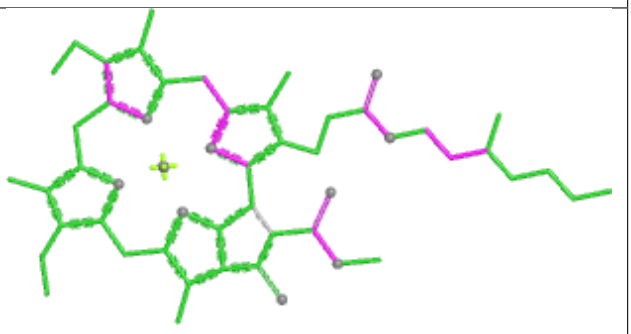
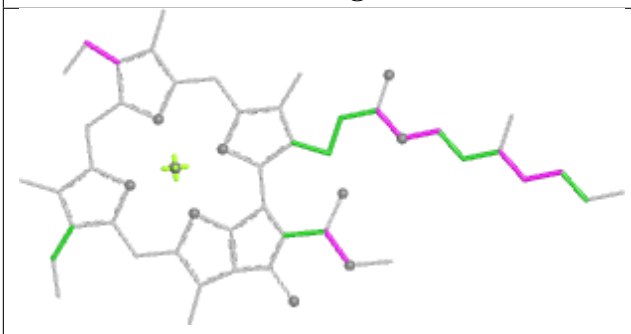
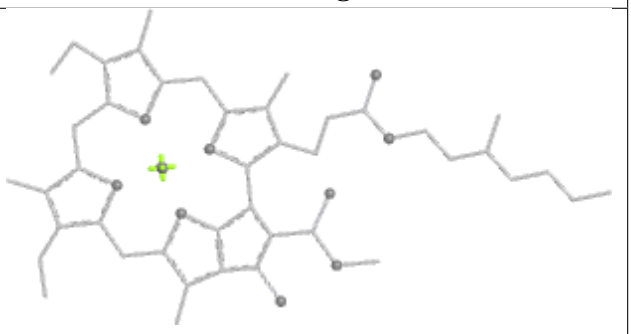
Torsions

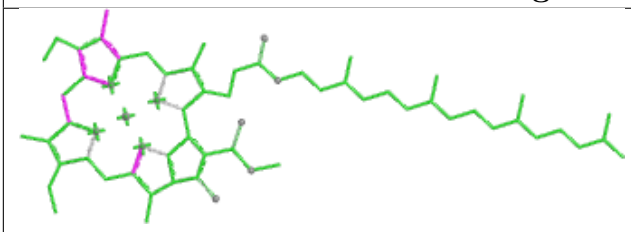
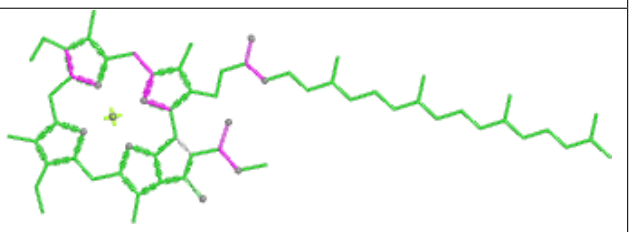
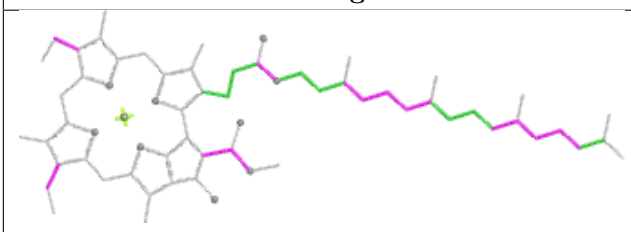
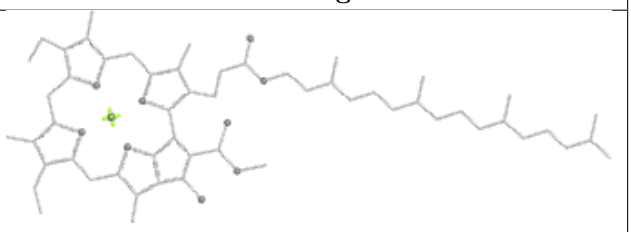


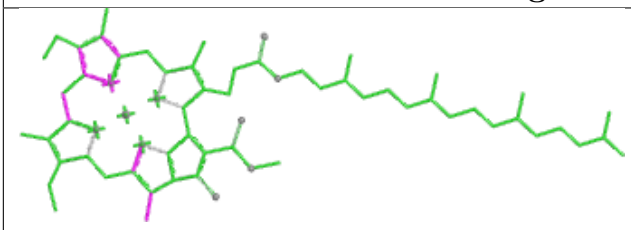
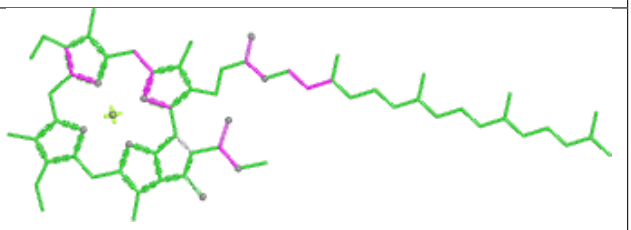
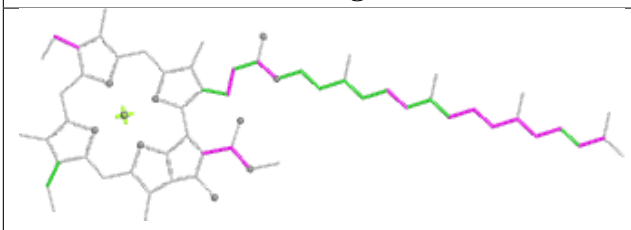
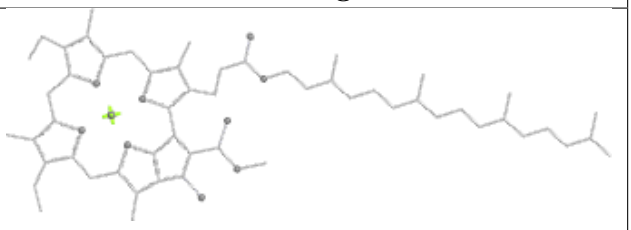
Rings

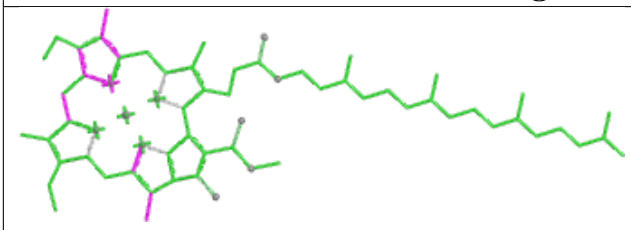
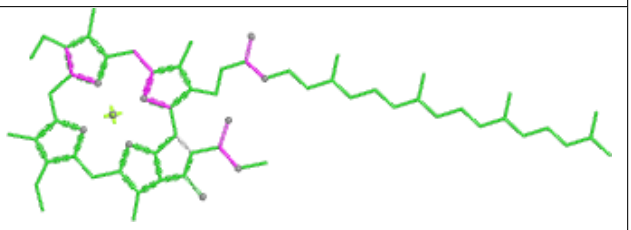
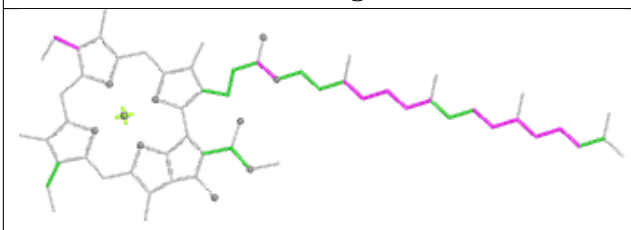
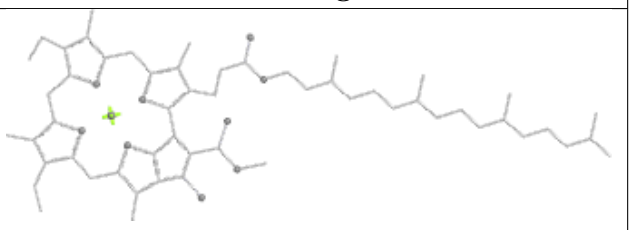
Ligand KC1 F 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 728	
	
Bond lengths	Bond angles
	
Torsions	Rings

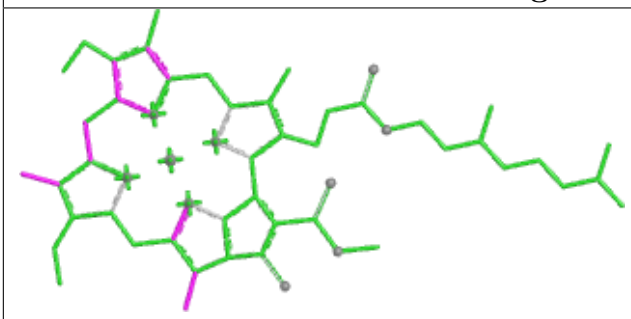
Ligand CLA M 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA l 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

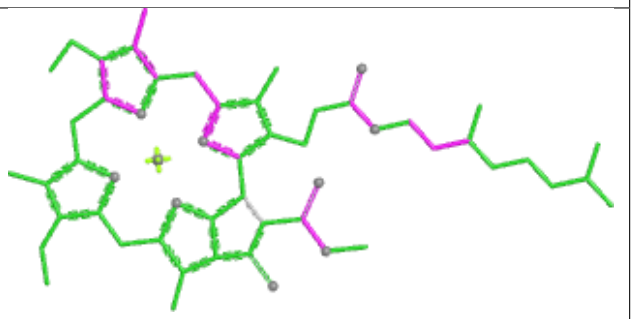
Ligand CLA a 721	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA I 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

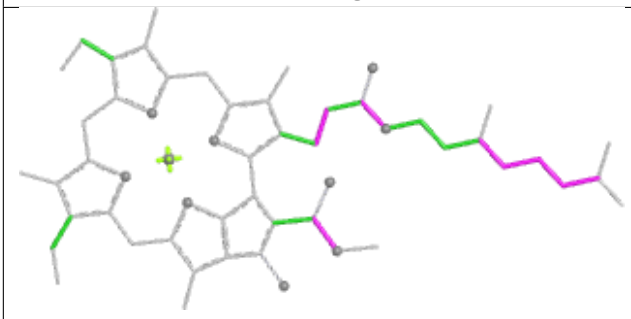
Ligand CLA I 313



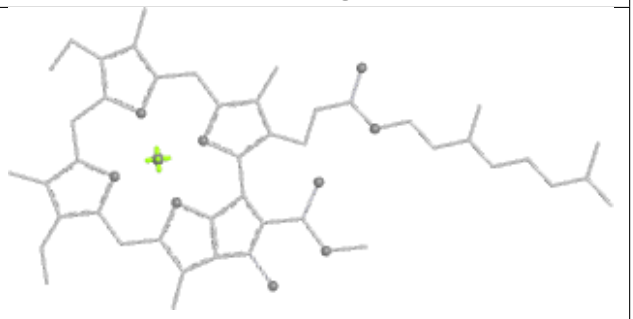
Bond lengths



Bond angles

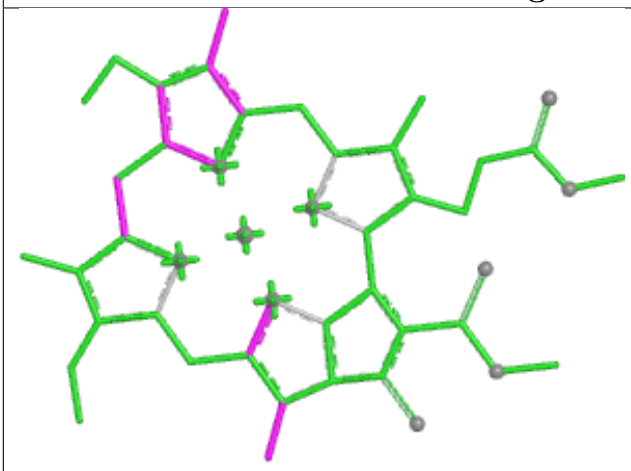


Torsions



Rings

Ligand CLA a 727



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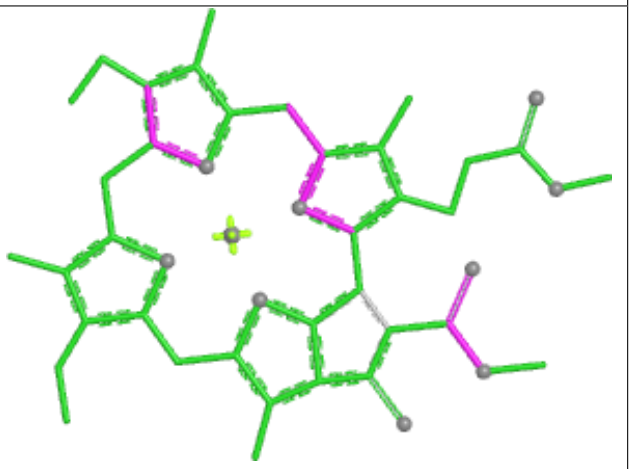
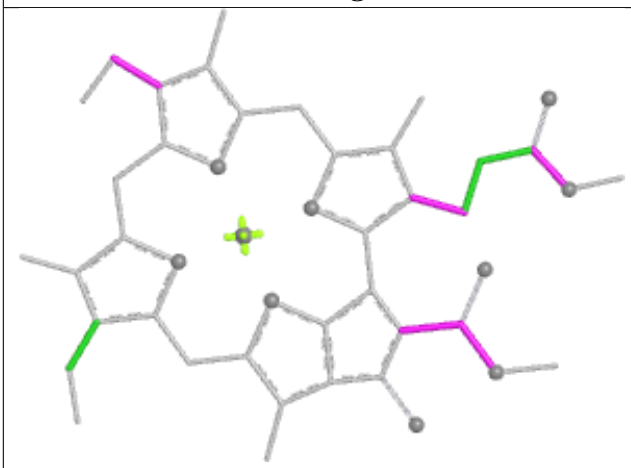


Bond angles



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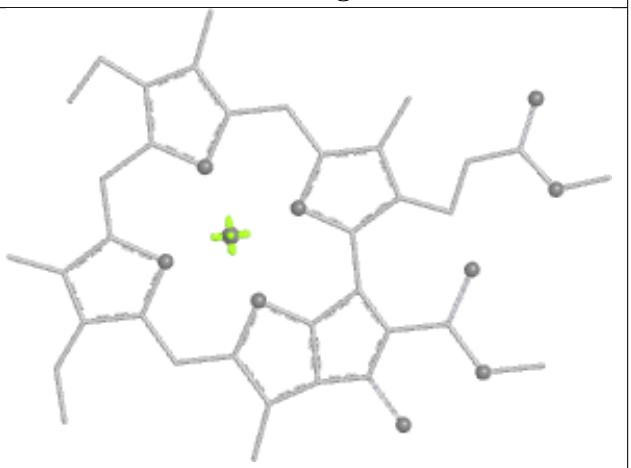
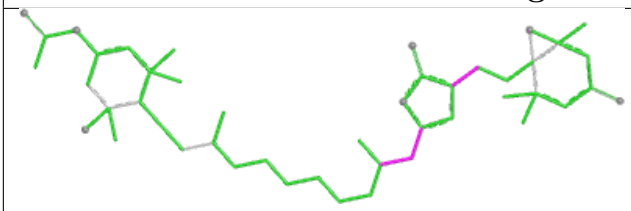


Rings

Ligand PID H 301



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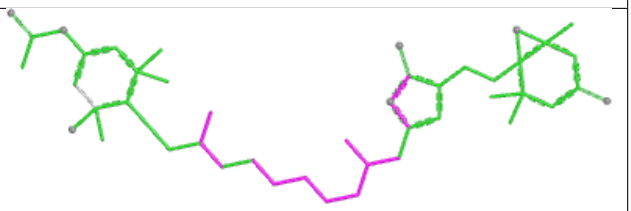
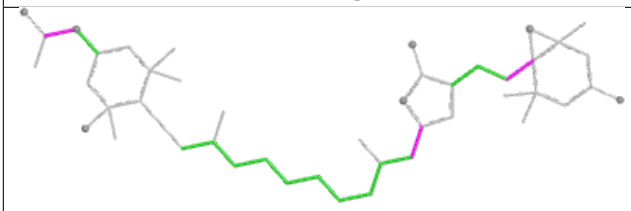


Bond angles



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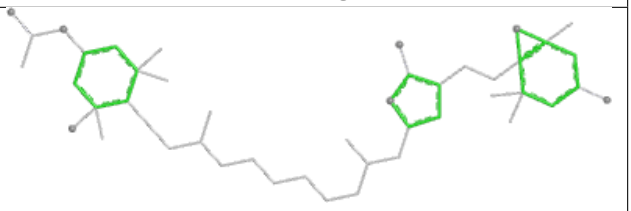
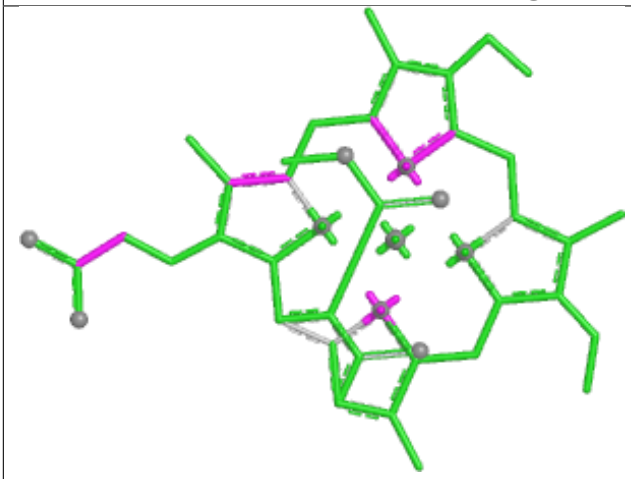


Rings

Ligand KC1 K 314



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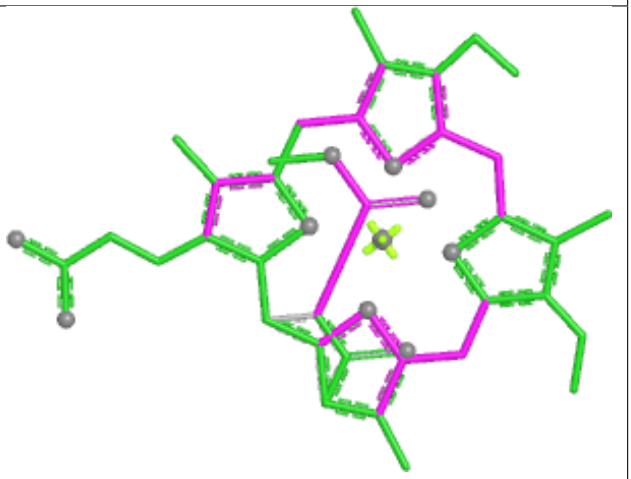
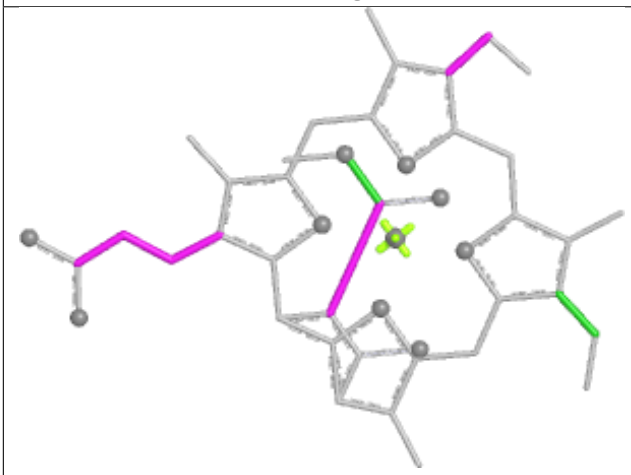


Bond angles



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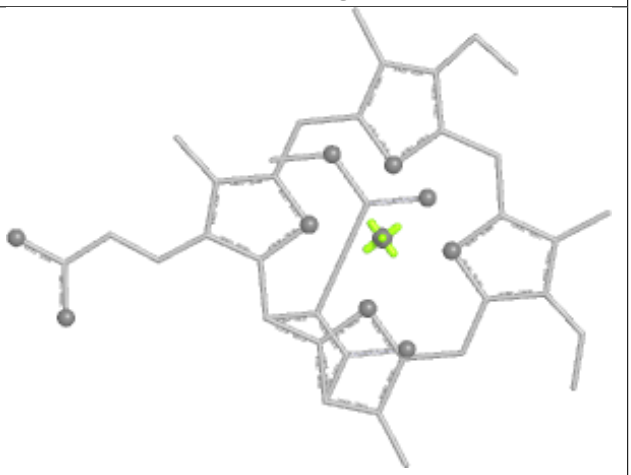
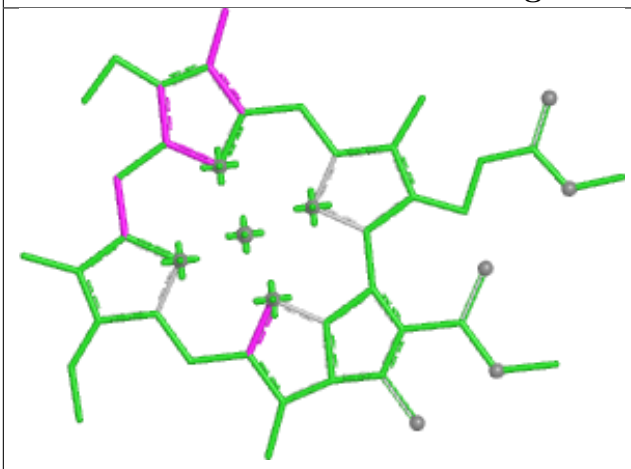
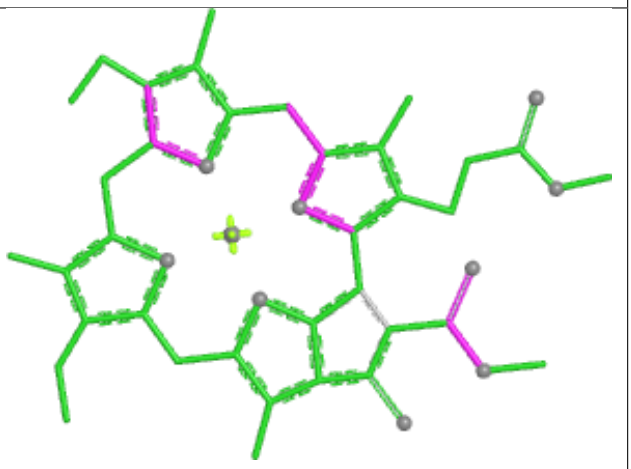


Rings

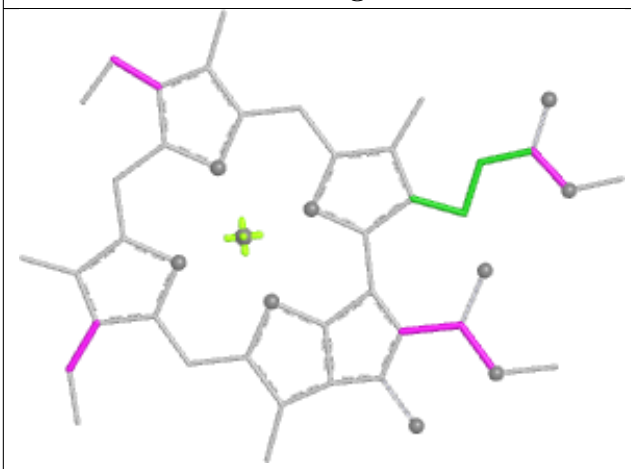
Ligand CLA B 316



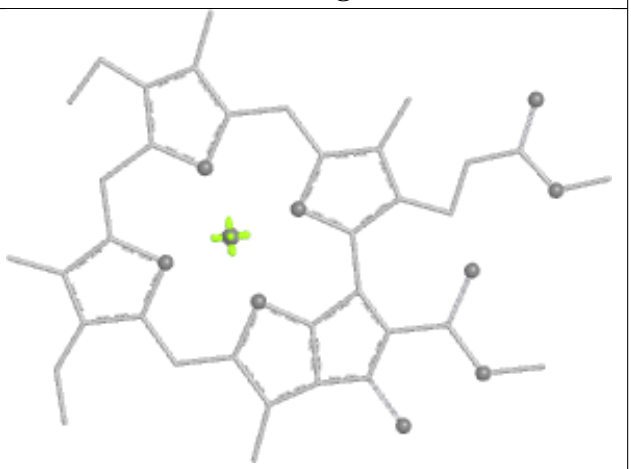
Bond lengths



Bond angles

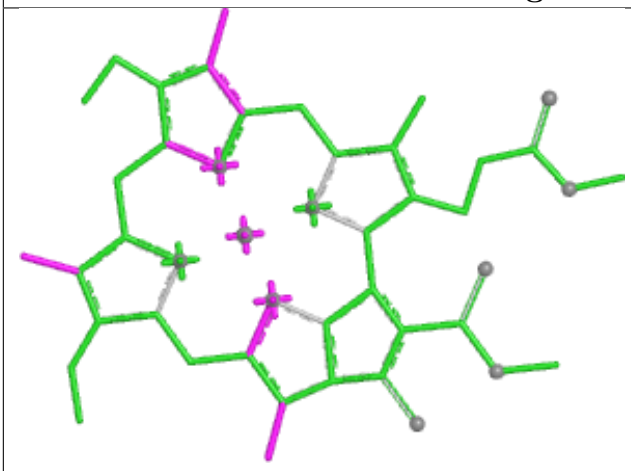


Torsions



Rings

Ligand CLA F 312



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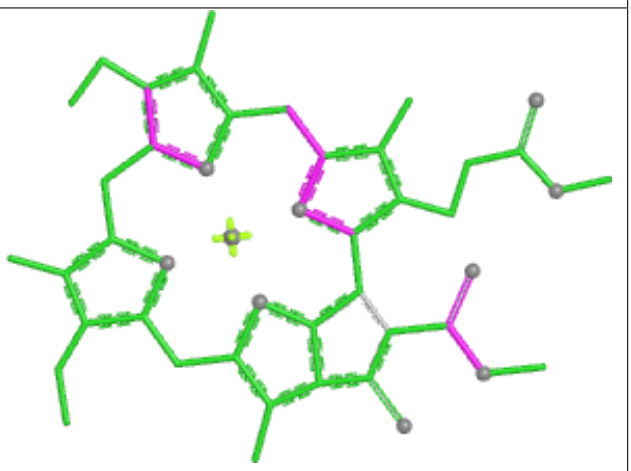
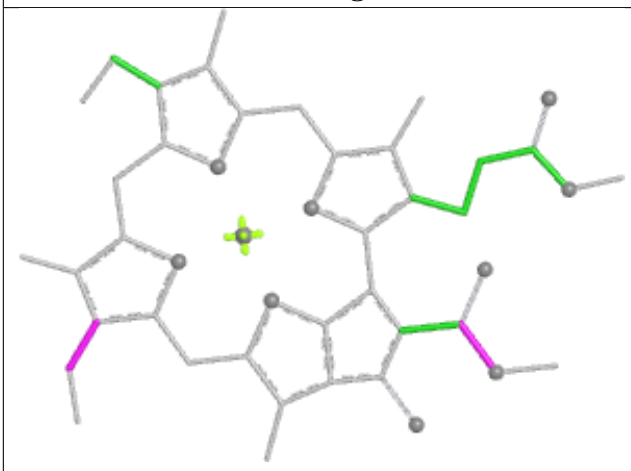
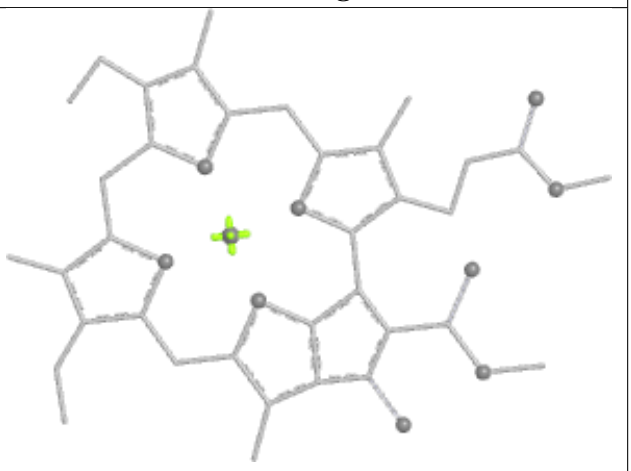


Bond angles

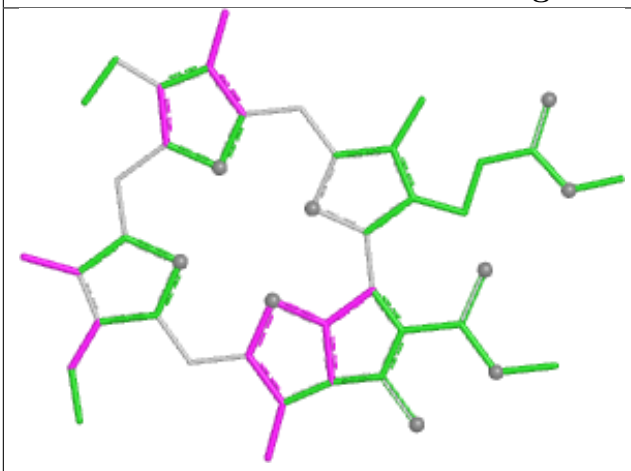


Torsions

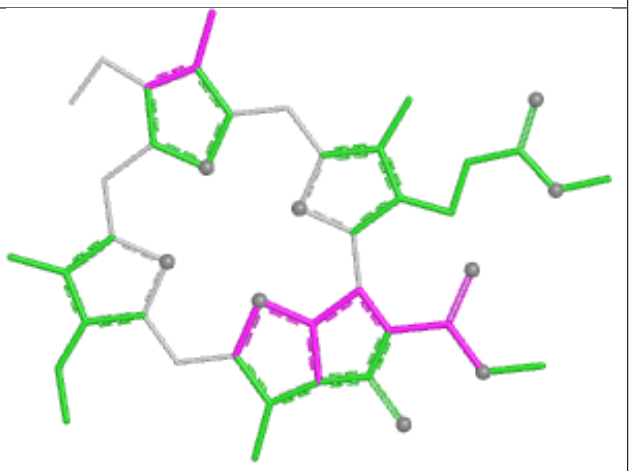


Rings

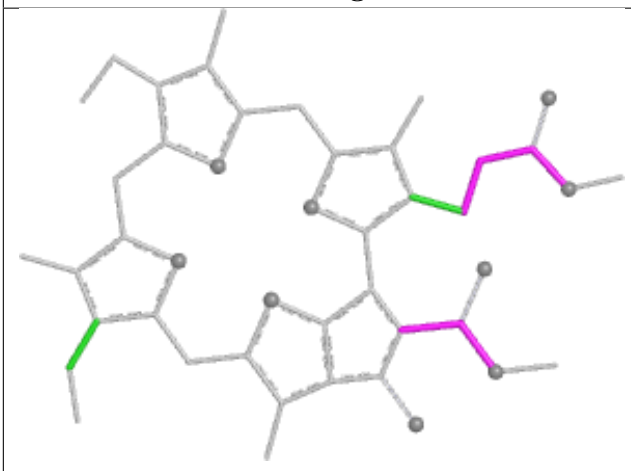
Ligand CLA l 310



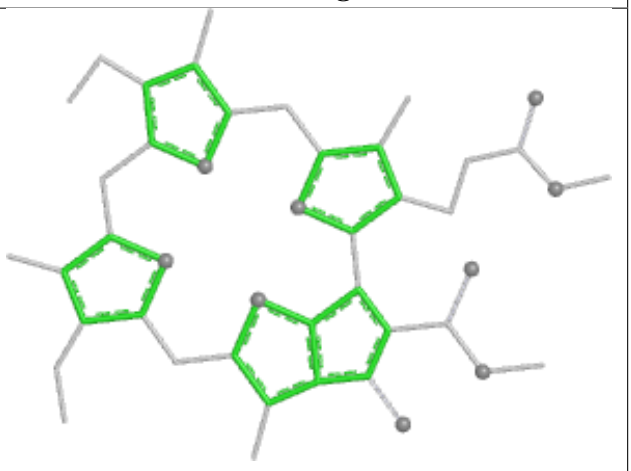
Bond lengths



Bond angles

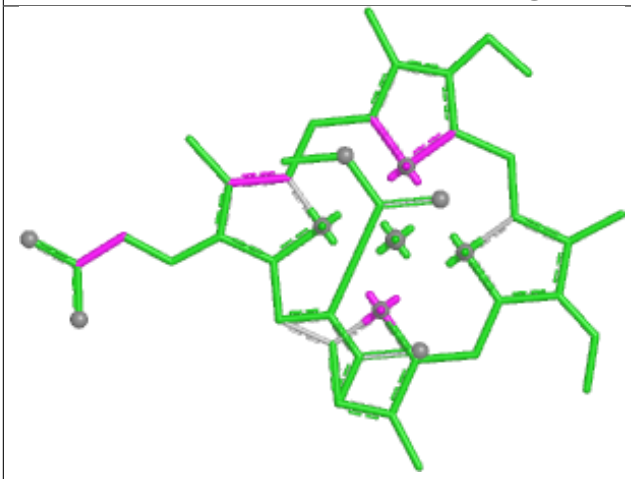


Torsions



Rings

Ligand KC1 O 310



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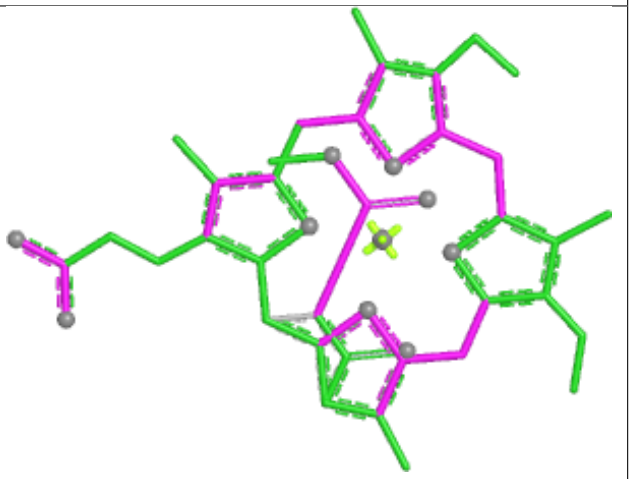
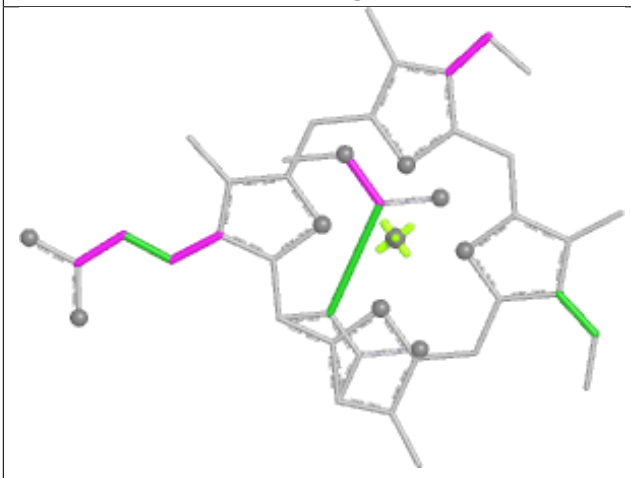


Bond angles



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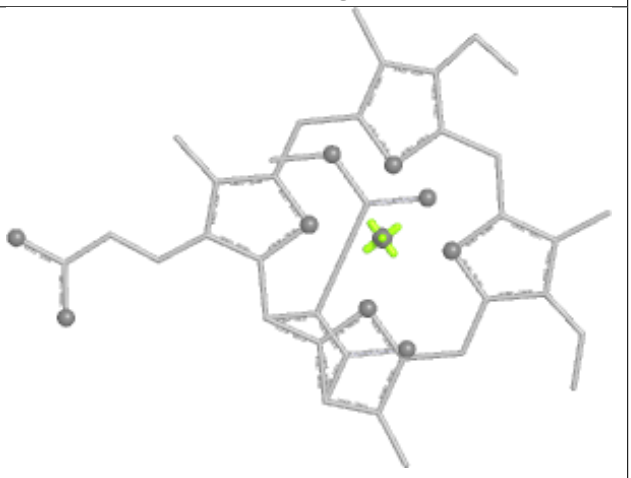
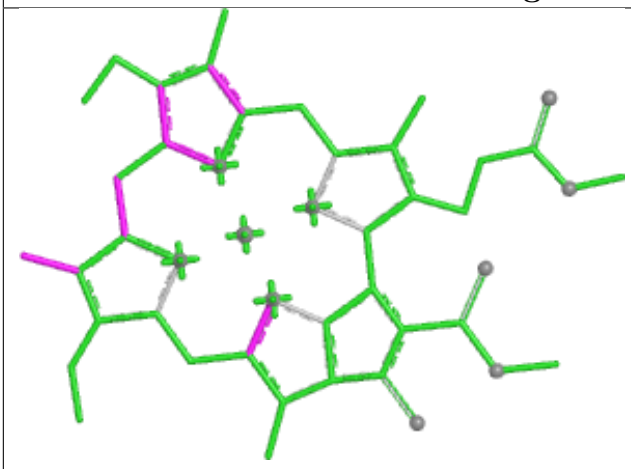


Rings

Ligand CLA D 311



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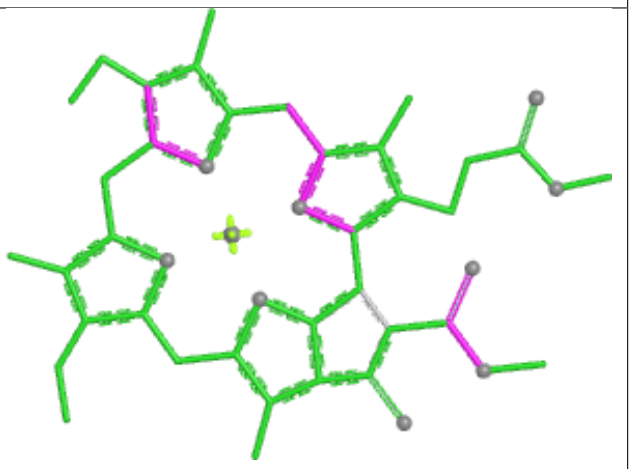
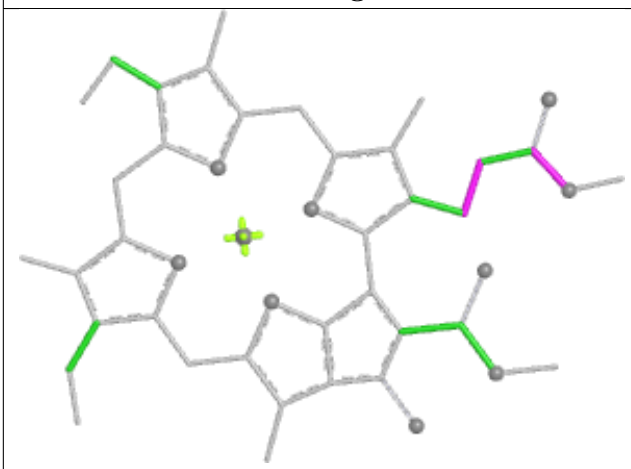
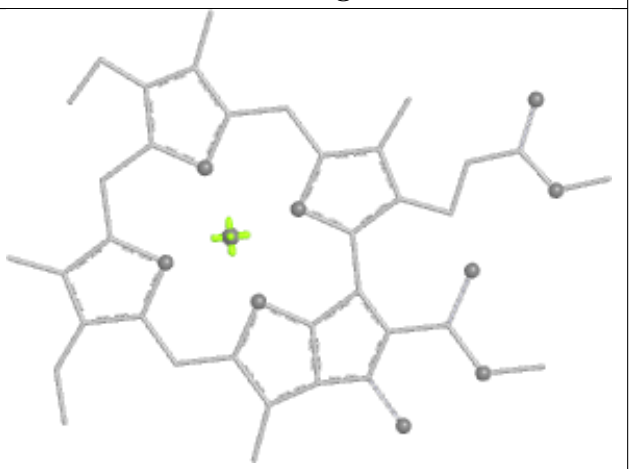


Bond angles

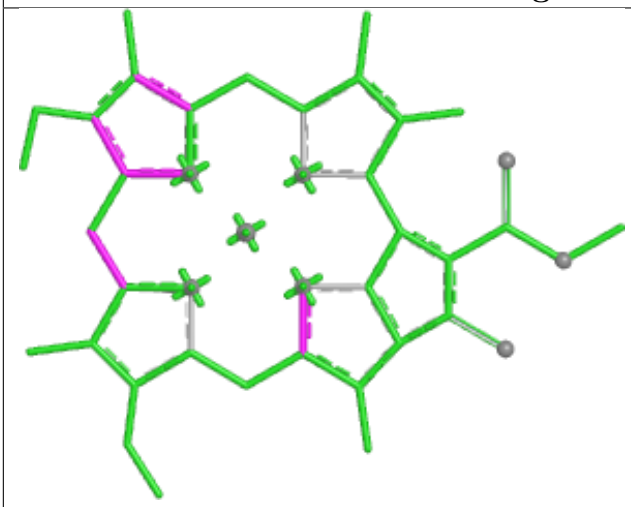


Torsions

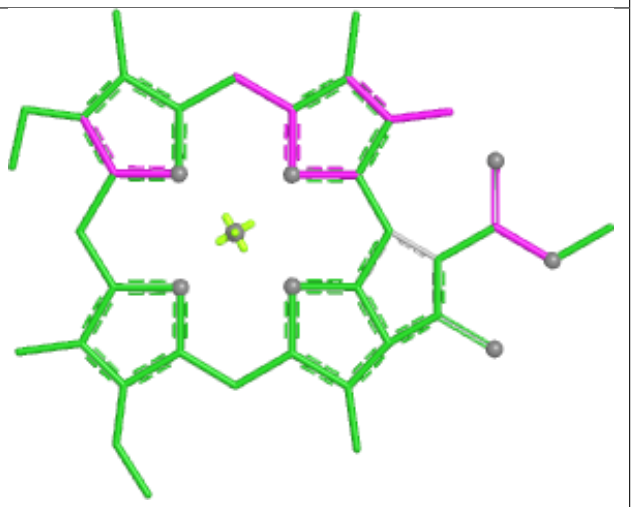


Rings

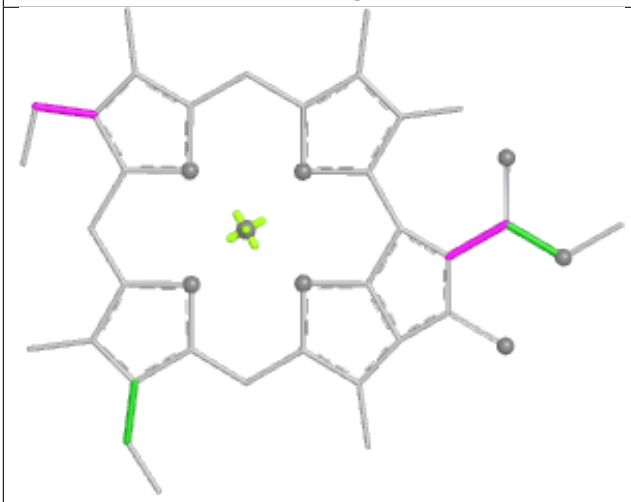
Ligand CLA l 309



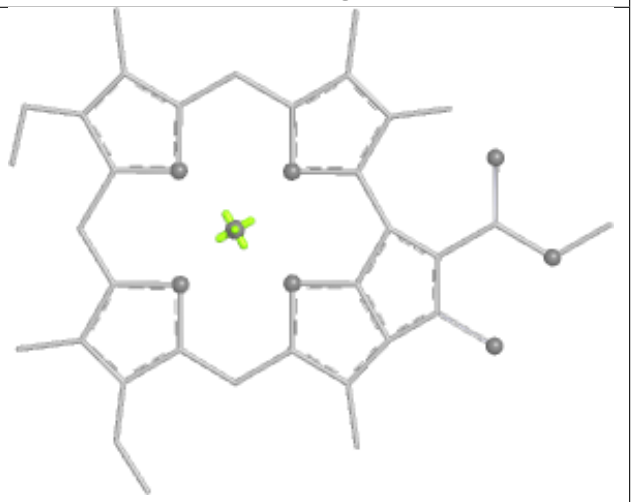
Bond lengths



Bond angles

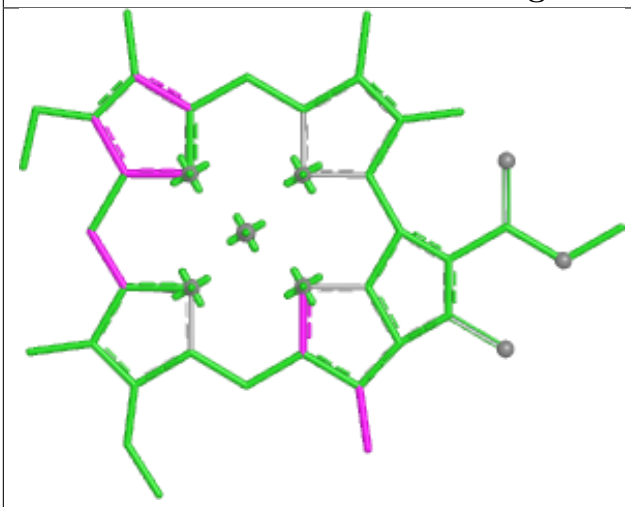


Torsions

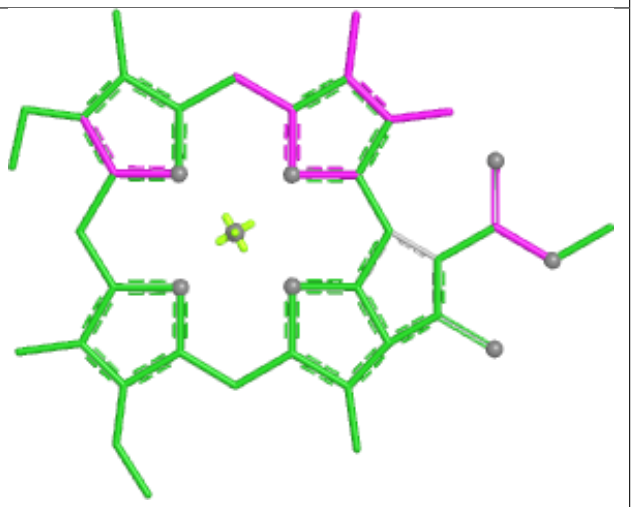


Rings

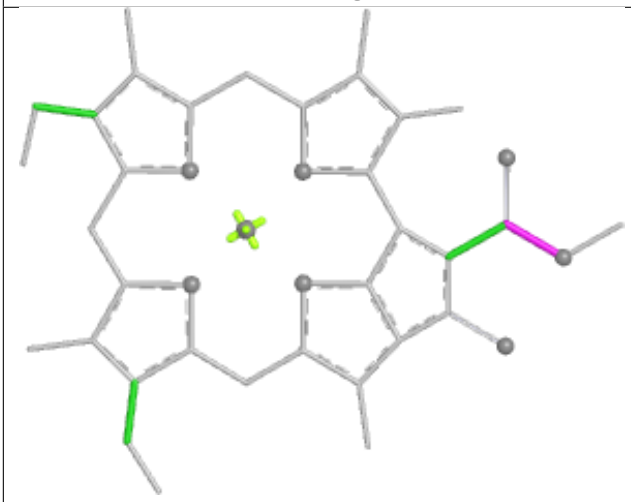
Ligand CLA J 314



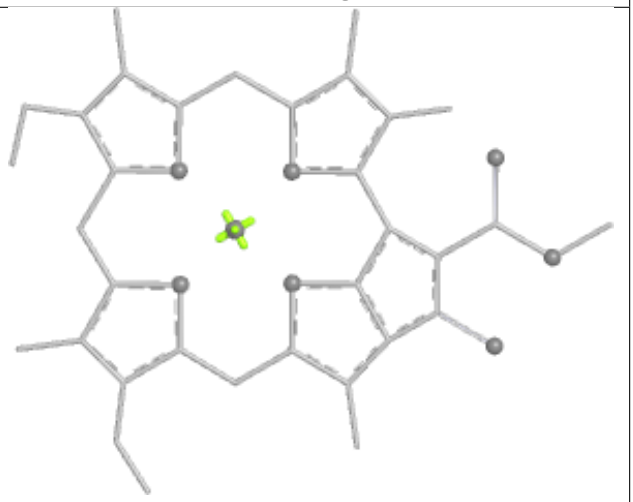
Bond lengths



Bond angles

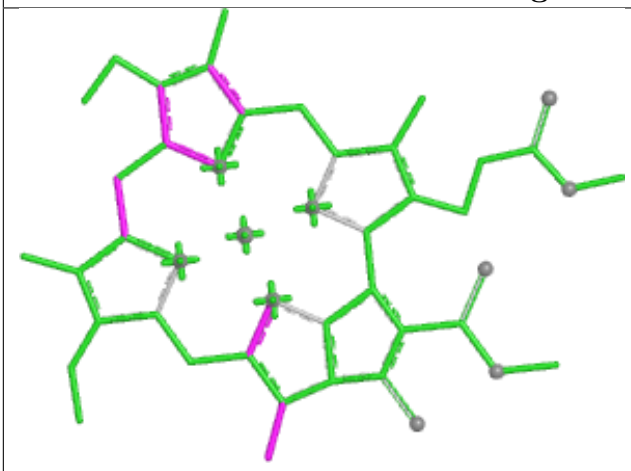


Torsions



Rings

Ligand CLA I 307



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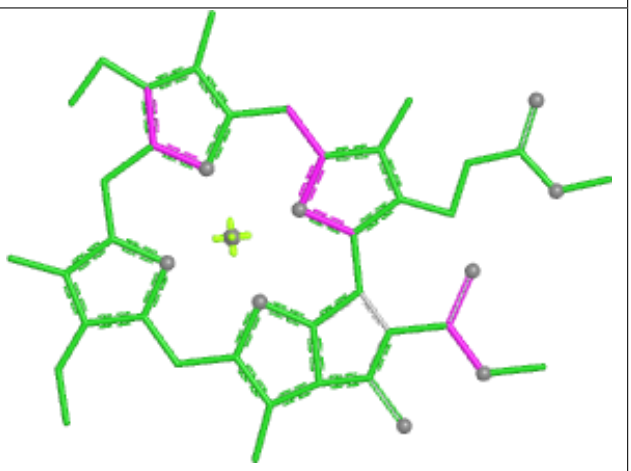

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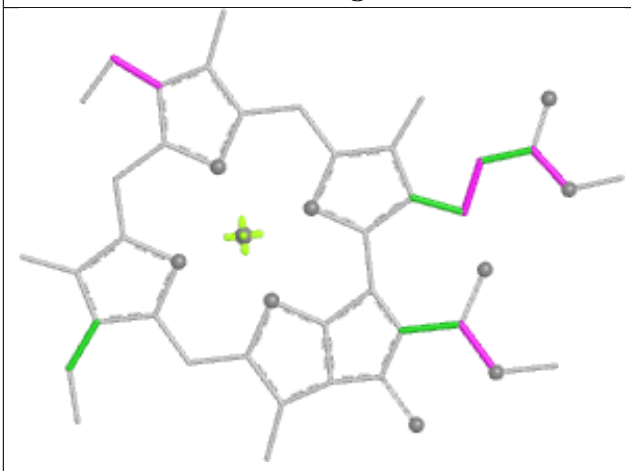

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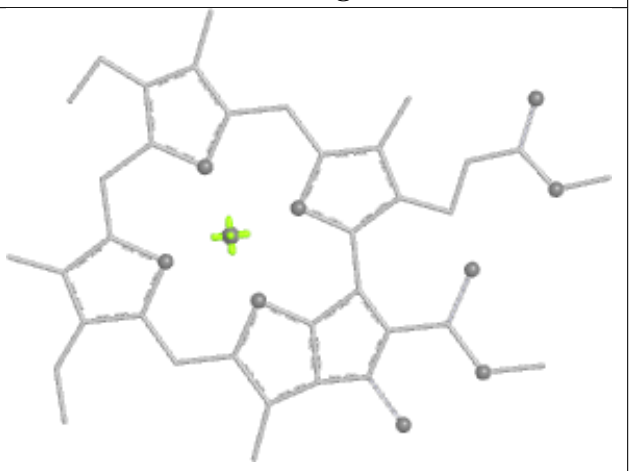
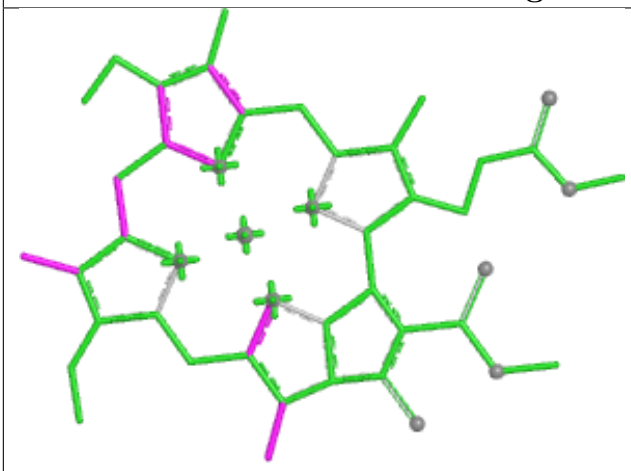


Rings

Ligand CLA F 313



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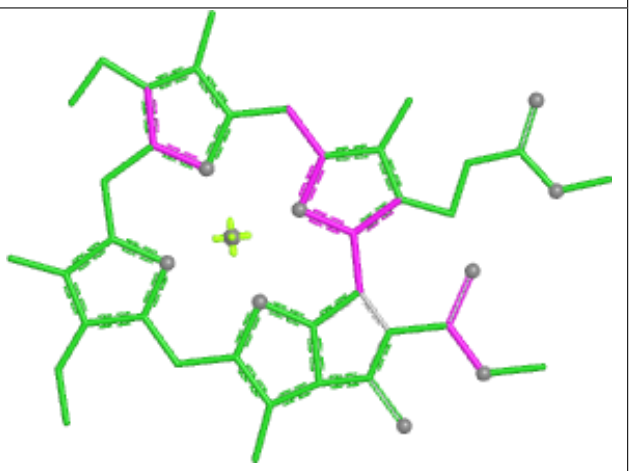
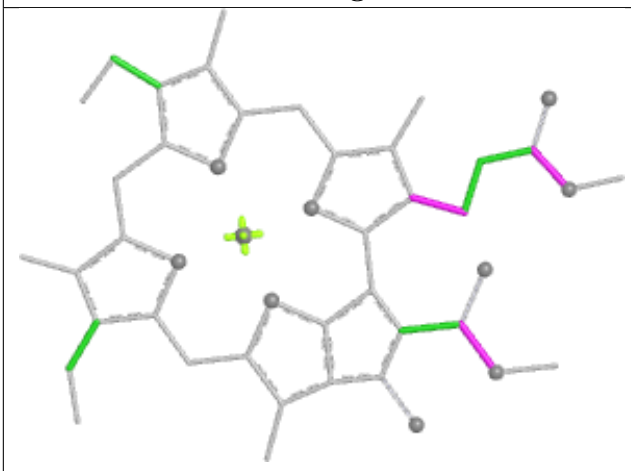


Bond angles



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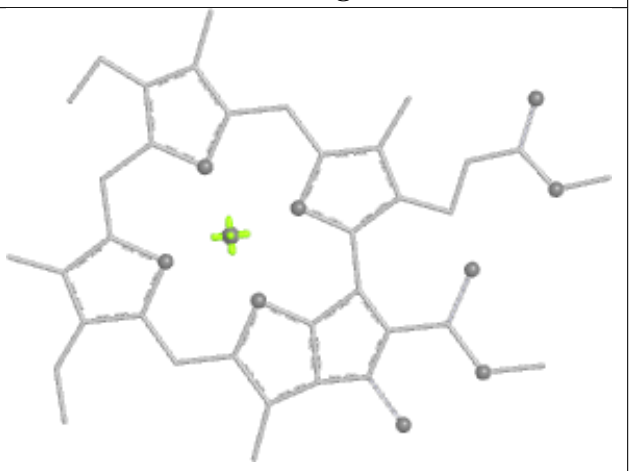
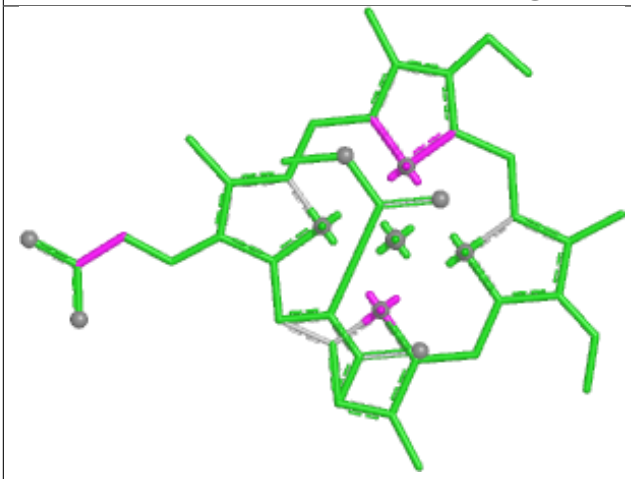


Rings

Ligand KC1 B 314



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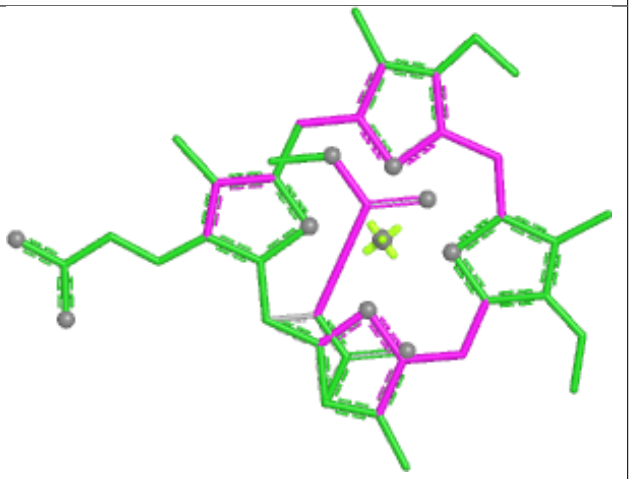

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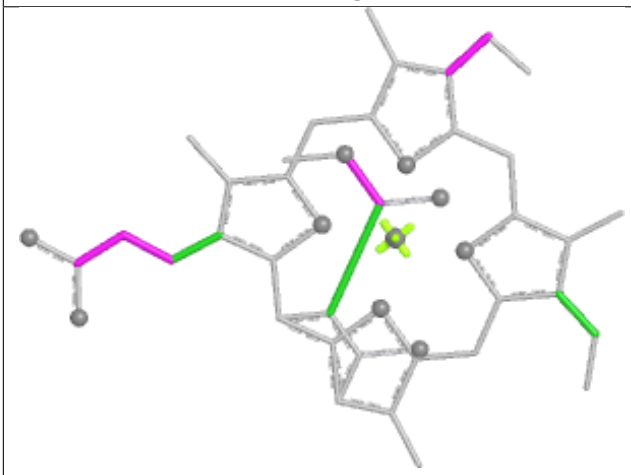

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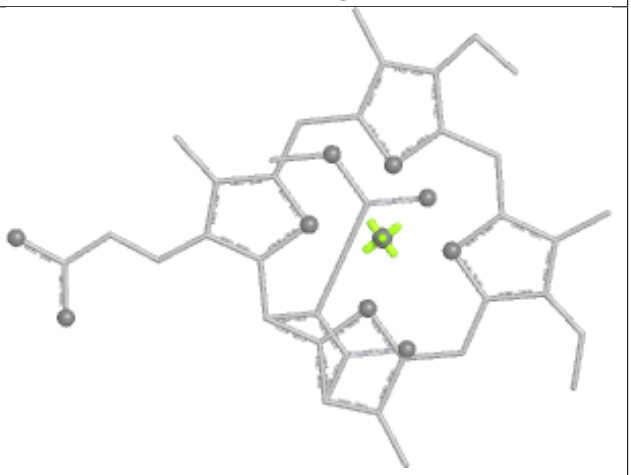
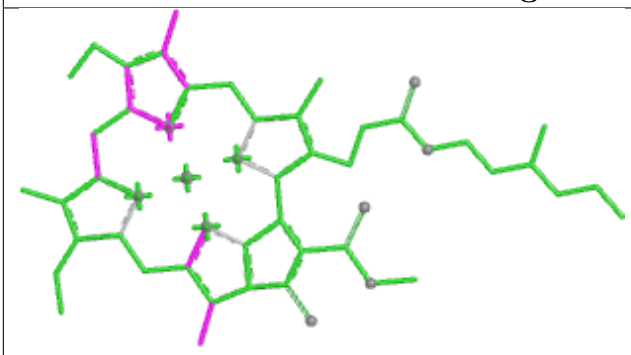
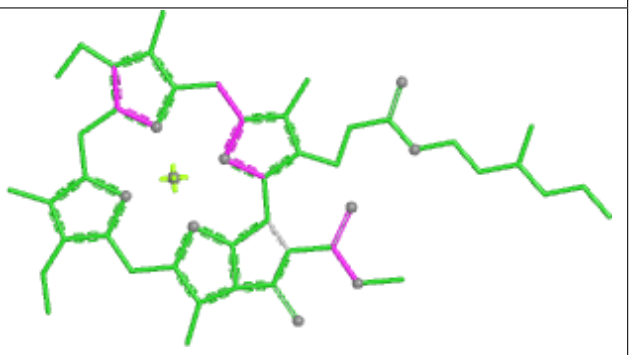


Rings

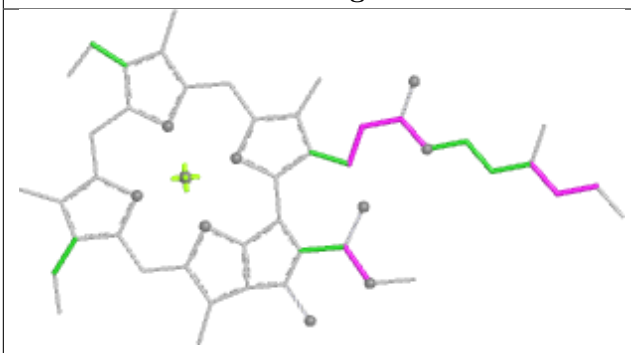
Ligand CLA M 316



Bond lengths



Bond angles



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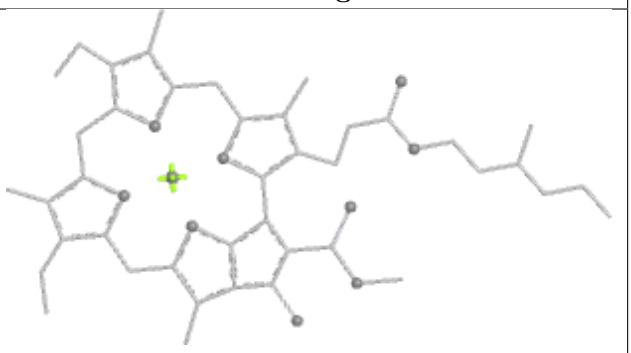
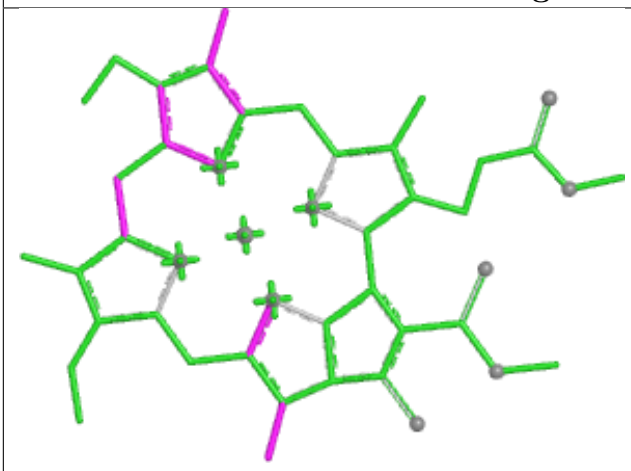


Rings

Ligand CLA l 312



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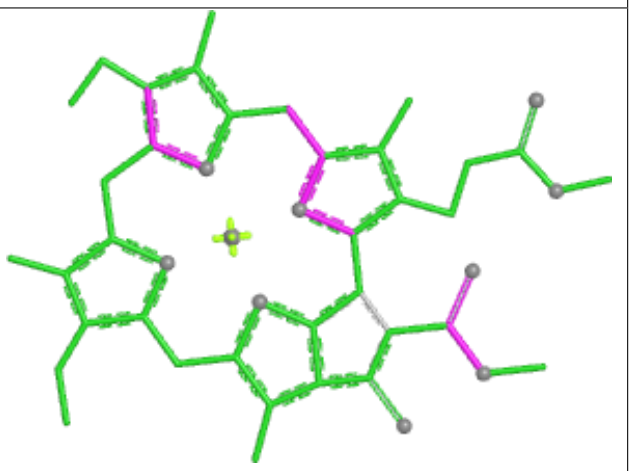
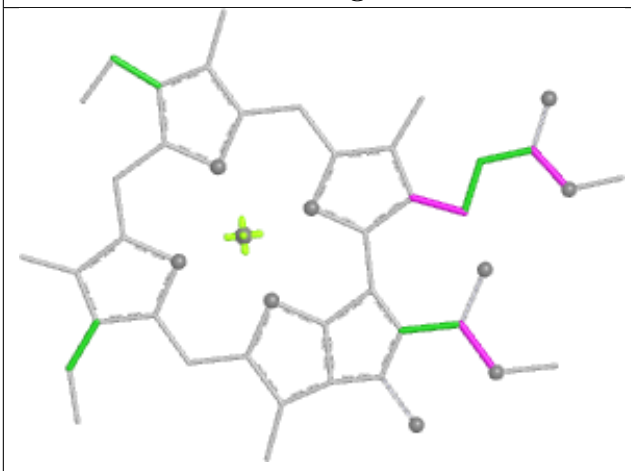


Bond angles



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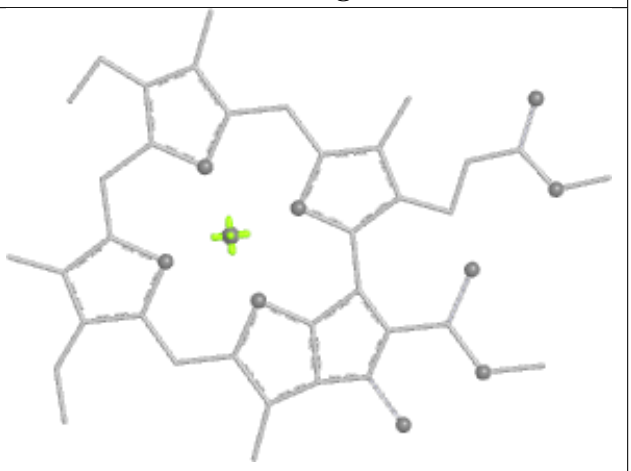
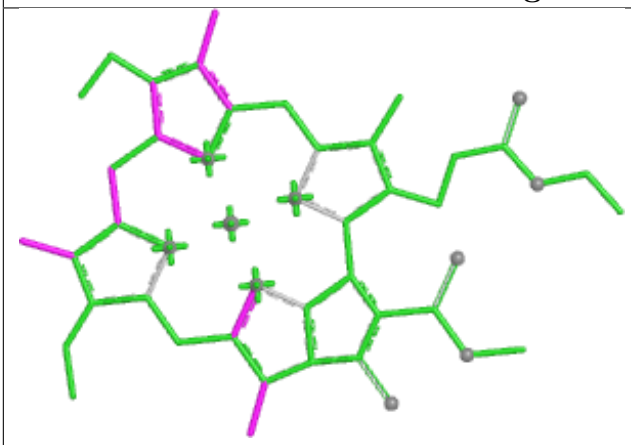


Rings

Ligand CLA O 314



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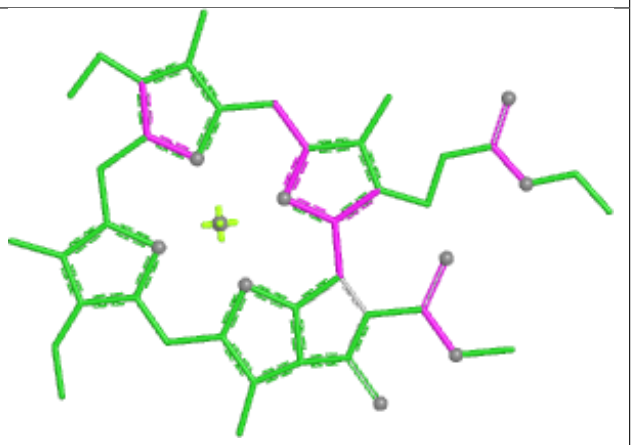
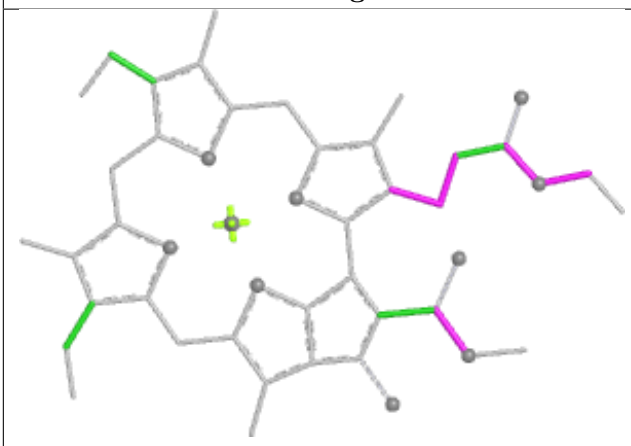


Bond angles



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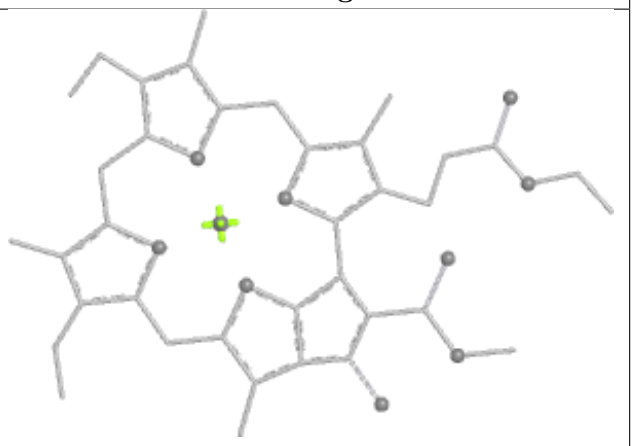
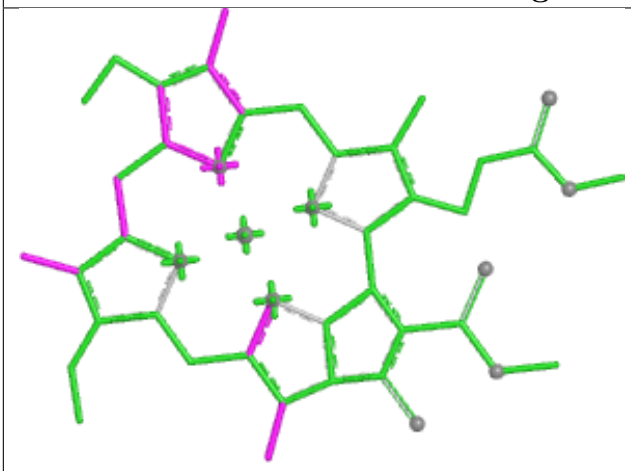


Rings

Ligand CLA f 303



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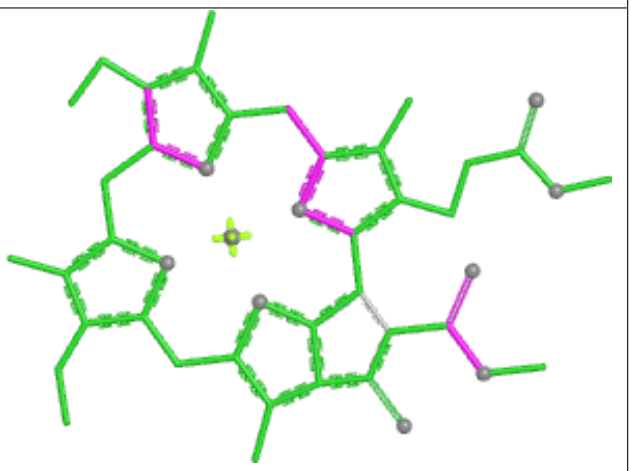
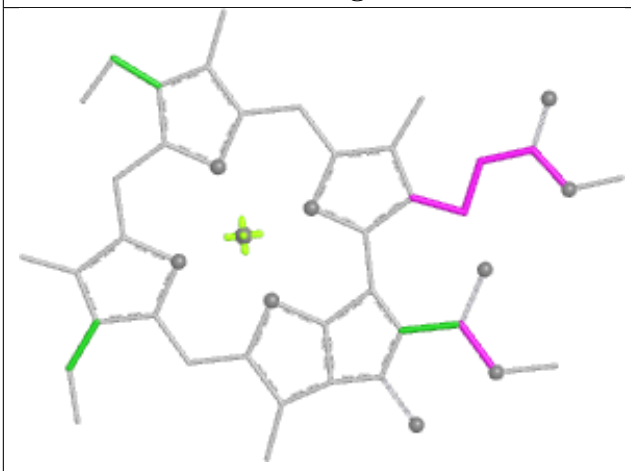


Bond angles



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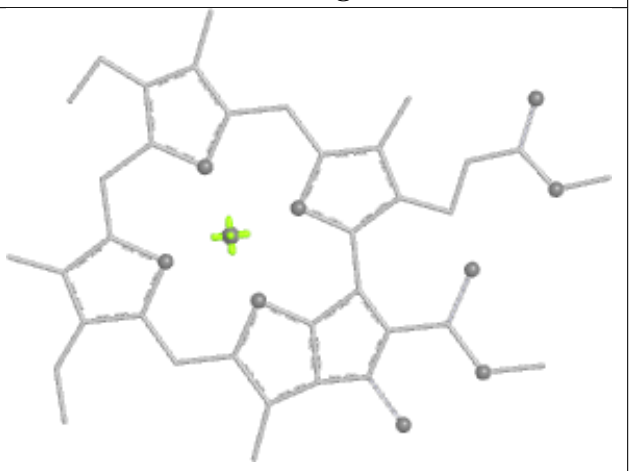
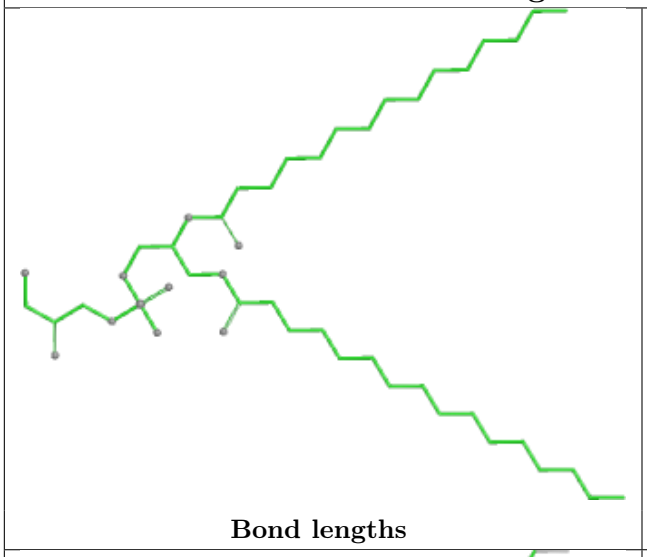


Rings

Ligand LHG a 733



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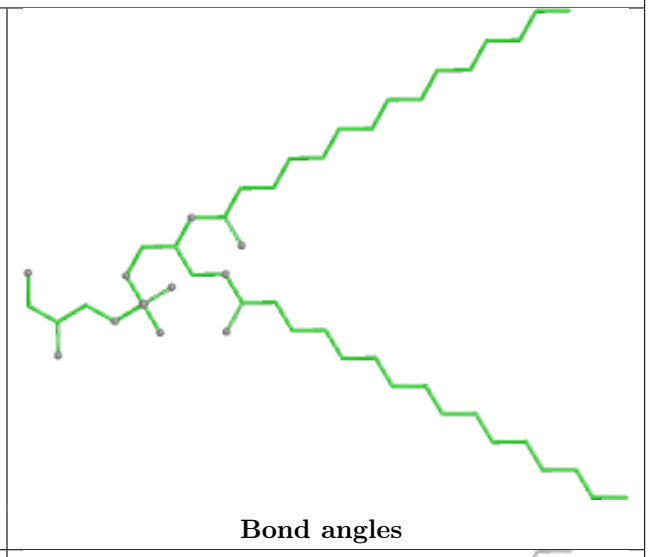
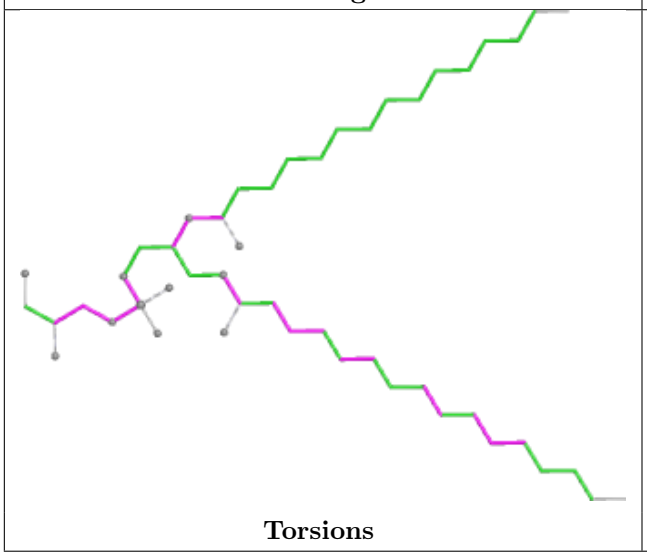
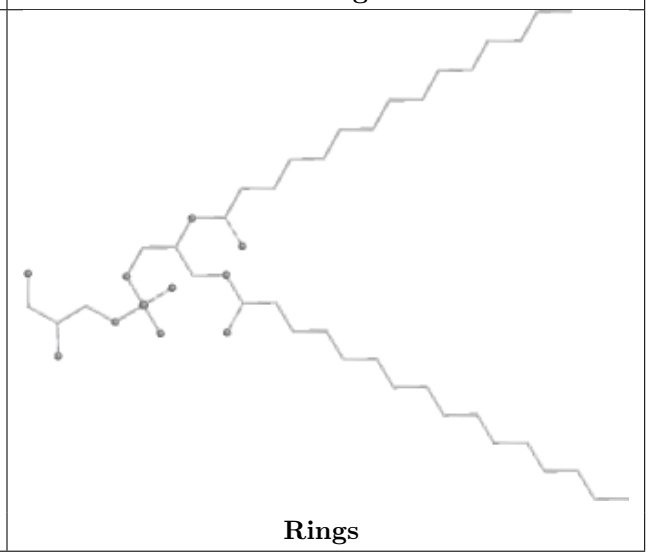


Bond angles

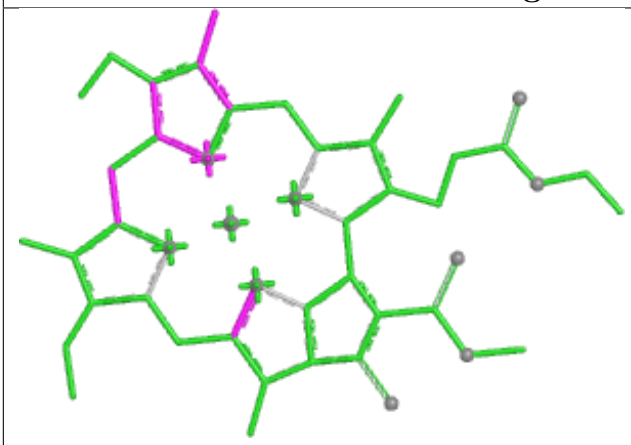


Torsions



Rings

Ligand CLA H 309



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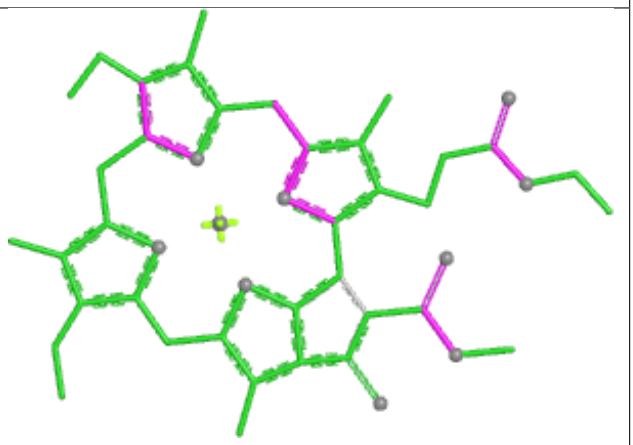
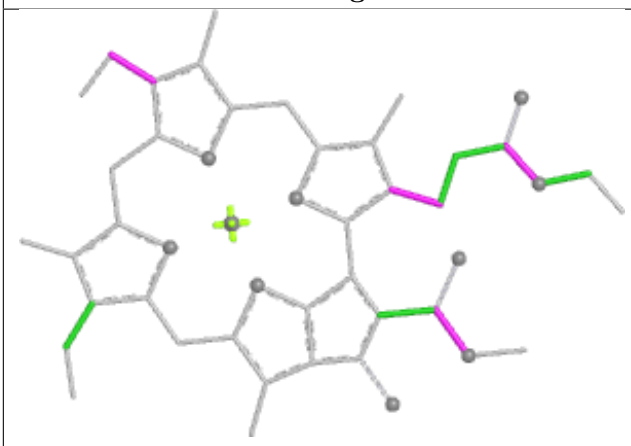


Bond angles



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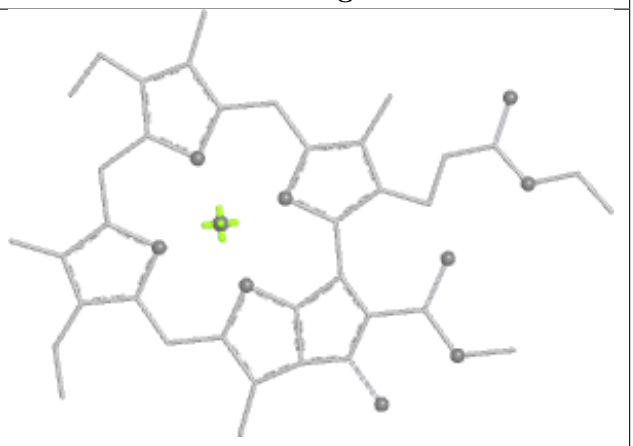
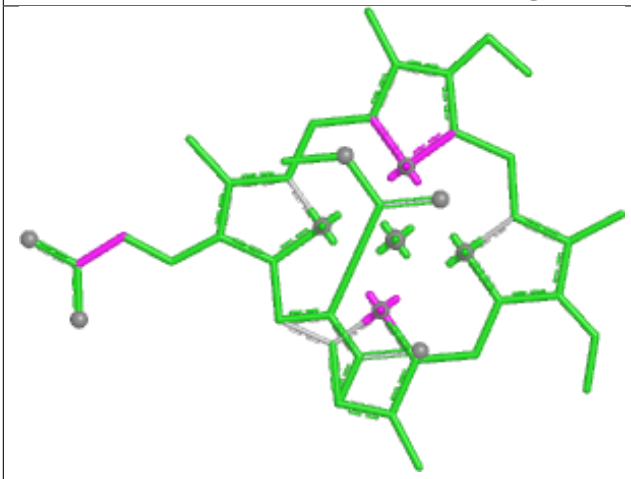


Rings

Ligand KC1 H 306



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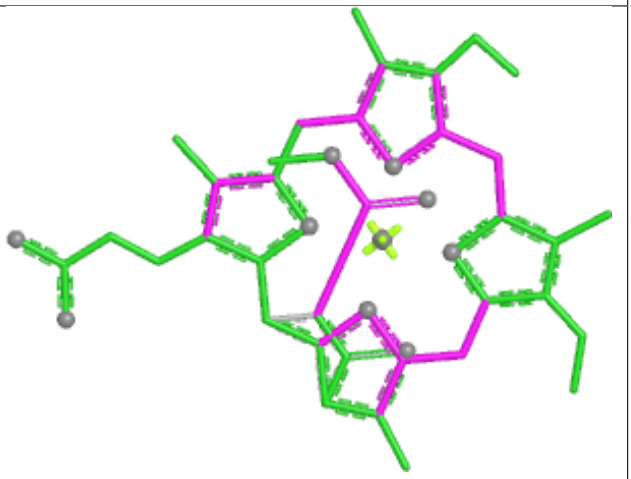
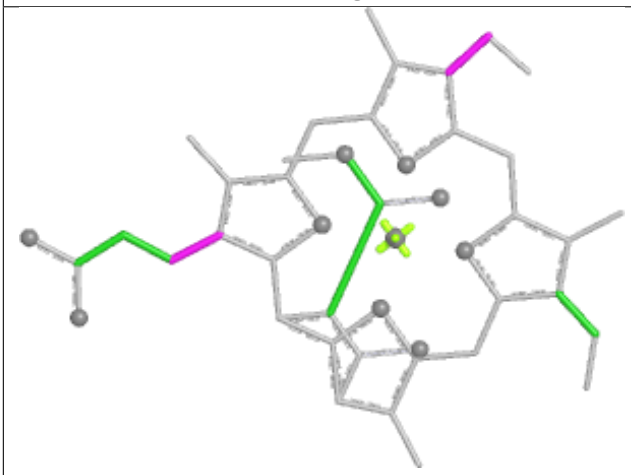


Bond angles



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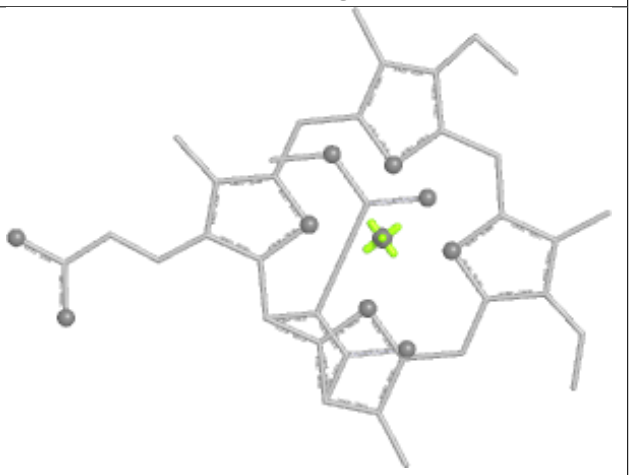
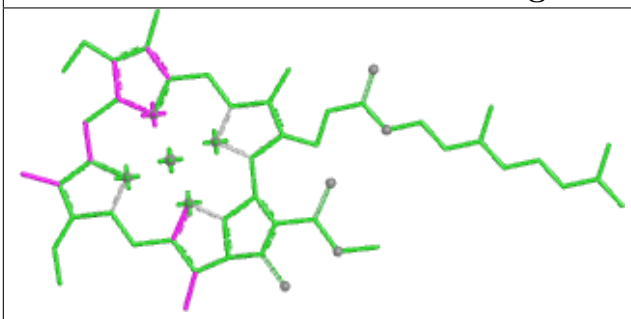


Rings

Ligand CLA a 710



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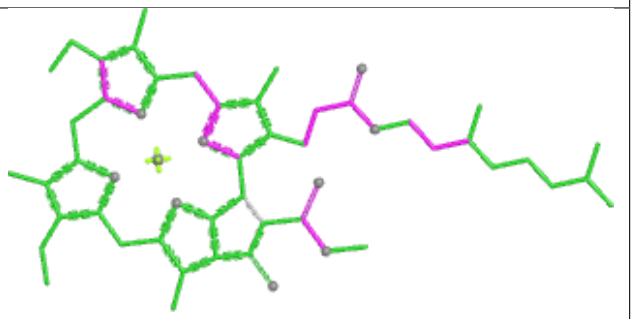
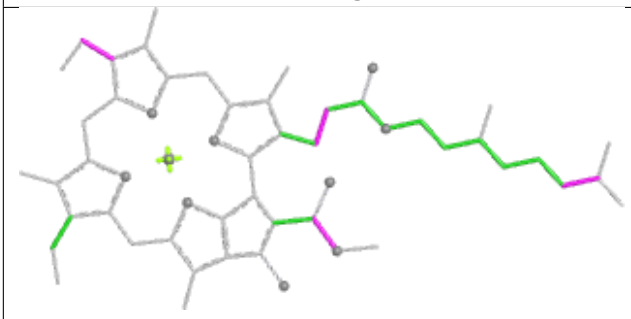


Bond angles



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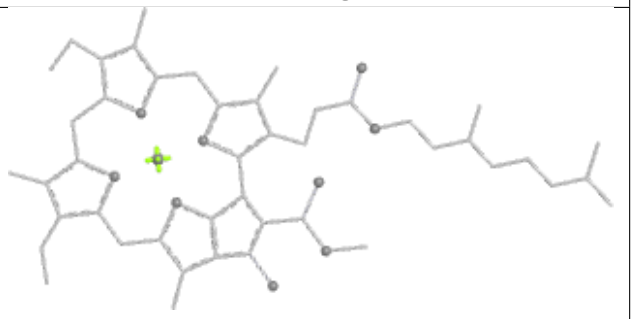
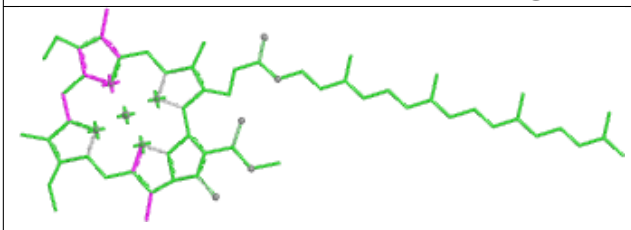
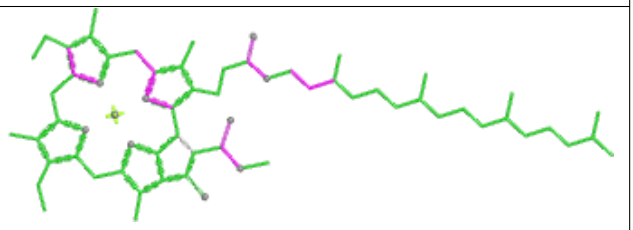


Rings

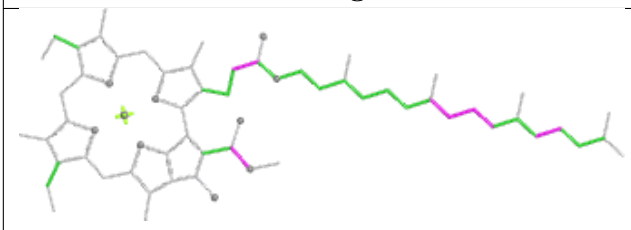
Ligand CLA b 713



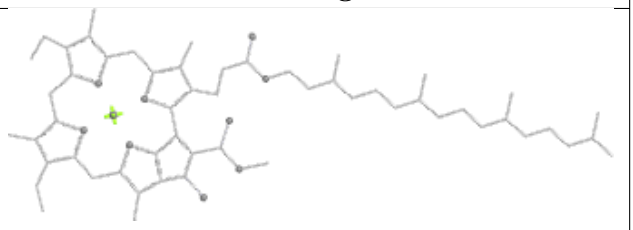
Bond lengths



Bond angles

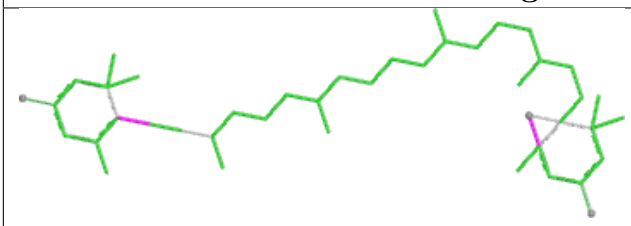


Torsions



Rings

Ligand DD6 M 306



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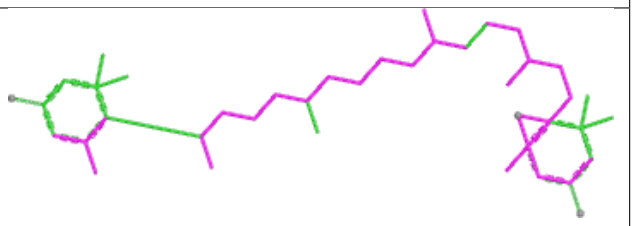
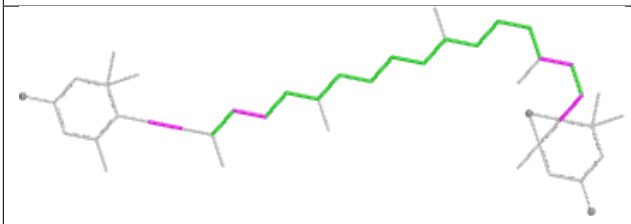
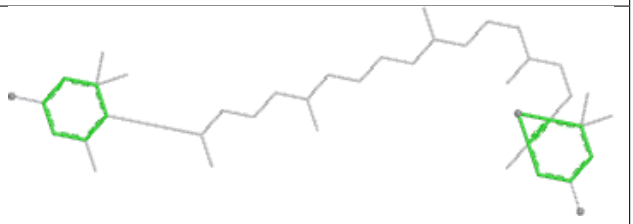


Bond angles

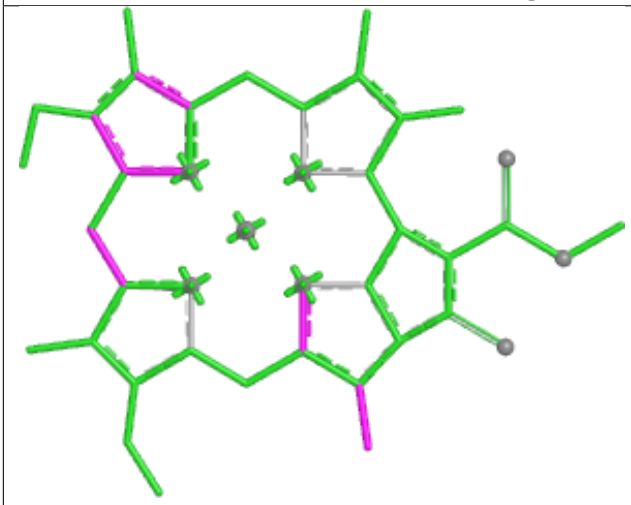


Torsions

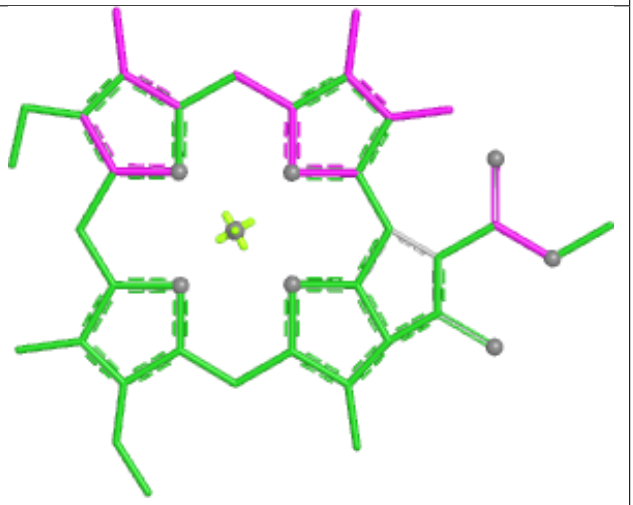


Rings

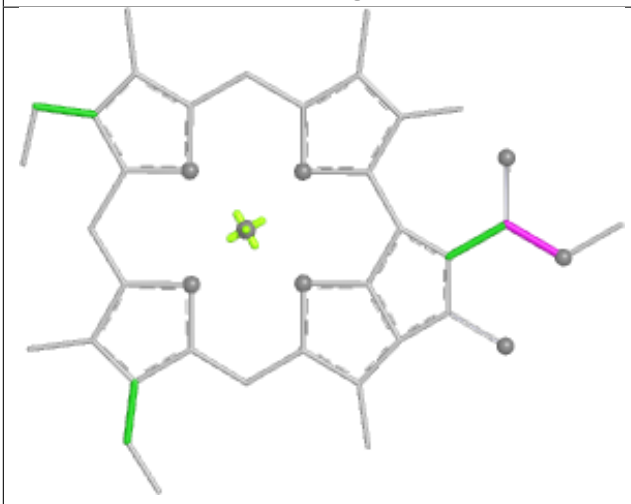
Ligand CLA K 315



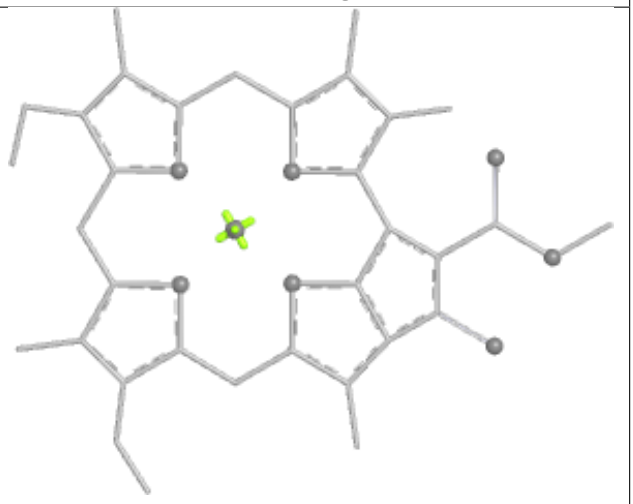
Bond lengths



Bond angles

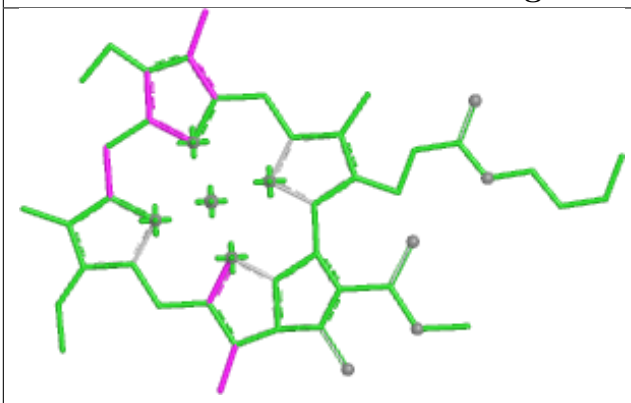


Torsions

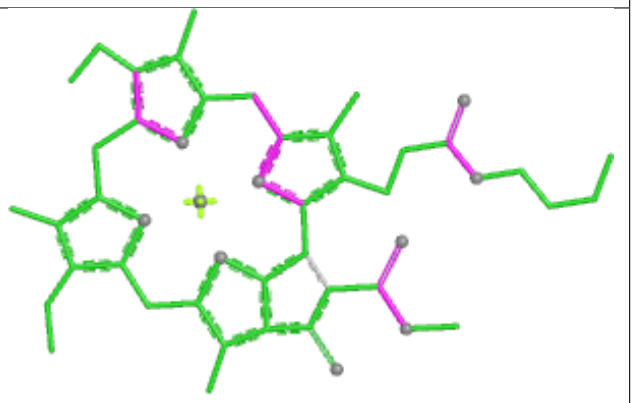


Rings

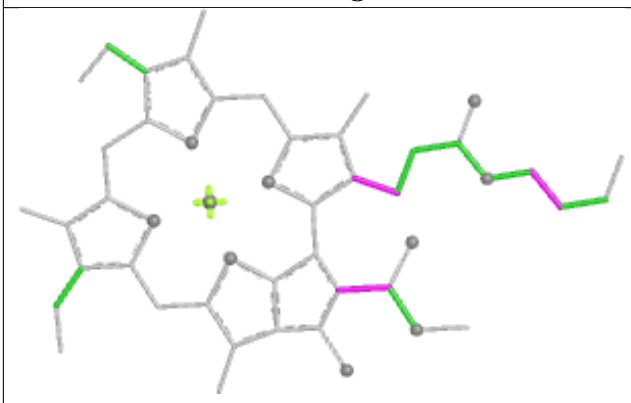
Ligand CLA B 307



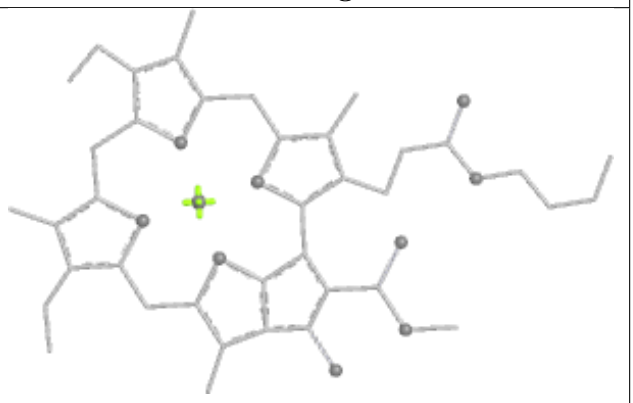
Bond lengths



Bond angles

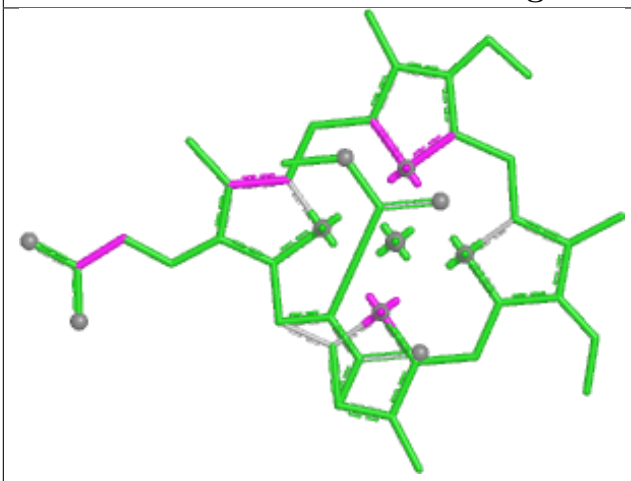


Torsions

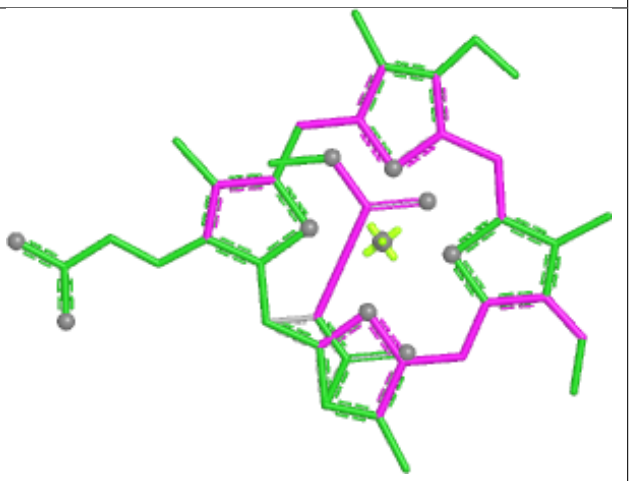


Rings

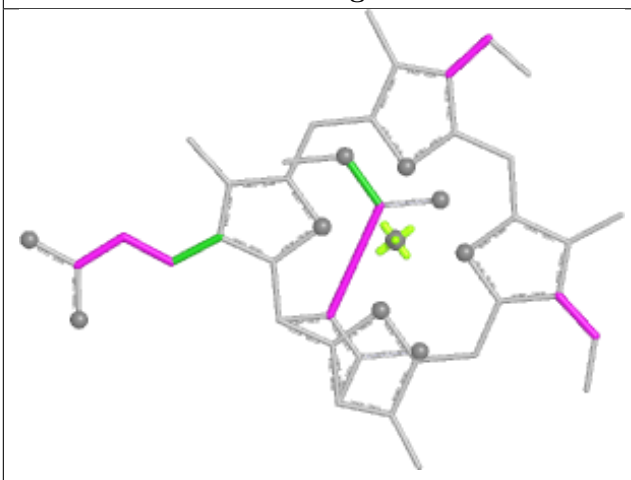
Ligand KC1 P 213



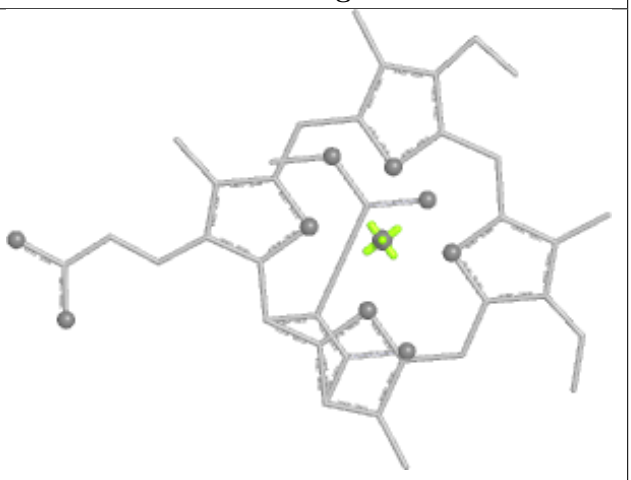
Bond lengths



Bond angles

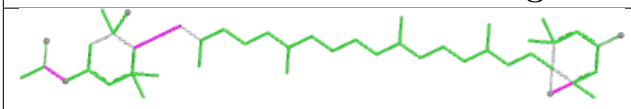


Torsions

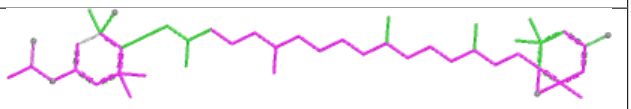


Rings

Ligand UIX K 302

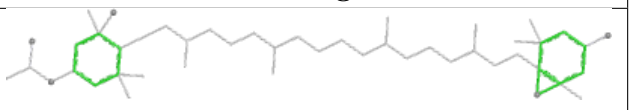


Bond lengths



Bond angles

Torsions

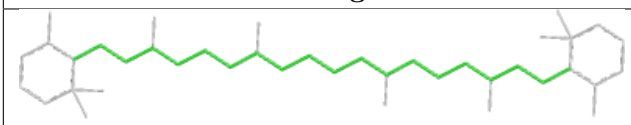


Rings

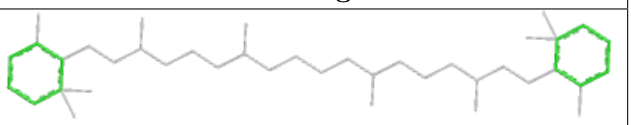
Ligand BCR b 732

Bond lengths

Bond angles

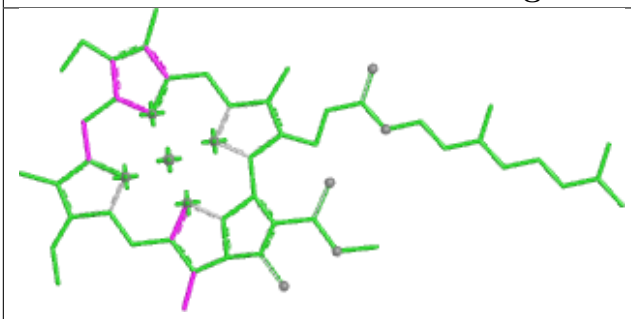


Torsions

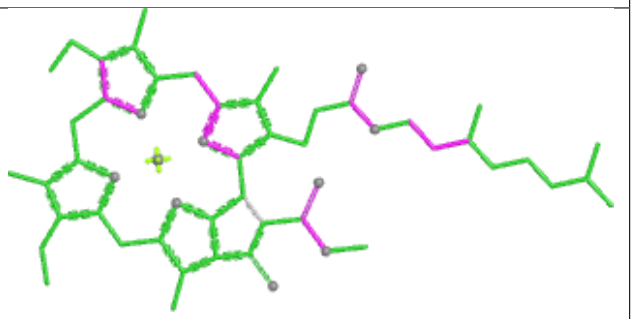


Rings

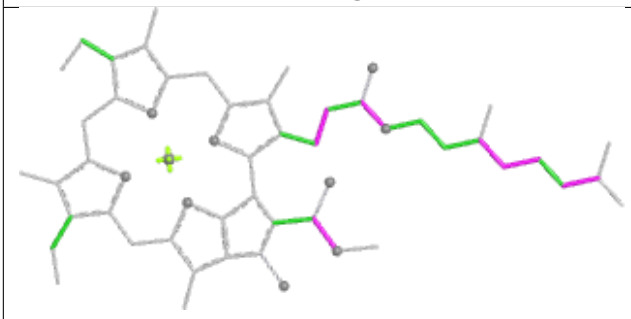
Ligand CLA A 313



Bond lengths



Bond angles



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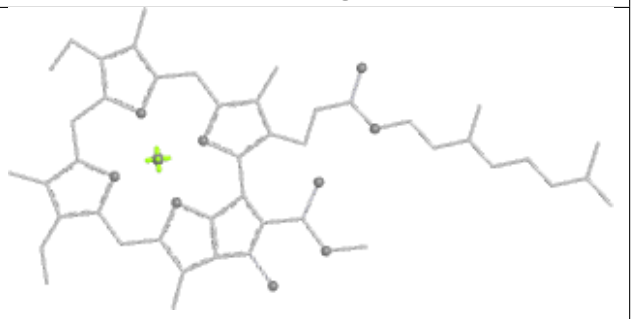
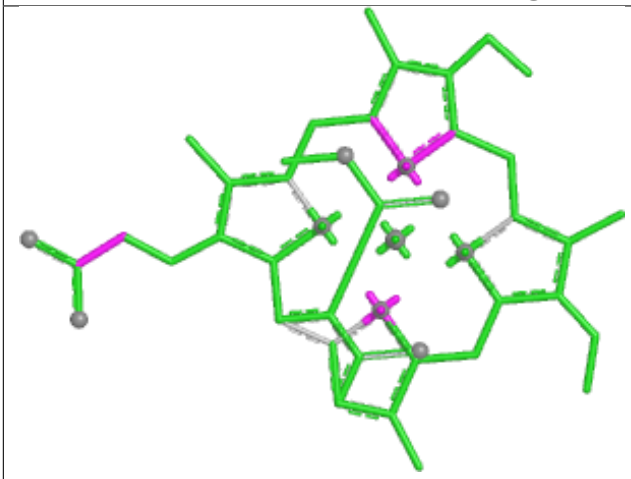
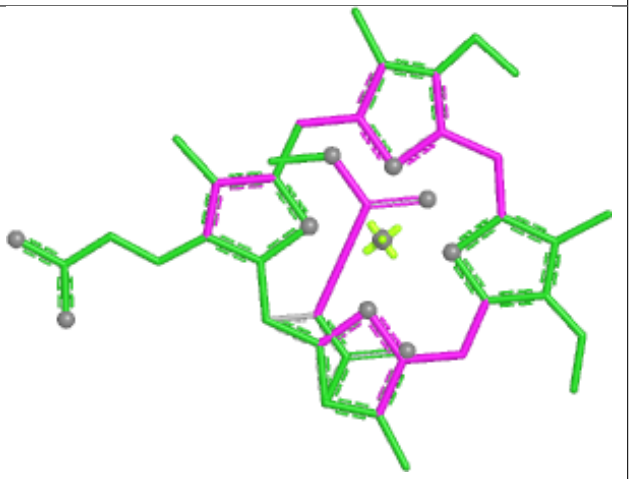


Rings

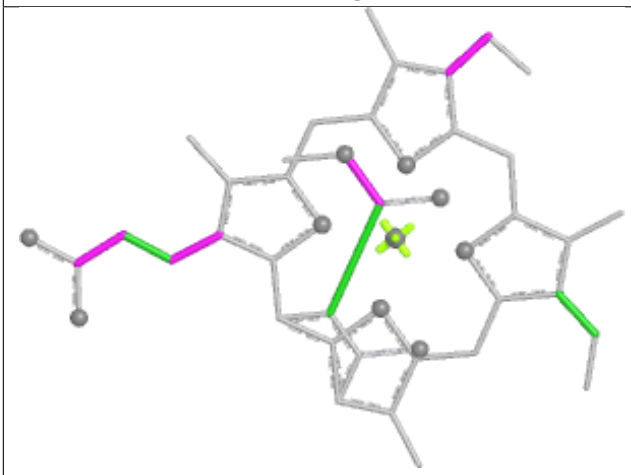
Ligand KC1 N 306



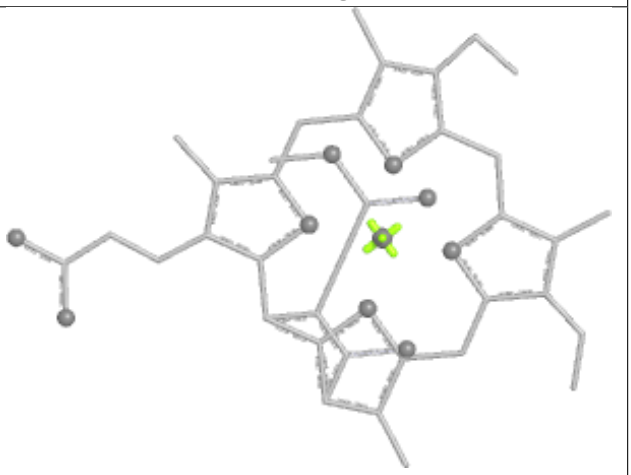
Bond lengths



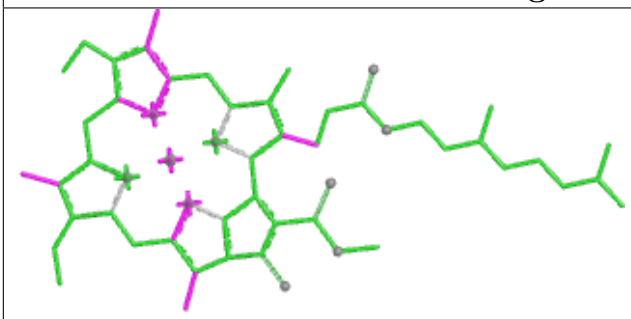
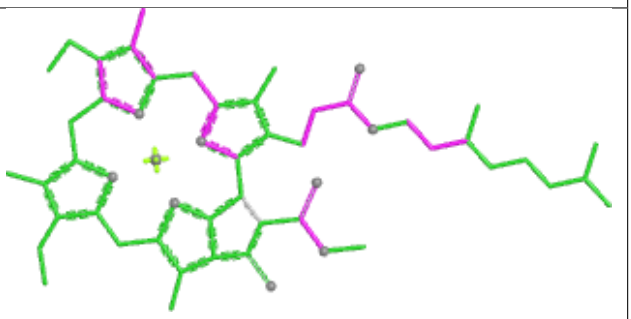
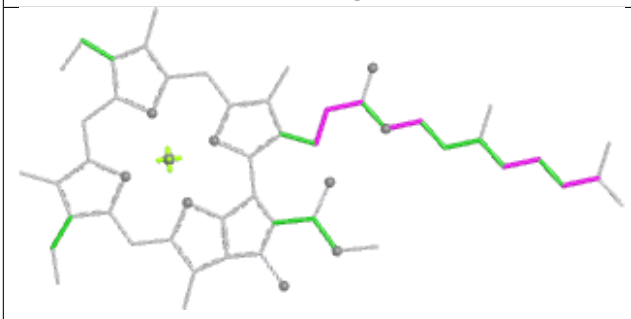
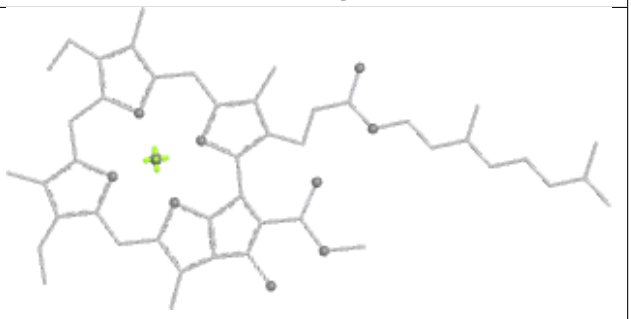
Bond angles

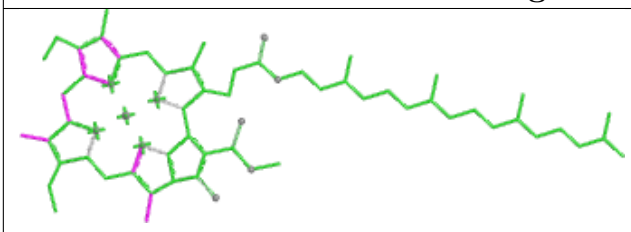
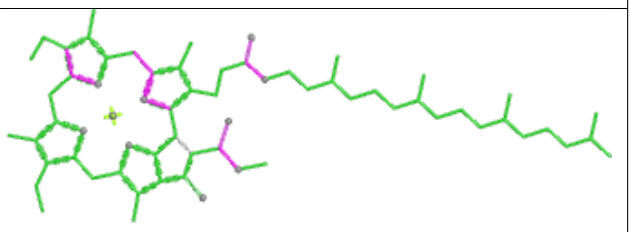
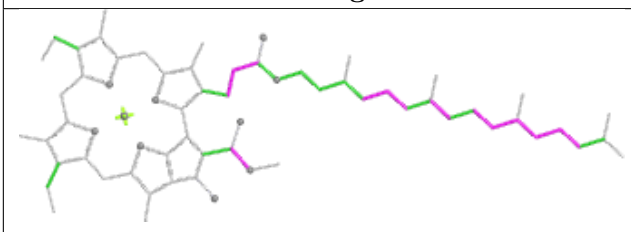
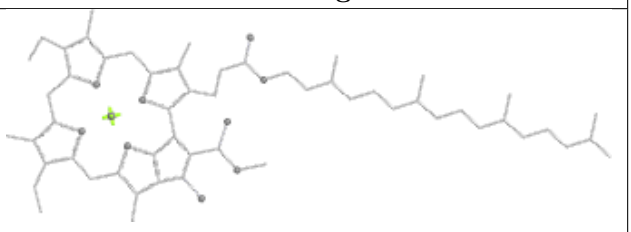


Torsions

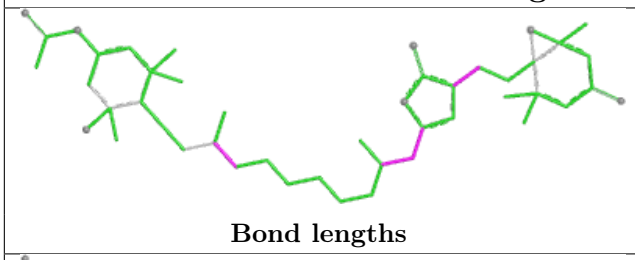


Rings

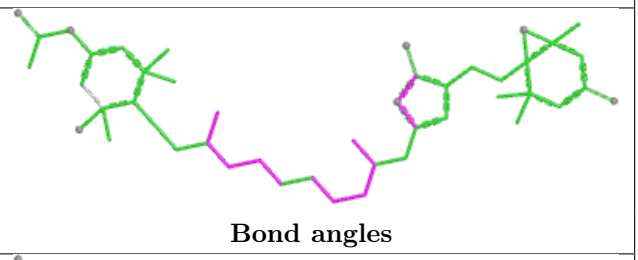
Ligand CLA a 703	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 723	
	
Bond lengths	Bond angles
	
Torsions	Rings

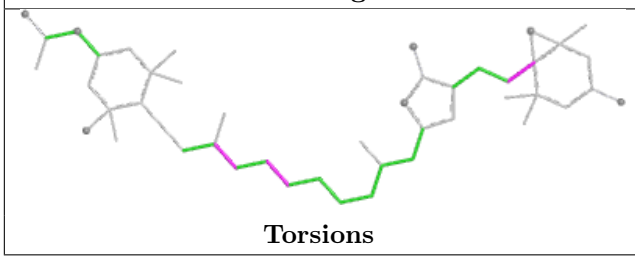
Ligand PID D 307



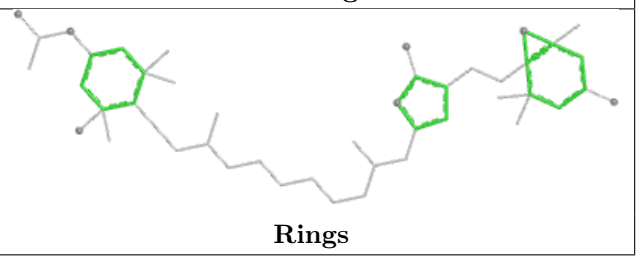
Bond lengths



Bond angles

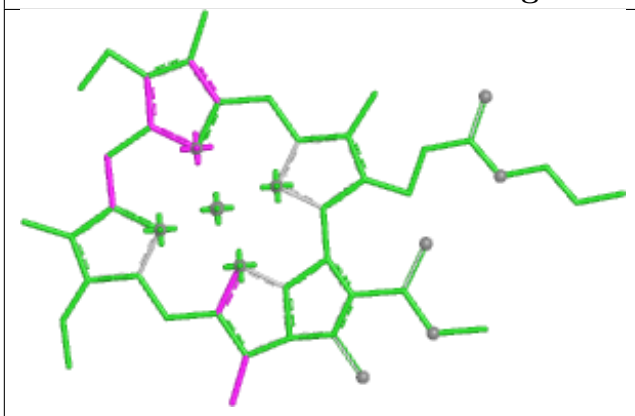


Torsions

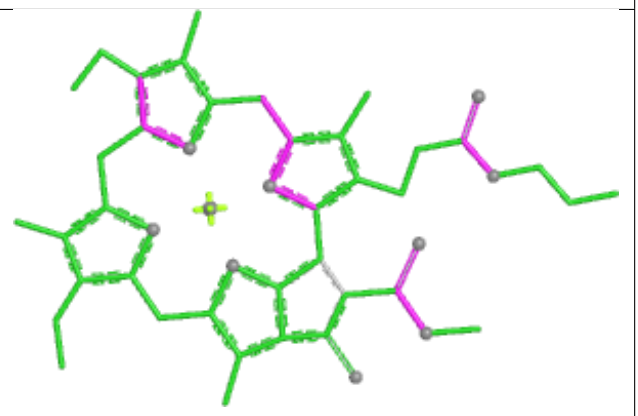


Rings

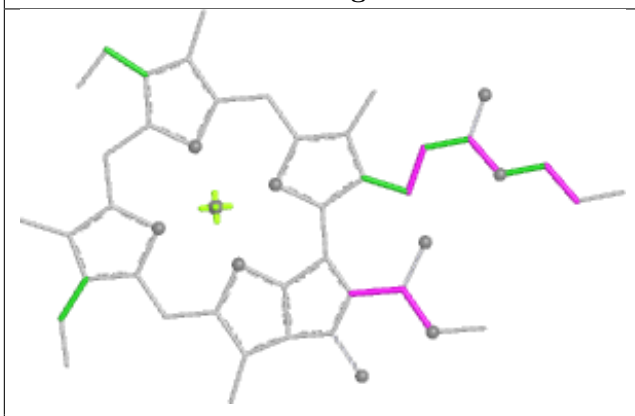
Ligand CLA M 310



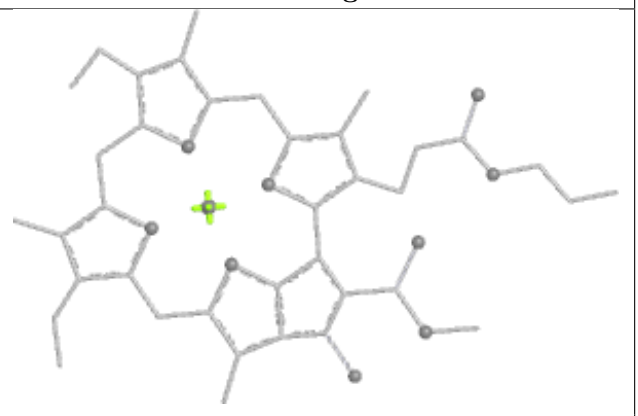
Bond lengths



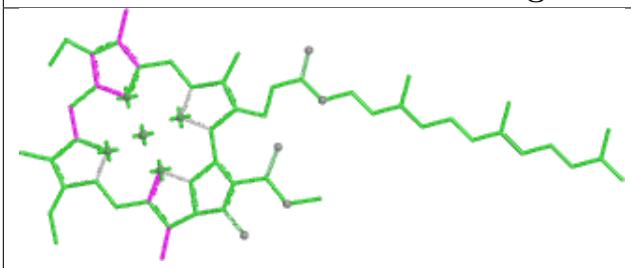
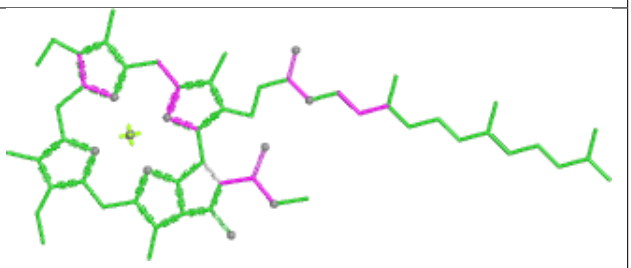
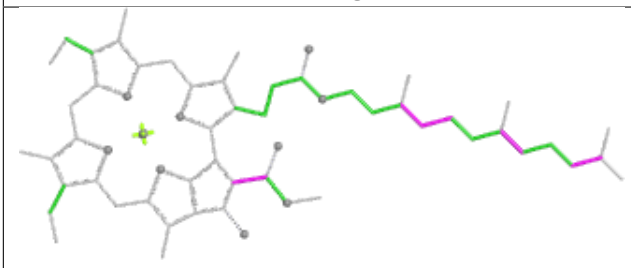
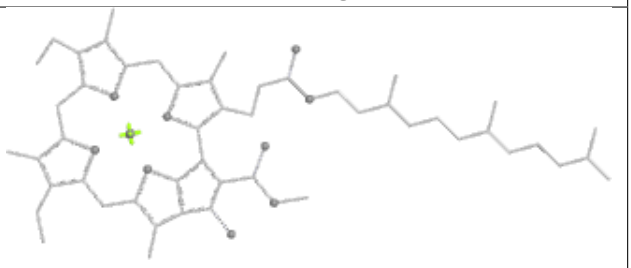
Bond angles

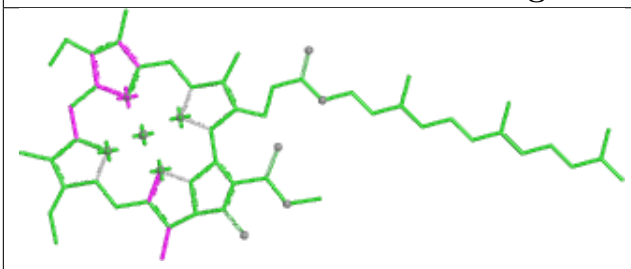
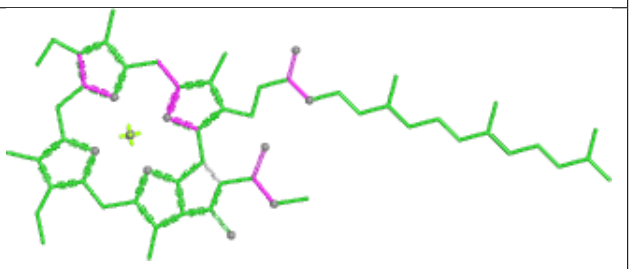
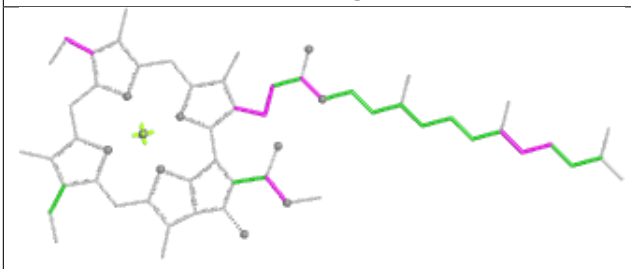
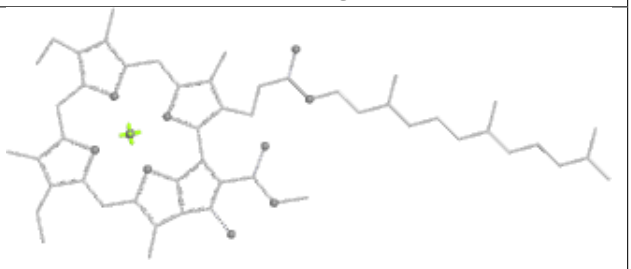


Torsions

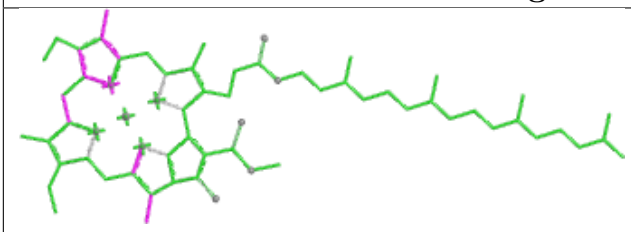


Rings

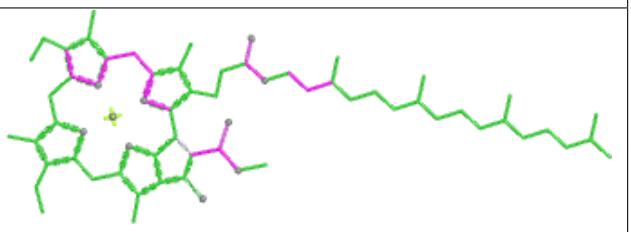
Ligand CLA b 709	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA J 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

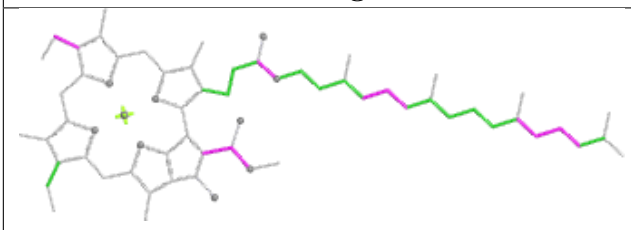
Ligand CLA a 726



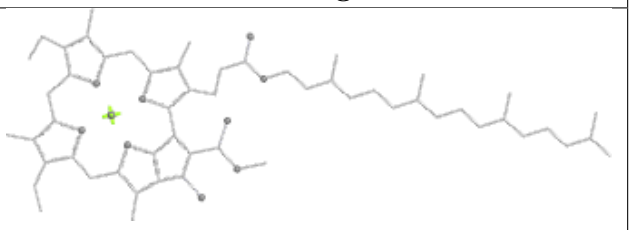
Bond lengths



Bond angles

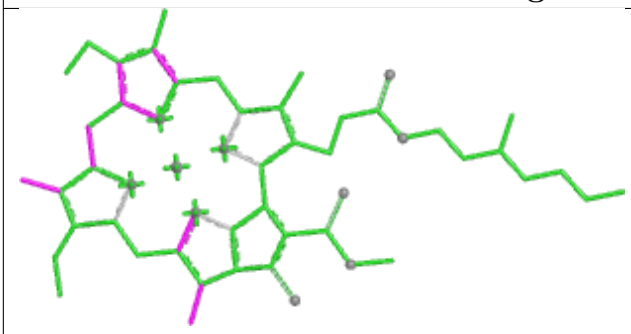


Torsions

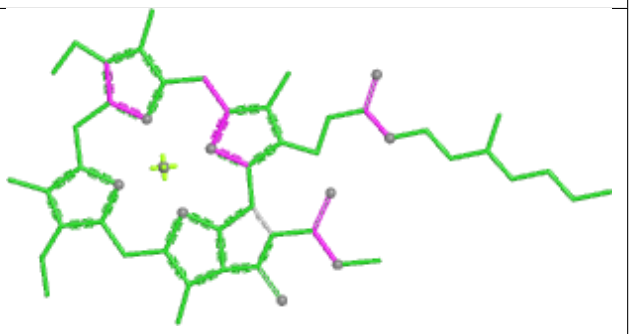


Rings

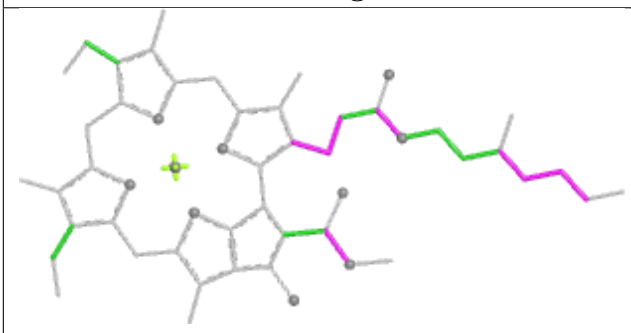
Ligand CLA b 720



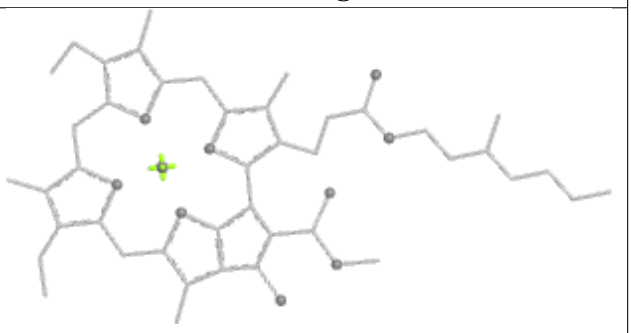
Bond lengths



Bond angles

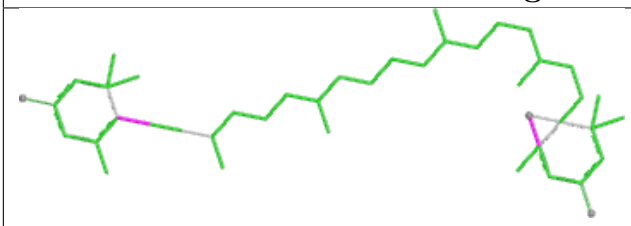


Torsions

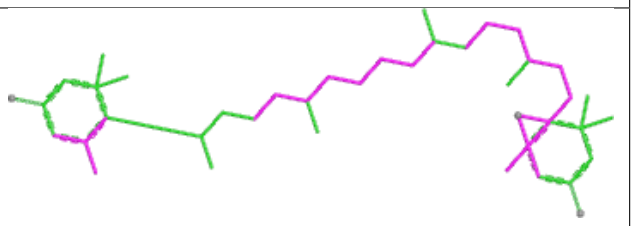


Rings

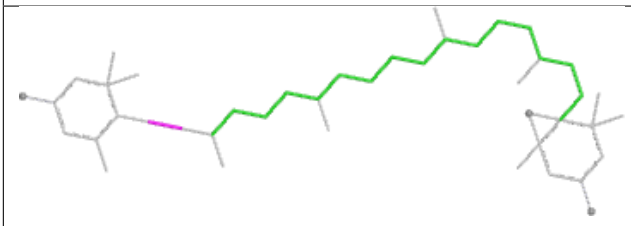
Ligand DD6 G 508



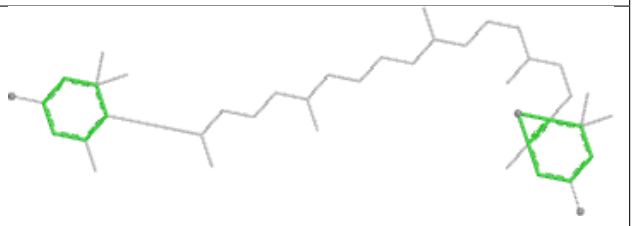
Bond lengths



Bond angles

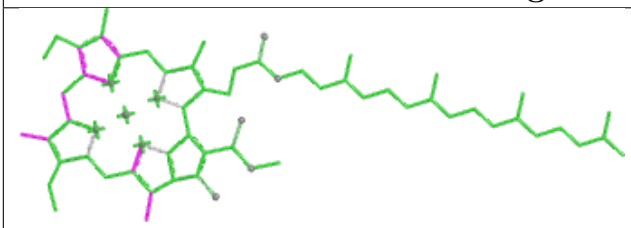


Torsions



Rings

Ligand CLA b 703



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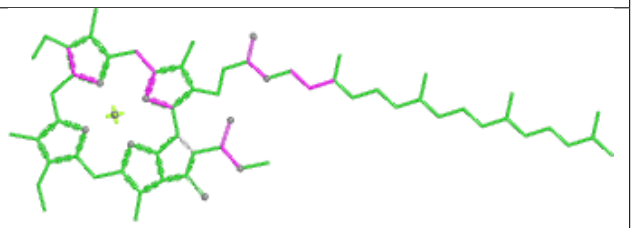
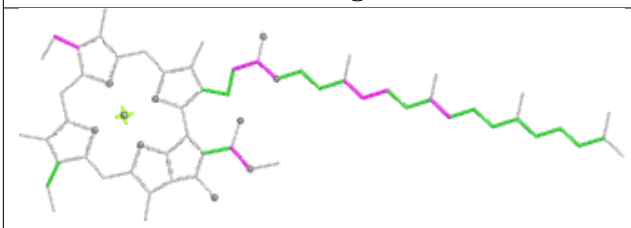
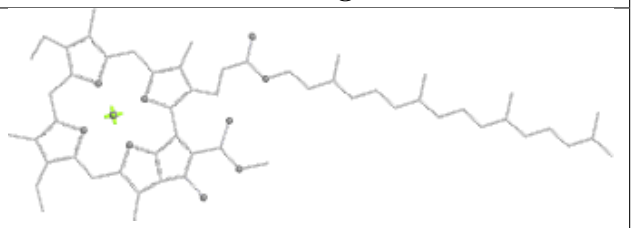


Bond angles

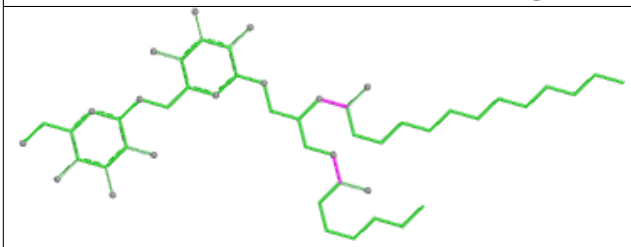


Torsions



Rings

Ligand DGD l 301



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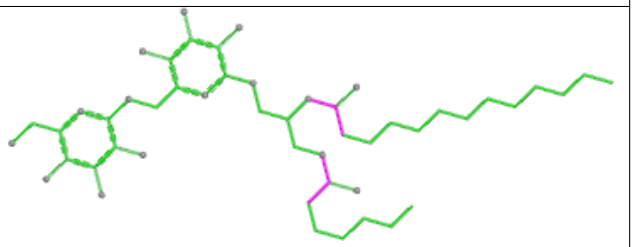
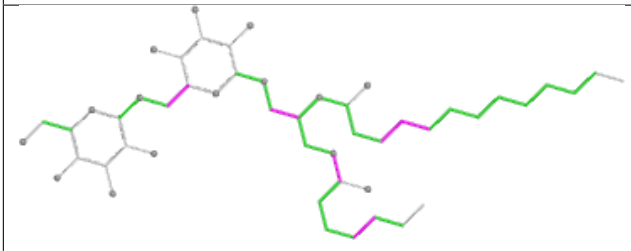


Bond angles



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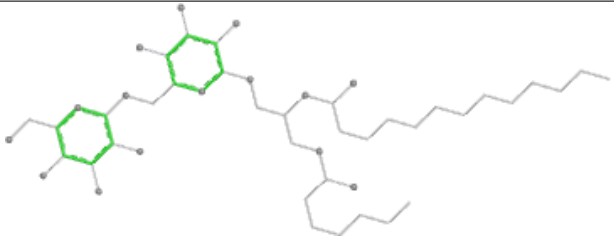
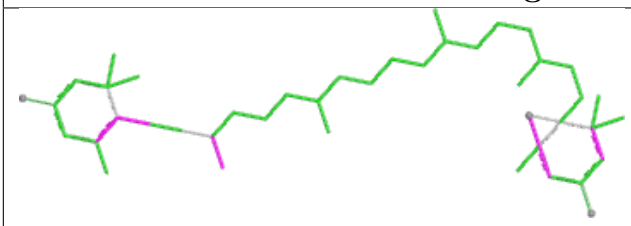


Rings

Ligand DD6 G 504



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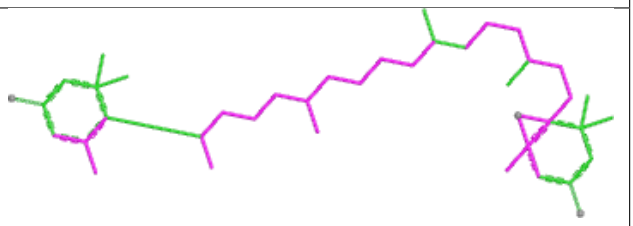
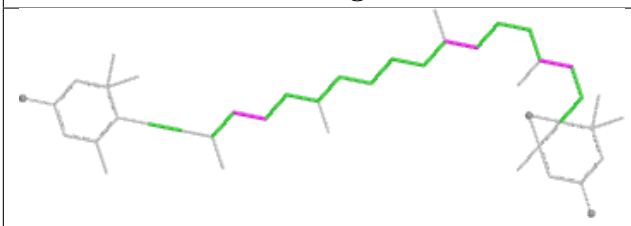


Bond angles



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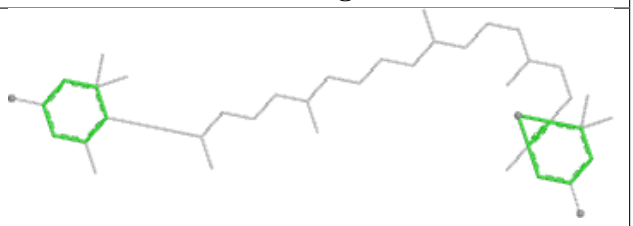
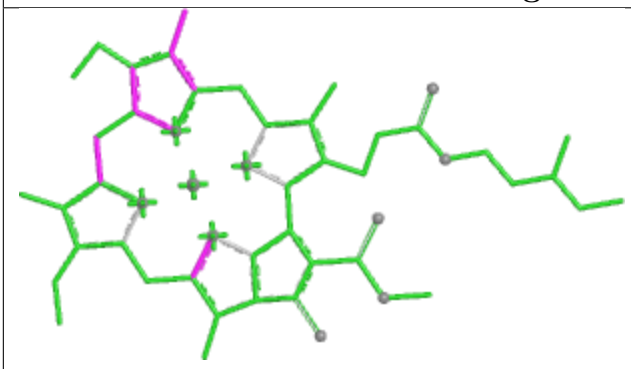


Rings

Ligand CLA G 509



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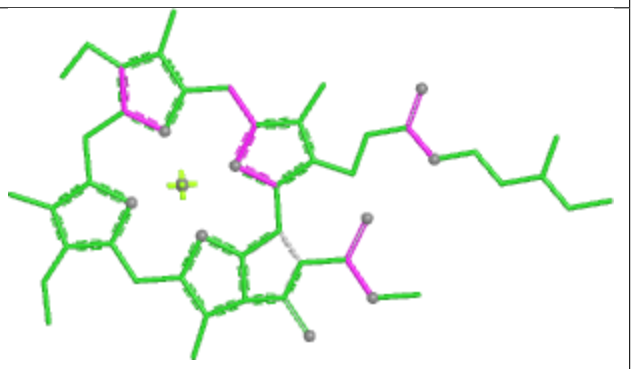
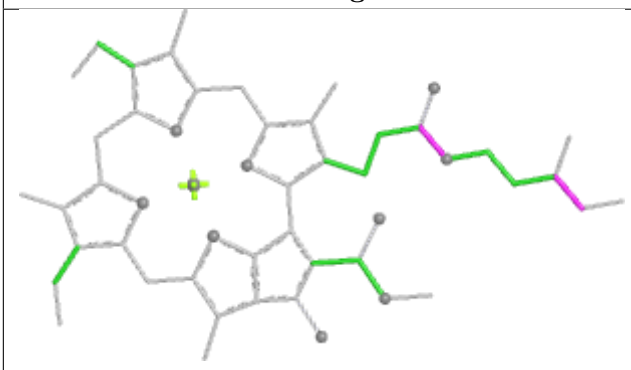


Bond angles



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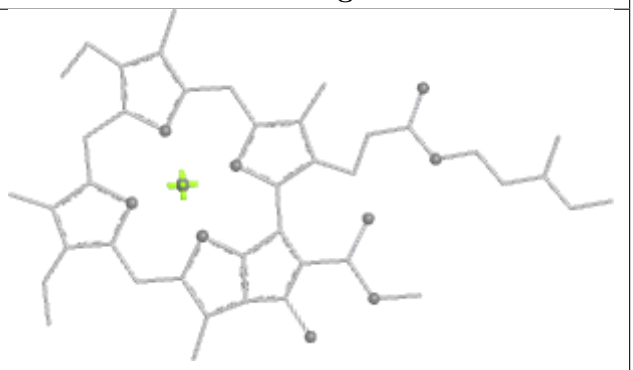
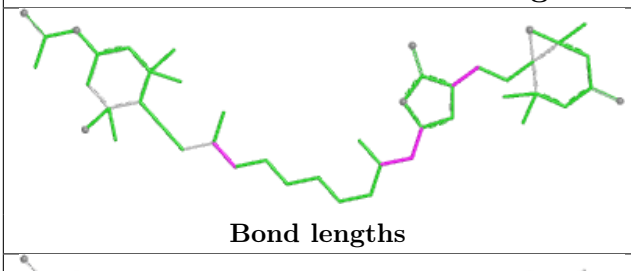


Rings

Ligand PID F 305



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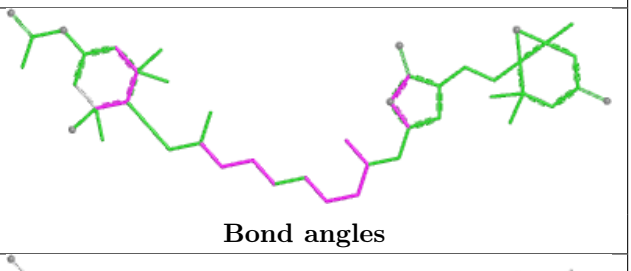
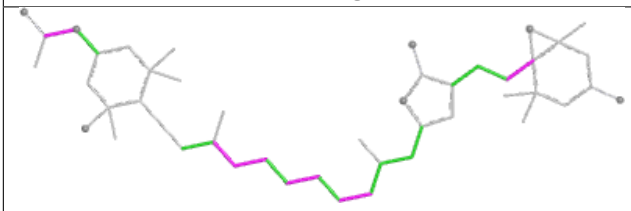


Bond angles



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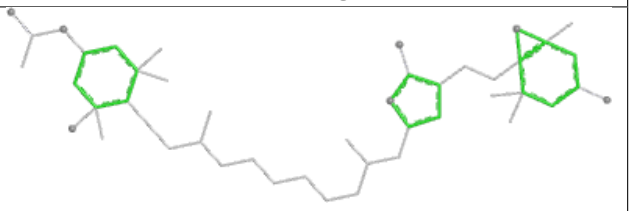
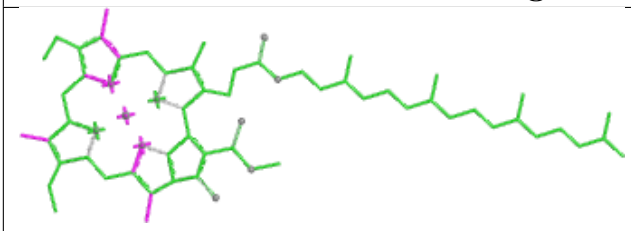


Rings

Ligand CLA b 704



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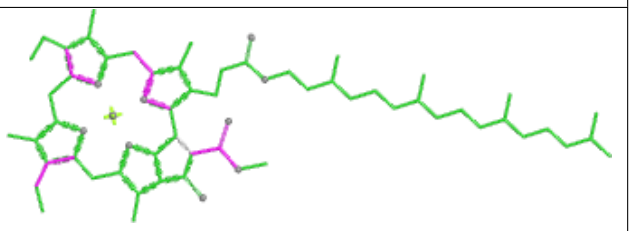
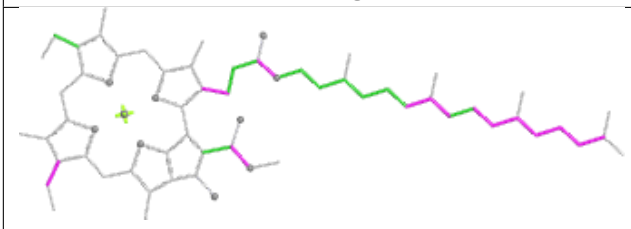


Bond angles



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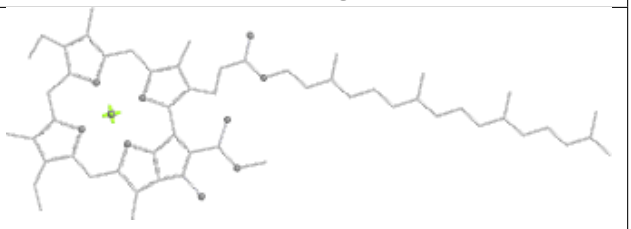
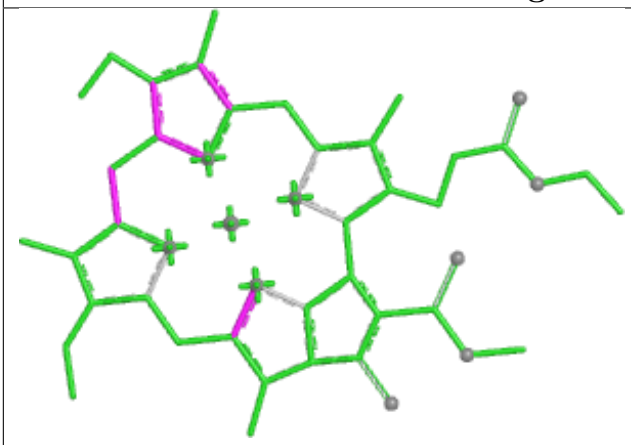


Rings

Ligand CLA J 311



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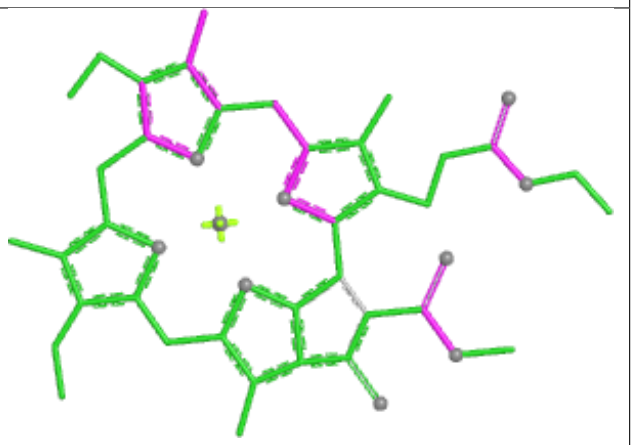
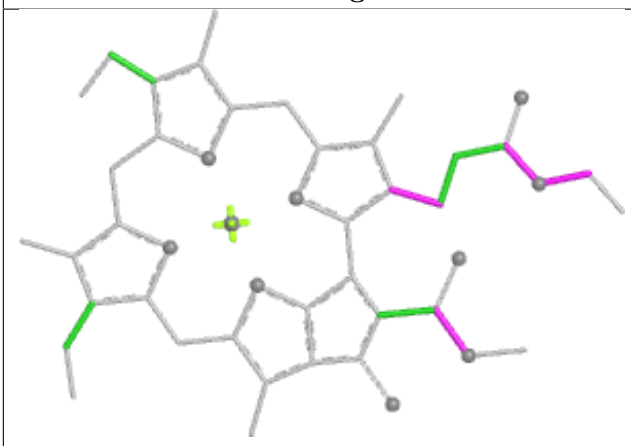


Bond angles



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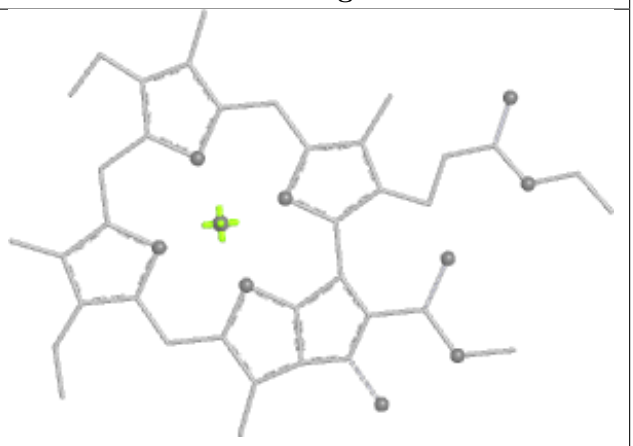
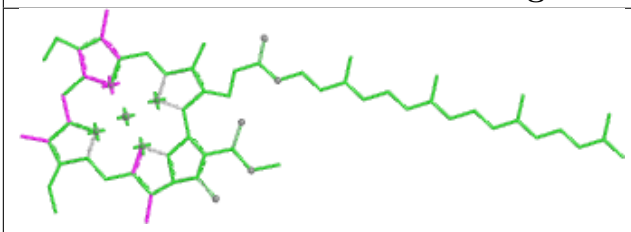


Rings

Ligand CLA b 717



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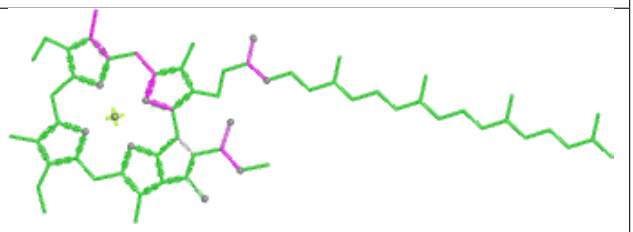
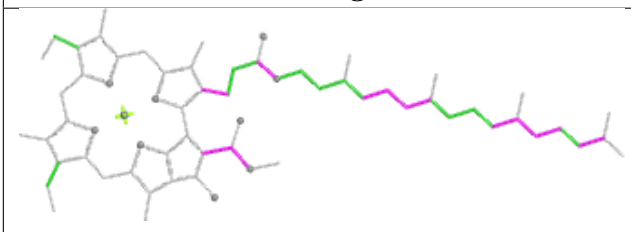


Bond angles



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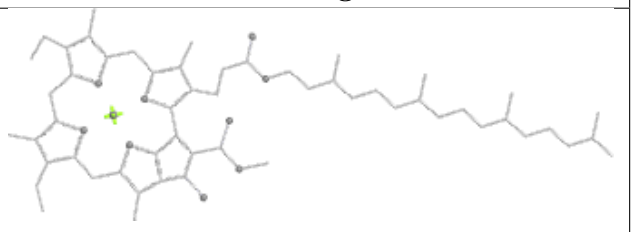
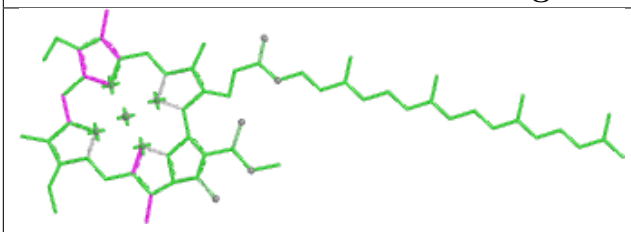


Rings

Ligand CLA l 303



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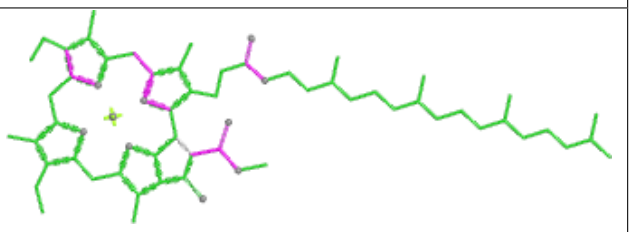
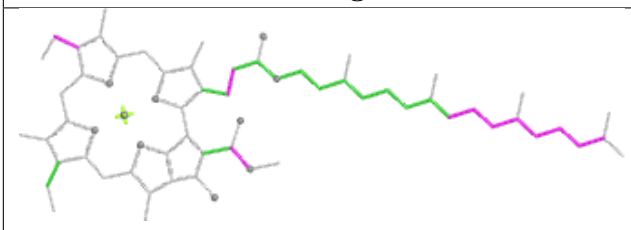


Bond angles



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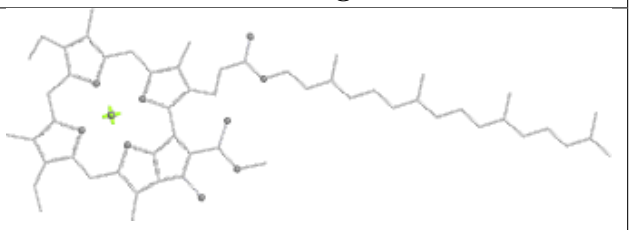
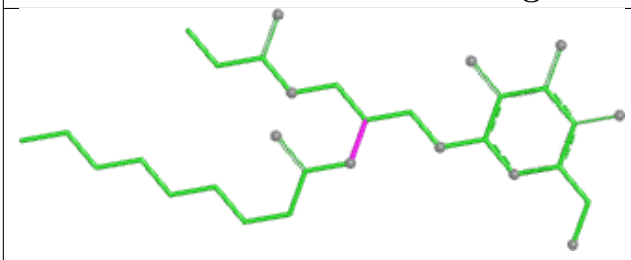


Rings

Ligand LMG b 734



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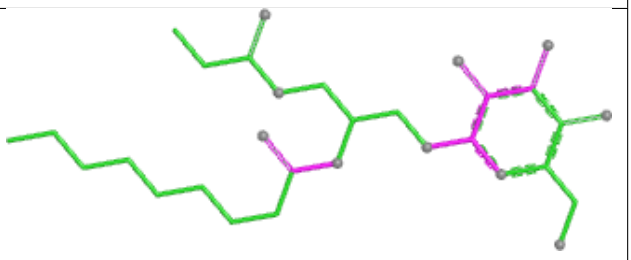
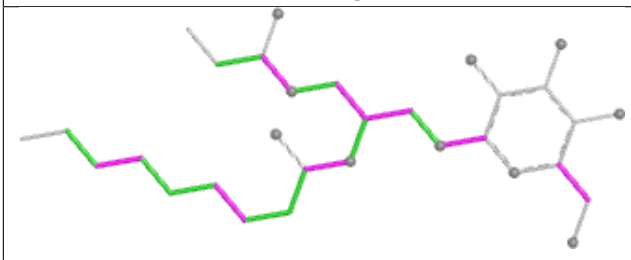


Bond angles



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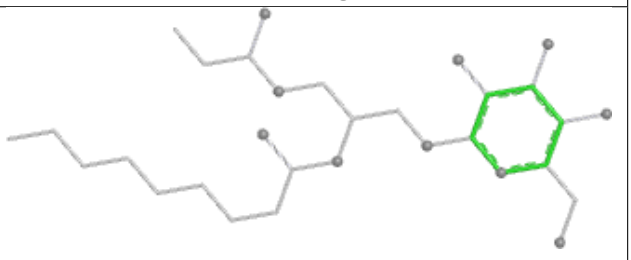
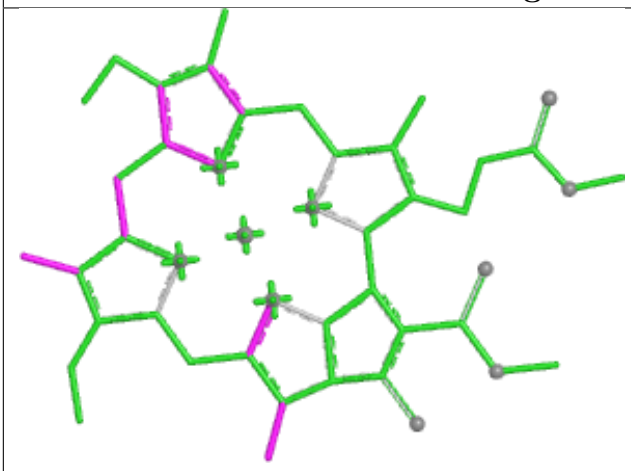


Rings

Ligand CLA A 319



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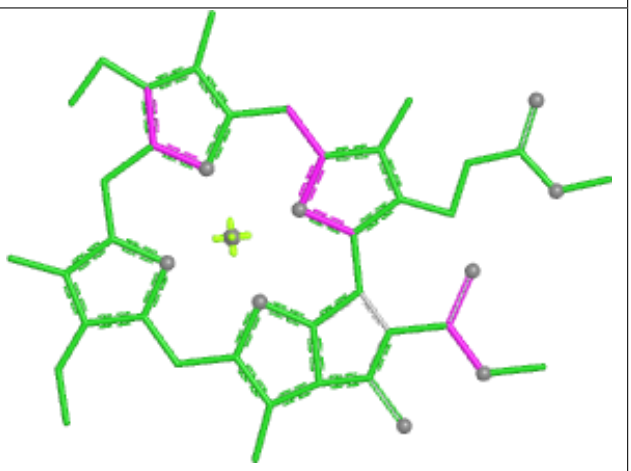
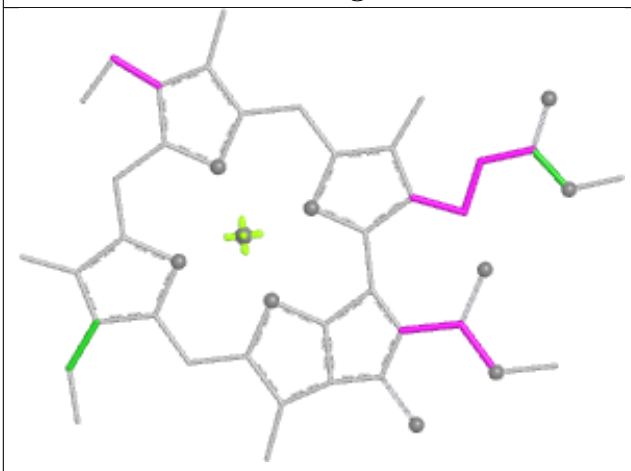
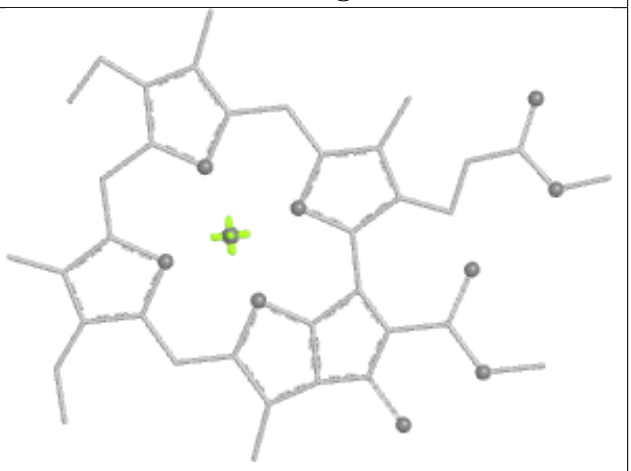


Bond angles

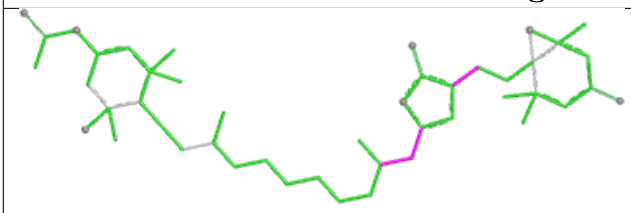


Torsions



Rings

Ligand PID D 306



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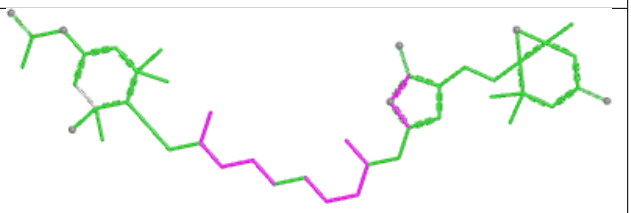
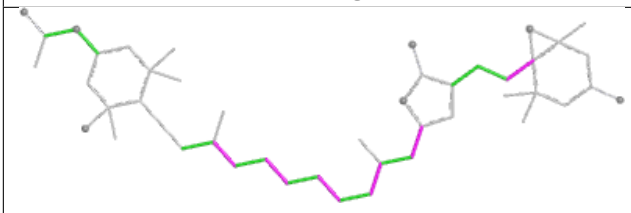
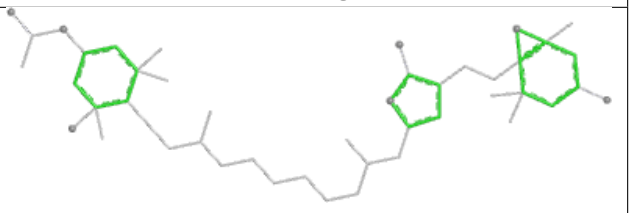


Bond angles

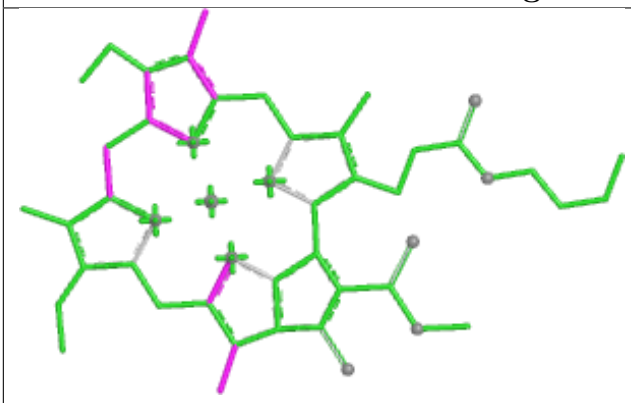


Torsions

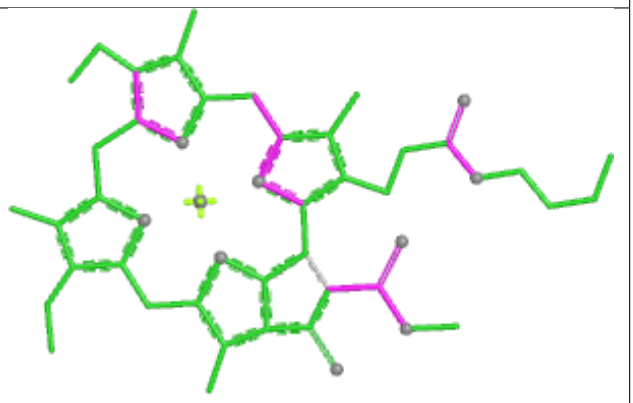


Rings

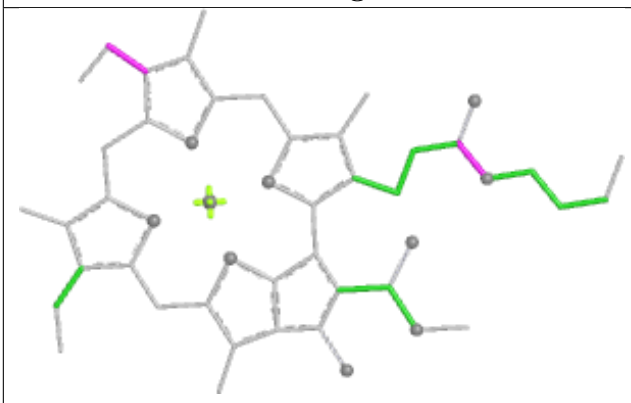
Ligand CLA K 306



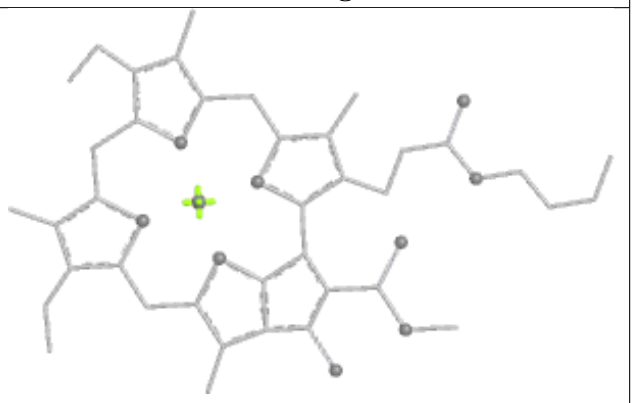
Bond lengths



Bond angles

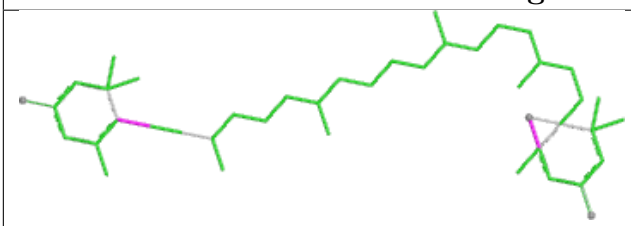


Torsions



Rings

Ligand DD6 L 305



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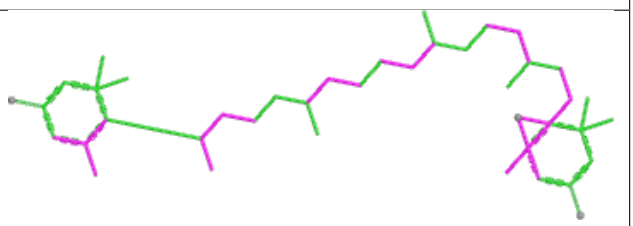

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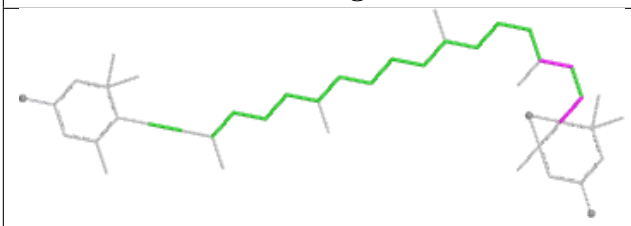
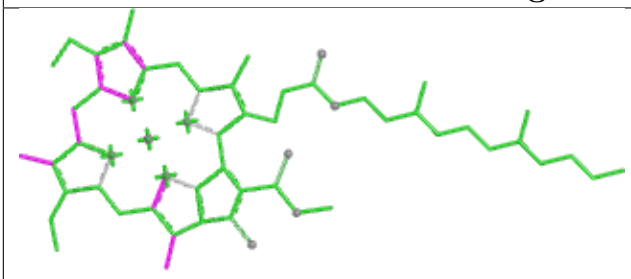


Torsions

Rings

Ligand CLA a 722



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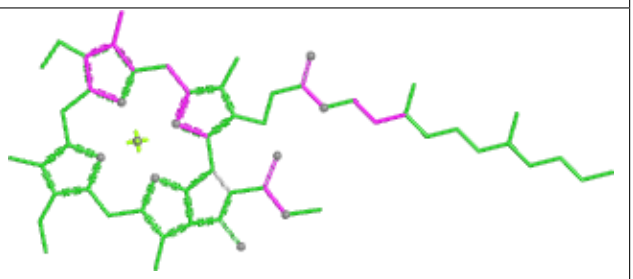

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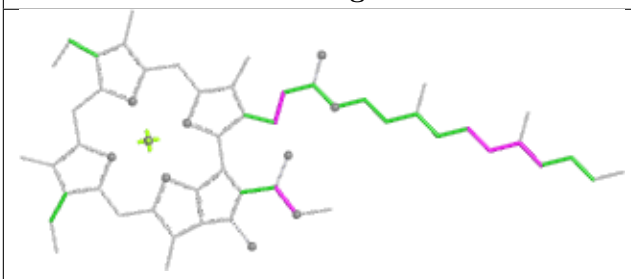

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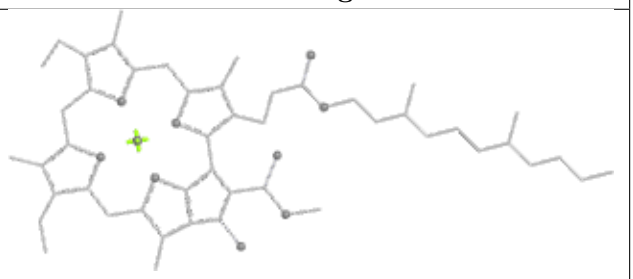
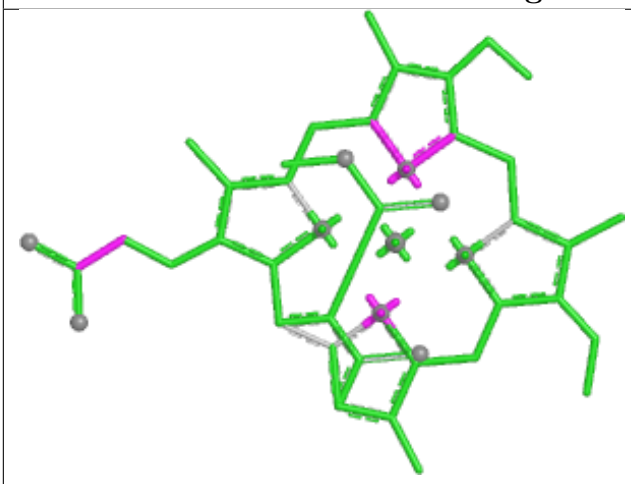


Rings

Ligand KC1 H 310



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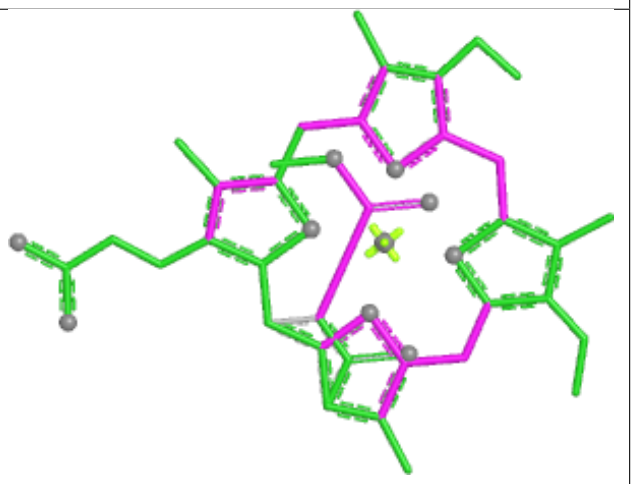

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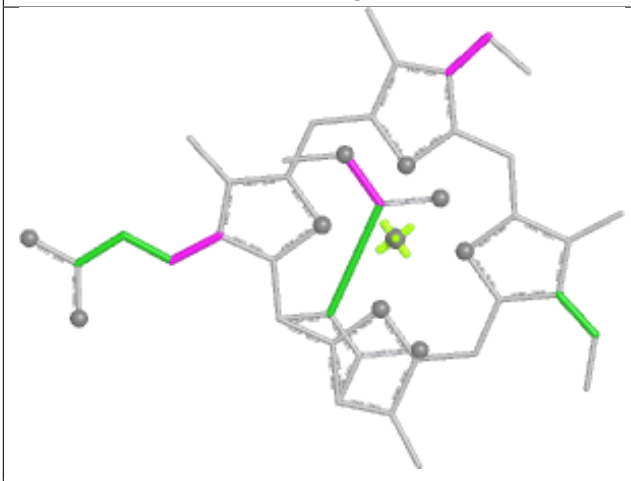

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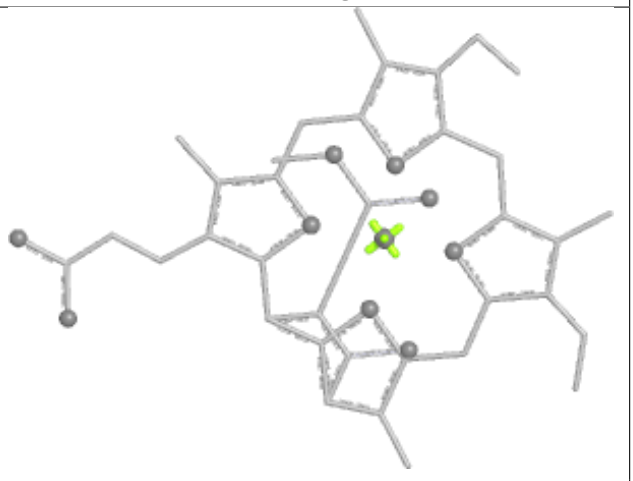
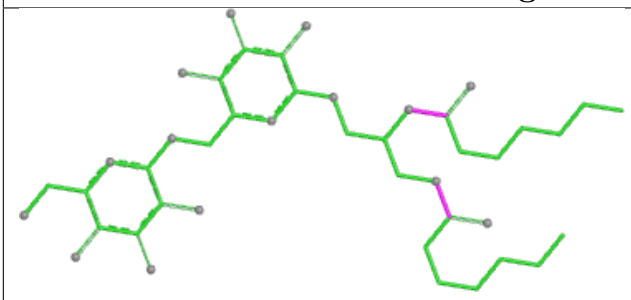


Rings

Ligand DGD G 521



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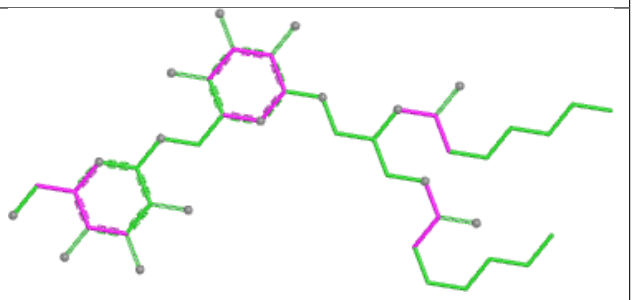

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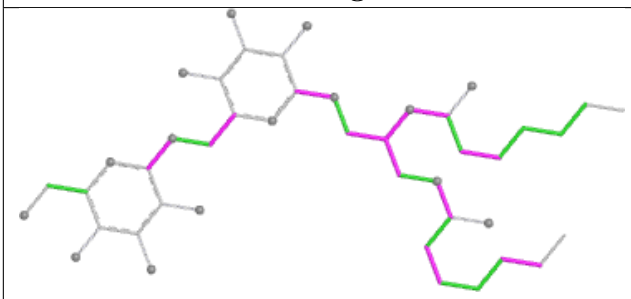

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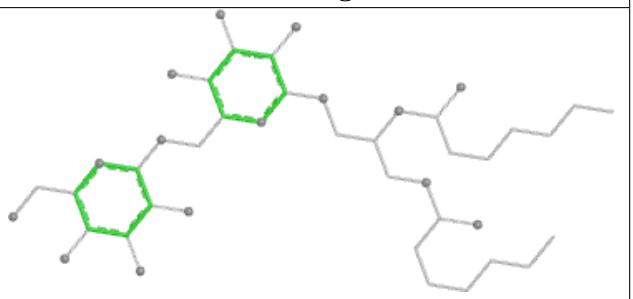
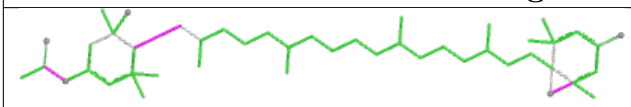


Rings

Ligand UIX A 304



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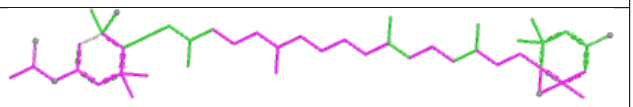
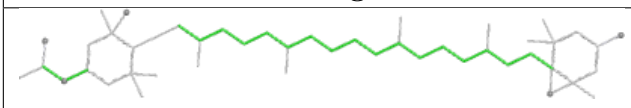


Bond angles



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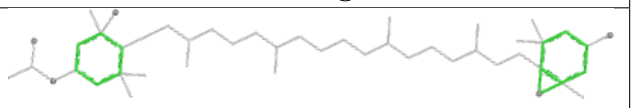
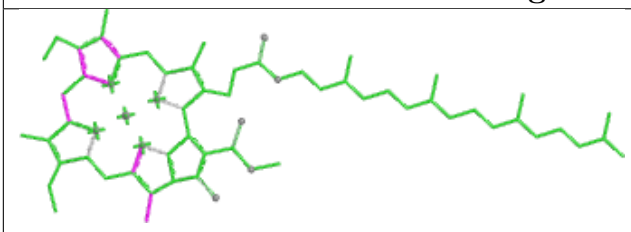


Rings

Ligand CLA a 707



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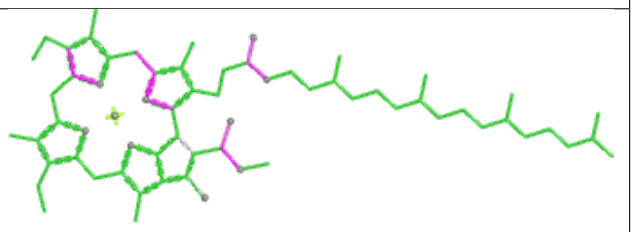
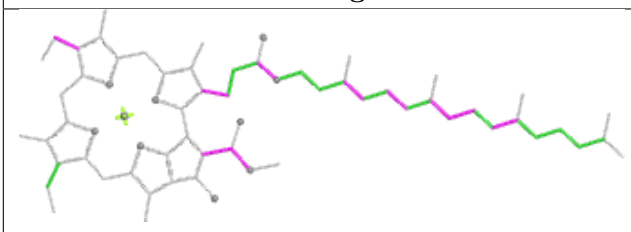


Bond angles



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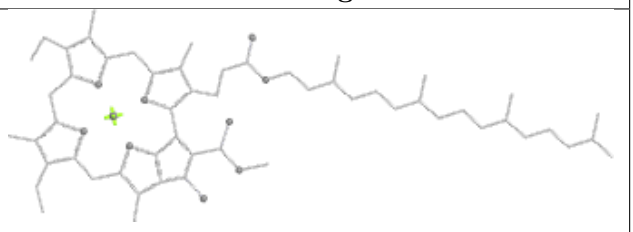
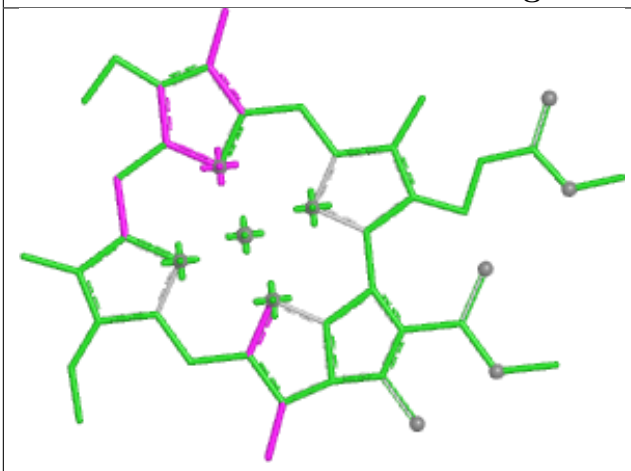


Rings

Ligand CLA D 312



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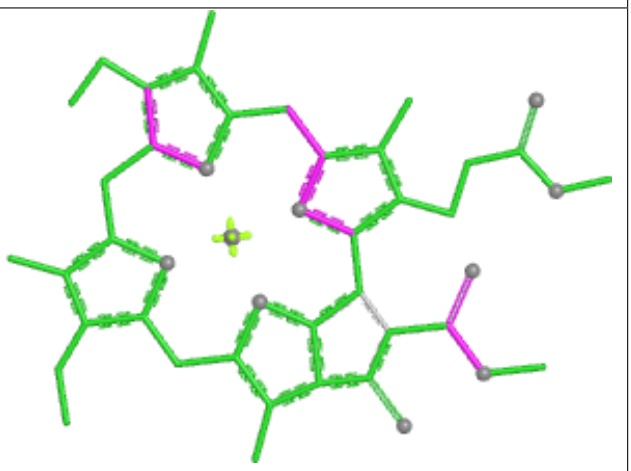
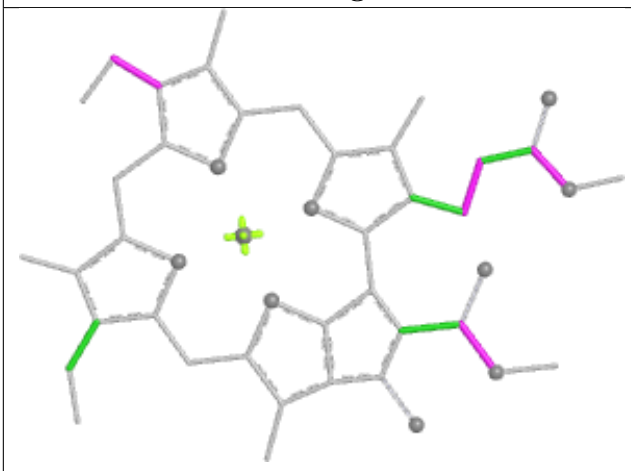


Bond angles



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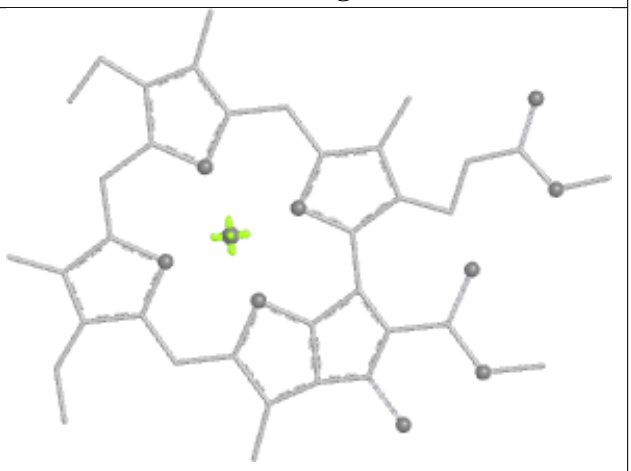
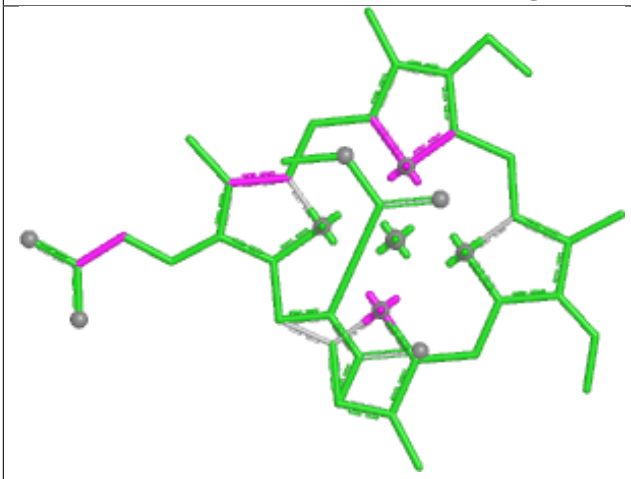


Rings

Ligand KC1 G 515



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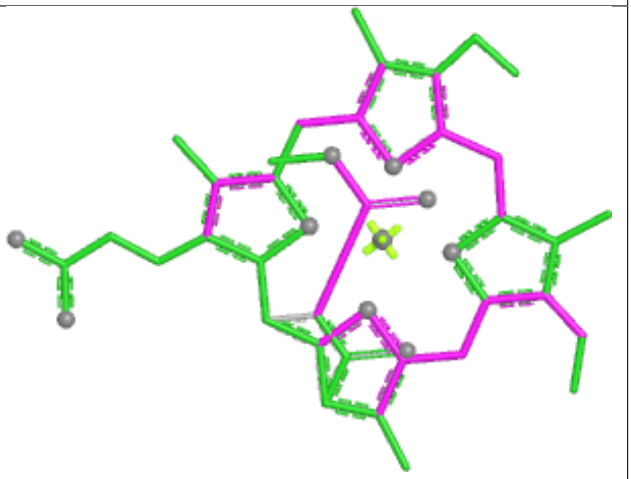
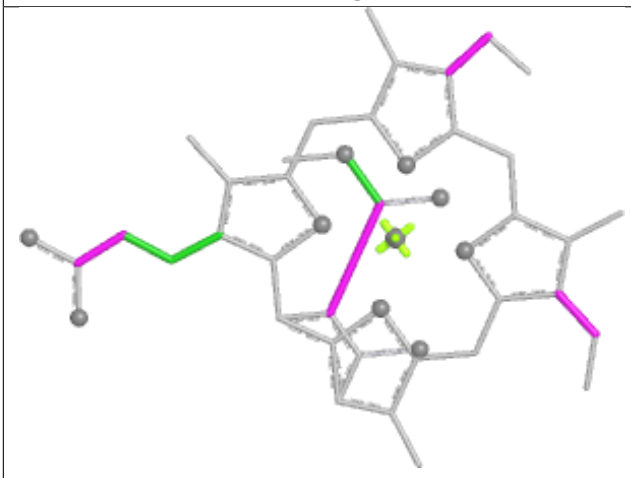


Bond angles



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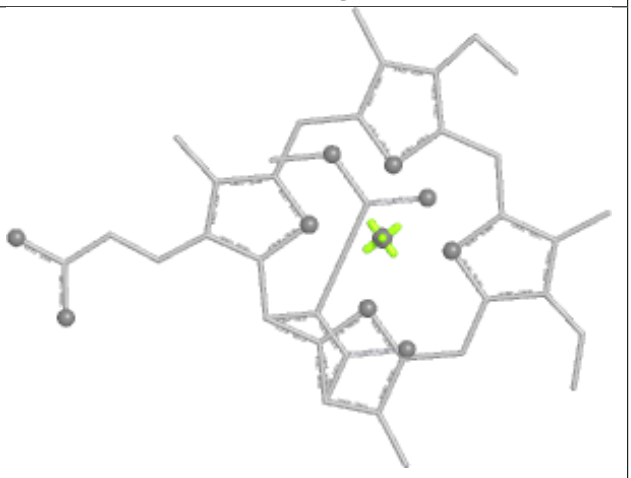
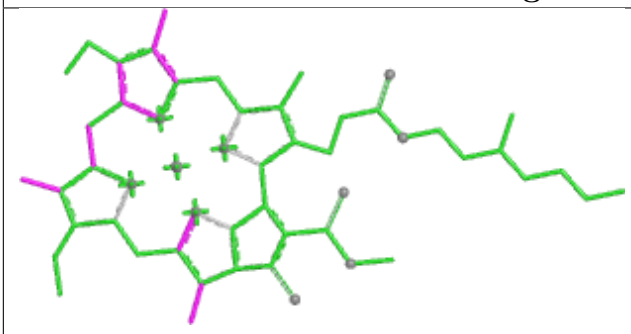


Rings

Ligand CLA G 514



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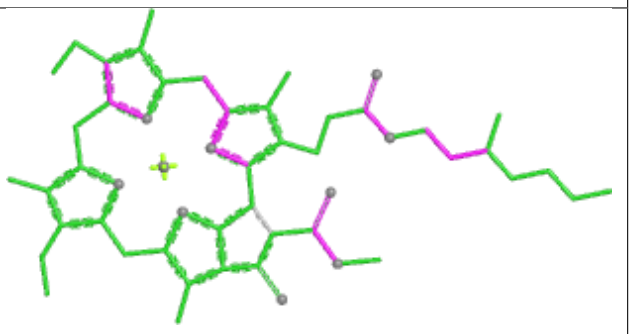
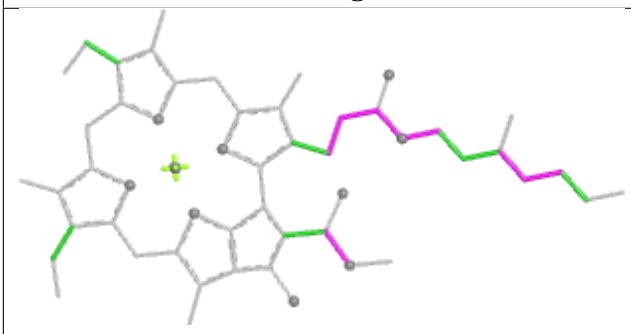
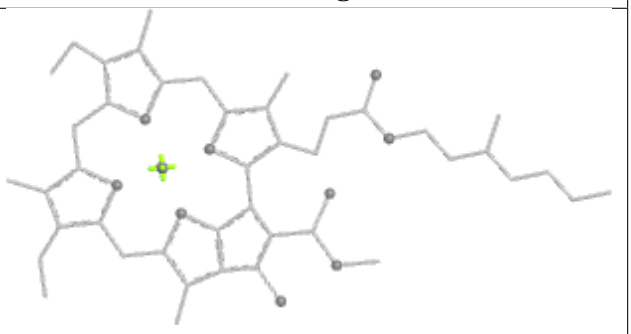


Bond angles

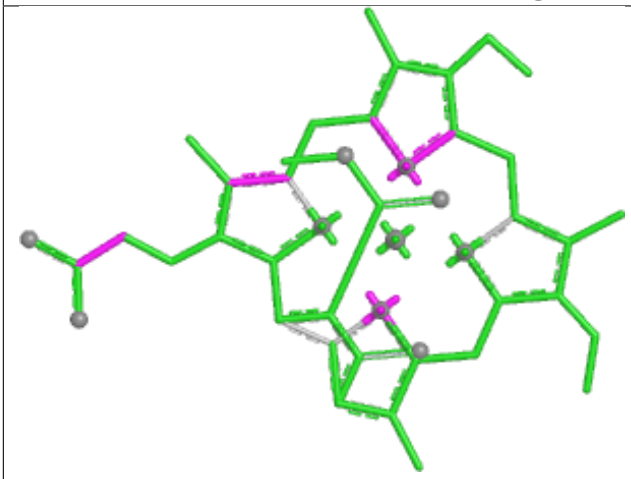


Torsions



Rings

Ligand KC1 J 313



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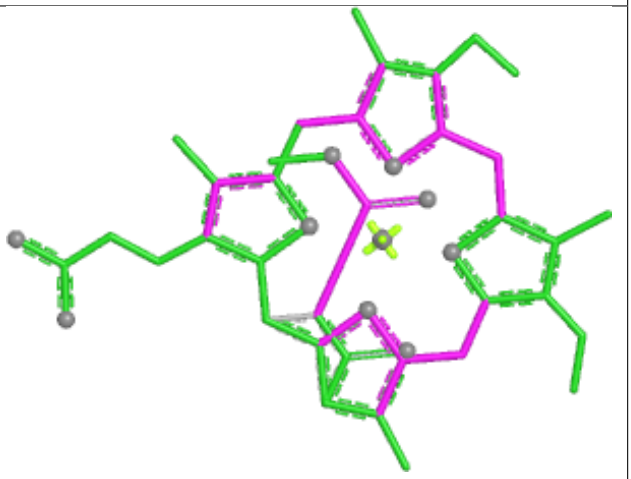
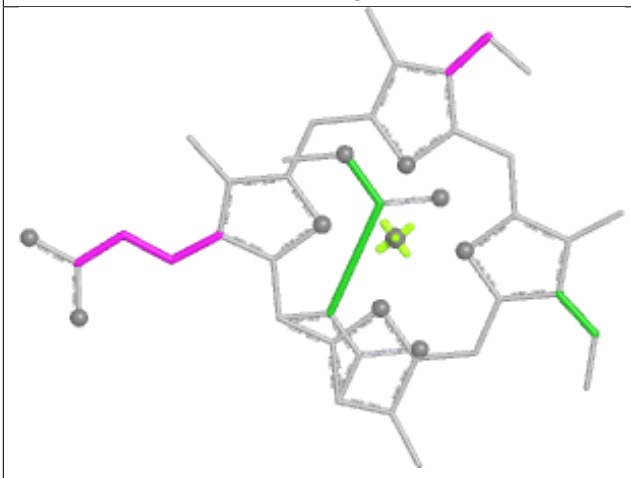


Bond angles



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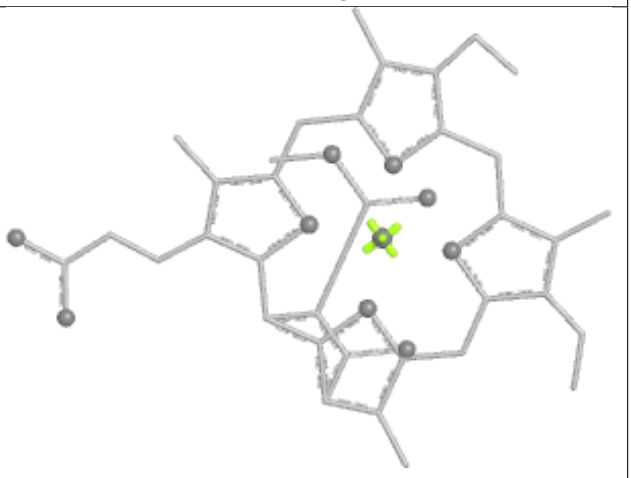
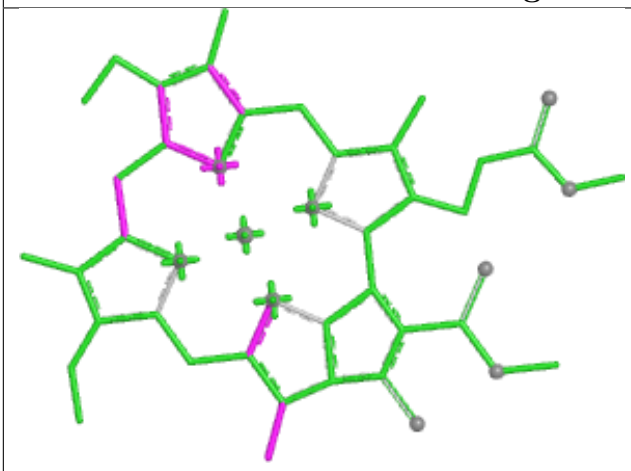


Rings

Ligand CLA H 308



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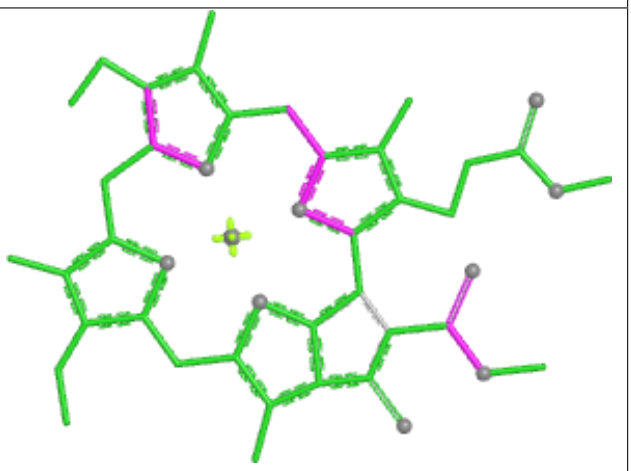
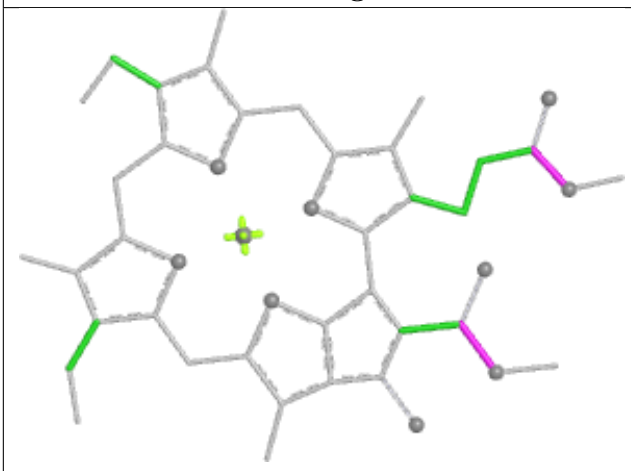


Bond angles



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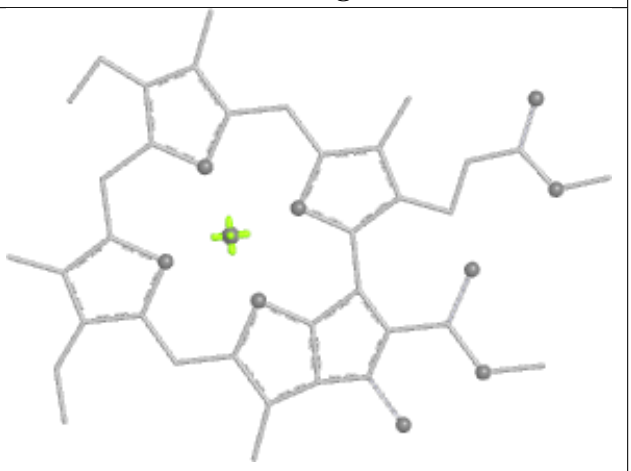
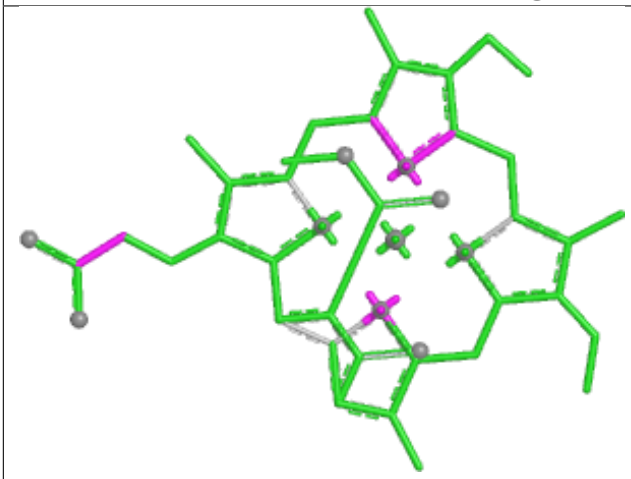


Rings

Ligand KC1 L 315



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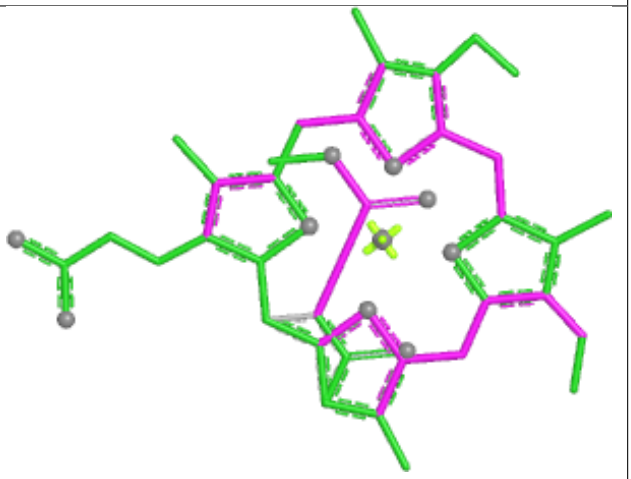
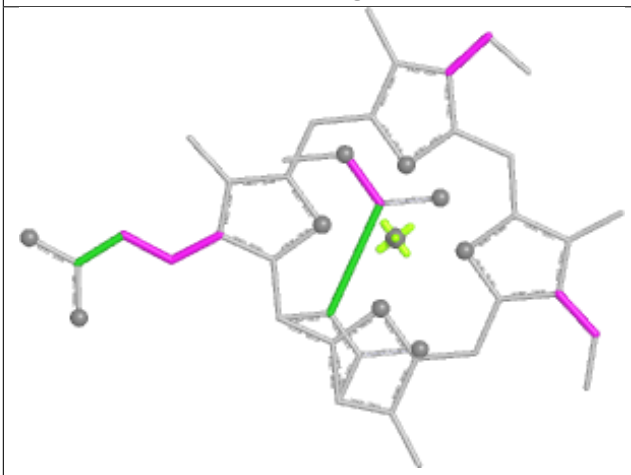


Bond angles



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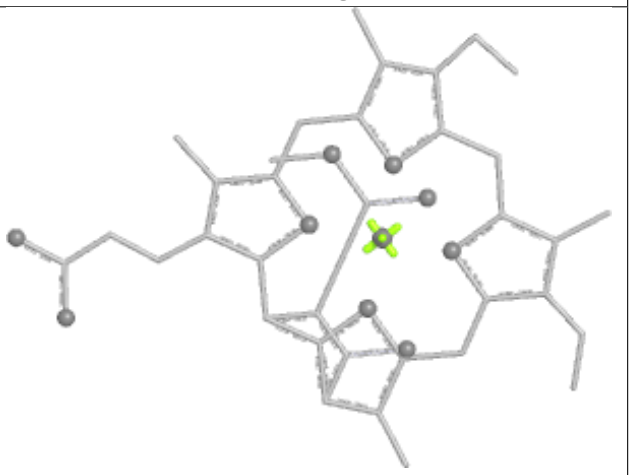
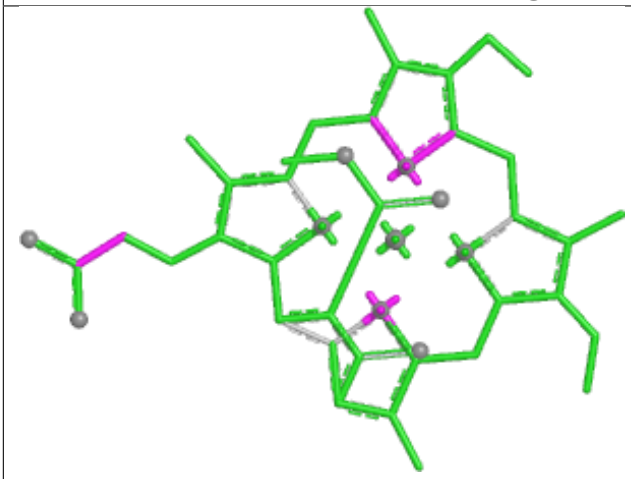


Rings

Ligand KC1 N 311



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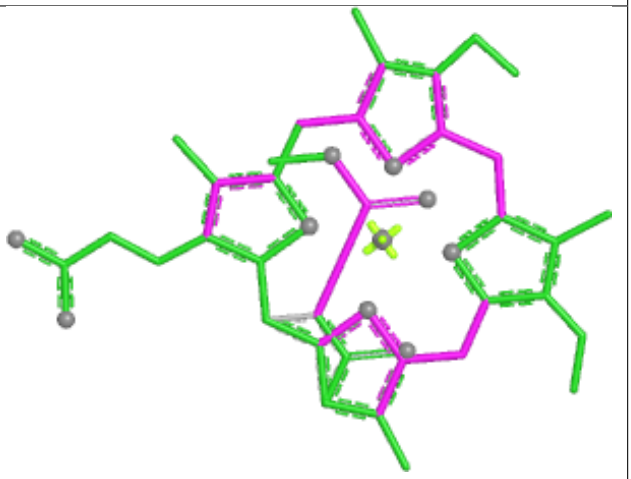
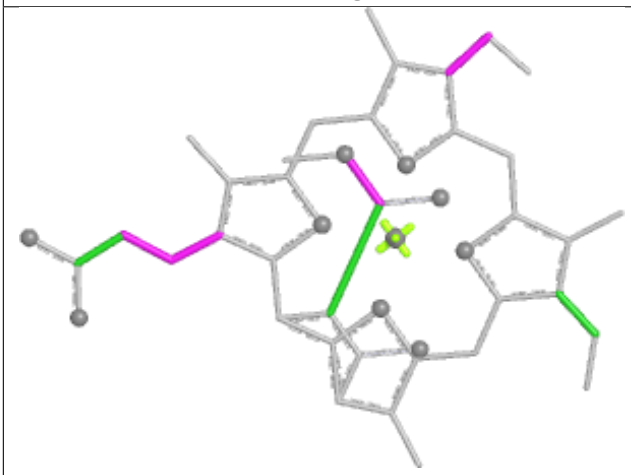


Bond angles



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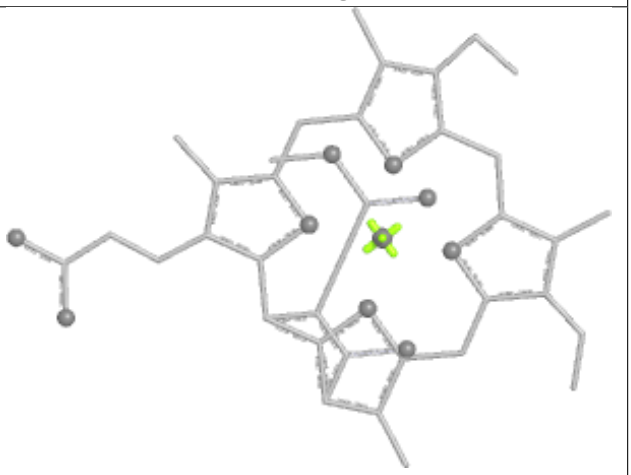
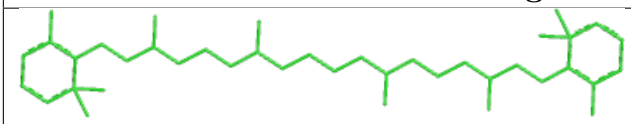


Rings

Ligand BCR b 730



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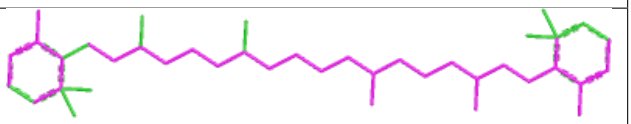
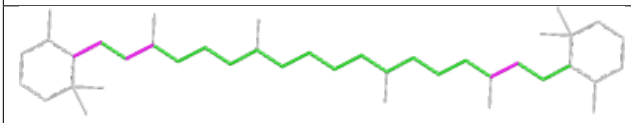
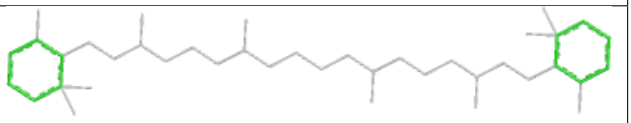


Bond angles

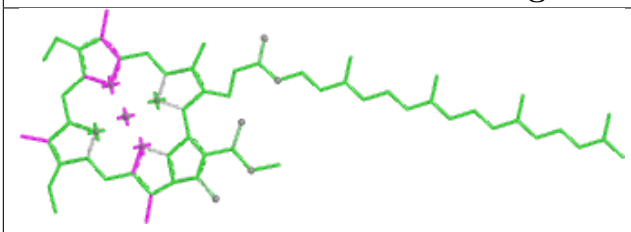


Torsions

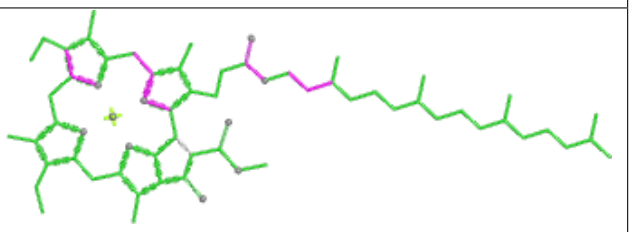


Rings

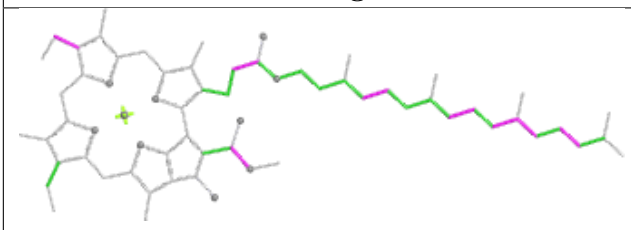
Ligand CLA a 702



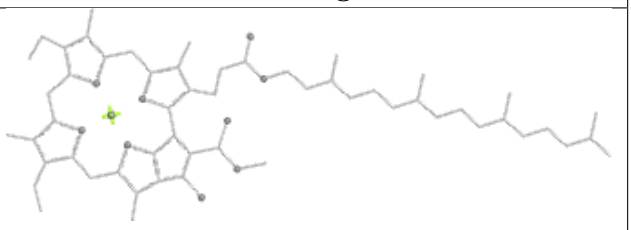
Bond lengths



Bond angles



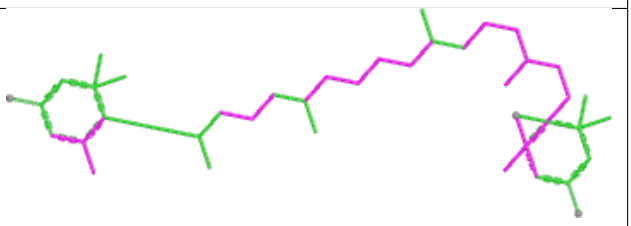
Torsions



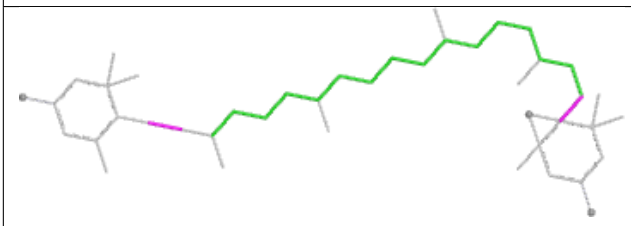
Rings

Ligand DD6 B 303

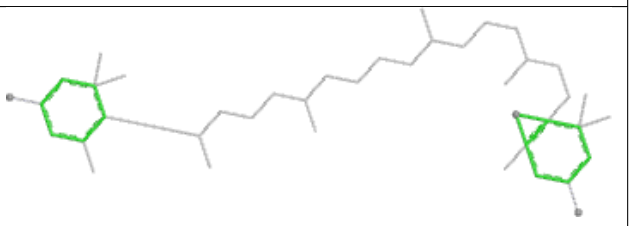
Bond lengths



Bond angles

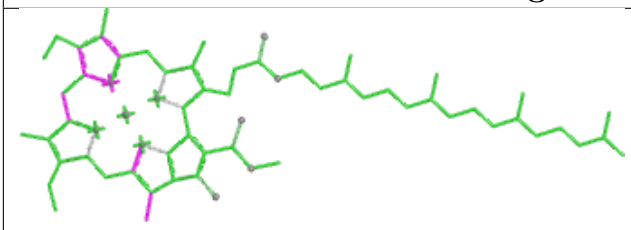


Torsions

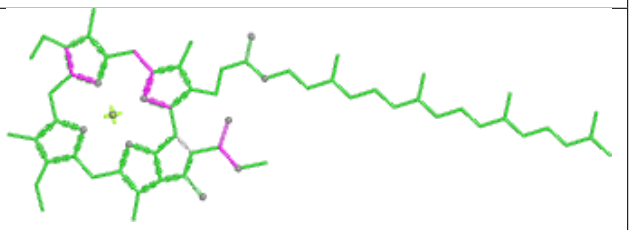


Rings

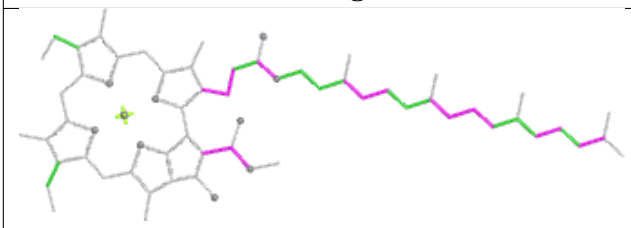
Ligand CLA J 307



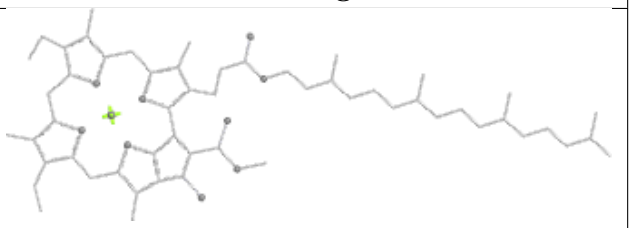
Bond lengths



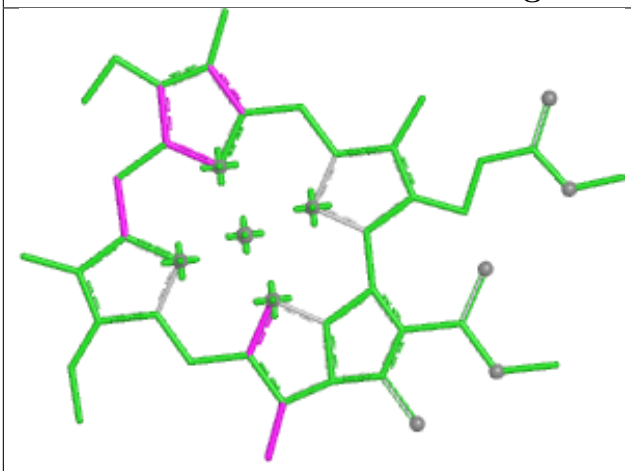
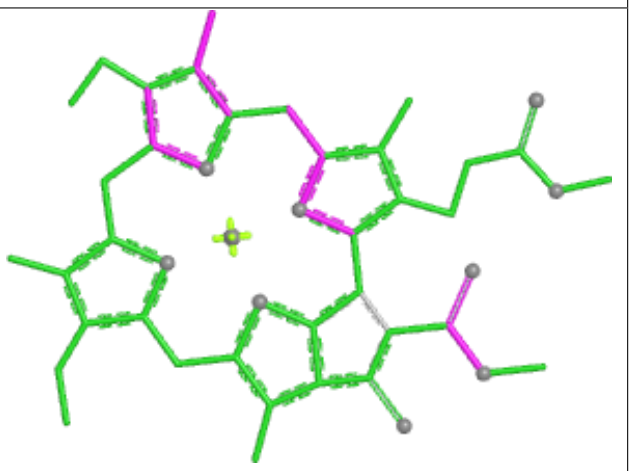
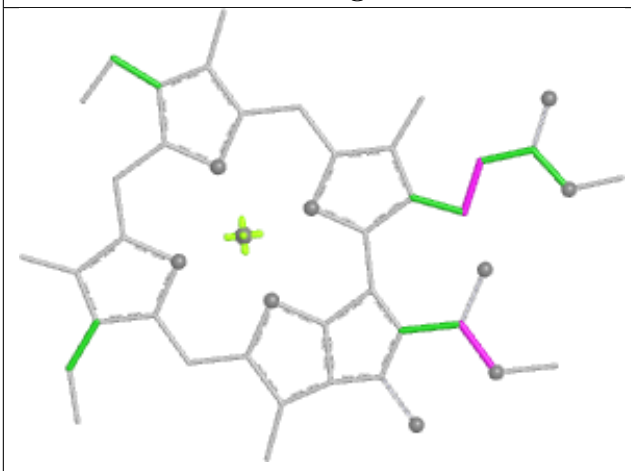
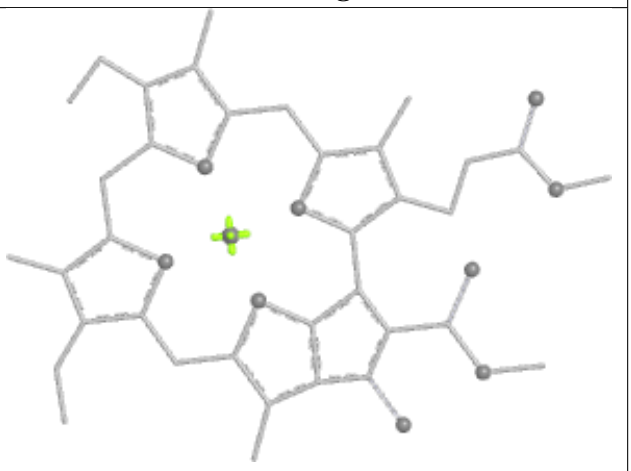
Bond angles

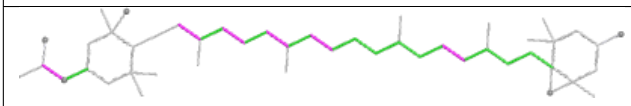
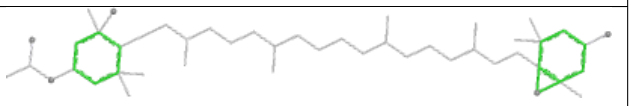


Torsions

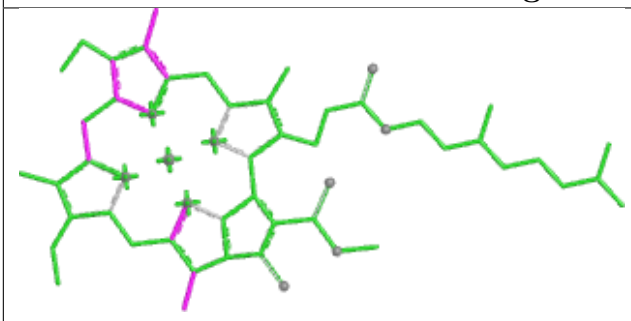


Rings

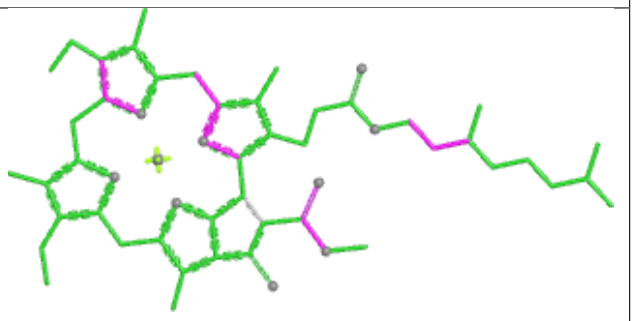
Ligand CLA O 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand UIX P 207	
Bond lengths	Bond angles
	
Torsions	Rings

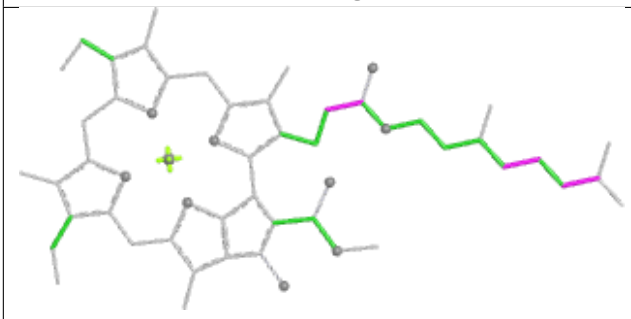
Ligand CLA G 511



Bond lengths



Bond angles



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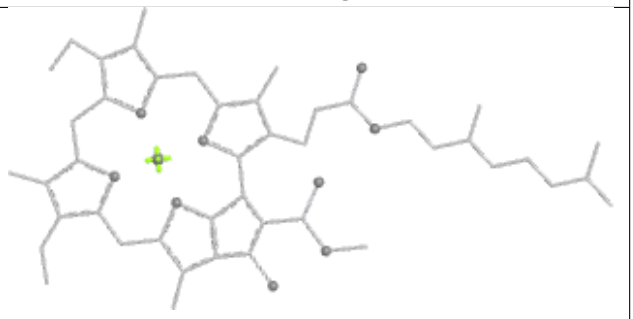
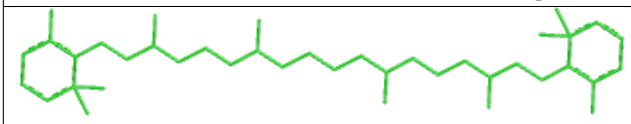
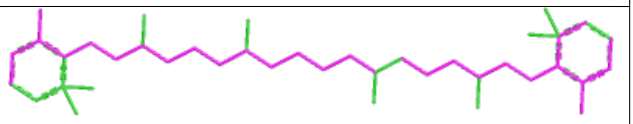


Rings

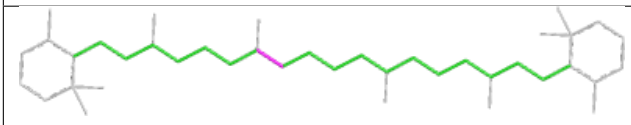
Ligand BCR f 304



Bond lengths



Bond angles



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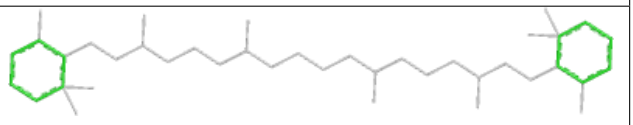
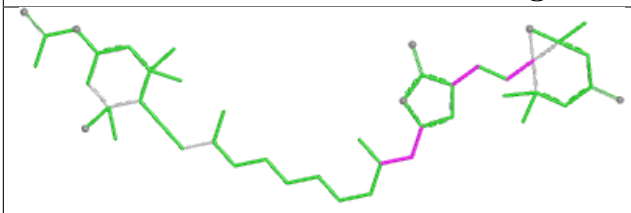
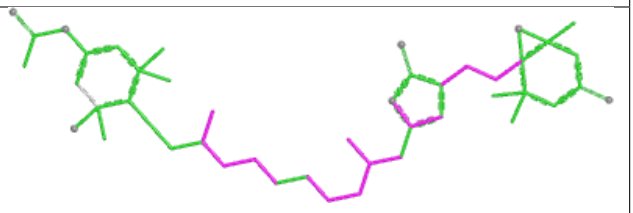


Rings

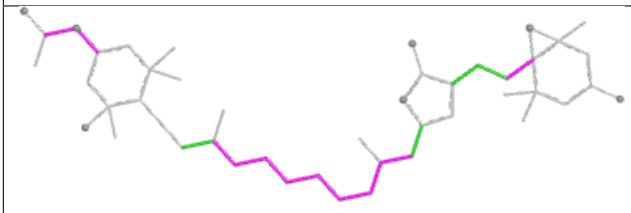
Ligand PID O 305



Bond lengths



Bond angles



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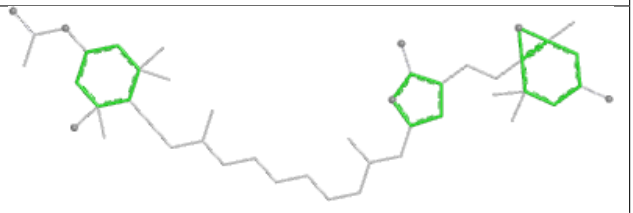
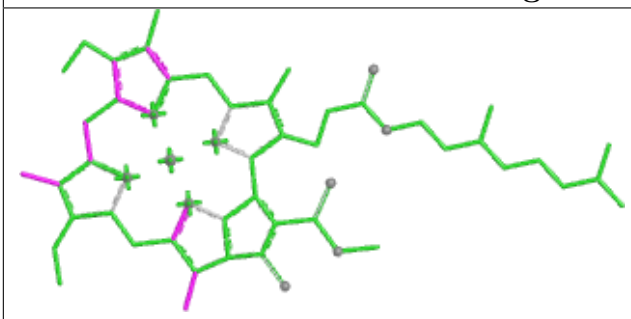
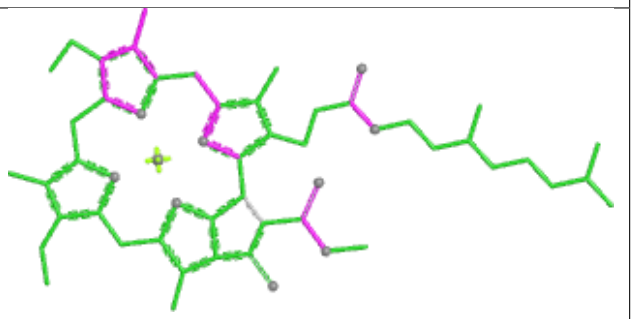


Rings

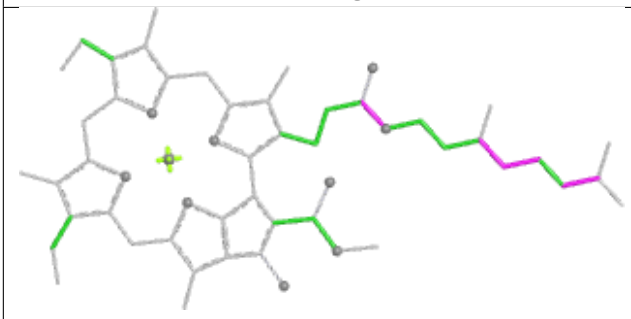
Ligand CLA K 313



Bond lengths



Bond angles



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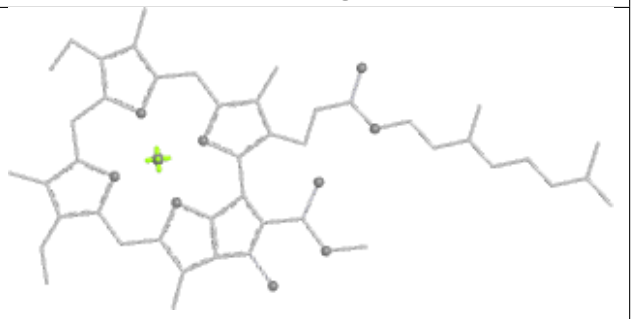
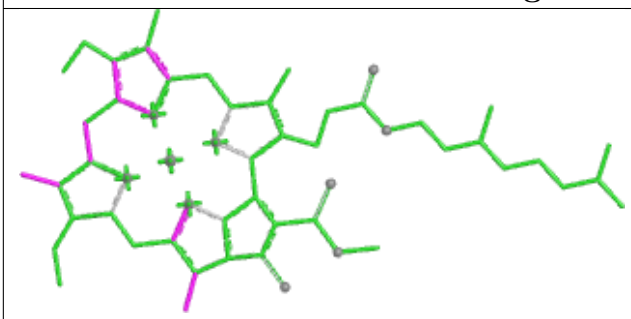


Rings

Ligand CLA A 312



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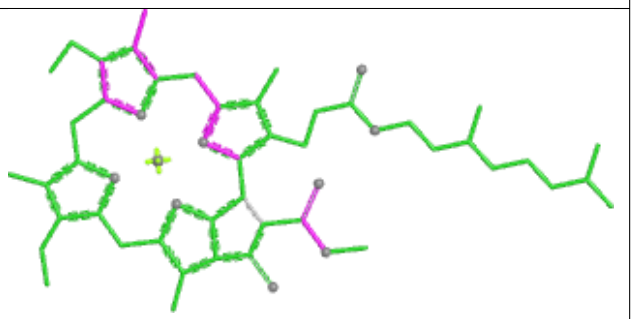
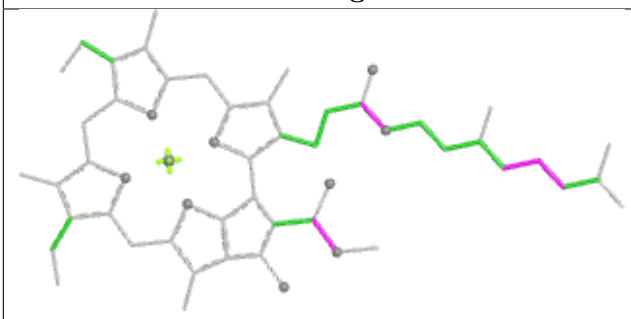


Bond angles



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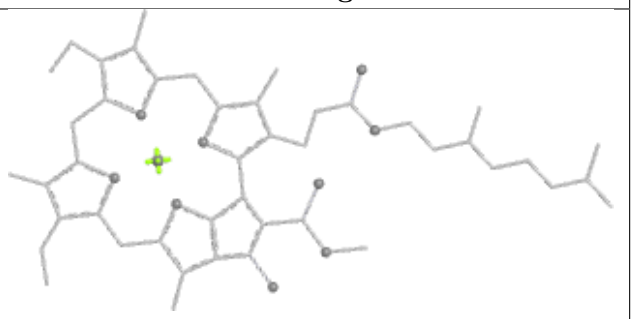
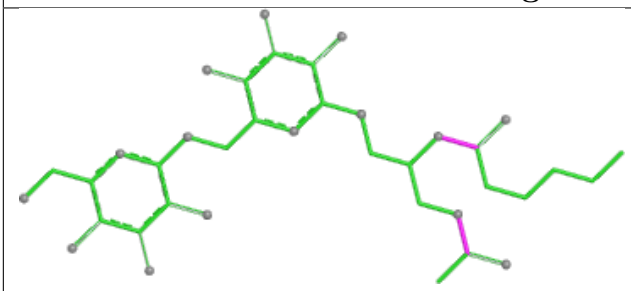


Rings

Ligand DGD L 301



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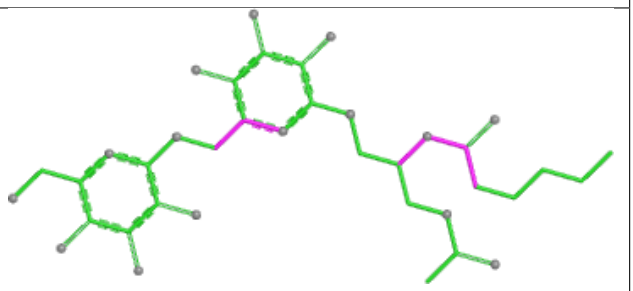
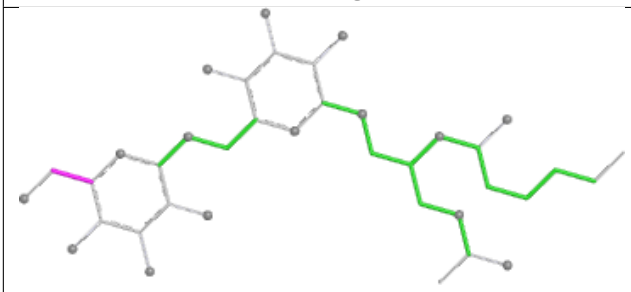
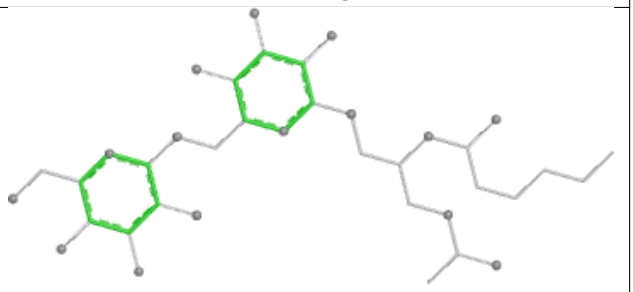


Bond angles

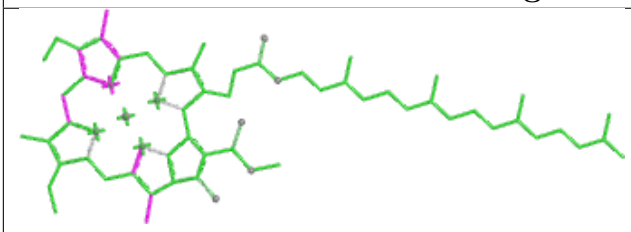


Torsions



Rings

Ligand CLA A 310



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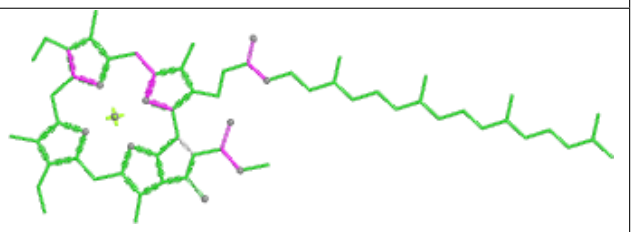
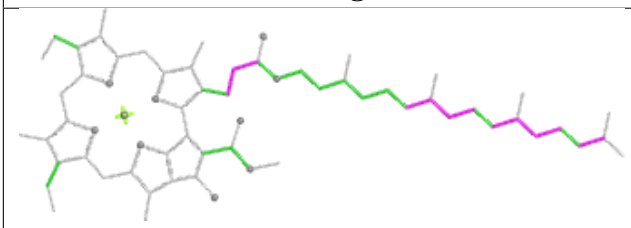
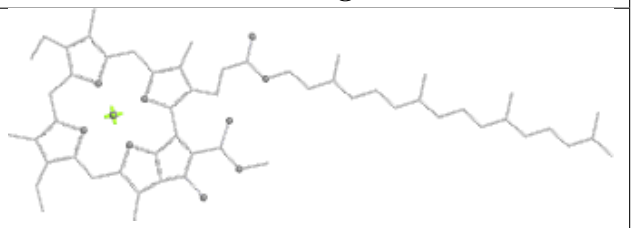


Bond angles

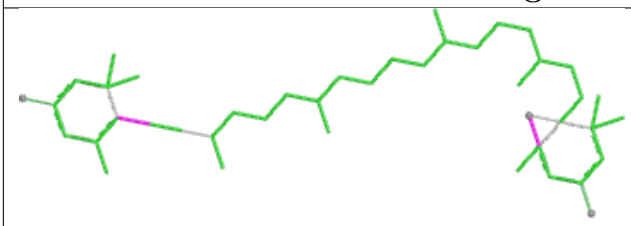


Torsions

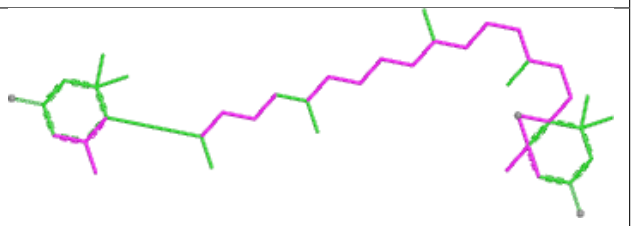


Rings

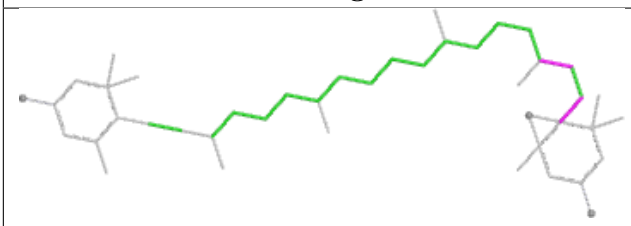
Ligand DD6 A 301



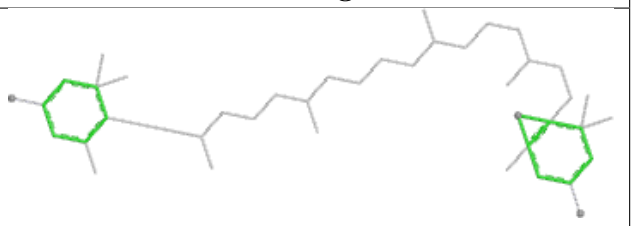
Bond lengths



Bond angles

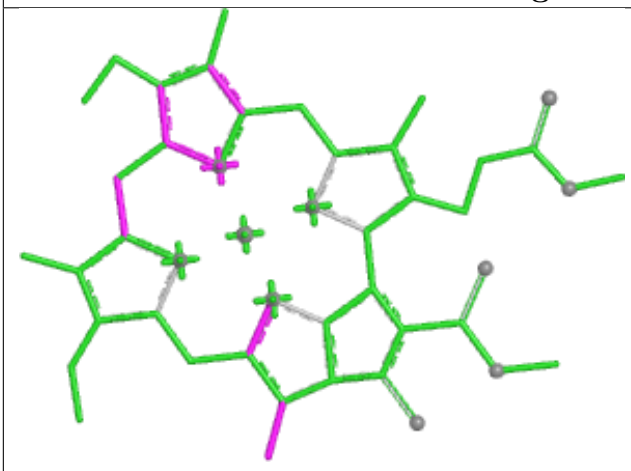


Torsions

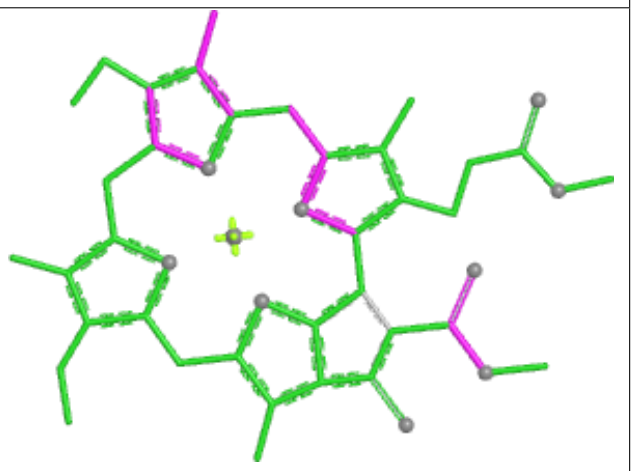


Rings

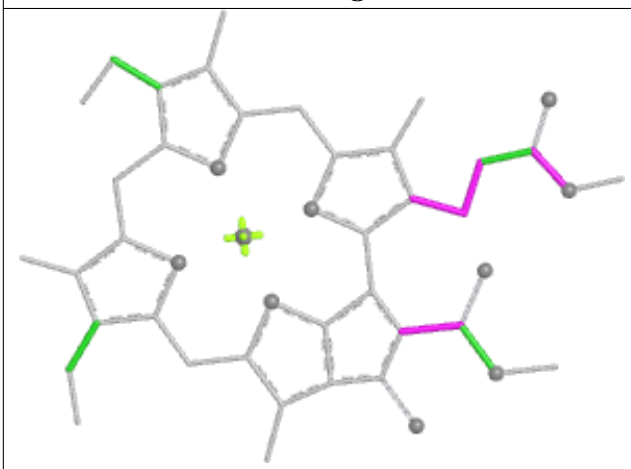
Ligand CLA f 302



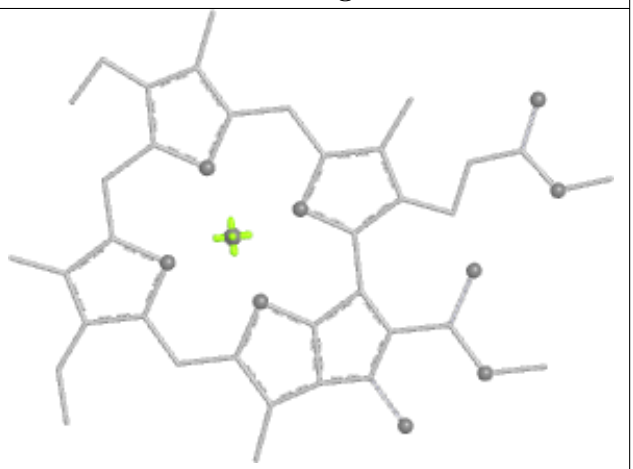
Bond lengths



Bond angles

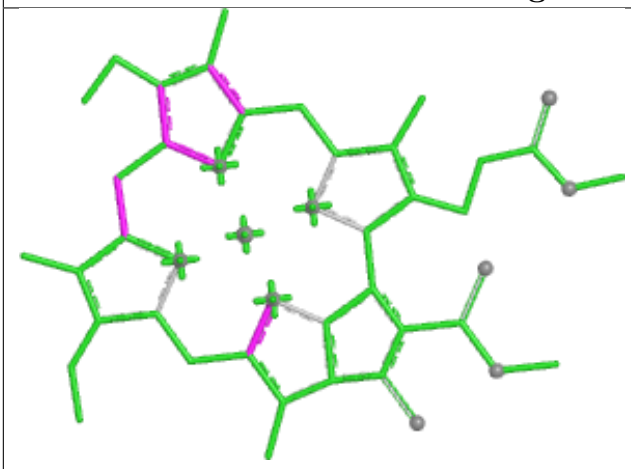


Torsions

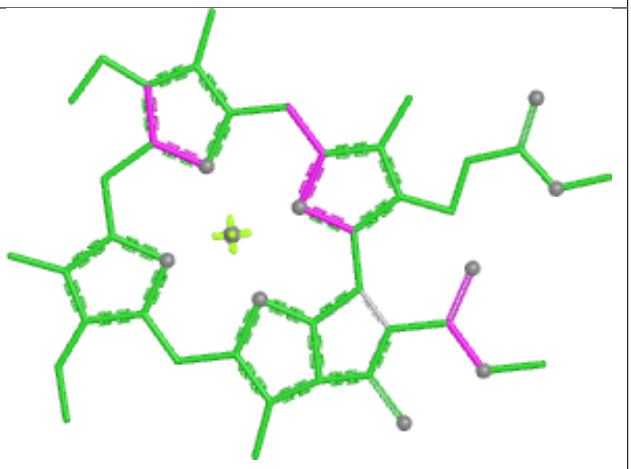


Rings

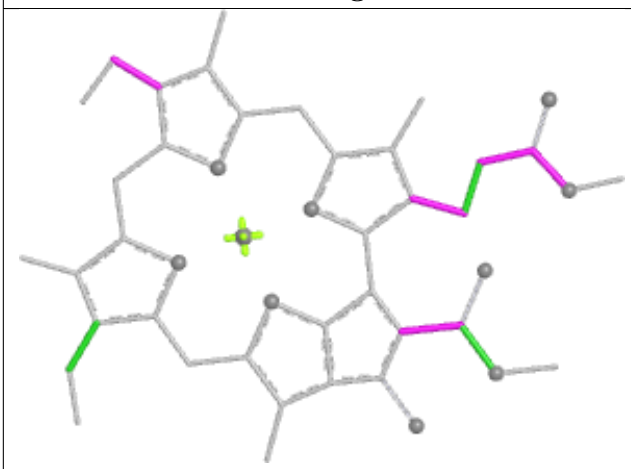
Ligand CLA a 718



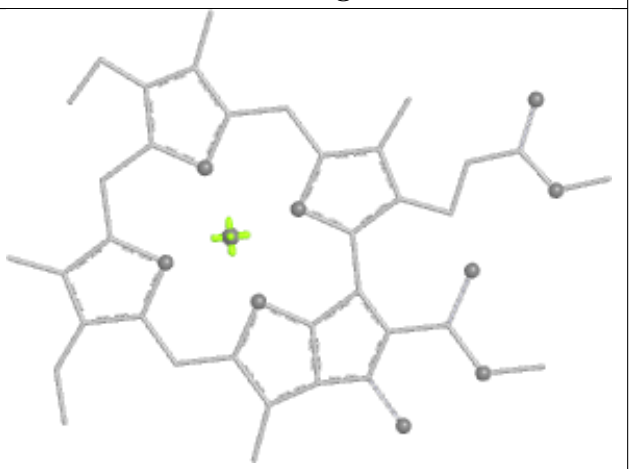
Bond lengths



Bond angles

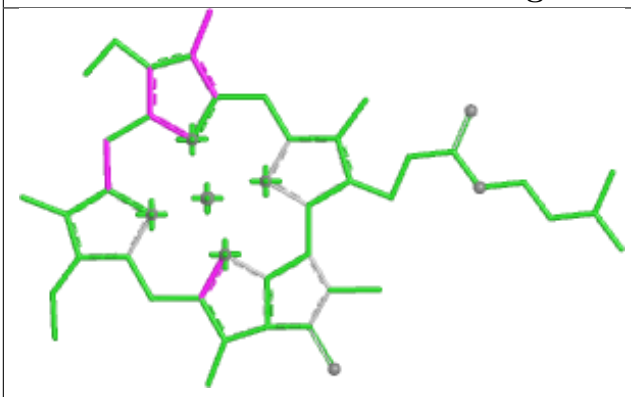


Torsions



Rings

Ligand CLA L 308



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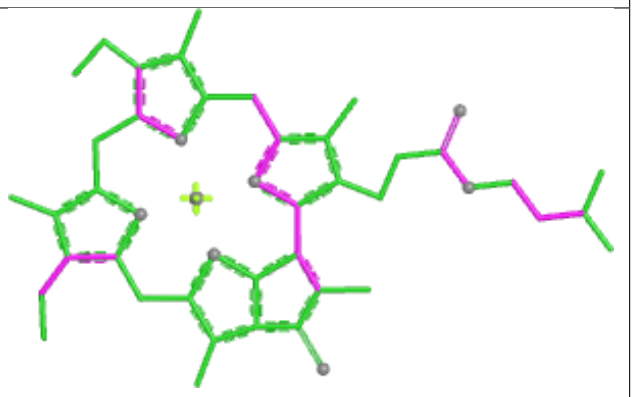
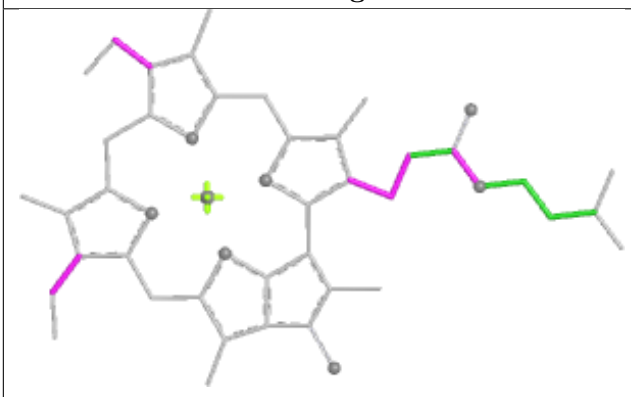
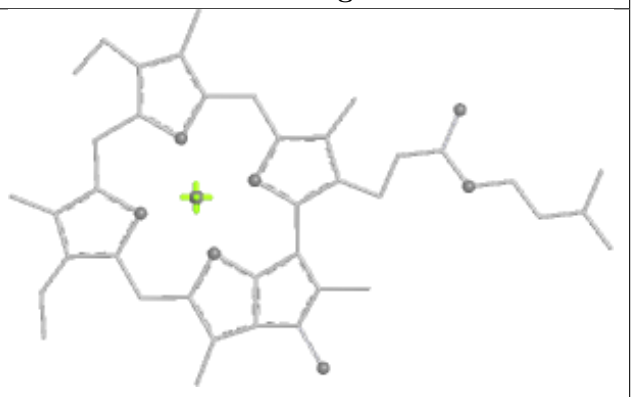


Bond angles



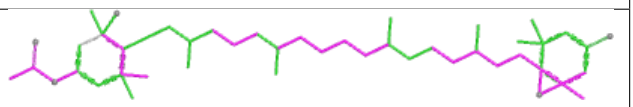
Torsions



Rings

Ligand UIX B 305

Bond lengths

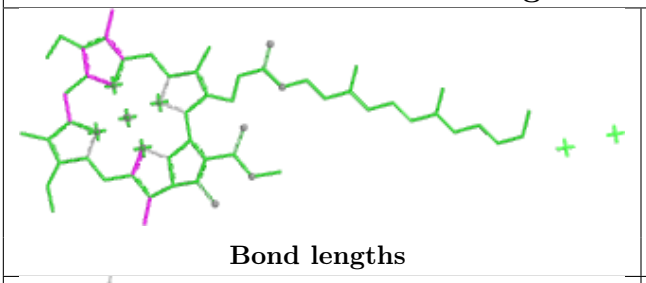


Bond angles

Torsions

Rings

Ligand CLA G 519



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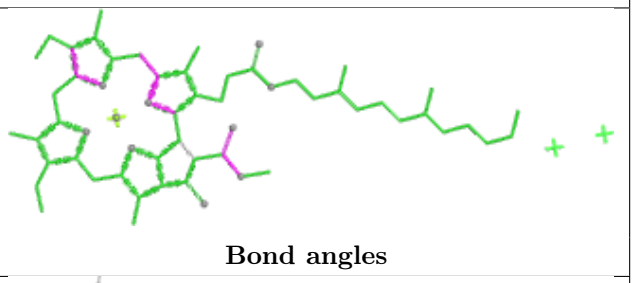
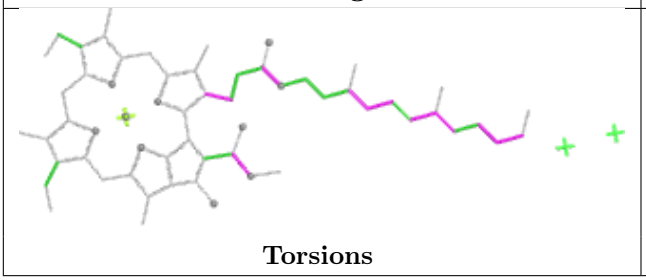


Bond angles



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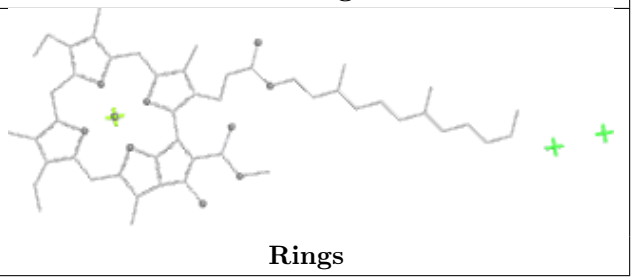
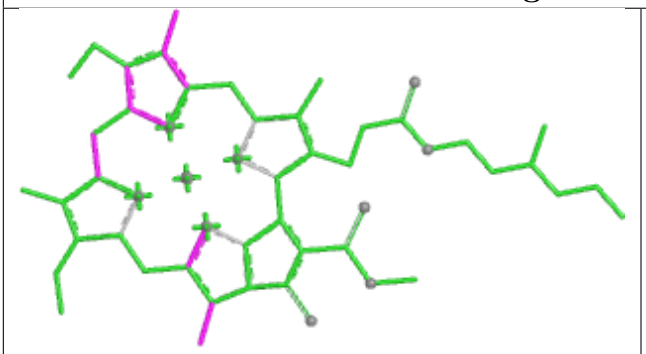
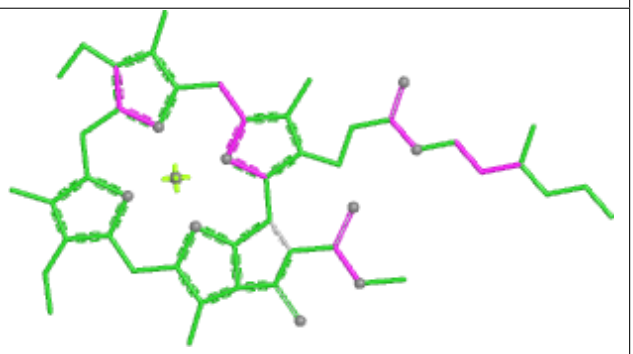


Rings

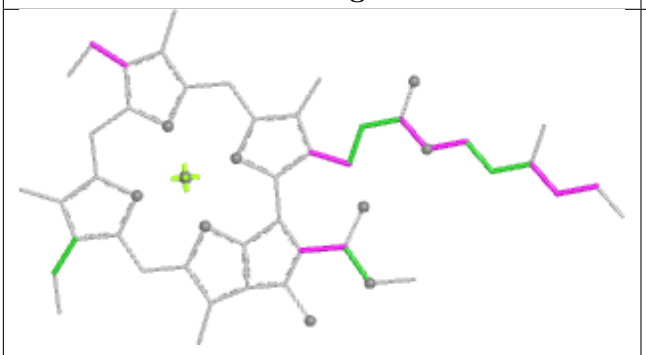
Ligand CLA K 311



Bond lengths



Bond angles



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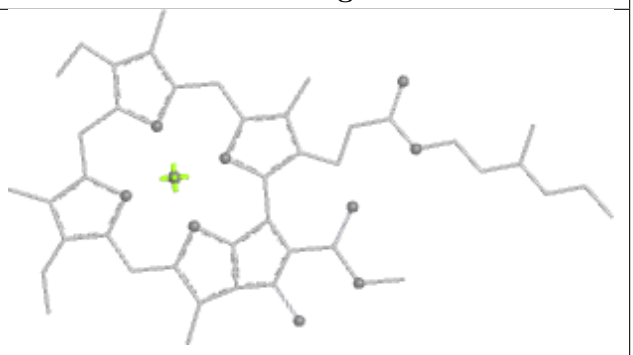
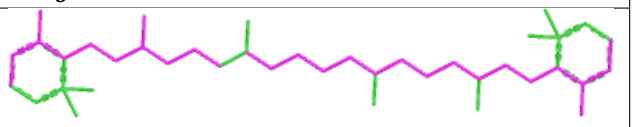


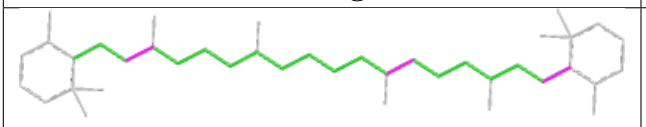
Rings

Ligand BCR j 102

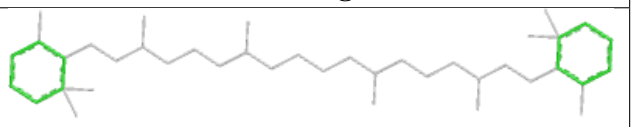
Bond lengths



Bond angles

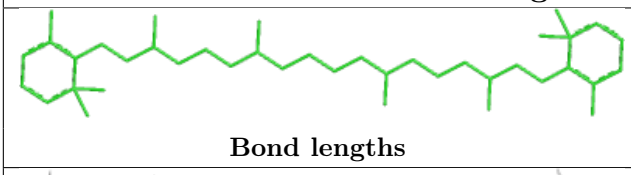


Torsions



Rings

Ligand BCR l 306



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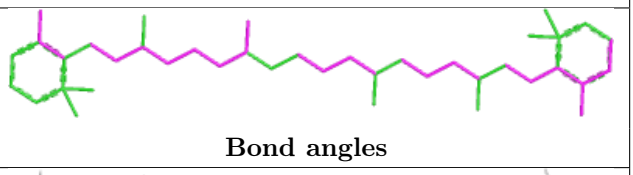
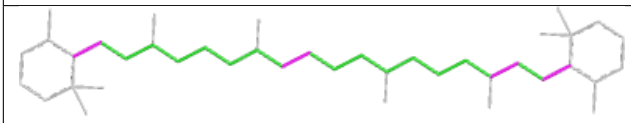


Bond angles



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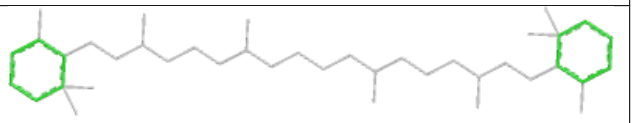
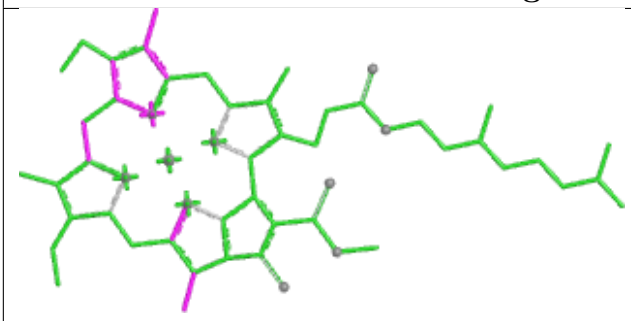


Rings

Ligand CLA K 310



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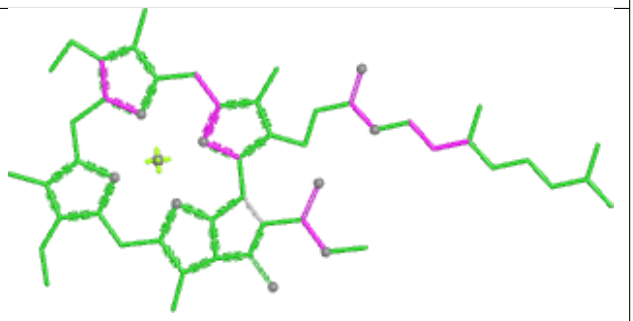
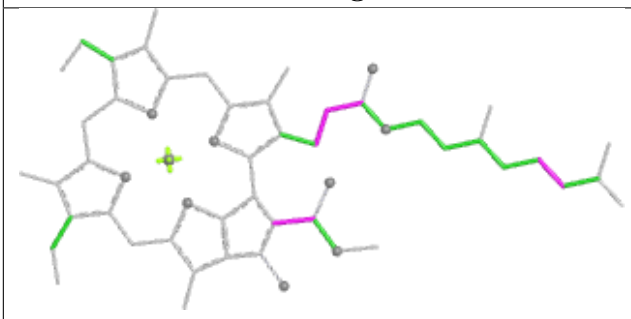


Bond angles



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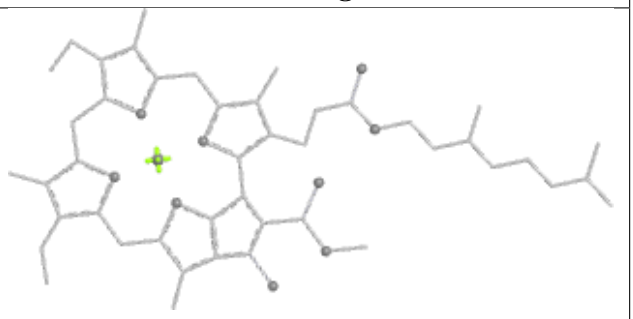
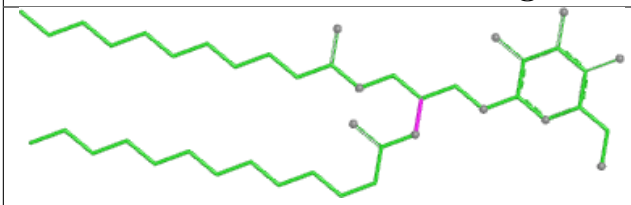


Rings

Ligand LMG K 317



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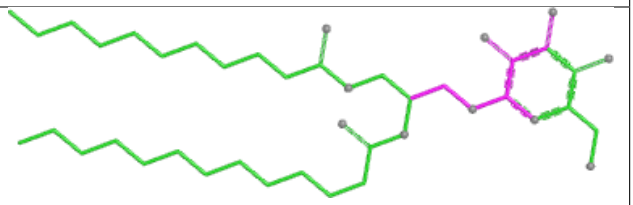
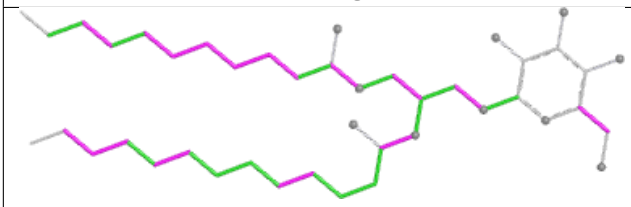


Bond angles



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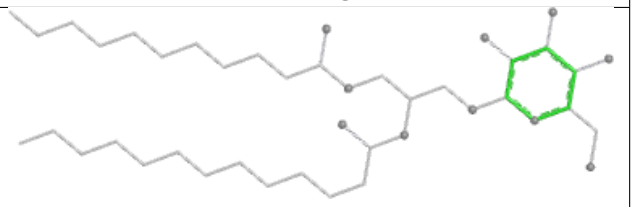
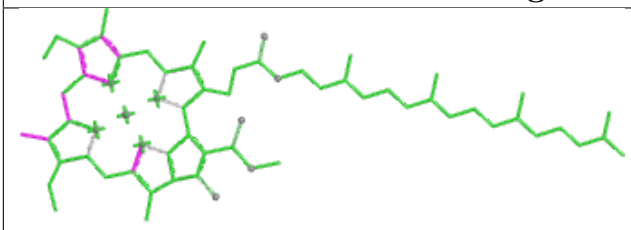
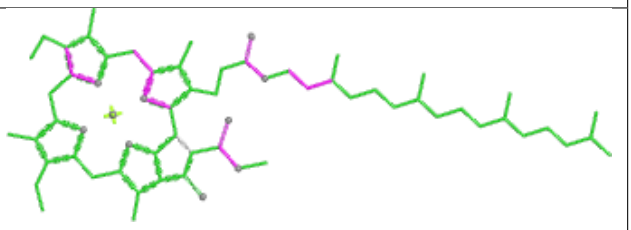


Rings

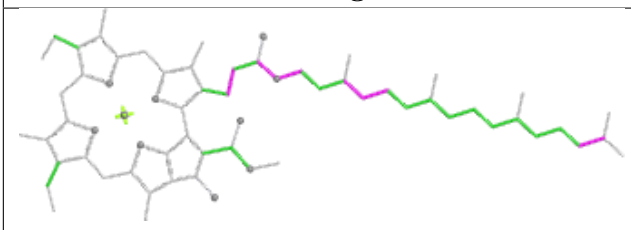
Ligand CLA b 725



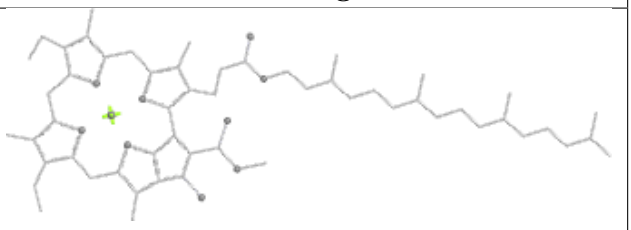
Bond lengths



Bond angles

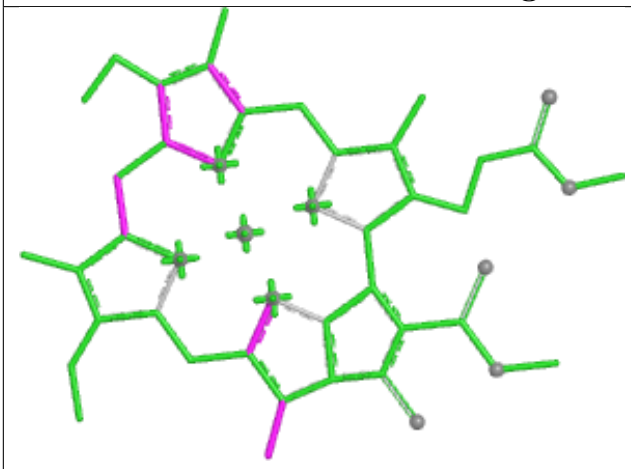


Torsions



Rings

Ligand CLA M 317



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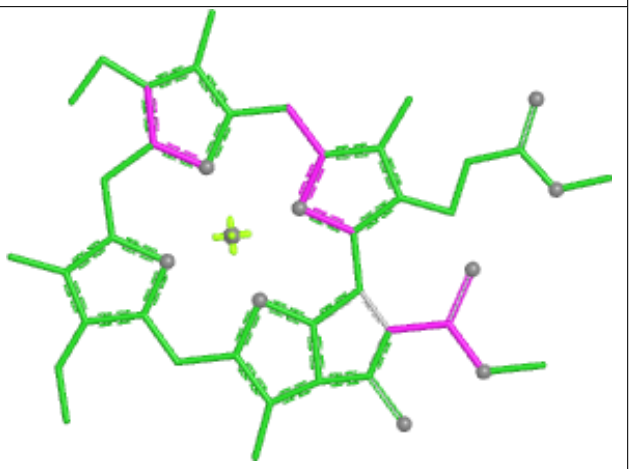
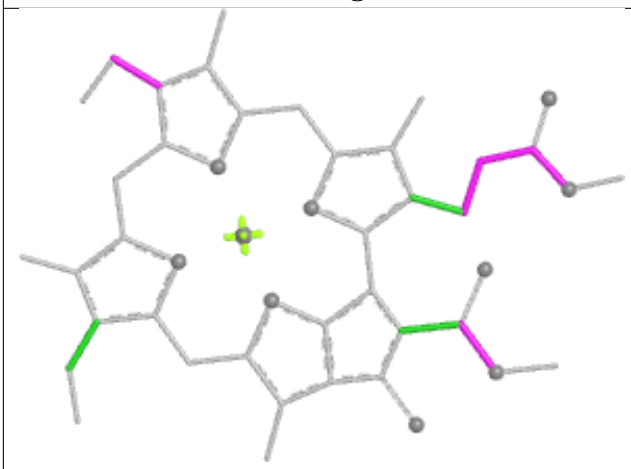


Bond angles



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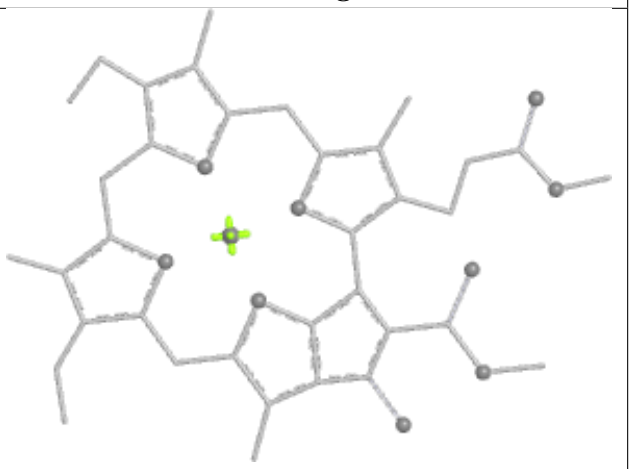
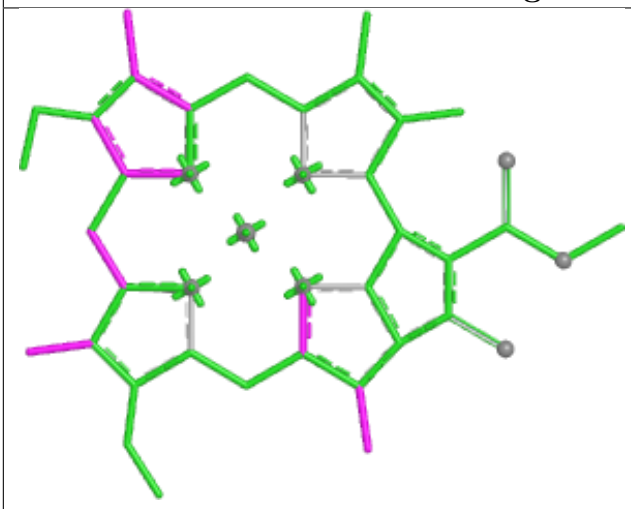


Rings

Ligand CLA A 317



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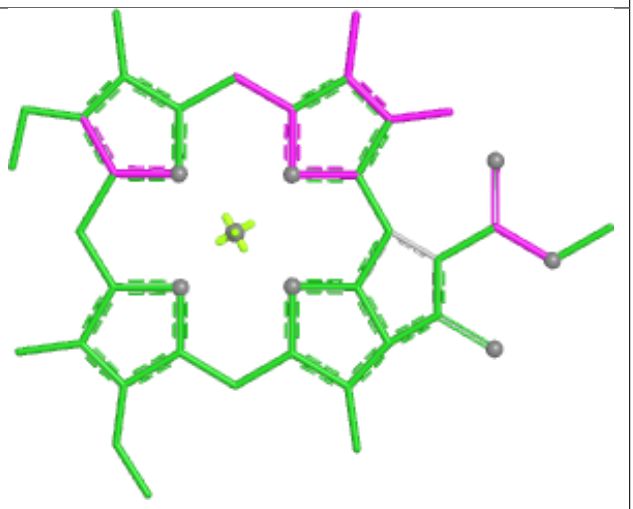
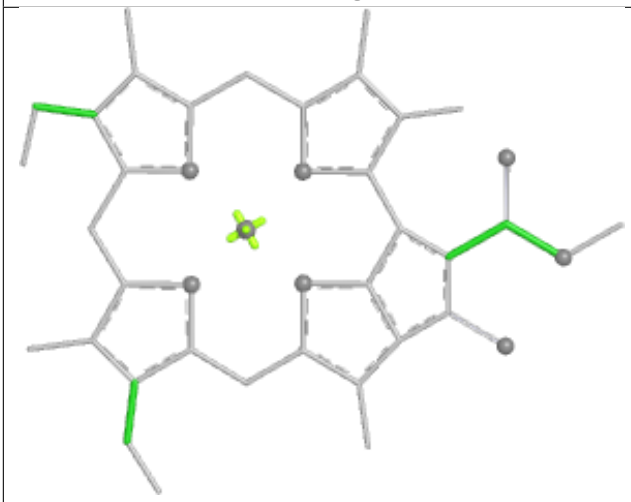


Bond angles



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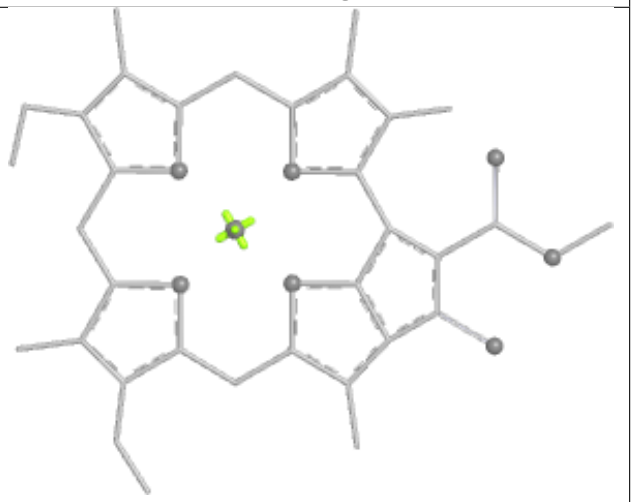
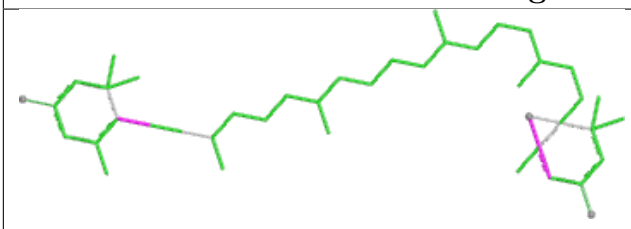


Rings

Ligand DD6 J 303



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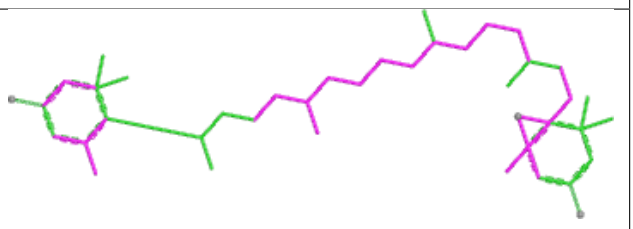
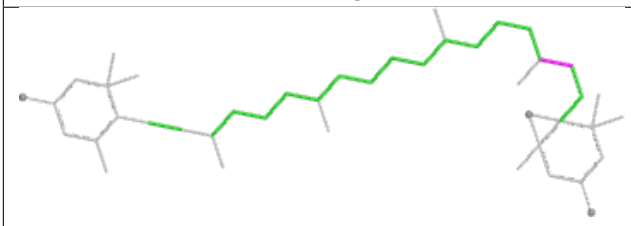


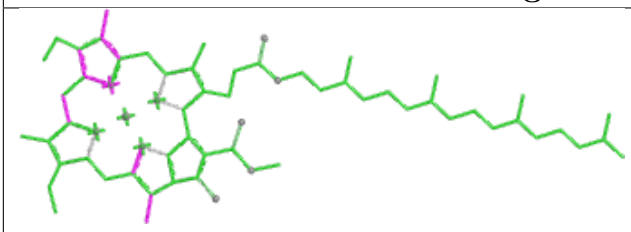
Bond angles



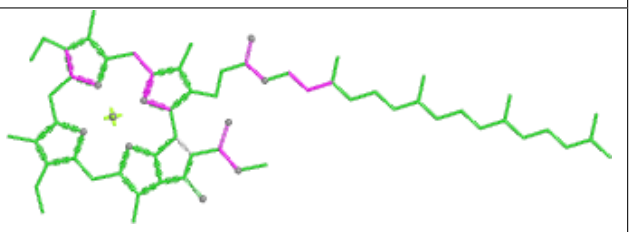
Torsions

Rings

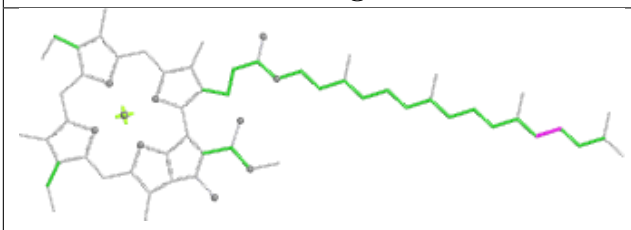
Ligand CLA O 309



Bond lengths



Bond angles



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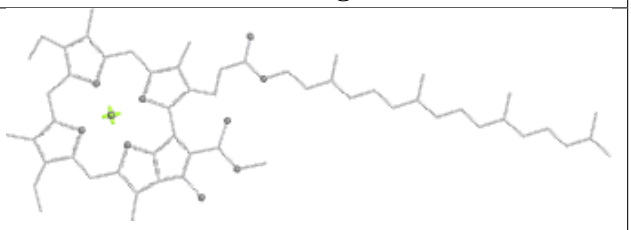
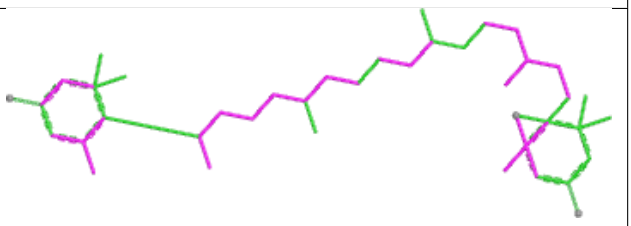


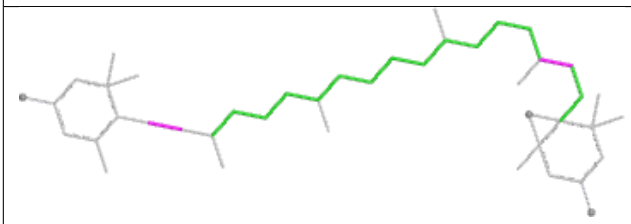
Rings

Ligand DD6 J 302

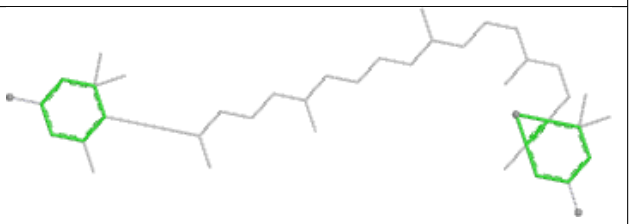
Bond lengths



Bond angles

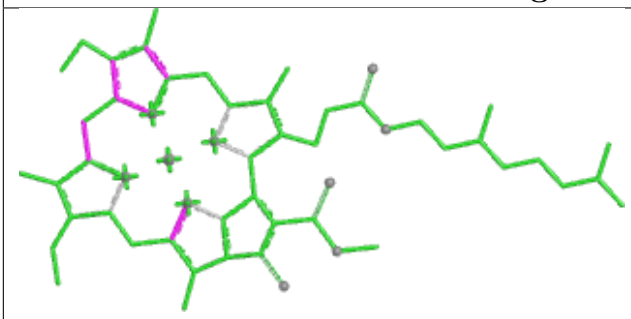


Torsions

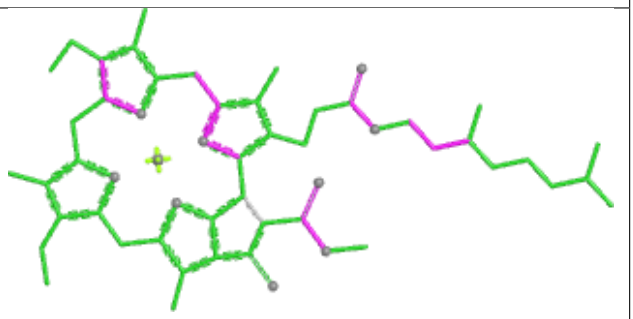


Rings

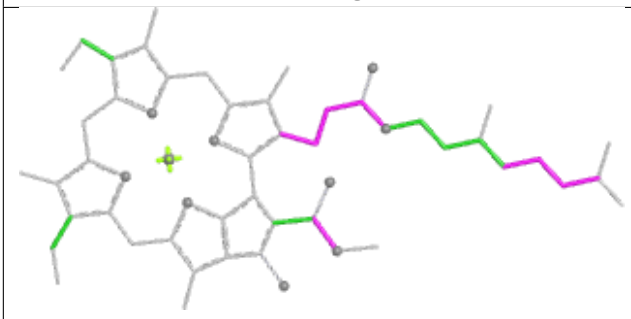
Ligand CLA I 316



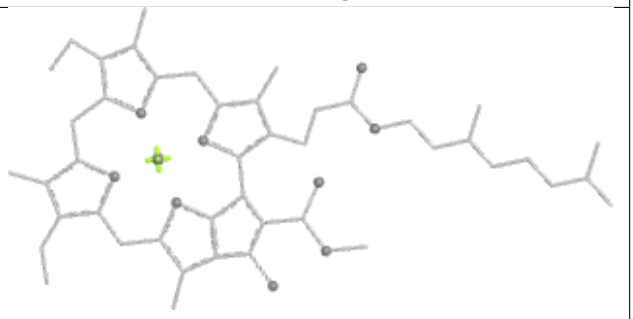
Bond lengths



Bond angles

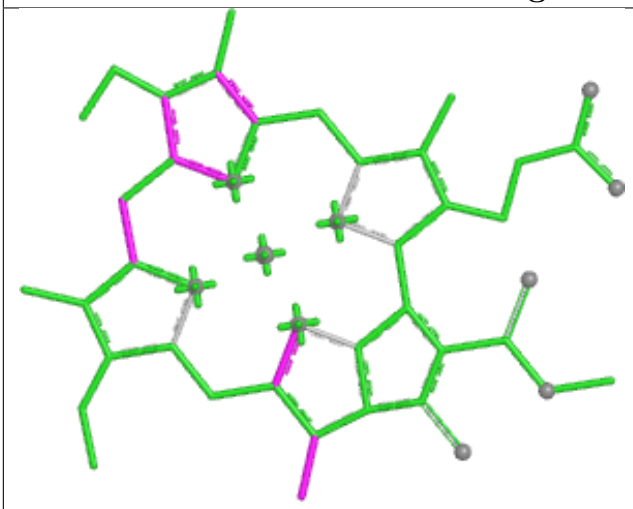


Torsions

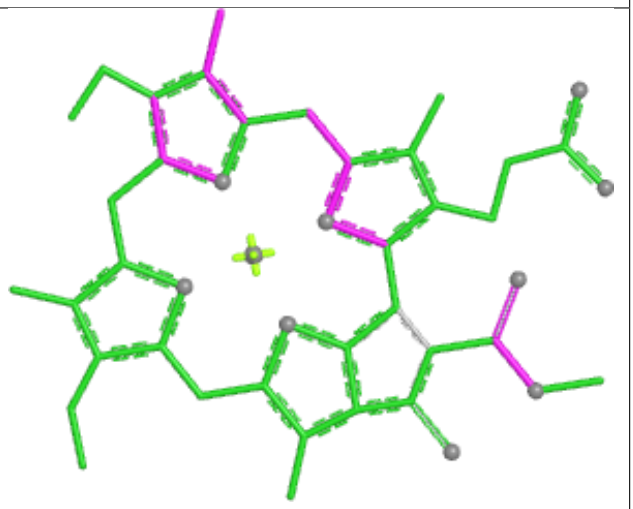


Rings

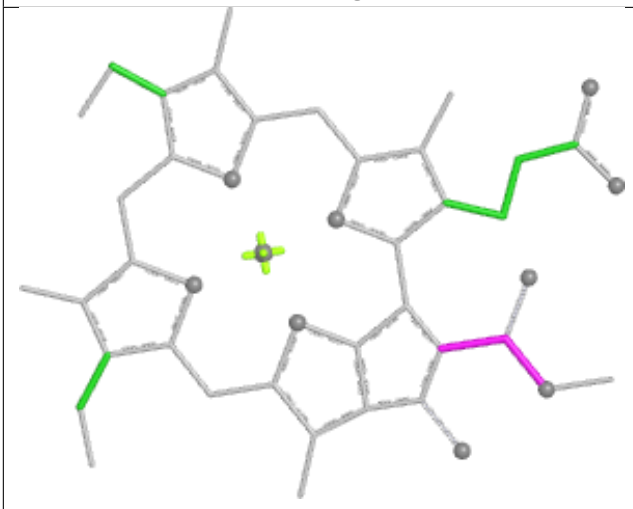
Ligand CLA a 714



Bond lengths



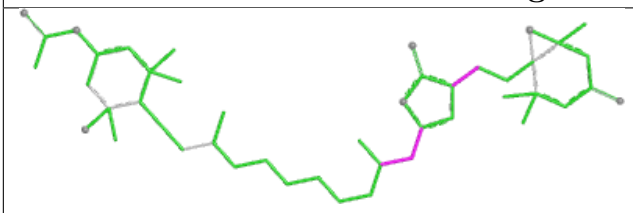
Bond angles



Torsions

Rings

Ligand PID D 302



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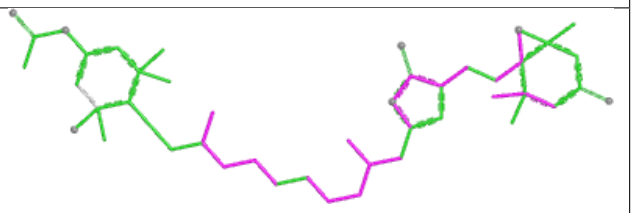
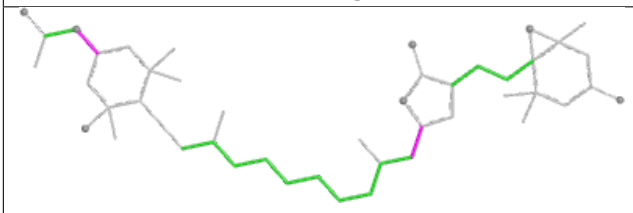


Bond angles



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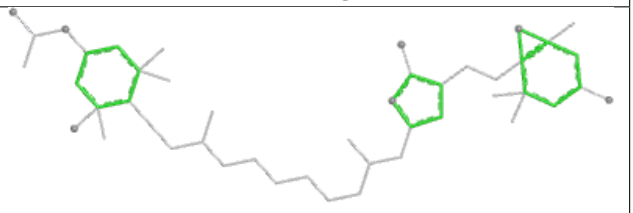
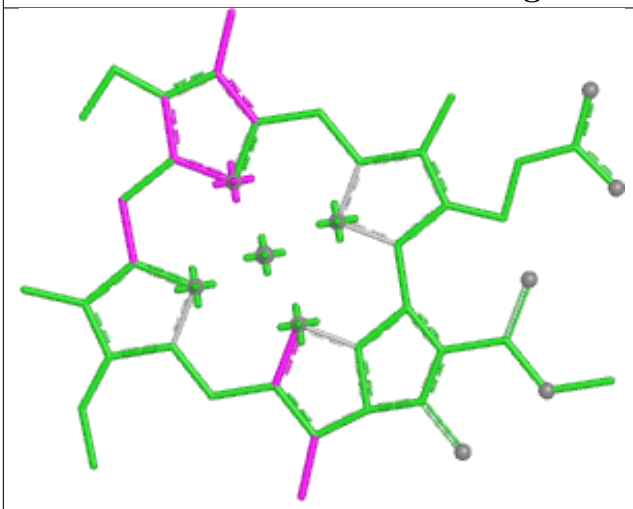


Rings

Ligand CLA D 313



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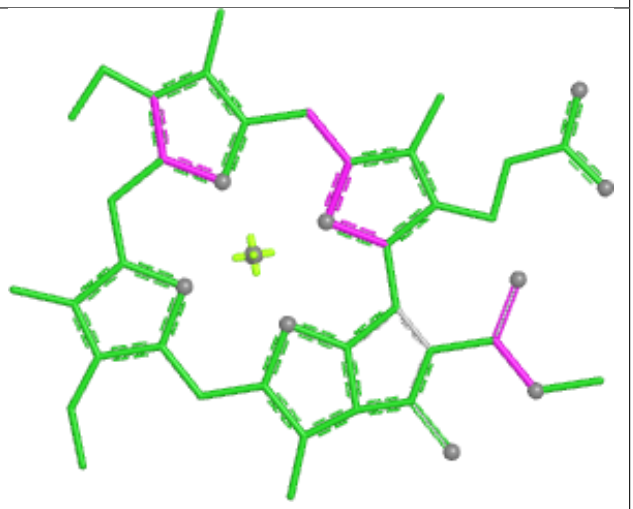
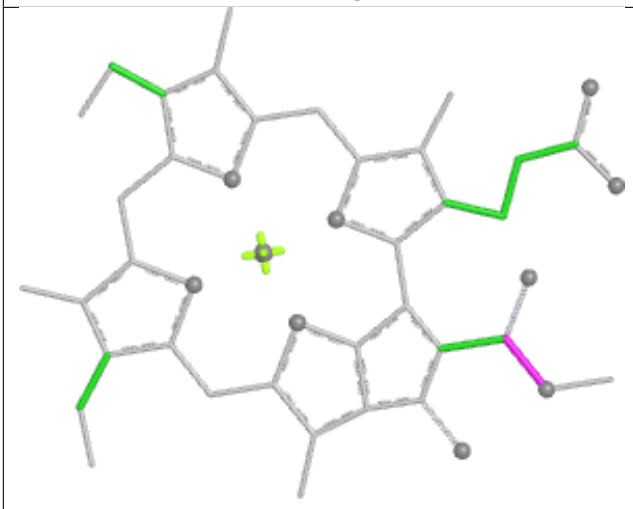


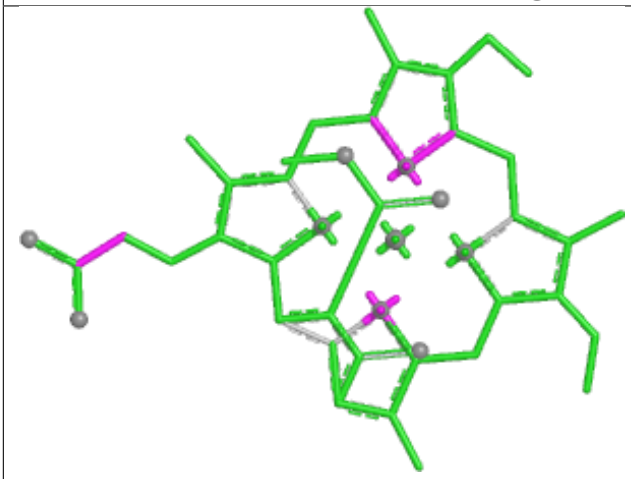
Bond angles



Torsions

Rings

Ligand KC1 L 307



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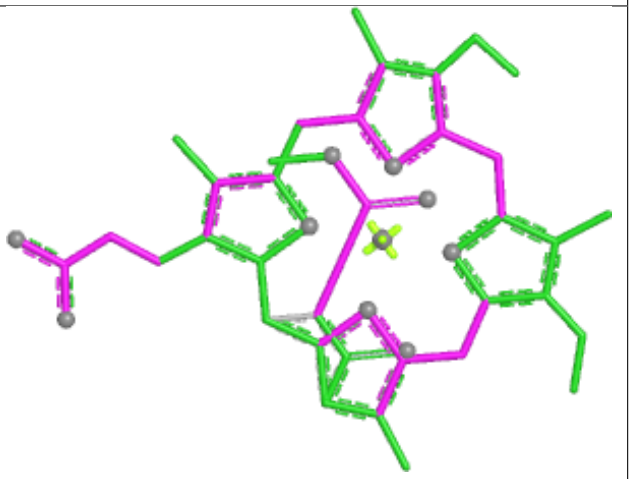
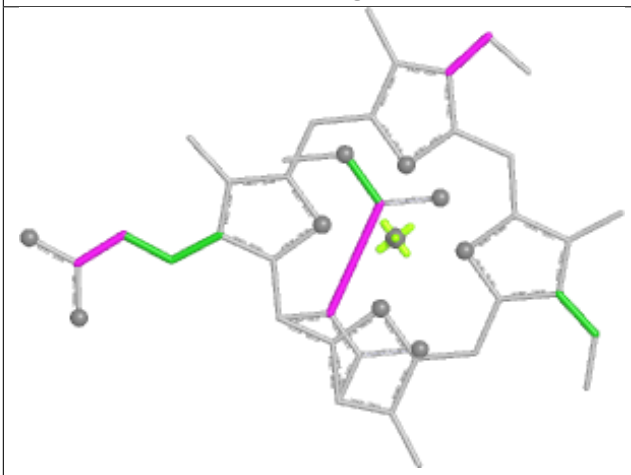
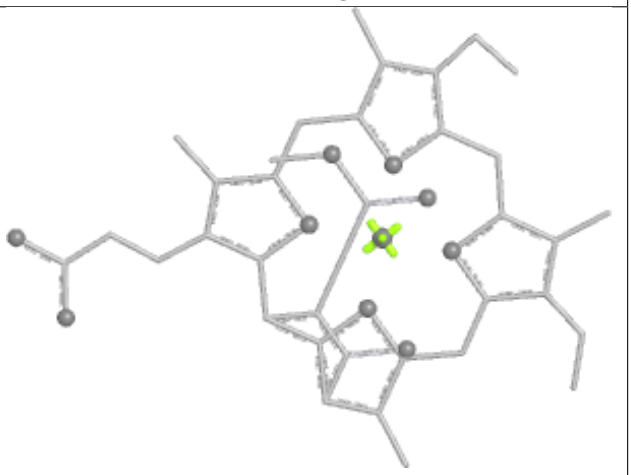


Bond angles

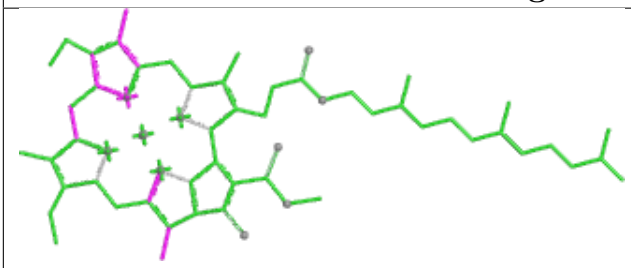


Torsions



Rings

Ligand CLA a 712



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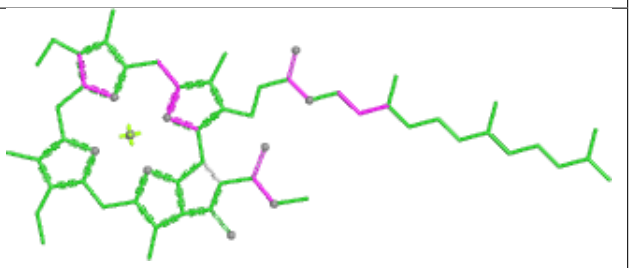
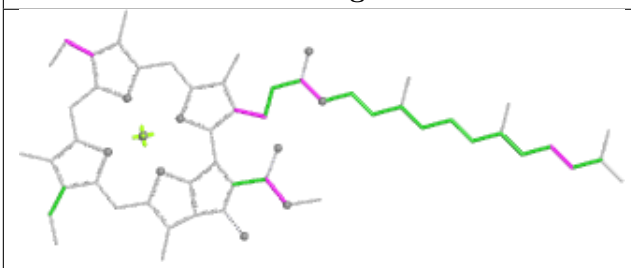


Bond angles



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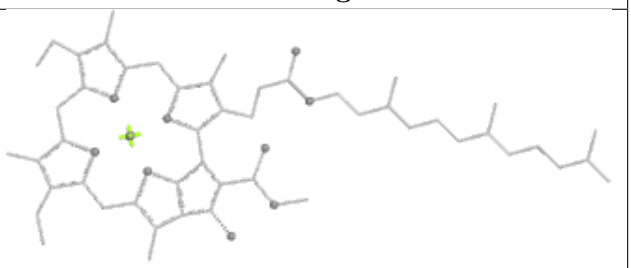
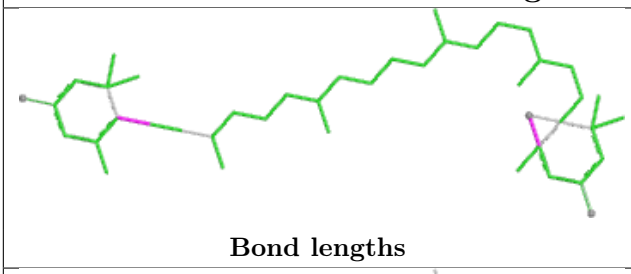


Rings

Ligand DD6 N 303



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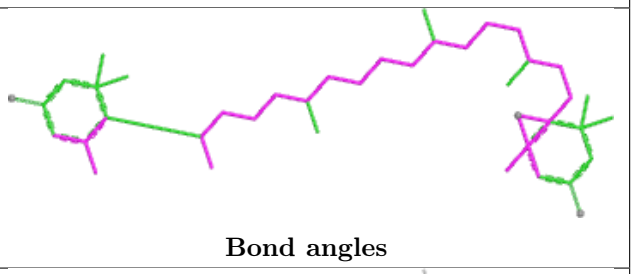
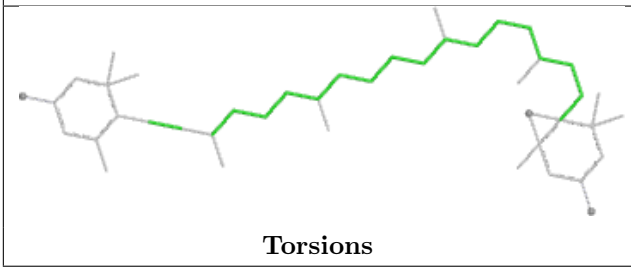
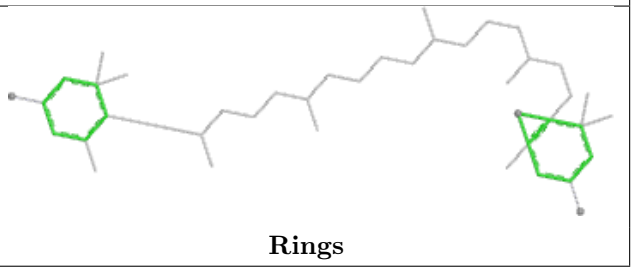


Bond angles

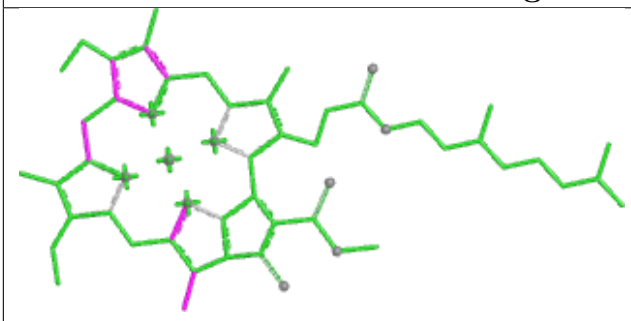


Torsions



Rings

Ligand CLA A 308



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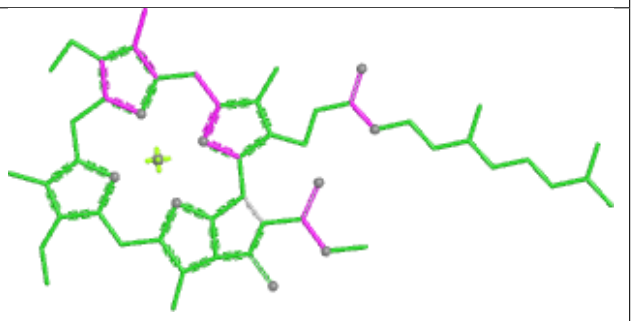
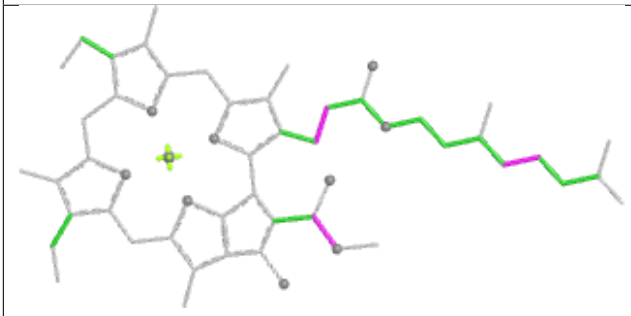


Bond angles



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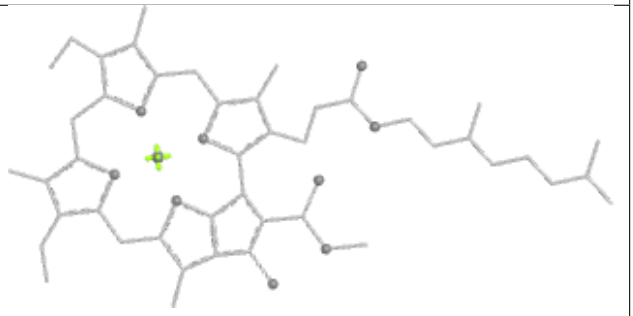
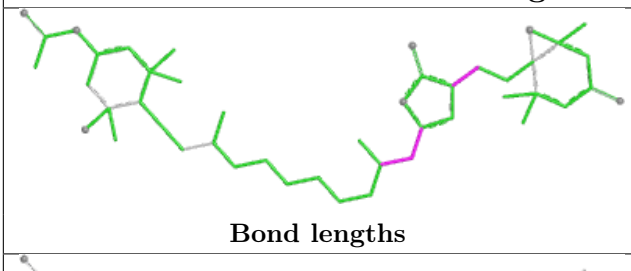


Rings

Ligand PID O 302



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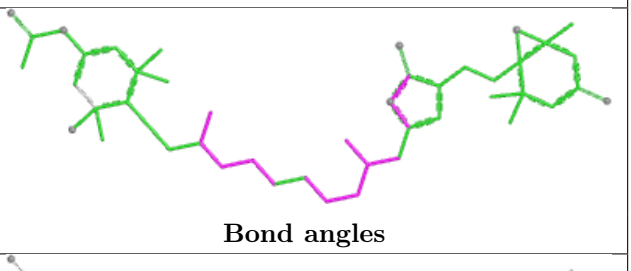
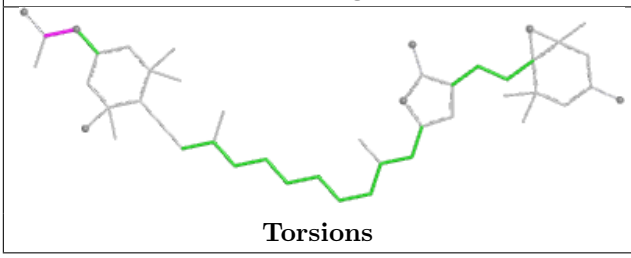


Bond angles



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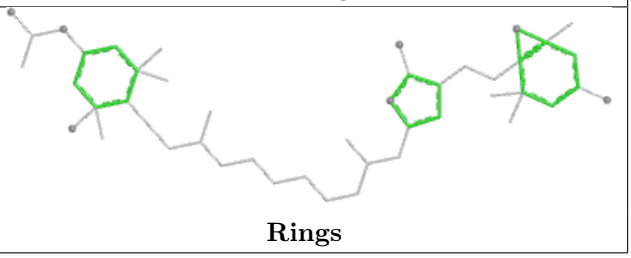
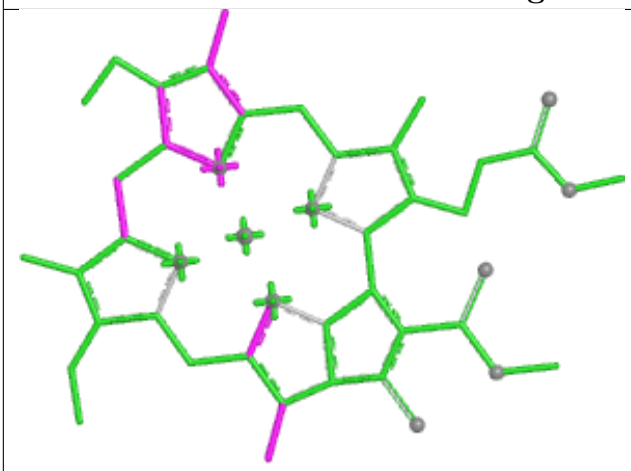


Rings

Ligand CLA b 719



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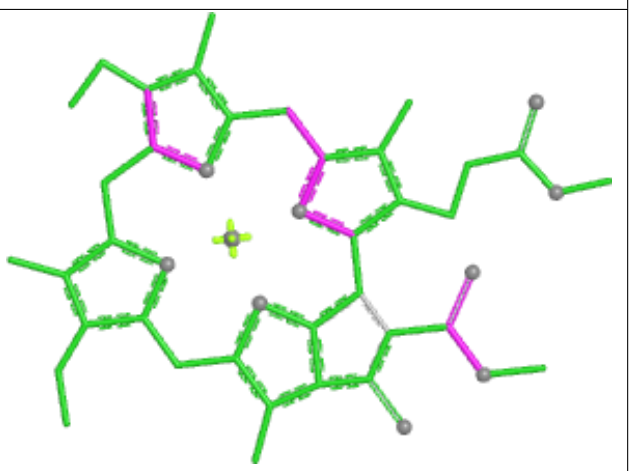
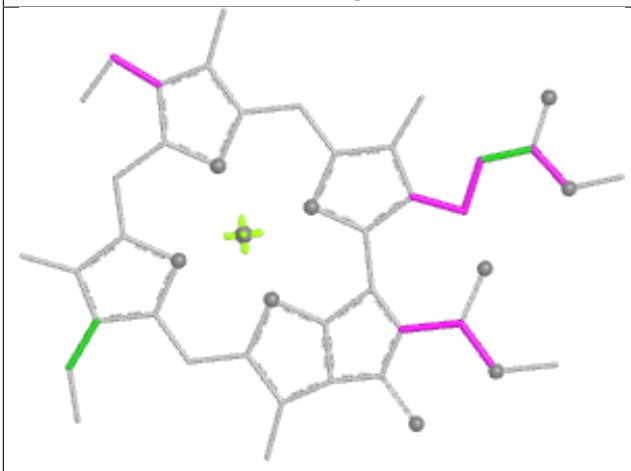
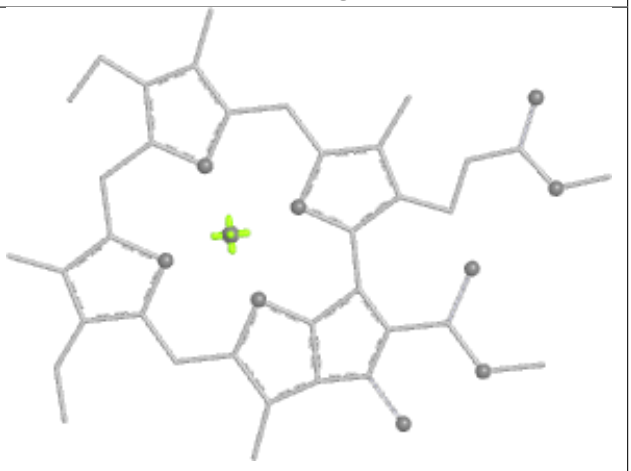


Bond angles

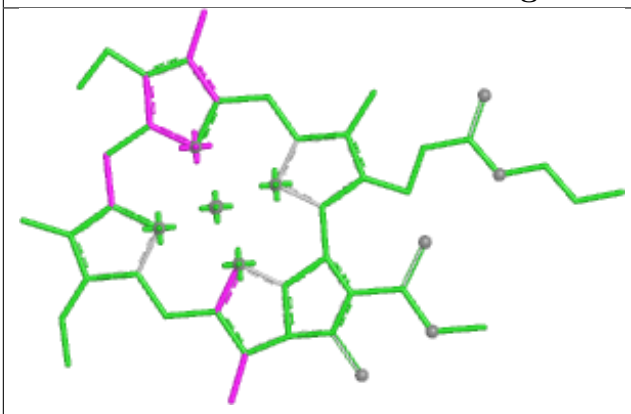


Torsions



Rings

Ligand CLA M 312



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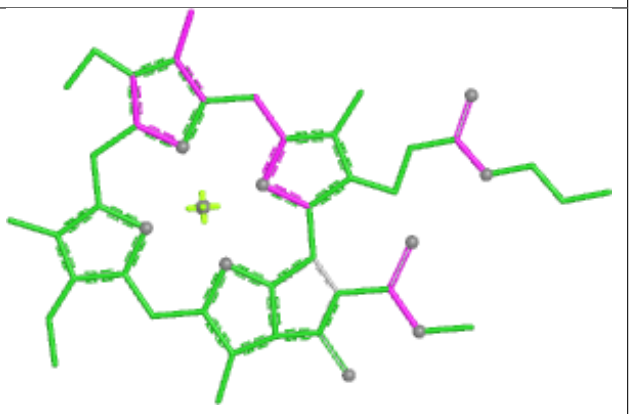
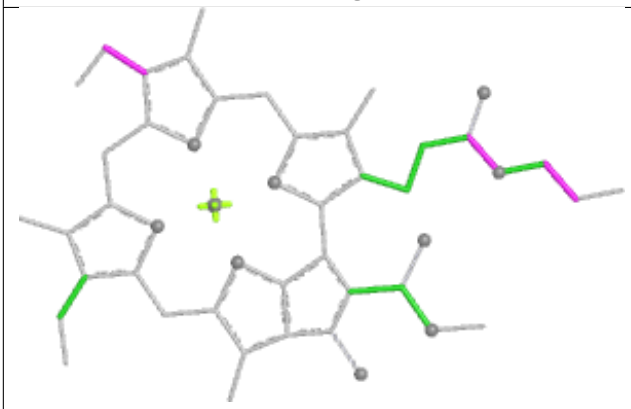


Bond angles



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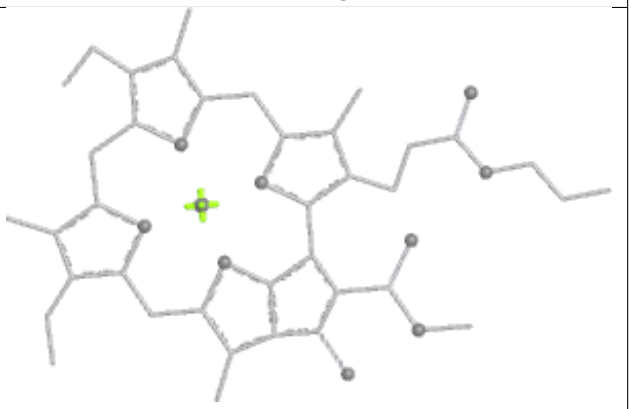
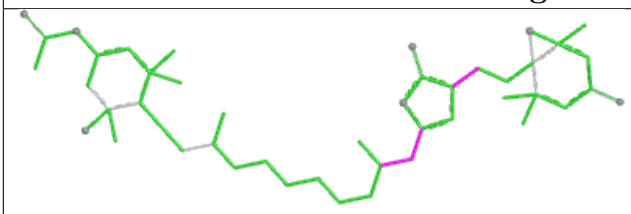


Rings

Ligand PID P 202



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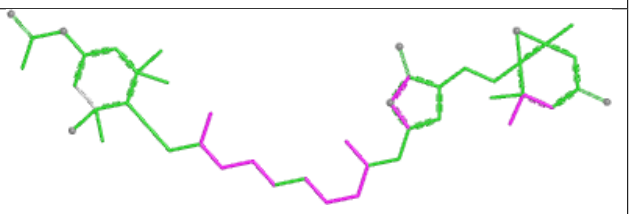
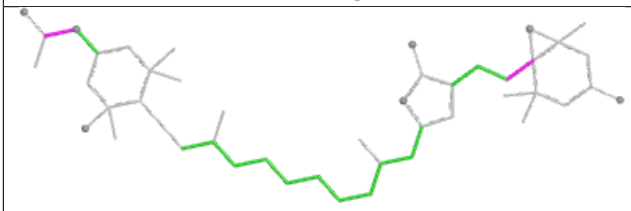


Bond angles



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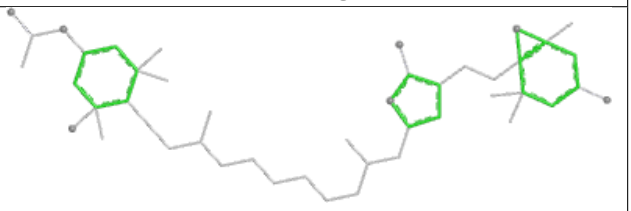
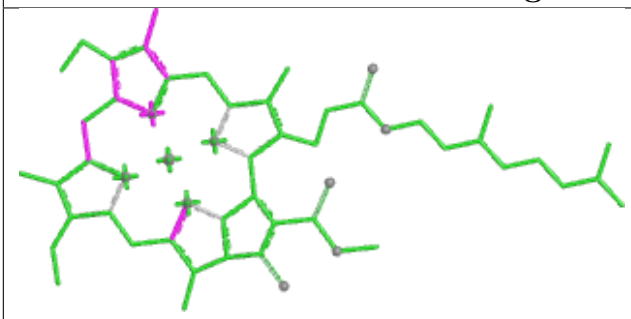


Rings

Ligand CLA B 310



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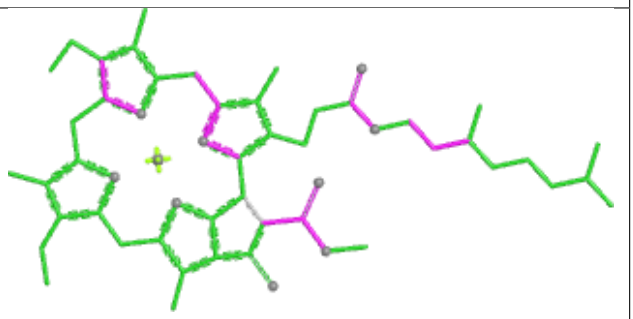
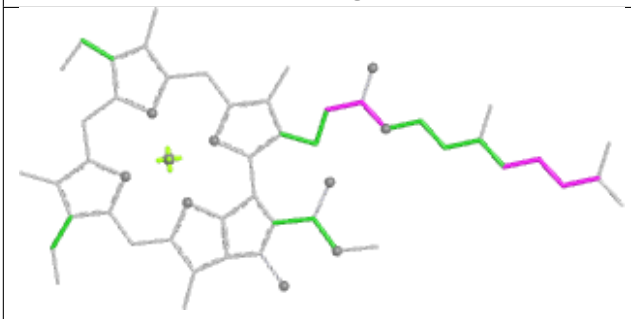
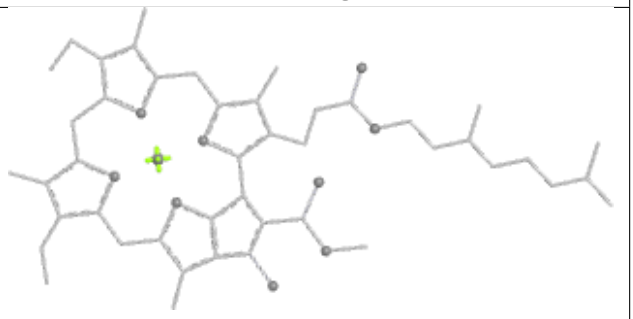


Bond angles

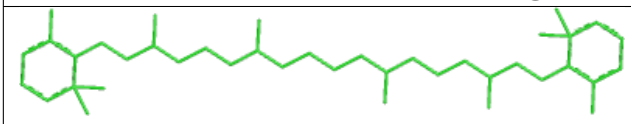


Torsions



Rings

Ligand BCR a 736



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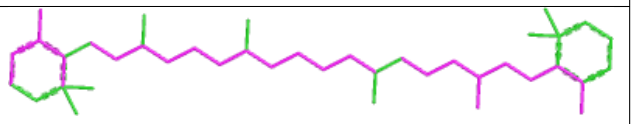
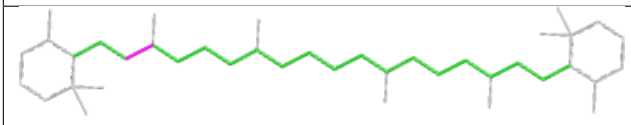
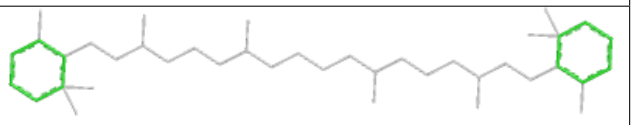


Bond angles

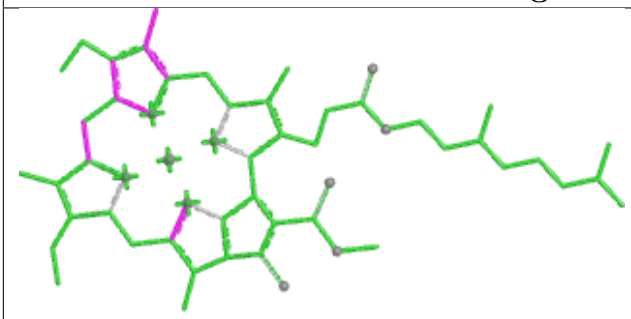


Torsions



Rings

Ligand CLA I 311



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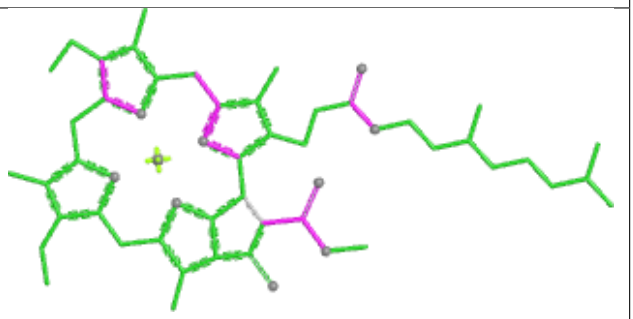
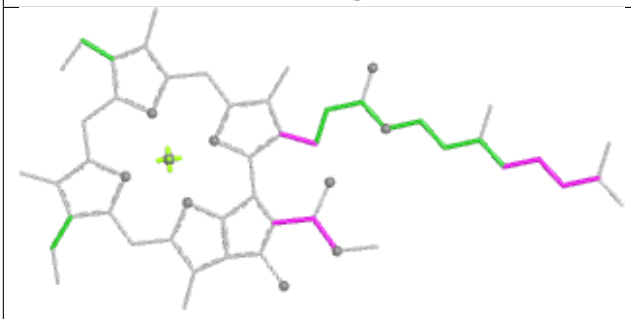
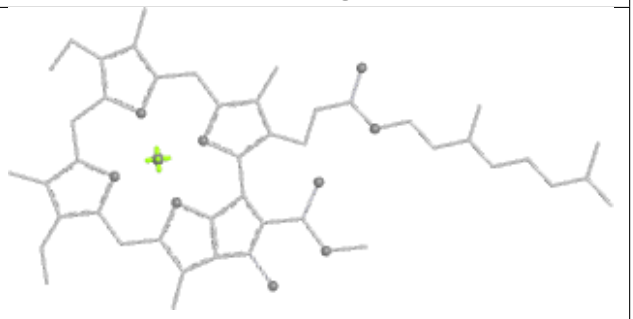


Bond angles

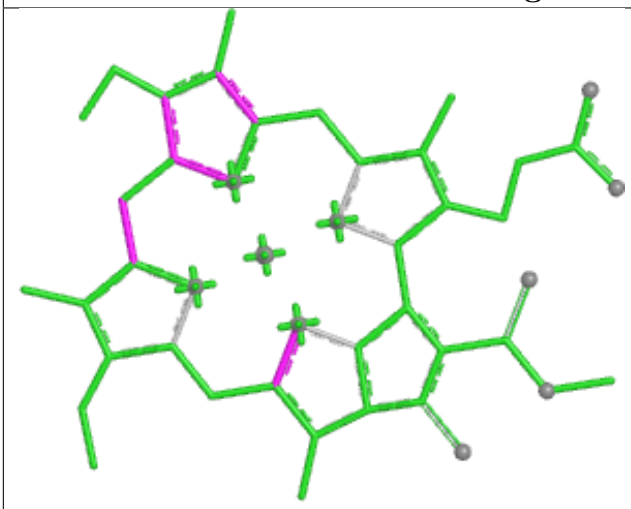


Torsions

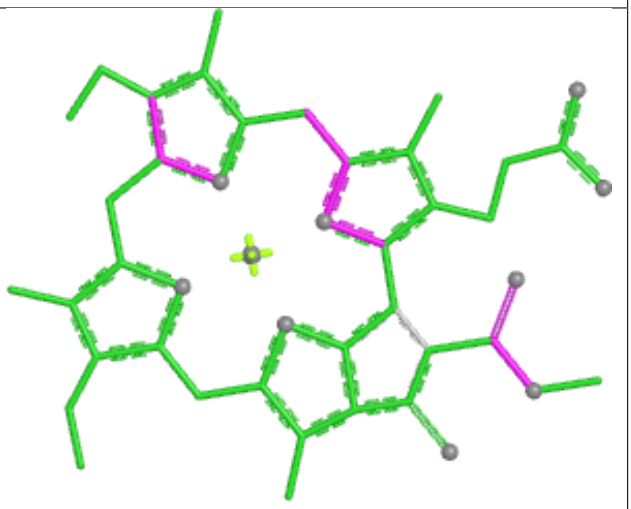


Rings

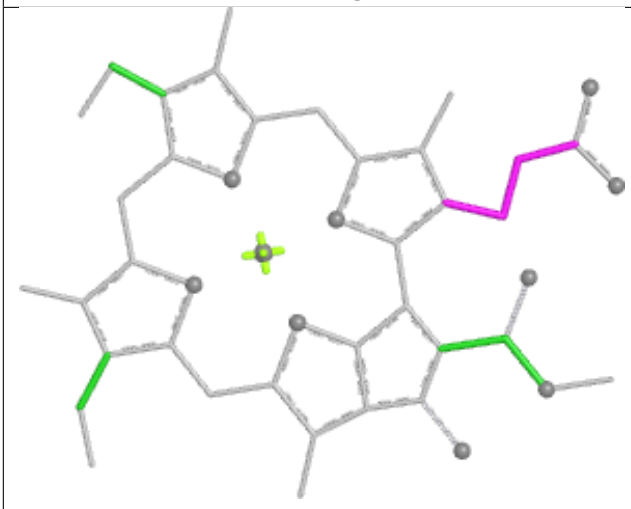
Ligand CLA B 308



Bond lengths



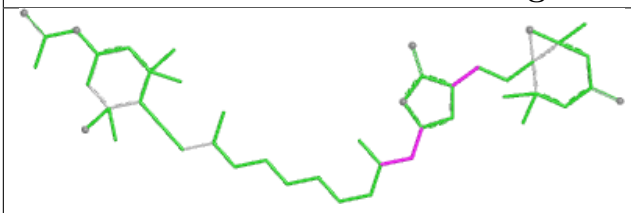
Bond angles



Torsions

Rings

Ligand PID D 301



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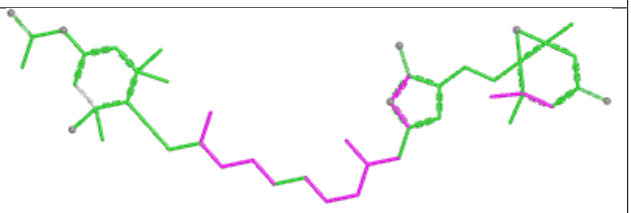
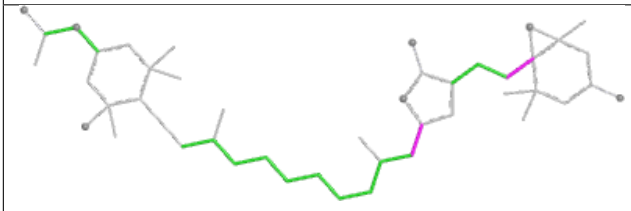


Bond angles



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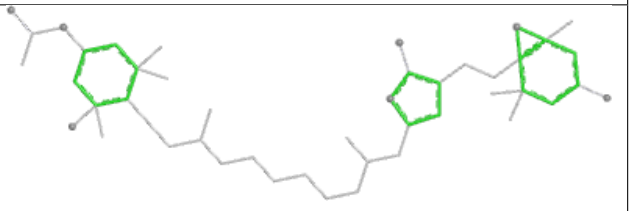
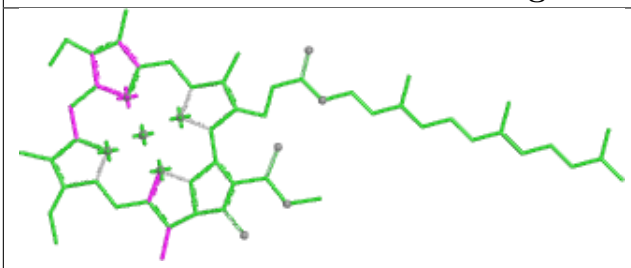


Rings

Ligand CLA a 713



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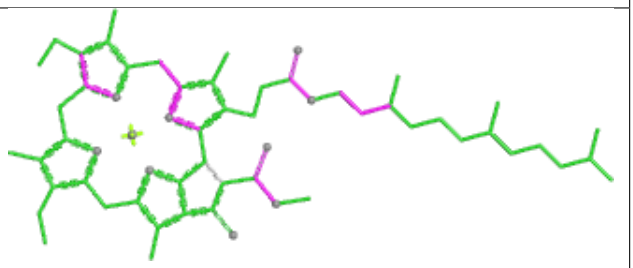
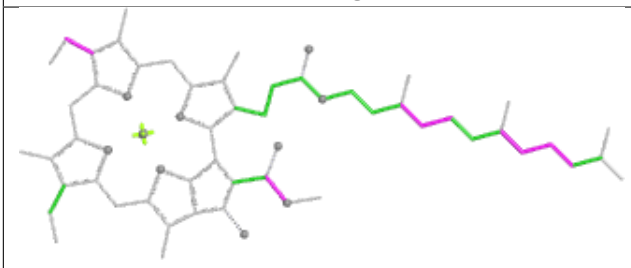


Bond angles



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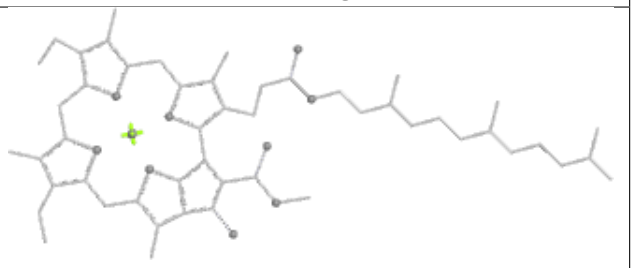
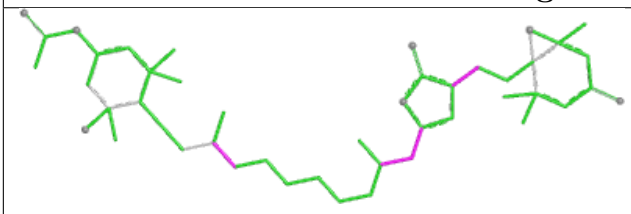


Rings

Ligand PID j 105



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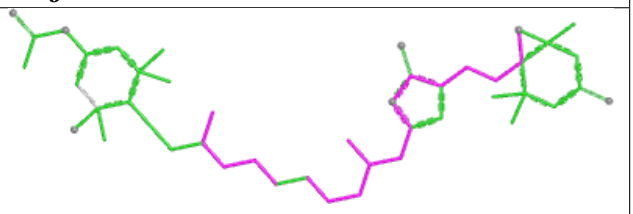
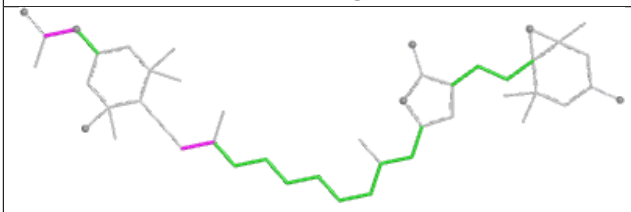


Bond angles



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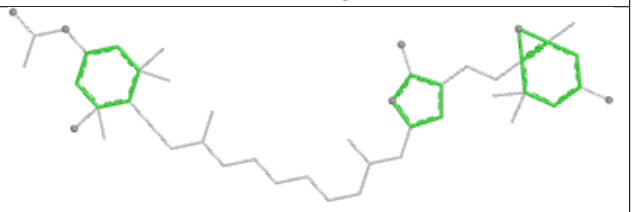
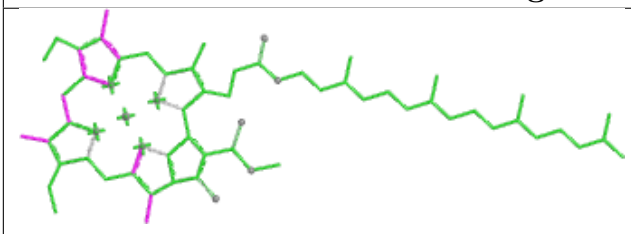


Rings

Ligand CLA b 705



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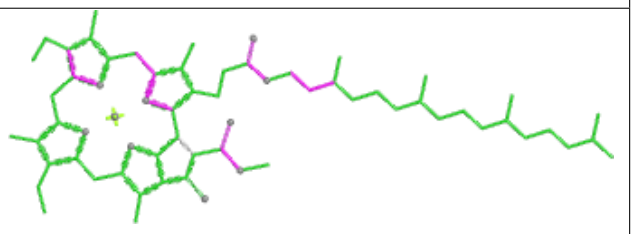
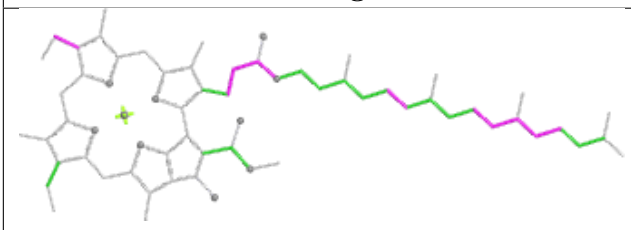


Bond angles



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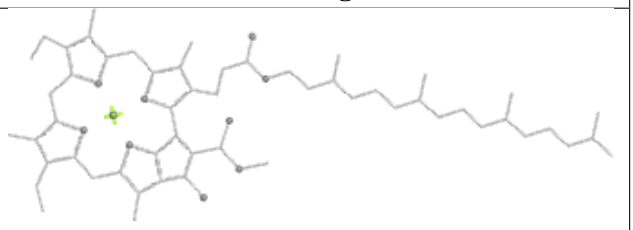
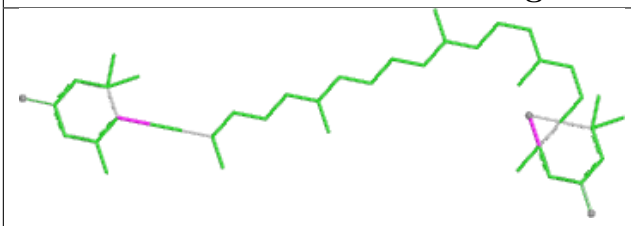


Rings

Ligand DD6 B 306



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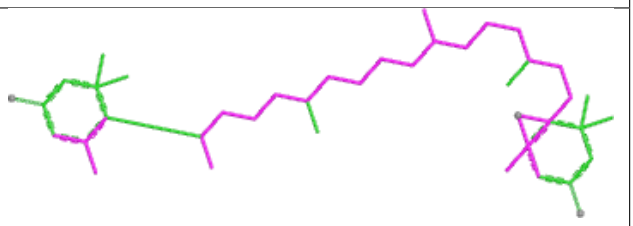
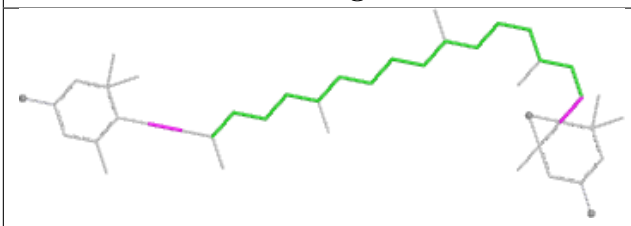


Bond angles



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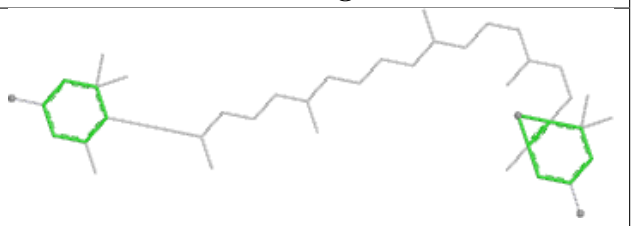
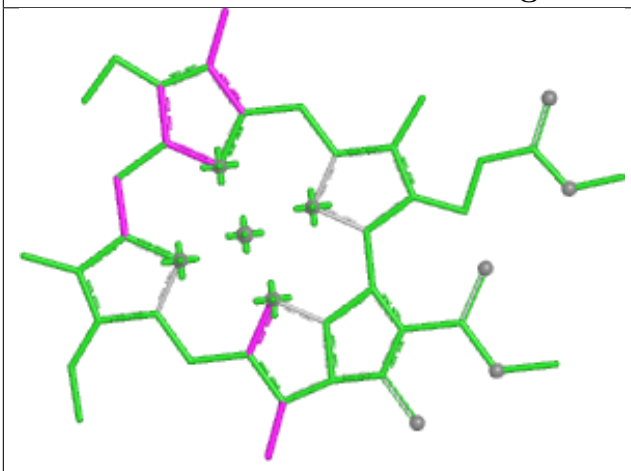


Rings

Ligand CLA M 313



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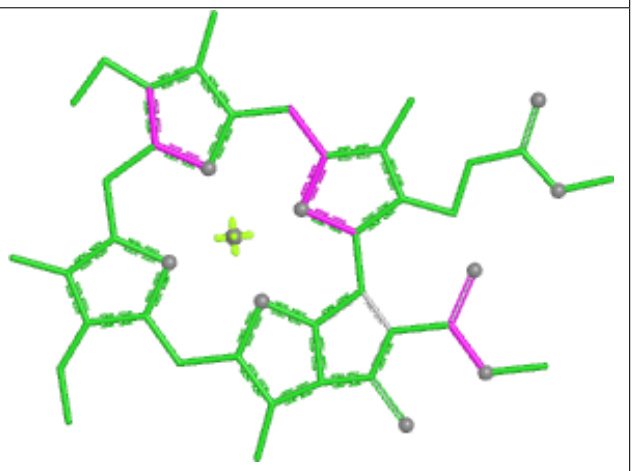
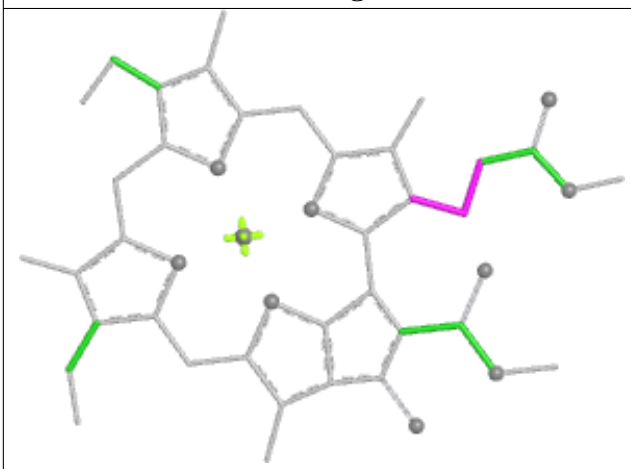
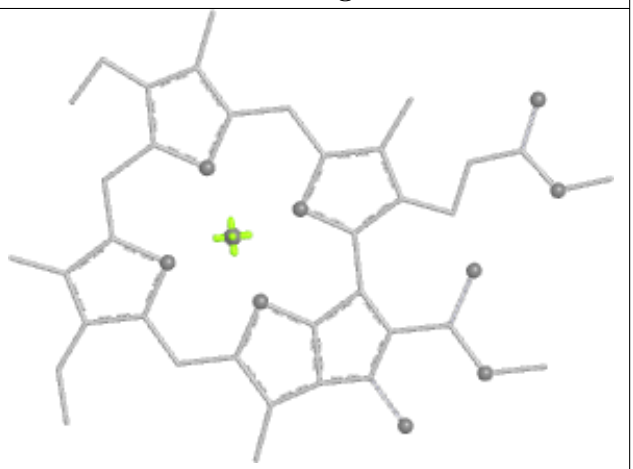


Bond angles

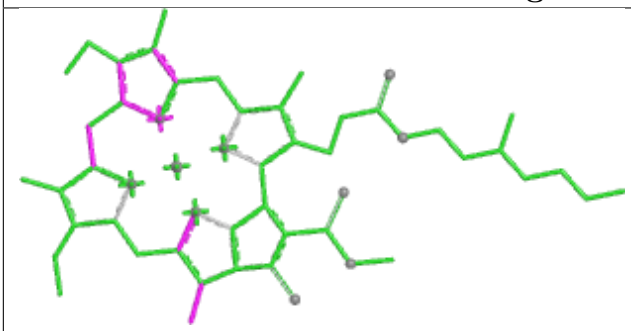


Torsions



Rings

Ligand CLA L 314



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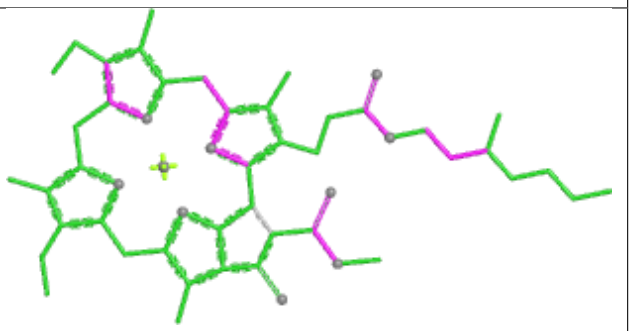
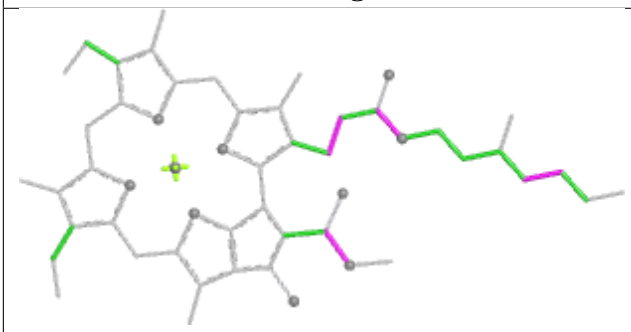


Bond angles



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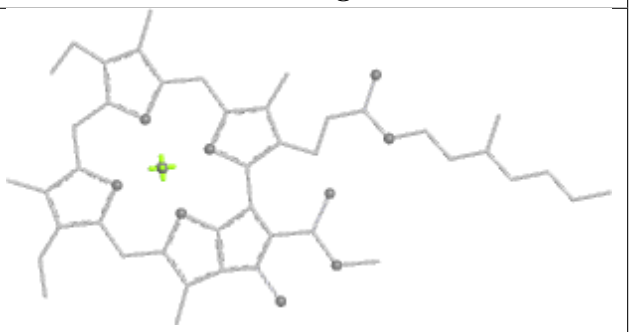
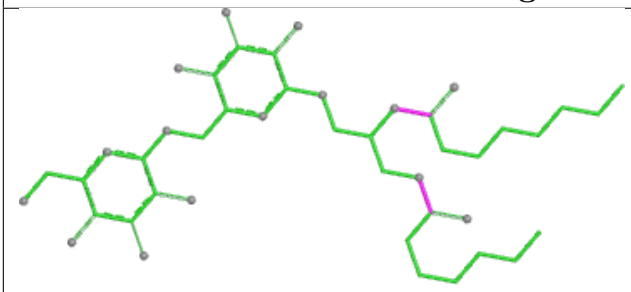


Rings

Ligand DGD G 501



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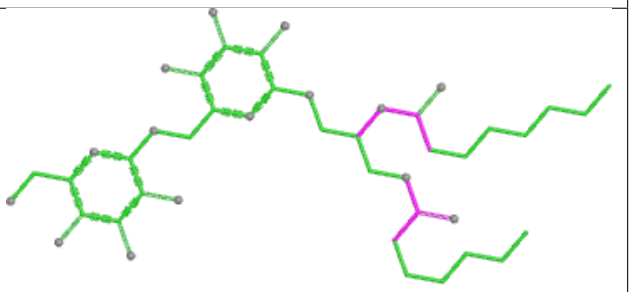
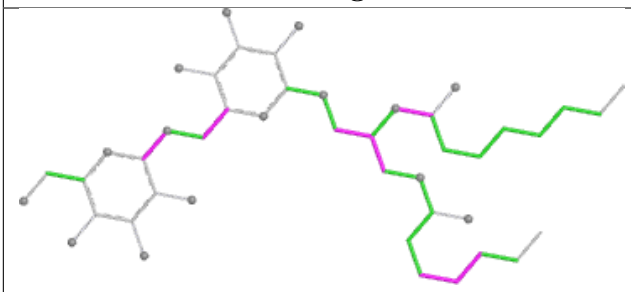


Bond angles



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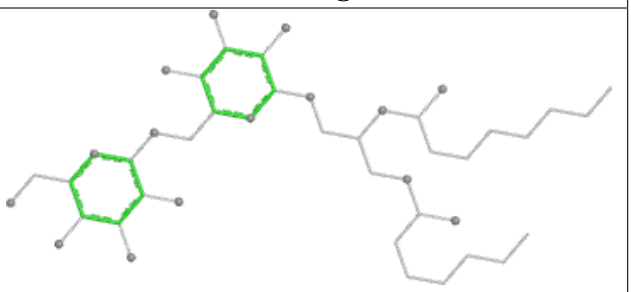
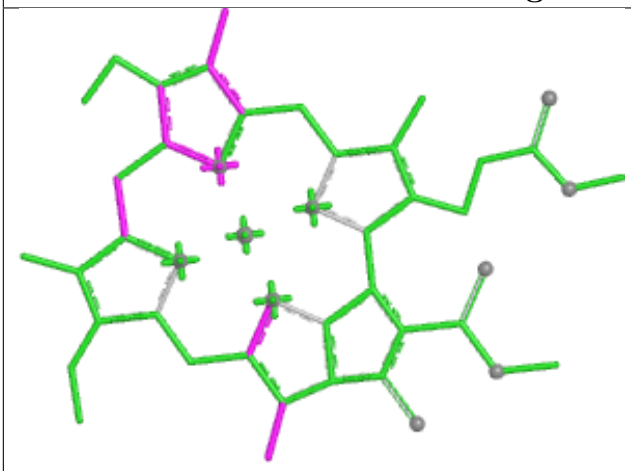


Rings

Ligand CLA F 307



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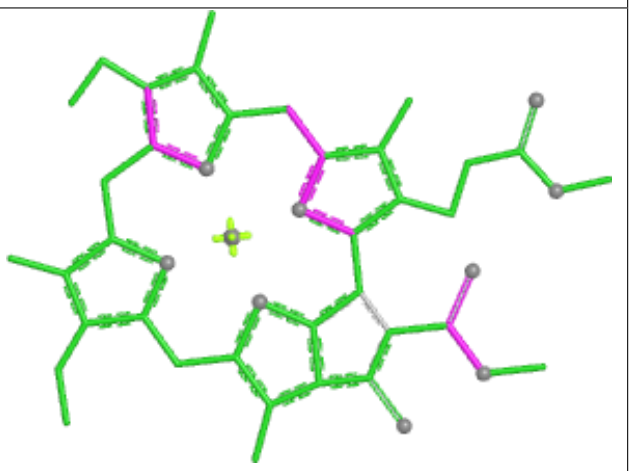
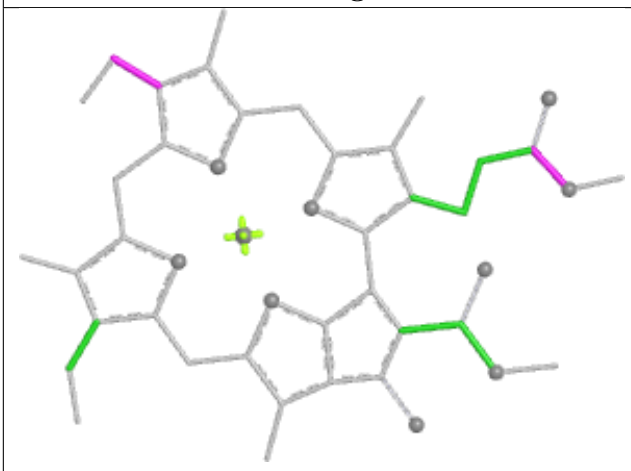


Bond angles



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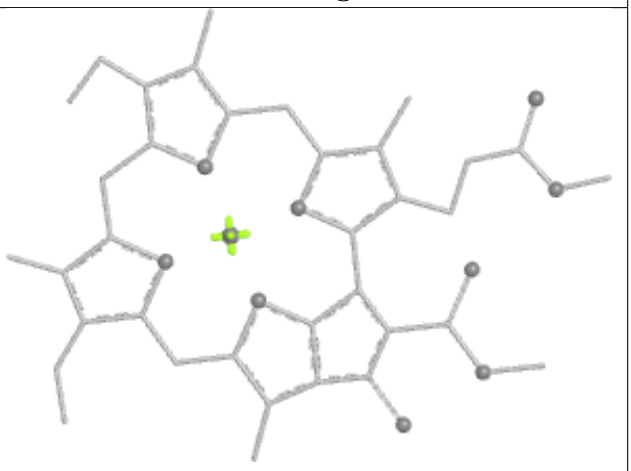
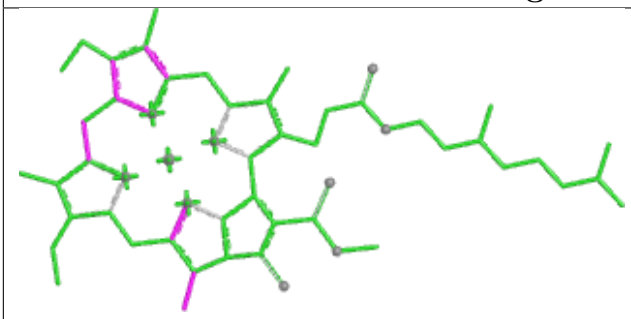


Rings

Ligand CLA L 311



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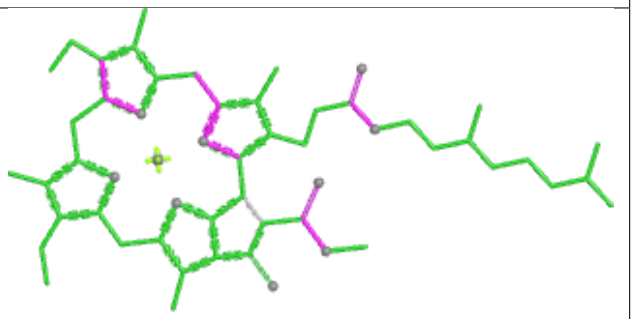
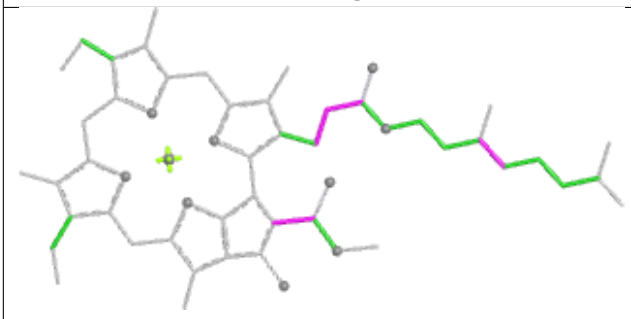


Bond angles



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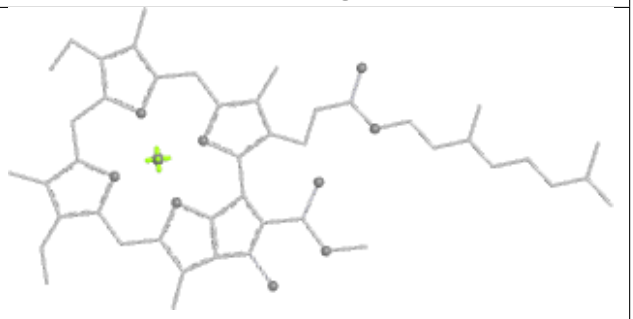
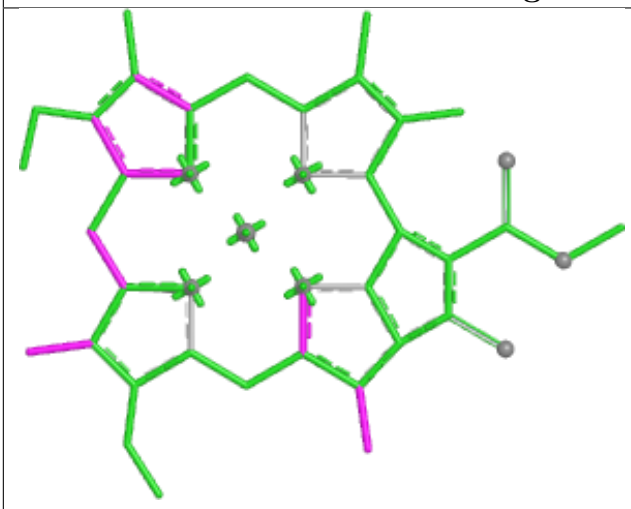
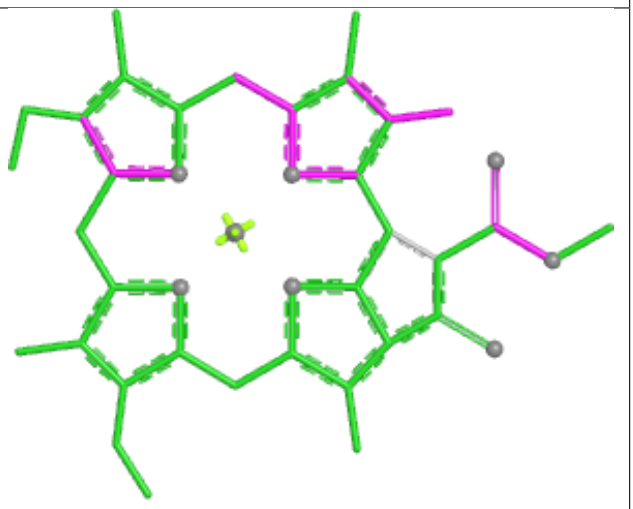


Rings

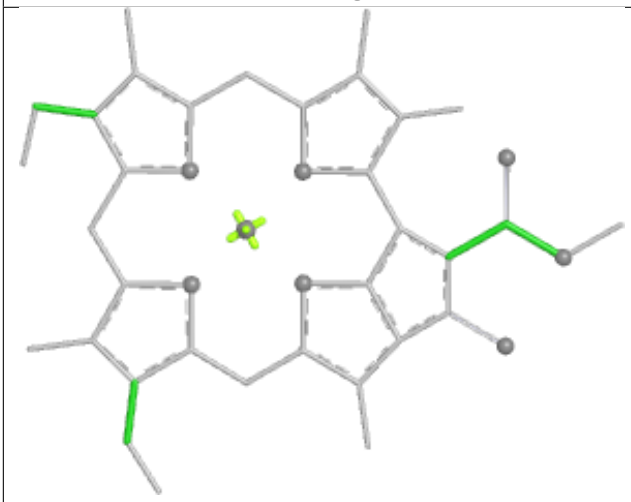
Ligand CLA D 316



Bond lengths



Bond angles



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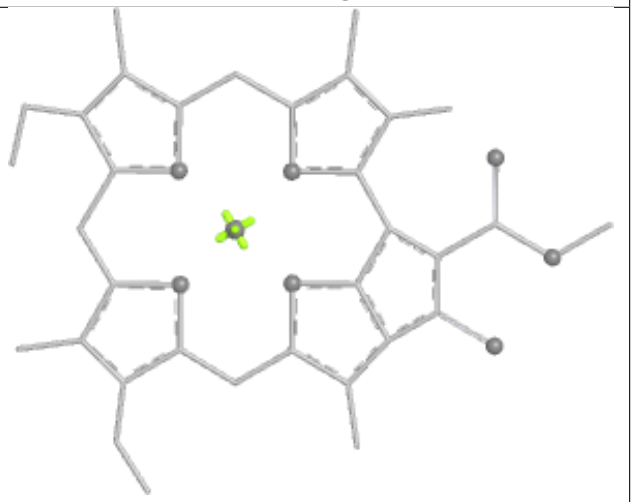
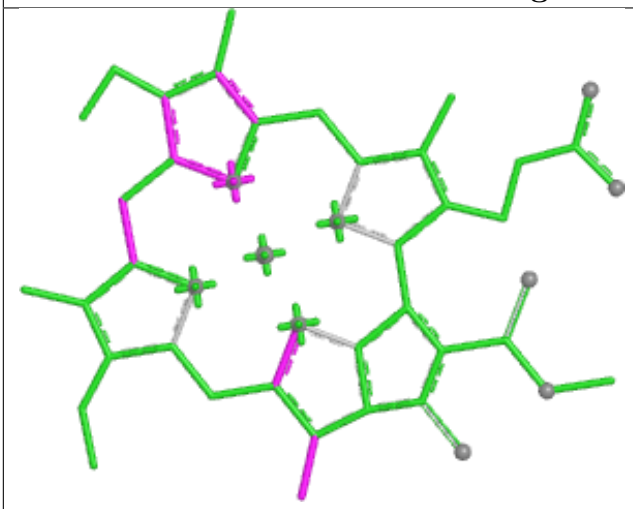


Rings

Ligand CLA I 319



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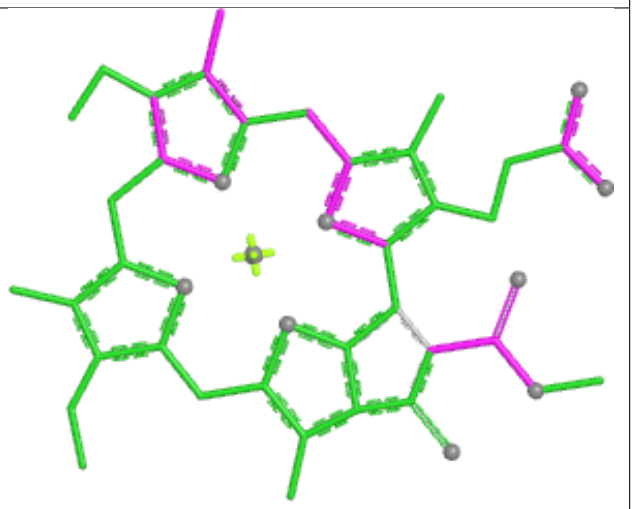
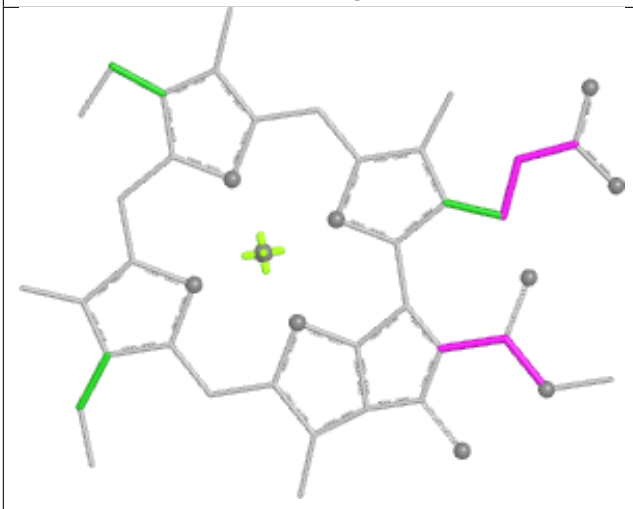


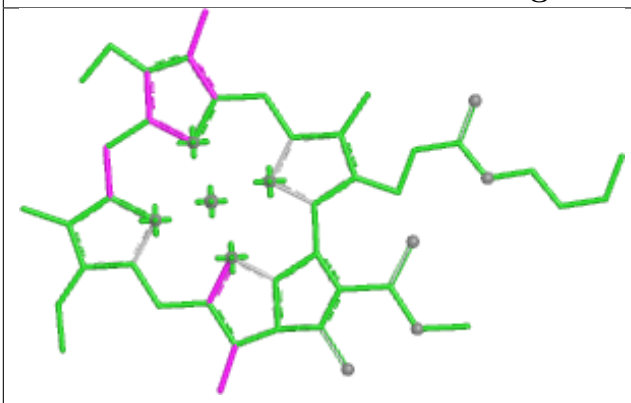
Bond angles



Torsions

Rings

Ligand CLA I 306



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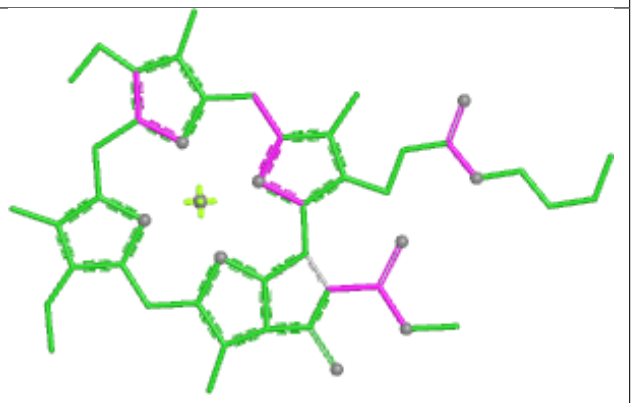
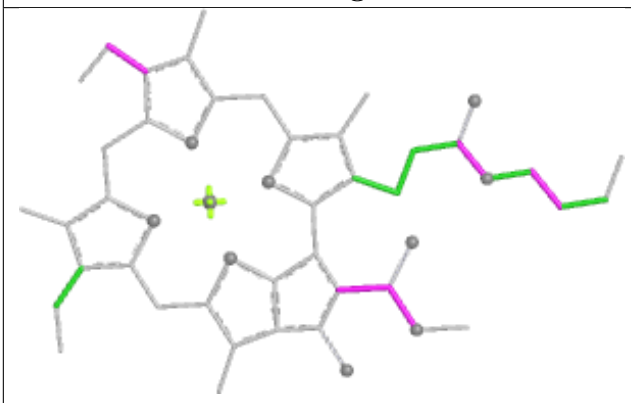
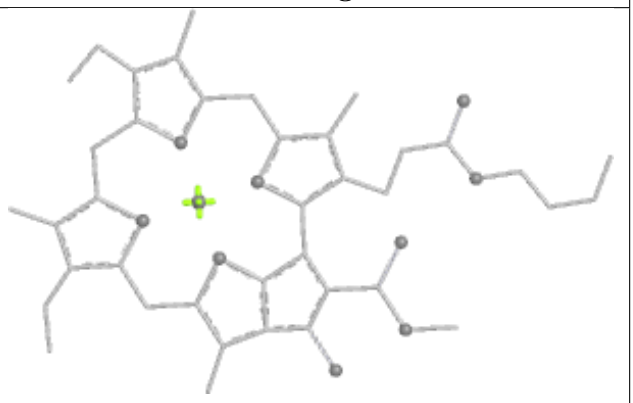


Bond angles

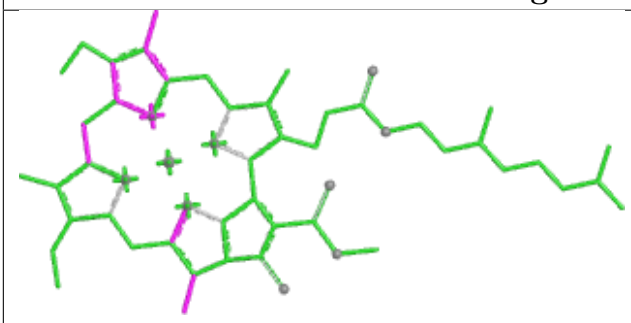


Torsions

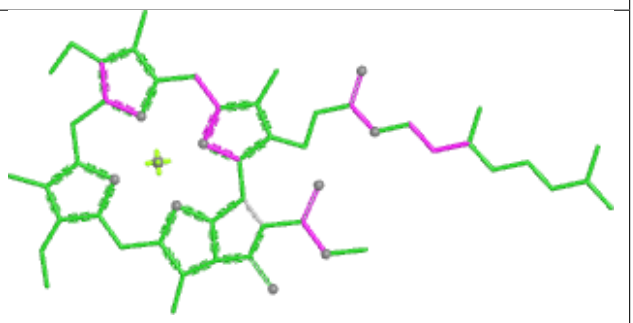


Rings

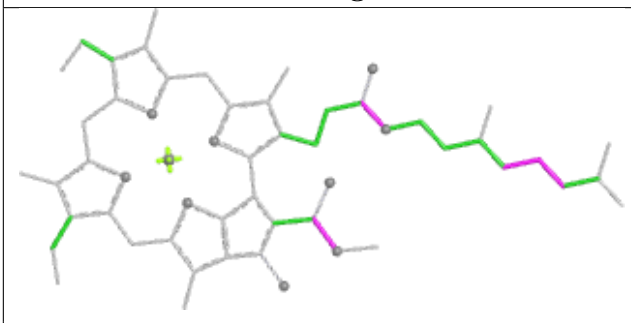
Ligand CLA I 309



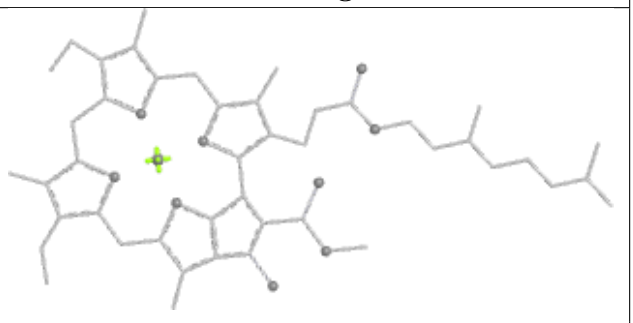
Bond lengths



Bond angles

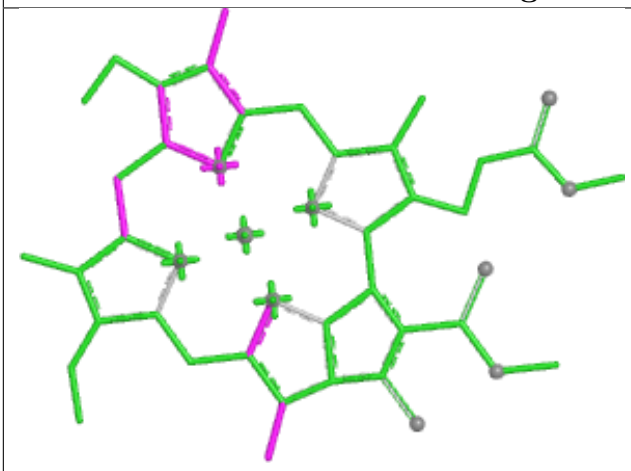


Torsions

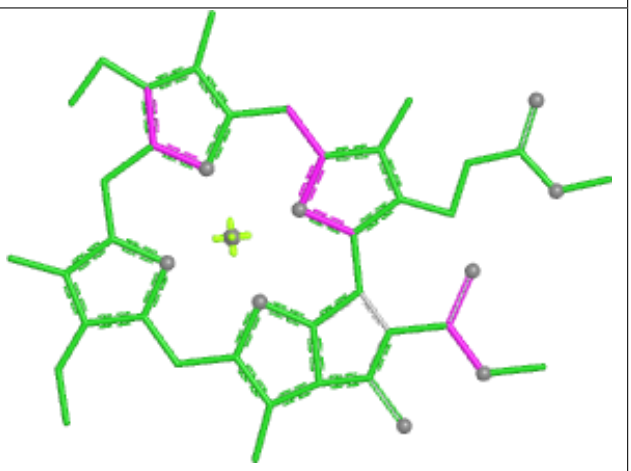


Rings

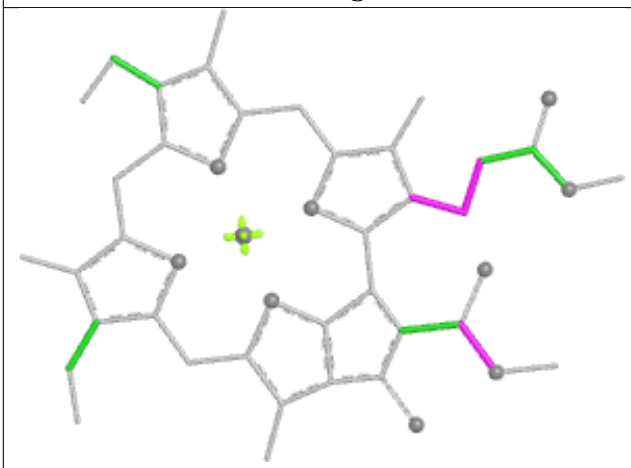
Ligand CLA M 311



Bond lengths



Bond angles



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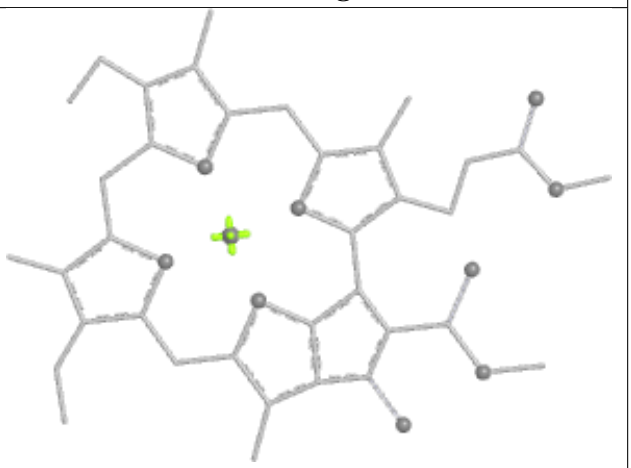
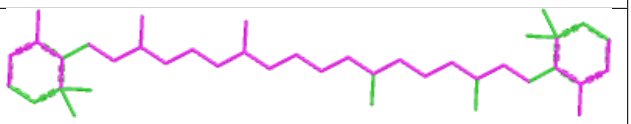


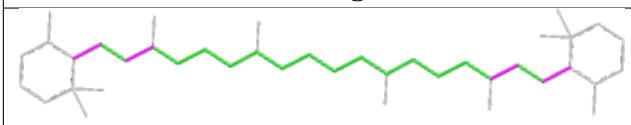
Rings

Ligand BCR i 201

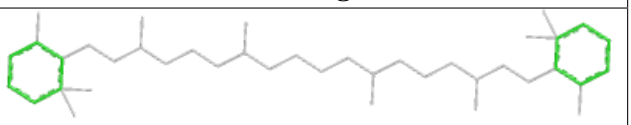
Bond lengths



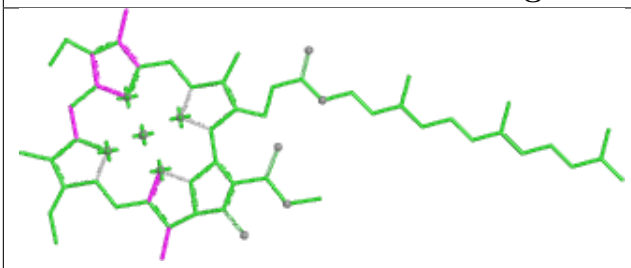
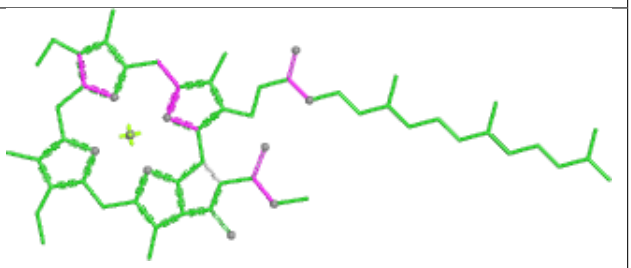
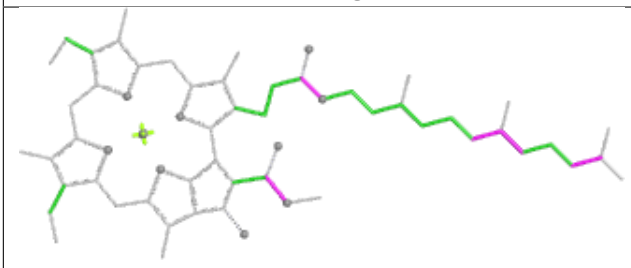
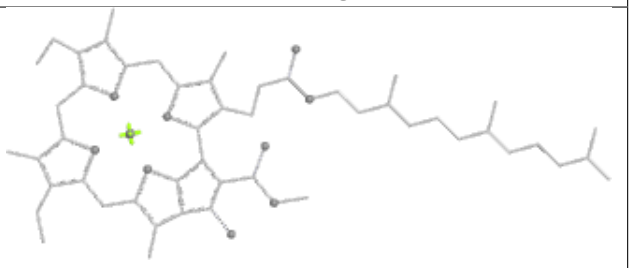
Bond angles

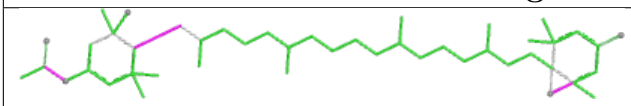
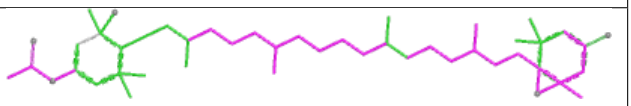
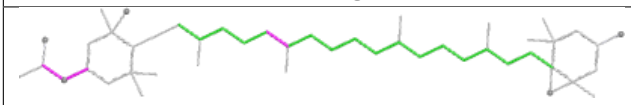
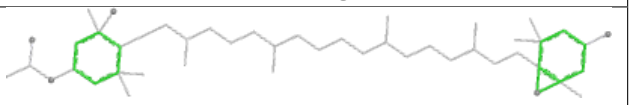


Torsions

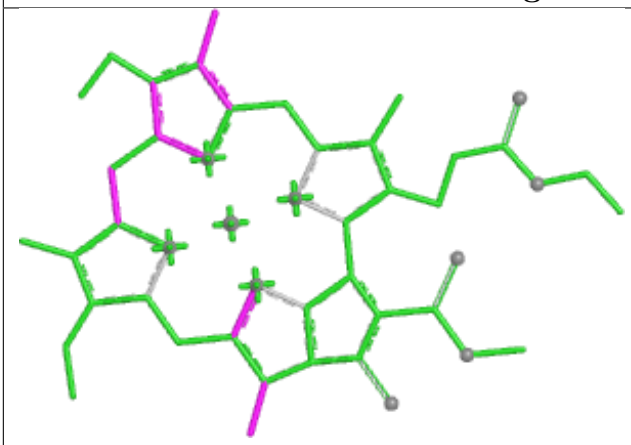


Rings

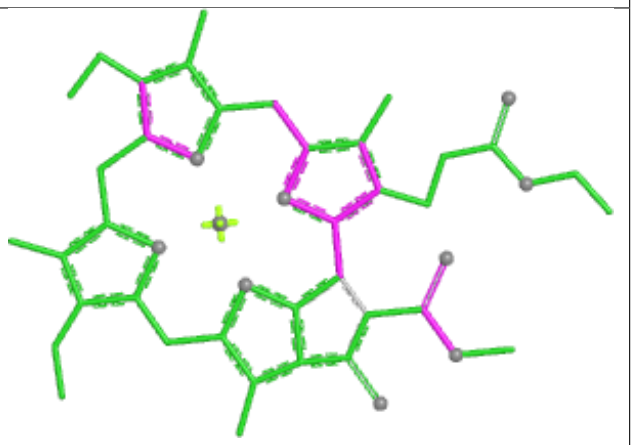
Ligand CLA B 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand UIX G 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

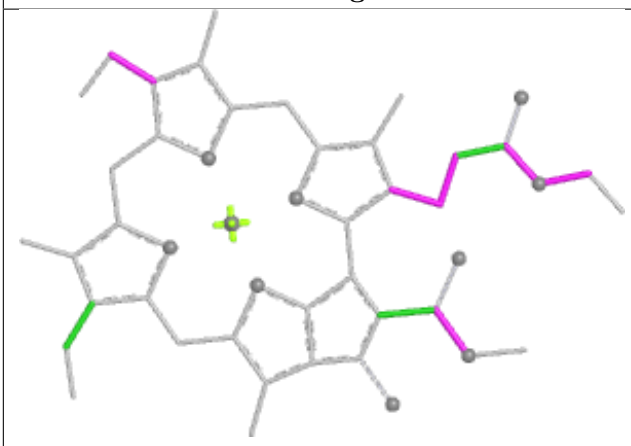
Ligand CLA N 310



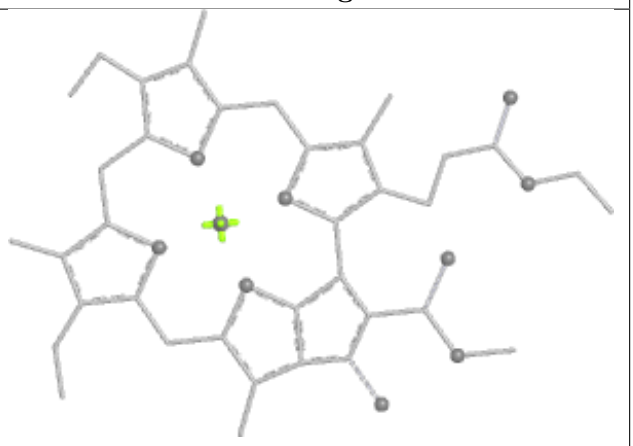
Bond lengths



Bond angles

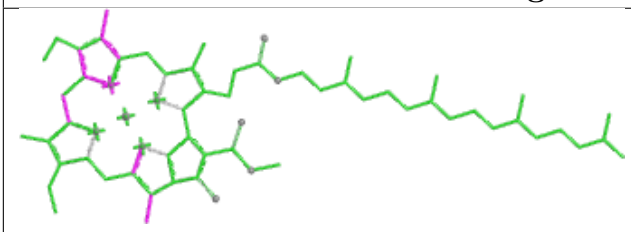


Torsions

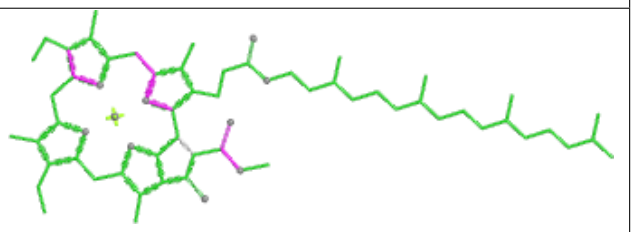


Rings

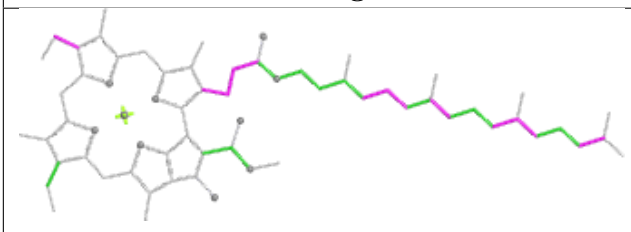
Ligand CLA b 724



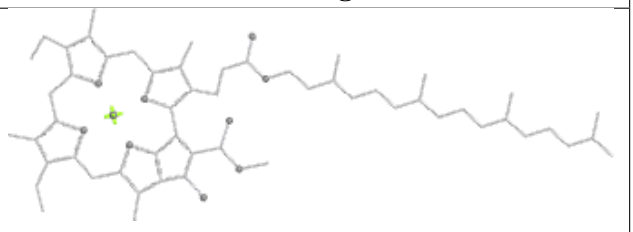
Bond lengths



Bond angles

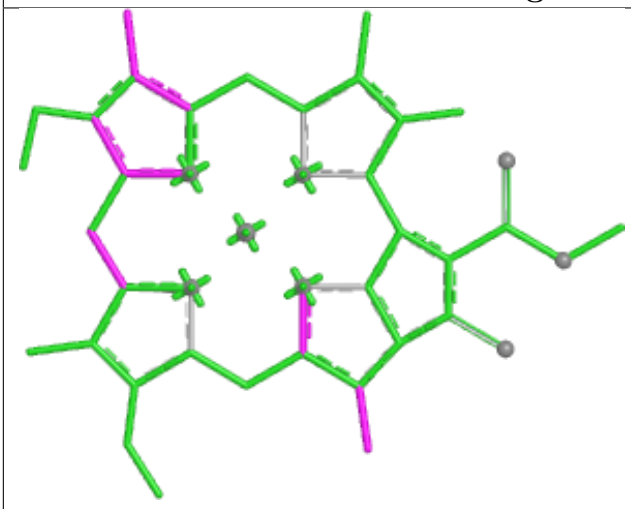


Torsions

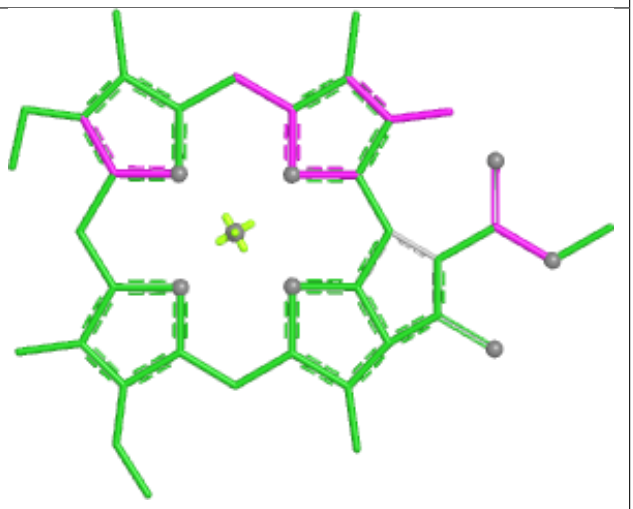


Rings

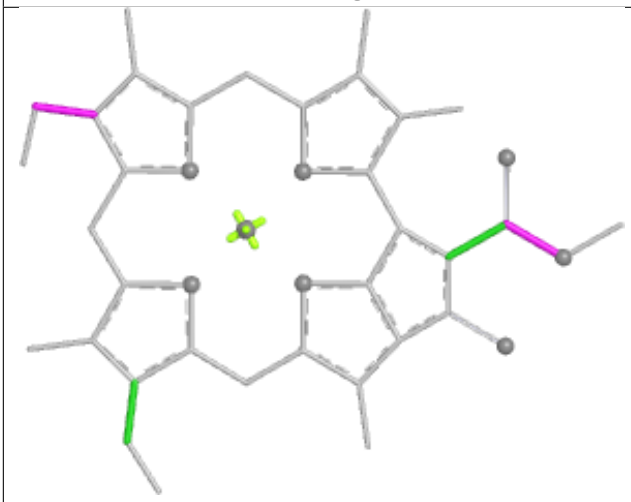
Ligand CLA L 316



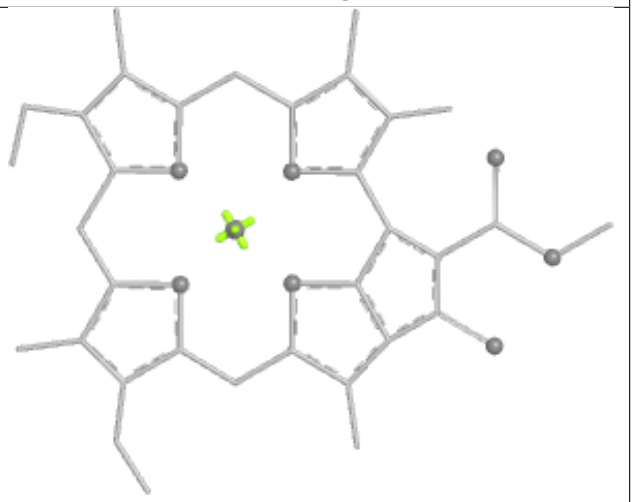
Bond lengths



Bond angles

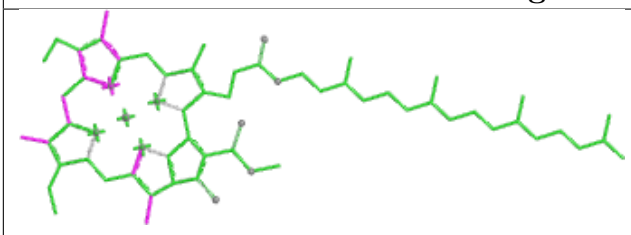


Torsions

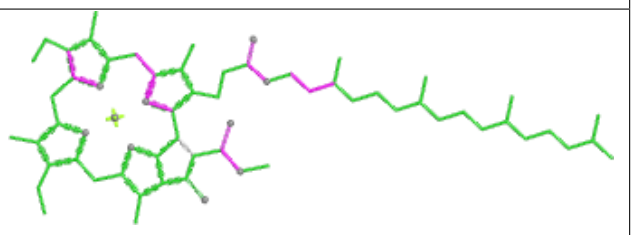


Rings

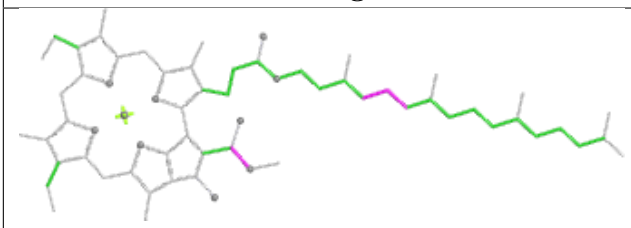
Ligand CLA a 730



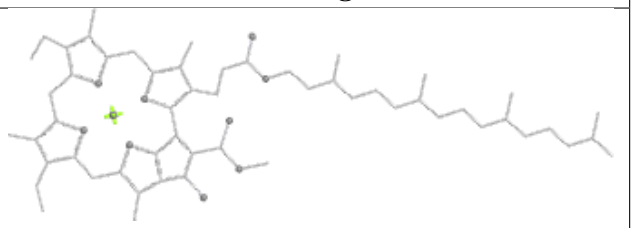
Bond lengths



Bond angles

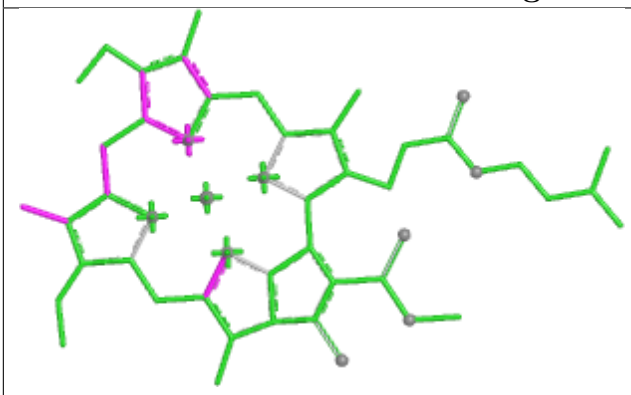


Torsions



Rings

Ligand CLA K 309



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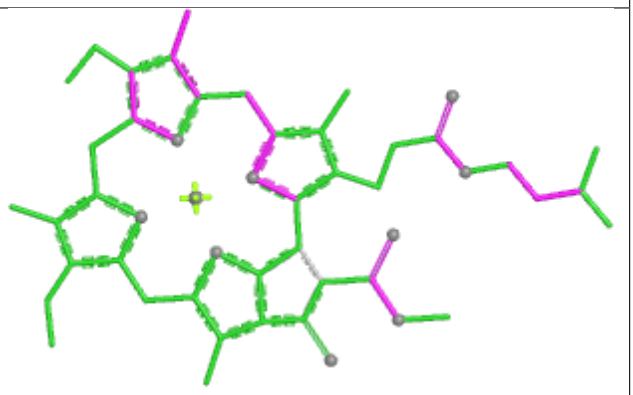
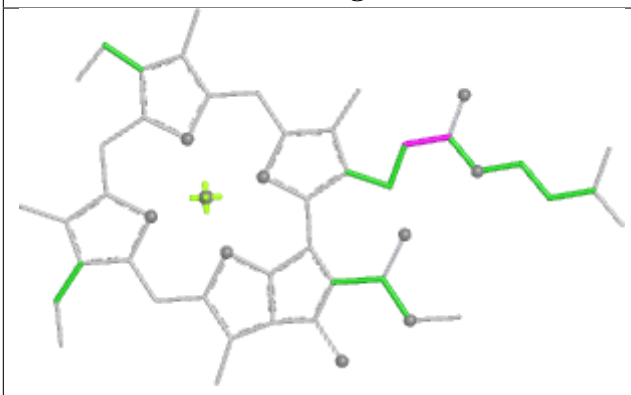
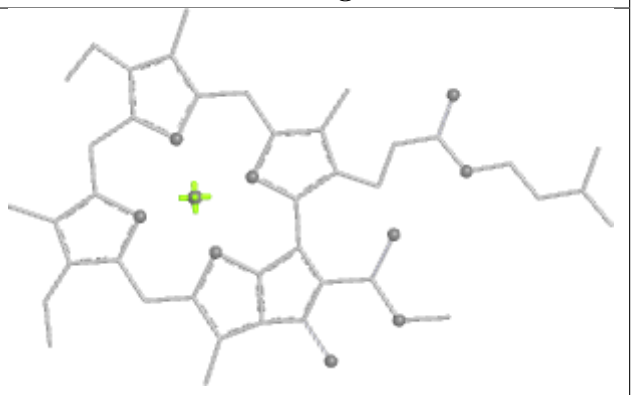


Bond angles

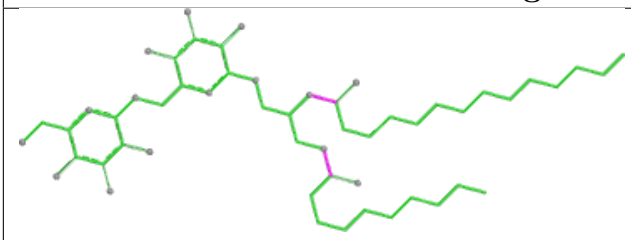


Torsions

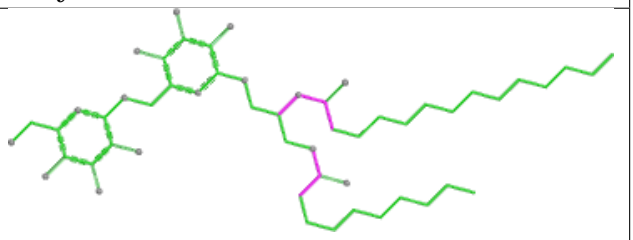


Rings

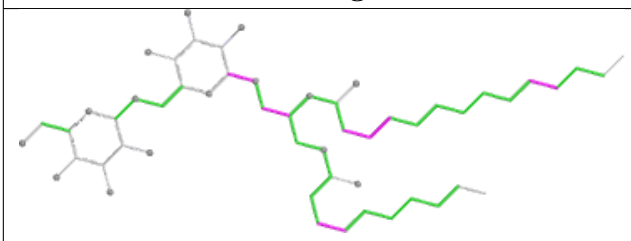
Ligand DGD y 201



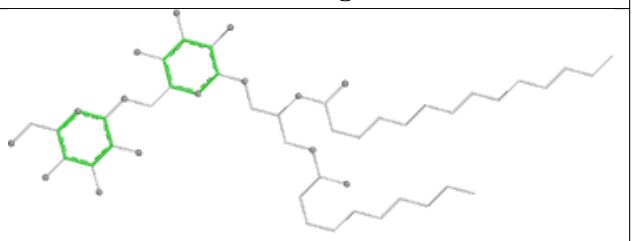
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

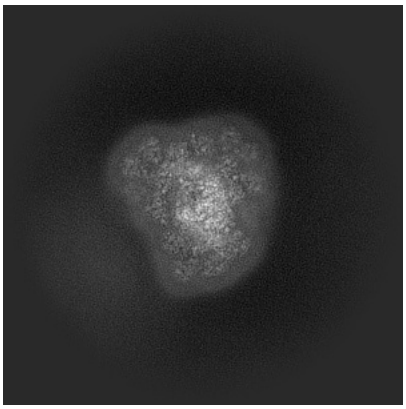
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36742. These allow visual inspection of the internal detail of the map and identification of artifacts.

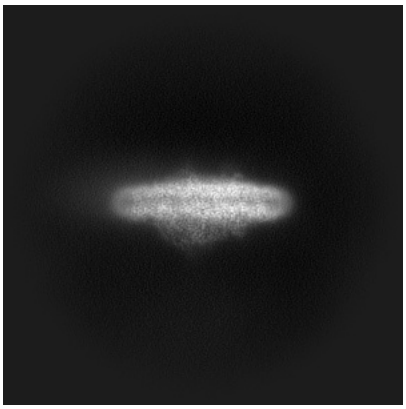
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

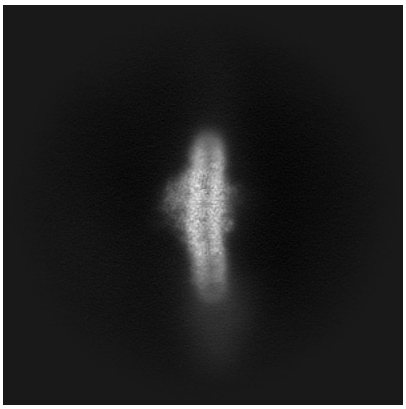
6.1.1 Primary map



X

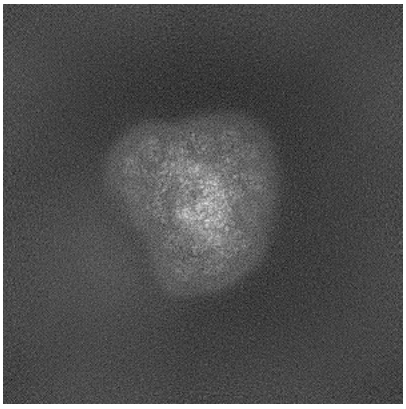


Y

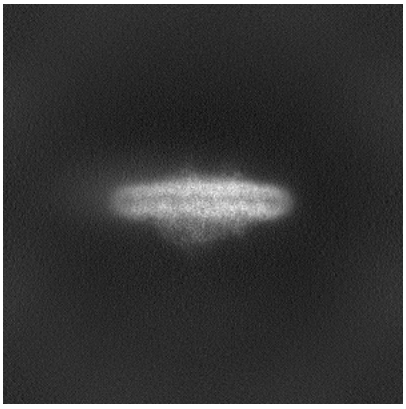


Z

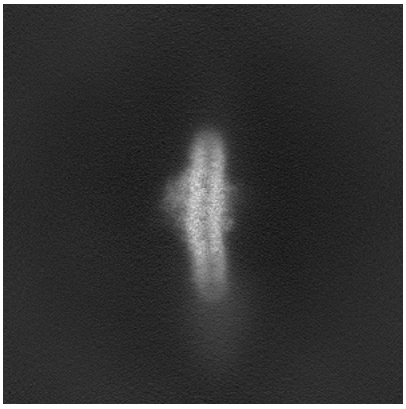
6.1.2 Raw map



X



Y

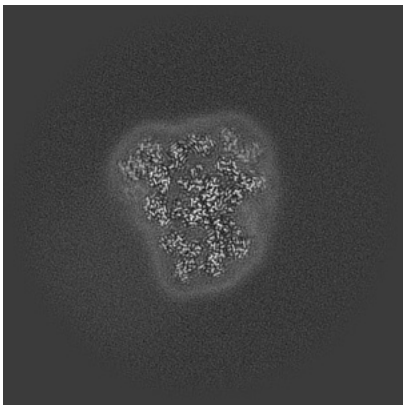


Z

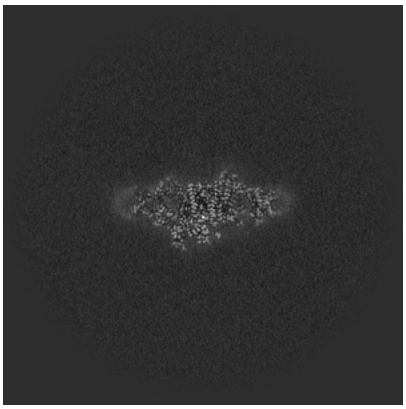
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

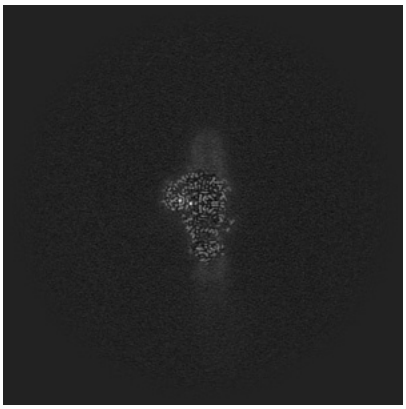
6.2.1 Primary map



X Index: 256

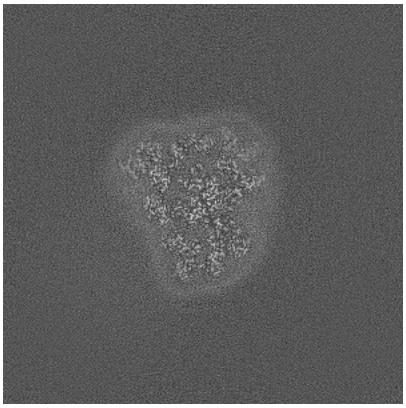


Y Index: 256

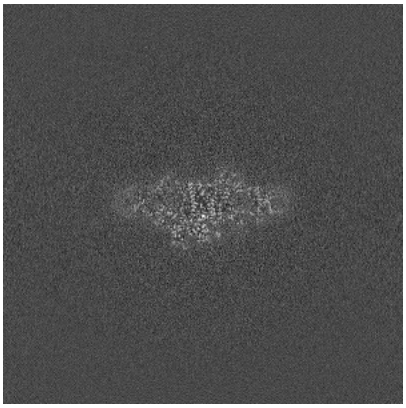


Z Index: 256

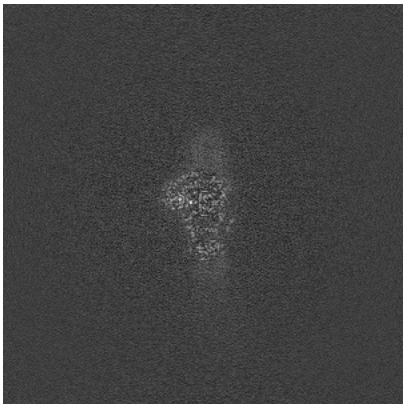
6.2.2 Raw map



X Index: 256



Y Index: 256

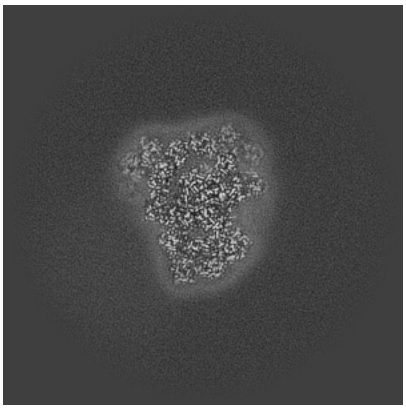


Z Index: 256

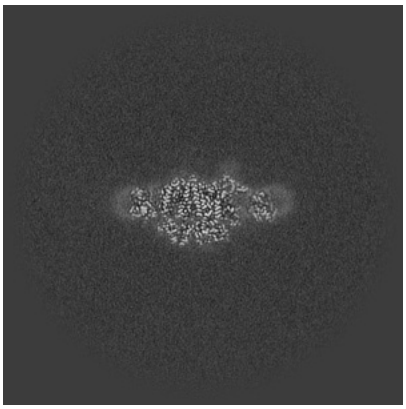
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

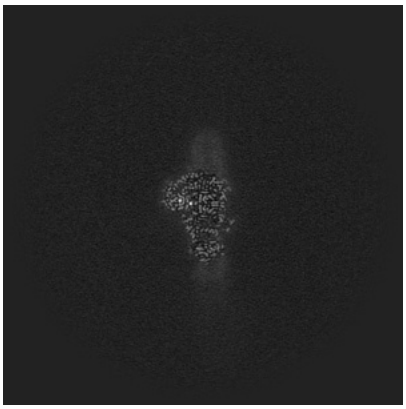
6.3.1 Primary map



X Index: 250

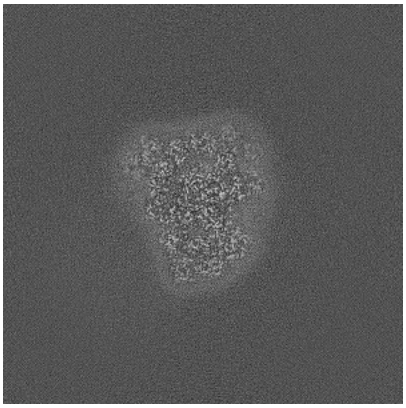


Y Index: 264

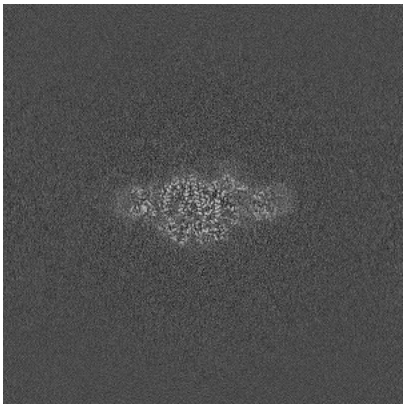


Z Index: 256

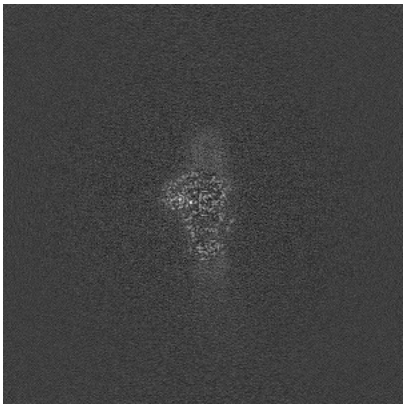
6.3.2 Raw map



X Index: 250



Y Index: 264

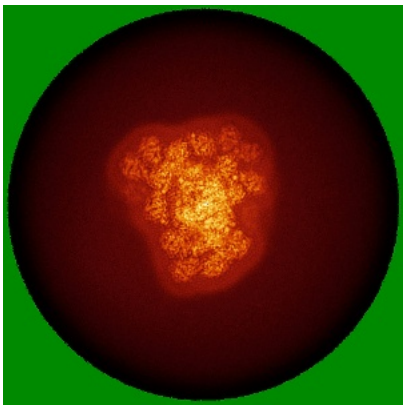


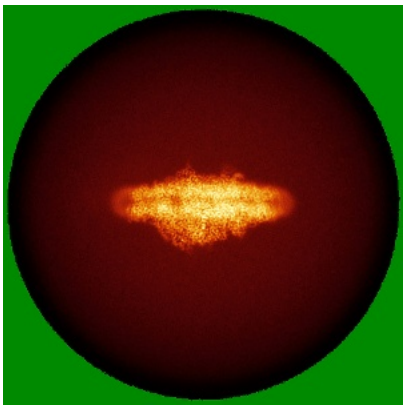
Z Index: 256

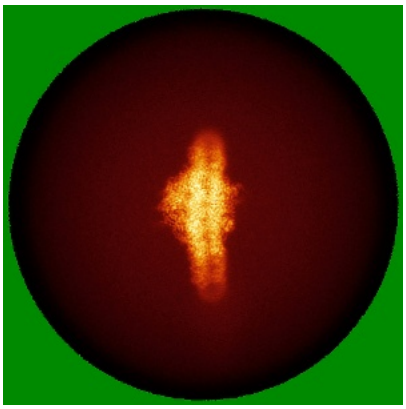
The images above show the largest variance slices of the map in three orthogonal directions.

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

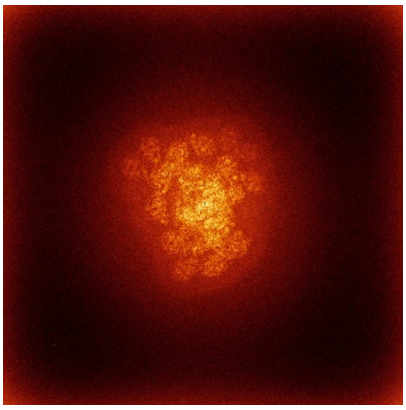
6.4.1 Primary map

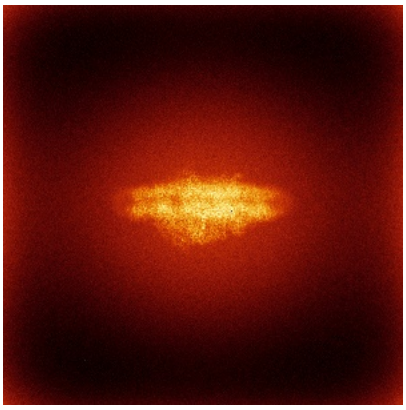

X

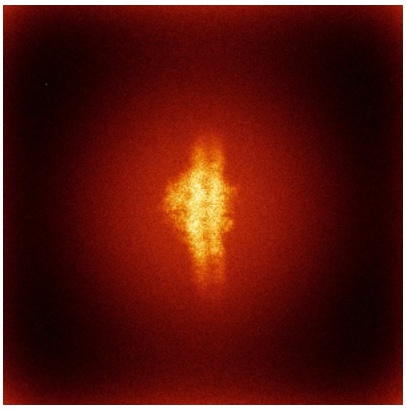

Y


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)

This section was not generated.

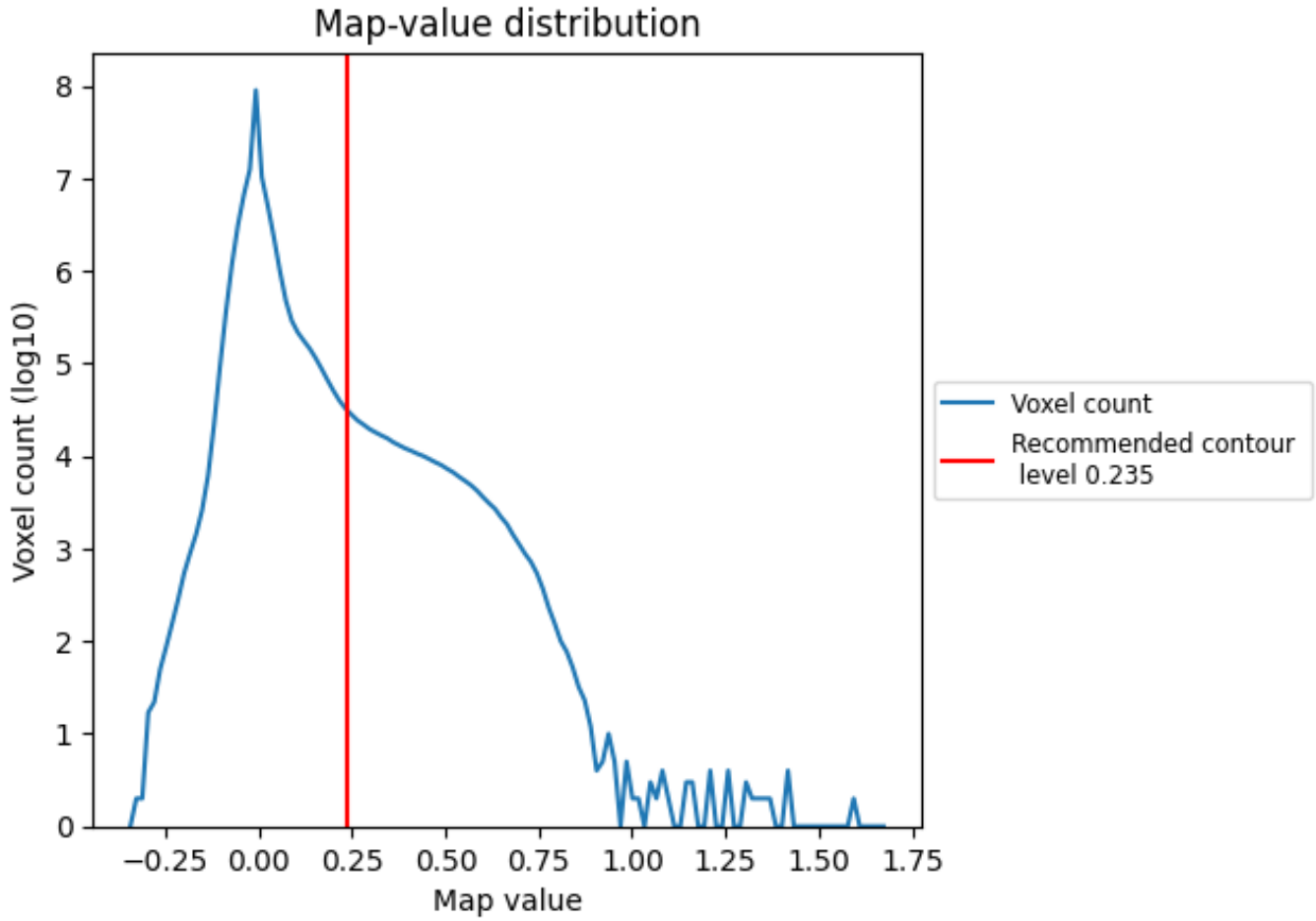
6.6 Mask visualisation (i)

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

7 Map analysis

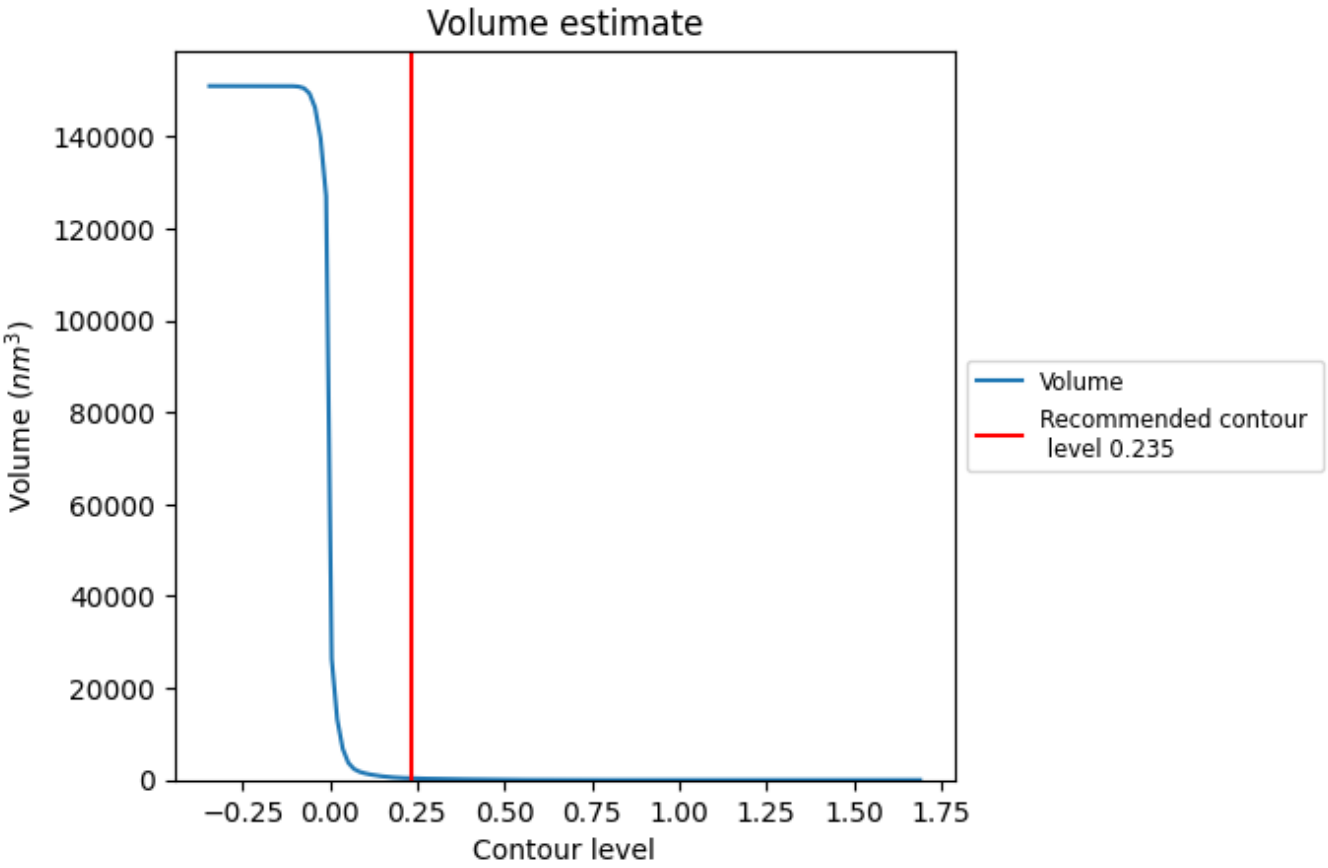
This section contains the results of statistical analysis of the map.

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.

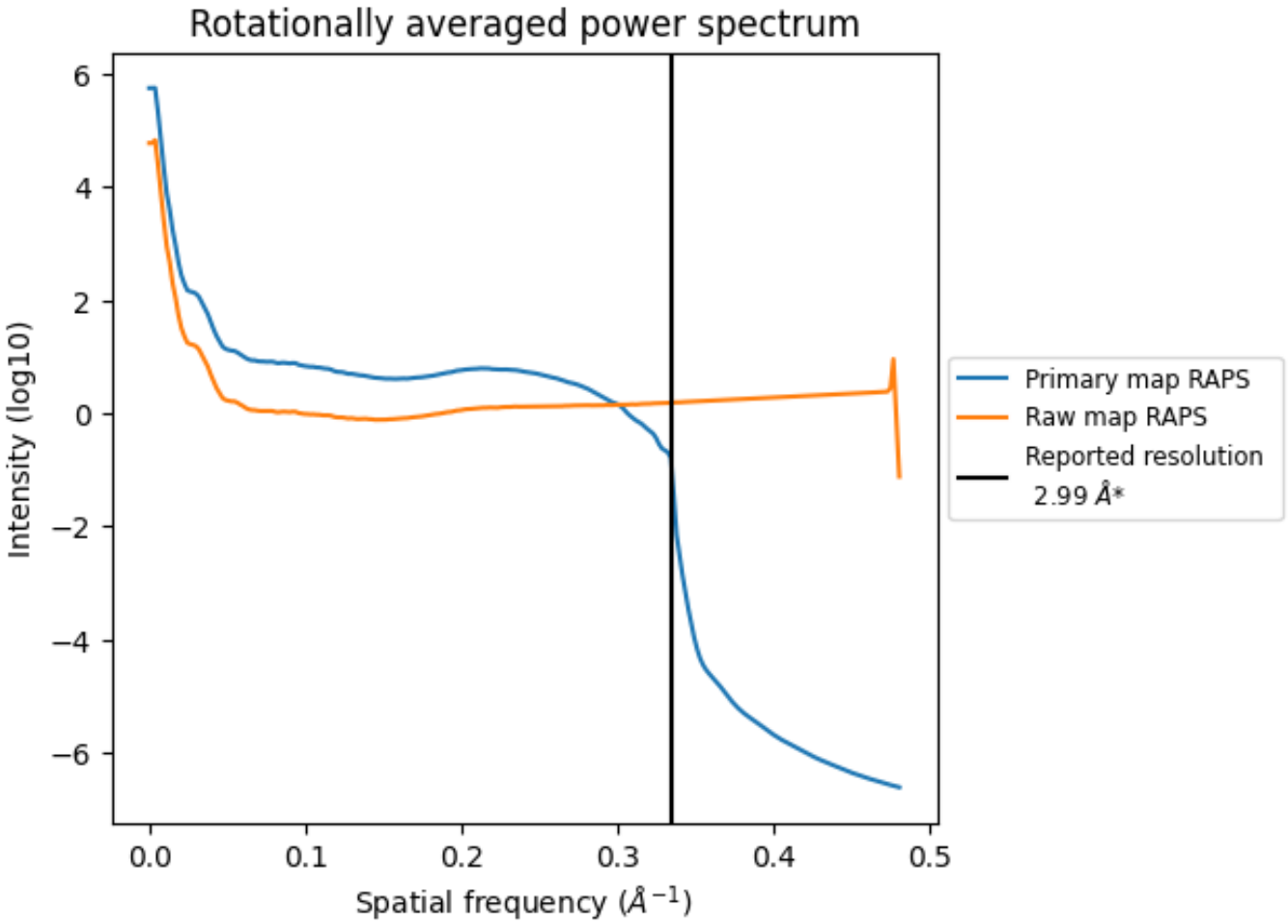
7.2 Volume estimate



The volume at the recommended contour level is 363 nm^3; this corresponds to an approximate mass of 328 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)

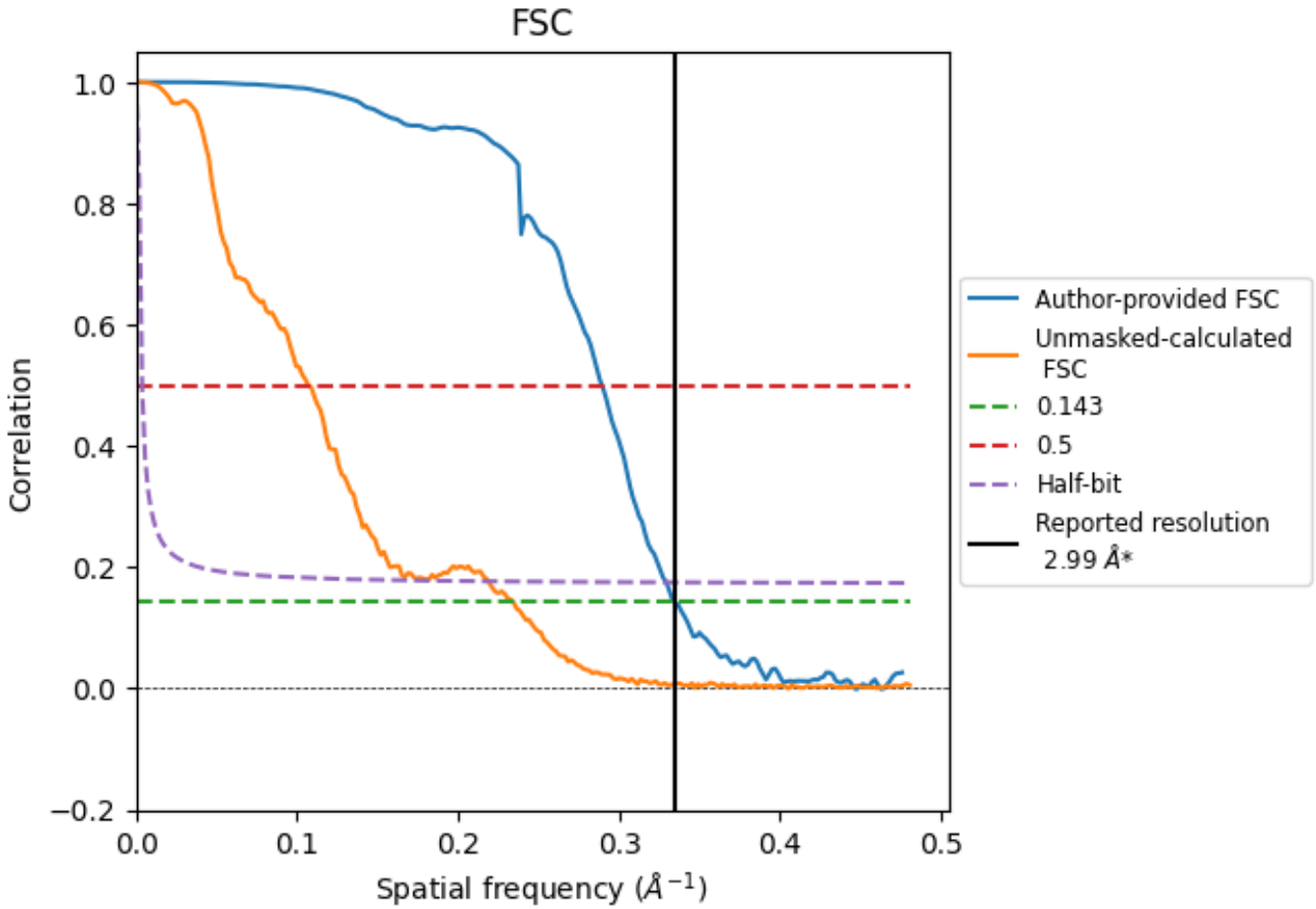


*Reported resolution corresponds to spatial frequency of 0.334 Å^{-1}

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 0.334 $Å^{-1}$

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.45	3.03
Unmasked-calculated*	4.27	9.35	4.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 2.99 by more than 10 %

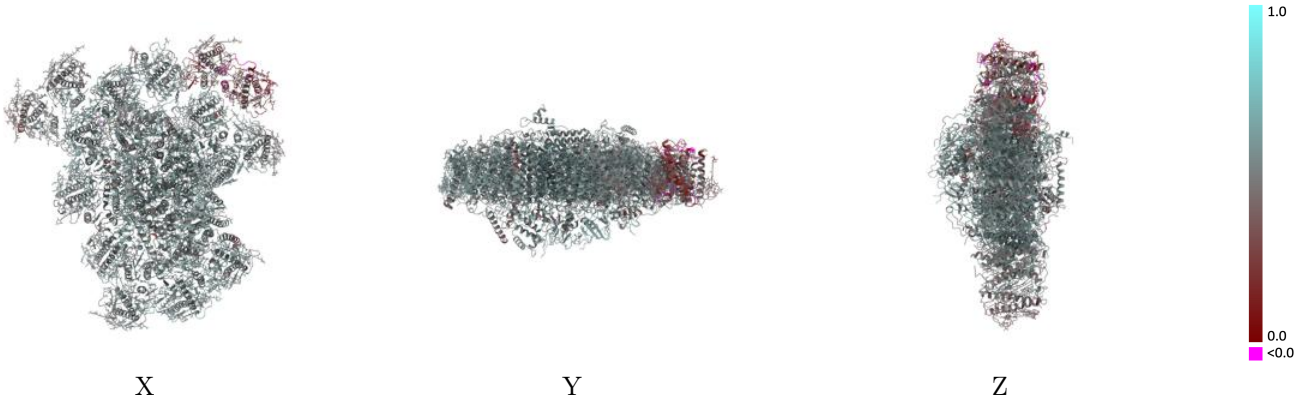
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36742 and PDB model 8JZE. Per-residue inclusion information can be found in section 3 on page 36.

9.1 Map-model overlay

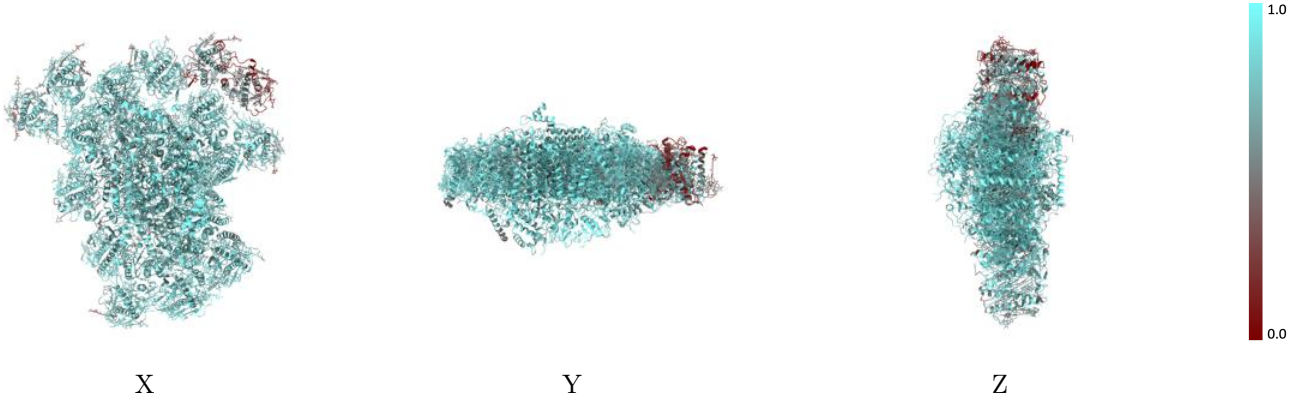
This section was not generated.

9.2 Q-score mapped to coordinate model



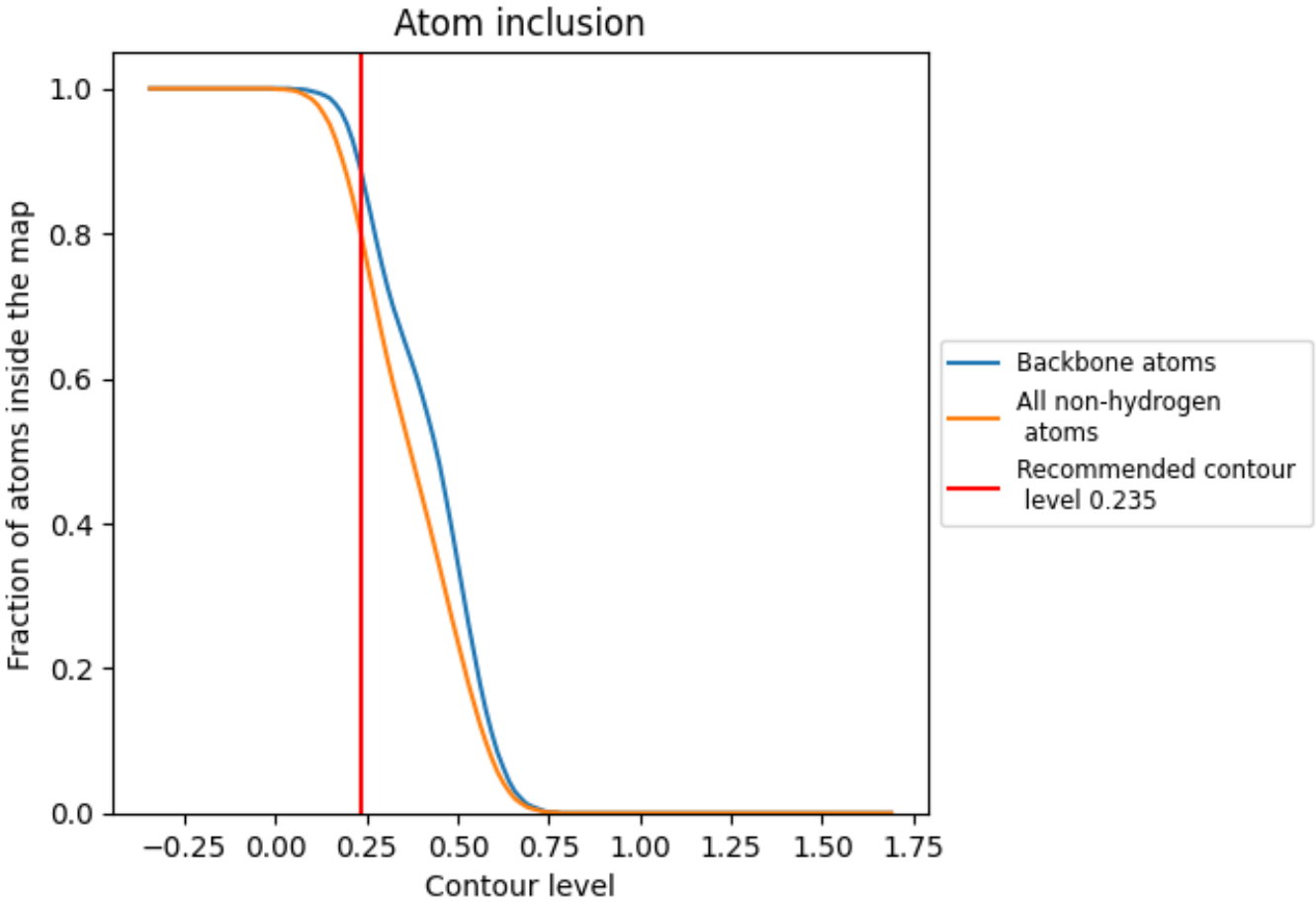
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.235).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.5180
A	0.8360	0.5390
B	0.7940	0.5260
D	0.7490	0.5080
F	0.7320	0.4980
G	0.8000	0.5170
H	0.3060	0.2340
I	0.7850	0.5140
J	0.8410	0.5330
K	0.8600	0.5510
L	0.8440	0.5460
M	0.7800	0.5200
N	0.4940	0.3650
O	0.6780	0.4560
P	0.7250	0.4850
a	0.8560	0.5470
b	0.8710	0.5530
c	0.9280	0.5570
d	0.8550	0.5450
e	0.8990	0.5640
f	0.8330	0.5420
h	0.8660	0.5480
i	0.8360	0.5320
j	0.7800	0.5310
l	0.8610	0.5490
m	0.8270	0.5380
y	0.8670	0.5260
z	0.9150	0.5230