Full wwPDB EM Validation Report ⓘ

Aug 12, 2026 – 11:26 PM JST

PDB ID	:	8XR6 / pdb_00008xr6
EMDB ID	:	EMD-38596
Title	:	Cryo-EM structure of cryptophyte photosystem II
Authors	:	Li, K.; Zhao, L.S.; Zhang, Y.Z.; Liu, L.N.
Deposited on	:	2024-01-06
Resolution	:	2.53 Å(reported)

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

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

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

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

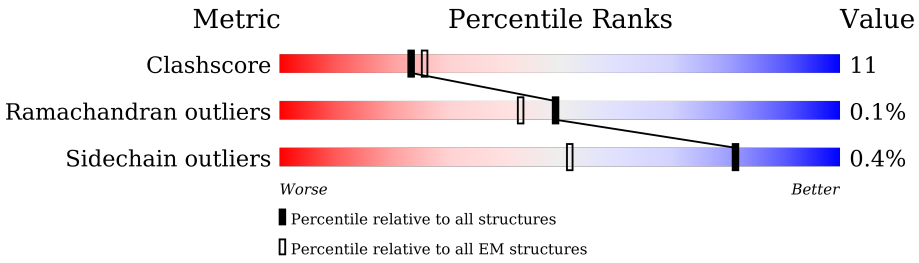
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

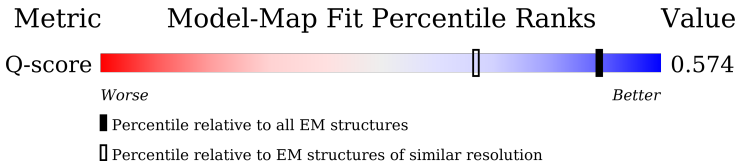
1 Overall quality at a glance

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

The reported resolution of this entry is 2.53 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	7309 (2.03 - 3.03)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	80% 13% 7%
1	a	360	81% 11% 7%
2	0	219	33% 42% 5% 19%
2	4	219	36% 41% • 19%

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Mol	Chain	Length	Quality of chain
3	1	218	71% 9% 20%
3	7	218	72% 9% 20%
4	2	200	78% 15% 6%
4	8	200	80% 14% 6%
5	3	229	72% 8% 19%
5	9	229	71% 8% 19%
6	5	216	58% 19% 21%
6	g	216	57% 21% 21%
7	6	234	35% 36% 11% 18%
7	p	234	37% 38% 7% 18%
8	B	509	86% 13%
8	b	509	85% 13%
9	C	473	85% 11% 5%
9	c	473	85% 10% 5%
10	D	351	85% 12%
10	d	351	85% 12%
11	E	84	70% 19% 11%
11	e	84	71% 18% 11%
12	F	42	57% 12% 31%
12	f	42	60% 10% 31%
13	H	67	84% 13%
13	h	67	85% 12%
14	I	38	79% 13% 8%
14	i	38	79% 13% 8%
15	J	39	77% 10% 13%

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Mol	Chain	Length	Quality of chain
15	j	39	77% 10% 13%
16	K	45	82% 18%
16	k	45	82% 18%
17	L	38	79% 18%
17	l	38	82% 16%
18	M	37	73% 27%
18	m	37	70% 30%
19	N	297	47% 14% 36%
19	n	297	49% 12% 36%
20	O	300	5% 77% 10% 13%
20	o	300	5% 77% 9% 13%
21	Q	144	10% 94% 6%
21	q	144	12% 92% 8%
22	T	32	81% 16%
22	t	32	81% 16%
23	U	121	64% 12% 23%
23	u	121	65% 12% 23%
24	V	163	77% 7% 16%
24	v	163	80% 16%
25	W	130	32% 6% 62%
25	w	130	32% 6% 62%
26	X	39	95% 5%
26	x	39	95% 5%
27	Y	34	79% 21%
27	y	34	85% 15%

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Mol	Chain	Length	Quality of chain
28	Z	62	92% 6%
28	z	62	95%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	N	303	-	-	X	-

2 Entry composition (i)

There are 45 unique types of molecules in this entry. The entry contains 82310 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	334	Total	C	N	O	S	0	0
			2617	1712	430	463	12		
1	A	334	Total	C	N	O	S	0	0
			2617	1712	430	463	12		

- Molecule 2 is a protein called ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	177	Total	C	N	O	S	0	0
			1365	882	229	245	9		
2	4	177	Total	C	N	O	S	0	0
			1365	882	229	245	9		

- Molecule 3 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	175	Total	C	N	O	S	0	0
			1360	886	223	243	8		
3	7	175	Total	C	N	O	S	0	0
			1360	886	223	243	8		

- Molecule 4 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	187	Total	C	N	O	S	0	0
			1469	955	243	266	5		
4	8	187	Total	C	N	O	S	0	0
			1469	955	243	266	5		

- Molecule 5 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	185	Total	C	N	O	S	0	0
			1400	904	240	247	9		
5	9	185	Total	C	N	O	S	0	0
			1400	904	240	247	9		

- Molecule 6 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	170	Total	C	N	O	S	0	0
			1339	885	218	233	3		
6	g	170	Total	C	N	O	S	0	0
			1339	885	218	233	3		

- Molecule 7 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	192	Total	C	N	O	S	0	0
			1455	933	254	260	8		
7	p	192	Total	C	N	O	S	0	0
			1455	933	254	260	8		

- Molecule 8 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	503	Total	C	N	O	S	0	0
			3953	2581	674	687	11		
8	b	503	Total	C	N	O	S	0	0
			3953	2581	674	687	11		

- Molecule 9 is a protein called PsbC_CP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	451	Total	C	N	O	S	0	0
			3503	2290	589	614	10		
9	c	451	Total	C	N	O	S	0	0
			3503	2290	589	614	10		

- Molecule 10 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		

- Molecule 11 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	E	75	Total	C	N	O	0	0
			616	402	102	112		
11	e	75	Total	C	N	O	0	0
			616	402	102	112		

- Molecule 12 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	29	Total	C	N	O	S	0	0
			235	159	40	35	1		
12	f	29	Total	C	N	O	S	0	0
			235	159	40	35	1		

- Molecule 13 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	65	Total	C	N	O	S	0	0
			515	344	81	88	2		
13	h	65	Total	C	N	O	S	0	0
			515	344	81	88	2		

- Molecule 14 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	35	Total	C	N	O	S	0	0
			287	191	46	49	1		
14	i	35	Total	C	N	O	S	0	0
			287	191	46	49	1		

- Molecule 15 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	J	34	Total	C	N	O	0	0
			249	168	38	43		
15	j	34	Total	C	N	O	0	0
			249	168	38	43		

- Molecule 16 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	K	37	Total	C	N	O	0	0
			296	209	44	43		
16	k	37	Total	C	N	O	0	0
			296	209	44	43		

- Molecule 17 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	L	37	Total	C	N	O	0	0
			301	204	47	50		
17	l	37	Total	C	N	O	0	0
			301	204	47	50		

- Molecule 18 is a protein called PsbM.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	37	Total	C	N	O	S	0	0
			276	182	43	50	1		
18	m	37	Total	C	N	O	S	0	0
			276	182	43	50	1		

- Molecule 19 is a protein called Psb-gama_linker.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	190	Total	C	N	O	S	0	0
			1474	954	234	283	3		
19	n	190	Total	C	N	O	S	0	0
			1474	954	234	283	3		

- Molecule 20 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	262	Total	C	N	O	S	0	0
			1993	1253	326	408	6		
20	o	262	Total	C	N	O	S	0	0
			1993	1253	326	408	6		

- Molecule 21 is a protein called PsbQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	143	Total	C	N	O	S	0	0
			1102	698	190	211	3		
21	q	143	Total	C	N	O	S	0	0
			1102	698	190	211	3		

- Molecule 22 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	31	Total	C	N	O	S	0	0
			250	173	38	38	1		
22	t	31	Total	C	N	O	S	0	0
			250	173	38	38	1		

- Molecule 23 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	93	Total	C	N	O	S	0	0
			741	476	122	141	2		
23	u	93	Total	C	N	O	S	0	0
			741	476	122	141	2		

- Molecule 24 is a protein called Photosystem II cytochrome c550.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	137	Total	C	N	O	S	0	0
			1043	653	177	209	4		
24	v	137	Total	C	N	O	S	0	0
			1043	653	177	209	4		

- Molecule 25 is a protein called PsbW.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	49	Total	C	N	O	0	0
			391	251	61	79		
25	w	49	Total	C	N	O	0	0
			391	251	61	79		

- Molecule 26 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	39	Total	C	N	O	S	0	0
			291	192	47	51	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	x	39	Total	C	N	O	S	0	0
			291	192	47	51	1		

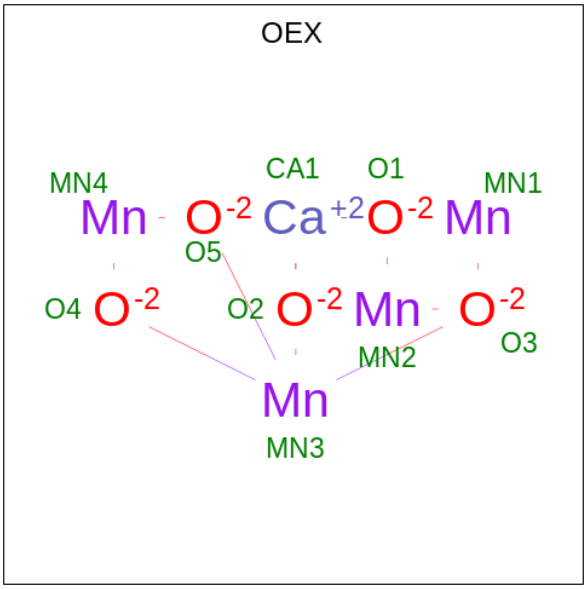
- Molecule 27 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	34	Total	C	N	O	S	0	0
			265	180	43	41	1		
27	y	34	Total	C	N	O	S	0	0
			265	180	43	41	1		

- Molecule 28 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		
28	z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).

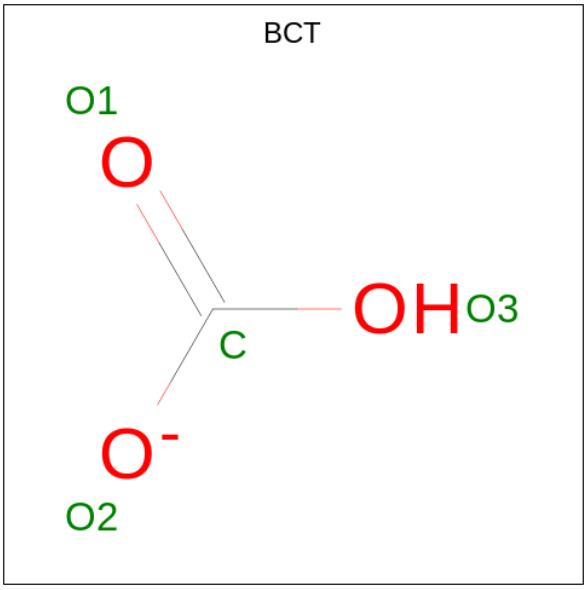


Mol	Chain	Residues	Atoms				AltConf
29	a	1	Total	Ca	Mn	O	0
			10	1	4	5	
29	A	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
30	a	1	Total Fe 1 1	0
30	A	1	Total Fe 1 1	0

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).

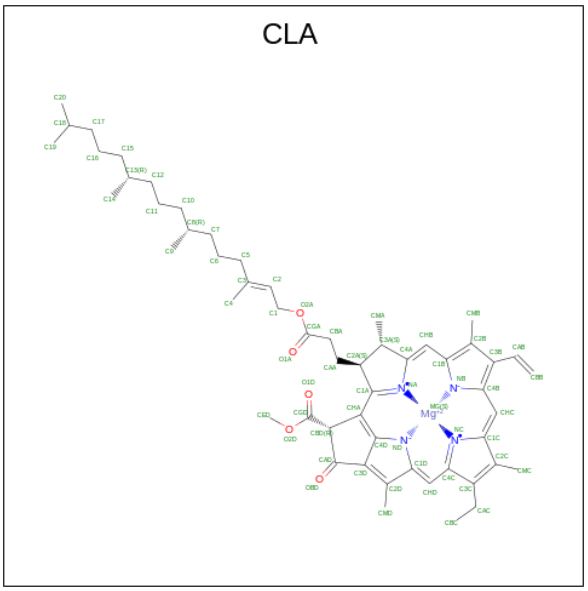


Mol	Chain	Residues	Atoms	AltConf
31	a	1	Total C O 4 1 3	0
31	A	1	Total C O 4 1 3	0

- Molecule 32 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total Cl 1 1	0
32	A	1	Total Cl 1 1	0

- Molecule 33 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
33	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	0	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	0	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
33	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	9	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	b	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
33	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
33	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	g	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	g	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
33	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	n	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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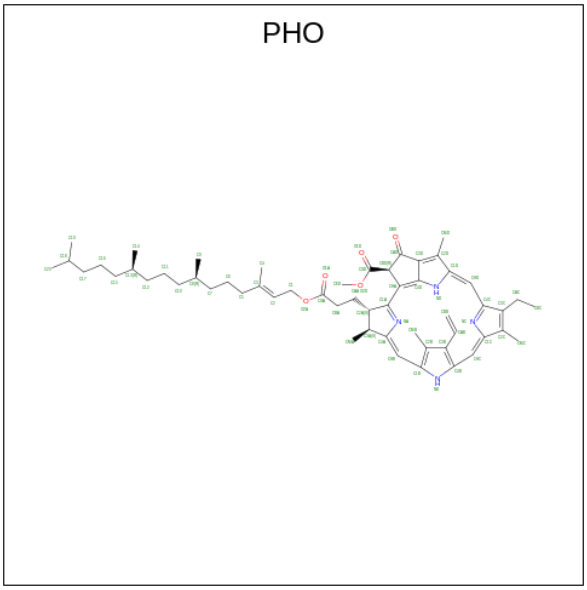
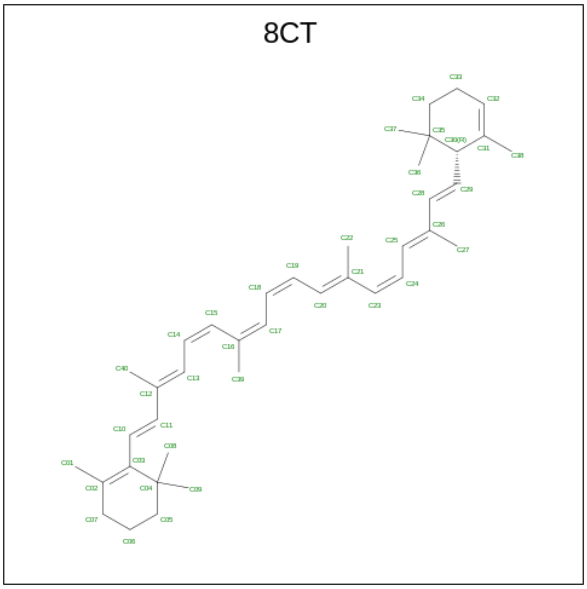
Mol	Chain	Residues	Atoms					AltConf
33	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
34	a	1	Total	C	N	O	0
			64	55	4	5	
34	A	1	Total	C	N	O	0
			64	55	4	5	
34	D	1	Total	C	N	O	0
			64	55	4	5	
34	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 35 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
35	a	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	0	1	Total C 40 40	0
35	1	1	Total C 40 40	0
35	4	1	Total C 40 40	0
35	7	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	C	1	Total C 40 40	0
35	C	1	Total C 40 40	0
35	C	1	Total C 40 40	0

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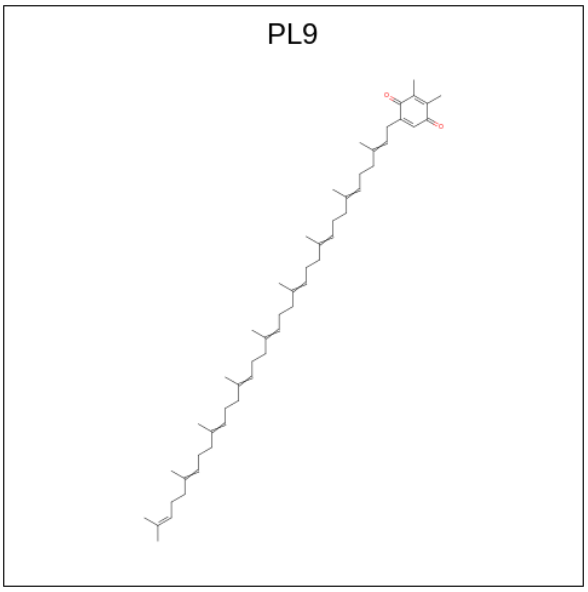
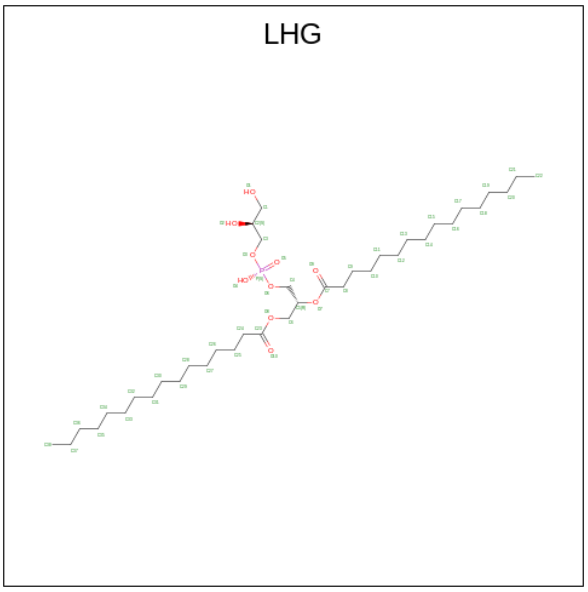
Mol	Chain	Residues	Atoms	AltConf
35	D	1	Total C 40 40	0
35	H	1	Total C 40 40	0
35	Y	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	c	1	Total C 40 40	0
35	c	1	Total C 40 40	0
35	c	1	Total C 40 40	0
35	d	1	Total C 40 40	0
35	h	1	Total C 40 40	0
35	y	1	Total C 40 40	0

- Molecule 36 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms	AltConf
36	a	1	Total C O 30 28 2	0
36	A	1	Total C O 30 28 2	0
36	D	1	Total C O 55 53 2	0
36	d	1	Total C O 55 53 2	0

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
37	a	1	Total	C	O	P	0
			24	13	10	1	
37	A	1	Total	C	O	P	0
			24	13	10	1	
37	0	1	Total	C	O	P	0
			24	13	10	1	
37	1	1	Total	C	O	P	0
			49	38	10	1	
37	2	1	Total	C	O	P	0
			46	35	10	1	
37	3	1	Total	C	O	P	0
			41	30	10	1	
37	3	1	Total	C	O	P	0
			24	13	10	1	
37	3	1	Total	C	O	P	0
			41	30	10	1	
37	4	1	Total	C	O	P	0
			24	13	10	1	
37	5	1	Total	C	O	P	0
			22	12	9	1	
37	7	1	Total	C	O	P	0
			49	38	10	1	
37	8	1	Total	C	O	P	0
			46	35	10	1	
37	9	1	Total	C	O	P	0
			41	30	10	1	
37	9	1	Total	C	O	P	0
			24	13	10	1	
37	9	1	Total	C	O	P	0
			41	30	10	1	
37	B	1	Total	C	O	P	0
			49	38	10	1	
37	D	1	Total	C	O	P	0
			46	35	10	1	
37	D	1	Total	C	O	P	0
			47	36	10	1	
37	D	1	Total	C	O	P	0
			49	38	10	1	
37	b	1	Total	C	O	P	0
			49	38	10	1	
37	d	1	Total	C	O	P	0
			46	35	10	1	
37	d	1	Total	C	O	P	0
			47	36	10	1	

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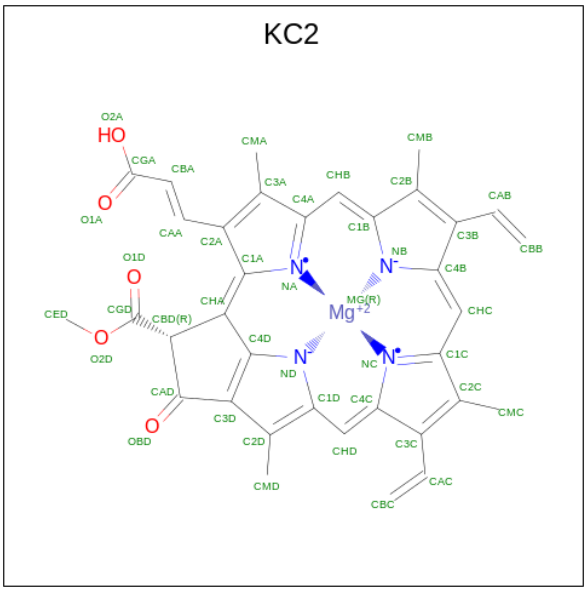
Mol	Chain	Residues	Atoms	AltConf
37	d	1	Total C O P 49 38 10 1	0
37	g	1	Total C O P 22 12 9 1	0

- Molecule 38 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
38	0	1	Total C Mg N O 45 35 1 4 5	0
38	1	1	Total C Mg N O 45 35 1 4 5	0
38	1	1	Total C Mg N O 45 35 1 4 5	0
38	2	1	Total C Mg N O 45 35 1 4 5	0
38	3	1	Total C Mg N O 45 35 1 4 5	0
38	4	1	Total C Mg N O 45 35 1 4 5	0
38	5	1	Total C Mg N O 45 35 1 4 5	0
38	6	1	Total C Mg N O 45 35 1 4 5	0
38	7	1	Total C Mg N O 45 35 1 4 5	0

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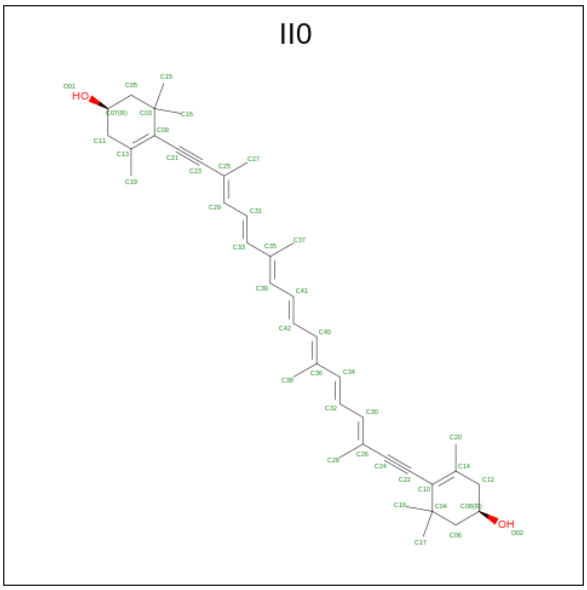
Mol	Chain	Residues	Atoms					AltConf
38	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 39 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: $C_{40}H_{52}O_2$).



Mol	Chain	Residues	Atoms			AltConf
39	0	1	Total	C	O	0
			42	40	2	
39	0	1	Total	C	O	0
			42	40	2	
39	0	1	Total	C	O	0
			42	40	2	
39	0	1	Total	C	O	0
			42	40	2	
39	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
39	1	1	Total C O 42 40 2	0
39	1	1	Total C O 42 40 2	0
39	1	1	Total C O 42 40 2	0
39	2	1	Total C O 42 40 2	0
39	2	1	Total C O 42 40 2	0
39	2	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	4	1	Total C O 42 40 2	0
39	4	1	Total C O 42 40 2	0
39	4	1	Total C O 42 40 2	0
39	4	1	Total C O 42 40 2	0
39	5	1	Total C O 42 40 2	0
39	5	1	Total C O 42 40 2	0
39	5	1	Total C O 42 40 2	0
39	6	1	Total C O 42 40 2	0
39	6	1	Total C O 42 40 2	0
39	6	1	Total C O 42 40 2	0

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Mol	Chain	Residues	Atoms			AltConf
39	6	1	Total	C	O	0
			42	40	2	
39	6	1	Total	C	O	0
			42	40	2	
39	7	1	Total	C	O	0
			42	40	2	
39	7	1	Total	C	O	0
			42	40	2	
39	7	1	Total	C	O	0
			42	40	2	
39	7	1	Total	C	O	0
			42	40	2	
39	8	1	Total	C	O	0
			42	40	2	
39	8	1	Total	C	O	0
			42	40	2	
39	8	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	p	1	Total	C	O	0
			42	40	2	
39	p	1	Total	C	O	0
			42	40	2	
39	p	1	Total	C	O	0
			42	40	2	
39	p	1	Total	C	O	0
			42	40	2	

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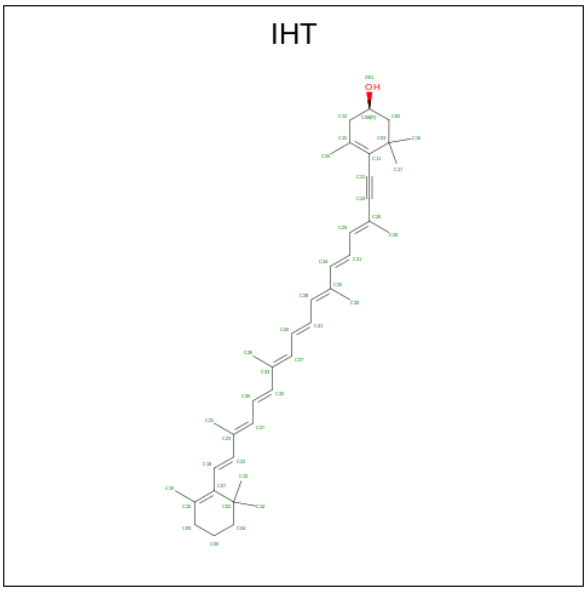
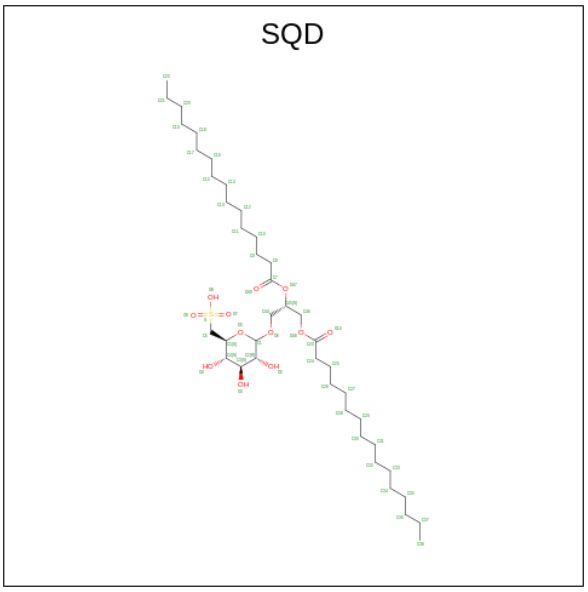
Mol	Chain	Residues	Atoms			AltConf
39	p	1	Total	C	O	0
			42	40	2	

- Molecule 40 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: $C_{40}H_{54}O$).



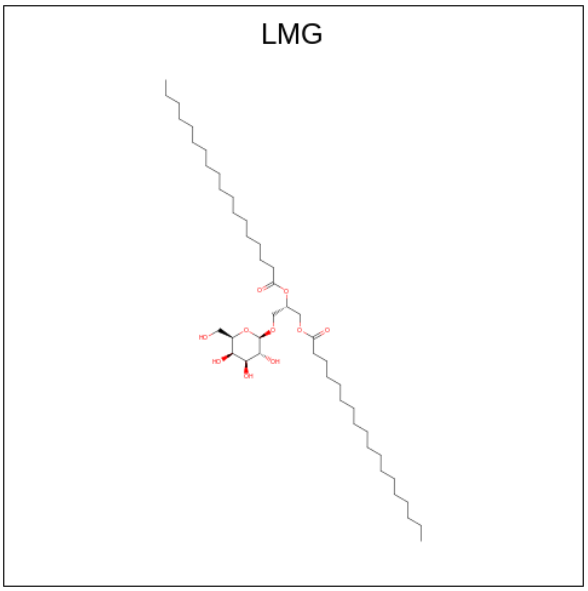
Mol	Chain	Residues	Atoms			AltConf
40	2	1	Total	C	O	0
			41	40	1	
40	3	1	Total	C	O	0
			41	40	1	
40	5	1	Total	C	O	0
			41	40	1	
40	6	1	Total	C	O	0
			41	40	1	
40	8	1	Total	C	O	0
			41	40	1	
40	9	1	Total	C	O	0
			41	40	1	
40	g	1	Total	C	O	0
			41	40	1	
40	p	1	Total	C	O	0
			41	40	1	

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



Mol	Chain	Residues	Atoms				AltConf
41	B	1	Total	C	O	S	0
			38	25	12	1	
41	C	1	Total	C	O	S	0
			42	29	12	1	
41	J	1	Total	C	O	S	0
			46	33	12	1	
41	L	1	Total	C	O	S	0
			54	41	12	1	
41	b	1	Total	C	O	S	0
			38	25	12	1	
41	c	1	Total	C	O	S	0
			42	29	12	1	
41	j	1	Total	C	O	S	0
			46	33	12	1	
41	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 42 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
42	B	1	Total	C	O	0
			49	39	10	
42	B	1	Total	C	O	0
			43	33	10	
42	C	1	Total	C	O	0
			51	41	10	
42	D	1	Total	C	O	0
			46	36	10	
42	D	1	Total	C	O	0
			46	36	10	
42	T	1	Total	C	O	0
			43	33	10	
42	W	1	Total	C	O	0
			47	37	10	
42	b	1	Total	C	O	0
			49	39	10	
42	b	1	Total	C	O	0
			43	33	10	
42	c	1	Total	C	O	0
			51	41	10	
42	d	1	Total	C	O	0
			46	36	10	
42	d	1	Total	C	O	0
			46	36	10	
42	l	1	Total	C	O	0
			38	28	10	
42	m	1	Total	C	O	0
			38	28	10	

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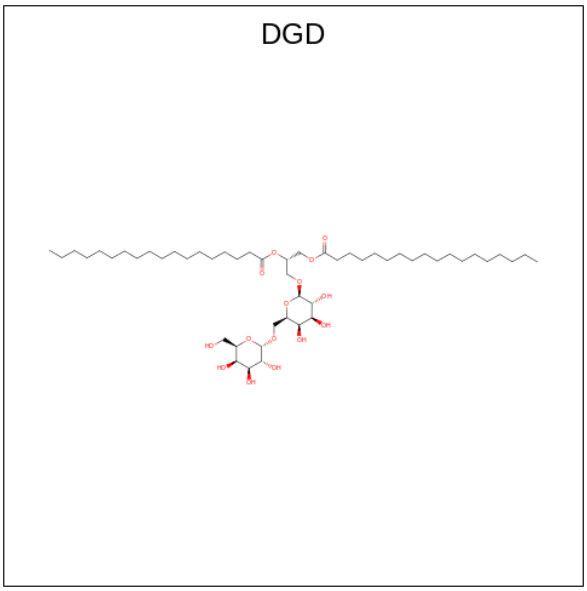
Mol	Chain	Residues	Atoms	AltConf
42	t	1	Total C O 43 33 10	0
42	w	1	Total C O 47 37 10	0

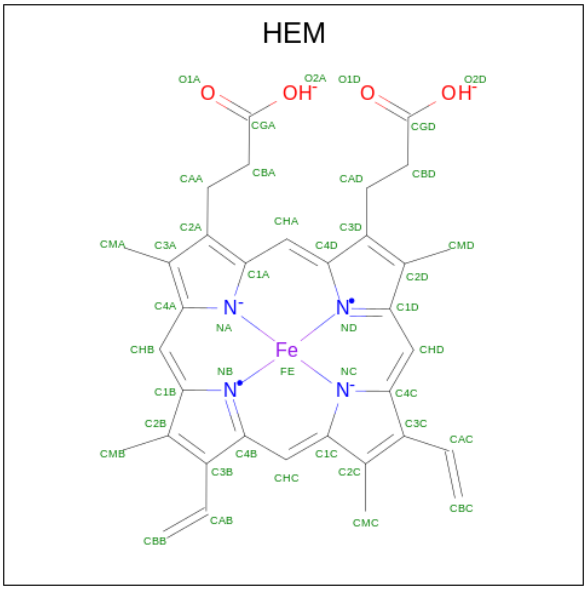
- Molecule 43 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	AltConf
43	C	1	Total C O 55 40 15	0
43	C	1	Total C O 62 47 15	0
43	C	1	Total C O 62 47 15	0
43	H	1	Total C O 60 45 15	0
43	c	1	Total C O 55 40 15	0
43	c	1	Total C O 62 47 15	0
43	c	1	Total C O 62 47 15	0
43	h	1	Total C O 60 45 15	0

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

$C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
44	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 45 is water.

Mol	Chain	Residues	Atoms		AltConf
45	a	24	Total	O	0
			24	24	
45	A	24	Total	O	0
			24	24	
45	B	3	Total	O	0
			3	3	
45	C	11	Total	O	0
			11	11	
45	O	1	Total	O	0
			1	1	
45	U	2	Total	O	0
			2	2	
45	W	1	Total	O	0
			1	1	

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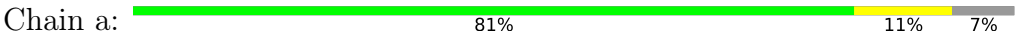
Mol	Chain	Residues	Atoms	AltConf
45	b	3	Total O 3 3	0
45	c	11	Total O 11 11	0
45	o	1	Total O 1 1	0
45	u	2	Total O 2 2	0
45	w	1	Total O 1 1	0

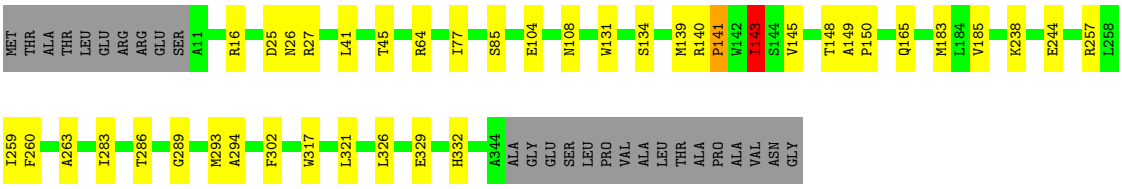
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

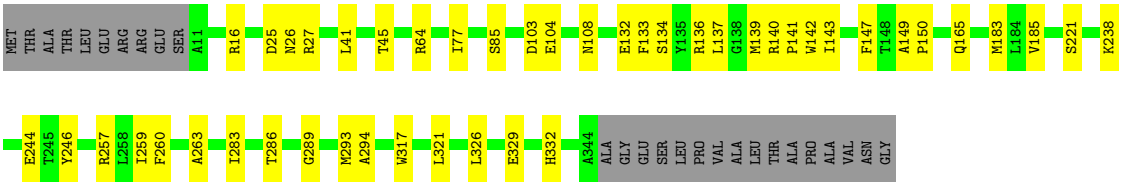
Chain a:





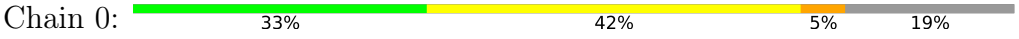
• Molecule 1: Photosystem II protein D1

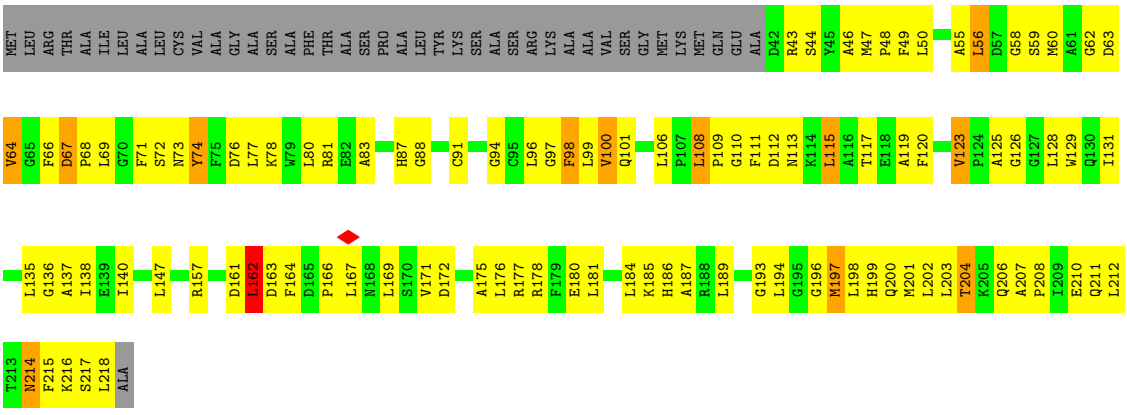
Chain A:



• Molecule 2: ACPII-4

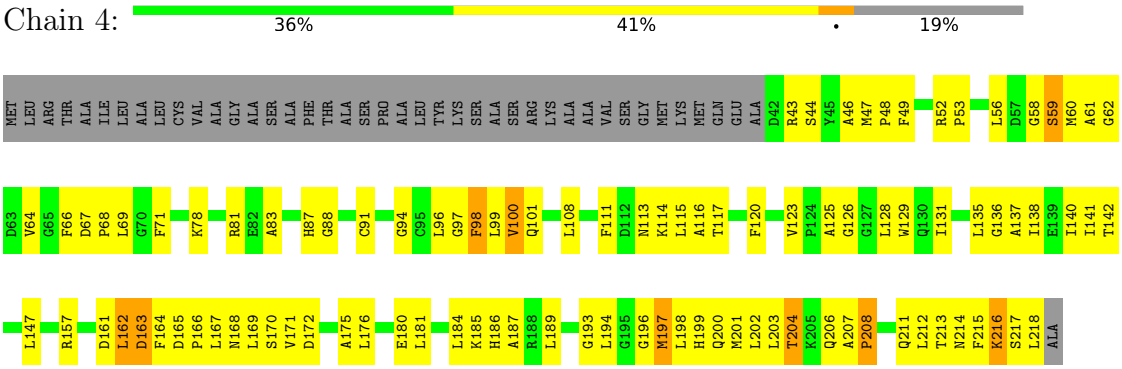
Chain 0:





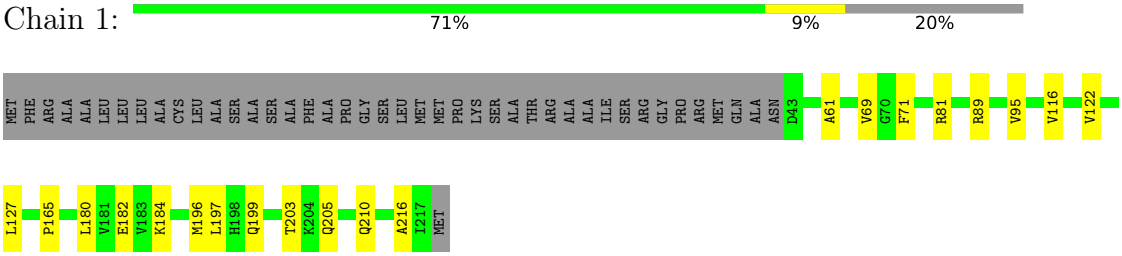
• Molecule 2: ACPII-4

Chain 4:



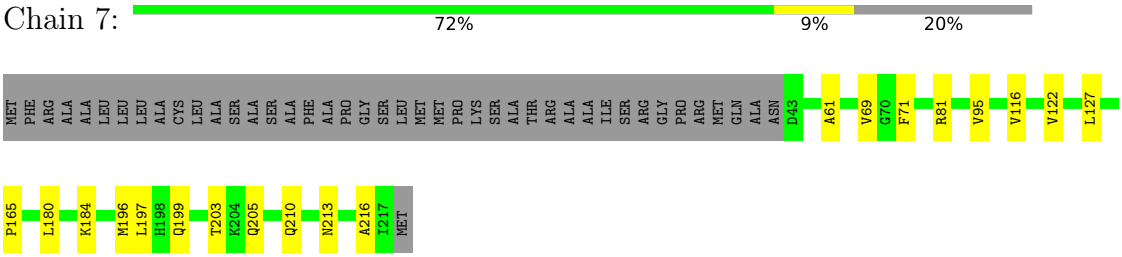
• Molecule 3: ACPII-1

Chain 1:



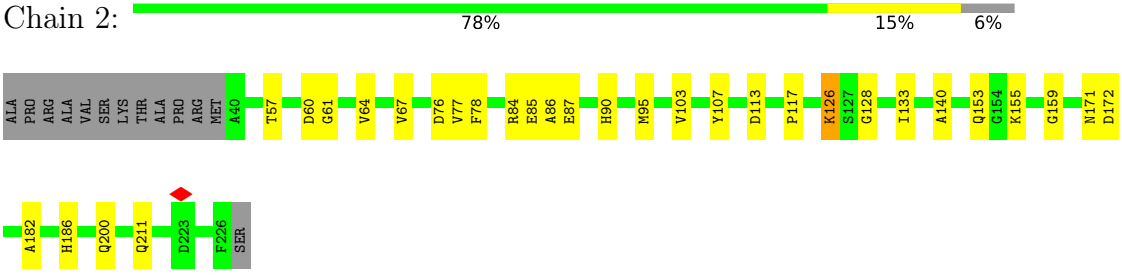
• Molecule 3: ACPII-1

Chain 7:



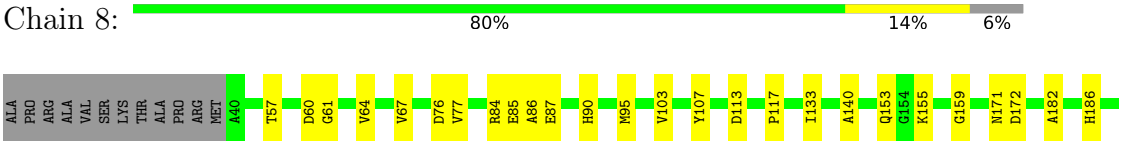
• Molecule 4: ACPII-2

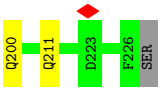
Chain 2:



• Molecule 4: ACPII-2

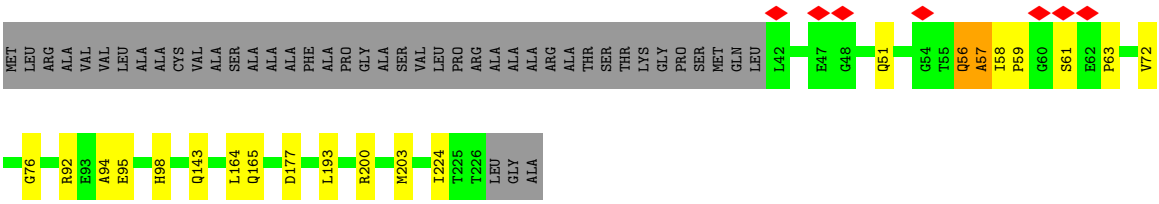
Chain 8:





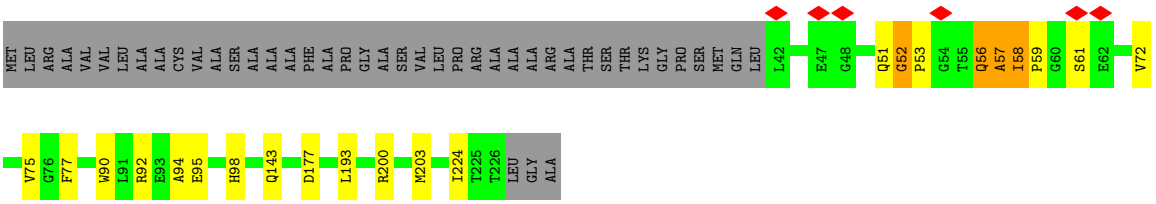
• Molecule 5: ACPII-3

Chain 3:



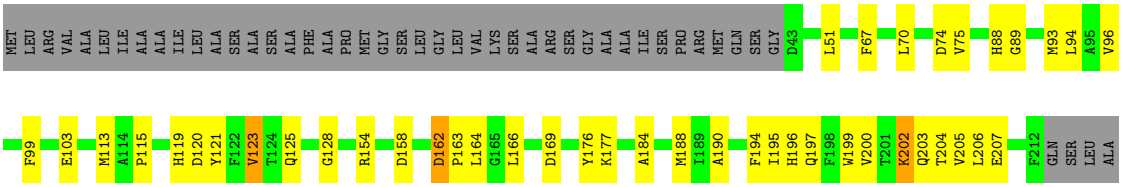
• Molecule 5: ACPII-3

Chain 9:



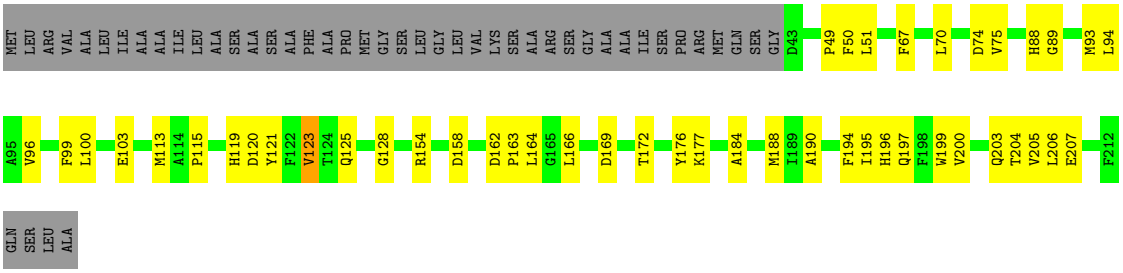
• Molecule 6: ACPII-5

Chain 5:



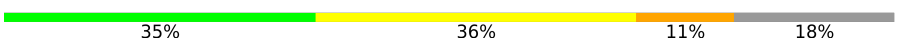
• Molecule 6: ACPII-5

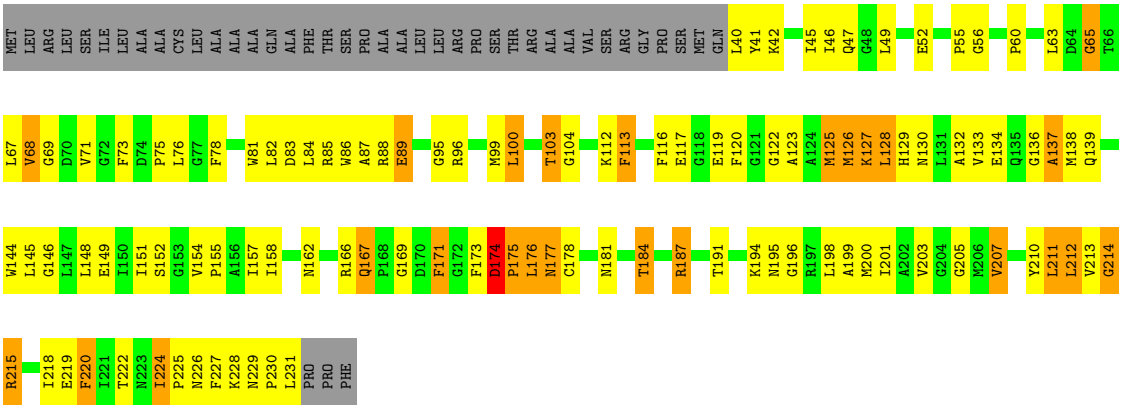
Chain g:



• Molecule 7: ACPII-6

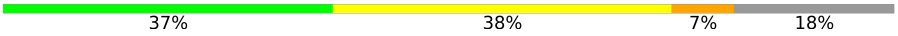
Chain 6:

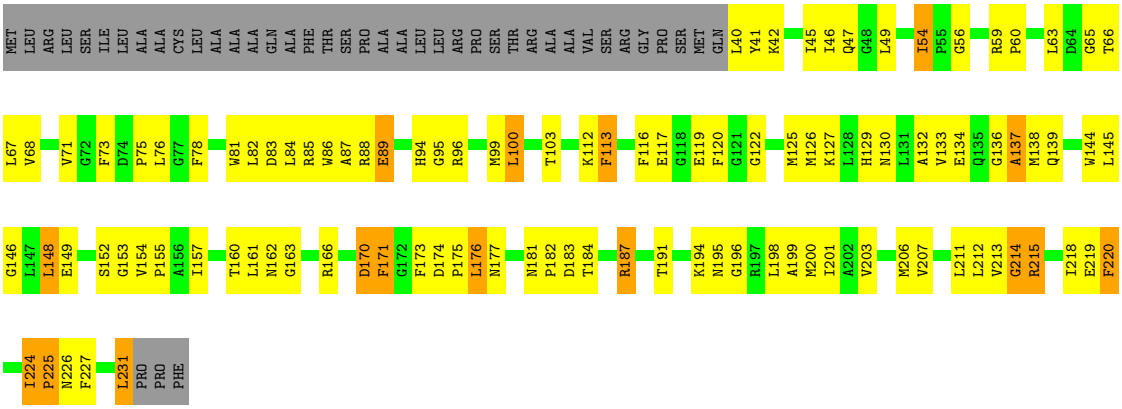




• Molecule 7: ACPII-6

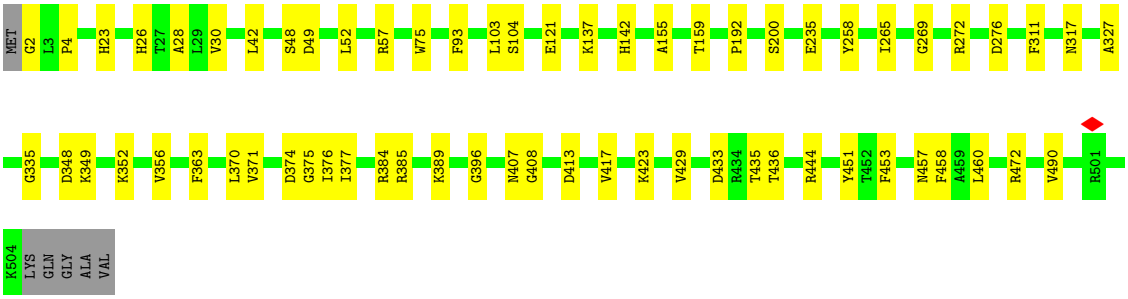
Chain p:





• Molecule 8: Photosystem II CP47 reaction center protein

Chain B:

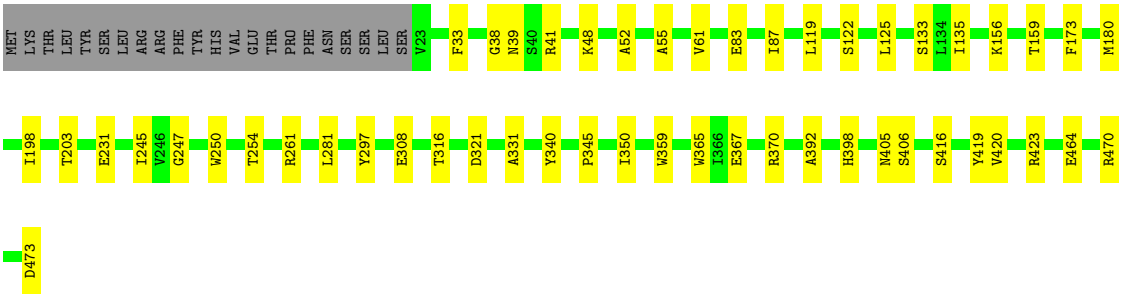


• Molecule 8: Photosystem II CP47 reaction center protein

Chain b:

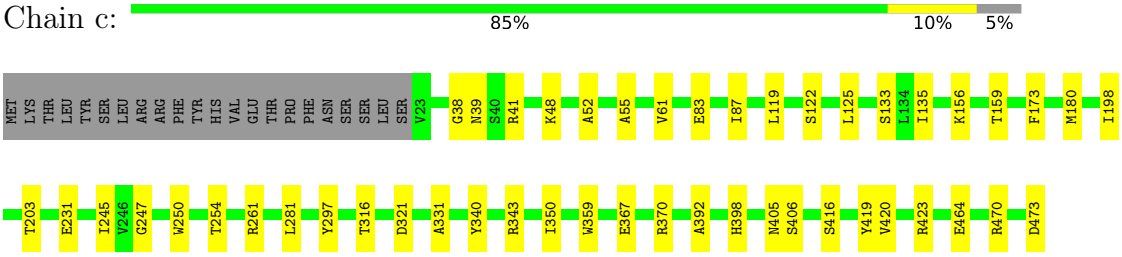
• Molecule 9: PsbC_CP43

Chain C:



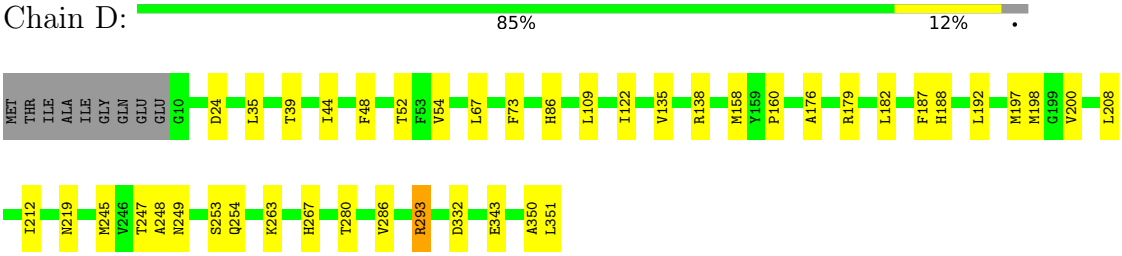
• Molecule 9: PsbC_CP43

Chain c:



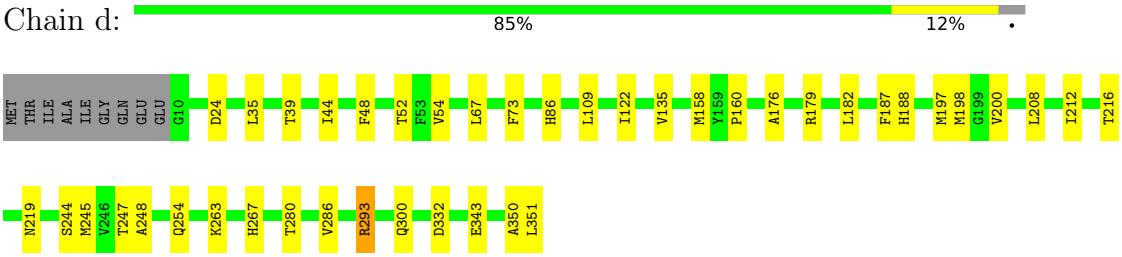
• Molecule 10: Photosystem II D2 protein

Chain D:



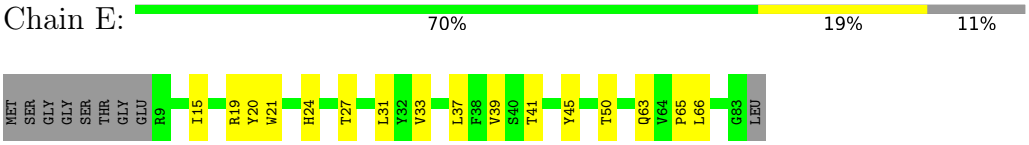
• Molecule 10: Photosystem II D2 protein

Chain d:



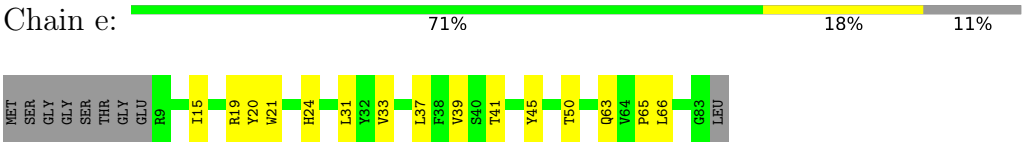
• Molecule 11: Cytochrome b559 subunit alpha

Chain E:



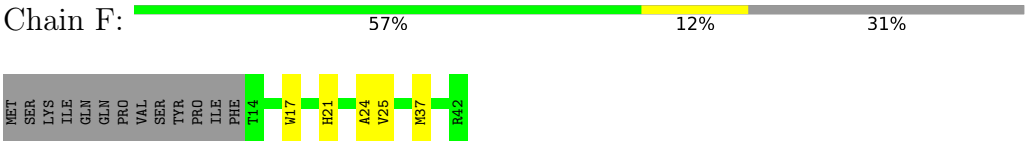
• Molecule 11: Cytochrome b559 subunit alpha

Chain e:



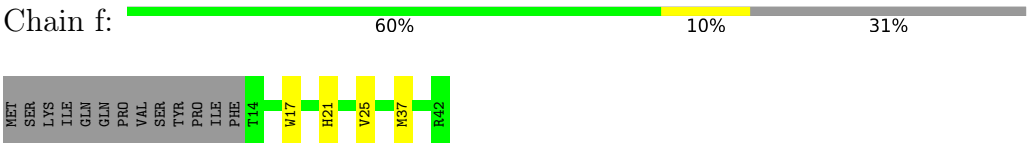
• Molecule 12: Cytochrome b559 subunit beta

Chain F:



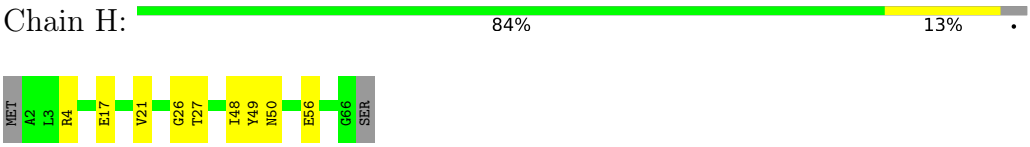
• Molecule 12: Cytochrome b559 subunit beta

Chain f:



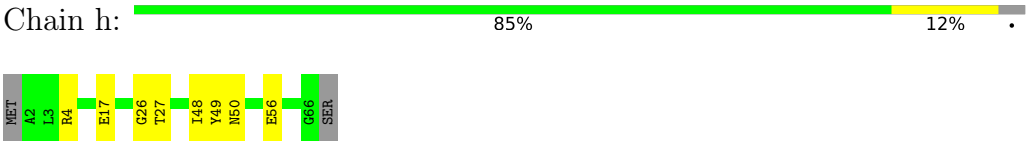
• Molecule 13: Photosystem II reaction center protein H

Chain H:



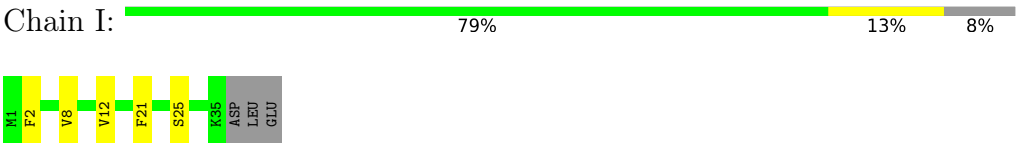
• Molecule 13: Photosystem II reaction center protein H

Chain h:



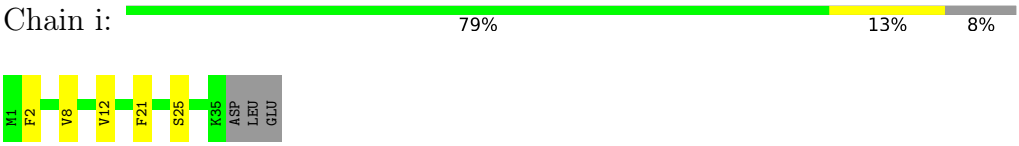
• Molecule 14: Photosystem II reaction center protein I

Chain I:



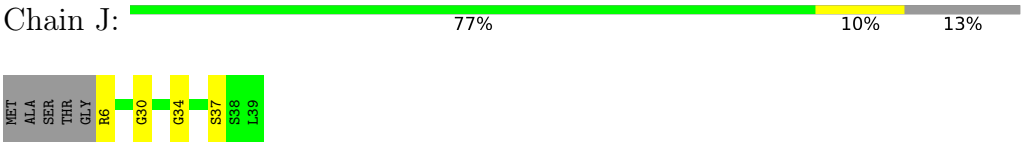
• Molecule 14: Photosystem II reaction center protein I

Chain i:



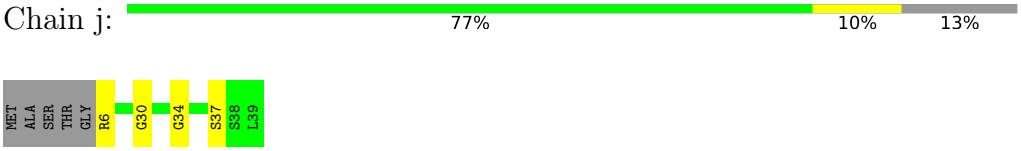
• Molecule 15: Photosystem II reaction center protein J

Chain J:



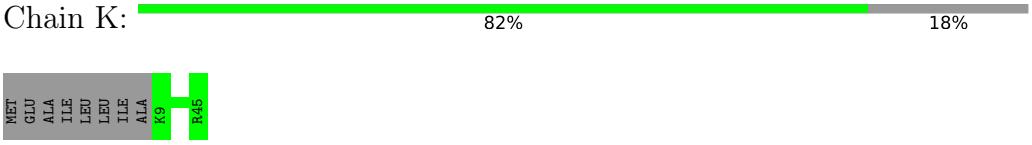
• Molecule 15: Photosystem II reaction center protein J

Chain j:



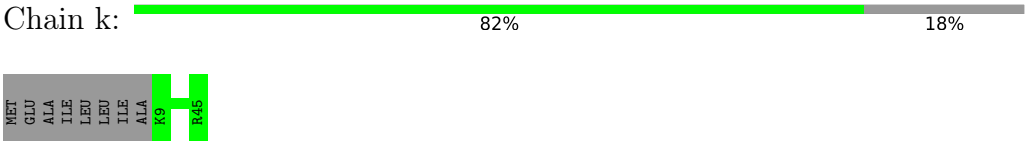
• Molecule 16: Photosystem II reaction center protein K

Chain K:



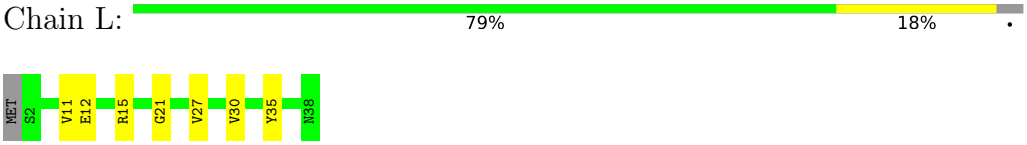
• Molecule 16: Photosystem II reaction center protein K

Chain k:



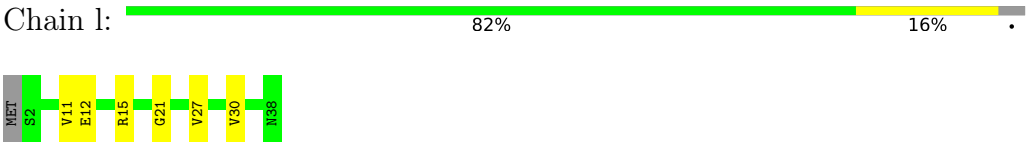
• Molecule 17: Photosystem II reaction center protein L

Chain L:



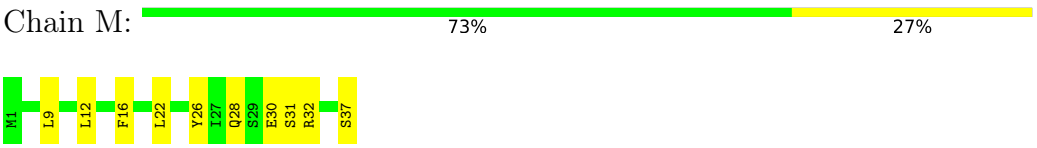
• Molecule 17: Photosystem II reaction center protein L

Chain l:



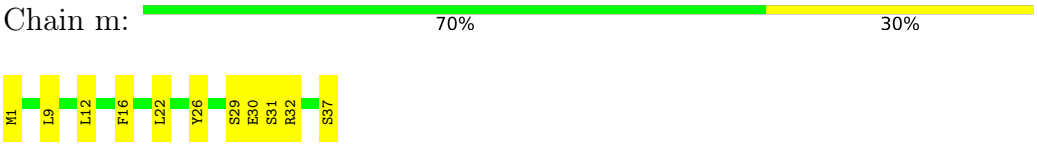
• Molecule 18: PsbM

Chain M:



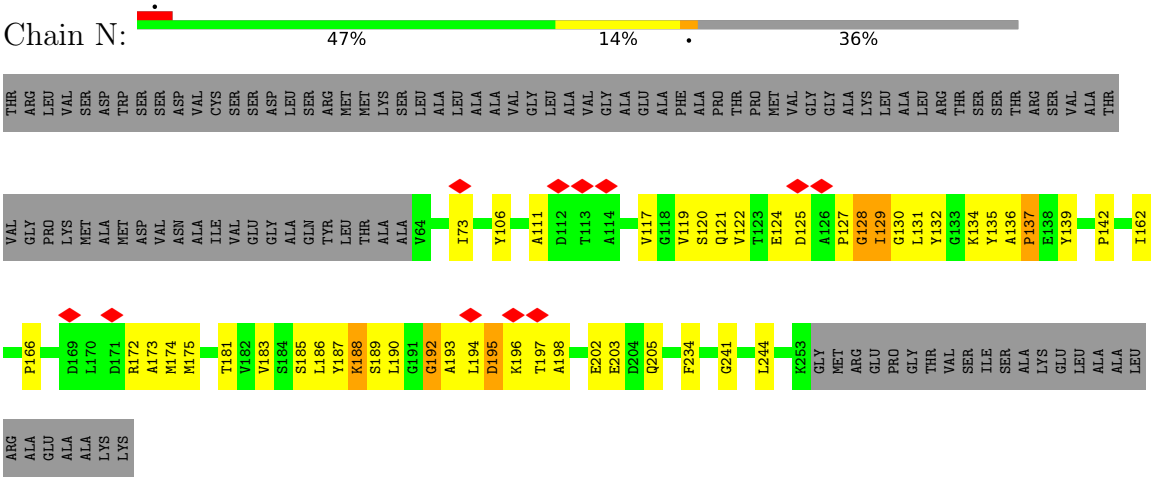
• Molecule 18: PsbM

Chain m:



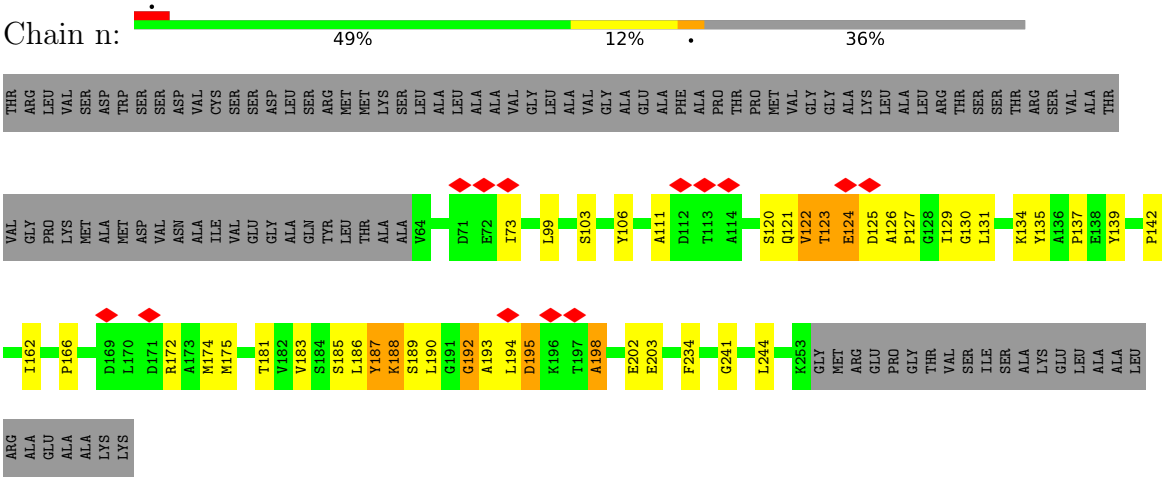
• Molecule 19: Psb-gama_linker

Chain N:



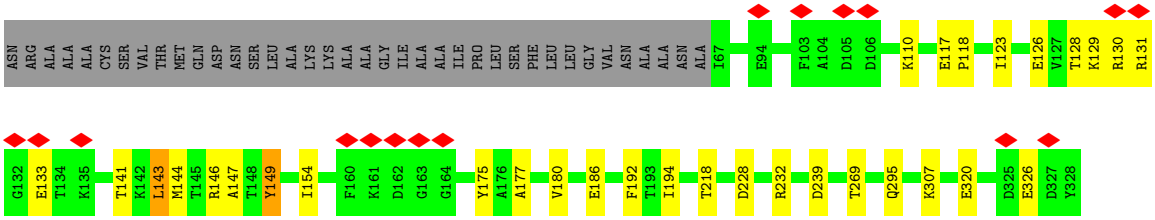
• Molecule 19: Psb-gama_linker

Chain n:

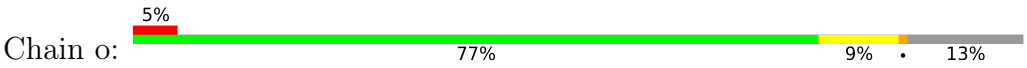


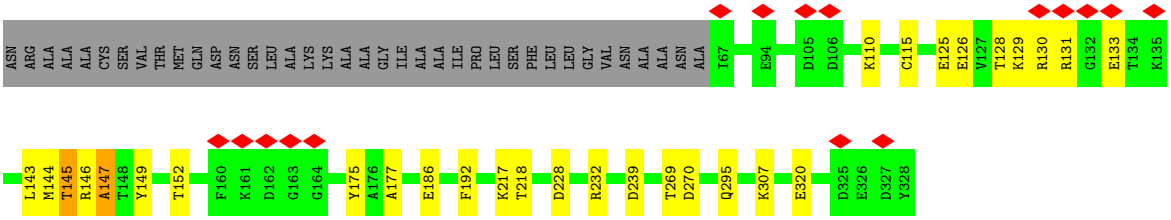
• Molecule 20: PsbO

Chain O:

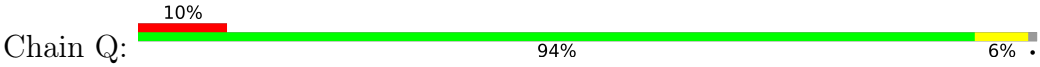


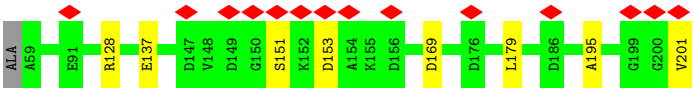
• Molecule 20: PsbO



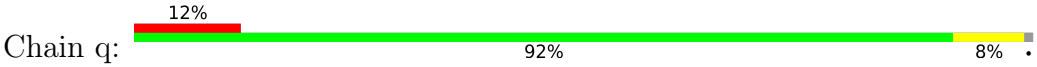


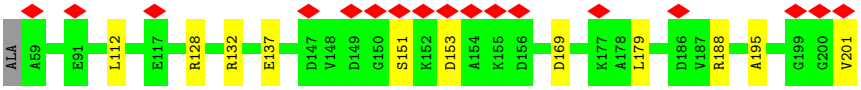
• Molecule 21: PsbQ



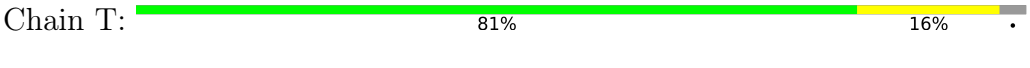


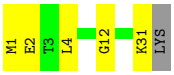
• Molecule 21: PsbQ



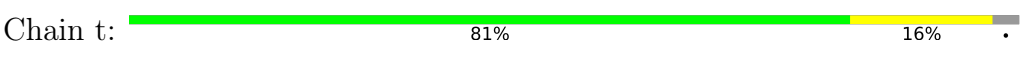


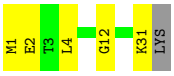
• Molecule 22: Photosystem II reaction center protein T





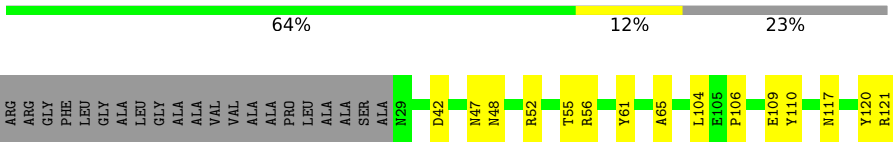
• Molecule 22: Photosystem II reaction center protein T





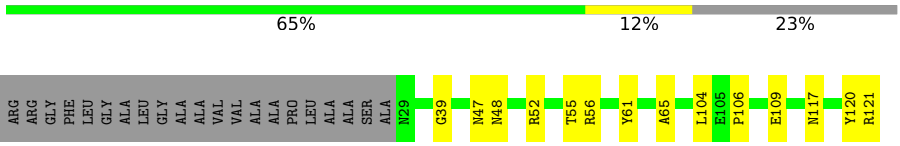
• Molecule 23: PsbU

Chain U:



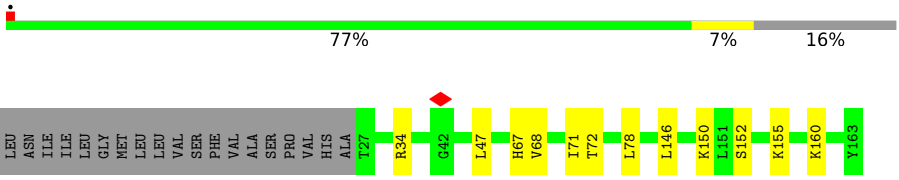
• Molecule 23: PsbU

Chain u:



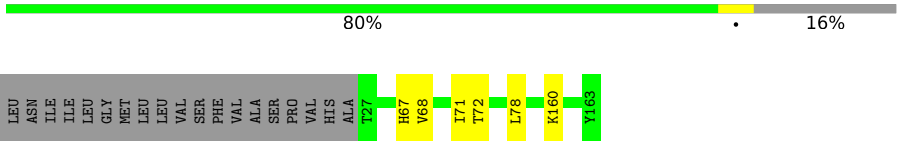
• Molecule 24: Photosystem II cytochrome c550

Chain V:



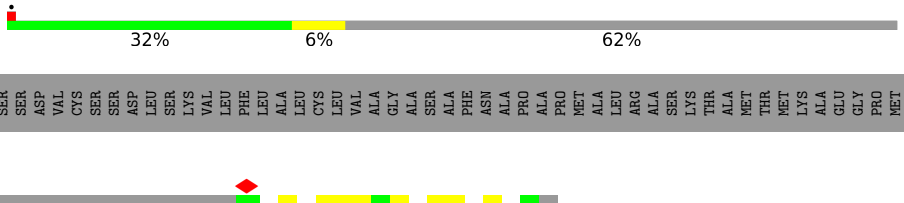
• Molecule 24: Photosystem II cytochrome c550

Chain v:



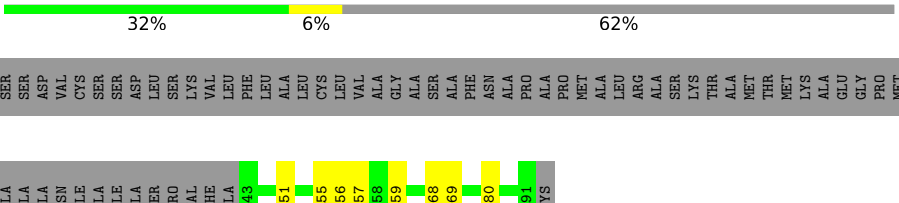
• Molecule 25: PsbW

Chain W:



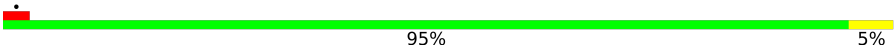
• Molecule 25: PsbW

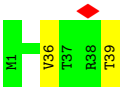
Chain w:



• Molecule 26: Photosystem II reaction center protein X

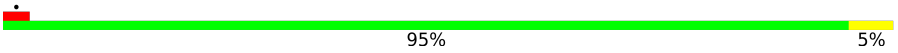
Chain X:

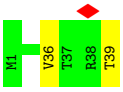




• Molecule 26: Photosystem II reaction center protein X

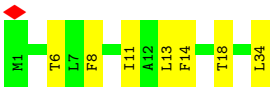
Chain x:





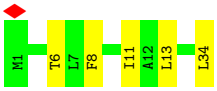
• Molecule 27: Photosystem II reaction center protein Psb30

Chain Y:



• Molecule 27: Photosystem II reaction center protein Psb30

Chain y:

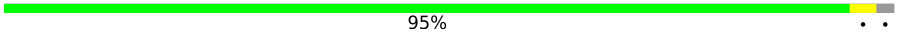


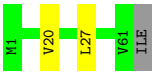
• Molecule 28: Photosystem II reaction center protein Z

Chain Z:

• Molecule 28: Photosystem II reaction center protein Z

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168683	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.868	Depositor
Minimum map value	0.000	Depositor
Average map value	0.088	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, LHG, PL9, BCT, KC2, LMG, PHO, CL, OEX, SQD, IHT, 8CT, CLA, DGD, FE2, II0

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.30	0/2701	0.50	1/3687 (0.0%)
1	a	0.26	0/2701	0.47	1/3687 (0.0%)
2	0	0.79	0/1398	1.14	19/1888 (1.0%)
2	4	0.80	1/1398 (0.1%)	1.05	13/1888 (0.7%)
3	1	0.24	0/1396	0.43	0/1892
3	7	0.24	0/1396	0.44	0/1892
4	2	0.27	0/1508	0.49	1/2044 (0.0%)
4	8	0.27	0/1508	0.47	1/2044 (0.0%)
5	3	0.29	0/1434	0.52	1/1943 (0.1%)
5	9	0.32	0/1434	0.65	6/1943 (0.3%)
6	5	0.64	0/1376	0.71	3/1862 (0.2%)
6	g	0.63	0/1376	0.69	2/1862 (0.1%)
7	6	1.09	2/1487 (0.1%)	1.44	34/2014 (1.7%)
7	p	1.09	3/1487 (0.2%)	1.36	26/2014 (1.3%)
8	B	0.22	0/4084	0.42	4/5558 (0.1%)
8	b	0.23	0/4084	0.45	3/5558 (0.1%)
9	C	0.21	0/3618	0.41	1/4937 (0.0%)
9	c	0.21	0/3618	0.41	1/4937 (0.0%)
10	D	0.21	0/2806	0.42	1/3823 (0.0%)
10	d	0.21	0/2806	0.42	1/3823 (0.0%)
11	E	0.31	0/634	0.59	0/865
11	e	0.30	0/634	0.59	0/865
12	F	0.25	0/242	0.52	0/328
12	f	0.25	0/242	0.52	0/328
13	H	0.23	0/527	0.52	2/717 (0.3%)
13	h	0.24	0/527	0.55	2/717 (0.3%)
14	I	0.19	0/294	0.38	0/397
14	i	0.19	0/294	0.38	0/397
15	J	0.34	0/255	0.57	1/348 (0.3%)
15	j	0.35	0/255	0.56	1/348 (0.3%)
16	K	0.30	0/307	0.52	0/421
16	k	0.40	0/307	0.65	0/421

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	L	0.21	0/311	0.37	0/424
17	l	0.21	0/311	0.37	0/424
18	M	0.38	0/280	0.49	0/381
18	m	0.35	0/280	0.49	0/381
19	N	0.38	0/1516	0.81	10/2070 (0.5%)
19	n	0.37	0/1516	0.77	8/2070 (0.4%)
20	O	0.26	0/2024	0.54	2/2722 (0.1%)
20	o	0.24	0/2024	0.52	4/2722 (0.1%)
21	Q	0.20	0/1121	0.39	0/1508
21	q	0.20	0/1121	0.39	0/1508
22	T	0.27	0/257	0.42	1/348 (0.3%)
22	t	0.27	0/257	0.42	1/348 (0.3%)
23	U	0.26	0/757	0.53	0/1031
23	u	0.27	0/757	0.50	0/1031
24	V	0.22	0/1063	0.40	0/1443
24	v	0.22	0/1063	0.41	0/1443
25	W	0.31	0/398	0.57	0/541
25	w	0.32	0/398	0.57	0/541
26	X	0.23	0/295	0.41	0/402
26	x	0.22	0/295	0.41	0/402
27	Y	0.29	0/270	0.51	0/367
27	y	0.29	0/270	0.51	0/367
28	Z	0.23	0/467	0.43	0/638
28	z	0.23	0/467	0.43	0/638
All	All	0.39	6/65652 (0.0%)	0.61	151/89198 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	p	170	ASP	CA-C	-6.11	1.46	1.53
7	p	148	LEU	C-O	-5.70	1.17	1.24
7	6	148	LEU	C-O	-5.68	1.17	1.24
2	4	113	ASN	CA-C	-5.13	1.47	1.52
7	p	137	ALA	CA-C	-5.09	1.46	1.52
7	6	137	ALA	CA-C	-5.08	1.46	1.52

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	143	ILE	N-CA-C	-10.79	99.61	110.62
7	p	65	GLY	N-CA-C	10.59	125.44	112.73
7	6	65	GLY	N-CA-C	10.18	124.95	112.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	p	198	LEU	N-CA-C	-9.86	100.54	111.28
7	6	198	LEU	N-CA-C	-9.85	100.55	111.28
7	6	89	GLU	N-CA-C	-9.29	101.14	111.07
7	p	89	GLU	N-CA-C	-9.28	101.14	111.07
5	9	56	GLN	N-CA-C	9.21	121.40	111.36
7	p	113	PHE	N-CA-C	-9.01	98.38	109.83
7	6	215	ARG	N-CA-C	9.01	123.29	110.23
19	N	195	ASP	N-CA-C	8.83	122.91	108.52
7	p	215	ARG	N-CA-C	8.58	122.67	110.23
7	p	125	MET	CB-CA-C	-8.56	106.70	116.63
7	6	228	LYS	N-CA-C	-8.51	102.08	111.36
1	a	143	ILE	N-CA-C	-8.47	100.09	111.44
7	6	162	ASN	N-CA-C	-8.40	102.12	111.28
19	n	130	GLY	N-CA-C	8.38	121.17	111.36
19	n	188	LYS	N-CA-C	-8.37	102.12	111.07
2	0	214	ASN	N-CA-C	-8.22	102.26	111.14
7	6	113	PHE	N-CA-C	-8.22	99.39	109.83
19	N	188	LYS	N-CA-C	-8.15	102.40	111.28
20	o	149	TYR	N-CA-C	7.92	122.20	112.54
20	o	145	THR	N-CA-C	-7.88	99.39	110.50
7	p	176	LEU	N-CA-C	-7.83	103.45	113.16
7	6	222	THR	N-CA-C	-7.78	100.25	110.53
7	6	171	PHE	N-CA-C	-7.74	100.31	110.53
2	0	74	TYR	N-CA-C	7.69	119.66	111.28
7	6	100	LEU	N-CA-C	-7.69	101.64	111.02
7	p	100	LEU	N-CA-C	-7.67	101.67	111.02
7	p	171	PHE	N-CA-C	-7.65	100.46	110.33
7	6	167	GLN	CA-C-N	-7.54	111.99	119.76
7	6	167	GLN	C-N-CA	-7.54	111.99	119.76
7	6	127	LYS	N-CA-C	7.48	120.31	111.71
7	6	103	THR	N-CA-C	-7.42	103.19	111.28
7	p	103	THR	N-CA-C	-7.41	103.20	111.28
2	0	98	PHE	N-CA-C	-7.41	102.22	111.11
2	4	98	PHE	N-CA-C	-7.38	102.26	111.11
7	6	128	LEU	N-CA-C	-7.37	103.25	111.28
20	O	149	TYR	N-CA-C	7.26	119.20	111.28
2	0	112	ASP	N-CA-C	7.18	120.81	109.39
5	9	61	SER	N-CA-C	7.14	120.58	110.23
8	b	373	LYS	CB-CA-C	-7.08	107.60	117.23
5	9	58	ILE	N-CA-C	-7.07	102.02	108.95
2	4	216	LYS	N-CA-C	-7.07	99.20	109.59
19	n	195	ASP	N-CA-C	7.06	120.23	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	p	195	ASN	N-CA-C	-7.05	103.60	111.28
7	6	195	ASN	N-CA-C	-7.03	103.61	111.28
19	n	192	GLY	N-CA-C	-6.96	103.64	112.54
2	0	123	VAL	N-CA-C	-6.93	101.34	108.96
2	4	123	VAL	N-CA-C	-6.92	101.35	108.96
2	4	204	THR	N-CA-C	-6.83	97.76	108.90
20	O	143	LEU	N-CA-C	6.81	119.67	109.25
7	p	163	GLY	N-CA-C	6.80	124.41	115.36
7	6	175	PRO	N-CA-C	-6.79	104.10	113.53
19	N	192	GLY	N-CA-C	-6.72	103.93	112.54
20	o	146	ARG	N-CA-C	-6.64	101.19	110.35
2	4	163	ASP	N-CA-CB	-6.55	102.24	112.13
2	0	197	MET	N-CA-C	-6.53	104.08	111.07
2	4	197	MET	N-CA-C	-6.53	104.08	111.07
13	h	48	ILE	N-CA-C	6.53	116.68	110.42
2	0	204	THR	N-CA-C	-6.49	98.32	108.90
19	N	198	ALA	N-CA-C	6.48	119.62	110.23
2	0	199	HIS	N-CA-C	-6.43	104.36	111.82
2	4	199	HIS	N-CA-C	-6.42	104.38	111.82
7	p	194	LYS	N-CA-C	6.41	118.34	111.36
7	6	194	LYS	N-CA-C	6.40	118.33	111.36
7	p	225	PRO	N-CA-C	-6.38	104.34	113.47
6	5	162	ASP	N-CA-C	-6.38	99.58	109.79
7	p	71	VAL	N-CA-C	-6.35	105.49	112.80
7	6	71	VAL	N-CA-C	-6.35	105.50	112.80
19	N	125	ASP	N-CA-C	-6.33	104.46	111.36
2	0	67	ASP	N-CA-C	-6.23	97.97	108.94
7	p	56	GLY	N-CA-C	-6.13	107.39	114.69
2	4	123	VAL	CA-C-N	-6.13	113.66	119.85
2	4	123	VAL	C-N-CA	-6.13	113.66	119.85
2	0	123	VAL	CA-C-N	-6.10	113.69	119.85
2	0	123	VAL	C-N-CA	-6.10	113.69	119.85
7	6	56	GLY	N-CA-C	-5.97	107.42	115.36
7	6	211	LEU	N-CA-C	5.96	117.44	111.07
15	J	30	GLY	N-CA-C	-5.94	106.97	114.16
15	j	30	GLY	N-CA-C	-5.93	106.98	114.16
7	p	224	ILE	CA-C-N	-5.91	112.83	118.97
7	p	224	ILE	C-N-CA	-5.91	112.83	118.97
2	0	162	LEU	N-CA-C	-5.91	105.65	112.92
2	4	99	LEU	N-CA-C	5.84	117.45	111.14
8	B	376	ILE	N-CA-C	-5.83	102.05	109.58
2	0	99	LEU	N-CA-C	5.83	117.43	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	n	198	ALA	N-CA-C	5.76	118.59	110.23
8	b	374	ASP	N-CA-C	-5.70	105.16	111.71
7	p	137	ALA	N-CA-C	-5.68	104.30	111.11
7	p	182	PRO	N-CA-C	-5.68	107.04	114.03
2	4	66	PHE	N-CA-C	5.68	118.65	107.98
7	6	137	ALA	N-CA-C	-5.68	104.30	111.11
20	o	147	ALA	N-CA-C	5.66	122.86	110.80
8	B	374	ASP	N-CA-C	-5.66	105.88	112.89
7	6	205	GLY	N-CA-C	-5.60	106.00	112.50
13	h	50	ASN	N-CA-C	-5.59	105.72	112.54
5	3	56	GLN	N-CA-C	5.55	119.37	112.59
19	n	123	THR	N-CA-C	-5.54	102.81	110.35
7	p	203	VAL	N-CA-C	-5.50	104.58	110.36
19	n	187	TYR	N-CA-CB	-5.49	103.56	111.91
2	0	58	GLY	N-CA-C	5.47	119.50	112.83
7	6	126	MET	N-CA-C	5.47	120.34	111.37
7	6	214	GLY	N-CA-C	5.47	119.29	112.73
7	6	212	LEU	N-CA-C	5.46	119.66	112.89
5	9	57	ALA	N-CA-C	-5.44	98.88	108.08
2	0	64	VAL	N-CA-C	-5.39	107.22	112.29
7	p	220	PHE	N-CA-C	5.38	117.14	111.28
6	5	123	VAL	N-CA-C	-5.36	105.78	113.07
7	6	220	PHE	N-CA-C	5.36	117.12	111.28
8	B	375	GLY	N-CA-C	5.36	123.46	115.64
13	H	48	ILE	N-CA-C	5.36	115.56	110.42
6	g	123	VAL	N-CA-C	-5.35	105.79	113.07
19	N	129	ILE	N-CA-C	5.35	116.48	109.58
2	0	100	VAL	N-CA-C	5.31	115.53	110.53
2	4	100	VAL	N-CA-C	5.31	115.52	110.53
7	6	203	VAL	N-CA-C	-5.31	104.57	110.62
7	6	207	VAL	CB-CA-C	-5.30	104.98	112.14
7	6	184	THR	N-CA-C	-5.29	105.52	111.28
7	p	187	ARG	N-CA-C	-5.25	105.55	111.28
19	n	122	VAL	N-CA-C	5.22	120.20	109.34
7	6	187	ARG	N-CA-C	-5.21	105.60	111.28
4	2	67	VAL	N-CA-C	-5.19	107.29	111.91
13	H	50	ASN	N-CA-C	-5.19	106.21	112.54
2	4	162	LEU	N-CA-C	-5.19	105.41	112.26
2	0	210	GLU	N-CA-C	5.16	116.90	111.28
7	6	177	ASN	N-CA-C	-5.16	99.82	110.80
4	8	67	VAL	N-CA-C	-5.15	107.33	111.91
7	p	66	THR	N-CA-C	5.14	116.88	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	0	56	LEU	CB-CA-C	-5.10	104.47	112.12
19	N	125	ASP	CA-C-N	-5.10	116.97	123.15
19	N	125	ASP	C-N-CA	-5.10	116.97	123.15
19	N	125	ASP	N-CA-CB	5.09	117.70	110.16
2	0	59	SER	N-CA-C	5.09	116.83	111.28
5	9	52	GLY	CA-C-N	-5.08	114.71	119.89
5	9	52	GLY	C-N-CA	-5.08	114.71	119.89
10	d	293	ARG	N-CA-C	5.07	117.76	109.59
7	6	224	ILE	CA-C-N	-5.07	113.70	118.97
7	6	224	ILE	C-N-CA	-5.07	113.70	118.97
10	D	293	ARG	N-CA-C	5.06	117.74	109.59
22	T	2	GLU	N-CA-C	-5.05	105.86	112.23
8	B	363	PHE	N-CA-C	5.04	116.96	109.25
6	5	125	GLN	N-CA-C	-5.03	105.80	111.28
8	b	363	PHE	N-CA-C	5.03	116.95	109.25
9	c	419	TYR	N-CA-C	5.03	121.51	110.80
7	p	214	GLY	N-CA-C	5.03	118.76	112.73
7	p	207	VAL	CB-CA-C	-5.03	105.36	112.14
9	C	419	TYR	N-CA-C	5.02	121.49	110.80
22	t	2	GLU	N-CA-C	-5.02	105.91	112.23
19	N	128	GLY	N-CA-C	-5.01	104.74	113.76
6	g	125	GLN	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2514	70	0
1	a	2617	0	2514	64	0
2	0	1365	0	1365	183	0
2	4	1365	0	1365	154	0
3	1	1360	0	1337	15	0
3	7	1360	0	1337	16	0
4	2	1469	0	1443	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	8	1469	0	1443	17	0
5	3	1400	0	1414	20	0
5	9	1400	0	1414	17	0
6	5	1339	0	1324	51	0
6	g	1339	0	1324	60	0
7	6	1455	0	1461	148	0
7	p	1455	0	1461	131	0
8	B	3953	0	3845	62	0
8	b	3953	0	3845	81	0
9	C	3503	0	3421	38	0
9	c	3503	0	3421	41	0
10	D	2713	0	2613	70	0
10	d	2713	0	2613	69	0
11	E	616	0	604	17	0
11	e	616	0	604	16	0
12	F	235	0	241	5	0
12	f	235	0	241	3	0
13	H	515	0	535	28	0
13	h	515	0	535	26	0
14	I	287	0	293	3	0
14	i	287	0	293	3	0
15	J	249	0	258	2	0
15	j	249	0	258	2	0
16	K	296	0	312	0	0
16	k	296	0	312	0	0
17	L	301	0	301	10	0
17	l	301	0	301	10	0
18	M	276	0	294	28	0
18	m	276	0	294	30	0
19	N	1474	0	1433	96	0
19	n	1474	0	1433	77	0
20	O	1993	0	1962	40	0
20	o	1993	0	1962	42	0
21	Q	1102	0	1115	5	0
21	q	1102	0	1115	7	0
22	T	250	0	265	9	0
22	t	250	0	265	10	0
23	U	741	0	743	12	0
23	u	741	0	743	8	0
24	V	1043	0	1036	7	0
24	v	1043	0	1036	4	0
25	W	391	0	373	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	w	391	0	373	10	0
26	X	291	0	318	1	0
26	x	291	0	318	1	0
27	Y	265	0	293	5	0
27	y	265	0	293	4	0
28	Z	457	0	501	3	0
28	z	457	0	501	2	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	1	0	0	0	0
30	a	1	0	0	0	0
31	A	4	0	1	1	0
31	a	4	0	1	0	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	0	478	0	373	39	0
33	1	506	0	471	5	0
33	2	488	0	433	2	0
33	3	564	0	446	0	0
33	4	431	0	338	32	0
33	5	504	0	391	28	0
33	6	515	0	382	51	0
33	7	506	0	471	5	0
33	8	488	0	433	2	0
33	9	564	0	446	6	0
33	A	239	0	242	17	0
33	B	1040	0	1095	14	0
33	C	836	0	915	12	0
33	D	130	0	144	1	0
33	N	378	0	345	25	0
33	a	239	0	242	16	0
33	b	1040	0	1095	15	0
33	c	836	0	915	12	0
33	d	130	0	144	1	0
33	g	504	0	391	34	0
33	n	331	0	310	1	0
33	p	515	0	382	47	0
34	A	64	0	74	5	0
34	D	64	0	74	1	0
34	a	64	0	74	4	0
34	d	64	0	74	1	0
35	0	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	1	40	0	0	0	0
35	4	40	0	0	1	0
35	7	40	0	0	0	0
35	A	40	0	0	0	0
35	B	120	0	0	0	0
35	C	120	0	0	1	0
35	D	40	0	0	0	0
35	H	40	0	0	0	0
35	Y	40	0	0	0	0
35	a	40	0	0	0	0
35	b	120	0	0	0	0
35	c	120	0	0	1	0
35	d	40	0	0	0	0
35	h	40	0	0	0	0
35	y	40	0	0	0	0
36	A	30	0	37	0	0
36	D	55	0	80	6	0
36	a	30	0	37	0	0
36	d	55	0	80	5	0
37	0	24	0	18	0	0
37	1	49	0	74	2	0
37	2	46	0	65	2	0
37	3	106	0	122	2	0
37	4	24	0	18	0	0
37	5	22	0	20	0	0
37	7	49	0	74	2	0
37	8	46	0	65	2	0
37	9	106	0	122	2	0
37	A	24	0	18	8	0
37	B	49	0	74	10	0
37	D	142	0	206	4	0
37	a	24	0	18	7	0
37	b	49	0	74	10	0
37	d	142	0	206	5	0
37	g	22	0	20	0	0
38	0	45	0	0	4	0
38	1	90	0	0	0	0
38	2	45	0	0	0	0
38	3	45	0	0	0	0
38	4	45	0	0	0	0
38	5	45	0	0	0	0
38	6	45	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	7	90	0	0	0	0
38	8	45	0	0	0	0
38	9	45	0	0	0	0
38	g	45	0	0	0	0
38	p	45	0	0	1	0
39	0	168	0	0	21	0
39	1	168	0	0	3	0
39	2	126	0	0	4	0
39	3	210	0	0	2	0
39	4	168	0	0	13	0
39	5	126	0	0	14	0
39	6	210	0	0	21	0
39	7	168	0	0	3	0
39	8	126	0	0	4	0
39	9	210	0	0	2	0
39	g	126	0	0	15	0
39	p	210	0	0	19	0
40	2	41	0	0	0	0
40	3	41	0	0	0	0
40	5	41	0	0	0	0
40	6	41	0	0	5	0
40	8	41	0	0	0	0
40	9	41	0	0	0	0
40	g	41	0	0	0	0
40	p	41	0	0	8	0
41	B	38	0	40	1	0
41	C	42	0	48	0	0
41	J	46	0	56	1	0
41	L	54	0	78	2	0
41	b	38	0	40	1	0
41	c	42	0	48	0	0
41	j	46	0	56	1	0
41	l	54	0	78	2	0
42	B	92	0	124	1	0
42	C	51	0	72	4	0
42	D	92	0	124	4	0
42	T	43	0	56	7	0
42	W	47	0	64	1	0
42	b	92	0	124	1	0
42	c	51	0	72	4	0
42	d	92	0	124	3	0
42	l	38	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	m	38	0	46	0	0
42	t	43	0	56	7	0
42	w	47	0	64	1	0
43	C	179	0	232	11	0
43	H	60	0	78	20	0
43	c	179	0	232	13	0
43	h	60	0	78	16	0
44	F	43	0	30	3	0
44	V	43	0	30	2	0
44	f	43	0	30	3	0
44	v	43	0	30	2	0
45	A	24	0	0	3	0
45	B	3	0	0	0	0
45	C	11	0	0	1	0
45	O	1	0	0	0	0
45	U	2	0	0	0	0
45	W	1	0	0	0	0
45	a	24	0	0	3	0
45	b	3	0	0	0	0
45	c	11	0	0	1	0
45	o	1	0	0	0	0
45	u	2	0	0	0	0
45	w	1	0	0	0	0
All	All	82310	0	77514	1750	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 11.

All (1750) 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)
1:a:317:TRP:CE3	10:d:179:ARG:CD	1.85	1.60
1:A:317:TRP:CE3	10:D:179:ARG:CD	1.85	1.60
1:a:317:TRP:CZ3	10:d:179:ARG:NE	1.70	1.59
1:A:317:TRP:CZ3	10:D:179:ARG:NE	1.70	1.59
1:A:317:TRP:CZ3	10:D:179:ARG:CZ	1.93	1.50
1:a:317:TRP:CZ3	10:d:179:ARG:CZ	1.93	1.50
18:M:12:LEU:O	18:M:16:PHE:CD2	1.67	1.46
18:m:12:LEU:O	18:m:16:PHE:CD2	1.67	1.46
13:H:49:TYR:HD2	43:H:101:DGD:C1B	1.34	1.40
1:a:317:TRP:HZ3	10:d:179:ARG:CZ	1.29	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TRP:HZ3	10:D:179:ARG:CZ	1.29	1.39
6:g:75:VAL:HG21	19:n:183:VAL:CG1	1.51	1.38
6:5:75:VAL:HG21	19:N:183:VAL:CG1	1.53	1.37
13:H:49:TYR:CD2	43:H:101:DGD:C1B	2.09	1.35
13:H:49:TYR:CE2	43:H:101:DGD:HB31	1.61	1.33
20:O:128:THR:CG2	8:b:49:ASP:HB2	1.60	1.32
8:B:49:ASP:HB2	20:o:128:THR:CG2	1.60	1.32
1:A:317:TRP:CE3	10:D:179:ARG:HD2	1.57	1.30
1:a:317:TRP:CE3	10:d:179:ARG:HD2	1.57	1.29
2:0:69:LEU:HD12	2:0:71:PHE:CE2	1.68	1.28
13:H:49:TYR:CE2	43:H:101:DGD:O2G	1.88	1.26
2:4:61:ALA:HA	19:N:130:GLY:CA	1.66	1.25
4:2:77:VAL:CG1	2:4:167:LEU:HD22	1.65	1.24
2:0:177:ARG:O	19:n:129:ILE:HD11	1.37	1.23
13:h:49:TYR:HD2	43:h:101:DGD:C1B	1.52	1.23
18:M:9:LEU:CD1	18:m:9:LEU:HD12	1.70	1.22
6:5:75:VAL:CG2	19:N:183:VAL:HG12	1.70	1.21
18:M:9:LEU:HD12	18:m:9:LEU:CD1	1.71	1.21
10:d:187:PHE:O	10:d:293:ARG:NH1	1.72	1.21
10:D:187:PHE:O	10:D:293:ARG:NH1	1.72	1.20
10:D:188:HIS:ND1	10:D:293:ARG:HD3	1.53	1.20
10:d:188:HIS:ND1	10:d:293:ARG:HD3	1.54	1.19
6:g:75:VAL:CG2	19:n:183:VAL:HG12	1.72	1.18
13:h:49:TYR:CE2	43:h:101:DGD:HG32	1.78	1.18
18:M:12:LEU:HB3	18:M:16:PHE:HE2	1.07	1.18
8:b:258:TYR:HB3	13:h:49:TYR:OH	1.43	1.17
18:m:12:LEU:HB3	18:m:16:PHE:HE2	1.07	1.16
7:p:126:MET:SD	40:p:318:IHT:C11	2.34	1.16
13:h:49:TYR:CE2	43:h:101:DGD:O2G	1.98	1.15
7:p:126:MET:SD	40:p:318:IHT:C15	2.34	1.15
19:n:190:LEU:O	19:n:190:LEU:HD23	1.46	1.14
2:0:117:THR:HG21	2:0:202:LEU:CD2	1.76	1.14
22:t:1:MET:HG2	42:t:101:LMG:HC91	1.28	1.14
18:M:9:LEU:CD1	18:m:9:LEU:CD1	2.27	1.13
22:T:1:MET:HG2	42:T:101:LMG:HC91	1.28	1.13
1:A:317:TRP:CZ3	10:D:179:ARG:CD	2.20	1.13
7:6:112:LYS:HE2	7:6:122:GLY:HA2	1.31	1.12
19:N:122:VAL:HG21	33:N:303:CLA:HMA2	1.32	1.12
2:4:203:LEU:HD23	2:4:204:THR:HG23	1.29	1.12
8:b:258:TYR:CB	13:h:49:TYR:OH	1.98	1.11
10:D:67:LEU:CD2	11:E:50:THR:HG21	1.81	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:h:49:TYR:CD2	43:h:101:DGD:C1B	2.34	1.11
2:0:49:PHE:CE1	2:0:50:LEU:HG	1.86	1.11
2:0:60:MET:HE1	19:n:137:PRO:CD	1.81	1.10
10:d:67:LEU:CD2	11:e:50:THR:HG21	1.81	1.10
1:a:317:TRP:CZ3	10:d:179:ARG:CD	2.20	1.10
7:6:176:LEU:HD23	39:6:314:II0:C06	1.82	1.10
2:4:61:ALA:HA	19:N:130:GLY:HA2	1.17	1.09
10:D:67:LEU:HD23	11:E:50:THR:HG21	1.13	1.09
19:N:121:GLN:HG2	33:N:303:CLA:HBA1	1.11	1.09
7:p:215:ARG:HG2	7:p:219:GLU:CD	1.78	1.09
19:N:122:VAL:HG21	33:N:303:CLA:CMA	1.83	1.08
7:p:215:ARG:HG2	7:p:219:GLU:OE2	1.51	1.08
2:0:69:LEU:HB2	2:0:71:PHE:CE2	1.88	1.08
2:4:200:GLN:NE2	33:4:309:CLA:NA	2.02	1.08
2:0:117:THR:HG21	2:0:202:LEU:HD23	1.27	1.08
2:0:200:GLN:NE2	33:0:310:CLA:NA	2.02	1.08
2:0:108:LEU:HD13	39:0:316:II0:C05	1.84	1.07
18:M:9:LEU:HD12	18:m:9:LEU:HD11	1.37	1.07
1:a:317:TRP:CE3	10:d:179:ARG:HD3	1.82	1.06
2:0:69:LEU:CD1	2:0:71:PHE:CE2	2.36	1.06
7:6:173:PHE:HE2	39:6:314:II0:C20	1.68	1.06
8:B:49:ASP:HB2	20:o:128:THR:HG23	1.31	1.06
8:B:258:TYR:HB2	13:H:49:TYR:OH	1.54	1.06
18:M:9:LEU:HD11	18:m:9:LEU:HD12	1.37	1.06
10:d:67:LEU:HD23	11:e:50:THR:HG21	1.13	1.06
20:O:128:THR:HG23	8:b:49:ASP:HB2	1.31	1.05
1:A:317:TRP:CE3	10:D:179:ARG:HD3	1.82	1.05
19:N:121:GLN:HG2	33:N:303:CLA:CBA	1.85	1.05
1:A:317:TRP:CE3	10:D:179:ARG:NE	2.11	1.05
1:a:317:TRP:CE3	10:d:179:ARG:NE	2.11	1.04
22:T:1:MET:HG3	42:T:101:LMG:O10	1.55	1.04
6:g:162:ASP:OD1	33:g:307:CLA:HBA2	1.57	1.04
22:t:1:MET:HG3	42:t:101:LMG:O10	1.55	1.04
7:6:215:ARG:HG2	7:6:219:GLU:CD	1.81	1.04
2:0:108:LEU:HD22	39:0:316:II0:C16	1.89	1.02
2:4:117:THR:HG21	2:4:202:LEU:CD2	1.90	1.02
7:6:215:ARG:HG2	7:6:219:GLU:OE2	1.59	1.02
7:p:112:LYS:HE3	7:p:122:GLY:HA2	1.38	1.02
22:t:1:MET:HG2	42:t:101:LMG:C9	1.89	1.01
13:H:49:TYR:CE2	43:H:101:DGD:C3B	2.43	1.01
22:T:1:MET:HG2	42:T:101:LMG:C9	1.89	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:12:LEU:HB3	18:M:16:PHE:CE2	1.95	1.01
1:a:317:TRP:HZ3	10:d:179:ARG:NE	1.24	1.01
18:m:12:LEU:HB3	18:m:16:PHE:CE2	1.95	1.00
13:h:49:TYR:CD2	43:h:101:DGD:O2G	2.14	1.00
20:O:128:THR:CG2	8:b:49:ASP:CB	2.39	0.99
4:2:77:VAL:HG12	2:4:167:LEU:HD22	1.00	0.99
1:A:317:TRP:HZ3	10:D:179:ARG:NE	1.24	0.99
7:p:166:ARG:HD2	7:p:170:ASP:O	1.60	0.99
19:N:122:VAL:HG11	33:N:303:CLA:HHB	1.45	0.98
9:c:343:ARG:NH2	20:o:152:THR:HG23	1.79	0.98
2:4:117:THR:HG21	2:4:202:LEU:HD23	1.42	0.98
8:B:49:ASP:CB	20:o:128:THR:CG2	2.39	0.98
2:0:69:LEU:CD1	2:0:71:PHE:CZ	2.47	0.97
13:h:49:TYR:CE2	43:h:101:DGD:C3G	2.48	0.97
4:2:77:VAL:HG12	2:4:167:LEU:CD2	1.93	0.97
8:B:258:TYR:CB	13:H:49:TYR:OH	2.13	0.96
7:6:173:PHE:CE2	39:6:314:II0:C20	2.48	0.96
18:M:12:LEU:C	18:M:16:PHE:CD2	2.43	0.95
10:d:188:HIS:HA	10:d:293:ARG:HD2	1.47	0.95
19:N:122:VAL:CG2	33:N:303:CLA:HMA2	1.97	0.95
2:0:69:LEU:HD12	2:0:71:PHE:HE2	1.06	0.95
18:m:12:LEU:O	18:m:16:PHE:HD2	1.13	0.95
18:m:12:LEU:C	18:m:16:PHE:CD2	2.43	0.94
20:O:128:THR:HG23	8:b:49:ASP:CB	1.98	0.94
8:B:49:ASP:CB	20:o:128:THR:HG23	1.98	0.94
18:M:12:LEU:O	18:M:16:PHE:HD2	1.13	0.94
7:6:212:LEU:CD1	7:6:213:VAL:HG23	1.95	0.94
13:H:49:TYR:CD2	43:H:101:DGD:O2G	2.16	0.94
10:D:188:HIS:HA	10:D:293:ARG:HD2	1.47	0.93
13:h:49:TYR:HE2	43:h:101:DGD:O2G	1.46	0.93
19:N:121:GLN:CG	33:N:303:CLA:HBA1	1.99	0.93
13:H:49:TYR:CD2	43:H:101:DGD:C2B	2.50	0.93
9:c:343:ARG:HH22	20:o:152:THR:CG2	1.82	0.93
18:m:12:LEU:CB	18:m:16:PHE:HE2	1.82	0.93
18:M:12:LEU:CB	18:M:16:PHE:HE2	1.82	0.93
2:4:212:LEU:HD12	2:4:213:THR:N	1.84	0.93
7:6:173:PHE:HE2	39:6:314:II0:C14	1.81	0.92
10:D:67:LEU:HD23	11:E:50:THR:CG2	2.00	0.92
10:d:67:LEU:HD23	11:e:50:THR:CG2	2.00	0.92
2:0:212:LEU:HD21	39:0:313:II0:O01	1.68	0.92
18:m:12:LEU:C	18:m:16:PHE:HD2	1.76	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TRP:HE3	10:D:179:ARG:HD2	1.15	0.91
7:6:211:LEU:HD13	33:6:313:CLA:HMD1	1.51	0.91
18:M:12:LEU:C	18:M:16:PHE:HD2	1.76	0.91
2:0:214:ASN:OD1	2:0:216:LYS:HG3	1.70	0.91
2:4:61:ALA:HA	19:N:130:GLY:HA3	1.51	0.91
10:d:179:ARG:NH2	10:d:332:ASP:OD1	2.04	0.91
10:D:179:ARG:NH2	10:D:332:ASP:OD1	2.04	0.90
13:H:49:TYR:HE2	43:H:101:DGD:O2G	1.39	0.90
2:0:60:MET:HE1	19:n:137:PRO:HD3	1.52	0.90
19:n:125:ASP:OD1	19:n:126:ALA:N	2.04	0.90
1:a:317:TRP:HE3	10:d:179:ARG:HD2	1.15	0.90
7:6:212:LEU:HD12	7:6:213:VAL:HG23	1.51	0.90
17:L:15:ARG:HD2	41:l:101:SQD:H241	1.54	0.89
7:6:126:MET:SD	40:6:318:IHT:C16	2.60	0.89
1:a:16:ARG:NH2	37:a:411:LHG:O1	2.03	0.89
2:4:169:LEU:HD11	2:4:171:VAL:HG13	1.55	0.89
41:L:101:SQD:H241	17:l:15:ARG:HD2	1.53	0.89
19:N:122:VAL:CG2	33:N:303:CLA:CMA	2.50	0.89
20:O:129:LYS:HG3	8:b:48:SER:CB	2.03	0.89
8:B:48:SER:CB	20:o:129:LYS:HG3	2.03	0.89
1:A:16:ARG:NH2	37:A:411:LHG:O1	2.04	0.88
2:0:69:LEU:CD1	2:0:71:PHE:HE2	1.82	0.88
2:0:69:LEU:HD13	2:0:71:PHE:CZ	2.07	0.88
8:b:258:TYR:CB	13:h:49:TYR:HH	1.85	0.88
5:3:164:LEU:HB2	19:N:119:VAL:HG11	1.54	0.87
2:0:69:LEU:HD12	2:0:71:PHE:CZ	2.08	0.87
2:4:78:LYS:HG2	19:N:137:PRO:HD2	1.57	0.86
2:4:200:GLN:HE22	33:4:309:CLA:C4A	1.87	0.86
20:O:192:PHE:HA	20:O:295:GLN:HE22	1.38	0.86
20:O:129:LYS:HG3	8:b:48:SER:HB3	1.57	0.86
20:o:192:PHE:HA	20:o:295:GLN:HE22	1.39	0.86
8:B:48:SER:HB3	20:o:129:LYS:HG3	1.58	0.86
8:b:258:TYR:HB3	13:h:49:TYR:HH	1.40	0.86
2:0:69:LEU:CB	2:0:71:PHE:CE2	2.58	0.86
2:0:200:GLN:HE22	33:0:310:CLA:C4A	1.87	0.86
20:O:128:THR:HG21	8:b:49:ASP:CG	2.00	0.86
1:A:317:TRP:CH2	10:D:179:ARG:CZ	2.58	0.85
1:a:317:TRP:CH2	10:d:179:ARG:CZ	2.58	0.85
19:N:127:PRO:HG2	19:N:129:ILE:HB	1.59	0.85
6:5:162:ASP:OD1	6:5:162:ASP:O	1.95	0.85
7:6:173:PHE:CE2	39:6:314:II0:C14	2.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:49:ASP:CG	20:o:128:THR:HG21	2.00	0.85
7:p:126:MET:SD	40:p:318:IHT:C20	2.65	0.85
7:6:138:MET:HE1	33:6:305:CLA:HMA1	1.59	0.85
7:p:138:MET:HE1	33:p:305:CLA:HMA1	1.59	0.85
19:N:187:TYR:HB2	19:N:193:ALA:HA	1.59	0.84
19:N:187:TYR:CD1	19:N:190:LEU:HD12	2.13	0.84
7:6:211:LEU:HD13	33:6:313:CLA:CMD	2.07	0.84
8:B:371:VAL:HG12	8:B:377:ILE:HD13	1.59	0.84
2:0:60:MET:CE	19:n:137:PRO:HG3	2.08	0.84
2:4:200:GLN:HE21	33:4:309:CLA:C4D	1.89	0.83
13:H:49:TYR:CE2	43:H:101:DGD:C1B	2.52	0.83
2:0:108:LEU:CD1	39:0:316:II0:C05	2.55	0.83
1:a:16:ARG:HH22	37:a:411:LHG:C2	1.91	0.83
1:a:317:TRP:CZ3	10:d:179:ARG:NH1	2.45	0.83
1:A:16:ARG:HH22	37:A:411:LHG:C2	1.91	0.83
2:0:200:GLN:HE21	33:0:310:CLA:C4D	1.89	0.83
7:6:211:LEU:CD1	33:6:313:CLA:CMD	2.57	0.83
27:y:8:PHE:HA	27:y:11:ILE:HD12	1.60	0.83
2:0:177:ARG:O	19:n:129:ILE:CD1	2.22	0.82
13:h:49:TYR:CZ	43:h:101:DGD:HG32	2.15	0.82
20:O:143:LEU:HD12	20:O:180:VAL:HG12	1.60	0.82
1:A:317:TRP:CZ3	10:D:179:ARG:NH1	2.45	0.82
2:4:108:LEU:HB2	2:4:111:PHE:CD1	2.14	0.82
10:d:176:ALA:O	10:d:179:ARG:HG2	1.79	0.82
6:g:50:PHE:HA	7:p:166:ARG:NE	1.94	0.82
22:t:1:MET:CG	42:t:101:LMG:O10	2.28	0.82
7:6:123:ALA:HB1	7:6:127:LYS:HD2	1.59	0.82
10:D:176:ALA:O	10:D:179:ARG:HG2	1.79	0.82
22:T:1:MET:CG	42:T:101:LMG:O10	2.27	0.82
7:p:126:MET:SD	40:p:318:IHT:C21	2.67	0.82
1:a:317:TRP:CH2	10:d:179:ARG:NH1	2.48	0.81
7:6:212:LEU:HD12	7:6:213:VAL:N	1.95	0.81
2:0:117:THR:HG21	2:0:202:LEU:HD21	1.61	0.81
1:A:317:TRP:CH2	10:D:179:ARG:NH1	2.48	0.81
19:N:122:VAL:CG1	33:N:303:CLA:HHB	2.09	0.81
7:6:224:ILE:H	7:6:224:ILE:HD12	1.45	0.80
2:0:69:LEU:HB2	2:0:71:PHE:CD2	2.17	0.80
33:7:305:CLA:HBB1	33:c:514:CLA:H142	1.62	0.80
7:6:127:LYS:HA	7:6:130:ASN:HD22	1.45	0.79
6:g:200:VAL:HG13	33:g:311:CLA:HED2	1.63	0.79
2:0:166:PRO:HA	19:n:106:TYR:CE2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:213:ASN:OD1	3:7:213:ASN:O	2.01	0.79
7:p:211:LEU:HD13	33:p:313:CLA:HMD1	1.64	0.79
33:1:305:CLA:HBB1	33:C:514:CLA:H142	1.62	0.79
27:Y:8:PHE:HA	27:Y:11:ILE:HD12	1.63	0.79
2:0:49:PHE:CE1	2:0:50:LEU:CG	2.65	0.78
8:B:258:TYR:CB	13:H:49:TYR:HH	1.95	0.78
2:0:108:LEU:HG	2:0:109:PRO:HD2	1.66	0.78
1:A:16:ARG:NH1	37:A:411:LHG:O2	2.16	0.78
19:n:190:LEU:O	19:n:190:LEU:CD2	2.30	0.78
1:a:16:ARG:NH1	37:a:411:LHG:O2	2.16	0.78
7:p:173:PHE:CE2	39:p:314:II0:C14	2.67	0.78
19:n:187:TYR:HB2	19:n:193:ALA:HA	1.66	0.78
13:h:49:TYR:CE2	43:h:101:DGD:C2G	2.67	0.77
13:H:49:TYR:HE2	43:H:101:DGD:HB31	1.40	0.77
19:N:183:VAL:HG13	19:N:188:LYS:HE2	1.64	0.77
2:0:215:PHE:O	2:0:215:PHE:CD2	2.37	0.77
2:0:69:LEU:HD13	2:0:71:PHE:HZ	1.50	0.77
2:0:164:PHE:HE2	39:0:313:II0:C20	1.98	0.77
1:A:317:TRP:CZ3	10:D:179:ARG:HD3	2.05	0.77
6:g:75:VAL:CG2	19:n:183:VAL:CG1	2.45	0.77
4:8:64:VAL:O	4:8:84:ARG:NH2	2.18	0.77
10:d:67:LEU:CD2	11:e:50:THR:CG2	2.62	0.76
33:4:308:CLA:HMC3	33:4:308:CLA:HBC2	1.67	0.76
4:2:64:VAL:O	4:2:84:ARG:NH2	2.18	0.76
33:0:309:CLA:HBC2	33:0:309:CLA:HMC3	1.67	0.76
3:7:165:PRO:O	39:7:313:II0:O02	2.03	0.76
33:A:412:CLA:H102	37:D:408:LHG:H191	1.68	0.76
2:0:60:MET:HE1	19:n:137:PRO:CG	2.15	0.76
18:M:28:GLN:HG2	18:m:31:SER:OG	1.85	0.76
33:a:412:CLA:H102	37:d:408:LHG:H191	1.68	0.75
2:0:111:PHE:CZ	38:0:305:KC2:OBD	2.39	0.75
3:1:165:PRO:O	39:1:313:II0:O02	2.04	0.75
10:D:67:LEU:CD2	11:E:50:THR:CG2	2.62	0.75
6:g:75:VAL:HG21	19:n:183:VAL:HG12	0.77	0.75
2:0:167:LEU:HD22	4:8:77:VAL:HG12	1.68	0.75
2:4:211:GLN:O	2:4:215:PHE:N	2.18	0.75
19:N:122:VAL:HG11	33:N:303:CLA:HMA1	1.68	0.75
9:c:343:ARG:HH22	20:o:152:THR:HG21	1.52	0.75
2:4:100:VAL:HG11	33:4:304:CLA:HAC2	1.67	0.75
5:3:165:GLN:HB3	19:N:119:VAL:CG2	2.16	0.75
7:6:126:MET:HB2	7:6:210:TYR:HE2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:119:HIS:O	6:5:123:VAL:HG13	1.87	0.74
1:A:16:ARG:HH12	37:A:411:LHG:H02	1.34	0.74
5:3:164:LEU:CB	19:N:119:VAL:HG11	2.17	0.74
19:N:173:ALA:HA	19:N:190:LEU:HD21	1.69	0.74
2:0:100:VAL:HG11	33:0:304:CLA:HAC2	1.67	0.74
2:4:169:LEU:HB3	19:N:111:ALA:HB3	1.68	0.74
5:3:72:VAL:O	5:3:92:ARG:NH2	2.21	0.74
9:c:343:ARG:NH2	20:o:152:THR:CG2	2.44	0.74
5:9:72:VAL:O	5:9:92:ARG:NH2	2.21	0.74
19:N:122:VAL:HG21	33:N:303:CLA:HMA1	1.70	0.73
6:g:119:HIS:O	6:g:123:VAL:HG13	1.87	0.73
4:2:77:VAL:CG1	2:4:167:LEU:CD2	2.58	0.73
4:2:78:PHE:CZ	2:4:167:LEU:HD11	2.23	0.73
8:B:192:PRO:HG3	13:H:49:TYR:HD1	1.53	0.73
13:h:49:TYR:HE2	43:h:101:DGD:C3G	1.96	0.73
1:A:64:ARG:NH1	20:O:177:ALA:O	2.22	0.73
6:g:200:VAL:HG11	39:p:301:II0:C19	2.17	0.73
9:c:343:ARG:HH22	20:o:152:THR:HG23	1.46	0.73
2:0:117:THR:CG2	2:0:202:LEU:HD21	2.18	0.73
7:6:196:GLY:O	7:6:199:ALA:HB3	1.89	0.73
33:6:319:CLA:HED2	33:6:319:CLA:C3D	2.19	0.73
6:g:164:LEU:HG	6:g:164:LEU:O	1.89	0.73
7:p:196:GLY:O	7:p:199:ALA:HB3	1.89	0.73
1:a:64:ARG:NH1	20:o:177:ALA:O	2.22	0.73
21:Q:128:ARG:NH1	21:Q:169:ASP:OD1	2.22	0.73
22:T:1:MET:CG	42:T:101:LMG:HC91	2.14	0.73
19:n:139:TYR:OH	19:n:142:PRO:O	2.07	0.73
6:5:164:LEU:O	6:5:164:LEU:HG	1.88	0.72
19:n:183:VAL:HG13	19:n:188:LYS:HE2	1.71	0.72
19:N:139:TYR:OH	19:N:142:PRO:O	2.07	0.72
33:p:319:CLA:C3D	33:p:319:CLA:HED2	2.19	0.72
2:0:117:THR:CG2	2:0:202:LEU:CD2	2.62	0.72
1:a:317:TRP:CZ3	10:d:179:ARG:HD3	2.05	0.72
21:q:128:ARG:NH1	21:q:169:ASP:OD1	2.22	0.72
4:2:84:ARG:NH1	4:2:87:GLU:OE1	2.23	0.72
7:6:211:LEU:CD1	33:6:313:CLA:HMD1	2.20	0.72
33:6:312:CLA:CAA	33:6:319:CLA:C4B	2.68	0.72
2:4:117:THR:HG21	2:4:202:LEU:HD21	1.69	0.71
4:8:84:ARG:NH1	4:8:87:GLU:OE1	2.23	0.71
19:N:120:SER:HB2	33:N:303:CLA:HAA2	1.70	0.71
8:b:258:TYR:HB2	13:h:49:TYR:OH	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:162:ASP:OD1	33:g:307:CLA:CBA	2.37	0.71
7:p:211:LEU:CD1	33:p:313:CLA:CMD	2.68	0.71
2:4:115:LEU:HD11	2:4:201:MET:HB3	1.72	0.71
21:Q:151:SER:OG	21:Q:153:ASP:OD1	2.07	0.71
10:D:188:HIS:CA	10:D:293:ARG:HD2	2.21	0.71
22:t:1:MET:CG	42:t:101:LMG:HC91	2.14	0.71
2:0:60:MET:CE	19:n:137:PRO:HD3	2.21	0.71
8:B:49:ASP:HB2	20:o:128:THR:HG21	1.66	0.71
33:p:312:CLA:CAA	33:p:319:CLA:C4B	2.67	0.71
21:q:151:SER:OG	21:q:153:ASP:OD1	2.07	0.71
10:d:188:HIS:CA	10:d:293:ARG:HD2	2.21	0.71
4:8:153:GLN:OE1	4:8:155:LYS:NZ	2.23	0.70
1:a:16:ARG:HH22	37:a:411:LHG:C1	2.04	0.70
7:6:211:LEU:CD1	33:6:313:CLA:C2D	2.68	0.70
4:2:117:PRO:O	39:2:312:II0:O02	2.08	0.70
4:2:153:GLN:OE1	4:2:155:LYS:NZ	2.23	0.70
1:A:16:ARG:HH22	37:A:411:LHG:C1	2.05	0.70
2:0:47:MET:HE2	2:0:68:PRO:HB3	1.74	0.70
2:0:49:PHE:CD1	2:0:50:LEU:HG	2.26	0.70
19:N:173:ALA:HA	19:N:190:LEU:CD2	2.21	0.70
33:p:312:CLA:CAA	33:p:319:CLA:CHC	2.70	0.70
1:a:16:ARG:HH12	37:a:411:LHG:H02	1.38	0.70
2:0:115:LEU:O	2:0:119:ALA:HB2	1.92	0.70
2:4:185:LYS:NZ	33:N:303:CLA:HMA3	2.06	0.70
7:6:176:LEU:O	7:6:177:ASN:C	2.35	0.70
2:0:185:LYS:NZ	33:0:308:CLA:HMA3	2.06	0.69
7:6:176:LEU:CD2	39:6:314:II0:C18	2.70	0.69
33:6:312:CLA:CAA	33:6:319:CLA:CHC	2.69	0.69
7:6:211:LEU:HD13	33:6:313:CLA:C2D	2.22	0.69
6:5:75:VAL:CG2	19:N:183:VAL:CG1	2.47	0.69
7:6:138:MET:HE1	33:6:305:CLA:CMA	2.22	0.69
1:A:27:ARG:NE	9:C:473:ASP:OD1	2.25	0.69
6:5:67:PHE:CE2	39:5:313:II0:C17	2.76	0.69
7:p:138:MET:HE1	33:p:305:CLA:CMA	2.22	0.69
5:3:165:GLN:HB3	19:N:119:VAL:HG21	1.74	0.69
20:O:128:THR:HG21	8:b:49:ASP:HB2	1.65	0.69
2:0:211:GLN:O	2:0:215:PHE:N	2.24	0.69
7:6:176:LEU:CD2	39:6:314:II0:C06	2.68	0.69
8:b:372:ASP:HB2	8:b:378:ARG:HG3	1.73	0.69
1:a:27:ARG:NE	9:c:473:ASP:OD1	2.25	0.69
3:7:216:ALA:HB1	39:8:313:II0:C17	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:188:HIS:ND1	10:D:293:ARG:CD	2.46	0.69
6:g:67:PHE:CE2	39:g:313:II0:C17	2.76	0.68
6:5:75:VAL:HG21	19:N:183:VAL:HG12	0.74	0.68
37:B:623:LHG:O1	17:L:12:GLU:O	2.11	0.68
2:0:60:MET:CE	19:n:137:PRO:CD	2.67	0.68
7:6:127:LYS:HA	7:6:130:ASN:ND2	2.08	0.68
5:9:143:GLN:OE1	37:9:322:LHG:O2	2.09	0.68
37:b:623:LHG:O1	17:l:12:GLU:O	2.11	0.68
2:4:215:PHE:CD2	2:4:215:PHE:O	2.47	0.68
8:B:348:ASP:OD1	8:B:352:LYS:N	2.27	0.68
6:5:75:VAL:HA	19:N:189:SER:HB3	1.76	0.68
7:6:82:LEU:HD23	7:6:83:ASP:N	2.08	0.68
8:b:348:ASP:OD1	8:b:352:LYS:N	2.27	0.68
8:B:311:PHE:O	8:B:317:ASN:ND2	2.27	0.68
7:p:82:LEU:HD23	7:p:83:ASP:N	2.08	0.68
7:p:211:LEU:CD1	33:p:313:CLA:HMD1	2.25	0.67
10:d:188:HIS:ND1	10:d:293:ARG:CD	2.46	0.67
18:m:12:LEU:O	18:m:16:PHE:CE2	2.41	0.67
7:6:212:LEU:HD12	7:6:212:LEU:C	2.20	0.67
13:H:49:TYR:HD2	43:H:101:DGD:C2B	1.95	0.67
8:b:311:PHE:O	8:b:317:ASN:ND2	2.27	0.67
3:7:216:ALA:CB	39:8:313:II0:C17	2.73	0.67
8:B:384:ARG:NH2	23:U:117:ASN:O	2.28	0.67
18:M:12:LEU:O	18:M:16:PHE:CE2	2.41	0.67
2:0:60:MET:CE	19:n:137:PRO:CG	2.73	0.67
5:3:143:GLN:OE1	37:3:322:LHG:O2	2.09	0.67
8:b:384:ARG:NH2	23:u:117:ASN:O	2.28	0.67
33:A:412:CLA:H42	10:D:208:LEU:HD23	1.76	0.66
7:6:126:MET:HB2	7:6:210:TYR:CE2	2.30	0.66
7:p:127:LYS:HA	7:p:130:ASN:HD22	1.60	0.66
24:V:67:HIS:ND1	24:V:71:ILE:O	2.29	0.66
4:2:78:PHE:HZ	2:4:167:LEU:HD11	1.59	0.66
33:a:412:CLA:H42	10:d:208:LEU:HD23	1.76	0.66
19:n:192:GLY:HA3	19:n:195:ASP:HB3	1.77	0.66
2:4:59:SER:HB2	19:N:135:TYR:CG	2.30	0.66
5:3:92:ARG:NH1	5:3:95:GLU:OE1	2.29	0.65
7:6:126:MET:SD	40:6:318:IHT:C11	2.84	0.65
20:o:218:THR:OG1	20:o:269:THR:OG1	2.14	0.65
24:v:67:HIS:ND1	24:v:71:ILE:O	2.29	0.65
5:9:92:ARG:NH1	5:9:95:GLU:OE1	2.29	0.65
20:O:218:THR:OG1	20:O:269:THR:OG1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:327:ALA:O	8:B:444:ARG:NH1	2.30	0.65
7:p:211:LEU:HD13	33:p:313:CLA:CMD	2.25	0.65
2:4:61:ALA:CA	19:N:130:GLY:HA3	2.26	0.65
8:B:49:ASP:HB2	20:o:128:THR:HG22	1.74	0.65
3:1:122:VAL:HG11	3:1:127:LEU:HD21	1.78	0.65
20:O:128:THR:HG22	8:b:49:ASP:HB2	1.74	0.65
1:A:137:LEU:HB2	1:A:139:MET:HG2	1.79	0.65
8:B:389:LYS:N	10:D:343:GLU:OE2	2.30	0.65
8:b:327:ALA:O	8:b:444:ARG:NH1	2.30	0.65
1:A:27:ARG:HD3	9:C:473:ASP:OD1	1.96	0.65
2:0:68:PRO:HD2	39:0:314:II0:O02	1.97	0.65
8:B:137:LYS:NZ	13:H:17:GLU:OE2	2.29	0.65
19:N:121:GLN:CG	33:N:303:CLA:CBA	2.68	0.64
8:b:389:LYS:N	10:d:343:GLU:OE2	2.30	0.64
6:g:75:VAL:HG21	19:n:183:VAL:HG11	1.72	0.64
7:p:173:PHE:CE2	39:p:314:II0:C20	2.81	0.64
1:A:317:TRP:HZ3	10:D:179:ARG:NH2	1.90	0.64
3:7:122:VAL:HG11	3:7:127:LEU:HD21	1.78	0.64
9:C:345:PRO:O	20:O:147:ALA:HB3	1.97	0.64
2:4:168:ASN:OD1	33:4:307:CLA:H2	1.98	0.64
8:b:57:ARG:NH2	8:b:335:GLY:O	2.31	0.64
1:a:317:TRP:HZ3	10:d:179:ARG:NH2	1.90	0.64
2:4:48:PRO:HG2	33:4:301:CLA:HMB3	1.78	0.64
37:b:623:LHG:O4	37:d:408:LHG:O1	2.14	0.64
10:d:351:LEU:HD12	10:d:351:LEU:O	1.97	0.64
7:p:126:MET:HE1	40:p:318:IHT:C20	2.28	0.64
1:a:27:ARG:HD3	9:c:473:ASP:OD1	1.96	0.64
20:O:130:ARG:NH2	8:b:52:LEU:HD12	2.13	0.64
6:g:50:PHE:HA	7:p:166:ARG:CZ	2.28	0.64
7:p:166:ARG:CD	7:p:170:ASP:O	2.43	0.64
8:B:57:ARG:NH2	8:B:335:GLY:O	2.31	0.64
8:b:137:LYS:NZ	13:h:17:GLU:OE2	2.29	0.64
10:d:176:ALA:O	10:d:179:ARG:CG	2.45	0.64
7:6:211:LEU:HD11	33:6:313:CLA:CMD	2.28	0.63
7:6:212:LEU:CD2	33:6:312:CLA:HMD2	2.28	0.63
20:O:128:THR:HG21	8:b:49:ASP:CB	2.17	0.63
3:1:216:ALA:HB1	39:2:313:II0:C17	2.29	0.63
8:B:52:LEU:HD12	20:o:130:ARG:NH2	2.12	0.63
12:F:17:TRP:HD1	44:F:101:HEM:HBA1	1.63	0.63
18:M:12:LEU:C	18:M:16:PHE:CE2	2.76	0.63
18:M:31:SER:OG	18:m:32:ARG:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:173:PHE:HB3	33:6:309:CLA:CAD	2.28	0.63
18:m:12:LEU:C	18:m:16:PHE:CE2	2.76	0.63
1:a:27:ARG:CD	9:c:473:ASP:OD1	2.46	0.63
33:7:305:CLA:HBB1	33:c:514:CLA:C14	2.28	0.63
10:D:176:ALA:O	10:D:179:ARG:CG	2.45	0.63
7:p:113:PHE:HE2	33:p:305:CLA:H11	1.61	0.63
7:6:173:PHE:HB3	33:6:309:CLA:OBD	1.98	0.63
7:p:174:ASP:CG	7:p:177:ASN:HA	2.24	0.63
1:A:27:ARG:CD	9:C:473:ASP:OD1	2.46	0.63
2:4:56:LEU:HD11	2:4:67:ASP:HB2	1.80	0.63
6:5:197:GLN:NE2	33:5:310:CLA:HMA3	2.14	0.63
37:B:623:LHG:O4	37:D:408:LHG:O1	2.14	0.63
1:A:25:ASP:OD2	9:C:470:ARG:NH2	2.32	0.62
2:0:218:LEU:HD23	33:g:304:CLA:HED3	1.80	0.62
3:1:216:ALA:CB	39:2:313:II0:C17	2.77	0.62
33:1:305:CLA:HBB1	33:C:514:CLA:C14	2.28	0.62
8:B:142:HIS:ND1	33:B:611:CLA:OBD	2.31	0.62
1:a:183:MET:HE3	33:a:412:CLA:HHD	1.81	0.62
1:A:183:MET:HE3	33:A:412:CLA:HHD	1.81	0.62
5:9:57:ALA:HB2	5:9:75:VAL:O	1.99	0.62
7:6:113:PHE:HE2	33:6:305:CLA:H11	1.62	0.62
2:4:142:THR:HB	2:4:162:LEU:HB3	1.80	0.62
42:b:622:LMG:O5	42:b:622:LMG:O4	2.12	0.62
6:g:197:GLN:NE2	33:g:310:CLA:HMA3	2.14	0.62
1:a:25:ASP:OD2	9:c:470:ARG:NH2	2.32	0.62
33:a:405:CLA:H41	33:a:412:CLA:HBB1	1.82	0.62
8:b:142:HIS:ND1	33:b:611:CLA:OBD	2.31	0.62
7:p:225:PRO:HG3	33:p:319:CLA:HMD3	1.81	0.62
3:1:184:LYS:NZ	37:1:317:LHG:O5	2.32	0.62
19:N:122:VAL:HG13	33:N:303:CLA:H3A	1.81	0.62
1:a:317:TRP:CD2	10:d:179:ARG:HD3	2.34	0.62
33:A:405:CLA:H41	33:A:412:CLA:HBB1	1.82	0.62
3:7:184:LYS:NZ	37:7:317:LHG:O5	2.32	0.62
9:C:367:GLU:OE2	9:C:370:ARG:NH1	2.32	0.62
20:O:117:GLU:HG3	20:O:149:TYR:HE1	1.65	0.62
8:b:28:ALA:O	8:b:104:SER:OG	2.13	0.62
1:A:317:TRP:CD2	10:D:179:ARG:HD3	2.34	0.62
7:6:42:LYS:HB3	7:6:45:ILE:HB	1.82	0.62
10:d:300:GLN:HG2	18:m:1:MET:HE1	1.81	0.62
7:p:42:LYS:HB3	7:p:45:ILE:HB	1.82	0.62
13:H:49:TYR:CE2	43:H:101:DGD:C2B	2.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:176:LEU:HD21	19:n:134:LYS:HG2	1.82	0.61
37:9:302:LHG:O1	37:9:302:LHG:O3	2.09	0.61
20:O:192:PHE:HA	20:O:295:GLN:NE2	2.11	0.61
7:6:120:PHE:CE1	7:6:132:ALA:HA	2.35	0.61
8:b:192:PRO:HG3	13:h:49:TYR:HD1	1.64	0.61
19:n:192:GLY:CA	19:n:195:ASP:HB3	2.30	0.61
37:3:302:LHG:O1	37:3:302:LHG:O3	2.09	0.61
2:4:62:GLY:HA3	2:4:184:LEU:CD2	2.31	0.61
2:4:69:LEU:HD12	2:4:71:PHE:CE2	2.34	0.61
11:e:45:TYR:CD1	11:e:50:THR:HG23	2.35	0.61
1:A:238:LYS:NZ	19:n:241:GLY:O	2.33	0.61
2:0:48:PRO:HG2	33:0:301:CLA:HMB3	1.82	0.61
2:0:69:LEU:CD1	2:0:71:PHE:HZ	2.06	0.61
7:6:212:LEU:HD12	7:6:213:VAL:CG2	2.26	0.61
37:B:623:LHG:H101	37:B:623:LHG:H242	1.82	0.61
37:b:623:LHG:H242	37:b:623:LHG:H101	1.82	0.61
9:c:250:TRP:O	9:c:254:THR:OG1	2.11	0.61
9:c:367:GLU:OE2	9:c:370:ARG:NH1	2.32	0.61
2:0:164:PHE:CE2	39:0:313:II0:C14	2.83	0.61
2:0:167:LEU:HA	19:n:106:TYR:CE1	2.35	0.61
8:B:28:ALA:O	8:B:104:SER:OG	2.13	0.61
9:C:321:ASP:OD2	9:C:340:TYR:OH	2.16	0.61
1:a:238:LYS:NZ	19:N:241:GLY:O	2.33	0.61
11:E:45:TYR:CD1	11:E:50:THR:HG23	2.35	0.61
2:4:169:LEU:CD1	2:4:171:VAL:HG13	2.30	0.61
42:B:622:LMG:O4	42:B:622:LMG:O5	2.12	0.61
15:j:6:ARG:NE	15:j:6:ARG:O	2.33	0.61
33:5:305:CLA:HBD	33:5:317:CLA:CMD	2.30	0.61
15:J:6:ARG:O	15:J:6:ARG:NE	2.33	0.61
9:C:52:ALA:HB2	33:C:512:CLA:HMA2	1.81	0.60
2:0:56:LEU:CD1	33:0:302:CLA:HBD	2.31	0.60
20:O:123:ILE:HG12	20:O:141:THR:HG21	1.82	0.60
7:p:211:LEU:HD11	33:p:313:CLA:CMD	2.31	0.60
2:0:56:LEU:HD13	33:0:302:CLA:HBD	1.81	0.60
8:B:49:ASP:CB	20:o:128:THR:HG21	2.17	0.60
33:c:505:CLA:C14	42:c:520:LMG:H422	2.31	0.60
33:g:305:CLA:HBD	33:g:317:CLA:CMD	2.30	0.60
20:o:192:PHE:HA	20:o:295:GLN:NE2	2.11	0.60
2:4:62:GLY:HA3	2:4:184:LEU:HD23	1.82	0.60
6:5:99:PHE:CE1	6:5:115:PRO:HB2	2.37	0.60
7:p:49:LEU:O	7:p:59:ARG:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:C:505:CLA:C14	42:C:520:LMG:H422	2.32	0.60
7:p:126:MET:CE	40:p:318:IHT:C20	2.80	0.60
23:u:47:ASN:ND2	23:u:104:LEU:O	2.35	0.60
1:A:259:ILE:HG22	1:A:260:PHE:CD2	2.37	0.60
2:4:212:LEU:HD12	2:4:212:LEU:C	2.26	0.60
11:e:20:TYR:O	11:e:24:HIS:ND1	2.34	0.60
7:p:120:PHE:CE1	7:p:132:ALA:HA	2.37	0.60
1:a:259:ILE:HG22	1:a:260:PHE:CD2	2.37	0.60
2:0:166:PRO:O	19:n:106:TYR:CG	2.54	0.60
2:4:166:PRO:HD2	39:4:312:II0:C06	2.32	0.60
6:g:99:PHE:CE1	6:g:115:PRO:HB2	2.37	0.60
7:p:112:LYS:HE3	7:p:122:GLY:CA	2.24	0.60
2:4:176:LEU:HD21	19:N:134:LYS:HG3	1.84	0.60
37:B:623:LHG:H261	17:L:21:GLY:HA2	1.82	0.60
6:g:75:VAL:HA	19:n:189:SER:HB3	1.84	0.60
19:N:124:GLU:HA	19:N:127:PRO:HG3	1.83	0.59
37:b:623:LHG:H261	17:l:21:GLY:HA2	1.82	0.59
7:p:211:LEU:CD1	33:p:313:CLA:C2D	2.80	0.59
2:4:78:LYS:HD3	19:N:136:ALA:HB1	1.83	0.59
23:U:47:ASN:ND2	23:U:104:LEU:O	2.35	0.59
7:p:95:GLY:O	7:p:99:MET:HE2	2.02	0.59
22:t:1:MET:HG2	42:t:101:LMG:HC92	1.83	0.59
2:4:69:LEU:CD1	2:4:71:PHE:CE2	2.85	0.59
7:6:112:LYS:HB3	7:6:117:GLU:HB2	1.84	0.59
24:V:72:THR:OG1	24:V:78:LEU:O	2.15	0.59
10:D:351:LEU:HD12	10:D:351:LEU:O	2.01	0.59
11:E:20:TYR:O	11:E:24:HIS:ND1	2.34	0.59
7:p:126:MET:HE1	39:p:315:II0:C17	2.32	0.59
6:5:203:GLN:O	6:5:204:THR:C	2.46	0.59
10:D:176:ALA:C	10:D:179:ARG:HG2	2.27	0.59
6:g:197:GLN:NE2	33:g:310:CLA:NA	2.51	0.59
2:0:200:GLN:NE2	33:0:310:CLA:C1A	2.65	0.59
2:4:59:SER:HB3	19:N:132:TYR:HD2	1.68	0.59
2:4:211:GLN:NE2	2:4:215:PHE:HA	2.18	0.59
6:5:197:GLN:NE2	33:5:310:CLA:NA	2.51	0.59
2:0:215:PHE:O	2:0:215:PHE:CG	2.54	0.59
2:4:200:GLN:NE2	33:4:309:CLA:C1A	2.65	0.59
19:n:174:MET:HA	19:n:174:MET:HE3	1.85	0.59
13:H:49:TYR:CD2	43:H:101:DGD:HB31	2.30	0.59
20:O:128:THR:CG2	8:b:49:ASP:CG	2.70	0.59
22:T:1:MET:HG2	42:T:101:LMG:HC92	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:145:VAL:O	1:a:148:THR:OG1	2.20	0.59
42:D:410:LMG:HO4	42:D:410:LMG:HO5	1.48	0.59
19:N:192:GLY:HA3	19:N:195:ASP:HB3	1.85	0.59
19:N:202:GLU:HG2	19:N:203:GLU:N	2.16	0.59
9:c:52:ALA:HB2	33:c:512:CLA:HMA1	1.85	0.59
2:4:166:PRO:HD2	39:4:312:II0:O02	2.03	0.59
7:6:95:GLY:O	7:6:99:MET:HE2	2.02	0.59
7:p:82:LEU:HD22	7:p:87:ALA:HB2	1.84	0.59
2:0:62:GLY:HA3	2:0:184:LEU:HD22	1.85	0.58
2:0:164:PHE:CE2	39:0:313:II0:C20	2.83	0.58
5:3:164:LEU:CB	19:N:119:VAL:CG1	2.81	0.58
2:4:117:THR:CG2	2:4:202:LEU:HD21	2.31	0.58
4:8:200:GLN:OE1	4:8:211:GLN:NE2	2.36	0.58
8:b:369:ILE:HD12	8:b:377:ILE:HD11	1.83	0.58
7:p:173:PHE:HE2	39:p:314:II0:C14	2.16	0.58
33:p:308:CLA:HBC3	39:p:317:II0:C15	2.33	0.58
10:d:176:ALA:C	10:d:179:ARG:HG2	2.27	0.58
7:6:176:LEU:O	7:6:178:CYS:N	2.37	0.58
33:6:308:CLA:HBC3	39:6:317:II0:C15	2.33	0.58
10:d:48:PHE:O	10:d:52:THR:OG1	2.18	0.58
10:d:176:ALA:HA	10:d:179:ARG:HG2	1.85	0.58
6:g:113:MET:SD	6:g:121:TYR:HB2	2.43	0.58
1:a:140:ARG:HH22	37:d:401:LHG:HC41	1.68	0.58
1:a:183:MET:HE3	33:a:412:CLA:HAC1	1.85	0.58
2:4:96:LEU:O	2:4:100:VAL:HG12	2.02	0.58
7:6:82:LEU:HD22	7:6:87:ALA:HB2	1.84	0.58
18:M:26:TYR:O	18:M:30:GLU:HG2	2.04	0.58
19:N:174:MET:HA	19:N:174:MET:HE3	1.85	0.58
9:c:39:ASN:ND2	33:c:511:CLA:O1A	2.35	0.58
43:c:521:DGD:HA62	10:d:73:PHE:CZ	2.38	0.58
2:0:111:PHE:HA	2:0:123:VAL:HG22	1.85	0.58
8:B:49:ASP:CG	20:o:128:THR:CG2	2.70	0.58
7:p:174:ASP:O	7:p:177:ASN:OD1	2.22	0.58
10:D:176:ALA:HA	10:D:179:ARG:HG2	1.85	0.58
6:g:203:GLN:O	6:g:204:THR:C	2.47	0.58
1:A:183:MET:HE3	33:A:412:CLA:HAC1	1.85	0.58
2:0:96:LEU:O	2:0:100:VAL:HG12	2.03	0.58
4:2:200:GLN:OE1	4:2:211:GLN:NE2	2.36	0.58
33:B:610:CLA:OBD	13:H:27:THR:OG1	2.22	0.58
10:D:245:MET:HE3	36:D:407:PL9:H523	1.85	0.58
7:p:212:LEU:HD23	7:p:213:VAL:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:51:LEU:HD21	7:p:155:PRO:HB2	1.86	0.58
2:0:164:PHE:CE2	39:0:313:II0:C12	2.86	0.58
11:E:63:GLN:OE1	11:E:63:GLN:N	2.37	0.58
11:e:63:GLN:OE1	11:e:63:GLN:N	2.37	0.58
2:4:87:HIS:CD2	33:4:306:CLA:HMD2	2.39	0.58
7:p:213:VAL:HG11	7:p:226:ASN:HB3	1.85	0.58
2:0:87:HIS:CD2	33:0:306:CLA:HMD2	2.39	0.57
2:4:69:LEU:HD12	2:4:71:PHE:HE2	1.68	0.57
43:C:521:DGD:HA62	10:D:73:PHE:CZ	2.38	0.57
23:U:42:ASP:O	23:U:56:ARG:NH2	2.37	0.57
13:h:56:GLU:OE2	13:h:56:GLU:N	2.37	0.57
24:v:72:THR:OG1	24:v:78:LEU:O	2.16	0.57
2:4:61:ALA:CA	19:N:130:GLY:HA2	2.11	0.57
2:4:200:GLN:OE1	39:4:312:II0:C11	2.52	0.57
8:B:451:TYR:OH	33:B:605:CLA:O2D	2.23	0.57
19:N:183:VAL:HG13	19:N:188:LYS:CE	2.32	0.57
18:m:26:TYR:O	18:m:30:GLU:HG2	2.03	0.57
2:0:200:GLN:OE1	39:0:313:II0:C11	2.52	0.57
2:4:200:GLN:NE2	33:4:309:CLA:ND	2.45	0.57
9:C:39:ASN:ND2	33:C:511:CLA:O1A	2.35	0.57
11:E:37:LEU:O	11:E:41:THR:OG1	2.10	0.57
7:p:132:ALA:HB3	7:p:138:MET:HE2	1.85	0.57
8:b:451:TYR:OH	33:b:605:CLA:O2D	2.23	0.57
1:A:165:GLN:NE2	1:A:294:ALA:O	2.37	0.57
11:E:27:THR:HB	44:F:101:HEM:HAB	1.86	0.57
33:b:610:CLA:OBD	13:h:27:THR:OG1	2.21	0.57
13:h:49:TYR:HE2	43:h:101:DGD:C2G	2.11	0.57
2:4:44:SER:OG	2:4:47:MET:O	2.22	0.57
13:H:56:GLU:N	13:H:56:GLU:OE2	2.37	0.57
7:p:112:LYS:HB3	7:p:117:GLU:HB2	1.85	0.57
2:4:203:LEU:HD23	2:4:204:THR:CG2	2.20	0.57
10:d:245:MET:HE3	36:d:407:PL9:H523	1.85	0.57
7:6:129:HIS:HA	7:6:138:MET:HE3	1.86	0.57
19:n:126:ALA:HB3	19:n:127:PRO:HD3	1.86	0.57
1:A:141:PRO:O	10:D:219:ASN:ND2	2.38	0.57
2:4:59:SER:HA	19:N:131:LEU:O	2.05	0.57
2:4:169:LEU:HD13	19:N:106:TYR:OH	2.05	0.57
5:9:56:GLN:HB2	33:9:306:CLA:CMA	2.35	0.56
6:g:89:GLY:HA3	6:g:184:ALA:HB1	1.86	0.56
13:h:49:TYR:CE2	43:h:101:DGD:HB31	2.40	0.56
7:p:49:LEU:HA	7:p:59:ARG:CZ	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:94:ALA:O	5:3:98:HIS:ND1	2.37	0.56
2:4:211:GLN:HE22	2:4:215:PHE:HA	1.70	0.56
7:6:99:MET:HE3	33:6:309:CLA:HMC3	1.87	0.56
7:6:112:LYS:HE2	7:6:122:GLY:CA	2.21	0.56
7:6:157:ILE:HD12	33:6:308:CLA:HMA2	1.87	0.56
7:6:173:PHE:CG	7:6:173:PHE:O	2.57	0.56
8:B:371:VAL:HG12	8:B:377:ILE:CD1	2.30	0.56
8:B:490:VAL:HG23	10:D:135:VAL:HG13	1.87	0.56
9:c:48:LYS:NZ	9:c:133:SER:O	2.36	0.56
19:n:124:GLU:O	19:n:127:PRO:HD2	2.05	0.56
7:p:201:ILE:HG21	39:p:316:II0:C31	2.35	0.56
1:a:165:GLN:NE2	1:a:294:ALA:O	2.37	0.56
2:4:60:MET:HG3	33:4:302:CLA:HED1	1.87	0.56
2:4:100:VAL:HG11	33:4:304:CLA:CAC	2.35	0.56
6:5:89:GLY:HA3	6:5:184:ALA:HB1	1.86	0.56
8:b:371:VAL:HB	8:b:375:GLY:HA2	1.87	0.56
2:0:76:ASP:O	2:0:80:LEU:HG	2.05	0.56
2:0:100:VAL:HG11	33:0:304:CLA:CAC	2.35	0.56
7:6:173:PHE:O	7:6:175:PRO:HD3	2.05	0.56
9:c:405:ASN:HB3	43:c:521:DGD:HG2	1.87	0.56
2:0:140:ILE:HD11	25:w:68:PHE:HE2	1.71	0.56
13:H:49:TYR:CD2	43:H:101:DGD:HB22	2.40	0.56
8:b:490:VAL:HG23	10:d:135:VAL:HG13	1.87	0.56
2:0:200:GLN:NE2	33:0:310:CLA:ND	2.45	0.56
7:6:201:ILE:HG21	39:6:316:II0:C31	2.35	0.56
33:B:618:CLA:HHC	33:B:618:CLA:HBB1	1.88	0.56
9:C:297:TYR:O	9:C:423:ARG:NH2	2.37	0.56
44:f:101:HEM:HMC2	44:f:101:HEM:HBC2	1.87	0.56
7:p:99:MET:HE3	33:p:309:CLA:HMC3	1.87	0.56
2:4:140:ILE:HD11	25:W:68:PHE:HE2	1.71	0.56
7:p:175:PRO:HD2	39:p:314:II0:C12	2.36	0.56
6:5:162:ASP:OD1	6:5:162:ASP:C	2.46	0.56
5:9:94:ALA:O	5:9:98:HIS:ND1	2.37	0.56
2:0:169:LEU:HB3	19:n:111:ALA:HB3	1.89	0.55
7:6:132:ALA:HB3	7:6:138:MET:HE2	1.87	0.55
7:6:176:LEU:HD23	39:6:314:II0:C04	2.36	0.55
13:H:49:TYR:HE2	43:H:101:DGD:C3B	2.02	0.55
19:N:187:TYR:HD1	19:N:190:LEU:HD12	1.67	0.55
9:c:297:TYR:O	9:c:423:ARG:NH2	2.37	0.55
7:p:42:LYS:HB2	7:p:46:ILE:HG22	1.87	0.55
1:A:317:TRP:CD2	10:D:179:ARG:CD	2.76	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:e:37:LEU:O	11:e:41:THR:OG1	2.10	0.55
1:a:317:TRP:CD2	10:d:179:ARG:CD	2.76	0.55
7:6:225:PRO:HG3	33:6:319:CLA:HMD3	1.87	0.55
5:9:59:PRO:HD3	33:9:306:CLA:C4B	2.36	0.55
9:C:405:ASN:HB3	43:C:521:DGD:HG2	1.87	0.55
5:9:56:GLN:HB2	33:9:306:CLA:HMA1	1.89	0.55
6:g:199:TRP:HE3	33:g:311:CLA:HED3	1.70	0.55
1:a:141:PRO:O	10:d:219:ASN:ND2	2.40	0.55
5:3:56:GLN:O	5:3:58:ILE:N	2.40	0.55
2:4:117:THR:OG1	2:4:201:MET:HE3	2.07	0.55
2:4:169:LEU:HD12	2:4:170:SER:H	1.72	0.55
8:B:155:ALA:O	8:B:159:THR:OG1	2.25	0.55
8:b:26:HIS:O	8:b:30:VAL:HG23	2.07	0.55
8:B:48:SER:HB3	20:o:129:LYS:CG	2.34	0.55
8:b:155:ALA:O	8:b:159:THR:OG1	2.25	0.55
33:g:305:CLA:HBD	33:g:317:CLA:HMD3	1.89	0.55
19:n:181:THR:O	19:n:185:SER:HB3	2.07	0.55
33:5:305:CLA:HBD	33:5:317:CLA:HMD3	1.89	0.55
8:B:26:HIS:O	8:B:30:VAL:HG23	2.07	0.55
9:C:48:LYS:NZ	9:C:133:SER:O	2.36	0.55
19:n:135:TYR:HE1	19:n:137:PRO:HB3	1.72	0.55
7:6:100:LEU:HD13	33:6:305:CLA:H92	1.87	0.55
9:c:321:ASP:OD2	9:c:340:TYR:OH	2.16	0.55
7:p:100:LEU:HD13	33:p:305:CLA:H92	1.88	0.55
2:0:111:PHE:HZ	38:0:305:KC2:CAD	2.19	0.55
7:6:154:VAL:HB	7:6:155:PRO:HD3	1.87	0.55
9:C:119:LEU:O	9:C:122:SER:OG	2.19	0.55
9:c:331:ALA:O	20:o:175:TYR:OH	2.25	0.55
6:g:93:MET:HE2	33:g:307:CLA:HMC3	1.89	0.55
33:a:412:CLA:HBB1	33:a:412:CLA:HHC	1.89	0.54
1:A:77:ILE:HD13	17:L:30:VAL:HG13	1.89	0.54
2:0:97:GLY:O	2:0:98:PHE:C	2.49	0.54
33:0:304:CLA:CGA	33:0:304:CLA:C1A	2.86	0.54
2:4:97:GLY:O	2:4:98:PHE:C	2.49	0.54
33:a:412:CLA:HED2	10:d:197:MET:SD	2.47	0.54
33:4:304:CLA:C1A	33:4:304:CLA:CGA	2.86	0.54
8:B:272:ARG:NH1	8:B:276:ASP:OD2	2.41	0.54
9:C:331:ALA:O	20:O:175:TYR:OH	2.25	0.54
19:N:173:ALA:CA	19:N:190:LEU:HD21	2.38	0.54
19:N:196:LYS:HG2	19:N:197:THR:HG23	1.88	0.54
7:6:215:ARG:N	7:6:231:LEU:HD12	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:458:PHE:HB3	33:B:605:CLA:HBC2	1.90	0.54
8:b:272:ARG:NH1	8:b:276:ASP:OD2	2.41	0.54
2:0:212:LEU:O	2:0:215:PHE:HB2	2.08	0.54
33:0:306:CLA:H92	33:0:306:CLA:H51	1.90	0.54
19:n:202:GLU:HG2	19:n:203:GLU:N	2.21	0.54
33:4:306:CLA:H51	33:4:306:CLA:H92	1.90	0.54
19:N:181:THR:O	19:N:185:SER:HB3	2.07	0.54
20:O:129:LYS:CG	8:b:48:SER:HB3	2.34	0.54
1:a:77:ILE:HD13	17:l:30:VAL:HG13	1.89	0.54
33:A:412:CLA:HBB1	33:A:412:CLA:HHC	1.89	0.54
2:4:59:SER:HB2	19:N:135:TYR:CD1	2.42	0.54
2:4:98:PHE:HD2	2:4:197:MET:HB3	1.73	0.54
6:5:93:MET:HE2	33:5:307:CLA:HMC3	1.89	0.54
4:8:60:ASP:OD1	4:8:61:GLY:N	2.41	0.54
8:b:458:PHE:HB3	33:b:605:CLA:HBC2	1.90	0.54
9:c:343:ARG:HH21	20:o:152:THR:HG23	1.65	0.54
6:g:99:PHE:CE2	6:g:194:PHE:HB3	2.42	0.54
6:g:197:GLN:HE22	33:g:310:CLA:HMA3	1.71	0.54
7:p:129:HIS:HA	7:p:138:MET:HE3	1.90	0.54
2:0:98:PHE:HD2	2:0:197:MET:HB3	1.73	0.54
4:2:60:ASP:OD1	4:2:61:GLY:N	2.41	0.54
7:6:231:LEU:HD13	7:6:231:LEU:C	2.32	0.54
10:d:263:LYS:O	10:d:267:HIS:ND1	2.41	0.54
2:0:68:PRO:HG2	39:0:314:II0:C06	2.38	0.54
6:5:99:PHE:CE2	6:5:194:PHE:HB3	2.42	0.54
7:6:119:GLU:OE2	39:6:317:II0:C06	2.56	0.54
10:D:263:LYS:O	10:D:267:HIS:ND1	2.41	0.54
20:o:217:LYS:NZ	20:o:270:ASP:OD1	2.37	0.54
33:A:412:CLA:HED2	10:D:197:MET:SD	2.47	0.54
2:4:61:ALA:CA	19:N:130:GLY:CA	2.61	0.54
1:A:134:SER:HA	1:A:139:MET:HG3	1.89	0.54
5:3:164:LEU:HB3	19:N:119:VAL:CG1	2.38	0.54
33:5:307:CLA:H2	39:5:312:II0:C15	2.37	0.54
7:6:128:LEU:HG	33:6:305:CLA:HMA2	1.89	0.54
9:c:119:LEU:O	9:c:122:SER:OG	2.19	0.54
33:g:307:CLA:H2	39:g:312:II0:C15	2.38	0.54
6:5:162:ASP:O	6:5:162:ASP:CG	2.50	0.53
18:m:12:LEU:CA	18:m:16:PHE:CE2	2.91	0.53
18:m:12:LEU:CA	18:m:16:PHE:HE2	2.22	0.53
7:p:173:PHE:HB3	33:p:309:CLA:CAD	2.38	0.53
2:0:166:PRO:HA	19:n:106:TYR:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:166:PRO:HD2	39:4:312:II0:C08	2.38	0.53
3:7:216:ALA:HB2	39:8:313:II0:C17	2.38	0.53
42:D:410:LMG:O5	42:D:410:LMG:O4	2.12	0.53
18:M:12:LEU:CA	18:M:16:PHE:HE2	2.22	0.53
6:g:194:PHE:CD1	6:g:205:VAL:HG11	2.44	0.53
6:5:197:GLN:HE22	33:5:310:CLA:HMA3	1.71	0.53
7:6:230:PRO:O	7:6:231:LEU:C	2.51	0.53
6:g:196:HIS:HA	6:g:199:TRP:CE3	2.43	0.53
7:p:146:GLY:HA2	33:p:308:CLA:CAB	2.38	0.53
2:4:108:LEU:HD12	2:4:111:PHE:CZ	2.44	0.53
18:M:12:LEU:CA	18:M:16:PHE:CE2	2.92	0.53
7:p:181:ASN:HB2	7:p:184:THR:HG23	1.89	0.53
7:p:211:LEU:HD13	33:p:313:CLA:C2D	2.39	0.53
7:6:112:LYS:CE	7:6:122:GLY:HA2	2.23	0.53
18:M:9:LEU:HD12	18:m:9:LEU:HD12	1.44	0.53
1:A:103:ASP:HB3	20:O:144:MET:HE1	1.91	0.53
1:A:185:VAL:HG12	45:A:511:HOH:O	2.09	0.53
7:6:146:GLY:HA2	33:6:308:CLA:CAB	2.38	0.53
8:B:48:SER:HB2	20:o:129:LYS:HG3	1.87	0.53
19:N:192:GLY:CA	19:N:195:ASP:HB3	2.39	0.53
1:a:104:GLU:HB2	20:o:144:MET:O	2.09	0.53
2:0:211:GLN:HG3	2:0:212:LEU:HD23	1.91	0.53
7:p:173:PHE:CD2	39:p:314:II0:C20	2.92	0.53
7:p:215:ARG:CG	7:p:219:GLU:CD	2.69	0.53
1:a:185:VAL:HG12	45:a:511:HOH:O	2.09	0.53
1:a:260:PHE:CZ	1:a:263:ALA:HB2	2.44	0.53
2:0:69:LEU:CG	2:0:71:PHE:CE2	2.92	0.53
2:4:147:LEU:CD1	25:W:69:ILE:HG23	2.39	0.53
7:6:123:ALA:CB	7:6:127:LYS:HD2	2.35	0.53
1:A:260:PHE:CZ	1:A:263:ALA:HB2	2.44	0.52
7:6:212:LEU:HD23	33:6:312:CLA:HMD2	1.91	0.52
1:A:132:GLU:O	1:A:136:ARG:HG2	2.09	0.52
2:0:111:PHE:CZ	38:0:305:KC2:CAD	2.92	0.52
33:0:309:CLA:HMC3	33:0:309:CLA:CBC	2.39	0.52
33:4:308:CLA:HMC3	33:4:308:CLA:CBC	2.39	0.52
19:N:122:VAL:CG1	33:N:303:CLA:HMA1	2.38	0.52
7:p:214:GLY:HA3	7:p:231:LEU:C	2.34	0.52
2:0:117:THR:OG1	2:0:201:MET:HE3	2.10	0.52
7:6:175:PRO:HD2	7:6:176:LEU:H	1.72	0.52
8:B:4:PRO:HB3	37:B:623:LHG:HC2	1.91	0.52
1:A:149:ALA:HB3	1:A:150:PRO:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:120:PHE:CE2	2:0:128:LEU:HD23	2.45	0.52
2:0:218:LEU:HD21	39:0:315:II0:C06	2.40	0.52
2:4:120:PHE:CE2	2:4:128:LEU:HD23	2.45	0.52
6:5:51:LEU:HD21	7:6:155:PRO:HB2	1.91	0.52
7:6:42:LYS:HB2	7:6:46:ILE:HG22	1.90	0.52
20:O:129:LYS:HG3	8:b:48:SER:HB2	1.87	0.52
20:O:154:ILE:HG12	20:O:194:ILE:HD11	1.91	0.52
6:g:163:PRO:HD2	39:g:312:II0:C07	2.38	0.52
34:A:407:PHO:C3B	33:A:412:CLA:H12	2.39	0.52
7:6:126:MET:SD	40:6:318:IHT:C21	2.97	0.52
8:B:23:HIS:ND1	33:B:616:CLA:OBD	2.41	0.52
8:B:75:TRP:O	41:B:601:SQD:O9	2.28	0.52
11:E:19:ARG:NE	11:E:19:ARG:HA	2.25	0.52
8:b:4:PRO:HB3	37:b:623:LHG:HC2	1.91	0.52
6:5:196:HIS:HA	6:5:199:TRP:CE3	2.45	0.52
20:O:118:PRO:HD2	20:O:149:TYR:HD1	1.74	0.52
1:A:140:ARG:HH22	37:D:401:LHG:HC41	1.74	0.52
2:0:47:MET:HE3	2:0:49:PHE:CZ	2.44	0.52
2:0:60:MET:HE2	19:n:137:PRO:HG3	1.88	0.52
2:0:147:LEU:CD1	25:w:69:ILE:HG23	2.40	0.52
2:4:157:ARG:HD2	2:4:161:ASP:O	2.10	0.52
2:4:212:LEU:O	2:4:215:PHE:HB2	2.10	0.52
7:6:76:LEU:HB2	7:6:78:PHE:CE1	2.45	0.52
7:6:86:TRP:CE2	33:6:308:CLA:CED	2.93	0.52
42:d:410:LMG:O5	42:d:410:LMG:O4	2.12	0.52
7:p:86:TRP:CE2	33:p:308:CLA:CED	2.93	0.52
1:A:104:GLU:O	1:A:108:ASN:ND2	2.40	0.52
2:0:157:ARG:HD2	2:0:161:ASP:O	2.10	0.52
7:6:120:PHE:CZ	7:6:132:ALA:HA	2.45	0.52
8:b:75:TRP:O	41:b:601:SQD:O9	2.28	0.52
11:e:19:ARG:NE	11:e:19:ARG:HA	2.25	0.52
6:g:154:ARG:NH1	6:g:158:ASP:O	2.42	0.52
34:a:407:PHO:C3B	33:a:412:CLA:H12	2.40	0.52
7:p:76:LEU:HB2	7:p:78:PHE:CE1	2.45	0.52
41:L:101:SQD:H362	22:t:12:GLY:HA2	1.91	0.52
8:b:265:ILE:O	8:b:269:GLY:N	2.42	0.52
33:g:307:CLA:HMC2	39:g:312:II0:C31	2.39	0.52
7:p:119:GLU:OE2	39:p:317:II0:C06	2.58	0.52
7:p:176:LEU:O	7:p:177:ASN:C	2.53	0.52
1:a:104:GLU:O	1:a:108:ASN:ND2	2.40	0.51
18:M:12:LEU:HD12	18:m:9:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:c:519:DGD:O5E	43:c:519:DGD:O4E	2.25	0.51
5:3:58:ILE:HD12	5:3:61:SER:HB2	1.91	0.51
2:4:167:LEU:H	39:4:312:II0:C08	2.23	0.51
2:4:172:ASP:HB3	2:4:175:ALA:HB3	1.92	0.51
7:6:211:LEU:HD11	33:6:313:CLA:HMD3	1.91	0.51
5:9:177:ASP:OD1	39:9:317:II0:O02	2.28	0.51
22:T:12:GLY:HA2	41:l:101:SQD:H362	1.91	0.51
23:U:52:ARG:O	23:U:55:THR:OG1	2.16	0.51
8:b:375:GLY:O	8:b:376:ILE:C	2.51	0.51
6:5:194:PHE:CD1	6:5:205:VAL:HG11	2.46	0.51
33:5:307:CLA:HMC2	39:5:312:II0:C31	2.39	0.51
19:N:166:PRO:HB3	19:N:189:SER:HA	1.92	0.51
8:b:23:HIS:ND1	33:b:616:CLA:OBD	2.41	0.51
1:a:45:THR:HG22	34:a:407:PHO:H71	1.92	0.51
2:0:49:PHE:CE1	2:0:50:LEU:CD2	2.94	0.51
5:3:164:LEU:HB2	19:N:119:VAL:CG1	2.35	0.51
6:5:113:MET:SD	6:5:121:TYR:HB2	2.50	0.51
18:M:9:LEU:HD21	18:m:12:LEU:HD12	1.91	0.51
10:d:200:VAL:HG12	33:d:404:CLA:C1B	2.41	0.51
6:g:177:LYS:HG3	33:g:307:CLA:HMA1	1.92	0.51
7:p:112:LYS:CE	7:p:122:GLY:HA2	2.27	0.51
5:3:177:ASP:OD1	39:3:317:II0:O02	2.28	0.51
6:5:154:ARG:NH1	6:5:158:ASP:O	2.42	0.51
11:e:45:TYR:HA	11:e:50:THR:HG22	1.92	0.51
6:g:103:GLU:CD	6:g:204:THR:HB	2.35	0.51
7:p:126:MET:SD	40:p:318:IHT:C16	2.98	0.51
1:A:45:THR:HG22	34:A:407:PHO:H71	1.92	0.51
2:0:63:ASP:HB2	33:0:302:CLA:HED2	1.93	0.51
7:6:136:GLY:O	7:6:137:ALA:C	2.51	0.51
10:D:200:VAL:HG12	33:D:404:CLA:C1B	2.41	0.51
11:E:45:TYR:HA	11:E:50:THR:HG22	1.92	0.51
23:U:42:ASP:HA	23:U:56:ARG:NH2	2.24	0.51
7:p:183:ASP:O	7:p:184:THR:C	2.54	0.51
1:a:143:ILE:HD11	10:d:216:THR:HA	1.93	0.51
2:0:169:LEU:HG	2:0:171:VAL:HG13	1.93	0.51
7:6:227:PHE:CE2	33:6:312:CLA:HED2	2.45	0.51
8:B:265:ILE:O	8:B:269:GLY:N	2.42	0.51
43:C:519:DGD:O1A	43:C:521:DGD:HB21	2.10	0.51
8:b:200:SER:OG	33:b:603:CLA:CMB	2.59	0.51
23:u:52:ARG:O	23:u:55:THR:OG1	2.16	0.51
2:4:69:LEU:HD13	2:4:71:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:132:ALA:CB	7:6:138:MET:HE2	2.41	0.51
8:B:48:SER:CB	20:o:129:LYS:CG	2.85	0.51
43:c:519:DGD:HA72	43:c:521:DGD:HB62	1.93	0.51
7:p:136:GLY:O	7:p:137:ALA:C	2.51	0.51
1:a:26:ASN:O	10:d:254:GLN:NE2	2.44	0.51
1:A:26:ASN:O	10:D:254:GLN:NE2	2.44	0.51
5:3:56:GLN:OE1	5:3:76:GLY:HA3	2.10	0.51
6:5:103:GLU:CD	6:5:204:THR:HB	2.35	0.51
6:5:177:LYS:HG3	33:5:307:CLA:HMA1	1.92	0.51
8:B:385:ARG:NH2	20:O:239:ASP:OD1	2.44	0.51
43:C:519:DGD:O5E	43:C:519:DGD:O4E	2.25	0.51
23:u:120:TYR:O	23:u:121:ARG:HB2	2.11	0.51
2:0:106:LEU:HD22	2:0:111:PHE:CE2	2.45	0.51
2:0:172:ASP:HB3	2:0:175:ALA:HB3	1.92	0.51
4:2:57:THR:OG1	4:2:76:ASP:OD1	2.29	0.51
2:4:215:PHE:O	2:4:215:PHE:CG	2.60	0.51
8:b:372:ASP:H	8:b:375:GLY:HA2	1.75	0.51
6:g:75:VAL:HG13	19:n:189:SER:HB3	1.93	0.51
2:4:60:MET:O	2:4:61:ALA:HB3	2.11	0.50
33:5:307:CLA:HMC2	39:5:312:II0:C29	2.41	0.50
23:U:120:TYR:O	23:U:121:ARG:HB2	2.11	0.50
19:n:192:GLY:H	19:n:195:ASP:HB3	1.75	0.50
2:0:176:LEU:HG	2:0:180:GLU:CD	2.35	0.50
9:C:52:ALA:HB1	33:C:510:CLA:HBB1	1.92	0.50
9:C:345:PRO:HB3	20:O:146:ARG:HE	1.75	0.50
8:b:385:ARG:NH2	20:o:239:ASP:OD1	2.43	0.50
7:p:132:ALA:CB	7:p:138:MET:HE2	2.41	0.50
2:4:176:LEU:HG	2:4:180:GLU:CD	2.35	0.50
19:N:187:TYR:CB	19:N:193:ALA:HA	2.38	0.50
2:4:52:ARG:NH1	2:4:56:LEU:O	2.44	0.50
6:5:163:PRO:HD2	39:5:312:II0:C07	2.41	0.50
7:6:144:TRP:CD1	33:6:306:CLA:C2C	2.95	0.50
8:B:49:ASP:OD2	20:o:128:THR:HG21	2.09	0.50
43:c:519:DGD:O1A	43:c:521:DGD:HB21	2.10	0.50
7:p:144:TRP:CD1	33:p:306:CLA:C2C	2.95	0.50
8:B:356:VAL:HG22	8:B:370:LEU:HG	1.93	0.50
43:C:519:DGD:HA72	43:C:521:DGD:HB62	1.93	0.50
11:e:45:TYR:HD1	11:e:50:THR:HG23	1.77	0.50
19:n:187:TYR:HB3	19:n:190:LEU:HB3	1.94	0.50
7:p:157:ILE:HD12	33:p:308:CLA:HMA2	1.94	0.50
1:a:149:ALA:HB3	1:a:150:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:216:ALA:HB2	39:2:313:II0:C17	2.41	0.50
4:2:85:GLU:OE1	4:2:159:GLY:N	2.43	0.50
4:8:57:THR:OG1	4:8:76:ASP:OD1	2.29	0.50
13:H:49:TYR:CD2	43:H:101:DGD:C3B	2.84	0.50
20:O:128:THR:HG21	8:b:49:ASP:OD2	2.09	0.50
20:O:129:LYS:CG	8:b:48:SER:CB	2.85	0.50
9:c:52:ALA:HB1	33:c:510:CLA:HBB1	1.92	0.50
9:c:55:ALA:HB1	35:c:516:8CT:C40	2.42	0.50
7:p:126:MET:CE	39:p:315:II0:C17	2.90	0.50
2:0:181:LEU:HD21	19:n:127:PRO:HB3	1.93	0.50
2:4:125:ALA:O	2:4:126:GLY:C	2.55	0.50
7:6:89:GLU:CD	7:6:166:ARG:HH22	2.20	0.50
11:E:45:TYR:HD1	11:E:50:THR:HG23	1.77	0.50
7:p:116:PHE:HD1	7:p:120:PHE:HE2	1.59	0.50
1:A:137:LEU:CB	1:A:139:MET:HG2	2.42	0.50
2:0:60:MET:HE1	19:n:137:PRO:HD2	1.84	0.50
2:0:166:PRO:O	2:0:167:LEU:HD23	2.12	0.50
2:0:169:LEU:HD11	2:0:171:VAL:HG13	1.93	0.50
9:C:55:ALA:HB1	35:C:516:8CT:C40	2.42	0.50
43:c:521:DGD:HA41	42:d:409:LMG:H122	1.94	0.50
33:g:307:CLA:HMC2	39:g:312:II0:C29	2.42	0.50
2:0:68:PRO:HD2	39:0:314:II0:C08	2.42	0.50
8:B:200:SER:OG	33:B:603:CLA:CMB	2.60	0.50
19:N:187:TYR:CE1	19:N:190:LEU:HD12	2.46	0.50
9:c:52:ALA:HB1	33:c:510:CLA:CBB	2.42	0.50
11:e:65:PRO:O	11:e:66:LEU:HD12	2.11	0.50
7:6:215:ARG:HD2	7:6:226:ASN:OD1	2.11	0.49
5:9:58:ILE:HG23	33:9:306:CLA:C2C	2.42	0.49
42:C:520:LMG:H152	27:Y:13:LEU:HD22	1.93	0.49
11:E:65:PRO:O	11:E:66:LEU:HD12	2.11	0.49
42:c:520:LMG:H152	27:y:13:LEU:HD22	1.93	0.49
43:c:521:DGD:HA41	42:d:409:LMG:C12	2.42	0.49
6:g:197:GLN:NE2	33:g:310:CLA:C4A	2.75	0.49
7:p:41:TYR:CD1	7:p:46:ILE:HG21	2.47	0.49
2:0:125:ALA:O	2:0:126:GLY:C	2.55	0.49
2:0:186:HIS:NE2	33:0:309:CLA:ND	2.61	0.49
2:4:186:HIS:NE2	33:4:308:CLA:ND	2.61	0.49
6:5:197:GLN:NE2	33:5:310:CLA:C4A	2.75	0.49
33:5:305:CLA:HED3	33:5:317:CLA:HMD1	1.93	0.49
43:C:521:DGD:HA41	42:D:409:LMG:H122	1.94	0.49
9:c:281:LEU:HD13	33:c:507:CLA:H201	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:146:GLY:CA	33:p:308:CLA:CAB	2.91	0.49
5:3:57:ALA:O	5:3:59:PRO:HD3	2.12	0.49
7:6:116:PHE:HD1	7:6:120:PHE:HE2	1.58	0.49
7:6:146:GLY:CA	33:6:308:CLA:CAB	2.91	0.49
43:C:521:DGD:HA41	42:D:409:LMG:C12	2.42	0.49
20:O:131:ARG:NH1	8:b:435:THR:OG1	2.45	0.49
33:4:310:CLA:C4A	33:4:310:CLA:CBA	2.91	0.49
8:B:49:ASP:OD2	20:o:130:ARG:NE	2.45	0.49
20:O:128:THR:HG23	8:b:49:ASP:CA	2.42	0.49
5:3:224:ILE:HD13	39:3:317:II0:C05	2.42	0.49
2:4:165:ASP:N	2:4:166:PRO:HD3	2.27	0.49
2:4:206:GLN:NE2	2:4:211:GLN:HA	2.27	0.49
33:5:307:CLA:C2	39:5:312:II0:C15	2.91	0.49
9:C:52:ALA:HB1	33:C:510:CLA:CBB	2.42	0.49
9:C:156:LYS:O	9:C:159:THR:OG1	2.27	0.49
6:g:188:MET:HE2	39:g:313:II0:C40	2.43	0.49
33:g:307:CLA:C2	39:g:312:II0:C15	2.91	0.49
1:a:329:GLU:O	1:a:332:HIS:ND1	2.46	0.49
7:6:60:PRO:HG2	7:6:63:LEU:HD12	1.93	0.49
4:8:85:GLU:OE1	4:8:159:GLY:N	2.43	0.49
8:B:435:THR:OG1	20:o:131:ARG:NH1	2.45	0.49
19:N:172:ARG:HB3	19:N:175:MET:HB3	1.94	0.49
6:g:169:ASP:HB3	6:g:172:THR:OG1	2.13	0.49
7:p:60:PRO:HG2	7:p:63:LEU:HD12	1.93	0.49
7:p:120:PHE:CZ	7:p:132:ALA:HA	2.48	0.49
1:a:16:ARG:HH22	37:a:411:LHG:HC2	1.76	0.49
2:4:157:ARG:NH1	2:4:161:ASP:O	2.39	0.49
7:6:212:LEU:HD13	7:6:213:VAL:HG23	1.86	0.49
5:9:224:ILE:HD13	39:9:317:II0:C05	2.42	0.49
33:g:305:CLA:HED3	33:g:317:CLA:HMD1	1.93	0.49
7:p:175:PRO:HD2	39:p:314:II0:O02	2.13	0.49
2:0:167:LEU:CA	19:n:106:TYR:CE1	2.96	0.49
6:5:188:MET:HE2	39:5:313:II0:C40	2.43	0.49
6:5:199:TRP:HE3	33:5:311:CLA:HED3	1.76	0.49
7:6:73:PHE:CD2	7:6:73:PHE:O	2.66	0.49
7:6:151:ILE:O	7:6:155:PRO:HG2	2.13	0.49
9:C:281:LEU:HD13	33:C:507:CLA:H201	1.93	0.49
22:T:31:LYS:HD3	19:n:234:PHE:CE2	2.48	0.49
11:e:33:VAL:O	11:e:37:LEU:HD22	2.13	0.49
7:p:86:TRP:CE2	33:p:308:CLA:HED3	2.48	0.49
7:p:212:LEU:CD2	7:p:213:VAL:HG23	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:166:PRO:O	2:0:167:LEU:HG	2.12	0.49
2:4:214:ASN:ND2	2:4:216:LYS:HD2	2.28	0.49
7:6:86:TRP:CE2	33:6:308:CLA:HED3	2.48	0.49
19:N:234:PHE:CE2	22:t:31:LYS:HD3	2.48	0.49
7:p:112:LYS:CD	7:p:117:GLU:HG2	2.43	0.49
33:0:311:CLA:CBA	33:0:311:CLA:C4A	2.91	0.49
10:D:48:PHE:O	10:D:52:THR:OG1	2.17	0.49
11:E:33:VAL:O	11:E:37:LEU:HD22	2.13	0.49
9:c:156:LYS:O	9:c:159:THR:OG1	2.27	0.49
10:d:158:MET:HE2	10:d:286:VAL:HG22	1.95	0.49
14:i:2:PHE:CE2	25:w:55:ARG:CZ	2.96	0.49
7:p:73:PHE:O	7:p:73:PHE:CD2	2.66	0.49
3:1:61:ALA:O	3:1:81:ARG:NH2	2.46	0.48
2:4:58:GLY:C	19:N:131:LEU:HB3	2.38	0.48
7:6:207:VAL:HG21	40:6:318:IHT:C28	2.42	0.48
19:n:166:PRO:HB3	19:n:189:SER:HA	1.94	0.48
1:A:329:GLU:O	1:A:332:HIS:ND1	2.46	0.48
7:6:99:MET:O	7:6:100:LEU:C	2.54	0.48
37:8:315:LHG:HC2	37:8:315:LHG:O5	2.09	0.48
10:D:158:MET:HE2	10:D:286:VAL:HG22	1.95	0.48
20:o:115:CYS:SG	20:o:152:THR:HG22	2.53	0.48
7:6:173:PHE:CD2	39:6:314:II0:C20	2.95	0.48
37:B:623:LHG:H261	17:L:21:GLY:CA	2.44	0.48
14:I:2:PHE:CE2	25:W:55:ARG:CZ	2.96	0.48
23:U:42:ASP:C	23:U:56:ARG:HH22	2.21	0.48
33:g:305:CLA:HBD	33:g:317:CLA:HMD1	1.94	0.48
14:i:21:PHE:O	14:i:25:SER:OG	2.30	0.48
19:n:172:ARG:HB3	19:n:175:MET:HB3	1.94	0.48
6:5:74:ASP:OD1	19:N:172:ARG:HG3	2.14	0.48
7:p:99:MET:O	7:p:100:LEU:C	2.54	0.48
1:A:133:PHE:CE2	10:D:254:GLN:HB2	2.49	0.48
7:6:175:PRO:HD2	7:6:176:LEU:HD22	1.94	0.48
7:p:87:ALA:HB1	33:p:303:CLA:H3A	1.95	0.48
7:p:213:VAL:HB	7:p:220:PHE:HE1	1.77	0.48
1:A:16:ARG:HH22	37:A:411:LHG:HC2	1.76	0.48
2:0:176:LEU:HD21	19:n:134:LYS:CG	2.44	0.48
8:B:52:LEU:HD12	20:o:130:ARG:CZ	2.44	0.48
37:b:623:LHG:H261	17:l:21:GLY:CA	2.44	0.48
19:n:192:GLY:N	19:n:195:ASP:HB3	2.28	0.48
1:a:257:ARG:NH2	10:d:24:ASP:OD2	2.46	0.48
6:5:197:GLN:HE21	33:5:310:CLA:C1A	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:73:PHE:CE1	7:6:75:PRO:HG2	2.48	0.48
6:g:74:ASP:OD1	19:n:172:ARG:HG3	2.14	0.48
1:A:257:ARG:NH2	10:D:24:ASP:OD2	2.46	0.48
2:0:43:ARG:NH2	2:0:49:PHE:O	2.47	0.48
2:0:136:GLY:CA	33:0:306:CLA:CBB	2.92	0.48
2:4:43:ARG:NH2	2:4:49:PHE:O	2.47	0.48
33:5:305:CLA:HBD	33:5:317:CLA:HMD1	1.94	0.48
7:6:87:ALA:HB1	33:6:303:CLA:H3A	1.95	0.48
10:D:248:ALA:HB3	36:D:407:PL9:H522	1.96	0.48
8:b:371:VAL:HB	8:b:375:GLY:CA	2.44	0.48
6:g:164:LEU:O	6:g:164:LEU:CG	2.61	0.48
7:p:73:PHE:CE1	7:p:75:PRO:HG2	2.48	0.48
7:p:112:LYS:HD2	7:p:117:GLU:HG2	1.96	0.48
34:a:407:PHO:CAB	33:a:412:CLA:H12	2.44	0.48
2:0:169:LEU:CG	2:0:171:VAL:HG13	2.44	0.48
2:4:114:LYS:O	2:4:115:LEU:C	2.55	0.48
2:4:136:GLY:CA	33:4:306:CLA:CBB	2.92	0.48
2:4:207:ALA:HB1	2:4:208:PRO:HD2	1.95	0.48
9:C:203:THR:HG23	9:C:231:GLU:HB3	1.96	0.48
44:V:201:HEM:HBD2	44:V:201:HEM:HHA	1.95	0.48
8:b:372:ASP:N	8:b:375:GLY:HA2	2.29	0.48
9:c:203:THR:HG23	9:c:231:GLU:HB3	1.96	0.48
6:g:197:GLN:HE21	33:g:310:CLA:C1A	2.26	0.48
34:A:407:PHO:CAB	33:A:412:CLA:H12	2.44	0.48
6:5:202:LYS:N	6:5:202:LYS:HD2	2.28	0.48
11:e:31:LEU:HD13	12:f:25:VAL:HG13	1.96	0.48
7:p:88:ARG:O	7:p:89:GLU:C	2.54	0.48
2:0:72:SER:O	2:0:73:ASN:C	2.56	0.47
2:0:208:PRO:O	2:0:212:LEU:HG	2.13	0.47
7:6:88:ARG:O	7:6:89:GLU:C	2.54	0.47
5:9:57:ALA:HB1	5:9:77:PHE:HB2	1.95	0.47
14:I:21:PHE:O	14:I:25:SER:OG	2.30	0.47
19:N:194:LEU:HB3	13:h:26:GLY:O	2.14	0.47
9:c:261:ARG:NH2	25:w:80:ASN:O	2.47	0.47
7:p:227:PHE:CE2	33:p:312:CLA:HED2	2.49	0.47
2:4:161:ASP:CG	2:4:163:ASP:H	2.21	0.47
9:C:38:GLY:O	9:C:41:ARG:HG3	2.14	0.47
43:C:521:DGD:HA42	10:D:73:PHE:HE1	1.78	0.47
20:O:130:ARG:CZ	8:b:52:LEU:HD12	2.44	0.47
10:d:248:ALA:HB3	36:d:407:PL9:H522	1.96	0.47
2:0:81:ARG:CZ	2:0:184:LEU:HD21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:91:CYS:SG	39:0:314:II0:C39	3.02	0.47
2:0:207:ALA:HB1	2:0:208:PRO:HD2	1.95	0.47
2:4:81:ARG:CZ	2:4:184:LEU:HD21	2.44	0.47
2:4:169:LEU:HD12	2:4:170:SER:N	2.29	0.47
33:4:304:CLA:HBA2	33:4:304:CLA:NA	2.29	0.47
7:6:176:LEU:C	7:6:177:ASN:OD1	2.57	0.47
11:E:31:LEU:HD13	12:F:25:VAL:HG13	1.96	0.47
13:H:49:TYR:CE2	43:H:101:DGD:HG32	2.49	0.47
2:4:60:MET:SD	19:N:135:TYR:HD1	2.36	0.47
7:6:181:ASN:HB2	7:6:184:THR:HG23	1.95	0.47
10:d:198:MET:HE2	10:d:280:THR:HG21	1.97	0.47
2:0:113:ASN:HD22	2:0:119:ALA:HA	1.79	0.47
2:0:166:PRO:CA	19:n:106:TYR:CE2	2.95	0.47
2:4:91:CYS:SG	39:4:313:II0:C39	3.02	0.47
33:5:303:CLA:CMB	33:5:305:CLA:HMC2	2.45	0.47
7:6:176:LEU:HB2	39:6:314:II0:O02	2.15	0.47
10:D:198:MET:HE2	10:D:280:THR:HG21	1.97	0.47
44:v:201:HEM:HBD2	44:v:201:HEM:HHA	1.95	0.47
2:0:68:PRO:CG	39:0:314:II0:C06	2.93	0.47
2:0:185:LYS:HZ2	33:0:308:CLA:HMA3	1.78	0.47
33:6:307:CLA:HMB1	40:6:318:IHT:C24	2.44	0.47
9:C:261:ARG:NH2	25:W:80:ASN:O	2.47	0.47
43:c:521:DGD:HA42	10:d:73:PHE:HE1	1.78	0.47
6:g:75:VAL:HA	19:n:189:SER:CB	2.44	0.47
7:p:73:PHE:CE1	7:p:75:PRO:CG	2.98	0.47
7:p:225:PRO:O	7:p:226:ASN:HB2	2.15	0.47
2:0:46:ALA:HB2	2:0:64:VAL:HG23	1.97	0.47
2:0:164:PHE:CZ	39:0:313:II0:C14	2.97	0.47
33:0:304:CLA:NA	33:0:304:CLA:HBA2	2.29	0.47
3:1:199:GLN:NE2	39:1:313:II0:O01	2.48	0.47
2:4:196:GLY:O	2:4:200:GLN:HG3	2.15	0.47
6:5:75:VAL:HG21	19:N:183:VAL:HG11	1.77	0.47
7:6:176:LEU:C	7:6:178:CYS:N	2.67	0.47
8:B:49:ASP:CA	20:o:128:THR:HG23	2.43	0.47
10:D:44:ILE:HD11	34:D:403:PHO:H41	1.97	0.47
19:N:117:VAL:HG23	19:N:117:VAL:O	2.14	0.47
25:W:51:ILE:HG21	25:W:57:ILE:HD11	1.96	0.47
10:d:176:ALA:CA	10:d:179:ARG:HG2	2.43	0.47
6:g:50:PHE:HA	7:p:166:ARG:HE	1.75	0.47
19:n:99:LEU:O	19:n:103:SER:OG	2.30	0.47
33:p:307:CLA:HMB1	40:p:318:IHT:C24	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PHE:CE1	1:A:263:ALA:HB2	2.50	0.47
4:2:171:ASN:OD1	4:2:172:ASP:N	2.47	0.47
2:4:167:LEU:HB2	39:4:312:II0:C17	2.44	0.47
2:4:212:LEU:HD12	2:4:213:THR:CA	2.43	0.47
6:5:204:THR:O	6:5:207:GLU:N	2.48	0.47
8:b:192:PRO:HG3	13:h:49:TYR:CD1	2.48	0.47
10:d:44:ILE:HD11	34:d:403:PHO:H41	1.97	0.47
33:g:303:CLA:CMB	33:g:305:CLA:HMC2	2.45	0.47
20:o:143:LEU:HD23	20:o:145:THR:O	2.15	0.47
1:a:260:PHE:CE1	1:a:263:ALA:HB2	2.50	0.47
33:a:406:CLA:HED1	43:c:521:DGD:HAE1	1.97	0.47
2:0:196:GLY:O	2:0:200:GLN:HG3	2.15	0.47
6:5:204:THR:O	6:5:205:VAL:C	2.58	0.47
8:B:349:LYS:N	8:B:396:GLY:O	2.48	0.47
8:b:349:LYS:N	8:b:396:GLY:O	2.48	0.47
11:e:15:ILE:O	11:e:21:TRP:NE1	2.48	0.47
7:p:67:LEU:HD12	7:p:67:LEU:HA	1.65	0.47
2:4:83:ALA:O	2:4:87:HIS:ND1	2.48	0.47
7:6:133:VAL:O	7:6:139:GLN:NE2	2.48	0.47
7:6:227:PHE:CE2	33:6:319:CLA:H3A	2.51	0.47
9:C:406:SER:HA	9:C:420:VAL:HG23	1.97	0.47
42:C:520:LMG:HC91	42:C:520:LMG:H112	1.97	0.47
11:E:15:ILE:O	11:E:21:TRP:NE1	2.48	0.47
9:c:38:GLY:O	9:c:41:ARG:HG3	2.14	0.47
9:c:406:SER:HA	9:c:420:VAL:HG23	1.97	0.47
42:c:520:LMG:H112	42:c:520:LMG:HC91	1.97	0.47
19:n:187:TYR:CB	19:n:193:ALA:HA	2.40	0.47
20:o:192:PHE:CA	20:o:295:GLN:HE22	2.20	0.47
1:a:183:MET:CE	33:a:412:CLA:HAC1	2.45	0.46
2:4:114:LYS:O	2:4:116:ALA:N	2.48	0.46
33:5:307:CLA:HBC1	39:5:314:II0:C18	2.46	0.46
7:6:73:PHE:CE1	7:6:75:PRO:CG	2.98	0.46
4:8:171:ASN:OD1	4:8:172:ASP:N	2.47	0.46
20:O:126:GLU:HB3	20:O:133:GLU:HG2	1.97	0.46
8:b:372:ASP:HB3	8:b:378:ARG:HH11	1.79	0.46
2:4:185:LYS:HZ2	33:N:303:CLA:HMA3	1.78	0.46
43:C:519:DGD:C1A	43:C:521:DGD:HB21	2.46	0.46
10:D:176:ALA:CA	10:D:179:ARG:HG2	2.43	0.46
10:D:249:ASN:O	10:D:253:SER:OG	2.31	0.46
8:b:372:ASP:OD1	8:b:373:LYS:HG3	2.15	0.46
33:g:307:CLA:HBC1	39:g:314:II0:C18	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:40:LEU:O	7:p:41:TYR:C	2.58	0.46
7:p:113:PHE:CZ	33:p:305:CLA:H42	2.50	0.46
7:p:133:VAL:O	7:p:139:GLN:NE2	2.48	0.46
7:p:227:PHE:CE2	33:p:319:CLA:H3A	2.50	0.46
2:0:164:PHE:HD2	33:0:307:CLA:C2D	2.27	0.46
2:0:207:ALA:HB1	2:0:208:PRO:CD	2.46	0.46
33:0:308:CLA:HAA2	19:n:120:SER:HB2	1.97	0.46
6:5:164:LEU:O	6:5:164:LEU:CG	2.60	0.46
3:7:199:GLN:NE2	39:7:313:II0:O01	2.48	0.46
37:B:623:LHG:H101	37:B:623:LHG:O8	2.15	0.46
22:T:4:LEU:HD13	42:T:101:LMG:H171	1.98	0.46
9:c:83:GLU:OE2	9:c:398:HIS:NE2	2.48	0.46
43:c:519:DGD:C1A	43:c:521:DGD:HB21	2.46	0.46
10:d:86:HIS:NE2	10:d:160:PRO:O	2.44	0.46
6:g:204:THR:O	6:g:207:GLU:N	2.48	0.46
7:p:154:VAL:HG22	33:p:308:CLA:HMA1	1.98	0.46
25:w:51:ILE:HG21	25:w:57:ILE:HD11	1.96	0.46
33:A:406:CLA:HED1	43:C:521:DGD:HAE1	1.97	0.46
3:7:116:VAL:HG11	3:7:197:LEU:HD12	1.98	0.46
19:N:196:LYS:HG2	19:N:197:THR:N	2.29	0.46
19:n:162:ILE:HB	33:n:306:CLA:HED1	1.98	0.46
20:o:126:GLU:HB3	20:o:133:GLU:HG2	1.97	0.46
1:a:41:LEU:O	1:a:45:THR:HG23	2.16	0.46
1:A:16:ARG:NH2	37:A:411:LHG:C2	2.71	0.46
2:0:55:ALA:HB3	2:0:72:SER:OG	2.15	0.46
2:0:203:LEU:CD2	2:0:204:THR:HG23	2.45	0.46
33:0:309:CLA:CBC	33:0:309:CLA:CMC	2.94	0.46
3:1:116:VAL:HG11	3:1:197:LEU:HD12	1.98	0.46
2:4:59:SER:HB3	19:N:132:TYR:CD2	2.47	0.46
2:4:111:PHE:O	33:4:304:CLA:HED3	2.15	0.46
2:4:198:LEU:HA	2:4:201:MET:HE2	1.96	0.46
7:6:211:LEU:HD13	33:6:313:CLA:C3D	2.46	0.46
6:g:164:LEU:HB3	6:g:166:LEU:CD2	2.46	0.46
7:p:224:ILE:O	7:p:226:ASN:ND2	2.49	0.46
1:a:16:ARG:NH2	37:a:411:LHG:C2	2.71	0.46
33:a:405:CLA:HBD	33:a:412:CLA:HAC2	1.97	0.46
33:A:405:CLA:HBD	33:A:412:CLA:HAC2	1.97	0.46
2:0:83:ALA:O	2:0:87:HIS:ND1	2.48	0.46
33:4:308:CLA:CBC	33:4:308:CLA:CMC	2.94	0.46
7:6:224:ILE:H	7:6:224:ILE:CD1	2.21	0.46
19:N:162:ILE:HB	33:N:307:CLA:HED1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:125:ALA:HB1	2:0:129:TRP:CD1	2.50	0.46
2:0:135:LEU:HA	2:0:138:ILE:HG12	1.98	0.46
2:4:207:ALA:HB1	2:4:208:PRO:CD	2.46	0.46
7:6:113:PHE:CE2	33:6:305:CLA:H11	2.48	0.46
37:b:623:LHG:H101	37:b:623:LHG:O8	2.15	0.46
1:A:183:MET:CE	33:A:412:CLA:HAC1	2.45	0.46
2:0:44:SER:OG	2:0:47:MET:O	2.31	0.46
2:0:203:LEU:HD23	2:0:203:LEU:C	2.41	0.46
2:4:78:LYS:CG	19:N:137:PRO:HD2	2.37	0.46
2:4:212:LEU:CD1	2:4:213:THR:N	2.70	0.46
7:6:67:LEU:HG	7:6:88:ARG:NH2	2.30	0.46
23:U:121:ARG:HD3	23:U:121:ARG:HA	1.73	0.46
8:b:433:ASP:OD2	8:b:436:THR:OG1	2.30	0.46
2:4:69:LEU:HD13	2:4:71:PHE:CE2	2.51	0.46
7:6:40:LEU:O	7:6:41:TYR:C	2.58	0.46
7:6:113:PHE:CZ	33:6:305:CLA:H42	2.51	0.46
9:C:83:GLU:OE2	9:C:398:HIS:NE2	2.48	0.46
2:4:64:VAL:HG12	19:N:128:GLY:HA3	1.97	0.46
2:4:218:LEU:HD12	2:4:218:LEU:N	2.30	0.46
7:6:112:LYS:CD	7:6:117:GLU:HG2	2.46	0.46
7:6:154:VAL:O	7:6:158:ILE:HG12	2.16	0.46
7:6:175:PRO:CD	7:6:176:LEU:H	2.29	0.46
43:c:521:DGD:HBE1	43:c:521:DGD:HBF1	1.63	0.46
6:g:93:MET:CE	33:g:307:CLA:CHC	2.94	0.46
6:g:204:THR:O	6:g:205:VAL:C	2.57	0.46
15:j:34:GLY:O	15:j:37:SER:OG	2.33	0.46
22:t:4:LEU:HD13	42:t:101:LMG:H171	1.98	0.46
2:0:56:LEU:CD1	2:0:67:ASP:HB2	2.46	0.45
2:0:162:LEU:O	2:0:163:ASP:HB2	2.16	0.45
2:0:197:MET:HE2	39:0:313:II0:C16	2.46	0.45
33:0:304:CLA:CGA	33:0:304:CLA:CHA	2.95	0.45
5:3:200:ARG:HA	5:3:203:MET:HE3	1.99	0.45
2:4:135:LEU:HA	2:4:138:ILE:HG12	1.98	0.45
33:4:304:CLA:CGA	33:4:304:CLA:CHA	2.94	0.45
6:5:197:GLN:HA	6:5:200:VAL:HG12	1.98	0.45
10:D:35:LEU:O	10:D:39:THR:OG1	2.32	0.45
8:b:235:GLU:OE2	8:b:472:ARG:NE	2.47	0.45
33:c:505:CLA:H141	42:c:520:LMG:H422	1.98	0.45
12:f:17:TRP:O	12:f:21:HIS:ND1	2.50	0.45
1:a:321:LEU:HD12	10:d:182:LEU:HD12	1.99	0.45
1:A:41:LEU:O	1:A:45:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:HD12	10:D:182:LEU:HD12	1.99	0.45
2:0:109:PRO:O	2:0:110:GLY:C	2.58	0.45
2:4:197:MET:HE2	39:4:312:II0:C16	2.47	0.45
7:6:89:GLU:OE1	7:6:169:GLY:N	2.49	0.45
5:9:200:ARG:HA	5:9:203:MET:HE3	1.99	0.45
37:B:623:LHG:H211	17:L:27:VAL:HG11	1.98	0.45
23:U:61:TYR:O	23:U:65:ALA:HB3	2.16	0.45
7:p:173:PHE:HE2	39:p:314:II0:C20	2.25	0.45
6:5:93:MET:CE	33:5:307:CLA:CHC	2.94	0.45
7:6:212:LEU:HD12	7:6:213:VAL:CB	2.46	0.45
37:b:623:LHG:H211	17:l:27:VAL:HG11	1.98	0.45
18:m:12:LEU:CB	18:m:16:PHE:CE2	2.74	0.45
23:u:61:TYR:O	23:u:65:ALA:HB3	2.16	0.45
1:a:131:TRP:O	1:a:134:SER:OG	2.22	0.45
1:A:289:GLY:O	1:A:293:MET:HE2	2.16	0.45
2:0:74:TYR:CD2	2:0:74:TYR:N	2.85	0.45
2:0:140:ILE:HD11	25:w:68:PHE:CE2	2.50	0.45
7:6:213:VAL:HB	7:6:220:PHE:HE1	1.80	0.45
43:C:521:DGD:HA22	43:C:521:DGD:HG11	1.34	0.45
12:F:17:TRP:O	12:F:21:HIS:ND1	2.50	0.45
25:W:56:LEU:O	25:W:59:PRO:HD2	2.16	0.45
7:p:215:ARG:HD2	7:p:226:ASN:OD1	2.16	0.45
25:w:56:LEU:O	25:w:59:PRO:HD2	2.16	0.45
2:0:98:PHE:HD2	2:0:197:MET:CB	2.28	0.45
2:4:98:PHE:HD2	2:4:197:MET:CB	2.28	0.45
2:4:125:ALA:HB1	2:4:129:TRP:CD1	2.50	0.45
2:4:135:LEU:HD12	33:4:306:CLA:HMC2	1.99	0.45
6:5:120:ASP:O	6:5:123:VAL:HG22	2.17	0.45
7:6:67:LEU:HD12	7:6:67:LEU:HA	1.70	0.45
9:C:247:GLY:CA	33:C:507:CLA:HBC2	2.46	0.45
33:C:505:CLA:H141	42:C:520:LMG:H422	1.98	0.45
10:D:54:VAL:HG21	10:D:109:LEU:HD22	1.97	0.45
14:I:8:VAL:O	14:I:12:VAL:HG23	2.16	0.45
19:N:135:TYR:CE1	19:N:137:PRO:HB3	2.52	0.45
19:N:202:GLU:OE1	19:N:202:GLU:N	2.50	0.45
37:b:623:LHG:HC81	37:d:402:LHG:HC92	1.98	0.45
10:d:54:VAL:HG21	10:d:109:LEU:HD22	1.97	0.45
19:n:192:GLY:C	19:n:195:ASP:H	2.24	0.45
2:0:193:GLY:O	2:0:194:LEU:C	2.57	0.45
2:4:166:PRO:CD	39:4:312:II0:O02	2.64	0.45
2:4:193:GLY:O	2:4:194:LEU:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:4:310:CLA:C4A	33:4:310:CLA:HBA1	2.46	0.45
10:D:192:LEU:O	17:L:35:TYR:OH	2.32	0.45
20:O:110:LYS:NZ	20:O:320:GLU:HB2	2.31	0.45
25:W:51:ILE:HD13	25:W:57:ILE:HG13	1.98	0.45
9:c:247:GLY:CA	33:c:507:CLA:HBC2	2.47	0.45
7:p:215:ARG:HB3	7:p:219:GLU:HB3	1.98	0.45
2:0:69:LEU:CG	2:0:71:PHE:HE2	2.30	0.45
4:2:126:LYS:C	4:2:128:GLY:H	2.24	0.45
2:4:194:LEU:HD12	2:4:194:LEU:HA	1.89	0.45
6:5:197:GLN:HE22	33:5:310:CLA:CMA	2.30	0.45
33:6:319:CLA:CAA	33:6:319:CLA:CBD	2.95	0.45
9:C:250:TRP:O	9:C:254:THR:OG1	2.11	0.45
10:D:245:MET:HE3	36:D:407:PL9:C52	2.47	0.45
43:H:101:DGD:O5D	43:H:101:DGD:O4D	2.26	0.45
23:U:48:ASN:HD22	23:U:106:PRO:HA	1.82	0.45
8:b:2:GLY:N	17:l:12:GLU:OE2	2.49	0.45
10:d:245:MET:HE3	36:d:407:PL9:C52	2.47	0.45
6:g:162:ASP:OD1	33:g:307:CLA:CAA	2.65	0.45
25:w:51:ILE:HD13	25:w:57:ILE:HG13	1.97	0.45
33:0:306:CLA:HBB1	33:0:306:CLA:HHC	1.99	0.45
2:4:167:LEU:N	39:4:312:II0:O02	2.43	0.45
8:B:200:SER:OG	33:B:603:CLA:HMB1	2.17	0.45
37:B:623:LHG:HC81	37:D:402:LHG:HC92	1.98	0.45
43:c:521:DGD:HA22	43:c:521:DGD:HG11	1.34	0.45
6:g:120:ASP:O	6:g:123:VAL:HG22	2.17	0.45
14:i:8:VAL:O	14:i:12:VAL:HG23	2.16	0.45
19:n:122:VAL:HG22	19:n:127:PRO:HD3	1.98	0.45
7:p:112:LYS:CB	7:p:117:GLU:HB2	2.47	0.45
1:a:329:GLU:HG3	45:a:524:HOH:O	2.16	0.45
33:a:412:CLA:H52	33:a:412:CLA:H92	1.98	0.45
2:0:194:LEU:HD12	2:0:194:LEU:HA	1.89	0.45
2:0:206:GLN:NE2	2:0:211:GLN:HA	2.32	0.45
2:4:71:PHE:CD2	33:4:302:CLA:H2	2.52	0.45
8:B:2:GLY:N	17:L:12:GLU:OE2	2.49	0.45
19:N:122:VAL:HG22	33:N:303:CLA:HMA2	1.92	0.45
10:d:188:HIS:CG	10:d:293:ARG:HD3	2.45	0.45
1:A:329:GLU:HG3	45:A:524:HOH:O	2.16	0.45
2:0:135:LEU:HD12	33:0:306:CLA:HMC2	1.99	0.45
2:0:200:GLN:NE2	33:0:310:CLA:C4D	2.70	0.45
2:0:201:MET:SD	2:0:208:PRO:HD3	2.56	0.45
33:0:311:CLA:C4A	33:0:311:CLA:HBA1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:4:306:CLA:HHC	33:4:306:CLA:HBB1	1.99	0.45
7:6:138:MET:HG3	33:6:307:CLA:CHD	2.47	0.45
4:8:86:ALA:O	4:8:90:HIS:ND1	2.50	0.45
21:Q:195:ALA:HB1	21:Q:201:VAL:HG23	1.99	0.45
6:g:197:GLN:HE22	33:g:310:CLA:CMA	2.30	0.45
19:n:183:VAL:HG13	19:n:188:LYS:CE	2.45	0.45
1:a:289:GLY:O	1:a:293:MET:HE2	2.16	0.44
1:A:244:GLU:OE2	10:D:263:LYS:NZ	2.50	0.44
33:A:412:CLA:H52	33:A:412:CLA:H92	1.98	0.44
2:0:49:PHE:CD1	2:0:50:LEU:CD2	3.00	0.44
2:4:120:PHE:CD1	2:4:120:PHE:C	2.95	0.44
20:O:186:GLU:OE2	20:O:307:LYS:NZ	2.50	0.44
23:U:42:ASP:C	23:U:56:ARG:NH2	2.75	0.44
9:c:464:GLU:OE2	10:d:247:THR:OG1	2.35	0.44
10:d:208:LEU:HD11	10:d:212:ILE:HD12	1.99	0.44
6:g:162:ASP:O	6:g:163:PRO:C	2.60	0.44
6:g:205:VAL:HG23	6:g:206:LEU:N	2.32	0.44
33:p:319:CLA:CBD	33:p:319:CLA:CAA	2.95	0.44
23:u:48:ASN:HD22	23:u:106:PRO:HA	1.82	0.44
2:0:178:ARG:HH21	19:n:124:GLU:CD	2.25	0.44
7:6:215:ARG:CG	7:6:219:GLU:CD	2.72	0.44
10:D:86:HIS:NE2	10:D:160:PRO:O	2.44	0.44
33:b:611:CLA:H143	33:b:611:CLA:HBD	2.00	0.44
20:o:110:LYS:NZ	20:o:320:GLU:HB2	2.31	0.44
20:o:125:GLU:OE2	20:o:307:LYS:NZ	2.41	0.44
1:a:244:GLU:OE2	10:d:263:LYS:NZ	2.50	0.44
1:A:326:LEU:HD21	24:V:160:LYS:HB3	1.99	0.44
2:0:68:PRO:HD2	39:0:314:II0:C06	2.48	0.44
2:0:218:LEU:HD23	33:g:304:CLA:CED	2.46	0.44
4:2:86:ALA:O	4:2:90:HIS:ND1	2.50	0.44
5:9:52:GLY:O	5:9:53:PRO:C	2.56	0.44
10:D:208:LEU:HD11	10:D:212:ILE:HD12	1.99	0.44
10:d:351:LEU:HD12	10:d:351:LEU:C	2.42	0.44
23:u:121:ARG:HD3	23:u:121:ARG:HA	1.73	0.44
33:B:611:CLA:HBD	33:B:611:CLA:H143	2.00	0.44
20:O:130:ARG:NE	8:b:49:ASP:OD2	2.44	0.44
8:b:356:VAL:HG22	8:b:370:LEU:HG	2.00	0.44
7:p:138:MET:HG3	33:p:307:CLA:CHD	2.47	0.44
21:q:195:ALA:HB1	21:q:201:VAL:HG23	1.99	0.44
1:a:283:ILE:HA	1:a:286:THR:HG22	1.99	0.44
1:A:16:ARG:NH2	37:A:411:LHG:HO1	2.13	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:167:LEU:N	19:n:106:TYR:CE1	2.86	0.44
2:0:198:LEU:HA	2:0:201:MET:HE2	1.99	0.44
4:2:95:MET:HE3	4:2:186:HIS:HB3	1.99	0.44
2:4:88:GLY:HA3	2:4:187:ALA:HB1	1.99	0.44
7:6:41:TYR:CD1	7:6:46:ILE:HG21	2.53	0.44
5:9:51:GLN:HG2	5:9:193:LEU:HD22	1.99	0.44
8:B:235:GLU:OE2	8:B:472:ARG:NE	2.47	0.44
27:Y:34:LEU:HD23	27:Y:34:LEU:HA	1.88	0.44
33:c:512:CLA:H141	28:z:20:VAL:HG13	2.00	0.44
7:p:145:LEU:HD12	33:p:308:CLA:HBC2	1.99	0.44
1:A:246:TYR:OH	31:A:403:BCT:O2	2.28	0.44
2:0:204:THR:O	2:0:206:GLN:N	2.51	0.44
7:6:174:ASP:HA	39:6:314:II0:C12	2.48	0.44
3:7:213:ASN:OD1	3:7:213:ASN:C	2.59	0.44
9:c:87:ILE:HG12	45:c:607:HOH:O	2.17	0.44
11:e:39:VAL:HG21	12:f:37:MET:HG3	1.99	0.44
1:a:326:LEU:HD21	24:v:160:LYS:HB3	1.99	0.44
2:0:56:LEU:HD11	2:0:67:ASP:HB2	1.99	0.44
2:0:120:PHE:CD1	2:0:120:PHE:C	2.95	0.44
2:4:189:LEU:HD13	33:N:303:CLA:HAC2	2.00	0.44
7:6:176:LEU:O	7:6:177:ASN:OD1	2.36	0.44
9:C:87:ILE:HG12	45:C:607:HOH:O	2.17	0.44
33:C:512:CLA:H141	28:Z:20:VAL:HG13	2.00	0.44
10:D:188:HIS:CG	10:D:293:ARG:HD3	2.44	0.44
2:0:46:ALA:HB2	2:0:64:VAL:CG2	2.48	0.44
2:0:189:LEU:HD13	33:0:308:CLA:HAC2	2.00	0.44
11:E:39:VAL:HG21	12:F:37:MET:HG3	1.99	0.44
9:c:416:SER:HB2	24:v:68:VAL:HG23	2.00	0.44
10:d:35:LEU:O	10:d:39:THR:OG1	2.31	0.44
6:g:70:LEU:HB2	39:g:313:II0:O02	2.18	0.44
43:h:101:DGD:O5D	43:h:101:DGD:O4D	2.26	0.44
20:o:186:GLU:OE2	20:o:307:LYS:NZ	2.50	0.44
7:p:224:ILE:O	7:p:225:PRO:C	2.60	0.44
1:A:221:SER:OG	10:D:138:ARG:O	2.30	0.44
2:0:166:PRO:O	2:0:167:LEU:CG	2.66	0.44
2:0:169:LEU:CD1	2:0:171:VAL:HG13	2.48	0.44
37:2:315:LHG:H281	37:2:315:LHG:H252	1.82	0.44
8:B:413:ASP:O	8:B:417:VAL:HG23	2.18	0.44
8:B:460:LEU:HD12	10:D:286:VAL:HG21	1.99	0.44
10:D:351:LEU:HD12	10:D:351:LEU:C	2.43	0.44
8:b:200:SER:OG	33:b:603:CLA:HMB1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:215:ARG:HD3	7:p:219:GLU:HG2	1.98	0.44
2:0:111:PHE:HE1	39:0:316:II0:C16	2.31	0.43
2:4:147:LEU:HD13	25:W:69:ILE:HG23	2.00	0.43
33:4:306:CLA:H61	33:4:306:CLA:H41	1.77	0.43
6:5:70:LEU:HB2	39:5:313:II0:O02	2.18	0.43
6:5:197:GLN:HE22	33:5:310:CLA:C4A	2.31	0.43
33:5:302:CLA:H11	39:5:313:II0:C18	2.48	0.43
4:8:95:MET:HE3	4:8:186:HIS:HB3	1.99	0.43
8:b:460:LEU:HD12	10:d:286:VAL:HG21	1.99	0.43
6:g:197:GLN:HE22	33:g:310:CLA:C4A	2.31	0.43
18:m:37:SER:O	18:m:37:SER:OG	2.29	0.43
7:p:157:ILE:O	7:p:161:LEU:HD13	2.17	0.43
23:u:39:GLY:O	23:u:56:ARG:NH2	2.51	0.43
1:A:150:PRO:HG3	34:A:407:PHO:C4C	2.48	0.43
2:0:64:VAL:HG22	33:0:302:CLA:HMD1	1.99	0.43
2:0:77:LEU:O	2:0:78:LYS:C	2.55	0.43
2:0:88:GLY:HA3	2:0:187:ALA:HB1	1.99	0.43
2:0:203:LEU:HD23	2:0:204:THR:HG23	1.99	0.43
2:4:61:ALA:CB	19:N:130:GLY:HA3	2.47	0.43
2:4:140:ILE:HD11	25:W:68:PHE:CE2	2.51	0.43
3:7:61:ALA:O	3:7:81:ARG:NH2	2.46	0.43
19:N:122:VAL:HG13	33:N:303:CLA:C3A	2.48	0.43
19:N:122:VAL:HG22	33:N:303:CLA:CMA	2.44	0.43
8:b:413:ASP:O	8:b:417:VAL:HG23	2.18	0.43
33:g:302:CLA:H11	39:g:313:II0:C18	2.48	0.43
33:0:306:CLA:H61	33:0:306:CLA:H41	1.77	0.43
4:2:103:VAL:O	4:2:107:TYR:N	2.44	0.43
2:4:136:GLY:O	2:4:137:ALA:C	2.58	0.43
6:5:128:GLY:HA3	33:5:305:CLA:HMD3	2.00	0.43
9:C:416:SER:HB2	24:V:68:VAL:HG23	2.00	0.43
13:H:26:GLY:O	19:n:194:LEU:HB3	2.18	0.43
44:f:101:HEM:HMD1	44:f:101:HEM:O1D	2.18	0.43
6:g:49:PRO:O	7:p:166:ARG:NH2	2.51	0.43
7:p:153:GLY:HA2	7:p:171:PHE:HZ	1.83	0.43
4:2:126:LYS:C	4:2:128:GLY:N	2.75	0.43
7:6:52:GLU:O	7:6:55:PRO:HD3	2.19	0.43
7:6:83:ASP:C	7:6:85:ARG:N	2.74	0.43
17:L:12:GLU:HB3	19:n:244:LEU:HD12	2.01	0.43
19:n:190:LEU:O	19:n:192:GLY:O	2.37	0.43
7:p:54:ILE:HG12	33:p:302:CLA:HBC2	2.01	0.43
2:0:109:PRO:C	2:0:111:PHE:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:147:LEU:HD13	25:w:69:ILE:HG23	2.01	0.43
33:1:305:CLA:HBC1	39:1:316:II0:C27	2.48	0.43
2:4:181:LEU:HD22	19:N:129:ILE:HA	2.00	0.43
7:6:176:LEU:HD23	39:6:314:II0:C18	2.42	0.43
9:C:350:ILE:HG21	9:C:359:TRP:HB2	2.01	0.43
13:H:49:TYR:CE2	43:H:101:DGD:C2G	2.95	0.43
9:c:350:ILE:HG21	9:c:359:TRP:HB2	2.01	0.43
7:p:119:GLU:OE2	39:p:317:II0:C12	2.67	0.43
7:p:149:GLU:OE2	33:p:308:CLA:NB	2.51	0.43
7:6:99:MET:HE3	33:6:309:CLA:CMC	2.49	0.43
7:6:145:LEU:HD12	33:6:308:CLA:HBC2	1.99	0.43
23:U:109:GLU:HG3	23:U:110:TYR:CD2	2.53	0.43
33:b:611:CLA:H141	33:b:613:CLA:HBD	2.01	0.43
1:A:283:ILE:HA	1:A:286:THR:HG22	1.99	0.43
2:0:217:SER:OG	39:g:314:II0:C15	2.66	0.43
33:4:310:CLA:HMB1	35:4:311:8CT:C39	2.49	0.43
33:7:305:CLA:HBC1	39:7:316:II0:C27	2.48	0.43
10:D:212:ILE:HG21	36:D:407:PL9:HC8	2.01	0.43
6:g:128:GLY:HA3	33:g:305:CLA:HMD3	2.00	0.43
6:g:195:ILE:HG23	6:g:196:HIS:N	2.34	0.43
7:p:83:ASP:C	7:p:85:ARG:N	2.74	0.43
7:p:200:MET:HB3	39:p:315:II0:C41	2.48	0.43
7:6:96:ARG:HG2	33:6:309:CLA:C3C	2.49	0.43
7:6:215:ARG:HD3	7:6:219:GLU:HG2	1.99	0.43
33:7:305:CLA:CBB	33:c:514:CLA:H13	2.48	0.43
8:B:103:LEU:HD21	33:B:606:CLA:HMC3	2.00	0.43
9:C:135:ILE:HG12	28:Z:27:LEU:HD22	1.99	0.43
8:b:103:LEU:HD21	33:b:606:CLA:HMC3	2.00	0.43
7:p:96:ARG:HG2	33:p:309:CLA:C3C	2.49	0.43
1:A:183:MET:HG2	33:A:412:CLA:HBC1	2.00	0.43
6:5:205:VAL:HG23	6:5:206:LEU:N	2.33	0.43
7:6:149:GLU:OE2	33:6:308:CLA:NB	2.51	0.43
7:6:200:MET:HB3	39:6:315:II0:C41	2.48	0.43
8:B:433:ASP:OD2	8:B:436:THR:OG1	2.30	0.43
19:N:244:LEU:HD12	17:l:12:GLU:HB3	2.01	0.43
33:g:302:CLA:C1	39:g:313:II0:C18	2.97	0.43
2:0:128:LEU:HA	2:0:131:ILE:HG12	2.00	0.43
2:0:161:ASP:HB2	19:n:134:LYS:HE3	2.00	0.43
6:5:195:ILE:HG23	6:5:196:HIS:N	2.34	0.43
37:8:315:LHG:H281	37:8:315:LHG:H252	1.82	0.43
19:N:192:GLY:H	19:N:195:ASP:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:41:TYR:HD1	7:p:46:ILE:HG21	1.84	0.43
7:p:99:MET:HE3	33:p:309:CLA:CMC	2.49	0.43
2:0:100:VAL:HG13	2:0:101:GLN:N	2.34	0.42
2:0:115:LEU:HD11	2:0:201:MET:HB3	2.00	0.42
33:0:311:CLA:HMB1	35:0:312:8CT:C39	2.49	0.42
7:6:191:THR:OG1	33:6:310:CLA:HED1	2.19	0.42
7:6:212:LEU:CD1	7:6:212:LEU:C	2.88	0.42
3:7:95:VAL:HG13	3:7:196:MET:HE1	2.01	0.42
18:M:9:LEU:HD21	18:m:12:LEU:CD1	2.49	0.42
18:M:12:LEU:CB	18:M:16:PHE:CE2	2.74	0.42
20:o:228:ASP:OD1	20:o:232:ARG:N	2.46	0.42
2:0:136:GLY:O	2:0:137:ALA:C	2.58	0.42
2:0:167:LEU:HA	19:n:106:TYR:CD1	2.54	0.42
33:1:305:CLA:CBB	33:C:514:CLA:H13	2.48	0.42
2:4:46:ALA:HB2	2:4:64:VAL:HG23	2.01	0.42
2:4:200:GLN:NE2	33:4:309:CLA:C4D	2.70	0.42
7:6:152:SER:HB2	7:6:171:PHE:HE2	1.84	0.42
9:C:61:VAL:HG21	9:C:125:LEU:HD12	2.00	0.42
33:N:303:CLA:HBB1	33:N:303:CLA:HMB3	2.01	0.42
21:Q:137:GLU:N	21:Q:137:GLU:OE2	2.52	0.42
8:b:372:ASP:O	8:b:375:GLY:N	2.42	0.42
10:d:212:ILE:HG21	36:d:407:PL9:HC8	2.01	0.42
7:p:191:THR:OG1	33:p:310:CLA:HED1	2.19	0.42
21:q:132:ARG:NH1	21:q:169:ASP:OD2	2.45	0.42
1:A:104:GLU:HB2	20:O:144:MET:O	2.18	0.42
33:B:618:CLA:HHC	33:B:618:CLA:CBB	2.49	0.42
8:b:453:PHE:O	8:b:457:ASN:ND2	2.53	0.42
6:g:88:HIS:HB3	6:g:188:MET:HE1	2.01	0.42
13:h:49:TYR:CD2	43:h:101:DGD:C2G	2.99	0.42
33:0:308:CLA:HBB1	33:0:308:CLA:HMB3	2.01	0.42
6:5:88:HIS:HB3	6:5:188:MET:HE1	2.01	0.42
33:5:302:CLA:C1	39:5:313:II0:C18	2.97	0.42
3:7:180:LEU:HD11	3:7:184:LYS:HD2	2.01	0.42
33:B:611:CLA:H141	33:B:613:CLA:HBD	2.01	0.42
12:F:24:ALA:HB1	44:F:101:HEM:HAC	2.01	0.42
41:J:101:SQD:O10	27:Y:6:THR:HG23	2.20	0.42
18:M:32:ARG:HG3	18:m:31:SER:O	2.19	0.42
19:N:124:GLU:O	19:N:127:PRO:HD3	2.19	0.42
19:N:173:ALA:HA	19:N:190:LEU:HD22	1.99	0.42
19:N:175:MET:O	19:N:175:MET:SD	2.78	0.42
9:c:135:ILE:HG12	28:z:27:LEU:HD22	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:n:122:VAL:CG2	19:n:126:ALA:HB3	2.50	0.42
19:n:192:GLY:O	19:n:193:ALA:C	2.61	0.42
1:a:183:MET:HG2	33:a:412:CLA:HBC1	2.00	0.42
2:0:166:PRO:C	19:n:106:TYR:CE2	2.98	0.42
3:1:95:VAL:HG13	3:1:196:MET:HE1	2.01	0.42
7:6:214:GLY:C	7:6:231:LEU:HD12	2.44	0.42
4:8:117:PRO:O	39:8:312:II0:O02	2.37	0.42
17:l:12:GLU:HA	18:m:29:SER:HB3	2.02	0.42
21:q:112:LEU:HB3	21:q:188:ARG:HG2	2.01	0.42
2:0:56:LEU:HD11	33:0:302:CLA:HAA1	2.02	0.42
2:4:128:LEU:HA	2:4:131:ILE:HG12	2.00	0.42
24:V:152:SER:CB	24:V:155:LYS:HB2	2.49	0.42
41:j:101:SQD:O10	27:y:6:THR:HG23	2.20	0.42
7:p:83:ASP:O	7:p:84:LEU:C	2.63	0.42
33:p:306:CLA:CHD	39:p:317:II0:C38	2.97	0.42
21:q:137:GLU:N	21:q:137:GLU:OE2	2.52	0.42
2:4:108:LEU:HB2	2:4:111:PHE:CG	2.54	0.42
8:B:453:PHE:O	8:B:457:ASN:ND2	2.53	0.42
42:W:101:LMG:H171	42:W:101:LMG:H202	1.18	0.42
9:c:464:GLU:OE2	10:d:244:SER:OG	2.32	0.42
7:p:40:LEU:HD12	7:p:47:GLN:NE2	2.35	0.42
4:2:133:ILE:HA	33:2:305:CLA:HBC3	2.02	0.42
5:3:56:GLN:HE22	5:3:63:PRO:HG3	1.85	0.42
2:4:100:VAL:HG13	2:4:101:GLN:N	2.34	0.42
2:4:164:PHE:CZ	2:4:166:PRO:HG2	2.55	0.42
33:6:306:CLA:CHD	39:6:317:II0:C38	2.97	0.42
10:D:350:ALA:O	10:D:351:LEU:C	2.62	0.42
24:V:146:LEU:O	24:V:150:LYS:NZ	2.52	0.42
9:c:61:VAL:HG21	9:c:125:LEU:HD12	2.00	0.42
1:a:85:SER:HB2	45:a:506:HOH:O	2.20	0.42
1:A:147:PHE:C	1:A:150:PRO:HD2	2.45	0.42
2:0:214:ASN:O	2:0:215:PHE:C	2.62	0.42
39:5:314:II0:C11	39:5:314:II0:C15	2.96	0.42
7:6:83:ASP:O	7:6:84:LEU:C	2.63	0.42
4:8:133:ILE:HA	33:8:305:CLA:HBC3	2.02	0.42
10:d:350:ALA:O	10:d:351:LEU:C	2.62	0.42
19:n:175:MET:O	19:n:175:MET:SD	2.78	0.42
1:a:134:SER:O	1:a:139:MET:HG2	2.19	0.42
2:0:108:LEU:HB3	2:0:111:PHE:CD1	2.55	0.42
2:0:164:PHE:CZ	39:0:313:II0:C12	3.03	0.42
2:4:60:MET:CB	33:4:302:CLA:HED2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B:623:LHG:H282	18:M:22:LEU:HD21	2.02	0.42
9:C:464:GLU:OE2	10:D:247:THR:OG1	2.35	0.42
18:M:12:LEU:CD1	18:m:9:LEU:HD21	2.50	0.42
6:g:94:LEU:CD1	33:g:307:CLA:HMC1	2.50	0.42
33:p:319:CLA:CAA	33:p:319:CLA:HBD	2.50	0.42
2:0:63:ASP:HB2	33:0:302:CLA:CED	2.49	0.41
37:2:315:LHG:O5	37:2:315:LHG:HC2	2.09	0.41
2:4:212:LEU:CD1	2:4:213:THR:HG23	2.50	0.41
7:6:95:GLY:N	7:6:200:MET:HE2	2.35	0.41
33:6:319:CLA:CAA	33:6:319:CLA:HBD	2.50	0.41
3:7:203:THR:O	3:7:205:GLN:N	2.53	0.41
4:8:113:ASP:OD1	4:8:113:ASP:C	2.63	0.41
18:M:37:SER:O	18:M:37:SER:OG	2.29	0.41
9:c:173:PHE:HE2	9:c:245:ILE:HD12	1.84	0.41
33:a:412:CLA:H92	33:a:412:CLA:C5	2.50	0.41
3:1:180:LEU:HD11	3:1:184:LYS:HD2	2.02	0.41
33:2:303:CLA:CMC	33:2:303:CLA:HBC3	2.50	0.41
2:4:204:THR:O	2:4:206:GLN:N	2.53	0.41
7:6:40:LEU:HD12	7:6:47:GLN:NE2	2.35	0.41
7:6:116:PHE:HD1	7:6:120:PHE:CE2	2.35	0.41
5:9:90:TRP:CD1	19:n:121:GLN:OE1	2.73	0.41
20:O:228:ASP:OD1	20:O:232:ARG:N	2.46	0.41
28:Z:56:ALA:O	28:Z:59:SER:OG	2.33	0.41
7:p:160:THR:C	7:p:162:ASN:N	2.77	0.41
7:p:206:MET:HG2	39:p:314:II0:C11	2.49	0.41
44:v:201:HEM:HMC2	44:v:201:HEM:HBC2	2.01	0.41
3:1:203:THR:O	3:1:205:GLN:N	2.53	0.41
5:3:51:GLN:HG2	5:3:193:LEU:HD22	2.02	0.41
2:4:43:ARG:HH21	2:4:49:PHE:HA	1.86	0.41
7:6:119:GLU:OE2	39:6:317:II0:C12	2.68	0.41
33:8:303:CLA:CMC	33:8:303:CLA:HBC3	2.50	0.41
33:B:615:CLA:OBD	17:L:11:VAL:HG21	2.21	0.41
13:H:21:VAL:C	19:n:198:ALA:HB1	2.46	0.41
19:N:173:ALA:HB2	19:N:196:LYS:HE2	2.01	0.41
19:N:186:LEU:O	19:N:187:TYR:HB2	2.20	0.41
6:g:100:LEU:CD2	6:g:205:VAL:HG21	2.50	0.41
19:n:186:LEU:O	19:n:187:TYR:HB2	2.19	0.41
7:p:132:ALA:C	7:p:134:GLU:N	2.77	0.41
33:A:412:CLA:H92	33:A:412:CLA:C5	2.50	0.41
2:0:46:ALA:HB3	2:0:66:PHE:HB2	2.02	0.41
2:4:140:ILE:CD1	25:W:68:PHE:HE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:94:LEU:CD1	33:5:307:CLA:HMC1	2.50	0.41
6:5:176:TYR:CE1	33:5:307:CLA:H43	2.55	0.41
33:6:305:CLA:CGA	33:6:305:CLA:C1A	2.98	0.41
6:g:176:TYR:CE1	33:g:307:CLA:H43	2.55	0.41
33:g:302:CLA:H12	39:g:313:II0:C06	2.51	0.41
7:p:95:GLY:N	7:p:200:MET:HE2	2.35	0.41
2:0:140:ILE:CD1	25:w:68:PHE:HE2	2.34	0.41
7:6:99:MET:HB3	39:6:314:II0:C42	2.51	0.41
8:B:121:GLU:OE1	13:H:4:ARG:NH1	2.54	0.41
9:C:173:PHE:HE2	9:C:245:ILE:HD12	1.84	0.41
44:V:201:HEM:HMC2	44:V:201:HEM:HBC2	2.01	0.41
37:b:623:LHG:H282	18:m:22:LEU:HD21	2.02	0.41
19:n:73:ILE:HB	21:q:179:LEU:HD13	2.02	0.41
7:p:211:LEU:HD11	33:p:313:CLA:HMD3	2.01	0.41
1:A:85:SER:HB2	45:A:506:HOH:O	2.20	0.41
34:A:407:PHO:C2B	33:A:412:CLA:H12	2.50	0.41
2:4:94:GLY:C	2:4:194:LEU:HD13	2.46	0.41
7:6:120:PHE:HD2	33:6:305:CLA:O1D	2.03	0.41
4:8:103:VAL:O	4:8:107:TYR:N	2.44	0.41
5:9:58:ILE:HG12	33:9:306:CLA:C3C	2.50	0.41
19:N:73:ILE:HB	21:Q:179:LEU:HD13	2.02	0.41
19:N:205:GLN:OE1	8:b:232:GLY:N	2.54	0.41
33:b:615:CLA:OBD	17:l:11:VAL:HG21	2.21	0.41
10:d:248:ALA:CB	36:d:407:PL9:H522	2.50	0.41
2:0:94:GLY:C	2:0:194:LEU:HD13	2.46	0.41
2:0:211:GLN:O	2:0:215:PHE:CA	2.69	0.41
2:4:116:ALA:O	2:4:117:THR:C	2.63	0.41
2:4:214:ASN:HD21	2:4:216:LYS:HD2	1.84	0.41
33:5:302:CLA:H12	39:5:313:II0:C06	2.51	0.41
7:6:227:PHE:HZ	33:6:312:CLA:OBD	2.04	0.41
33:6:313:CLA:H3A	39:6:316:II0:C26	2.51	0.41
8:B:407:ASN:OD1	8:B:408:GLY:N	2.53	0.41
10:D:248:ALA:CB	36:D:407:PL9:H522	2.50	0.41
33:b:614:CLA:H42	33:b:614:CLA:HMA2	2.03	0.41
39:g:314:II0:C15	39:g:314:II0:C11	2.96	0.41
13:h:49:TYR:CD2	43:h:101:DGD:C2B	3.00	0.41
7:p:99:MET:HB3	39:p:314:II0:C42	2.51	0.41
33:p:310:CLA:CAA	33:p:310:CLA:CBD	2.99	0.41
42:w:101:LMG:H171	42:w:101:LMG:H202	1.18	0.41
1:A:141:PRO:O	1:A:142:TRP:HB2	2.20	0.41
1:A:147:PHE:O	1:A:150:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:166:PRO:C	19:n:106:TYR:CD2	2.99	0.41
6:5:164:LEU:HB3	6:5:166:LEU:CD2	2.51	0.41
15:J:34:GLY:O	15:J:37:SER:OG	2.33	0.41
19:N:122:VAL:CG1	33:N:303:CLA:H3A	2.50	0.41
19:N:122:VAL:HG22	33:N:303:CLA:H3A	2.03	0.41
33:p:319:CLA:HED2	33:p:319:CLA:C4D	2.51	0.41
2:0:49:PHE:CD1	2:0:50:LEU:CG	2.99	0.41
4:2:78:PHE:CZ	2:4:167:LEU:CD1	3.00	0.41
4:2:78:PHE:CZ	2:4:167:LEU:HD21	2.56	0.41
4:2:113:ASP:OD1	4:2:113:ASP:C	2.63	0.41
4:2:182:ALA:O	4:2:186:HIS:ND1	2.50	0.41
2:4:53:PRO:HG2	2:4:56:LEU:HD12	2.03	0.41
2:4:60:MET:SD	19:N:135:TYR:CD1	3.13	0.41
2:4:167:LEU:H	39:4:312:II0:C06	2.33	0.41
33:6:310:CLA:CBD	33:6:310:CLA:CAA	2.99	0.41
33:6:319:CLA:HED2	33:6:319:CLA:C4D	2.51	0.41
9:C:180:MET:O	9:C:198:ILE:HG23	2.21	0.41
10:D:122:ILE:HD11	43:H:101:DGD:HAE1	2.02	0.41
24:V:34:ARG:NH1	24:V:47:LEU:O	2.49	0.41
26:X:36:VAL:HG23	26:X:39:THR:OG1	2.21	0.41
8:b:121:GLU:OE1	13:h:4:ARG:NH1	2.54	0.41
8:b:376:ILE:H	8:b:376:ILE:HG13	1.76	0.41
19:n:122:VAL:HG22	19:n:123:THR:O	2.20	0.41
7:p:59:ARG:O	7:p:60:PRO:C	2.64	0.41
7:p:148:LEU:O	7:p:152:SER:OG	2.34	0.41
33:p:305:CLA:CGA	33:p:305:CLA:C1A	2.98	0.41
33:p:313:CLA:H3A	39:p:316:II0:C26	2.51	0.41
34:a:407:PHO:C2B	33:a:412:CLA:H12	2.50	0.41
2:4:98:PHE:CD2	2:4:197:MET:CB	3.04	0.41
2:4:138:ILE:HA	2:4:141:ILE:HB	2.03	0.41
7:6:103:THR:O	7:6:104:GLY:C	2.62	0.41
7:6:116:PHE:CZ	39:6:317:II0:C30	3.04	0.41
7:6:132:ALA:C	7:6:134:GLU:N	2.77	0.41
4:8:182:ALA:O	4:8:186:HIS:ND1	2.50	0.41
8:B:423:LYS:HG2	8:B:429:VAL:HG23	2.03	0.41
10:D:188:HIS:HA	10:D:293:ARG:CD	2.34	0.41
27:Y:14:PHE:O	27:Y:18:THR:HG23	2.20	0.41
8:b:200:SER:OG	33:b:603:CLA:HMB3	2.20	0.41
8:b:377:ILE:HD13	8:b:377:ILE:HA	1.75	0.41
8:b:423:LYS:HG2	8:b:429:VAL:HG23	2.03	0.41
7:p:42:LYS:CB	7:p:46:ILE:HG22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:113:PHE:CE2	33:p:305:CLA:H11	2.50	0.41
1:a:317:TRP:CD2	10:d:179:ARG:HD2	2.38	0.40
2:0:98:PHE:CD2	2:0:197:MET:CB	3.04	0.40
2:0:177:ARG:HH12	19:n:131:LEU:HD23	1.86	0.40
38:0:305:KC2:CHD	39:0:316:II0:C35	2.99	0.40
3:1:210:GLN:NE2	33:1:308:CLA:O1D	2.54	0.40
37:1:317:LHG:H322	4:2:140:ALA:HB1	2.02	0.40
2:4:172:ASP:HB3	2:4:175:ALA:CB	2.51	0.40
7:6:68:VAL:HG22	7:6:69:GLY:N	2.37	0.40
3:7:210:GLN:NE2	33:7:308:CLA:O1D	2.54	0.40
37:7:317:LHG:H322	4:8:140:ALA:HB1	2.02	0.40
9:C:316:THR:HG23	9:C:392:ALA:HB1	2.02	0.40
8:b:372:ASP:CB	8:b:378:ARG:HG3	2.45	0.40
9:c:180:MET:O	9:c:198:ILE:HG23	2.21	0.40
7:p:67:LEU:HG	7:p:88:ARG:NH2	2.36	0.40
27:y:34:LEU:HA	27:y:34:LEU:HD23	1.88	0.40
33:A:412:CLA:HED1	36:D:407:PL9:H351	2.03	0.40
3:1:69:VAL:HG21	3:1:71:PHE:CE2	2.56	0.40
2:4:217:SER:HB3	2:4:218:LEU:HD12	2.03	0.40
33:4:302:CLA:H42	33:4:302:CLA:C2B	2.51	0.40
7:6:187:ARG:NH2	38:6:311:KC2:OBD	2.54	0.40
8:B:42:LEU:HD21	8:B:93:PHE:CB	2.51	0.40
8:b:42:LEU:HD21	8:b:93:PHE:CB	2.50	0.40
8:b:369:ILE:O	8:b:369:ILE:HG13	2.21	0.40
8:b:376:ILE:HB	8:b:378:ARG:NH2	2.36	0.40
8:b:407:ASN:OD1	8:b:408:GLY:N	2.53	0.40
44:f:101:HEM:HBB2	44:f:101:HEM:HMB1	2.03	0.40
33:g:307:CLA:CMC	39:g:312:II0:C31	3.00	0.40
7:p:187:ARG:NH2	38:p:311:KC2:OBD	2.54	0.40
26:x:36:VAL:HG23	26:x:39:THR:OG1	2.21	0.40
2:4:167:LEU:O	39:4:312:II0:O02	2.39	0.40
2:4:196:GLY:O	2:4:200:GLN:CG	2.70	0.40
6:5:96:VAL:HG21	6:5:190:ALA:HB3	2.03	0.40
3:7:69:VAL:HG21	3:7:71:PHE:CE2	2.56	0.40
9:C:33:PHE:O	9:C:41:ARG:NH1	2.55	0.40
9:C:308:GLU:OE2	9:C:365:TRP:NE1	2.52	0.40
20:O:146:ARG:HG3	20:O:146:ARG:O	2.21	0.40
9:c:316:THR:HG23	9:c:392:ALA:HB1	2.02	0.40
2:0:196:GLY:O	2:0:200:GLN:CG	2.70	0.40
33:0:302:CLA:H42	33:0:302:CLA:C2B	2.51	0.40
3:1:89:ARG:NE	3:1:182:GLU:OE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:4:304:CLA:HBA2	33:4:304:CLA:C4A	2.52	0.40
33:9:309:CLA:H62	33:9:309:CLA:H41	1.96	0.40
8:B:103:LEU:HD22	33:B:607:CLA:H41	2.04	0.40
19:N:234:PHE:CD2	22:t:31:LYS:HD3	2.56	0.40
8:b:462:PHE:CE2	33:b:614:CLA:HMB3	2.57	0.40
1:a:140:ARG:HH22	37:d:401:LHG:C4	2.34	0.40
1:a:302:PHE:CZ	43:c:521:DGD:HG12	2.56	0.40
33:0:304:CLA:HBA2	33:0:304:CLA:C4A	2.52	0.40
2:4:68:PRO:HD2	39:4:313:II0:O02	2.21	0.40
33:5:307:CLA:CMC	39:5:312:II0:C31	3.00	0.40
7:6:49:LEU:HD21	7:6:65:GLY:CA	2.52	0.40
7:6:125:MET:HE3	7:6:125:MET:HB3	1.77	0.40
7:6:212:LEU:HD12	7:6:213:VAL:CA	2.52	0.40
8:b:103:LEU:HD22	33:b:607:CLA:H41	2.04	0.40
10:d:122:ILE:HD11	43:h:101:DGD:HAE1	2.02	0.40
6:g:96:VAL:HG21	6:g:190:ALA:HB3	2.03	0.40
19:n:135:TYR:CE1	19:n:137:PRO:HB3	2.54	0.40
7:p:94:HIS:CD2	33:p:303:CLA:HBB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/360 (92%)	322 (97%)	10 (3%)	0	100	100
1	a	332/360 (92%)	322 (97%)	9 (3%)	1 (0%)	36	53
2	0	175/219 (80%)	167 (95%)	8 (5%)	0	100	100
2	4	175/219 (80%)	165 (94%)	9 (5%)	1 (1%)	21	36
3	1	173/218 (79%)	171 (99%)	2 (1%)	0	100	100
3	7	173/218 (79%)	171 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	2	185/200 (92%)	180 (97%)	5 (3%)	0	100	100
4	8	185/200 (92%)	181 (98%)	4 (2%)	0	100	100
5	3	183/229 (80%)	173 (94%)	9 (5%)	1 (0%)	24	41
5	9	183/229 (80%)	173 (94%)	10 (6%)	0	100	100
6	5	168/216 (78%)	164 (98%)	4 (2%)	0	100	100
6	g	168/216 (78%)	163 (97%)	5 (3%)	0	100	100
7	6	190/234 (81%)	181 (95%)	8 (4%)	1 (0%)	24	41
7	p	190/234 (81%)	183 (96%)	7 (4%)	0	100	100
8	B	501/509 (98%)	490 (98%)	11 (2%)	0	100	100
8	b	501/509 (98%)	488 (97%)	13 (3%)	0	100	100
9	C	449/473 (95%)	439 (98%)	10 (2%)	0	100	100
9	c	449/473 (95%)	439 (98%)	10 (2%)	0	100	100
10	D	340/351 (97%)	330 (97%)	10 (3%)	0	100	100
10	d	340/351 (97%)	330 (97%)	10 (3%)	0	100	100
11	E	73/84 (87%)	73 (100%)	0	0	100	100
11	e	73/84 (87%)	73 (100%)	0	0	100	100
12	F	27/42 (64%)	27 (100%)	0	0	100	100
12	f	27/42 (64%)	27 (100%)	0	0	100	100
13	H	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
13	h	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
14	I	33/38 (87%)	33 (100%)	0	0	100	100
14	i	33/38 (87%)	33 (100%)	0	0	100	100
15	J	32/39 (82%)	32 (100%)	0	0	100	100
15	j	32/39 (82%)	32 (100%)	0	0	100	100
16	K	35/45 (78%)	33 (94%)	2 (6%)	0	100	100
16	k	35/45 (78%)	33 (94%)	2 (6%)	0	100	100
17	L	35/38 (92%)	35 (100%)	0	0	100	100
17	l	35/38 (92%)	35 (100%)	0	0	100	100
18	M	35/37 (95%)	35 (100%)	0	0	100	100
18	m	35/37 (95%)	35 (100%)	0	0	100	100
19	N	188/297 (63%)	171 (91%)	16 (8%)	1 (0%)	24	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	n	188/297 (63%)	172 (92%)	16 (8%)	0	100	100
20	O	260/300 (87%)	256 (98%)	4 (2%)	0	100	100
20	o	260/300 (87%)	255 (98%)	4 (2%)	1 (0%)	30	47
21	Q	141/144 (98%)	138 (98%)	3 (2%)	0	100	100
21	q	141/144 (98%)	138 (98%)	3 (2%)	0	100	100
22	T	29/32 (91%)	29 (100%)	0	0	100	100
22	t	29/32 (91%)	29 (100%)	0	0	100	100
23	U	91/121 (75%)	87 (96%)	4 (4%)	0	100	100
23	u	91/121 (75%)	87 (96%)	4 (4%)	0	100	100
24	V	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
24	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
25	W	47/130 (36%)	47 (100%)	0	0	100	100
25	w	47/130 (36%)	47 (100%)	0	0	100	100
26	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
26	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
27	Y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
27	y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
28	Z	59/62 (95%)	59 (100%)	0	0	100	100
28	z	59/62 (95%)	59 (100%)	0	0	100	100
All	All	8096/9442 (86%)	7858 (97%)	232 (3%)	6 (0%)	49	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	3	57	ALA
20	o	147	ALA
7	6	174	ASP
1	a	141	PRO
2	4	208	PRO
19	N	137	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/289 (93%)	270 (100%)	0	100	100
1	a	270/289 (93%)	269 (100%)	1 (0%)	84	92
2	0	143/171 (84%)	140 (98%)	3 (2%)	47	72
2	4	143/171 (84%)	142 (99%)	1 (1%)	76	89
3	1	143/173 (83%)	143 (100%)	0	100	100
3	7	143/173 (83%)	143 (100%)	0	100	100
4	2	156/166 (94%)	155 (99%)	1 (1%)	78	90
4	8	156/166 (94%)	156 (100%)	0	100	100
5	3	145/172 (84%)	145 (100%)	0	100	100
5	9	145/172 (84%)	145 (100%)	0	100	100
6	5	136/167 (81%)	134 (98%)	2 (2%)	57	79
6	g	136/167 (81%)	136 (100%)	0	100	100
7	6	147/178 (83%)	139 (95%)	8 (5%)	20	39
7	p	147/178 (83%)	142 (97%)	5 (3%)	32	57
8	B	400/404 (99%)	400 (100%)	0	100	100
8	b	400/404 (99%)	398 (100%)	2 (0%)	81	91
9	C	356/378 (94%)	356 (100%)	0	100	100
9	c	356/378 (94%)	356 (100%)	0	100	100
10	D	274/281 (98%)	274 (100%)	0	100	100
10	d	274/281 (98%)	274 (100%)	0	100	100
11	E	67/73 (92%)	67 (100%)	0	100	100
11	e	67/73 (92%)	67 (100%)	0	100	100
12	F	24/37 (65%)	24 (100%)	0	100	100
12	f	24/37 (65%)	24 (100%)	0	100	100
13	H	56/58 (97%)	56 (100%)	0	100	100
13	h	56/58 (97%)	56 (100%)	0	100	100
14	I	33/36 (92%)	33 (100%)	0	100	100
14	i	33/36 (92%)	33 (100%)	0	100	100
15	J	26/29 (90%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	j	26/29 (90%)	26 (100%)	0	100 100
16	K	30/36 (83%)	30 (100%)	0	100 100
16	k	30/36 (83%)	30 (100%)	0	100 100
17	L	34/35 (97%)	34 (100%)	0	100 100
17	l	34/35 (97%)	34 (100%)	0	100 100
18	M	31/31 (100%)	31 (100%)	0	100 100
18	m	31/31 (100%)	31 (100%)	0	100 100
19	N	153/231 (66%)	153 (100%)	0	100 100
19	n	153/231 (66%)	152 (99%)	1 (1%)	76 89
20	O	214/239 (90%)	213 (100%)	1 (0%)	81 91
20	o	214/239 (90%)	214 (100%)	0	100 100
21	Q	113/113 (100%)	113 (100%)	0	100 100
21	q	113/113 (100%)	113 (100%)	0	100 100
22	T	26/27 (96%)	26 (100%)	0	100 100
22	t	26/27 (96%)	26 (100%)	0	100 100
23	U	80/96 (83%)	80 (100%)	0	100 100
23	u	80/96 (83%)	79 (99%)	1 (1%)	61 81
24	V	118/141 (84%)	118 (100%)	0	100 100
24	v	118/141 (84%)	118 (100%)	0	100 100
25	W	42/101 (42%)	42 (100%)	0	100 100
25	w	42/101 (42%)	42 (100%)	0	100 100
26	X	34/34 (100%)	34 (100%)	0	100 100
26	x	34/34 (100%)	34 (100%)	0	100 100
27	Y	29/29 (100%)	29 (100%)	0	100 100
27	y	29/29 (100%)	29 (100%)	0	100 100
28	Z	50/51 (98%)	50 (100%)	0	100 100
28	z	50/51 (98%)	50 (100%)	0	100 100
All	All	6660/7552 (88%)	6634 (100%)	26 (0%)	81 92

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	143	ILE

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Mol	Chain	Res	Type
2	0	108	LEU
2	0	115	LEU
2	0	162	LEU
4	2	126	LYS
2	4	59	SER
6	5	169	ASP
6	5	202	LYS
7	6	68	VAL
7	6	81	TRP
7	6	125	MET
7	6	167	GLN
7	6	174	ASP
7	6	176	LEU
7	6	218	ILE
7	6	229	ASN
20	O	326	GLU
8	b	373	LYS
8	b	377	ILE
19	n	124	GLU
7	p	54	ILE
7	p	68	VAL
7	p	81	TRP
7	p	218	ILE
7	p	231	LEU
23	u	109	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	303	ASN
1	A	303	ASN
2	0	73	ASN
2	0	101	GLN
2	0	105	ASN
2	0	143	ASN
2	0	200	GLN
2	0	206	GLN
2	0	211	GLN
3	1	199	GLN
5	3	112	GLN
2	4	101	GLN
2	4	143	ASN

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Mol	Chain	Res	Type
2	4	200	GLN
2	4	214	ASN
6	5	197	GLN
6	5	203	GLN
7	6	47	GLN
7	6	130	ASN
3	7	199	GLN
5	9	112	GLN
8	B	455	HIS
8	B	457	ASN
8	B	466	HIS
9	C	385	GLN
9	C	418	ASN
10	D	116	HIS
10	D	193	ASN
10	D	349	ASN
20	O	295	GLN
23	U	48	ASN
24	V	148	GLN
8	b	455	HIS
8	b	457	ASN
8	b	466	HIS
9	c	418	ASN
10	d	116	HIS
10	d	193	ASN
10	d	349	ASN
11	e	54	ASN
6	g	197	GLN
6	g	203	GLN
20	o	295	GLN
7	p	47	GLN
7	p	130	ASN
7	p	195	ASN
23	u	48	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 380 ligands modelled in this entry, 4 are monoatomic - leaving 376 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	CLA	8	307	-	64,68,73	1.81	9 (14%)	77,107,113	1.43	6 (7%)
33	CLA	5	301	6	46,50,73	2.14	9 (19%)	55,85,113	1.69	8 (14%)
33	CLA	7	306	-	64,68,73	1.80	9 (14%)	77,107,113	1.46	6 (7%)
39	II0	5	314	-	39,43,43	0.37	0	50,60,60	1.06	2 (4%)
41	SQD	L	101	-	53,54,54	1.20	4 (7%)	62,65,65	1.08	4 (6%)
33	CLA	B	611	45	69,73,73	1.77	9 (13%)	83,113,113	1.46	11 (13%)
33	CLA	p	306	-	49,53,73	2.00	9 (18%)	59,89,113	1.67	11 (18%)
40	IHT	8	314	-	40,42,42	0.19	0	53,58,58	0.55	1 (1%)
38	KC2	0	305	-	49,53,53	1.85	4 (8%)	62,89,89	1.47	8 (12%)
35	8CT	b	619	-	40,41,41	0.21	0	50,56,56	0.42	0
39	II0	7	313	-	39,43,43	0.24	0	50,60,60	0.58	0
35	8CT	h	102	-	40,41,41	0.22	0	50,56,56	0.43	0
33	CLA	g	306	6	49,53,73	2.06	9 (18%)	59,89,113	1.67	7 (11%)
33	CLA	8	304	4	64,68,73	1.83	9 (14%)	77,107,113	1.49	7 (9%)
33	CLA	0	311	2	49,53,73	2.15	9 (18%)	59,89,113	1.85	10 (16%)
36	PL9	a	410	-	30,30,55	0.92	1 (3%)	38,39,69	1.33	6 (15%)
33	CLA	N	303	37	51,55,73	2.04	9 (17%)	61,91,113	1.92	13 (21%)
37	LHG	5	316	-	21,21,48	0.78	0	23,26,54	1.26	2 (8%)
33	CLA	9	314	5	45,49,73	2.27	10 (22%)	54,84,113	1.85	8 (14%)
33	CLA	A	412	-	69,73,73	1.79	9 (13%)	83,113,113	1.60	12 (14%)
33	CLA	1	304	-	59,63,73	1.89	9 (15%)	71,101,113	1.50	7 (9%)
33	CLA	0	308	37	51,55,73	2.04	9 (17%)	61,91,113	1.92	13 (21%)
33	CLA	B	618	33	43,48,73	2.27	9 (20%)	52,82,113	1.98	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	IHT	5	315	-	40,42,42	0.22	0	53,58,58	0.42	0
33	CLA	3	305	5	59,63,73	1.88	9 (15%)	71,101,113	1.48	6 (8%)
35	8CT	B	620	-	40,41,41	0.23	0	50,56,56	0.51	0
33	CLA	b	611	45	69,73,73	1.77	9 (13%)	83,113,113	1.46	11 (13%)
35	8CT	y	101	-	40,41,41	0.23	0	50,56,56	0.51	0
33	CLA	6	306	-	49,53,73	2.01	9 (18%)	59,89,113	1.68	11 (18%)
33	CLA	p	309	7	46,50,73	2.12	9 (19%)	55,85,113	1.83	10 (18%)
33	CLA	c	511	9	69,73,73	1.73	9 (13%)	83,113,113	1.37	6 (7%)
29	OEX	a	401	1,9,45	0,14,14	-	-	-		
33	CLA	B	610	-	69,73,73	1.72	9 (13%)	83,113,113	1.39	8 (9%)
33	CLA	3	307	5	49,53,73	2.08	9 (18%)	59,89,113	1.77	8 (13%)
39	II0	8	311	-	39,43,43	0.24	0	50,60,60	0.53	1 (2%)
37	LHG	d	402	-	46,46,48	0.69	0	49,52,54	1.14	3 (6%)
34	PHO	a	407	-	58,69,69	1.10	2 (3%)	56,99,99	1.20	7 (12%)
33	CLA	5	310	-	45,49,73	2.31	10 (22%)	54,84,113	1.85	8 (14%)
39	II0	7	315	-	39,43,43	0.18	0	50,60,60	0.60	2 (4%)
33	CLA	3	306	-	45,49,73	2.31	10 (22%)	54,84,113	1.91	8 (14%)
35	8CT	b	620	-	40,41,41	0.23	0	50,56,56	0.51	0
33	CLA	A	408	1	64,68,73	1.81	9 (14%)	77,107,113	1.47	6 (7%)
34	PHO	A	407	-	58,69,69	1.09	2 (3%)	56,99,99	1.20	7 (12%)
39	II0	3	301	-	39,43,43	0.22	0	50,60,60	0.52	0
33	CLA	5	305	6	43,48,73	2.20	9 (20%)	52,82,113	1.81	10 (19%)
39	II0	1	316	-	39,43,43	0.23	0	50,60,60	0.58	0
29	OEX	A	401	1,9,45	0,14,14	-	-	-		
33	CLA	4	302	2	55,59,73	1.95	9 (16%)	66,96,113	1.68	8 (12%)
38	KC2	8	309	4	49,53,53	1.90	4 (8%)	62,89,89	1.36	8 (12%)
33	CLA	1	306	-	64,68,73	1.80	9 (14%)	77,107,113	1.46	6 (7%)
33	CLA	7	304	-	59,63,73	1.88	9 (15%)	71,101,113	1.50	7 (9%)
39	II0	3	317	-	39,43,43	0.23	0	50,60,60	0.63	1 (2%)
33	CLA	7	301	3	49,53,73	2.09	9 (18%)	59,89,113	1.78	8 (13%)
39	II0	4	314	-	39,43,43	0.37	0	50,60,60	0.54	1 (2%)
33	CLA	C	514	9	69,73,73	1.78	9 (13%)	83,113,113	1.33	6 (7%)
33	CLA	B	606	8	69,73,73	1.76	10 (14%)	83,113,113	1.47	8 (9%)
33	CLA	B	608	-	69,73,73	1.74	9 (13%)	83,113,113	1.38	5 (6%)
33	CLA	N	305	-	59,63,73	1.93	9 (15%)	71,101,113	1.48	10 (14%)
33	CLA	8	308	-	59,63,73	1.87	9 (15%)	71,101,113	1.43	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	6	308	7	46,50,73	2.07	9 (19%)	55,85,113	1.83	11 (20%)
42	LMG	b	624	-	43,43,55	0.80	1 (2%)	51,51,63	1.25	5 (9%)
33	CLA	7	302	3	68,72,73	1.78	9 (13%)	81,111,113	1.58	11 (13%)
37	LHG	3	321	-	23,23,48	0.86	0	26,29,54	1.21	1 (3%)
39	II0	1	314	-	39,43,43	0.26	0	50,60,60	0.51	1 (2%)
33	CLA	C	507	9	69,73,73	1.74	9 (13%)	83,113,113	1.44	8 (9%)
33	CLA	4	303	2	54,58,73	2.00	9 (16%)	65,95,113	1.63	8 (12%)
33	CLA	3	310	-	45,49,73	2.23	10 (22%)	54,84,113	1.72	5 (9%)
33	CLA	5	306	6	49,53,73	2.06	9 (18%)	59,89,113	1.67	7 (11%)
33	CLA	0	302	2	55,59,73	1.94	9 (16%)	66,96,113	1.68	7 (10%)
33	CLA	g	301	6	46,50,73	2.14	9 (19%)	55,85,113	1.69	8 (14%)
42	LMG	d	409	-	46,46,55	0.77	0	54,54,63	1.21	2 (3%)
33	CLA	3	308	-	53,57,73	1.93	9 (16%)	62,93,113	1.64	9 (14%)
33	CLA	c	506	-	69,73,73	1.71	9 (13%)	83,113,113	1.37	7 (8%)
31	BCT	a	403	30	2,3,3	1.26	0	2,3,3	4.17	2 (100%)
39	II0	4	312	-	39,43,43	0.36	0	50,60,60	0.56	0
39	II0	3	316	-	39,43,43	0.28	0	50,60,60	0.63	1 (2%)
33	CLA	4	310	2	49,53,73	2.14	9 (18%)	59,89,113	1.84	9 (15%)
33	CLA	6	303	7	45,49,73	2.31	10 (22%)	54,84,113	1.88	9 (16%)
33	CLA	a	406	45	53,57,73	2.04	9 (16%)	62,93,113	1.65	8 (12%)
33	CLA	B	614	8	69,73,73	1.73	9 (13%)	83,113,113	1.43	11 (13%)
33	CLA	9	303	5	59,63,73	1.88	9 (15%)	71,101,113	1.58	10 (14%)
33	CLA	0	304	-	51,55,73	2.03	9 (17%)	61,91,113	1.69	8 (13%)
33	CLA	b	605	8	69,73,73	1.69	9 (13%)	83,113,113	1.33	6 (7%)
33	CLA	5	302	6	59,63,73	1.92	9 (15%)	71,101,113	1.67	13 (18%)
39	II0	8	312	-	39,43,43	0.20	0	50,60,60	0.87	3 (6%)
37	LHG	D	402	-	46,46,48	0.69	0	49,52,54	1.14	3 (6%)
43	DGD	C	518	-	56,56,67	0.88	1 (1%)	70,70,81	1.44	11 (15%)
33	CLA	A	406	45	53,57,73	2.04	9 (16%)	62,93,113	1.65	8 (12%)
33	CLA	2	310	-	50,54,73	2.08	9 (18%)	60,90,113	1.74	8 (13%)
33	CLA	n	303	6	45,49,73	2.31	10 (22%)	54,84,113	1.89	9 (16%)
33	CLA	C	504	-	69,73,73	1.73	9 (13%)	83,113,113	1.34	5 (6%)
33	CLA	5	317	-	43,48,73	2.28	9 (20%)	52,82,113	1.89	10 (19%)
37	LHG	0	317	33	23,23,48	0.90	0	26,29,54	1.23	1 (3%)
37	LHG	D	401	-	45,45,48	0.66	1 (2%)	48,51,54	1.18	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	KC2	7	311	-	49,53,53	1.88	4 (8%)	62,89,89	1.33	8 (12%)
43	DGD	c	518	-	56,56,67	0.88	1 (1%)	70,70,81	1.44	11 (15%)
38	KC2	p	311	7	49,53,53	1.83	4 (8%)	62,89,89	1.45	10 (16%)
33	CLA	1	309	3	59,63,73	1.88	9 (15%)	71,101,113	1.44	6 (8%)
33	CLA	C	513	9	60,64,73	1.89	9 (15%)	72,102,113	1.51	7 (9%)
43	DGD	c	521	-	63,63,67	0.92	2 (3%)	77,77,81	1.33	8 (10%)
33	CLA	c	507	9	69,73,73	1.74	9 (13%)	83,113,113	1.45	8 (9%)
33	CLA	N	307	-	54,58,73	2.01	9 (16%)	65,95,113	1.63	10 (15%)
40	IHT	p	318	-	40,42,42	0.32	0	53,58,58	0.45	0
35	8CT	c	515	-	40,41,41	0.45	1 (2%)	50,56,56	0.64	0
35	8CT	Y	101	-	40,41,41	0.22	0	50,56,56	0.51	0
33	CLA	B	615	8	49,53,73	2.12	9 (18%)	59,89,113	1.78	8 (13%)
33	CLA	g	317	-	43,48,73	2.27	9 (20%)	52,82,113	1.89	10 (19%)
37	LHG	D	408	-	48,48,48	0.66	1 (2%)	51,54,54	1.13	2 (3%)
33	CLA	g	310	-	45,49,73	2.30	10 (22%)	54,84,113	1.84	8 (14%)
33	CLA	B	612	-	69,73,73	1.75	9 (13%)	83,113,113	1.43	7 (8%)
33	CLA	9	307	5	49,53,73	2.09	9 (18%)	59,89,113	1.77	8 (13%)
33	CLA	n	305	-	59,63,73	1.89	9 (15%)	71,101,113	1.55	8 (11%)
41	SQD	b	601	-	37,38,54	1.40	4 (10%)	46,49,65	1.09	5 (10%)
39	II0	9	319	-	39,43,43	0.22	0	50,60,60	0.68	3 (6%)
33	CLA	3	309	5	59,63,73	1.92	9 (15%)	71,101,113	1.65	10 (14%)
33	CLA	6	302	7	45,49,73	2.38	10 (22%)	54,84,113	1.92	10 (18%)
33	CLA	1	302	3	68,72,73	1.78	9 (13%)	81,111,113	1.57	11 (13%)
39	II0	0	313	-	39,43,43	0.36	0	50,60,60	0.56	0
42	LMG	l	102	-	38,38,55	0.96	1 (2%)	46,46,63	1.23	6 (13%)
33	CLA	p	310	-	45,49,73	2.30	10 (22%)	54,84,113	1.76	11 (20%)
33	CLA	8	301	4	49,53,73	2.11	9 (18%)	59,89,113	1.71	8 (13%)
33	CLA	0	310	2	43,48,73	2.22	9 (20%)	52,82,113	2.03	12 (23%)
33	CLA	4	306	2	59,63,73	1.87	9 (15%)	71,101,113	1.50	11 (15%)
41	SQD	B	601	-	37,38,54	1.40	4 (10%)	46,49,65	1.09	5 (10%)
38	KC2	4	305	-	49,53,53	1.85	4 (8%)	62,89,89	1.47	9 (14%)
33	CLA	p	305	7	59,63,73	1.81	9 (15%)	71,101,113	1.45	8 (11%)
40	IHT	6	318	-	40,42,42	0.32	0	53,58,58	0.45	0
33	CLA	8	306	4	64,68,73	1.80	9 (14%)	77,107,113	1.54	9 (11%)
33	CLA	2	303	4	56,60,73	1.99	9 (16%)	67,97,113	1.78	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	B	603	-	69,73,73	1.74	9 (13%)	83,113,113	1.44	8 (9%)
33	CLA	d	404	-	69,73,73	1.73	9 (13%)	83,113,113	1.48	8 (9%)
37	LHG	3	322	-	40,40,48	0.70	2 (5%)	43,46,54	1.23	4 (9%)
33	CLA	B	602	33	54,58,73	1.98	9 (16%)	65,95,113	1.53	8 (12%)
33	CLA	D	405	-	69,73,73	1.74	9 (13%)	83,113,113	1.39	5 (6%)
33	CLA	N	304	6	45,49,73	2.31	10 (22%)	54,84,113	1.89	9 (16%)
35	8CT	C	516	-	40,41,41	0.19	0	50,56,56	0.39	0
39	II0	g	314	-	39,43,43	0.37	0	50,60,60	1.06	2 (4%)
33	CLA	8	302	4	59,63,73	1.91	9 (15%)	71,101,113	1.76	12 (16%)
33	CLA	g	308	-	45,49,73	2.29	10 (22%)	54,84,113	1.82	8 (14%)
33	CLA	C	505	-	69,73,73	1.78	9 (13%)	83,113,113	1.44	8 (9%)
33	CLA	3	312	5	59,63,73	1.89	9 (15%)	71,101,113	1.53	8 (11%)
39	II0	p	315	-	39,43,43	0.33	0	50,60,60	0.54	1 (2%)
35	8CT	0	312	-	40,41,41	0.32	0	50,56,56	0.35	0
37	LHG	1	317	-	48,48,48	0.62	0	51,54,54	1.24	6 (11%)
33	CLA	4	309	2	43,48,73	2.22	9 (20%)	52,82,113	2.03	12 (23%)
39	II0	9	301	-	39,43,43	0.22	0	50,60,60	0.52	0
39	II0	7	314	-	39,43,43	0.25	0	50,60,60	0.52	1 (2%)
40	IHT	2	314	-	40,42,42	0.19	0	53,58,58	0.55	1 (1%)
33	CLA	9	310	-	45,49,73	2.22	10 (22%)	54,84,113	1.71	5 (9%)
33	CLA	3	303	5	59,63,73	1.88	9 (15%)	71,101,113	1.58	10 (14%)
35	8CT	A	409	-	40,41,41	0.20	0	50,56,56	0.38	0
33	CLA	B	609	8	69,73,73	1.75	9 (13%)	83,113,113	1.43	9 (10%)
33	CLA	3	315	-	45,49,73	2.31	10 (22%)	54,84,113	1.65	7 (12%)
44	HEM	v	201	-	50,50,50	0.66	1 (2%)	66,82,82	0.63	0
39	II0	0	316	-	39,43,43	0.25	0	50,60,60	0.29	0
35	8CT	c	517	-	40,41,41	0.17	0	50,56,56	0.38	0
33	CLA	N	302	19	69,73,73	1.74	9 (13%)	83,113,113	1.42	7 (8%)
33	CLA	c	512	-	69,73,73	1.72	9 (13%)	83,113,113	1.32	8 (9%)
33	CLA	b	618	33	43,48,73	2.26	9 (20%)	52,82,113	1.95	11 (21%)
35	8CT	D	406	-	40,41,41	0.21	0	50,56,56	0.69	1 (2%)
37	LHG	7	317	-	48,48,48	0.62	0	51,54,54	1.25	6 (11%)
42	LMG	m	101	-	38,38,55	0.96	1 (2%)	46,46,63	1.23	6 (13%)
35	8CT	c	516	-	40,41,41	0.19	0	50,56,56	0.39	0
39	II0	6	315	-	39,43,43	0.33	0	50,60,60	0.54	1 (2%)
39	II0	2	313	-	39,43,43	0.20	0	50,60,60	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	C	508	-	69,73,73	1.73	9 (13%)	83,113,113	1.32	8 (9%)
33	CLA	C	506	-	69,73,73	1.72	9 (13%)	83,113,113	1.37	7 (8%)
39	II0	0	315	-	39,43,43	0.37	0	50,60,60	0.55	1 (2%)
33	CLA	g	305	6	43,48,73	2.19	9 (20%)	52,82,113	1.81	10 (19%)
33	CLA	0	307	2	59,63,73	1.92	9 (15%)	71,101,113	1.58	11 (15%)
33	CLA	n	302	19	69,73,73	1.74	9 (13%)	83,113,113	1.42	7 (8%)
38	KC2	5	309	6	49,53,53	1.84	4 (8%)	62,89,89	1.39	7 (11%)
33	CLA	c	513	9	60,64,73	1.89	9 (15%)	72,102,113	1.51	7 (9%)
37	LHG	2	315	-	45,45,48	0.62	0	48,51,54	1.21	4 (8%)
39	II0	5	313	-	39,43,43	0.32	0	50,60,60	0.92	2 (4%)
33	CLA	4	301	2	45,49,73	2.33	10 (22%)	54,84,113	1.88	10 (18%)
38	KC2	3	311	-	49,53,53	1.89	4 (8%)	62,89,89	1.31	9 (14%)
33	CLA	7	305	3	64,68,73	1.83	9 (14%)	77,107,113	1.39	7 (9%)
33	CLA	c	510	9	69,73,73	1.74	9 (13%)	83,113,113	1.40	8 (9%)
35	8CT	4	311	-	40,41,41	0.32	0	50,56,56	0.35	0
33	CLA	B	604	8	69,73,73	1.71	9 (13%)	83,113,113	1.40	6 (7%)
44	HEM	V	201	-	50,50,50	0.66	1 (2%)	66,82,82	0.63	0
43	DGD	h	101	-	61,61,67	0.88	1 (1%)	75,75,81	1.22	5 (6%)
33	CLA	C	503	-	69,73,73	1.69	9 (13%)	83,113,113	1.36	7 (8%)
33	CLA	B	613	8	69,73,73	1.75	9 (13%)	83,113,113	1.38	5 (6%)
35	8CT	B	621	-	40,41,41	0.18	0	50,56,56	0.36	0
39	II0	3	319	-	39,43,43	0.22	0	50,60,60	0.68	2 (4%)
33	CLA	b	612	-	69,73,73	1.76	9 (13%)	83,113,113	1.43	6 (7%)
43	DGD	C	521	-	63,63,67	0.92	2 (3%)	77,77,81	1.33	8 (10%)
37	LHG	b	623	-	48,48,48	0.64	1 (2%)	51,54,54	1.30	6 (11%)
35	8CT	H	102	-	40,41,41	0.22	0	50,56,56	0.43	0
42	LMG	B	622	-	49,49,55	0.77	0	57,57,63	1.21	5 (8%)
33	CLA	3	314	5	45,49,73	2.25	10 (22%)	54,84,113	1.84	8 (14%)
43	DGD	c	519	-	63,63,67	0.91	2 (3%)	77,77,81	1.26	5 (6%)
33	CLA	p	308	7	46,50,73	2.07	9 (19%)	55,85,113	1.83	11 (20%)
36	PL9	d	407	-	55,55,55	0.96	4 (7%)	68,69,69	1.45	11 (16%)
33	CLA	9	305	5	59,63,73	1.88	9 (15%)	71,101,113	1.48	6 (8%)
33	CLA	n	304	-	59,63,73	1.93	9 (15%)	71,101,113	1.47	9 (12%)
33	CLA	9	309	5	59,63,73	1.91	9 (15%)	71,101,113	1.64	10 (14%)
33	CLA	p	307	-	47,51,73	2.10	9 (19%)	56,86,113	1.79	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	g	302	6	59,63,73	1.92	9 (15%)	71,101,113	1.67	13 (18%)
33	CLA	5	307	-	59,63,73	1.88	9 (15%)	71,101,113	1.55	10 (14%)
33	CLA	6	307	7	47,51,73	2.10	9 (19%)	56,86,113	1.79	8 (14%)
33	CLA	C	512	-	69,73,73	1.72	9 (13%)	83,113,113	1.32	9 (10%)
41	SQD	l	101	-	53,54,54	1.20	4 (7%)	62,65,65	1.08	4 (6%)
33	CLA	c	505	-	69,73,73	1.78	9 (13%)	83,113,113	1.44	8 (9%)
33	CLA	8	310	-	50,54,73	2.08	9 (18%)	60,90,113	1.73	8 (13%)
33	CLA	p	319	-	45,49,73	2.31	10 (22%)	54,84,113	1.83	10 (18%)
33	CLA	6	310	-	45,49,73	2.30	10 (22%)	54,84,113	1.76	11 (20%)
35	8CT	C	515	-	40,41,41	0.45	1 (2%)	50,56,56	0.64	0
33	CLA	b	607	-	69,73,73	1.73	9 (13%)	83,113,113	1.38	7 (8%)
33	CLA	b	602	33	54,58,73	1.98	9 (16%)	65,95,113	1.54	7 (10%)
33	CLA	p	304	7	46,50,73	2.21	9 (19%)	55,85,113	1.71	8 (14%)
33	CLA	6	305	7	59,63,73	1.81	9 (15%)	71,101,113	1.45	8 (11%)
33	CLA	C	510	9	69,73,73	1.74	9 (13%)	83,113,113	1.39	8 (9%)
33	CLA	D	404	-	69,73,73	1.73	9 (13%)	83,113,113	1.48	8 (9%)
33	CLA	b	608	-	69,73,73	1.74	9 (13%)	83,113,113	1.38	6 (7%)
33	CLA	6	304	7	46,50,73	2.20	9 (19%)	55,85,113	1.71	8 (14%)
33	CLA	9	304	5	49,53,73	2.08	9 (18%)	59,89,113	1.64	7 (11%)
42	LMG	w	101	-	47,47,55	0.74	0	55,55,63	1.24	2 (3%)
39	II0	0	314	-	39,43,43	0.32	0	50,60,60	0.49	1 (2%)
39	II0	9	316	-	39,43,43	0.28	0	50,60,60	0.63	1 (2%)
39	II0	5	312	-	39,43,43	0.39	0	50,60,60	0.74	3 (6%)
33	CLA	B	607	-	69,73,73	1.73	9 (13%)	83,113,113	1.37	7 (8%)
33	CLA	9	306	5	45,49,73	2.31	10 (22%)	54,84,113	1.92	8 (14%)
37	LHG	a	411	-	23,23,48	0.86	1 (4%)	26,29,54	1.32	2 (7%)
40	IHT	g	315	-	40,42,42	0.22	0	53,58,58	0.41	0
37	LHG	A	411	-	23,23,48	0.86	1 (4%)	26,29,54	1.32	2 (7%)
39	II0	p	316	-	39,43,43	0.32	0	50,60,60	0.71	2 (4%)
33	CLA	p	303	7	45,49,73	2.30	10 (22%)	54,84,113	1.89	8 (14%)
33	CLA	4	308	2	51,55,73	2.05	9 (17%)	61,91,113	1.67	7 (11%)
39	II0	6	316	-	39,43,43	0.33	0	50,60,60	0.71	2 (4%)
39	II0	p	314	-	39,43,43	0.36	0	50,60,60	0.74	1 (2%)
41	SQD	J	101	-	45,46,54	1.26	4 (8%)	54,57,65	1.28	5 (9%)
44	HEM	F	101	11,12	50,50,50	1.59	9 (18%)	66,82,82	1.75	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	LHG	9	321	-	23,23,48	0.86	1 (4%)	26,29,54	1.21	1 (3%)
33	CLA	c	508	-	69,73,73	1.73	9 (13%)	83,113,113	1.32	8 (9%)
33	CLA	8	303	4	56,60,73	1.99	9 (16%)	67,97,113	1.79	9 (13%)
33	CLA	g	311	6	49,53,73	2.12	9 (18%)	59,89,113	1.71	9 (15%)
33	CLA	a	405	1	69,73,73	1.74	9 (13%)	83,113,113	1.43	9 (10%)
33	CLA	2	301	4	49,53,73	2.09	9 (18%)	59,89,113	1.71	7 (11%)
39	II0	9	318	-	39,43,43	0.22	0	50,60,60	0.61	2 (4%)
41	SQD	C	501	-	41,42,54	1.34	4 (9%)	50,53,65	1.26	5 (10%)
33	CLA	2	307	-	64,68,73	1.81	9 (14%)	77,107,113	1.43	6 (7%)
37	LHG	B	623	-	48,48,48	0.64	1 (2%)	51,54,54	1.30	6 (11%)
33	CLA	7	307	-	69,73,73	1.80	9 (13%)	83,113,113	1.51	9 (10%)
42	LMG	d	410	-	46,46,55	0.82	1 (2%)	54,54,63	1.32	6 (11%)
33	CLA	n	306	-	54,58,73	2.01	9 (16%)	65,95,113	1.63	10 (15%)
31	BCT	A	403	30	2,3,3	1.25	0	2,3,3	4.17	2 (100%)
33	CLA	9	312	5	59,63,73	1.89	9 (15%)	71,101,113	1.53	8 (11%)
39	II0	p	301	-	39,43,43	0.33	0	50,60,60	0.55	2 (4%)
39	II0	6	314	-	39,43,43	0.35	0	50,60,60	0.74	1 (2%)
33	CLA	5	308	-	45,49,73	2.29	10 (22%)	54,84,113	1.82	8 (14%)
33	CLA	0	306	2	59,63,73	1.87	9 (15%)	71,101,113	1.50	11 (15%)
33	CLA	2	305	-	59,63,73	1.87	9 (15%)	71,101,113	1.53	8 (11%)
42	LMG	c	520	-	51,51,55	0.72	1 (1%)	59,59,63	1.35	7 (11%)
33	CLA	b	615	8	49,53,73	2.12	9 (18%)	59,89,113	1.78	7 (11%)
33	CLA	g	307	-	59,63,73	1.88	9 (15%)	71,101,113	1.55	10 (14%)
33	CLA	2	304	4	64,68,73	1.83	9 (14%)	77,107,113	1.48	7 (9%)
37	LHG	9	322	-	40,40,48	0.70	2 (5%)	43,46,54	1.23	4 (9%)
33	CLA	b	616	8	69,73,73	1.71	9 (13%)	83,113,113	1.32	8 (9%)
33	CLA	9	313	5	45,49,73	2.22	10 (22%)	54,84,113	1.67	7 (12%)
43	DGD	C	519	-	63,63,67	0.91	2 (3%)	77,77,81	1.26	5 (6%)
34	PHO	d	403	-	58,69,69	1.00	1 (1%)	56,99,99	0.92	5 (8%)
33	CLA	C	502	9	69,73,73	1.74	9 (13%)	83,113,113	1.36	8 (9%)
38	KC2	1	311	-	49,53,53	1.89	4 (8%)	62,89,89	1.33	8 (12%)
33	CLA	A	405	1	69,73,73	1.73	9 (13%)	83,113,113	1.43	9 (10%)
33	CLA	5	303	-	59,63,73	1.94	10 (16%)	71,101,113	1.59	7 (9%)
33	CLA	6	309	7	46,50,73	2.11	9 (19%)	55,85,113	1.83	10 (18%)
33	CLA	1	305	3	64,68,73	1.83	9 (14%)	77,107,113	1.39	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	LMG	B	624	-	43,43,55	0.81	1 (2%)	51,51,63	1.25	5 (9%)
40	IHT	3	320	-	40,42,42	0.21	0	53,58,58	0.49	0
33	CLA	3	304	5	49,53,73	2.09	9 (18%)	59,89,113	1.64	6 (10%)
33	CLA	1	303	3	55,59,73	1.95	9 (16%)	66,96,113	1.52	5 (7%)
41	SQD	c	501	-	41,42,54	1.34	4 (9%)	50,53,65	1.26	5 (10%)
33	CLA	5	304	-	49,53,73	2.11	9 (18%)	59,89,113	1.74	7 (11%)
33	CLA	p	313	7	45,49,73	2.10	10 (22%)	54,84,113	1.77	10 (18%)
33	CLA	B	617	8	64,68,73	1.82	9 (14%)	77,107,113	1.42	8 (10%)
33	CLA	6	313	7	45,49,73	2.10	10 (22%)	54,84,113	1.77	10 (18%)
33	CLA	6	319	-	45,49,73	2.31	10 (22%)	54,84,113	1.83	10 (18%)
33	CLA	C	509	9	69,73,73	1.73	9 (13%)	83,113,113	1.33	6 (7%)
39	II0	2	311	-	39,43,43	0.24	0	50,60,60	0.53	1 (2%)
33	CLA	b	603	-	69,73,73	1.74	9 (13%)	83,113,113	1.45	8 (9%)
33	CLA	g	304	-	49,53,73	2.10	9 (18%)	59,89,113	1.73	7 (11%)
39	II0	1	313	-	39,43,43	0.24	0	50,60,60	0.58	0
33	CLA	N	301	-	69,73,73	1.73	9 (13%)	83,113,113	1.43	7 (8%)
33	CLA	b	613	8	69,73,73	1.75	9 (13%)	83,113,113	1.38	5 (6%)
43	DGD	H	101	-	61,61,67	0.88	1 (1%)	75,75,81	1.22	5 (6%)
33	CLA	n	301	-	69,73,73	1.73	9 (13%)	83,113,113	1.43	7 (8%)
33	CLA	N	306	-	59,63,73	1.89	9 (15%)	71,101,113	1.56	8 (11%)
34	PHO	D	403	-	58,69,69	1.00	1 (1%)	56,99,99	0.93	5 (8%)
33	CLA	9	315	-	45,49,73	2.30	10 (22%)	54,84,113	1.66	7 (12%)
33	CLA	c	509	9	69,73,73	1.73	9 (13%)	83,113,113	1.33	6 (7%)
37	LHG	8	315	-	45,45,48	0.62	0	48,51,54	1.21	4 (8%)
33	CLA	8	305	-	59,63,73	1.87	9 (15%)	71,101,113	1.52	8 (11%)
33	CLA	b	617	8	64,68,73	1.82	9 (14%)	77,107,113	1.42	8 (10%)
36	PL9	D	407	-	55,55,55	0.95	3 (5%)	68,69,69	1.44	11 (16%)
38	KC2	2	309	4	49,53,53	1.89	4 (8%)	62,89,89	1.36	8 (12%)
33	CLA	0	309	2	51,55,73	2.04	9 (17%)	61,91,113	1.67	7 (11%)
39	II0	4	313	-	39,43,43	0.32	0	50,60,60	0.49	1 (2%)
35	8CT	b	621	-	40,41,41	0.18	0	50,56,56	0.36	0
37	LHG	d	408	-	48,48,48	0.65	1 (2%)	51,54,54	1.13	2 (3%)
36	PL9	A	410	-	30,30,55	0.92	1 (3%)	38,39,69	1.33	6 (15%)
42	LMG	C	520	-	51,51,55	0.72	1 (1%)	59,59,63	1.35	7 (11%)
39	II0	8	313	-	39,43,43	0.20	0	50,60,60	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	b	604	8	69,73,73	1.71	9 (13%)	83,113,113	1.40	6 (7%)
37	LHG	3	302	-	40,40,48	0.69	1 (2%)	43,46,54	1.17	3 (6%)
33	CLA	2	308	-	59,63,73	1.87	9 (15%)	71,101,113	1.43	6 (8%)
33	CLA	p	312	7	45,49,73	2.16	10 (22%)	54,84,113	1.75	9 (16%)
38	KC2	g	309	6	49,53,53	1.84	4 (8%)	62,89,89	1.39	7 (11%)
35	8CT	1	312	-	40,41,41	0.21	0	50,56,56	0.42	0
33	CLA	c	504	-	69,73,73	1.73	9 (13%)	83,113,113	1.34	5 (6%)
37	LHG	d	401	-	45,45,48	0.67	1 (2%)	48,51,54	1.18	4 (8%)
33	CLA	b	609	8	69,73,73	1.75	9 (13%)	83,113,113	1.42	9 (10%)
40	IHT	9	320	-	40,42,42	0.21	0	53,58,58	0.49	0
33	CLA	c	503	-	69,73,73	1.69	9 (13%)	83,113,113	1.36	7 (8%)
35	8CT	B	619	-	40,41,41	0.21	0	50,56,56	0.42	0
33	CLA	2	306	4	64,68,73	1.80	9 (14%)	77,107,113	1.53	9 (11%)
41	SQD	j	101	-	45,46,54	1.26	4 (8%)	54,57,65	1.28	5 (9%)
35	8CT	C	517	-	40,41,41	0.17	0	50,56,56	0.38	0
42	LMG	D	409	-	46,46,55	0.77	0	54,54,63	1.21	2 (3%)
38	KC2	7	310	3	49,53,53	1.87	4 (8%)	62,89,89	1.36	8 (12%)
39	II0	g	313	-	39,43,43	0.33	0	50,60,60	0.92	2 (4%)
37	LHG	4	316	33	23,23,48	0.90	0	26,29,54	1.23	1 (3%)
33	CLA	1	308	-	55,59,73	1.95	9 (16%)	66,96,113	1.54	6 (9%)
33	CLA	5	311	6	49,53,73	2.12	9 (18%)	59,89,113	1.72	9 (15%)
39	II0	4	315	-	39,43,43	0.25	0	50,60,60	0.29	0
33	CLA	d	405	-	69,73,73	1.74	9 (13%)	83,113,113	1.38	6 (7%)
39	II0	6	301	-	39,43,43	0.33	0	50,60,60	0.56	2 (4%)
33	CLA	0	303	2	54,58,73	2.00	9 (16%)	65,95,113	1.63	7 (10%)
33	CLA	C	511	9	69,73,73	1.73	9 (13%)	83,113,113	1.37	7 (8%)
35	8CT	a	409	-	40,41,41	0.20	0	50,56,56	0.38	0
33	CLA	4	304	-	51,55,73	2.02	9 (17%)	61,91,113	1.69	8 (13%)
35	8CT	d	406	-	40,41,41	0.21	0	50,56,56	0.70	1 (2%)
42	LMG	b	622	-	49,49,55	0.77	0	57,57,63	1.21	5 (8%)
33	CLA	6	312	7	45,49,73	2.17	10 (22%)	54,84,113	1.75	9 (16%)
42	LMG	T	101	-	43,43,55	0.81	1 (2%)	51,51,63	1.40	9 (17%)
33	CLA	a	412	-	69,73,73	1.79	9 (13%)	83,113,113	1.60	12 (14%)
35	8CT	7	312	-	40,41,41	0.20	0	50,56,56	0.42	0
39	II0	1	315	-	39,43,43	0.18	0	50,60,60	0.60	2 (4%)
42	LMG	t	101	-	43,43,55	0.81	1 (2%)	51,51,63	1.40	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CLA	c	514	9	69,73,73	1.78	9 (13%)	83,113,113	1.33	6 (7%)
33	CLA	0	301	2	45,49,73	2.33	10 (22%)	54,84,113	1.87	10 (18%)
38	KC2	9	311	-	49,53,53	1.89	4 (8%)	62,89,89	1.32	8 (12%)
33	CLA	B	605	8	69,73,73	1.68	9 (13%)	83,113,113	1.33	6 (7%)
33	CLA	g	303	-	59,63,73	1.94	9 (15%)	71,101,113	1.60	7 (9%)
39	II0	p	317	-	39,43,43	0.31	0	50,60,60	0.62	1 (2%)
44	HEM	f	101	11	50,50,50	0.71	1 (2%)	66,82,82	0.56	0
39	II0	9	317	-	39,43,43	0.23	0	50,60,60	0.63	1 (2%)
37	LHG	g	316	-	21,21,48	0.78	0	23,26,54	1.26	2 (8%)
33	CLA	b	606	8	69,73,73	1.76	10 (14%)	83,113,113	1.47	8 (9%)
33	CLA	7	309	3	59,63,73	1.88	9 (15%)	71,101,113	1.43	6 (8%)
39	II0	3	318	-	39,43,43	0.22	0	50,60,60	0.61	2 (4%)
33	CLA	7	303	3	55,59,73	1.95	9 (16%)	66,96,113	1.53	5 (7%)
33	CLA	a	408	1	64,68,73	1.80	9 (14%)	77,107,113	1.47	6 (7%)
42	LMG	D	410	-	46,46,55	0.82	1 (2%)	54,54,63	1.32	6 (11%)
33	CLA	c	502	9	69,73,73	1.74	9 (13%)	83,113,113	1.36	8 (9%)
33	CLA	1	301	3	49,53,73	2.09	9 (18%)	59,89,113	1.79	8 (13%)
39	II0	2	312	-	39,43,43	0.20	0	50,60,60	0.87	3 (6%)
33	CLA	1	307	-	69,73,73	1.80	9 (13%)	83,113,113	1.51	9 (10%)
33	CLA	b	614	8	69,73,73	1.73	9 (13%)	83,113,113	1.44	11 (13%)
33	CLA	2	302	4	59,63,73	1.91	9 (15%)	71,101,113	1.77	12 (16%)
39	II0	6	317	-	39,43,43	0.31	0	50,60,60	0.62	1 (2%)
33	CLA	3	313	5	45,49,73	2.22	10 (22%)	54,84,113	1.67	6 (11%)
33	CLA	B	616	8	69,73,73	1.71	9 (13%)	83,113,113	1.31	8 (9%)
38	KC2	6	311	7	49,53,53	1.83	4 (8%)	62,89,89	1.46	10 (16%)
38	KC2	1	310	3	49,53,53	1.87	4 (8%)	62,89,89	1.36	8 (12%)
37	LHG	9	302	-	40,40,48	0.69	1 (2%)	43,46,54	1.17	3 (6%)
33	CLA	9	308	-	53,57,73	1.92	9 (16%)	62,93,113	1.64	9 (14%)
33	CLA	b	610	-	69,73,73	1.72	9 (13%)	83,113,113	1.38	8 (9%)
33	CLA	p	302	7	45,49,73	2.38	10 (22%)	54,84,113	1.91	10 (18%)
33	CLA	7	308	-	55,59,73	1.94	9 (16%)	66,96,113	1.54	6 (9%)
39	II0	g	312	-	39,43,43	0.40	0	50,60,60	0.74	3 (6%)
42	LMG	W	101	-	47,47,55	0.74	0	55,55,63	1.24	2 (3%)
33	CLA	4	307	2	59,63,73	1.92	9 (15%)	71,101,113	1.58	11 (15%)
39	II0	7	316	-	39,43,43	0.23	0	50,60,60	0.58	0

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
33	CLA	8	307	-	-	7/33/109/115	-
33	CLA	5	301	6	-	7/12/88/115	-
33	CLA	7	306	-	-	8/33/109/115	-
39	II0	5	314	-	-	0/21/67/67	0/2/2/2
41	SQD	L	101	-	-	19/49/69/69	0/1/1/1
33	CLA	B	611	45	-	6/39/115/115	-
33	CLA	p	306	-	-	8/15/91/115	-
40	IHT	8	314	-	-	0/25/65/65	0/2/2/2
38	KC2	0	305	-	-	9/15/71/71	-
35	8CT	b	619	-	-	3/29/63/63	0/2/2/2
39	II0	7	313	-	-	1/21/67/67	0/2/2/2
35	8CT	h	102	-	-	7/29/63/63	0/2/2/2
33	CLA	g	306	6	-	2/15/91/115	-
33	CLA	8	304	4	-	5/33/109/115	-
33	CLA	0	311	2	-	5/15/91/115	-
36	PL9	a	410	-	-	5/23/43/73	0/1/1/1
33	CLA	N	303	37	-	11/18/94/115	-
37	LHG	5	316	-	-	10/24/24/53	-
33	CLA	9	314	5	-	2/10/86/115	-
33	CLA	A	412	-	-	8/39/115/115	-
33	CLA	1	304	-	-	4/27/103/115	-
33	CLA	0	308	37	-	11/18/94/115	-
33	CLA	B	618	33	-	2/10/82/115	-
40	IHT	5	315	-	-	0/25/65/65	0/2/2/2
33	CLA	3	305	5	-	4/27/103/115	-
35	8CT	B	620	-	-	10/29/63/63	0/2/2/2
33	CLA	b	611	45	-	6/39/115/115	-
35	8CT	y	101	-	-	8/29/63/63	0/2/2/2
33	CLA	6	306	-	-	8/15/91/115	-
33	CLA	p	309	7	-	4/12/88/115	-
33	CLA	c	511	9	-	8/39/115/115	-
33	CLA	B	610	-	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	3	307	5	-	8/15/91/115	-
39	II0	8	311	-	-	0/21/67/67	0/2/2/2
37	LHG	d	402	-	-	19/51/51/53	-
34	PHO	a	407	-	-	10/37/103/103	0/5/6/6
33	CLA	5	310	-	-	0/10/86/115	-
39	II0	7	315	-	-	2/21/67/67	0/2/2/2
33	CLA	3	306	-	-	3/10/86/115	-
35	8CT	b	620	-	-	10/29/63/63	0/2/2/2
33	CLA	A	408	1	-	2/33/109/115	-
34	PHO	A	407	-	-	10/37/103/103	0/5/6/6
39	II0	3	301	-	-	1/21/67/67	0/2/2/2
33	CLA	5	305	6	-	2/10/82/115	-
39	II0	1	316	-	-	2/21/67/67	0/2/2/2
33	CLA	4	302	2	-	3/23/99/115	-
38	KC2	8	309	4	-	9/15/71/71	-
33	CLA	1	306	-	-	8/33/109/115	-
33	CLA	7	304	-	-	4/27/103/115	-
39	II0	3	317	-	-	0/21/67/67	0/2/2/2
33	CLA	7	301	3	-	5/15/91/115	-
39	II0	4	314	-	-	1/21/67/67	0/2/2/2
33	CLA	C	514	9	-	4/39/115/115	-
33	CLA	B	606	8	-	5/39/115/115	-
33	CLA	B	608	-	-	7/39/115/115	-
33	CLA	N	305	-	-	5/27/103/115	-
33	CLA	8	308	-	-	1/27/103/115	-
33	CLA	6	308	7	-	5/12/88/115	-
42	LMG	b	624	-	-	16/38/58/70	0/1/1/1
33	CLA	7	302	3	-	9/38/114/115	-
37	LHG	3	321	-	-	13/27/27/53	-
39	II0	1	314	-	-	1/21/67/67	0/2/2/2
33	CLA	C	507	9	-	10/39/115/115	-
33	CLA	4	303	2	-	7/21/97/115	-
33	CLA	3	310	-	-	4/10/86/115	-
33	CLA	5	306	6	-	2/15/91/115	-
33	CLA	0	302	2	-	3/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	g	301	6	-	7/12/88/115	-
42	LMG	d	409	-	-	17/41/61/70	0/1/1/1
33	CLA	3	308	-	-	2/20/96/115	-
33	CLA	c	506	-	-	7/39/115/115	-
39	II0	4	312	-	-	2/21/67/67	0/2/2/2
39	II0	3	316	-	-	3/21/67/67	0/2/2/2
33	CLA	4	310	2	-	5/15/91/115	-
33	CLA	6	303	7	-	2/10/86/115	-
33	CLA	a	406	45	-	8/20/96/115	-
33	CLA	B	614	8	-	8/39/115/115	-
33	CLA	9	303	5	-	8/27/103/115	-
33	CLA	0	304	-	-	6/18/94/115	-
33	CLA	b	605	8	-	14/39/115/115	-
33	CLA	5	302	6	-	8/27/103/115	-
39	II0	8	312	-	-	1/21/67/67	0/2/2/2
37	LHG	D	402	-	-	19/51/51/53	-
43	DGD	C	518	-	-	13/44/84/95	0/2/2/2
33	CLA	A	406	45	-	8/20/96/115	-
33	CLA	2	310	-	-	3/17/93/115	-
33	CLA	n	303	6	-	1/10/86/115	-
33	CLA	C	504	-	-	4/39/115/115	-
33	CLA	5	317	-	-	3/10/82/115	-
37	LHG	0	317	33	-	7/27/27/53	-
37	LHG	D	401	-	-	25/50/50/53	-
38	KC2	7	311	-	-	6/15/71/71	-
43	DGD	c	518	-	-	12/44/84/95	0/2/2/2
38	KC2	p	311	7	-	3/15/71/71	-
33	CLA	1	309	3	-	2/27/103/115	-
33	CLA	C	513	9	-	8/29/105/115	-
43	DGD	c	521	-	-	23/51/91/95	0/2/2/2
33	CLA	c	507	9	-	10/39/115/115	-
33	CLA	N	307	-	-	6/21/97/115	-
40	IHT	p	318	-	-	2/25/65/65	0/2/2/2
35	8CT	c	515	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	8CT	Y	101	-	-	8/29/63/63	0/2/2/2
33	CLA	B	615	8	-	4/15/91/115	-
33	CLA	g	317	-	-	3/10/82/115	-
37	LHG	D	408	-	-	21/53/53/53	-
33	CLA	g	310	-	-	0/10/86/115	-
33	CLA	B	612	-	-	3/39/115/115	-
33	CLA	9	307	5	-	8/15/91/115	-
33	CLA	n	305	-	-	4/27/103/115	-
41	SQD	b	601	-	-	11/33/53/69	0/1/1/1
39	II0	9	319	-	-	2/21/67/67	0/2/2/2
33	CLA	3	309	5	-	6/27/103/115	-
33	CLA	6	302	7	-	2/10/86/115	-
33	CLA	1	302	3	-	9/38/114/115	-
39	II0	0	313	-	-	2/21/67/67	0/2/2/2
42	LMG	l	102	-	-	9/33/53/70	0/1/1/1
33	CLA	p	310	-	-	7/10/86/115	-
33	CLA	8	301	4	-	6/15/91/115	-
33	CLA	0	310	2	-	10/10/82/115	-
33	CLA	4	306	2	-	9/27/103/115	-
41	SQD	B	601	-	-	11/33/53/69	0/1/1/1
38	KC2	4	305	-	-	9/15/71/71	-
33	CLA	p	305	7	-	4/27/103/115	-
40	IHT	6	318	-	-	2/25/65/65	0/2/2/2
33	CLA	8	306	4	-	5/33/109/115	-
33	CLA	2	303	4	-	15/24/100/115	-
33	CLA	B	603	-	-	6/39/115/115	-
33	CLA	d	404	-	-	1/39/115/115	-
37	LHG	3	322	-	-	19/45/45/53	-
33	CLA	B	602	33	-	8/21/97/115	-
33	CLA	D	405	-	-	9/39/115/115	-
33	CLA	N	304	6	-	1/10/86/115	-
35	8CT	C	516	-	-	5/29/63/63	0/2/2/2
39	II0	g	314	-	-	0/21/67/67	0/2/2/2
33	CLA	8	302	4	-	12/27/103/115	-
33	CLA	g	308	-	-	3/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	C	505	-	-	13/39/115/115	-
33	CLA	3	312	5	-	2/27/103/115	-
39	II0	p	315	-	-	2/21/67/67	0/2/2/2
35	8CT	0	312	-	-	4/29/63/63	0/2/2/2
37	LHG	1	317	-	-	21/53/53/53	-
33	CLA	4	309	2	-	10/10/82/115	-
39	II0	9	301	-	-	1/21/67/67	0/2/2/2
39	II0	7	314	-	-	1/21/67/67	0/2/2/2
40	IHT	2	314	-	-	0/25/65/65	0/2/2/2
33	CLA	9	310	-	-	4/10/86/115	-
33	CLA	3	303	5	-	8/27/103/115	-
35	8CT	A	409	-	-	3/29/63/63	0/2/2/2
33	CLA	B	609	8	-	2/39/115/115	-
33	CLA	3	315	-	-	6/10/86/115	-
44	HEM	v	201	-	-	3/14/54/54	-
39	II0	0	316	-	-	2/21/67/67	0/2/2/2
35	8CT	c	517	-	-	6/29/63/63	0/2/2/2
33	CLA	N	302	19	-	8/39/115/115	-
33	CLA	c	512	-	-	7/39/115/115	-
33	CLA	b	618	33	-	2/10/82/115	-
35	8CT	D	406	-	-	9/29/63/63	0/2/2/2
37	LHG	7	317	-	-	21/53/53/53	-
42	LMG	m	101	-	-	9/33/53/70	0/1/1/1
35	8CT	c	516	-	-	5/29/63/63	0/2/2/2
39	II0	6	315	-	-	2/21/67/67	0/2/2/2
39	II0	2	313	-	-	5/21/67/67	0/2/2/2
33	CLA	C	508	-	-	8/39/115/115	-
33	CLA	C	506	-	-	7/39/115/115	-
39	II0	0	315	-	-	1/21/67/67	0/2/2/2
33	CLA	g	305	6	-	2/10/82/115	-
33	CLA	0	307	2	-	12/27/103/115	-
33	CLA	n	302	19	-	8/39/115/115	-
38	KC2	5	309	6	-	4/15/71/71	-
33	CLA	c	513	9	-	8/29/105/115	-
37	LHG	2	315	-	-	35/50/50/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	II0	5	313	-	-	1/21/67/67	0/2/2/2
33	CLA	4	301	2	-	3/10/86/115	-
38	KC2	3	311	-	-	7/15/71/71	-
33	CLA	7	305	3	-	7/33/109/115	-
33	CLA	c	510	9	-	3/39/115/115	-
35	8CT	4	311	-	-	4/29/63/63	0/2/2/2
33	CLA	B	604	8	-	3/39/115/115	-
44	HEM	V	201	-	-	3/14/54/54	-
43	DGD	h	101	-	-	13/49/89/95	0/2/2/2
33	CLA	C	503	-	-	10/39/115/115	-
33	CLA	B	613	8	-	10/39/115/115	-
35	8CT	B	621	-	-	8/29/63/63	0/2/2/2
39	II0	3	319	-	-	2/21/67/67	0/2/2/2
33	CLA	b	612	-	-	3/39/115/115	-
43	DGD	C	521	-	-	23/51/91/95	0/2/2/2
37	LHG	b	623	-	-	28/53/53/53	-
35	8CT	H	102	-	-	7/29/63/63	0/2/2/2
42	LMG	B	622	-	-	21/44/64/70	0/1/1/1
33	CLA	3	314	5	-	2/10/86/115	-
43	DGD	c	519	-	-	23/51/91/95	0/2/2/2
33	CLA	p	308	7	-	5/12/88/115	-
36	PL9	d	407	-	-	18/53/73/73	0/1/1/1
33	CLA	9	305	5	-	4/27/103/115	-
33	CLA	n	304	-	-	5/27/103/115	-
33	CLA	9	309	5	-	6/27/103/115	-
33	CLA	p	307	-	-	1/13/89/115	-
33	CLA	g	302	6	-	8/27/103/115	-
33	CLA	5	307	-	-	10/27/103/115	-
33	CLA	6	307	7	-	1/13/89/115	-
33	CLA	C	512	-	-	7/39/115/115	-
41	SQD	l	101	-	-	18/49/69/69	0/1/1/1
33	CLA	c	505	-	-	13/39/115/115	-
33	CLA	8	310	-	-	3/17/93/115	-
33	CLA	p	319	-	-	8/10/86/115	-
33	CLA	6	310	-	-	7/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	8CT	C	515	-	-	8/29/63/63	0/2/2/2
33	CLA	b	607	-	-	11/39/115/115	-
33	CLA	b	602	33	-	8/21/97/115	-
33	CLA	p	304	7	-	4/12/88/115	-
33	CLA	6	305	7	-	4/27/103/115	-
33	CLA	C	510	9	-	3/39/115/115	-
33	CLA	D	404	-	-	1/39/115/115	-
33	CLA	b	608	-	-	7/39/115/115	-
33	CLA	6	304	7	-	4/12/88/115	-
33	CLA	9	304	5	-	1/15/91/115	-
42	LMG	w	101	-	-	26/42/62/70	0/1/1/1
39	II0	0	314	-	-	2/21/67/67	0/2/2/2
39	II0	9	316	-	-	3/21/67/67	0/2/2/2
39	II0	5	312	-	-	2/21/67/67	0/2/2/2
33	CLA	B	607	-	-	11/39/115/115	-
33	CLA	9	306	5	-	3/10/86/115	-
37	LHG	a	411	-	-	6/28/28/53	-
40	IHT	g	315	-	-	0/25/65/65	0/2/2/2
37	LHG	A	411	-	-	6/28/28/53	-
39	II0	p	316	-	-	0/21/67/67	0/2/2/2
33	CLA	p	303	7	-	2/10/86/115	-
33	CLA	4	308	2	-	11/18/94/115	-
39	II0	6	316	-	-	0/21/67/67	0/2/2/2
39	II0	p	314	-	-	0/21/67/67	0/2/2/2
41	SQD	J	101	-	-	20/41/61/69	0/1/1/1
44	HEM	F	101	11,12	-	8/14/54/54	-
37	LHG	9	321	-	-	13/27/27/53	-
33	CLA	c	508	-	-	8/39/115/115	-
33	CLA	8	303	4	-	15/24/100/115	-
33	CLA	g	311	6	-	9/15/91/115	-
33	CLA	a	405	1	-	4/39/115/115	-
33	CLA	2	301	4	-	6/15/91/115	-
39	II0	9	318	-	-	1/21/67/67	0/2/2/2
41	SQD	C	501	-	-	9/37/57/69	0/1/1/1
33	CLA	2	307	-	-	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	B	623	-	-	28/53/53/53	-
33	CLA	7	307	-	-	7/39/115/115	-
42	LMG	d	410	-	-	17/41/61/70	0/1/1/1
33	CLA	n	306	-	-	6/21/97/115	-
33	CLA	9	312	5	-	2/27/103/115	-
39	II0	p	301	-	-	0/21/67/67	0/2/2/2
39	II0	6	314	-	-	0/21/67/67	0/2/2/2
33	CLA	5	308	-	-	3/10/86/115	-
33	CLA	0	306	2	-	9/27/103/115	-
33	CLA	2	305	-	-	7/27/103/115	-
42	LMG	c	520	-	-	28/46/66/70	0/1/1/1
33	CLA	b	615	8	-	4/15/91/115	-
33	CLA	g	307	-	-	10/27/103/115	-
33	CLA	2	304	4	-	5/33/109/115	-
37	LHG	9	322	-	-	19/45/45/53	-
33	CLA	b	616	8	-	7/39/115/115	-
33	CLA	9	313	5	-	2/10/86/115	-
43	DGD	C	519	-	-	23/51/91/95	0/2/2/2
34	PHO	d	403	-	-	6/37/103/103	0/5/6/6
33	CLA	C	502	9	-	5/39/115/115	-
38	KC2	1	311	-	-	6/15/71/71	-
33	CLA	A	405	1	-	4/39/115/115	-
33	CLA	5	303	-	-	3/27/103/115	-
33	CLA	6	309	7	-	4/12/88/115	-
33	CLA	1	305	3	-	7/33/109/115	-
42	LMG	B	624	-	-	16/38/58/70	0/1/1/1
40	IHT	3	320	-	-	7/25/65/65	0/2/2/2
33	CLA	3	304	5	-	1/15/91/115	-
33	CLA	1	303	3	-	3/23/99/115	-
41	SQD	c	501	-	-	9/37/57/69	0/1/1/1
33	CLA	5	304	-	-	5/15/91/115	-
33	CLA	p	313	7	-	4/10/86/115	-
33	CLA	B	617	8	-	4/33/109/115	-
33	CLA	6	313	7	-	4/10/86/115	-
33	CLA	6	319	-	-	8/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	C	509	9	-	4/39/115/115	-
39	II0	2	311	-	-	0/21/67/67	0/2/2/2
33	CLA	b	603	-	-	6/39/115/115	-
33	CLA	g	304	-	-	5/15/91/115	-
39	II0	1	313	-	-	1/21/67/67	0/2/2/2
33	CLA	N	301	-	-	12/39/115/115	-
33	CLA	b	613	8	-	10/39/115/115	-
43	DGD	H	101	-	-	13/49/89/95	0/2/2/2
33	CLA	n	301	-	-	12/39/115/115	-
33	CLA	N	306	-	-	4/27/103/115	-
34	PHO	D	403	-	-	6/37/103/103	0/5/6/6
33	CLA	9	315	-	-	6/10/86/115	-
33	CLA	c	509	9	-	4/39/115/115	-
37	LHG	8	315	-	-	35/50/50/53	-
33	CLA	8	305	-	-	7/27/103/115	-
33	CLA	b	617	8	-	4/33/109/115	-
36	PL9	D	407	-	-	18/53/73/73	0/1/1/1
38	KC2	2	309	4	-	9/15/71/71	-
33	CLA	0	309	2	-	11/18/94/115	-
39	II0	4	313	-	-	2/21/67/67	0/2/2/2
35	8CT	b	621	-	-	8/29/63/63	0/2/2/2
37	LHG	d	408	-	-	20/53/53/53	-
36	PL9	A	410	-	-	5/23/43/73	0/1/1/1
42	LMG	C	520	-	-	28/46/66/70	0/1/1/1
39	II0	8	313	-	-	5/21/67/67	0/2/2/2
33	CLA	b	604	8	-	3/39/115/115	-
37	LHG	3	302	-	-	19/45/45/53	-
33	CLA	2	308	-	-	1/27/103/115	-
33	CLA	p	312	7	-	3/10/86/115	-
38	KC2	g	309	6	-	4/15/71/71	-
35	8CT	1	312	-	-	5/29/63/63	0/2/2/2
33	CLA	c	504	-	-	4/39/115/115	-
37	LHG	d	401	-	-	25/50/50/53	-
33	CLA	b	609	8	-	2/39/115/115	-
40	IHT	9	320	-	-	7/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	c	503	-	-	9/39/115/115	-
35	8CT	B	619	-	-	3/29/63/63	0/2/2/2
33	CLA	2	306	4	-	5/33/109/115	-
41	SQD	j	101	-	-	20/41/61/69	0/1/1/1
35	8CT	C	517	-	-	6/29/63/63	0/2/2/2
42	LMG	D	409	-	-	17/41/61/70	0/1/1/1
38	KC2	7	310	3	-	7/15/71/71	-
39	II0	g	313	-	-	1/21/67/67	0/2/2/2
37	LHG	4	316	33	-	7/27/27/53	-
33	CLA	1	308	-	-	6/23/99/115	-
33	CLA	5	311	6	-	9/15/91/115	-
39	II0	4	315	-	-	3/21/67/67	0/2/2/2
33	CLA	d	405	-	-	9/39/115/115	-
39	II0	6	301	-	-	0/21/67/67	0/2/2/2
33	CLA	0	303	2	-	7/21/97/115	-
33	CLA	C	511	9	-	8/39/115/115	-
35	8CT	a	409	-	-	3/29/63/63	0/2/2/2
33	CLA	4	304	-	-	6/18/94/115	-
35	8CT	d	406	-	-	9/29/63/63	0/2/2/2
42	LMG	b	622	-	-	21/44/64/70	0/1/1/1
33	CLA	6	312	7	-	3/10/86/115	-
42	LMG	T	101	-	-	15/38/58/70	0/1/1/1
33	CLA	a	412	-	-	8/39/115/115	-
35	8CT	7	312	-	-	5/29/63/63	0/2/2/2
39	II0	1	315	-	-	2/21/67/67	0/2/2/2
42	LMG	t	101	-	-	15/38/58/70	0/1/1/1
33	CLA	c	514	9	-	4/39/115/115	-
33	CLA	0	301	2	-	3/10/86/115	-
38	KC2	9	311	-	-	7/15/71/71	-
33	CLA	B	605	8	-	14/39/115/115	-
33	CLA	g	303	-	-	3/27/103/115	-
39	II0	p	317	-	-	2/21/67/67	0/2/2/2
44	HEM	f	101	11	-	0/14/54/54	-
39	II0	9	317	-	-	0/21/67/67	0/2/2/2
37	LHG	g	316	-	-	10/24/24/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	b	606	8	-	5/39/115/115	-
33	CLA	7	309	3	-	2/27/103/115	-
39	II0	3	318	-	-	1/21/67/67	0/2/2/2
33	CLA	7	303	3	-	3/23/99/115	-
33	CLA	a	408	1	-	2/33/109/115	-
42	LMG	D	410	-	-	17/41/61/70	0/1/1/1
33	CLA	c	502	9	-	5/39/115/115	-
33	CLA	1	301	3	-	5/15/91/115	-
39	II0	2	312	-	-	1/21/67/67	0/2/2/2
33	CLA	1	307	-	-	7/39/115/115	-
33	CLA	b	614	8	-	7/39/115/115	-
33	CLA	2	302	4	-	12/27/103/115	-
39	II0	6	317	-	-	2/21/67/67	0/2/2/2
33	CLA	3	313	5	-	2/10/86/115	-
33	CLA	B	616	8	-	7/39/115/115	-
38	KC2	6	311	7	-	3/15/71/71	-
38	KC2	1	310	3	-	7/15/71/71	-
37	LHG	9	302	-	-	19/45/45/53	-
33	CLA	9	308	-	-	2/20/96/115	-
33	CLA	b	610	-	-	10/39/115/115	-
33	CLA	p	302	7	-	2/10/86/115	-
33	CLA	7	308	-	-	6/23/99/115	-
39	II0	g	312	-	-	1/21/67/67	0/2/2/2
42	LMG	W	101	-	-	26/42/62/70	0/1/1/1
33	CLA	4	307	2	-	12/27/103/115	-
39	II0	7	316	-	-	2/21/67/67	0/2/2/2

All (2077) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	p	311	KC2	MG-ND	-10.71	1.84	2.05
38	6	311	KC2	MG-ND	-10.70	1.84	2.05
38	g	309	KC2	MG-ND	-10.63	1.84	2.05
38	5	309	KC2	MG-ND	-10.61	1.84	2.05
38	4	305	KC2	MG-ND	-10.39	1.85	2.05
38	0	305	KC2	MG-ND	-10.38	1.85	2.05
38	1	311	KC2	MG-ND	-10.01	1.85	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	7	311	KC2	MG-ND	-10.00	1.86	2.05
38	2	309	KC2	MG-ND	-9.92	1.86	2.05
38	8	309	KC2	MG-ND	-9.90	1.86	2.05
38	3	311	KC2	MG-ND	-9.80	1.86	2.05
38	9	311	KC2	MG-ND	-9.80	1.86	2.05
38	1	310	KC2	MG-ND	-9.67	1.86	2.05
38	7	310	KC2	MG-ND	-9.63	1.86	2.05
33	C	512	CLA	C1D-ND	7.65	1.47	1.37
33	c	512	CLA	C1D-ND	7.62	1.47	1.37
33	N	307	CLA	C1D-ND	7.45	1.46	1.37
33	n	304	CLA	C1D-ND	7.44	1.46	1.37
33	N	305	CLA	C1D-ND	7.42	1.46	1.37
33	p	304	CLA	C1D-ND	7.41	1.46	1.37
33	6	304	CLA	C1D-ND	7.41	1.46	1.37
33	n	306	CLA	C1D-ND	7.40	1.46	1.37
33	g	317	CLA	C1D-ND	7.40	1.46	1.37
33	5	317	CLA	C1D-ND	7.38	1.46	1.37
33	b	607	CLA	C1D-ND	7.36	1.46	1.37
33	1	309	CLA	C1D-ND	7.36	1.46	1.37
33	7	309	CLA	C1D-ND	7.35	1.46	1.37
33	8	310	CLA	C1D-ND	7.35	1.46	1.37
33	b	616	CLA	C1D-ND	7.33	1.46	1.37
33	b	617	CLA	C1D-ND	7.33	1.46	1.37
33	2	310	CLA	C1D-ND	7.33	1.46	1.37
33	B	616	CLA	C1D-ND	7.31	1.46	1.37
33	1	303	CLA	C1D-ND	7.30	1.46	1.37
33	B	607	CLA	C1D-ND	7.30	1.46	1.37
33	6	302	CLA	C1D-ND	7.28	1.46	1.37
33	B	617	CLA	C1D-ND	7.27	1.46	1.37
33	7	303	CLA	C1D-ND	7.27	1.46	1.37
33	p	302	CLA	C1D-ND	7.26	1.46	1.37
33	a	406	CLA	C1D-ND	7.26	1.46	1.37
33	B	614	CLA	C1D-ND	7.25	1.46	1.37
33	b	614	CLA	C1D-ND	7.25	1.46	1.37
33	b	602	CLA	C1D-ND	7.25	1.46	1.37
33	3	315	CLA	C1D-ND	7.23	1.46	1.37
33	B	602	CLA	C1D-ND	7.23	1.46	1.37
33	A	406	CLA	C1D-ND	7.23	1.46	1.37
33	9	315	CLA	C1D-ND	7.20	1.46	1.37
33	n	302	CLA	C1D-ND	7.18	1.46	1.37
33	c	508	CLA	C1D-ND	7.17	1.46	1.37
33	0	303	CLA	C1D-ND	7.17	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	3	313	CLA	C1D-ND	7.15	1.46	1.37
33	4	303	CLA	C1D-ND	7.14	1.46	1.37
33	C	508	CLA	C1D-ND	7.13	1.46	1.37
33	N	302	CLA	C1D-ND	7.13	1.46	1.37
33	g	301	CLA	C1D-ND	7.12	1.46	1.37
33	5	301	CLA	C1D-ND	7.11	1.46	1.37
33	3	304	CLA	C1D-ND	7.11	1.46	1.37
33	5	311	CLA	C1D-ND	7.11	1.46	1.37
33	C	505	CLA	C1D-ND	7.10	1.46	1.37
33	a	405	CLA	C1D-ND	7.10	1.46	1.37
33	9	313	CLA	C1D-ND	7.10	1.46	1.37
33	A	405	CLA	C1D-ND	7.10	1.46	1.37
33	b	611	CLA	C1D-ND	7.10	1.46	1.37
33	3	310	CLA	C1D-ND	7.10	1.46	1.37
33	9	310	CLA	C1D-ND	7.10	1.46	1.37
33	g	311	CLA	C1D-ND	7.08	1.46	1.37
33	B	611	CLA	C1D-ND	7.08	1.46	1.37
33	c	504	CLA	C1D-ND	7.08	1.46	1.37
33	c	505	CLA	C1D-ND	7.08	1.46	1.37
33	D	405	CLA	C1D-ND	7.06	1.46	1.37
33	9	305	CLA	C1D-ND	7.05	1.46	1.37
33	3	305	CLA	C1D-ND	7.04	1.46	1.37
33	d	405	CLA	C1D-ND	7.04	1.46	1.37
33	C	504	CLA	C1D-ND	7.03	1.46	1.37
33	5	308	CLA	C1D-ND	7.03	1.46	1.37
33	g	308	CLA	C1D-ND	7.03	1.46	1.37
33	8	301	CLA	C1D-ND	7.01	1.46	1.37
33	c	514	CLA	C1D-ND	7.01	1.46	1.37
33	9	306	CLA	C1D-ND	7.00	1.46	1.37
33	C	514	CLA	C1D-ND	7.00	1.46	1.37
33	3	306	CLA	C1D-ND	7.00	1.46	1.37
33	9	304	CLA	C1D-ND	7.00	1.46	1.37
33	c	513	CLA	C1D-ND	6.99	1.46	1.37
33	g	302	CLA	C1D-ND	6.97	1.46	1.37
33	C	502	CLA	C1D-ND	6.96	1.46	1.37
33	5	303	CLA	C1D-ND	6.95	1.46	1.37
33	C	513	CLA	C1D-ND	6.95	1.46	1.37
33	9	314	CLA	C1D-ND	6.95	1.46	1.37
33	5	302	CLA	C1D-ND	6.94	1.46	1.37
33	2	301	CLA	C1D-ND	6.94	1.46	1.37
33	B	618	CLA	C1D-ND	6.94	1.46	1.37
33	b	612	CLA	C1D-ND	6.94	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	609	CLA	C1D-ND	6.93	1.46	1.37
33	b	609	CLA	C1D-ND	6.92	1.46	1.37
33	c	502	CLA	C1D-ND	6.92	1.46	1.37
33	3	314	CLA	C1D-ND	6.92	1.46	1.37
33	g	303	CLA	C1D-ND	6.91	1.46	1.37
33	n	303	CLA	C1D-ND	6.91	1.46	1.37
33	B	612	CLA	C1D-ND	6.91	1.46	1.37
33	b	618	CLA	C1D-ND	6.89	1.46	1.37
33	g	310	CLA	C1D-ND	6.87	1.46	1.37
33	N	304	CLA	C1D-ND	6.87	1.46	1.37
33	N	301	CLA	C1D-ND	6.87	1.46	1.37
33	7	307	CLA	C1D-ND	6.85	1.46	1.37
33	n	301	CLA	C1D-ND	6.85	1.46	1.37
33	7	306	CLA	C1D-ND	6.84	1.46	1.37
33	5	310	CLA	C1D-ND	6.84	1.46	1.37
33	C	510	CLA	C1D-ND	6.84	1.46	1.37
33	c	510	CLA	C1D-ND	6.84	1.46	1.37
33	b	613	CLA	C1D-ND	6.83	1.46	1.37
33	B	615	CLA	C1D-ND	6.82	1.46	1.37
33	1	307	CLA	C1D-ND	6.82	1.46	1.37
33	A	408	CLA	C1D-ND	6.82	1.46	1.37
33	2	307	CLA	C1D-ND	6.82	1.46	1.37
33	8	304	CLA	C1D-ND	6.81	1.46	1.37
33	C	507	CLA	C1D-ND	6.81	1.46	1.37
33	1	308	CLA	C1D-ND	6.81	1.46	1.37
33	b	615	CLA	C1D-ND	6.81	1.46	1.37
33	1	306	CLA	C1D-ND	6.81	1.46	1.37
33	B	613	CLA	C1D-ND	6.80	1.46	1.37
33	1	304	CLA	C1D-ND	6.80	1.46	1.37
33	9	307	CLA	C1D-ND	6.80	1.46	1.37
33	0	307	CLA	C1D-ND	6.80	1.46	1.37
33	4	307	CLA	C1D-ND	6.79	1.46	1.37
33	b	605	CLA	C1D-ND	6.79	1.46	1.37
33	b	603	CLA	C1D-ND	6.78	1.46	1.37
33	7	308	CLA	C1D-ND	6.78	1.46	1.37
33	3	307	CLA	C1D-ND	6.78	1.46	1.37
33	B	605	CLA	C1D-ND	6.78	1.46	1.37
33	c	507	CLA	C1D-ND	6.78	1.46	1.37
33	b	608	CLA	C1D-ND	6.77	1.46	1.37
33	B	603	CLA	C1D-ND	6.77	1.46	1.37
33	B	610	CLA	C1D-ND	6.77	1.46	1.37
33	7	302	CLA	C1D-ND	6.76	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	7	304	CLA	C1D-ND	6.76	1.46	1.37
33	3	309	CLA	C1D-ND	6.76	1.46	1.37
33	9	309	CLA	C1D-ND	6.76	1.46	1.37
33	2	304	CLA	C1D-ND	6.76	1.46	1.37
33	a	408	CLA	C1D-ND	6.75	1.46	1.37
33	3	303	CLA	C1D-ND	6.75	1.46	1.37
33	b	610	CLA	C1D-ND	6.75	1.46	1.37
33	c	509	CLA	C1D-ND	6.75	1.46	1.37
33	2	302	CLA	C1D-ND	6.74	1.46	1.37
33	1	302	CLA	C1D-ND	6.74	1.46	1.37
33	8	307	CLA	C1D-ND	6.73	1.46	1.37
33	9	303	CLA	C1D-ND	6.73	1.46	1.37
33	B	608	CLA	C1D-ND	6.71	1.46	1.37
33	C	509	CLA	C1D-ND	6.71	1.46	1.37
33	8	302	CLA	C1D-ND	6.71	1.46	1.37
33	6	307	CLA	C1D-ND	6.69	1.46	1.37
33	p	307	CLA	C1D-ND	6.68	1.46	1.37
33	3	312	CLA	C1D-ND	6.65	1.46	1.37
33	A	412	CLA	C1D-ND	6.65	1.46	1.37
33	p	312	CLA	C1D-ND	6.65	1.46	1.37
33	9	312	CLA	C1D-ND	6.64	1.46	1.37
33	3	308	CLA	C1D-ND	6.64	1.45	1.37
33	9	308	CLA	C1D-ND	6.63	1.45	1.37
33	a	412	CLA	C1D-ND	6.61	1.45	1.37
33	p	309	CLA	C1D-ND	6.61	1.45	1.37
33	6	312	CLA	C1D-ND	6.58	1.45	1.37
33	g	306	CLA	C1D-ND	6.58	1.45	1.37
33	1	305	CLA	C1D-ND	6.57	1.45	1.37
33	4	302	CLA	C1D-ND	6.57	1.45	1.37
33	n	305	CLA	C1D-ND	6.57	1.45	1.37
33	5	306	CLA	C1D-ND	6.57	1.45	1.37
33	6	309	CLA	C1D-ND	6.56	1.45	1.37
33	N	306	CLA	C1D-ND	6.56	1.45	1.37
33	4	301	CLA	C1D-ND	6.55	1.45	1.37
33	8	303	CLA	C1D-ND	6.54	1.45	1.37
33	7	305	CLA	C1D-ND	6.54	1.45	1.37
33	7	301	CLA	C1D-ND	6.54	1.45	1.37
33	B	606	CLA	C1D-ND	6.53	1.45	1.37
33	0	302	CLA	C1D-ND	6.52	1.45	1.37
33	0	301	CLA	C1D-ND	6.52	1.45	1.37
33	1	301	CLA	C1D-ND	6.52	1.45	1.37
33	p	319	CLA	MG-ND	-6.51	1.92	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	6	306	CLA	C1D-ND	6.51	1.45	1.37
33	p	306	CLA	C1D-ND	6.51	1.45	1.37
33	2	308	CLA	C1D-ND	6.50	1.45	1.37
33	b	604	CLA	C1D-ND	6.50	1.45	1.37
33	2	303	CLA	C1D-ND	6.49	1.45	1.37
33	p	319	CLA	C1D-ND	6.49	1.45	1.37
33	6	319	CLA	MG-ND	-6.48	1.92	2.05
33	b	606	CLA	C1D-ND	6.47	1.45	1.37
33	N	303	CLA	C1D-ND	6.47	1.45	1.37
33	8	306	CLA	C1D-ND	6.46	1.45	1.37
33	4	308	CLA	C1D-ND	6.46	1.45	1.37
33	4	304	CLA	C1D-ND	6.46	1.45	1.37
33	0	304	CLA	C1D-ND	6.45	1.45	1.37
33	6	319	CLA	C1D-ND	6.45	1.45	1.37
33	8	308	CLA	C1D-ND	6.45	1.45	1.37
33	0	308	CLA	C1D-ND	6.44	1.45	1.37
33	B	604	CLA	C1D-ND	6.43	1.45	1.37
33	8	305	CLA	C1D-ND	6.42	1.45	1.37
33	C	506	CLA	C1D-ND	6.42	1.45	1.37
33	d	404	CLA	C1D-ND	6.41	1.45	1.37
33	2	305	CLA	C1D-ND	6.40	1.45	1.37
33	2	306	CLA	C1D-ND	6.39	1.45	1.37
33	6	310	CLA	C1D-ND	6.39	1.45	1.37
33	0	309	CLA	C1D-ND	6.39	1.45	1.37
33	c	506	CLA	C1D-ND	6.38	1.45	1.37
33	D	404	CLA	C1D-ND	6.38	1.45	1.37
33	p	310	CLA	C1D-ND	6.38	1.45	1.37
33	0	311	CLA	C1D-ND	6.37	1.45	1.37
33	4	310	CLA	C1D-ND	6.35	1.45	1.37
33	5	304	CLA	C1D-ND	6.30	1.45	1.37
33	g	304	CLA	C1D-ND	6.30	1.45	1.37
33	5	307	CLA	C1D-ND	6.28	1.45	1.37
33	g	307	CLA	C1D-ND	6.28	1.45	1.37
33	0	309	CLA	MG-NB	-6.26	1.93	2.05
34	a	407	PHO	C1D-C2D	6.24	1.46	1.39
34	A	407	PHO	C1D-C2D	6.24	1.46	1.39
33	4	308	CLA	MG-NB	-6.23	1.93	2.05
33	5	304	CLA	MG-ND	-6.22	1.93	2.05
34	D	403	PHO	C1D-C2D	6.21	1.46	1.39
33	c	503	CLA	C1D-ND	6.20	1.45	1.37
33	c	511	CLA	C1D-ND	6.20	1.45	1.37
33	g	304	CLA	MG-ND	-6.19	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	503	CLA	C1D-ND	6.19	1.45	1.37
33	g	305	CLA	MG-ND	-6.19	1.93	2.05
34	d	403	PHO	C1D-C2D	6.18	1.46	1.39
33	C	511	CLA	C1D-ND	6.17	1.45	1.37
33	5	305	CLA	MG-ND	-6.16	1.93	2.05
33	6	308	CLA	C1D-ND	6.14	1.45	1.37
33	p	308	CLA	C1D-ND	6.13	1.45	1.37
33	5	305	CLA	C1D-ND	6.12	1.45	1.37
33	0	310	CLA	MG-ND	-6.12	1.93	2.05
33	g	305	CLA	C1D-ND	6.11	1.45	1.37
33	p	302	CLA	C1B-NB	6.11	1.45	1.37
33	4	309	CLA	MG-ND	-6.11	1.93	2.05
33	p	313	CLA	C1D-ND	6.10	1.45	1.37
33	6	303	CLA	C1D-ND	6.09	1.45	1.37
33	6	302	CLA	C1B-NB	6.09	1.45	1.37
33	0	310	CLA	MG-NB	-6.08	1.93	2.05
33	0	304	CLA	MG-ND	-6.08	1.93	2.05
33	4	309	CLA	MG-NB	-6.08	1.93	2.05
38	3	311	KC2	C4B-NB	6.08	1.45	1.37
38	9	311	KC2	C4B-NB	6.07	1.45	1.37
33	p	303	CLA	C1D-ND	6.07	1.45	1.37
38	8	309	KC2	C4B-NB	6.06	1.45	1.37
33	6	313	CLA	C1D-ND	6.06	1.45	1.37
33	0	308	CLA	MG-NA	-6.06	1.91	2.06
33	0	301	CLA	MG-NA	-6.05	1.91	2.06
33	N	303	CLA	MG-NA	-6.05	1.91	2.06
33	p	319	CLA	MG-NB	-6.03	1.93	2.05
33	6	319	CLA	MG-NB	-6.03	1.93	2.05
33	4	304	CLA	MG-ND	-6.02	1.93	2.05
33	4	301	CLA	MG-NA	-6.02	1.92	2.06
33	0	311	CLA	MG-NB	-6.02	1.93	2.05
33	6	308	CLA	MG-ND	-6.01	1.93	2.05
33	6	303	CLA	MG-NB	-6.01	1.93	2.05
33	p	308	CLA	MG-ND	-6.01	1.93	2.05
38	2	309	KC2	C4B-NB	5.99	1.45	1.37
33	4	310	CLA	MG-NB	-5.99	1.93	2.05
33	p	303	CLA	MG-NB	-5.98	1.93	2.05
33	6	305	CLA	MG-ND	-5.98	1.93	2.05
33	8	303	CLA	MG-NB	-5.98	1.93	2.05
33	2	303	CLA	MG-NB	-5.97	1.94	2.05
33	a	412	CLA	MG-NA	-5.97	1.92	2.06
33	A	412	CLA	MG-NA	-5.96	1.92	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	p	303	CLA	C3A-C2A	-5.95	1.49	1.54
33	p	305	CLA	MG-ND	-5.95	1.94	2.05
33	4	306	CLA	C1D-ND	5.95	1.45	1.37
33	0	311	CLA	MG-ND	-5.95	1.94	2.05
33	0	306	CLA	C1D-ND	5.95	1.45	1.37
33	6	303	CLA	C3A-C2A	-5.95	1.49	1.54
33	7	305	CLA	MG-ND	-5.94	1.94	2.05
38	7	310	KC2	C4B-NB	5.94	1.45	1.37
33	4	306	CLA	MG-ND	-5.93	1.94	2.05
33	c	508	CLA	MG-ND	-5.93	1.94	2.05
38	1	310	KC2	C4B-NB	5.93	1.45	1.37
33	0	306	CLA	MG-ND	-5.93	1.94	2.05
33	4	310	CLA	MG-ND	-5.92	1.94	2.05
33	C	508	CLA	MG-ND	-5.92	1.94	2.05
33	g	304	CLA	MG-NB	-5.92	1.94	2.05
33	1	305	CLA	MG-ND	-5.92	1.94	2.05
33	0	310	CLA	MG-NA	-5.91	1.92	2.06
33	0	307	CLA	MG-NB	-5.91	1.94	2.05
33	5	304	CLA	MG-NB	-5.90	1.94	2.05
33	6	302	CLA	MG-ND	-5.89	1.94	2.05
33	4	309	CLA	MG-NA	-5.89	1.92	2.06
33	D	404	CLA	MG-ND	-5.88	1.94	2.05
33	4	307	CLA	MG-NB	-5.88	1.94	2.05
33	1	302	CLA	MG-NB	-5.88	1.94	2.05
33	8	306	CLA	MG-ND	-5.87	1.94	2.05
33	d	404	CLA	MG-ND	-5.87	1.94	2.05
33	p	302	CLA	MG-ND	-5.87	1.94	2.05
33	2	306	CLA	MG-ND	-5.86	1.94	2.05
33	c	511	CLA	MG-ND	-5.83	1.94	2.05
33	6	310	CLA	MG-ND	-5.82	1.94	2.05
33	7	301	CLA	MG-ND	-5.81	1.94	2.05
33	7	302	CLA	MG-NB	-5.81	1.94	2.05
33	6	319	CLA	MG-NA	-5.80	1.92	2.06
33	4	309	CLA	C1D-ND	5.80	1.44	1.37
33	5	306	CLA	MG-ND	-5.80	1.94	2.05
33	p	319	CLA	MG-NA	-5.80	1.92	2.06
33	p	310	CLA	MG-ND	-5.79	1.94	2.05
33	0	310	CLA	C1D-ND	5.79	1.44	1.37
33	g	308	CLA	C1B-NB	5.79	1.44	1.37
33	7	307	CLA	MG-ND	-5.78	1.94	2.05
33	5	308	CLA	C1B-NB	5.78	1.44	1.37
33	C	511	CLA	MG-ND	-5.78	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	g	306	CLA	MG-ND	-5.78	1.94	2.05
33	6	305	CLA	C1D-ND	5.78	1.44	1.37
33	b	611	CLA	MG-ND	-5.77	1.94	2.05
33	g	307	CLA	MG-ND	-5.77	1.94	2.05
33	1	301	CLA	MG-ND	-5.77	1.94	2.05
33	4	310	CLA	MG-NA	-5.76	1.92	2.06
33	5	307	CLA	MG-ND	-5.76	1.94	2.05
33	C	505	CLA	MG-NB	-5.76	1.94	2.05
33	1	307	CLA	MG-ND	-5.76	1.94	2.05
33	5	310	CLA	C1B-NB	5.76	1.44	1.37
33	c	505	CLA	MG-NB	-5.76	1.94	2.05
33	0	311	CLA	MG-NA	-5.75	1.92	2.06
33	6	302	CLA	MG-NB	-5.75	1.94	2.05
33	3	312	CLA	MG-ND	-5.75	1.94	2.05
33	3	306	CLA	C1B-NB	5.75	1.44	1.37
33	6	309	CLA	MG-ND	-5.75	1.94	2.05
33	p	309	CLA	MG-ND	-5.74	1.94	2.05
33	p	302	CLA	MG-NB	-5.74	1.94	2.05
33	B	611	CLA	MG-ND	-5.74	1.94	2.05
33	9	312	CLA	MG-ND	-5.74	1.94	2.05
33	9	308	CLA	MG-ND	-5.73	1.94	2.05
33	g	310	CLA	C1B-NB	5.73	1.44	1.37
33	3	308	CLA	MG-ND	-5.73	1.94	2.05
33	g	310	CLA	MG-ND	-5.73	1.94	2.05
33	p	305	CLA	C1D-ND	5.73	1.44	1.37
33	B	610	CLA	MG-ND	-5.73	1.94	2.05
33	5	311	CLA	C1B-NB	5.72	1.44	1.37
33	C	503	CLA	MG-ND	-5.72	1.94	2.05
33	3	315	CLA	MG-ND	-5.72	1.94	2.05
33	b	605	CLA	MG-ND	-5.72	1.94	2.05
33	9	306	CLA	C1B-NB	5.72	1.44	1.37
33	c	503	CLA	MG-ND	-5.72	1.94	2.05
33	8	305	CLA	MG-ND	-5.72	1.94	2.05
33	9	315	CLA	MG-ND	-5.71	1.94	2.05
33	b	610	CLA	MG-ND	-5.71	1.94	2.05
33	2	305	CLA	MG-ND	-5.71	1.94	2.05
33	c	514	CLA	C1B-NB	5.71	1.44	1.37
33	1	307	CLA	MG-NB	-5.71	1.94	2.05
33	B	605	CLA	MG-ND	-5.71	1.94	2.05
33	N	305	CLA	C1B-NB	5.71	1.44	1.37
33	n	304	CLA	C1B-NB	5.71	1.44	1.37
33	C	514	CLA	C1B-NB	5.70	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	310	CLA	MG-ND	-5.70	1.94	2.05
33	7	302	CLA	MG-ND	-5.69	1.94	2.05
33	g	311	CLA	C1B-NB	5.69	1.44	1.37
33	1	301	CLA	MG-NB	-5.68	1.94	2.05
33	1	302	CLA	MG-ND	-5.68	1.94	2.05
33	7	307	CLA	MG-NB	-5.68	1.94	2.05
33	p	309	CLA	MG-NB	-5.68	1.94	2.05
33	8	303	CLA	MG-ND	-5.67	1.94	2.05
33	9	314	CLA	MG-ND	-5.67	1.94	2.05
33	6	309	CLA	MG-NB	-5.67	1.94	2.05
33	p	313	CLA	MG-ND	-5.66	1.94	2.05
33	4	308	CLA	MG-NA	-5.66	1.92	2.06
33	n	303	CLA	MG-NA	-5.66	1.92	2.06
33	N	304	CLA	MG-ND	-5.66	1.94	2.05
33	g	302	CLA	MG-ND	-5.66	1.94	2.05
33	n	303	CLA	MG-NB	-5.66	1.94	2.05
33	N	304	CLA	MG-NA	-5.66	1.92	2.06
33	g	307	CLA	MG-NB	-5.65	1.94	2.05
33	5	307	CLA	MG-NB	-5.65	1.94	2.05
33	B	603	CLA	MG-ND	-5.65	1.94	2.05
33	0	309	CLA	MG-NA	-5.65	1.92	2.06
33	B	613	CLA	MG-ND	-5.65	1.94	2.05
33	8	303	CLA	C1B-NB	5.65	1.44	1.37
33	6	313	CLA	MG-ND	-5.65	1.94	2.05
33	b	613	CLA	MG-ND	-5.65	1.94	2.05
33	2	303	CLA	MG-ND	-5.65	1.94	2.05
33	b	603	CLA	MG-ND	-5.65	1.94	2.05
33	b	618	CLA	MG-NA	-5.64	1.92	2.06
33	N	304	CLA	MG-NB	-5.64	1.94	2.05
33	B	618	CLA	MG-NA	-5.64	1.92	2.06
33	b	614	CLA	MG-ND	-5.64	1.94	2.05
33	b	618	CLA	MG-ND	-5.64	1.94	2.05
33	7	301	CLA	MG-NB	-5.64	1.94	2.05
33	p	302	CLA	MG-NA	-5.63	1.92	2.06
33	9	309	CLA	C1B-NB	5.63	1.44	1.37
33	9	306	CLA	MG-ND	-5.63	1.94	2.05
33	p	304	CLA	C1B-NB	5.63	1.44	1.37
33	5	302	CLA	MG-ND	-5.63	1.94	2.05
33	b	604	CLA	MG-ND	-5.63	1.94	2.05
33	C	514	CLA	MG-NB	-5.63	1.94	2.05
33	7	306	CLA	MG-ND	-5.63	1.94	2.05
33	6	310	CLA	C3A-C2A	-5.63	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	4	301	CLA	MG-NB	-5.63	1.94	2.05
33	4	302	CLA	MG-NB	-5.63	1.94	2.05
33	8	306	CLA	MG-NB	-5.63	1.94	2.05
33	0	302	CLA	MG-NB	-5.63	1.94	2.05
33	p	310	CLA	C3A-C2A	-5.62	1.49	1.54
33	3	314	CLA	MG-ND	-5.62	1.94	2.05
33	2	303	CLA	C1B-NB	5.62	1.44	1.37
33	B	614	CLA	MG-ND	-5.62	1.94	2.05
33	3	309	CLA	C1B-NB	5.62	1.44	1.37
33	B	615	CLA	MG-NA	-5.62	1.92	2.06
33	c	514	CLA	MG-NB	-5.62	1.94	2.05
33	6	302	CLA	MG-NA	-5.62	1.92	2.06
33	n	303	CLA	MG-ND	-5.62	1.94	2.05
33	a	405	CLA	MG-ND	-5.62	1.94	2.05
33	B	609	CLA	MG-ND	-5.62	1.94	2.05
33	N	302	CLA	MG-ND	-5.62	1.94	2.05
33	2	306	CLA	MG-NB	-5.61	1.94	2.05
33	5	317	CLA	C1B-NB	5.61	1.44	1.37
33	b	612	CLA	MG-ND	-5.61	1.94	2.05
33	4	301	CLA	MG-ND	-5.61	1.94	2.05
33	1	306	CLA	MG-ND	-5.61	1.94	2.05
33	0	301	CLA	MG-NB	-5.61	1.94	2.05
33	0	301	CLA	MG-ND	-5.61	1.94	2.05
33	A	408	CLA	C1B-NB	5.61	1.44	1.37
33	3	306	CLA	MG-ND	-5.60	1.94	2.05
33	B	615	CLA	C1B-NB	5.60	1.44	1.37
33	n	303	CLA	C1B-NB	5.60	1.44	1.37
33	8	307	CLA	C1B-NB	5.60	1.44	1.37
33	g	301	CLA	MG-ND	-5.60	1.94	2.05
33	5	301	CLA	MG-ND	-5.60	1.94	2.05
33	b	615	CLA	C1B-NB	5.60	1.44	1.37
33	6	304	CLA	C1B-NB	5.60	1.44	1.37
33	b	615	CLA	MG-NA	-5.59	1.93	2.06
33	9	315	CLA	MG-NB	-5.59	1.94	2.05
33	B	612	CLA	MG-ND	-5.59	1.94	2.05
33	B	604	CLA	MG-ND	-5.59	1.94	2.05
33	b	609	CLA	MG-ND	-5.59	1.94	2.05
33	g	317	CLA	C1B-NB	5.59	1.44	1.37
33	a	408	CLA	C1B-NB	5.59	1.44	1.37
33	1	307	CLA	C1B-NB	5.59	1.44	1.37
33	8	302	CLA	MG-ND	-5.59	1.94	2.05
33	1	308	CLA	C1B-NB	5.59	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	n	302	CLA	MG-ND	-5.58	1.94	2.05
33	5	303	CLA	C1B-NB	5.58	1.44	1.37
33	2	302	CLA	MG-ND	-5.58	1.94	2.05
33	8	302	CLA	MG-NB	-5.58	1.94	2.05
33	4	304	CLA	MG-NA	-5.58	1.93	2.06
33	g	308	CLA	MG-ND	-5.58	1.94	2.05
33	7	307	CLA	C1B-NB	5.58	1.44	1.37
33	3	315	CLA	MG-NB	-5.58	1.94	2.05
33	B	618	CLA	MG-ND	-5.58	1.94	2.05
33	2	307	CLA	C1B-NB	5.57	1.44	1.37
33	g	302	CLA	C1B-NB	5.57	1.44	1.37
33	2	302	CLA	MG-NB	-5.57	1.94	2.05
33	5	308	CLA	MG-ND	-5.57	1.94	2.05
33	9	306	CLA	MG-NA	-5.57	1.93	2.06
33	9	305	CLA	MG-NB	-5.56	1.94	2.05
33	A	405	CLA	MG-ND	-5.56	1.94	2.05
33	3	305	CLA	MG-NB	-5.56	1.94	2.05
33	g	303	CLA	C1B-NB	5.56	1.44	1.37
33	b	606	CLA	C1B-NB	5.56	1.44	1.37
33	0	304	CLA	MG-NA	-5.56	1.93	2.06
33	6	310	CLA	MG-NA	-5.56	1.93	2.06
33	3	306	CLA	MG-NA	-5.56	1.93	2.06
33	D	405	CLA	C1B-NB	5.56	1.44	1.37
33	N	304	CLA	C1B-NB	5.56	1.44	1.37
38	1	311	KC2	C4B-NB	5.56	1.44	1.37
33	c	510	CLA	MG-ND	-5.56	1.94	2.05
33	3	307	CLA	MG-ND	-5.55	1.94	2.05
33	N	306	CLA	MG-ND	-5.55	1.94	2.05
33	n	305	CLA	MG-ND	-5.55	1.94	2.05
33	7	307	CLA	MG-NA	-5.55	1.93	2.06
33	p	310	CLA	MG-NA	-5.55	1.93	2.06
33	N	307	CLA	C1B-NB	5.55	1.44	1.37
33	c	513	CLA	MG-ND	-5.55	1.94	2.05
33	6	303	CLA	MG-ND	-5.55	1.94	2.05
33	B	606	CLA	C1B-NB	5.55	1.44	1.37
33	5	302	CLA	C1B-NB	5.55	1.44	1.37
33	n	306	CLA	C1B-NB	5.55	1.44	1.37
33	5	301	CLA	C1B-NB	5.54	1.44	1.37
33	3	303	CLA	MG-ND	-5.54	1.94	2.05
33	9	313	CLA	C1B-NB	5.54	1.44	1.37
33	9	307	CLA	MG-ND	-5.54	1.94	2.05
33	b	612	CLA	C1B-NB	5.54	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	9	304	CLA	MG-ND	-5.54	1.94	2.05
33	3	304	CLA	MG-ND	-5.54	1.94	2.05
33	p	303	CLA	MG-ND	-5.54	1.94	2.05
33	9	313	CLA	MG-ND	-5.54	1.94	2.05
33	A	406	CLA	C1B-NB	5.54	1.44	1.37
33	4	302	CLA	MG-ND	-5.53	1.94	2.05
33	g	310	CLA	MG-NA	-5.53	1.93	2.06
33	a	406	CLA	MG-NB	-5.53	1.94	2.05
33	9	303	CLA	MG-ND	-5.53	1.94	2.05
33	1	307	CLA	MG-NA	-5.53	1.93	2.06
33	C	510	CLA	MG-ND	-5.53	1.94	2.05
33	9	305	CLA	MG-ND	-5.53	1.94	2.05
33	C	506	CLA	MG-ND	-5.53	1.94	2.05
33	N	303	CLA	MG-ND	-5.53	1.94	2.05
33	8	310	CLA	MG-ND	-5.53	1.94	2.05
33	c	506	CLA	MG-ND	-5.53	1.94	2.05
33	7	308	CLA	C1B-NB	5.53	1.44	1.37
33	a	406	CLA	C1B-NB	5.52	1.44	1.37
33	C	513	CLA	MG-ND	-5.52	1.94	2.05
33	d	405	CLA	C1B-NB	5.52	1.44	1.37
33	C	513	CLA	C1B-NB	5.52	1.44	1.37
33	0	302	CLA	MG-ND	-5.52	1.94	2.05
33	c	514	CLA	MG-ND	-5.52	1.94	2.05
33	1	303	CLA	MG-ND	-5.52	1.94	2.05
33	2	304	CLA	MG-NB	-5.52	1.94	2.05
33	b	602	CLA	MG-ND	-5.51	1.94	2.05
33	7	303	CLA	MG-ND	-5.51	1.94	2.05
33	5	310	CLA	MG-NA	-5.51	1.93	2.06
33	p	303	CLA	MG-NA	-5.51	1.93	2.06
33	8	310	CLA	C1B-NB	5.51	1.44	1.37
33	8	304	CLA	MG-NB	-5.51	1.94	2.05
33	n	304	CLA	MG-ND	-5.51	1.94	2.05
33	2	304	CLA	C1B-NB	5.51	1.44	1.37
33	A	406	CLA	MG-NB	-5.51	1.94	2.05
33	0	307	CLA	MG-ND	-5.51	1.94	2.05
33	0	308	CLA	MG-ND	-5.51	1.94	2.05
33	3	309	CLA	MG-ND	-5.50	1.94	2.05
33	C	514	CLA	MG-ND	-5.50	1.94	2.05
33	2	307	CLA	MG-ND	-5.50	1.94	2.05
33	N	305	CLA	MG-ND	-5.50	1.94	2.05
33	B	615	CLA	MG-ND	-5.50	1.94	2.05
33	1	309	CLA	MG-ND	-5.50	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	502	CLA	MG-ND	-5.50	1.94	2.05
33	c	513	CLA	C1B-NB	5.50	1.44	1.37
33	g	301	CLA	C1B-NB	5.50	1.44	1.37
38	7	311	KC2	C4B-NB	5.49	1.44	1.37
33	6	307	CLA	MG-ND	-5.49	1.94	2.05
33	A	406	CLA	MG-ND	-5.49	1.94	2.05
33	7	309	CLA	MG-ND	-5.49	1.94	2.05
33	p	307	CLA	MG-ND	-5.49	1.94	2.05
33	9	310	CLA	MG-ND	-5.49	1.94	2.05
33	4	307	CLA	MG-ND	-5.49	1.94	2.05
33	b	615	CLA	MG-ND	-5.49	1.94	2.05
33	a	406	CLA	MG-ND	-5.49	1.94	2.05
33	a	412	CLA	MG-ND	-5.49	1.94	2.05
33	2	310	CLA	MG-ND	-5.49	1.94	2.05
33	5	302	CLA	MG-NB	-5.49	1.94	2.05
33	8	307	CLA	MG-ND	-5.49	1.94	2.05
33	3	310	CLA	C1B-NB	5.49	1.44	1.37
33	3	313	CLA	MG-ND	-5.49	1.94	2.05
33	g	305	CLA	MG-NA	-5.49	1.93	2.06
33	n	301	CLA	MG-ND	-5.49	1.94	2.05
33	2	301	CLA	MG-ND	-5.49	1.94	2.05
33	N	301	CLA	MG-ND	-5.48	1.94	2.05
33	8	301	CLA	MG-NB	-5.48	1.94	2.05
33	g	311	CLA	MG-ND	-5.48	1.94	2.05
33	B	602	CLA	MG-ND	-5.48	1.94	2.05
33	9	309	CLA	MG-ND	-5.48	1.94	2.05
33	2	308	CLA	MG-ND	-5.48	1.94	2.05
33	A	412	CLA	MG-ND	-5.48	1.94	2.05
33	5	305	CLA	MG-NA	-5.48	1.93	2.06
33	2	310	CLA	C1B-NB	5.48	1.44	1.37
33	9	314	CLA	C1B-NB	5.48	1.44	1.37
33	8	301	CLA	C1B-NB	5.47	1.44	1.37
33	8	301	CLA	MG-ND	-5.47	1.94	2.05
33	8	304	CLA	C1B-NB	5.47	1.44	1.37
33	B	612	CLA	C1B-NB	5.47	1.44	1.37
33	6	303	CLA	MG-NA	-5.47	1.93	2.06
33	5	301	CLA	MG-NB	-5.47	1.94	2.05
33	c	502	CLA	MG-ND	-5.47	1.94	2.05
33	g	303	CLA	MG-NA	-5.47	1.93	2.06
33	b	602	CLA	C1B-NB	5.47	1.44	1.37
33	b	603	CLA	C1B-NB	5.47	1.44	1.37
33	3	305	CLA	MG-ND	-5.47	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	3	314	CLA	C1B-NB	5.47	1.44	1.37
33	g	301	CLA	MG-NB	-5.47	1.95	2.05
33	b	618	CLA	MG-NB	-5.46	1.95	2.05
33	8	308	CLA	MG-ND	-5.46	1.95	2.05
33	B	602	CLA	C1B-NB	5.46	1.44	1.37
33	3	310	CLA	MG-ND	-5.46	1.95	2.05
33	3	313	CLA	C1B-NB	5.46	1.44	1.37
33	9	310	CLA	C1B-NB	5.46	1.44	1.37
33	n	302	CLA	C1B-NB	5.46	1.44	1.37
33	5	303	CLA	MG-NA	-5.45	1.93	2.06
33	g	302	CLA	MG-NB	-5.45	1.95	2.05
33	9	307	CLA	C1B-NB	5.45	1.44	1.37
33	4	303	CLA	C1B-NB	5.45	1.44	1.37
33	2	301	CLA	MG-NB	-5.45	1.95	2.05
33	9	314	CLA	MG-NB	-5.45	1.95	2.05
33	5	317	CLA	MG-ND	-5.44	1.95	2.05
33	5	311	CLA	MG-ND	-5.44	1.95	2.05
33	B	618	CLA	MG-NB	-5.44	1.95	2.05
33	6	305	CLA	MG-NA	-5.44	1.93	2.06
33	p	305	CLA	MG-NA	-5.44	1.93	2.06
33	b	616	CLA	MG-ND	-5.44	1.95	2.05
33	b	611	CLA	C1B-NB	5.44	1.44	1.37
33	5	310	CLA	MG-NB	-5.44	1.95	2.05
33	8	303	CLA	MG-NA	-5.44	1.93	2.06
33	6	307	CLA	MG-NB	-5.43	1.95	2.05
33	g	308	CLA	MG-NB	-5.43	1.95	2.05
33	5	308	CLA	MG-NB	-5.43	1.95	2.05
33	C	503	CLA	MG-NB	-5.43	1.95	2.05
33	p	307	CLA	MG-NB	-5.43	1.95	2.05
33	9	312	CLA	C1B-NB	5.43	1.44	1.37
33	9	309	CLA	MG-NB	-5.43	1.95	2.05
33	N	302	CLA	C1B-NB	5.43	1.44	1.37
33	c	511	CLA	MG-NA	-5.43	1.93	2.06
33	8	308	CLA	MG-NB	-5.43	1.95	2.05
33	g	317	CLA	MG-ND	-5.43	1.95	2.05
33	9	307	CLA	MG-NA	-5.43	1.93	2.06
33	B	606	CLA	MG-ND	-5.43	1.95	2.05
33	1	301	CLA	MG-NA	-5.42	1.93	2.06
33	7	301	CLA	MG-NA	-5.42	1.93	2.06
33	B	603	CLA	C1B-NB	5.42	1.44	1.37
33	3	307	CLA	C1B-NB	5.42	1.44	1.37
33	5	308	CLA	MG-NA	-5.42	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	308	CLA	MG-NB	-5.42	1.95	2.05
33	g	308	CLA	MG-NA	-5.42	1.93	2.06
33	0	307	CLA	MG-NA	-5.41	1.93	2.06
33	5	304	CLA	MG-NA	-5.41	1.93	2.06
33	5	307	CLA	MG-NA	-5.41	1.93	2.06
33	B	616	CLA	MG-ND	-5.41	1.95	2.05
33	2	303	CLA	MG-NA	-5.41	1.93	2.06
33	b	608	CLA	MG-ND	-5.41	1.95	2.05
33	3	314	CLA	MG-NB	-5.41	1.95	2.05
33	3	312	CLA	C1B-NB	5.41	1.44	1.37
33	g	310	CLA	MG-NB	-5.41	1.95	2.05
33	0	303	CLA	C1B-NB	5.41	1.44	1.37
33	3	309	CLA	MG-NB	-5.41	1.95	2.05
33	C	511	CLA	MG-NA	-5.41	1.93	2.06
33	c	503	CLA	MG-NB	-5.41	1.95	2.05
33	1	304	CLA	MG-NB	-5.41	1.95	2.05
33	b	606	CLA	MG-ND	-5.41	1.95	2.05
33	D	405	CLA	MG-ND	-5.40	1.95	2.05
33	p	310	CLA	MG-NB	-5.40	1.95	2.05
33	6	313	CLA	MG-NB	-5.40	1.95	2.05
33	4	302	CLA	MG-NA	-5.40	1.93	2.06
33	p	313	CLA	MG-NB	-5.40	1.95	2.05
33	3	307	CLA	MG-NA	-5.40	1.93	2.06
33	c	507	CLA	MG-ND	-5.40	1.95	2.05
33	g	304	CLA	MG-NA	-5.40	1.93	2.06
33	0	302	CLA	MG-NA	-5.39	1.93	2.06
33	4	307	CLA	MG-NA	-5.39	1.93	2.06
33	d	405	CLA	MG-ND	-5.39	1.95	2.05
33	g	303	CLA	MG-NB	-5.39	1.95	2.05
33	9	304	CLA	C1B-NB	5.39	1.44	1.37
33	5	311	CLA	MG-NB	-5.39	1.95	2.05
33	g	307	CLA	MG-NA	-5.39	1.93	2.06
33	p	304	CLA	MG-ND	-5.39	1.95	2.05
33	7	304	CLA	MG-NB	-5.38	1.95	2.05
33	B	611	CLA	C1B-NB	5.38	1.44	1.37
33	C	509	CLA	MG-ND	-5.38	1.95	2.05
33	3	304	CLA	C1B-NB	5.38	1.44	1.37
33	c	509	CLA	MG-ND	-5.38	1.95	2.05
33	A	408	CLA	MG-ND	-5.38	1.95	2.05
33	B	608	CLA	MG-ND	-5.38	1.95	2.05
33	C	507	CLA	C1B-NB	5.38	1.44	1.37
33	5	303	CLA	MG-NB	-5.38	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	612	CLA	MG-NB	-5.38	1.95	2.05
33	C	507	CLA	MG-ND	-5.37	1.95	2.05
33	C	504	CLA	MG-ND	-5.37	1.95	2.05
33	6	304	CLA	MG-ND	-5.37	1.95	2.05
33	9	306	CLA	MG-NB	-5.37	1.95	2.05
33	0	303	CLA	MG-ND	-5.37	1.95	2.05
33	6	304	CLA	MG-NB	-5.37	1.95	2.05
33	3	306	CLA	MG-NB	-5.37	1.95	2.05
33	C	509	CLA	MG-NB	-5.37	1.95	2.05
33	c	509	CLA	MG-NB	-5.37	1.95	2.05
33	b	606	CLA	MG-NB	-5.37	1.95	2.05
33	B	606	CLA	MG-NB	-5.36	1.95	2.05
33	3	310	CLA	MG-NB	-5.36	1.95	2.05
33	B	612	CLA	MG-NB	-5.36	1.95	2.05
33	b	613	CLA	C1B-NB	5.36	1.44	1.37
33	B	613	CLA	MG-NB	-5.36	1.95	2.05
33	7	309	CLA	C1B-NB	5.36	1.44	1.37
33	4	304	CLA	MG-NB	-5.36	1.95	2.05
33	B	610	CLA	MG-NB	-5.36	1.95	2.05
33	b	613	CLA	MG-NB	-5.36	1.95	2.05
33	p	304	CLA	MG-NB	-5.36	1.95	2.05
33	C	504	CLA	C1B-NB	5.35	1.44	1.37
33	C	505	CLA	MG-NA	-5.35	1.93	2.06
33	B	617	CLA	MG-ND	-5.35	1.95	2.05
33	6	310	CLA	MG-NB	-5.35	1.95	2.05
33	c	512	CLA	MG-ND	-5.35	1.95	2.05
33	2	301	CLA	C1B-NB	5.35	1.44	1.37
33	b	615	CLA	MG-NB	-5.35	1.95	2.05
33	B	609	CLA	C1B-NB	5.35	1.44	1.37
33	a	408	CLA	MG-ND	-5.35	1.95	2.05
33	c	507	CLA	C1B-NB	5.35	1.44	1.37
33	c	505	CLA	MG-NA	-5.35	1.93	2.06
33	b	617	CLA	MG-ND	-5.35	1.95	2.05
33	1	308	CLA	MG-ND	-5.34	1.95	2.05
33	B	611	CLA	MG-NB	-5.34	1.95	2.05
33	0	304	CLA	MG-NB	-5.34	1.95	2.05
33	b	609	CLA	C1B-NB	5.34	1.44	1.37
33	7	306	CLA	MG-NB	-5.34	1.95	2.05
33	0	306	CLA	MG-NB	-5.34	1.95	2.05
33	g	311	CLA	MG-NB	-5.34	1.95	2.05
33	7	303	CLA	MG-NB	-5.33	1.95	2.05
33	7	308	CLA	MG-ND	-5.33	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	4	301	CLA	C1B-NB	5.33	1.44	1.37
33	b	610	CLA	MG-NB	-5.33	1.95	2.05
33	B	613	CLA	C1B-NB	5.33	1.44	1.37
33	2	302	CLA	C1B-NB	5.33	1.44	1.37
33	b	611	CLA	MG-NB	-5.33	1.95	2.05
33	8	305	CLA	C1B-NB	5.33	1.44	1.37
33	1	305	CLA	MG-NB	-5.32	1.95	2.05
33	1	306	CLA	MG-NB	-5.32	1.95	2.05
33	3	307	CLA	MG-NB	-5.32	1.95	2.05
33	C	505	CLA	MG-ND	-5.32	1.95	2.05
33	2	302	CLA	MG-NA	-5.32	1.93	2.06
33	n	305	CLA	C1B-NB	5.32	1.44	1.37
33	C	507	CLA	MG-NA	-5.32	1.93	2.06
33	a	406	CLA	MG-NA	-5.32	1.93	2.06
33	B	607	CLA	C1B-NB	5.32	1.44	1.37
33	2	305	CLA	C1B-NB	5.32	1.44	1.37
33	9	307	CLA	MG-NB	-5.32	1.95	2.05
33	C	511	CLA	MG-NB	-5.32	1.95	2.05
33	p	312	CLA	MG-ND	-5.32	1.95	2.05
33	c	505	CLA	MG-ND	-5.32	1.95	2.05
33	c	507	CLA	MG-NA	-5.31	1.93	2.06
33	1	308	CLA	MG-NB	-5.31	1.95	2.05
33	C	506	CLA	C1B-NB	5.31	1.44	1.37
33	7	305	CLA	MG-NB	-5.31	1.95	2.05
33	N	301	CLA	C1B-NB	5.31	1.44	1.37
33	4	303	CLA	MG-ND	-5.31	1.95	2.05
33	6	306	CLA	MG-ND	-5.31	1.95	2.05
33	C	513	CLA	MG-NB	-5.31	1.95	2.05
33	1	303	CLA	MG-NB	-5.31	1.95	2.05
33	5	317	CLA	MG-NA	-5.31	1.93	2.06
33	b	607	CLA	C1B-NB	5.31	1.44	1.37
33	8	302	CLA	C1B-NB	5.31	1.44	1.37
33	c	513	CLA	MG-NB	-5.31	1.95	2.05
33	c	510	CLA	C1B-NB	5.31	1.44	1.37
33	6	312	CLA	MG-NB	-5.31	1.95	2.05
33	p	312	CLA	MG-NB	-5.31	1.95	2.05
33	4	306	CLA	MG-NB	-5.30	1.95	2.05
33	N	306	CLA	MG-NB	-5.30	1.95	2.05
33	C	505	CLA	C1B-NB	5.30	1.44	1.37
33	n	305	CLA	MG-NB	-5.30	1.95	2.05
33	B	618	CLA	C1B-NB	5.30	1.44	1.37
33	4	303	CLA	MG-NB	-5.30	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	504	CLA	MG-ND	-5.30	1.95	2.05
33	6	312	CLA	MG-ND	-5.30	1.95	2.05
33	C	512	CLA	MG-ND	-5.30	1.95	2.05
33	5	303	CLA	MG-ND	-5.30	1.95	2.05
33	b	608	CLA	MG-NB	-5.30	1.95	2.05
33	8	302	CLA	MG-NA	-5.30	1.93	2.06
33	A	406	CLA	MG-NA	-5.30	1.93	2.06
33	7	308	CLA	MG-NB	-5.30	1.95	2.05
33	9	310	CLA	MG-NB	-5.30	1.95	2.05
33	C	510	CLA	C1B-NB	5.30	1.44	1.37
33	c	502	CLA	MG-NB	-5.30	1.95	2.05
33	B	608	CLA	MG-NB	-5.29	1.95	2.05
33	g	317	CLA	MG-NA	-5.29	1.93	2.06
33	C	508	CLA	MG-NB	-5.29	1.95	2.05
33	1	309	CLA	C1B-NB	5.29	1.44	1.37
33	1	302	CLA	MG-NA	-5.29	1.93	2.06
33	c	508	CLA	MG-NB	-5.29	1.95	2.05
33	n	301	CLA	C1B-NB	5.29	1.44	1.37
33	g	306	CLA	MG-NB	-5.29	1.95	2.05
33	c	504	CLA	C1B-NB	5.29	1.44	1.37
33	7	309	CLA	MG-NB	-5.28	1.95	2.05
33	p	306	CLA	MG-ND	-5.28	1.95	2.05
33	c	502	CLA	C1B-NB	5.28	1.44	1.37
33	0	303	CLA	MG-NB	-5.28	1.95	2.05
33	g	317	CLA	MG-NB	-5.28	1.95	2.05
33	2	304	CLA	MG-ND	-5.28	1.95	2.05
33	9	304	CLA	MG-NB	-5.28	1.95	2.05
33	3	304	CLA	MG-NB	-5.28	1.95	2.05
33	0	306	CLA	MG-NA	-5.28	1.93	2.06
33	2	301	CLA	MG-NA	-5.28	1.93	2.06
33	c	504	CLA	MG-NB	-5.28	1.95	2.05
33	5	317	CLA	MG-NB	-5.28	1.95	2.05
33	7	302	CLA	MG-NA	-5.28	1.93	2.06
33	B	608	CLA	C1B-NB	5.28	1.44	1.37
33	B	615	CLA	MG-NB	-5.27	1.95	2.05
33	C	509	CLA	C1B-NB	5.27	1.44	1.37
33	N	306	CLA	C1B-NB	5.27	1.44	1.37
33	9	314	CLA	MG-NA	-5.27	1.93	2.06
33	B	607	CLA	MG-ND	-5.27	1.95	2.05
33	C	502	CLA	C1B-NB	5.27	1.44	1.37
33	C	502	CLA	MG-NB	-5.27	1.95	2.05
33	3	313	CLA	MG-NB	-5.27	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	511	CLA	MG-NB	-5.27	1.95	2.05
33	D	404	CLA	C1B-NB	5.26	1.44	1.37
33	8	304	CLA	MG-ND	-5.26	1.95	2.05
33	0	301	CLA	C1B-NB	5.26	1.44	1.37
33	9	303	CLA	MG-NB	-5.26	1.95	2.05
33	8	301	CLA	MG-NA	-5.26	1.93	2.06
33	c	506	CLA	C1B-NB	5.26	1.44	1.37
33	1	309	CLA	MG-NB	-5.26	1.95	2.05
33	c	509	CLA	C1B-NB	5.26	1.44	1.37
33	b	618	CLA	C1B-NB	5.26	1.44	1.37
33	c	505	CLA	C1B-NB	5.26	1.44	1.37
33	1	304	CLA	C1B-NB	5.26	1.44	1.37
33	C	511	CLA	C1B-NB	5.25	1.44	1.37
33	C	504	CLA	MG-NB	-5.25	1.95	2.05
33	B	604	CLA	MG-NB	-5.25	1.95	2.05
33	b	607	CLA	MG-ND	-5.25	1.95	2.05
33	4	306	CLA	MG-NA	-5.25	1.93	2.06
33	3	314	CLA	MG-NA	-5.25	1.93	2.06
33	5	306	CLA	MG-NB	-5.25	1.95	2.05
33	5	302	CLA	MG-NA	-5.25	1.93	2.06
33	7	304	CLA	C1B-NB	5.25	1.44	1.37
33	1	304	CLA	MG-NA	-5.25	1.93	2.06
33	9	313	CLA	MG-NB	-5.24	1.95	2.05
33	b	602	CLA	MG-NB	-5.24	1.95	2.05
33	2	308	CLA	C1B-NB	5.24	1.44	1.37
33	g	303	CLA	MG-ND	-5.24	1.95	2.05
33	B	617	CLA	C1B-NB	5.23	1.44	1.37
33	d	404	CLA	C1B-NB	5.23	1.44	1.37
33	D	404	CLA	MG-NB	-5.23	1.95	2.05
33	3	303	CLA	MG-NB	-5.23	1.95	2.05
33	B	602	CLA	MG-NB	-5.23	1.95	2.05
33	2	305	CLA	MG-NB	-5.23	1.95	2.05
33	b	604	CLA	MG-NB	-5.23	1.95	2.05
33	n	305	CLA	MG-NA	-5.23	1.93	2.06
33	d	404	CLA	MG-NB	-5.23	1.95	2.05
33	b	608	CLA	C1B-NB	5.23	1.44	1.37
33	8	305	CLA	MG-NA	-5.23	1.93	2.06
33	7	304	CLA	MG-NA	-5.22	1.93	2.06
33	1	302	CLA	C1B-NB	5.22	1.44	1.37
33	8	305	CLA	MG-NB	-5.22	1.95	2.05
33	N	306	CLA	MG-NA	-5.22	1.93	2.06
33	g	302	CLA	MG-NA	-5.22	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	305	CLA	MG-NA	-5.22	1.93	2.06
33	1	304	CLA	MG-ND	-5.22	1.95	2.05
33	7	301	CLA	C1B-NB	5.22	1.44	1.37
33	1	301	CLA	C1B-NB	5.21	1.44	1.37
33	9	303	CLA	C1B-NB	5.21	1.44	1.37
33	8	308	CLA	C1B-NB	5.21	1.44	1.37
33	p	304	CLA	MG-NA	-5.21	1.93	2.06
33	8	307	CLA	MG-NB	-5.21	1.95	2.05
33	2	307	CLA	MG-NB	-5.20	1.95	2.05
33	B	614	CLA	C1B-NB	5.20	1.44	1.37
33	0	303	CLA	MG-NA	-5.20	1.93	2.06
33	b	617	CLA	C1B-NB	5.20	1.44	1.37
33	2	304	CLA	MG-NA	-5.20	1.93	2.06
33	6	312	CLA	MG-NA	-5.19	1.93	2.06
33	9	312	CLA	MG-NB	-5.19	1.95	2.05
33	b	614	CLA	C1B-NB	5.19	1.44	1.37
33	C	506	CLA	MG-NB	-5.19	1.95	2.05
33	C	514	CLA	MG-NA	-5.19	1.93	2.06
33	c	511	CLA	C1B-NB	5.19	1.44	1.37
33	6	304	CLA	MG-NA	-5.19	1.93	2.06
33	B	606	CLA	MG-NA	-5.19	1.93	2.06
33	c	506	CLA	MG-NB	-5.19	1.95	2.05
33	4	303	CLA	MG-NA	-5.19	1.93	2.06
33	7	304	CLA	MG-ND	-5.19	1.95	2.05
33	b	617	CLA	MG-NB	-5.19	1.95	2.05
33	9	309	CLA	MG-NA	-5.18	1.94	2.06
33	7	302	CLA	C1B-NB	5.18	1.44	1.37
33	1	305	CLA	MG-NA	-5.18	1.94	2.06
33	3	309	CLA	MG-NA	-5.18	1.94	2.06
33	C	510	CLA	MG-NB	-5.18	1.95	2.05
33	c	510	CLA	MG-NB	-5.18	1.95	2.05
33	b	606	CLA	MG-NA	-5.18	1.94	2.06
33	a	412	CLA	C1B-NB	5.18	1.44	1.37
33	6	307	CLA	MG-NA	-5.18	1.94	2.06
33	p	307	CLA	MG-NA	-5.17	1.94	2.06
33	B	608	CLA	MG-NA	-5.17	1.94	2.06
33	p	312	CLA	MG-NA	-5.17	1.94	2.06
33	5	305	CLA	MG-NB	-5.17	1.95	2.05
33	3	303	CLA	C1B-NB	5.17	1.44	1.37
33	c	514	CLA	MG-NA	-5.17	1.94	2.06
33	B	617	CLA	MG-NB	-5.17	1.95	2.05
33	8	304	CLA	MG-NA	-5.16	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	608	CLA	MG-NA	-5.16	1.94	2.06
33	N	307	CLA	MG-ND	-5.16	1.95	2.05
33	d	405	CLA	MG-NB	-5.16	1.95	2.05
33	A	412	CLA	C1B-NB	5.16	1.44	1.37
33	7	305	CLA	MG-NA	-5.16	1.94	2.06
38	4	305	KC2	C4B-NB	5.16	1.44	1.37
33	g	305	CLA	MG-NB	-5.16	1.95	2.05
33	D	405	CLA	MG-NB	-5.15	1.95	2.05
33	6	306	CLA	MG-NA	-5.15	1.94	2.06
33	p	306	CLA	MG-NA	-5.15	1.94	2.06
38	0	305	KC2	C4B-NB	5.15	1.44	1.37
33	b	603	CLA	MG-NB	-5.14	1.95	2.05
33	p	305	CLA	MG-NB	-5.14	1.95	2.05
33	3	312	CLA	MG-NB	-5.14	1.95	2.05
33	9	305	CLA	C1B-NB	5.14	1.44	1.37
33	3	305	CLA	C1B-NB	5.14	1.44	1.37
33	2	310	CLA	MG-NB	-5.14	1.95	2.05
33	6	305	CLA	MG-NB	-5.14	1.95	2.05
33	B	605	CLA	C1B-NB	5.14	1.44	1.37
33	n	306	CLA	MG-ND	-5.14	1.95	2.05
33	b	616	CLA	C1B-NB	5.13	1.44	1.37
33	B	616	CLA	C1B-NB	5.12	1.44	1.37
33	b	610	CLA	C1B-NB	5.12	1.44	1.37
33	5	306	CLA	MG-NA	-5.12	1.94	2.06
33	g	306	CLA	MG-NA	-5.12	1.94	2.06
33	B	603	CLA	MG-NB	-5.12	1.95	2.05
33	N	302	CLA	MG-NB	-5.11	1.95	2.05
33	8	310	CLA	MG-NB	-5.11	1.95	2.05
33	C	507	CLA	MG-NB	-5.11	1.95	2.05
33	c	510	CLA	MG-NA	-5.11	1.94	2.06
33	a	408	CLA	MG-NA	-5.11	1.94	2.06
33	C	510	CLA	MG-NA	-5.11	1.94	2.06
33	a	405	CLA	C1B-NB	5.11	1.44	1.37
33	g	304	CLA	C1B-NB	5.10	1.44	1.37
33	3	315	CLA	C1B-NB	5.10	1.44	1.37
33	9	303	CLA	MG-NA	-5.10	1.94	2.06
33	n	302	CLA	MG-NB	-5.10	1.95	2.05
33	b	609	CLA	MG-NB	-5.10	1.95	2.05
33	a	405	CLA	MG-NA	-5.10	1.94	2.06
44	F	101	HEM	FE-NB	5.10	2.10	1.94
33	a	408	CLA	MG-NB	-5.10	1.95	2.05
33	b	605	CLA	C1B-NB	5.09	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	408	CLA	MG-NA	-5.09	1.94	2.06
33	B	610	CLA	C1B-NB	5.09	1.44	1.37
33	5	304	CLA	C1B-NB	5.09	1.44	1.37
33	B	609	CLA	MG-NB	-5.09	1.95	2.05
33	b	617	CLA	MG-NA	-5.09	1.94	2.06
33	3	315	CLA	C3A-C2A	-5.09	1.49	1.54
33	a	412	CLA	MG-NB	-5.09	1.95	2.05
33	C	509	CLA	MG-NA	-5.09	1.94	2.06
33	5	311	CLA	MG-NA	-5.09	1.94	2.06
33	c	507	CLA	MG-NB	-5.09	1.95	2.05
33	A	405	CLA	MG-NA	-5.09	1.94	2.06
33	c	509	CLA	MG-NA	-5.08	1.94	2.06
33	B	605	CLA	MG-NB	-5.08	1.95	2.05
33	9	315	CLA	C1B-NB	5.08	1.44	1.37
33	3	303	CLA	MG-NA	-5.08	1.94	2.06
33	A	412	CLA	MG-NB	-5.08	1.95	2.05
33	b	605	CLA	MG-NB	-5.08	1.95	2.05
33	7	305	CLA	C1B-NB	5.07	1.44	1.37
33	1	305	CLA	C1B-NB	5.07	1.44	1.37
33	A	408	CLA	MG-NB	-5.07	1.95	2.05
33	p	308	CLA	C1B-NB	5.07	1.44	1.37
33	N	305	CLA	MG-NB	-5.07	1.95	2.05
33	B	617	CLA	MG-NA	-5.06	1.94	2.06
33	9	315	CLA	C3A-C2A	-5.06	1.49	1.54
33	n	306	CLA	MG-NA	-5.06	1.94	2.06
33	g	311	CLA	MG-NA	-5.06	1.94	2.06
33	9	305	CLA	MG-NA	-5.06	1.94	2.06
33	N	307	CLA	MG-NA	-5.06	1.94	2.06
33	c	508	CLA	C1B-NB	5.06	1.44	1.37
33	3	305	CLA	MG-NA	-5.05	1.94	2.06
33	6	308	CLA	C1B-NB	5.05	1.44	1.37
33	7	303	CLA	C1B-NB	5.05	1.44	1.37
33	C	508	CLA	C1B-NB	5.05	1.44	1.37
33	7	306	CLA	C1B-NB	5.04	1.44	1.37
33	A	405	CLA	C1B-NB	5.04	1.44	1.37
33	n	304	CLA	MG-NB	-5.04	1.95	2.05
33	n	306	CLA	MG-NB	-5.03	1.95	2.05
33	B	611	CLA	MG-NA	-5.03	1.94	2.06
33	b	611	CLA	MG-NA	-5.02	1.94	2.06
33	3	308	CLA	C1B-NB	5.02	1.44	1.37
33	3	308	CLA	MG-NB	-5.02	1.95	2.05
33	1	308	CLA	MG-NA	-5.02	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	506	CLA	MG-NA	-5.01	1.94	2.06
33	N	307	CLA	MG-NB	-5.01	1.95	2.05
33	n	301	CLA	MG-NB	-5.01	1.95	2.05
33	A	405	CLA	MG-NB	-5.00	1.95	2.05
33	N	301	CLA	MG-NB	-5.00	1.95	2.05
33	8	307	CLA	MG-NA	-5.00	1.94	2.06
33	9	308	CLA	C1B-NB	5.00	1.43	1.37
33	2	306	CLA	MG-NA	-4.99	1.94	2.06
33	7	308	CLA	MG-NA	-4.99	1.94	2.06
33	c	506	CLA	MG-NA	-4.99	1.94	2.06
33	a	405	CLA	MG-NB	-4.99	1.95	2.05
33	1	303	CLA	C1B-NB	4.99	1.43	1.37
33	b	603	CLA	MG-NA	-4.99	1.94	2.06
33	2	307	CLA	MG-NA	-4.98	1.94	2.06
33	6	307	CLA	C1B-NB	4.98	1.43	1.37
38	g	309	KC2	C4B-NB	4.98	1.43	1.37
33	9	308	CLA	MG-NB	-4.98	1.95	2.05
38	5	309	KC2	C4B-NB	4.98	1.43	1.37
33	b	604	CLA	MG-NA	-4.98	1.94	2.06
33	C	512	CLA	MG-NB	-4.98	1.95	2.05
33	C	502	CLA	MG-NA	-4.98	1.94	2.06
33	B	602	CLA	MG-NA	-4.97	1.94	2.06
33	1	306	CLA	C1B-NB	4.97	1.43	1.37
33	p	307	CLA	C1B-NB	4.97	1.43	1.37
33	8	310	CLA	MG-NA	-4.97	1.94	2.06
33	D	404	CLA	MG-NA	-4.96	1.94	2.06
33	b	602	CLA	MG-NA	-4.96	1.94	2.06
33	c	512	CLA	C1B-NB	4.96	1.43	1.37
33	2	310	CLA	MG-NA	-4.96	1.94	2.06
33	n	301	CLA	MG-NA	-4.96	1.94	2.06
33	B	607	CLA	MG-NB	-4.95	1.96	2.05
33	c	513	CLA	MG-NA	-4.95	1.94	2.06
33	d	404	CLA	MG-NA	-4.95	1.94	2.06
33	7	306	CLA	MG-NA	-4.95	1.94	2.06
33	B	603	CLA	MG-NA	-4.95	1.94	2.06
33	B	604	CLA	MG-NA	-4.95	1.94	2.06
33	3	312	CLA	MG-NA	-4.95	1.94	2.06
33	8	306	CLA	MG-NA	-4.95	1.94	2.06
33	C	512	CLA	C1B-NB	4.95	1.43	1.37
33	c	512	CLA	MG-NB	-4.95	1.96	2.05
33	6	306	CLA	C1B-NB	4.95	1.43	1.37
33	B	616	CLA	MG-NB	-4.95	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	513	CLA	MG-NA	-4.95	1.94	2.06
33	9	312	CLA	MG-NA	-4.94	1.94	2.06
33	c	502	CLA	MG-NA	-4.94	1.94	2.06
33	b	607	CLA	MG-NB	-4.94	1.96	2.05
33	p	308	CLA	MG-NB	-4.94	1.96	2.05
33	6	308	CLA	MG-NB	-4.93	1.96	2.05
33	N	301	CLA	MG-NA	-4.93	1.94	2.06
33	1	306	CLA	MG-NA	-4.93	1.94	2.06
33	p	306	CLA	C1B-NB	4.93	1.43	1.37
33	N	303	CLA	MG-NB	-4.92	1.96	2.05
33	g	306	CLA	C1B-NB	4.92	1.43	1.37
33	p	313	CLA	MG-NA	-4.92	1.94	2.06
33	0	308	CLA	MG-NB	-4.91	1.96	2.05
33	b	616	CLA	MG-NB	-4.91	1.96	2.05
33	p	312	CLA	C1B-NB	4.91	1.43	1.37
33	B	609	CLA	MG-NA	-4.91	1.94	2.06
33	0	307	CLA	C1B-NB	4.91	1.43	1.37
33	5	306	CLA	C1B-NB	4.91	1.43	1.37
33	6	312	CLA	C1B-NB	4.90	1.43	1.37
33	4	307	CLA	C1B-NB	4.90	1.43	1.37
33	6	313	CLA	MG-NA	-4.90	1.94	2.06
33	d	405	CLA	MG-NA	-4.90	1.94	2.06
33	p	309	CLA	C1B-NB	4.88	1.43	1.37
33	7	303	CLA	MG-NA	-4.88	1.94	2.06
33	b	613	CLA	MG-NA	-4.88	1.94	2.06
33	p	308	CLA	MG-NA	-4.88	1.94	2.06
33	b	609	CLA	MG-NA	-4.88	1.94	2.06
33	B	604	CLA	C1B-NB	4.87	1.43	1.37
33	B	613	CLA	MG-NA	-4.87	1.94	2.06
33	D	405	CLA	MG-NA	-4.87	1.94	2.06
33	b	604	CLA	C1B-NB	4.87	1.43	1.37
33	1	303	CLA	MG-NA	-4.87	1.94	2.06
33	p	306	CLA	MG-NB	-4.87	1.96	2.05
33	6	308	CLA	MG-NA	-4.86	1.94	2.06
33	4	306	CLA	C1B-NB	4.86	1.43	1.37
33	N	305	CLA	MG-NA	-4.85	1.94	2.06
33	n	304	CLA	MG-NA	-4.85	1.94	2.06
33	6	306	CLA	MG-NB	-4.85	1.96	2.05
33	B	612	CLA	MG-NA	-4.85	1.94	2.06
33	B	607	CLA	MG-NA	-4.84	1.94	2.06
33	4	308	CLA	C1B-NB	4.84	1.43	1.37
33	b	612	CLA	MG-NA	-4.84	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	4	302	CLA	C1B-NB	4.84	1.43	1.37
33	b	607	CLA	MG-NA	-4.84	1.94	2.06
33	0	306	CLA	C1B-NB	4.83	1.43	1.37
33	5	305	CLA	C1B-NB	4.83	1.43	1.37
33	C	503	CLA	C1B-NB	4.83	1.43	1.37
33	8	308	CLA	MG-NA	-4.83	1.94	2.06
33	6	309	CLA	C1B-NB	4.83	1.43	1.37
33	2	308	CLA	MG-NA	-4.82	1.94	2.06
33	c	503	CLA	MG-NA	-4.81	1.94	2.06
33	C	503	CLA	MG-NA	-4.81	1.94	2.06
33	0	309	CLA	C1B-NB	4.81	1.43	1.37
33	g	305	CLA	C1B-NB	4.79	1.43	1.37
33	g	301	CLA	MG-NA	-4.79	1.94	2.06
33	9	313	CLA	MG-NA	-4.79	1.94	2.06
33	b	614	CLA	MG-NA	-4.78	1.94	2.06
33	B	614	CLA	MG-NA	-4.78	1.94	2.06
33	c	503	CLA	C1B-NB	4.78	1.43	1.37
33	3	313	CLA	MG-NA	-4.78	1.94	2.06
33	0	302	CLA	C1B-NB	4.78	1.43	1.37
33	5	301	CLA	MG-NA	-4.77	1.94	2.06
33	2	306	CLA	C1B-NB	4.76	1.43	1.37
33	c	504	CLA	MG-NA	-4.75	1.95	2.06
33	8	306	CLA	C1B-NB	4.75	1.43	1.37
33	3	304	CLA	MG-NA	-4.74	1.95	2.06
33	p	309	CLA	MG-NA	-4.74	1.95	2.06
33	3	315	CLA	MG-NA	-4.73	1.95	2.06
33	6	309	CLA	MG-NA	-4.72	1.95	2.06
33	9	315	CLA	MG-NA	-4.72	1.95	2.06
33	0	311	CLA	C1B-NB	4.72	1.43	1.37
33	C	504	CLA	MG-NA	-4.72	1.95	2.06
33	9	304	CLA	MG-NA	-4.71	1.95	2.06
33	N	302	CLA	MG-NA	-4.70	1.95	2.06
33	p	319	CLA	C1B-NB	4.69	1.43	1.37
33	b	614	CLA	MG-NB	-4.69	1.96	2.05
33	4	310	CLA	C1B-NB	4.68	1.43	1.37
33	B	614	CLA	MG-NB	-4.68	1.96	2.05
38	p	311	KC2	C4B-NB	4.68	1.43	1.37
33	n	302	CLA	MG-NA	-4.66	1.95	2.06
33	6	319	CLA	C1B-NB	4.65	1.43	1.37
33	5	307	CLA	C1B-NB	4.64	1.43	1.37
33	9	310	CLA	MG-NA	-4.63	1.95	2.06
33	g	307	CLA	C1B-NB	4.63	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	L	101	SQD	O8-S	4.63	1.64	1.47
41	l	101	SQD	O8-S	4.63	1.64	1.47
38	6	311	KC2	C4B-NB	4.62	1.43	1.37
41	b	601	SQD	O8-S	4.62	1.63	1.47
33	3	308	CLA	MG-NA	-4.61	1.95	2.06
33	3	310	CLA	MG-NA	-4.60	1.95	2.06
41	B	601	SQD	O8-S	4.60	1.63	1.47
41	j	101	SQD	O8-S	4.59	1.63	1.47
33	9	308	CLA	MG-NA	-4.59	1.95	2.06
41	c	501	SQD	O8-S	4.59	1.63	1.47
41	J	101	SQD	O8-S	4.58	1.63	1.47
41	C	501	SQD	O8-S	4.58	1.63	1.47
33	4	309	CLA	C1B-NB	4.58	1.43	1.37
33	B	610	CLA	MG-NA	-4.58	1.95	2.06
33	c	512	CLA	MG-NA	-4.58	1.95	2.06
33	b	610	CLA	MG-NA	-4.57	1.95	2.06
33	C	512	CLA	MG-NA	-4.57	1.95	2.06
33	0	310	CLA	C1B-NB	4.55	1.43	1.37
33	4	308	CLA	MG-ND	-4.55	1.96	2.05
33	0	309	CLA	MG-ND	-4.52	1.96	2.05
33	1	309	CLA	MG-NA	-4.51	1.95	2.06
33	0	301	CLA	C3A-C2A	-4.49	1.50	1.54
33	7	309	CLA	MG-NA	-4.48	1.95	2.06
33	6	303	CLA	C1B-NB	4.46	1.43	1.37
33	p	303	CLA	C1B-NB	4.46	1.43	1.37
33	N	303	CLA	MG-NC	-4.46	1.95	2.06
33	4	301	CLA	C3A-C2A	-4.45	1.50	1.54
33	0	308	CLA	MG-NC	-4.44	1.95	2.06
33	N	303	CLA	C1B-NB	4.41	1.43	1.37
33	A	412	CLA	MG-NC	-4.40	1.95	2.06
33	a	412	CLA	MG-NC	-4.40	1.95	2.06
33	4	301	CLA	MG-NC	-4.38	1.95	2.06
33	0	308	CLA	C1B-NB	4.38	1.43	1.37
33	0	301	CLA	MG-NC	-4.37	1.95	2.06
33	p	310	CLA	C1B-NB	4.34	1.43	1.37
33	C	508	CLA	MG-NA	-4.33	1.96	2.06
33	6	310	CLA	C1B-NB	4.33	1.43	1.37
33	c	508	CLA	MG-NA	-4.31	1.96	2.06
33	b	605	CLA	MG-NA	-4.31	1.96	2.06
41	l	101	SQD	O47-C7	4.30	1.46	1.34
33	B	605	CLA	MG-NA	-4.29	1.96	2.06
41	L	101	SQD	O47-C7	4.29	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	n	306	CLA	C4B-NB	4.27	1.43	1.37
41	C	501	SQD	O48-C23	4.26	1.45	1.33
33	N	307	CLA	C4B-NB	4.25	1.43	1.37
41	c	501	SQD	O48-C23	4.25	1.45	1.33
33	5	317	CLA	C4B-NB	4.23	1.43	1.37
33	g	317	CLA	C4B-NB	4.21	1.43	1.37
41	L	101	SQD	O48-C23	4.21	1.45	1.33
33	p	305	CLA	C1B-NB	4.21	1.43	1.37
33	B	616	CLA	MG-NA	-4.21	1.96	2.06
41	l	101	SQD	O48-C23	4.20	1.45	1.33
33	b	616	CLA	MG-NA	-4.20	1.96	2.06
33	9	310	CLA	C3A-C2A	-4.20	1.50	1.54
33	4	309	CLA	MG-NC	-4.19	1.96	2.06
33	3	310	CLA	C3A-C2A	-4.19	1.50	1.54
33	6	305	CLA	C1B-NB	4.19	1.42	1.37
41	B	601	SQD	O48-C23	4.17	1.45	1.33
33	0	310	CLA	MG-NC	-4.17	1.96	2.06
41	b	601	SQD	O48-C23	4.17	1.45	1.33
33	B	609	CLA	C4B-NB	4.15	1.42	1.37
33	b	609	CLA	C4B-NB	4.15	1.42	1.37
33	6	313	CLA	C1B-NB	4.14	1.42	1.37
33	N	305	CLA	C4B-NB	4.14	1.42	1.37
33	0	304	CLA	C1B-NB	4.13	1.42	1.37
33	p	313	CLA	C1B-NB	4.13	1.42	1.37
33	4	304	CLA	C1B-NB	4.13	1.42	1.37
33	g	310	CLA	C4B-NB	4.12	1.42	1.37
33	5	310	CLA	C4B-NB	4.11	1.42	1.37
33	5	311	CLA	C4B-NB	4.11	1.42	1.37
41	C	501	SQD	O47-C7	4.10	1.45	1.34
33	g	311	CLA	C4B-NB	4.10	1.42	1.37
33	n	304	CLA	C4B-NB	4.10	1.42	1.37
33	p	319	CLA	MG-NC	-4.09	1.96	2.06
41	c	501	SQD	O47-C7	4.09	1.45	1.34
33	B	618	CLA	MG-NC	-4.08	1.96	2.06
33	6	319	CLA	MG-NC	-4.08	1.96	2.06
33	9	306	CLA	C3A-C2A	-4.08	1.50	1.54
41	b	601	SQD	O47-C7	4.08	1.45	1.34
41	B	601	SQD	O47-C7	4.08	1.45	1.34
33	2	310	CLA	C4B-NB	4.07	1.42	1.37
33	g	308	CLA	C4B-NB	4.07	1.42	1.37
41	J	101	SQD	O48-C23	4.06	1.45	1.33
33	6	304	CLA	C4B-NB	4.05	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	311	KC2	C1B-NB	4.05	1.42	1.37
33	5	307	CLA	MG-NC	-4.05	1.96	2.06
38	7	311	KC2	C1B-NB	4.05	1.42	1.37
41	j	101	SQD	O48-C23	4.05	1.45	1.33
33	6	302	CLA	C4B-NB	4.04	1.42	1.37
33	g	307	CLA	MG-NC	-4.04	1.96	2.06
33	p	304	CLA	C4B-NB	4.04	1.42	1.37
33	6	303	CLA	MG-NC	-4.04	1.96	2.06
36	d	407	PL9	C3-C4	-4.03	1.42	1.49
33	3	306	CLA	C3A-C2A	-4.03	1.50	1.54
38	3	311	KC2	C1B-NB	4.02	1.42	1.37
33	p	303	CLA	MG-NC	-4.02	1.96	2.06
36	D	407	PL9	C3-C4	-4.02	1.42	1.49
33	6	319	CLA	C3A-C2A	-4.02	1.50	1.54
33	9	314	CLA	C3A-C2A	-4.02	1.50	1.54
33	C	513	CLA	C4B-NB	4.01	1.42	1.37
33	5	308	CLA	C4B-NB	4.01	1.42	1.37
33	8	308	CLA	C4B-NB	4.01	1.42	1.37
33	p	319	CLA	C3A-C2A	-4.01	1.50	1.54
33	p	302	CLA	C4B-NB	4.01	1.42	1.37
33	n	303	CLA	C3A-C2A	-4.01	1.50	1.54
33	8	310	CLA	C4B-NB	4.00	1.42	1.37
44	F	101	HEM	FE-NC	3.99	2.08	1.95
33	B	616	CLA	C4B-NB	3.99	1.42	1.37
38	7	311	KC2	C4C-NC	3.99	1.43	1.37
33	1	305	CLA	C4B-NB	3.99	1.42	1.37
33	N	304	CLA	C3A-C2A	-3.99	1.50	1.54
33	7	305	CLA	C4B-NB	3.98	1.42	1.37
33	b	616	CLA	C4B-NB	3.98	1.42	1.37
33	b	618	CLA	MG-NC	-3.98	1.96	2.06
33	C	512	CLA	C4B-NB	3.98	1.42	1.37
33	c	513	CLA	C4B-NB	3.98	1.42	1.37
41	j	101	SQD	O47-C7	3.98	1.45	1.34
33	2	308	CLA	C4B-NB	3.97	1.42	1.37
33	8	307	CLA	C4B-NB	3.97	1.42	1.37
38	7	310	KC2	C4C-NC	3.97	1.43	1.37
41	J	101	SQD	O47-C7	3.97	1.45	1.34
38	9	311	KC2	C1B-NB	3.97	1.42	1.37
33	b	605	CLA	C4B-NB	3.96	1.42	1.37
33	3	314	CLA	C3A-C2A	-3.96	1.50	1.54
38	1	310	KC2	C4C-NC	3.95	1.43	1.37
33	c	512	CLA	C4B-NB	3.95	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	618	CLA	C4B-NB	3.95	1.42	1.37
38	1	310	KC2	C1B-NB	3.95	1.42	1.37
38	1	311	KC2	C4C-NC	3.95	1.43	1.37
33	4	310	CLA	MG-NC	-3.94	1.96	2.06
33	0	311	CLA	MG-NC	-3.94	1.96	2.06
33	9	306	CLA	C4B-NB	3.94	1.42	1.37
33	B	605	CLA	C4B-NB	3.93	1.42	1.37
33	n	305	CLA	C4B-NB	3.93	1.42	1.37
33	3	306	CLA	C4B-NB	3.91	1.42	1.37
33	3	313	CLA	C4B-NB	3.91	1.42	1.37
33	N	306	CLA	C4B-NB	3.90	1.42	1.37
38	7	310	KC2	C1B-NB	3.90	1.42	1.37
33	9	312	CLA	C4B-NB	3.90	1.42	1.37
33	4	306	CLA	MG-NC	-3.90	1.97	2.06
33	2	307	CLA	C4B-NB	3.90	1.42	1.37
33	5	310	CLA	C3A-C2A	-3.89	1.50	1.54
33	c	502	CLA	C4B-NB	3.89	1.42	1.37
33	0	303	CLA	C4B-NB	3.89	1.42	1.37
33	c	504	CLA	C4B-NB	3.89	1.42	1.37
33	3	312	CLA	C4B-NB	3.89	1.42	1.37
33	4	303	CLA	C4B-NB	3.88	1.42	1.37
33	C	502	CLA	C4B-NB	3.88	1.42	1.37
33	3	310	CLA	C4B-NB	3.88	1.42	1.37
33	0	306	CLA	MG-NC	-3.87	1.97	2.06
33	3	304	CLA	C4B-NB	3.87	1.42	1.37
33	B	607	CLA	C4B-NB	3.86	1.42	1.37
33	b	614	CLA	C4B-NB	3.86	1.42	1.37
33	d	405	CLA	C4B-NB	3.86	1.42	1.37
33	9	304	CLA	C4B-NB	3.86	1.42	1.37
33	0	302	CLA	MG-NC	-3.85	1.97	2.06
33	C	504	CLA	C4B-NB	3.85	1.42	1.37
33	b	604	CLA	C4B-NB	3.85	1.42	1.37
33	b	617	CLA	C4B-NB	3.85	1.42	1.37
38	2	309	KC2	C1B-NB	3.84	1.42	1.37
33	9	315	CLA	C4B-NB	3.84	1.42	1.37
33	g	310	CLA	C3A-C2A	-3.84	1.50	1.54
33	c	506	CLA	C4B-NB	3.84	1.42	1.37
33	4	302	CLA	MG-NC	-3.83	1.97	2.06
33	2	304	CLA	C4B-NB	3.83	1.42	1.37
33	B	604	CLA	C4B-NB	3.83	1.42	1.37
33	8	304	CLA	C4B-NB	3.83	1.42	1.37
33	b	607	CLA	C4B-NB	3.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	9	313	CLA	C4B-NB	3.82	1.42	1.37
33	N	304	CLA	C4B-NB	3.82	1.42	1.37
33	9	310	CLA	C4B-NB	3.82	1.42	1.37
33	1	308	CLA	C4B-NB	3.82	1.42	1.37
33	B	617	CLA	C4B-NB	3.81	1.42	1.37
33	A	405	CLA	C4B-NB	3.81	1.42	1.37
33	3	315	CLA	C4B-NB	3.81	1.42	1.37
33	B	614	CLA	C4B-NB	3.81	1.42	1.37
33	C	506	CLA	C4B-NB	3.81	1.42	1.37
33	D	405	CLA	C4B-NB	3.81	1.42	1.37
33	b	618	CLA	C4B-NB	3.81	1.42	1.37
38	8	309	KC2	C1B-NB	3.80	1.42	1.37
33	4	306	CLA	C4B-NB	3.80	1.42	1.37
33	0	306	CLA	C4B-NB	3.80	1.42	1.37
33	b	612	CLA	C4B-NB	3.80	1.42	1.37
33	B	612	CLA	C4B-NB	3.80	1.42	1.37
33	g	306	CLA	C4B-NB	3.79	1.42	1.37
33	7	308	CLA	C4B-NB	3.79	1.42	1.37
33	0	309	CLA	C4B-NB	3.78	1.42	1.37
33	n	303	CLA	C4B-NB	3.78	1.42	1.37
33	8	301	CLA	C4B-NB	3.78	1.42	1.37
33	1	304	CLA	C4B-NB	3.77	1.42	1.37
33	5	306	CLA	C4B-NB	3.77	1.42	1.37
33	n	303	CLA	MG-NC	-3.77	1.97	2.06
33	2	301	CLA	C4B-NB	3.77	1.42	1.37
33	b	615	CLA	C4B-NB	3.77	1.42	1.37
33	0	304	CLA	MG-NC	-3.76	1.97	2.06
38	3	311	KC2	C4C-NC	3.76	1.43	1.37
33	a	405	CLA	C4B-NB	3.76	1.42	1.37
33	7	304	CLA	C4B-NB	3.76	1.42	1.37
33	N	304	CLA	MG-NC	-3.76	1.97	2.06
33	4	304	CLA	MG-NC	-3.76	1.97	2.06
33	5	301	CLA	C4B-NB	3.75	1.42	1.37
33	g	301	CLA	C4B-NB	3.75	1.42	1.37
33	a	412	CLA	C4B-NB	3.75	1.42	1.37
33	C	503	CLA	C4B-NB	3.75	1.42	1.37
33	3	309	CLA	C4B-NB	3.75	1.42	1.37
33	C	507	CLA	C4B-NB	3.74	1.42	1.37
33	9	309	CLA	C4B-NB	3.73	1.42	1.37
33	C	508	CLA	C4B-NB	3.73	1.42	1.37
33	B	602	CLA	C4B-NB	3.73	1.42	1.37
33	B	606	CLA	C4B-NB	3.73	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	g	303	CLA	MG-NC	-3.73	1.97	2.06
33	C	509	CLA	C4B-NB	3.73	1.42	1.37
33	5	305	CLA	MG-NC	-3.73	1.97	2.06
33	g	305	CLA	MG-NC	-3.73	1.97	2.06
33	g	317	CLA	MG-NC	-3.73	1.97	2.06
33	5	303	CLA	MG-NC	-3.73	1.97	2.06
33	c	508	CLA	C4B-NB	3.72	1.42	1.37
33	b	606	CLA	C4B-NB	3.72	1.42	1.37
33	1	307	CLA	C4B-NB	3.72	1.42	1.37
33	5	317	CLA	MG-NC	-3.72	1.97	2.06
38	8	309	KC2	C4C-NC	3.72	1.43	1.37
33	N	301	CLA	C4B-NB	3.72	1.42	1.37
33	4	308	CLA	C4B-NB	3.72	1.42	1.37
33	b	613	CLA	C4B-NB	3.72	1.42	1.37
33	n	301	CLA	C4B-NB	3.71	1.42	1.37
33	A	406	CLA	C4B-NB	3.71	1.42	1.37
33	3	307	CLA	C4B-NB	3.71	1.42	1.37
33	4	307	CLA	MG-NC	-3.71	1.97	2.06
33	c	507	CLA	C4B-NB	3.71	1.42	1.37
33	B	615	CLA	C4B-NB	3.71	1.42	1.37
33	b	602	CLA	C4B-NB	3.70	1.42	1.37
33	B	613	CLA	C4B-NB	3.70	1.42	1.37
33	a	406	CLA	C4B-NB	3.70	1.42	1.37
33	0	307	CLA	MG-NC	-3.70	1.97	2.06
33	9	307	CLA	C4B-NB	3.70	1.42	1.37
33	c	509	CLA	C4B-NB	3.69	1.42	1.37
38	2	309	KC2	C4C-NC	3.69	1.43	1.37
33	B	610	CLA	C4B-NB	3.69	1.42	1.37
33	9	303	CLA	C4B-NB	3.69	1.42	1.37
38	9	311	KC2	C4C-NC	3.69	1.43	1.37
33	B	608	CLA	C4B-NB	3.68	1.42	1.37
33	p	310	CLA	MG-NC	-3.67	1.97	2.06
33	a	408	CLA	C4B-NB	3.67	1.42	1.37
33	A	412	CLA	C4B-NB	3.67	1.42	1.37
33	7	307	CLA	C4B-NB	3.67	1.42	1.37
33	3	303	CLA	C4B-NB	3.67	1.42	1.37
33	6	306	CLA	MG-NC	-3.67	1.97	2.06
33	b	603	CLA	C4B-NB	3.67	1.42	1.37
33	6	310	CLA	MG-NC	-3.66	1.97	2.06
33	B	603	CLA	C4B-NB	3.66	1.42	1.37
33	9	313	CLA	C3A-C2A	-3.66	1.51	1.54
33	c	503	CLA	C4B-NB	3.66	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	408	CLA	C4B-NB	3.65	1.42	1.37
33	p	306	CLA	MG-NC	-3.65	1.97	2.06
33	5	308	CLA	C3A-C2A	-3.65	1.51	1.54
33	b	608	CLA	C4B-NB	3.65	1.42	1.37
33	5	303	CLA	C4B-NB	3.65	1.42	1.37
33	3	306	CLA	MG-NC	-3.65	1.97	2.06
33	9	306	CLA	MG-NC	-3.64	1.97	2.06
33	4	308	CLA	MG-NC	-3.64	1.97	2.06
33	1	303	CLA	C4B-NB	3.64	1.42	1.37
33	7	309	CLA	C4B-NB	3.64	1.42	1.37
33	B	611	CLA	C4B-NB	3.63	1.42	1.37
33	p	308	CLA	MG-NC	-3.63	1.97	2.06
33	1	306	CLA	C4B-NB	3.63	1.42	1.37
33	0	309	CLA	MG-NC	-3.63	1.97	2.06
33	1	309	CLA	C4B-NB	3.63	1.42	1.37
33	6	308	CLA	MG-NC	-3.62	1.97	2.06
33	9	314	CLA	C4B-NB	3.62	1.42	1.37
33	g	304	CLA	C4B-NB	3.62	1.42	1.37
33	c	511	CLA	C4B-NB	3.62	1.42	1.37
33	g	308	CLA	C3A-C2A	-3.61	1.51	1.54
33	b	610	CLA	C4B-NB	3.61	1.42	1.37
33	5	306	CLA	MG-NC	-3.60	1.97	2.06
33	p	309	CLA	MG-NC	-3.60	1.97	2.06
33	6	309	CLA	MG-NC	-3.60	1.97	2.06
33	p	313	CLA	MG-NC	-3.60	1.97	2.06
33	c	505	CLA	C4B-NB	3.60	1.42	1.37
33	6	313	CLA	MG-NC	-3.60	1.97	2.06
33	n	306	CLA	MG-NC	-3.60	1.97	2.06
33	D	404	CLA	C4B-NB	3.60	1.42	1.37
33	p	310	CLA	C4B-NB	3.59	1.42	1.37
33	N	307	CLA	MG-NC	-3.59	1.97	2.06
33	6	307	CLA	C4B-NB	3.59	1.42	1.37
33	5	304	CLA	C4B-NB	3.59	1.42	1.37
33	g	306	CLA	MG-NC	-3.59	1.97	2.06
33	7	306	CLA	C4B-NB	3.58	1.42	1.37
33	C	511	CLA	C4B-NB	3.58	1.42	1.37
33	1	307	CLA	MG-NC	-3.58	1.97	2.06
33	C	505	CLA	C4B-NB	3.58	1.42	1.37
33	g	303	CLA	C4B-NB	3.58	1.42	1.37
33	3	314	CLA	C4B-NB	3.57	1.42	1.37
33	7	307	CLA	MG-NC	-3.57	1.97	2.06
33	2	302	CLA	MG-NC	-3.57	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	6	310	CLA	C4B-NB	3.57	1.42	1.37
33	3	313	CLA	C3A-C2A	-3.57	1.51	1.54
33	p	307	CLA	C4B-NB	3.57	1.42	1.37
33	6	307	CLA	MG-NC	-3.56	1.97	2.06
33	7	305	CLA	MG-NC	-3.56	1.97	2.06
33	7	301	CLA	C4B-NB	3.56	1.42	1.37
33	5	310	CLA	MG-NC	-3.56	1.97	2.06
33	1	305	CLA	MG-NC	-3.55	1.97	2.06
33	C	514	CLA	C4B-NB	3.55	1.42	1.37
33	8	302	CLA	MG-NC	-3.55	1.97	2.06
33	p	307	CLA	MG-NC	-3.55	1.97	2.06
33	5	302	CLA	C4B-NB	3.55	1.42	1.37
33	1	301	CLA	C4B-NB	3.55	1.42	1.37
33	7	303	CLA	C4B-NB	3.55	1.42	1.37
33	8	302	CLA	C4B-NB	3.55	1.42	1.37
33	g	310	CLA	MG-NC	-3.54	1.97	2.06
33	p	313	CLA	C3A-C2A	-3.54	1.51	1.54
33	6	302	CLA	C3A-C2A	-3.53	1.51	1.54
33	c	510	CLA	C4B-NB	3.53	1.42	1.37
33	0	301	CLA	C4B-NB	3.53	1.42	1.37
33	4	301	CLA	C4B-NB	3.53	1.42	1.37
33	6	304	CLA	MG-NC	-3.52	1.97	2.06
33	c	514	CLA	C4B-NB	3.52	1.42	1.37
33	2	302	CLA	C4B-NB	3.52	1.42	1.37
33	0	307	CLA	C4B-NB	3.52	1.42	1.37
33	d	404	CLA	C4B-NB	3.52	1.42	1.37
33	g	302	CLA	C4B-NB	3.52	1.42	1.37
33	b	611	CLA	C4B-NB	3.52	1.42	1.37
33	g	308	CLA	MG-NC	-3.51	1.97	2.06
33	8	306	CLA	MG-NC	-3.51	1.97	2.06
33	6	313	CLA	C3A-C2A	-3.51	1.51	1.54
33	p	302	CLA	C3A-C2A	-3.51	1.51	1.54
33	N	302	CLA	C4B-NB	3.50	1.42	1.37
33	B	611	CLA	MG-NC	-3.50	1.97	2.06
33	1	302	CLA	C4B-NB	3.50	1.42	1.37
33	p	304	CLA	MG-NC	-3.50	1.98	2.06
33	4	307	CLA	C4B-NB	3.50	1.42	1.37
33	2	306	CLA	MG-NC	-3.50	1.98	2.06
33	C	510	CLA	C4B-NB	3.50	1.42	1.37
33	3	309	CLA	MG-NC	-3.49	1.98	2.06
33	7	302	CLA	MG-NC	-3.49	1.98	2.06
33	b	611	CLA	MG-NC	-3.49	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	308	CLA	MG-NC	-3.49	1.98	2.06
38	0	305	KC2	C1B-NB	3.49	1.42	1.37
33	c	505	CLA	MG-NC	-3.49	1.98	2.06
44	F	101	HEM	C1B-NB	-3.49	1.34	1.40
38	4	305	KC2	C1B-NB	3.48	1.42	1.37
33	3	312	CLA	MG-NC	-3.47	1.98	2.06
33	7	302	CLA	C4B-NB	3.47	1.42	1.37
33	9	309	CLA	MG-NC	-3.47	1.98	2.06
33	9	308	CLA	C4B-NB	3.46	1.42	1.37
33	n	302	CLA	C4B-NB	3.46	1.42	1.37
33	C	505	CLA	MG-NC	-3.46	1.98	2.06
33	A	406	CLA	MG-NC	-3.46	1.98	2.06
33	9	312	CLA	MG-NC	-3.46	1.98	2.06
33	3	308	CLA	C4B-NB	3.45	1.42	1.37
33	b	615	CLA	MG-NC	-3.45	1.98	2.06
33	B	615	CLA	MG-NC	-3.44	1.98	2.06
33	g	304	CLA	MG-NC	-3.44	1.98	2.06
33	5	304	CLA	MG-NC	-3.44	1.98	2.06
33	c	507	CLA	MG-NC	-3.44	1.98	2.06
33	1	302	CLA	MG-NC	-3.44	1.98	2.06
33	C	507	CLA	MG-NC	-3.44	1.98	2.06
33	a	406	CLA	MG-NC	-3.43	1.98	2.06
44	F	101	HEM	C4D-ND	-3.43	1.34	1.40
33	6	305	CLA	MG-NC	-3.43	1.98	2.06
33	p	305	CLA	MG-NC	-3.43	1.98	2.06
33	6	306	CLA	C4B-NB	3.43	1.42	1.37
33	2	304	CLA	MG-NC	-3.42	1.98	2.06
33	8	304	CLA	MG-NC	-3.42	1.98	2.06
33	9	307	CLA	MG-NC	-3.42	1.98	2.06
33	0	308	CLA	C4B-NB	3.41	1.42	1.37
33	7	304	CLA	MG-NC	-3.41	1.98	2.06
33	6	312	CLA	C4B-NB	3.41	1.42	1.37
33	p	306	CLA	C4B-NB	3.41	1.42	1.37
33	1	304	CLA	MG-NC	-3.41	1.98	2.06
33	2	305	CLA	C4B-NB	3.41	1.42	1.37
33	1	301	CLA	MG-NC	-3.40	1.98	2.06
33	6	312	CLA	MG-NC	-3.40	1.98	2.06
33	p	312	CLA	MG-NC	-3.40	1.98	2.06
33	N	303	CLA	C4B-NB	3.39	1.42	1.37
33	3	307	CLA	MG-NC	-3.39	1.98	2.06
33	7	301	CLA	MG-NC	-3.39	1.98	2.06
33	2	303	CLA	MG-NC	-3.39	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	301	CLA	MG-NC	-3.38	1.98	2.06
33	0	311	CLA	C4B-NB	3.38	1.41	1.37
33	9	305	CLA	C4B-NB	3.38	1.41	1.37
33	1	308	CLA	MG-NC	-3.38	1.98	2.06
33	A	405	CLA	MG-NC	-3.38	1.98	2.06
33	7	308	CLA	MG-NC	-3.38	1.98	2.06
33	g	302	CLA	MG-NC	-3.37	1.98	2.06
33	g	311	CLA	MG-NC	-3.37	1.98	2.06
33	8	301	CLA	MG-NC	-3.37	1.98	2.06
33	8	305	CLA	C4B-NB	3.36	1.41	1.37
33	5	311	CLA	MG-NC	-3.36	1.98	2.06
33	C	509	CLA	MG-NC	-3.36	1.98	2.06
33	N	306	CLA	MG-NC	-3.36	1.98	2.06
33	a	405	CLA	MG-NC	-3.36	1.98	2.06
33	6	302	CLA	MG-NC	-3.35	1.98	2.06
33	2	305	CLA	MG-NC	-3.35	1.98	2.06
33	n	305	CLA	MG-NC	-3.35	1.98	2.06
33	p	302	CLA	MG-NC	-3.35	1.98	2.06
33	4	310	CLA	C4B-NB	3.35	1.41	1.37
33	5	302	CLA	MG-NC	-3.35	1.98	2.06
33	p	312	CLA	C4B-NB	3.35	1.41	1.37
33	8	303	CLA	MG-NC	-3.34	1.98	2.06
33	9	303	CLA	MG-NC	-3.34	1.98	2.06
33	8	305	CLA	MG-NC	-3.33	1.98	2.06
33	3	303	CLA	MG-NC	-3.33	1.98	2.06
33	8	303	CLA	C4B-NB	3.33	1.41	1.37
33	2	303	CLA	C4B-NB	3.33	1.41	1.37
33	3	314	CLA	MG-NC	-3.33	1.98	2.06
33	3	305	CLA	C4B-NB	3.33	1.41	1.37
33	9	314	CLA	MG-NC	-3.33	1.98	2.06
33	4	303	CLA	MG-NC	-3.32	1.98	2.06
33	c	509	CLA	MG-NC	-3.32	1.98	2.06
33	0	304	CLA	C4B-NB	3.31	1.41	1.37
33	0	303	CLA	MG-NC	-3.31	1.98	2.06
33	B	617	CLA	MG-NC	-3.30	1.98	2.06
33	9	304	CLA	MG-NC	-3.29	1.98	2.06
33	4	304	CLA	C4B-NB	3.28	1.41	1.37
33	b	617	CLA	MG-NC	-3.28	1.98	2.06
33	3	304	CLA	MG-NC	-3.27	1.98	2.06
33	d	404	CLA	MG-NC	-3.27	1.98	2.06
33	8	306	CLA	C4B-NB	3.26	1.41	1.37
33	9	315	CLA	MG-NC	-3.26	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	404	CLA	MG-NC	-3.26	1.98	2.06
33	1	306	CLA	MG-NC	-3.25	1.98	2.06
33	3	315	CLA	MG-NC	-3.25	1.98	2.06
33	b	608	CLA	MG-NC	-3.25	1.98	2.06
33	c	503	CLA	MG-NC	-3.24	1.98	2.06
33	2	306	CLA	C4B-NB	3.24	1.41	1.37
33	B	608	CLA	MG-NC	-3.24	1.98	2.06
33	8	308	CLA	MG-NC	-3.24	1.98	2.06
33	2	310	CLA	MG-NC	-3.23	1.98	2.06
33	b	609	CLA	MG-NC	-3.23	1.98	2.06
33	8	310	CLA	MG-NC	-3.22	1.98	2.06
33	2	308	CLA	MG-NC	-3.22	1.98	2.06
33	5	305	CLA	C4B-NB	3.22	1.41	1.37
33	9	305	CLA	MG-NC	-3.22	1.98	2.06
34	a	407	PHO	C3A-C2A	3.22	1.57	1.54
33	9	308	CLA	MG-NC	-3.22	1.98	2.06
33	D	405	CLA	MG-NC	-3.22	1.98	2.06
33	B	609	CLA	MG-NC	-3.21	1.98	2.06
33	C	503	CLA	MG-NC	-3.21	1.98	2.06
33	3	305	CLA	MG-NC	-3.21	1.98	2.06
33	3	308	CLA	MG-NC	-3.21	1.98	2.06
33	A	408	CLA	MG-NC	-3.20	1.98	2.06
33	N	301	CLA	MG-NC	-3.20	1.98	2.06
33	b	606	CLA	MG-NC	-3.20	1.98	2.06
33	c	514	CLA	MG-NC	-3.20	1.98	2.06
33	g	305	CLA	C4B-NB	3.20	1.41	1.37
33	B	612	CLA	MG-NC	-3.19	1.98	2.06
33	n	301	CLA	MG-NC	-3.19	1.98	2.06
33	7	306	CLA	MG-NC	-3.19	1.98	2.06
33	9	313	CLA	MG-NC	-3.19	1.98	2.06
33	3	313	CLA	MG-NC	-3.19	1.98	2.06
33	c	513	CLA	MG-NC	-3.19	1.98	2.06
33	B	606	CLA	MG-NC	-3.18	1.98	2.06
33	a	408	CLA	MG-NC	-3.18	1.98	2.06
33	B	604	CLA	MG-NC	-3.18	1.98	2.06
33	b	602	CLA	MG-NC	-3.18	1.98	2.06
33	2	307	CLA	MG-NC	-3.18	1.98	2.06
33	d	405	CLA	MG-NC	-3.18	1.98	2.06
33	C	513	CLA	MG-NC	-3.18	1.98	2.06
33	C	514	CLA	MG-NC	-3.17	1.98	2.06
33	c	502	CLA	MG-NC	-3.17	1.98	2.06
33	N	305	CLA	MG-NC	-3.16	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	g	309	KC2	C4C-NC	3.16	1.42	1.37
33	B	602	CLA	MG-NC	-3.16	1.98	2.06
33	B	603	CLA	MG-NC	-3.15	1.98	2.06
33	b	604	CLA	MG-NC	-3.15	1.98	2.06
33	b	612	CLA	MG-NC	-3.15	1.98	2.06
33	8	307	CLA	MG-NC	-3.15	1.98	2.06
33	6	312	CLA	C3A-C2A	-3.15	1.51	1.54
38	5	309	KC2	C4C-NC	3.14	1.42	1.37
34	A	407	PHO	C3A-C2A	3.14	1.57	1.54
33	B	613	CLA	MG-NC	-3.14	1.98	2.06
33	C	502	CLA	MG-NC	-3.14	1.98	2.06
33	b	613	CLA	MG-NC	-3.14	1.98	2.06
33	n	304	CLA	MG-NC	-3.14	1.98	2.06
33	4	309	CLA	C4B-NB	3.14	1.41	1.37
33	6	309	CLA	C4B-NB	3.14	1.41	1.37
33	c	506	CLA	MG-NC	-3.14	1.98	2.06
33	b	607	CLA	MG-NC	-3.14	1.98	2.06
33	0	310	CLA	C4B-NB	3.13	1.41	1.37
33	b	603	CLA	MG-NC	-3.13	1.98	2.06
33	6	308	CLA	C4B-NB	3.13	1.41	1.37
33	7	303	CLA	MG-NC	-3.12	1.98	2.06
33	1	303	CLA	MG-NC	-3.12	1.98	2.06
33	p	305	CLA	C4B-NB	3.12	1.41	1.37
33	C	506	CLA	MG-NC	-3.12	1.98	2.06
33	p	308	CLA	C4B-NB	3.11	1.41	1.37
33	b	614	CLA	MG-NC	-3.11	1.98	2.06
33	B	614	CLA	MG-NC	-3.11	1.98	2.06
33	B	607	CLA	MG-NC	-3.11	1.98	2.06
42	m	101	LMG	C4-C5	3.10	1.59	1.53
33	6	305	CLA	C4B-NB	3.10	1.41	1.37
33	p	309	CLA	C4B-NB	3.10	1.41	1.37
33	C	511	CLA	MG-NC	-3.09	1.98	2.06
42	l	102	LMG	C4-C5	3.09	1.59	1.53
33	C	504	CLA	MG-NC	-3.09	1.98	2.06
33	c	511	CLA	MG-NC	-3.08	1.98	2.06
33	4	302	CLA	C4B-NB	3.06	1.41	1.37
33	C	510	CLA	MG-NC	-3.06	1.99	2.06
33	c	504	CLA	MG-NC	-3.06	1.99	2.06
33	c	510	CLA	MG-NC	-3.04	1.99	2.06
33	p	312	CLA	C3A-C2A	-3.03	1.51	1.54
33	0	302	CLA	C4B-NB	3.03	1.41	1.37
33	C	512	CLA	MG-NC	-2.99	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	3	310	CLA	MG-NC	-2.98	1.99	2.06
33	5	301	CLA	MG-NC	-2.98	1.99	2.06
33	g	301	CLA	MG-NC	-2.98	1.99	2.06
33	c	512	CLA	MG-NC	-2.96	1.99	2.06
44	f	101	HEM	FE-NB	2.95	2.04	1.94
33	9	310	CLA	MG-NC	-2.95	1.99	2.06
38	4	305	KC2	C4C-NC	2.94	1.42	1.37
41	C	501	SQD	C6-S	-2.93	1.66	1.77
38	0	305	KC2	C4C-NC	2.93	1.42	1.37
41	c	501	SQD	C6-S	-2.93	1.66	1.77
33	1	309	CLA	MG-NC	-2.92	1.99	2.06
33	7	309	CLA	MG-NC	-2.91	1.99	2.06
33	B	616	CLA	MG-NC	-2.91	1.99	2.06
33	g	307	CLA	C4B-NB	2.90	1.41	1.37
33	b	616	CLA	MG-NC	-2.90	1.99	2.06
33	B	610	CLA	MG-NC	-2.88	1.99	2.06
33	5	307	CLA	C4B-NB	2.88	1.41	1.37
41	b	601	SQD	C6-S	-2.87	1.66	1.77
33	b	610	CLA	MG-NC	-2.87	1.99	2.06
41	B	601	SQD	C6-S	-2.86	1.66	1.77
33	n	302	CLA	MG-NC	-2.84	1.99	2.06
38	6	311	KC2	C4C-NC	2.84	1.42	1.37
33	6	303	CLA	C4B-NB	2.83	1.41	1.37
41	l	101	SQD	C6-S	-2.82	1.67	1.77
33	p	303	CLA	C4B-NB	2.80	1.41	1.37
38	p	311	KC2	C4C-NC	2.80	1.42	1.37
33	N	302	CLA	MG-NC	-2.79	1.99	2.06
41	L	101	SQD	C6-S	-2.79	1.67	1.77
33	c	508	CLA	MG-NC	-2.78	1.99	2.06
33	C	508	CLA	MG-NC	-2.77	1.99	2.06
33	6	319	CLA	C4B-NB	2.76	1.41	1.37
33	p	319	CLA	C4B-NB	2.76	1.41	1.37
33	p	313	CLA	C4B-NB	2.75	1.41	1.37
41	J	101	SQD	C6-S	-2.73	1.67	1.77
41	j	101	SQD	C6-S	-2.73	1.67	1.77
38	5	309	KC2	C1B-NB	2.71	1.41	1.37
38	g	309	KC2	C1B-NB	2.68	1.41	1.37
33	6	313	CLA	C4B-NB	2.68	1.41	1.37
33	0	311	CLA	C3D-C4D	-2.65	1.38	1.44
43	C	521	DGD	O2G-C2G	-2.64	1.40	1.46
33	4	310	CLA	C3D-C4D	-2.63	1.38	1.44
38	6	311	KC2	C1B-NB	2.62	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	p	311	KC2	C1B-NB	2.62	1.41	1.37
43	c	521	DGD	O2G-C2G	-2.61	1.40	1.46
36	a	410	PL9	C3-C4	-2.60	1.45	1.49
36	A	410	PL9	C3-C4	-2.59	1.45	1.49
33	B	605	CLA	MG-NC	-2.57	2.00	2.06
33	b	605	CLA	MG-NC	-2.57	2.00	2.06
44	F	101	HEM	FE-ND	-2.56	1.86	1.94
44	F	101	HEM	C1C-C2C	-2.55	1.40	1.45
33	p	310	CLA	C3D-C4D	-2.55	1.38	1.44
33	6	310	CLA	C1D-C2D	-2.55	1.40	1.45
33	p	305	CLA	C1D-C2D	-2.54	1.40	1.45
33	p	310	CLA	C1D-C2D	-2.53	1.40	1.45
33	g	307	CLA	C3D-C4D	-2.51	1.38	1.44
42	B	624	LMG	C4-C5	2.51	1.58	1.53
33	6	305	CLA	C1D-C2D	-2.51	1.40	1.45
33	6	303	CLA	C3D-C4D	-2.51	1.38	1.44
33	6	310	CLA	C3D-C4D	-2.51	1.38	1.44
42	b	624	LMG	C4-C5	2.50	1.58	1.53
33	p	303	CLA	C3D-C4D	-2.50	1.38	1.44
33	5	307	CLA	C3D-C4D	-2.50	1.38	1.44
33	p	312	CLA	C1D-C2D	-2.50	1.40	1.45
33	p	308	CLA	C3D-C4D	-2.50	1.38	1.44
33	4	302	CLA	C3D-C4D	-2.50	1.38	1.44
33	4	308	CLA	C1D-C2D	-2.50	1.40	1.45
33	0	309	CLA	C1D-C2D	-2.49	1.40	1.45
33	4	309	CLA	C3D-C4D	-2.49	1.38	1.44
33	0	302	CLA	C3D-C4D	-2.49	1.38	1.44
33	0	310	CLA	C3D-C4D	-2.49	1.38	1.44
33	c	503	CLA	C1D-C2D	-2.49	1.40	1.45
33	6	312	CLA	C3D-C4D	-2.48	1.38	1.44
33	6	308	CLA	C3D-C4D	-2.48	1.38	1.44
33	p	312	CLA	C3D-C4D	-2.48	1.38	1.44
33	2	306	CLA	C3D-C4D	-2.48	1.38	1.44
33	C	508	CLA	C1D-C2D	-2.48	1.40	1.45
33	0	306	CLA	C1D-C2D	-2.48	1.40	1.45
33	6	312	CLA	C1D-C2D	-2.48	1.40	1.45
33	6	309	CLA	C3D-C4D	-2.47	1.38	1.44
33	4	306	CLA	C1D-C2D	-2.47	1.40	1.45
33	c	508	CLA	C1D-C2D	-2.46	1.40	1.45
35	c	515	8CT	C10-C03	2.46	1.53	1.45
33	2	308	CLA	C1D-C2D	-2.46	1.40	1.45
33	p	309	CLA	C3D-C4D	-2.46	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	0	306	CLA	C3D-C4D	-2.45	1.38	1.44
33	8	308	CLA	C1D-C2D	-2.45	1.40	1.45
33	C	503	CLA	C1D-C2D	-2.45	1.40	1.45
33	5	305	CLA	C3D-C4D	-2.45	1.38	1.44
33	6	313	CLA	C3D-C4D	-2.45	1.38	1.44
33	p	313	CLA	C3D-C4D	-2.45	1.38	1.44
42	d	410	LMG	C4-C5	2.45	1.58	1.53
33	4	306	CLA	C3D-C4D	-2.45	1.38	1.44
35	C	515	8CT	C10-C03	2.44	1.53	1.45
33	0	311	CLA	C1D-C2D	-2.44	1.40	1.45
33	4	310	CLA	C1D-C2D	-2.44	1.40	1.45
42	D	410	LMG	C4-C5	2.44	1.58	1.53
33	8	306	CLA	C3D-C4D	-2.43	1.38	1.44
33	b	613	CLA	C1D-C2D	-2.41	1.40	1.45
33	n	305	CLA	C1D-C2D	-2.41	1.40	1.45
33	0	308	CLA	C3D-C4D	-2.41	1.38	1.44
33	N	303	CLA	C3D-C4D	-2.41	1.38	1.44
33	0	309	CLA	C3D-C4D	-2.39	1.38	1.44
33	B	613	CLA	C1D-C2D	-2.39	1.40	1.45
33	p	303	CLA	C1D-C2D	-2.39	1.40	1.45
33	N	306	CLA	C1D-C2D	-2.39	1.40	1.45
33	g	305	CLA	C3D-C4D	-2.39	1.38	1.44
33	4	308	CLA	C3D-C4D	-2.39	1.38	1.44
33	g	306	CLA	C1D-C2D	-2.38	1.40	1.45
33	6	313	CLA	C1D-C2D	-2.38	1.40	1.45
33	B	604	CLA	C3D-C4D	-2.38	1.38	1.44
33	p	305	CLA	C3D-C4D	-2.38	1.38	1.44
33	p	313	CLA	C1D-C2D	-2.37	1.40	1.45
42	T	101	LMG	C7-C8	2.37	1.58	1.50
33	5	306	CLA	C1D-C2D	-2.37	1.40	1.45
33	p	319	CLA	C3D-C4D	-2.37	1.38	1.44
33	b	604	CLA	C3D-C4D	-2.37	1.38	1.44
33	4	304	CLA	C3D-C4D	-2.37	1.38	1.44
33	6	319	CLA	C3D-C4D	-2.37	1.38	1.44
33	6	307	CLA	C3D-C4D	-2.36	1.38	1.44
33	0	304	CLA	C3D-C4D	-2.36	1.38	1.44
33	6	305	CLA	C3D-C4D	-2.36	1.38	1.44
33	b	610	CLA	C1D-C2D	-2.36	1.40	1.45
33	6	303	CLA	C1D-C2D	-2.36	1.40	1.45
33	6	306	CLA	C3D-C4D	-2.36	1.38	1.44
42	t	101	LMG	C7-C8	2.36	1.57	1.50
33	c	506	CLA	C1D-C2D	-2.36	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	1	303	CLA	C1D-C2D	-2.35	1.40	1.45
33	b	616	CLA	C1D-C2D	-2.35	1.40	1.45
33	N	306	CLA	C3D-C4D	-2.35	1.38	1.44
33	1	305	CLA	C1D-C2D	-2.34	1.40	1.45
33	8	304	CLA	C3D-C4D	-2.34	1.38	1.44
33	b	612	CLA	C1D-C2D	-2.34	1.40	1.45
33	b	605	CLA	C1D-C2D	-2.34	1.40	1.45
33	7	301	CLA	C3D-C4D	-2.34	1.38	1.44
33	p	309	CLA	C1D-C2D	-2.34	1.40	1.45
33	p	319	CLA	C1D-C2D	-2.34	1.40	1.45
33	p	306	CLA	C3D-C4D	-2.34	1.38	1.44
33	6	319	CLA	C1D-C2D	-2.34	1.40	1.45
33	8	306	CLA	C1D-C2D	-2.34	1.40	1.45
33	7	303	CLA	C1D-C2D	-2.33	1.40	1.45
33	C	506	CLA	C1D-C2D	-2.33	1.40	1.45
33	p	307	CLA	C3D-C4D	-2.33	1.38	1.44
33	2	303	CLA	C3D-C4D	-2.33	1.38	1.44
33	B	616	CLA	C1D-C2D	-2.33	1.40	1.45
33	2	304	CLA	C3D-C4D	-2.33	1.38	1.44
33	B	610	CLA	C1D-C2D	-2.33	1.40	1.45
33	8	303	CLA	C3D-C4D	-2.32	1.38	1.44
33	1	309	CLA	C1D-C2D	-2.32	1.40	1.45
33	6	309	CLA	C1D-C2D	-2.32	1.40	1.45
33	B	612	CLA	C1D-C2D	-2.32	1.40	1.45
33	5	305	CLA	C1D-C2D	-2.32	1.40	1.45
33	5	307	CLA	C1D-C2D	-2.32	1.40	1.45
33	9	314	CLA	C1D-C2D	-2.32	1.40	1.45
33	3	315	CLA	C1D-C2D	-2.32	1.40	1.45
33	3	304	CLA	C1D-C2D	-2.32	1.40	1.45
33	b	606	CLA	C3D-C4D	-2.32	1.38	1.44
33	c	511	CLA	C1D-C2D	-2.32	1.40	1.45
33	C	502	CLA	C1D-C2D	-2.32	1.40	1.45
33	8	305	CLA	C3D-C4D	-2.31	1.39	1.44
43	C	521	DGD	O1G-C1G	-2.31	1.39	1.45
33	C	513	CLA	C1D-C2D	-2.31	1.40	1.45
33	9	315	CLA	C1D-C2D	-2.31	1.40	1.45
33	6	306	CLA	C1D-C2D	-2.31	1.40	1.45
33	9	304	CLA	C1D-C2D	-2.31	1.40	1.45
33	4	301	CLA	C1D-C2D	-2.31	1.40	1.45
33	c	502	CLA	C1D-C2D	-2.31	1.40	1.45
33	n	305	CLA	C3D-C4D	-2.31	1.39	1.44
33	6	302	CLA	C1D-C2D	-2.31	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	306	CLA	C1D-C2D	-2.31	1.40	1.45
33	C	509	CLA	C1D-C2D	-2.31	1.40	1.45
33	c	513	CLA	C1D-C2D	-2.31	1.40	1.45
33	8	307	CLA	C1D-C2D	-2.31	1.40	1.45
33	g	305	CLA	C1D-C2D	-2.31	1.40	1.45
33	b	604	CLA	C1D-C2D	-2.30	1.40	1.45
33	A	412	CLA	C3D-C4D	-2.30	1.39	1.44
33	2	307	CLA	C1D-C2D	-2.30	1.40	1.45
33	g	307	CLA	C1D-C2D	-2.30	1.40	1.45
33	9	312	CLA	C3D-C4D	-2.30	1.39	1.44
33	B	606	CLA	C1D-C2D	-2.30	1.40	1.45
33	B	605	CLA	C1D-C2D	-2.30	1.40	1.45
33	B	606	CLA	C3D-C4D	-2.30	1.39	1.44
33	c	504	CLA	C1D-C2D	-2.30	1.40	1.45
33	1	301	CLA	C3D-C4D	-2.30	1.39	1.44
33	0	304	CLA	C1D-C2D	-2.30	1.40	1.45
33	9	303	CLA	C3D-C4D	-2.30	1.39	1.44
33	B	603	CLA	C3D-C4D	-2.30	1.39	1.44
33	B	611	CLA	C1D-C2D	-2.30	1.40	1.45
33	1	308	CLA	C1D-C2D	-2.30	1.40	1.45
33	p	308	CLA	C1D-C2D	-2.30	1.40	1.45
43	C	519	DGD	O2G-C2G	-2.30	1.40	1.46
33	8	305	CLA	C1D-C2D	-2.30	1.40	1.45
33	b	603	CLA	C3D-C4D	-2.29	1.39	1.44
33	n	303	CLA	C3D-C4D	-2.29	1.39	1.44
33	5	304	CLA	C3D-C4D	-2.29	1.39	1.44
33	3	312	CLA	C3D-C4D	-2.29	1.39	1.44
33	6	308	CLA	C1D-C2D	-2.29	1.40	1.45
33	b	611	CLA	C1D-C2D	-2.29	1.40	1.45
33	B	614	CLA	C1D-C2D	-2.29	1.40	1.45
33	C	504	CLA	C1D-C2D	-2.29	1.40	1.45
33	p	302	CLA	C3D-C4D	-2.29	1.39	1.44
33	b	618	CLA	C1D-C2D	-2.29	1.40	1.45
33	4	307	CLA	C1D-C2D	-2.29	1.40	1.45
33	b	609	CLA	C1D-C2D	-2.29	1.40	1.45
33	9	304	CLA	C3D-C4D	-2.28	1.39	1.44
33	0	301	CLA	C1D-C2D	-2.28	1.40	1.45
33	p	306	CLA	C1D-C2D	-2.28	1.40	1.45
43	c	521	DGD	O1G-C1G	-2.28	1.39	1.45
33	0	301	CLA	C3D-C4D	-2.28	1.39	1.44
33	9	307	CLA	C1D-C2D	-2.28	1.40	1.45
33	C	511	CLA	C1D-C2D	-2.28	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	305	CLA	C3D-C4D	-2.28	1.39	1.44
33	4	304	CLA	C1D-C2D	-2.28	1.40	1.45
33	7	305	CLA	C1D-C2D	-2.28	1.40	1.45
33	7	309	CLA	C1D-C2D	-2.28	1.40	1.45
33	C	511	CLA	C3D-C4D	-2.28	1.39	1.44
33	1	306	CLA	C1D-C2D	-2.28	1.40	1.45
33	3	314	CLA	C1D-C2D	-2.28	1.40	1.45
33	3	307	CLA	C1D-C2D	-2.28	1.40	1.45
37	D	408	LHG	O7-C5	-2.28	1.40	1.46
33	B	609	CLA	C1D-C2D	-2.28	1.40	1.45
33	B	617	CLA	C1D-C2D	-2.28	1.40	1.45
33	c	511	CLA	C3D-C4D	-2.28	1.39	1.44
37	d	408	LHG	O7-C5	-2.28	1.40	1.46
33	g	310	CLA	C1D-C2D	-2.28	1.40	1.45
33	3	313	CLA	C1D-C2D	-2.27	1.40	1.45
33	7	306	CLA	C1D-C2D	-2.27	1.40	1.45
33	b	611	CLA	C3D-C4D	-2.27	1.39	1.44
33	p	302	CLA	C1D-C2D	-2.27	1.40	1.45
33	4	309	CLA	C1D-C2D	-2.27	1.40	1.45
33	B	615	CLA	C1D-C2D	-2.27	1.40	1.45
33	b	608	CLA	C1D-C2D	-2.27	1.40	1.45
33	B	604	CLA	C1D-C2D	-2.27	1.40	1.45
33	N	301	CLA	C3D-C4D	-2.27	1.39	1.44
43	c	519	DGD	O2G-C2G	-2.27	1.40	1.46
33	0	307	CLA	C1D-C2D	-2.27	1.40	1.45
33	c	514	CLA	C1D-C2D	-2.27	1.40	1.45
33	2	305	CLA	C1D-C2D	-2.26	1.40	1.45
33	C	514	CLA	C1D-C2D	-2.26	1.40	1.45
33	b	615	CLA	C1D-C2D	-2.26	1.40	1.45
33	b	614	CLA	C1D-C2D	-2.26	1.40	1.45
33	5	304	CLA	C1D-C2D	-2.26	1.40	1.45
33	N	305	CLA	C1D-C2D	-2.26	1.40	1.45
33	c	509	CLA	C1D-C2D	-2.26	1.40	1.45
33	3	303	CLA	C3D-C4D	-2.26	1.39	1.44
33	B	603	CLA	C1D-C2D	-2.26	1.40	1.45
33	b	603	CLA	C1D-C2D	-2.26	1.40	1.45
33	9	313	CLA	C1D-C2D	-2.26	1.40	1.45
33	1	305	CLA	C3D-C4D	-2.26	1.39	1.44
33	g	304	CLA	C3D-C4D	-2.26	1.39	1.44
33	a	412	CLA	C3D-C4D	-2.26	1.39	1.44
33	2	308	CLA	C3D-C4D	-2.26	1.39	1.44
33	B	618	CLA	C3D-C4D	-2.26	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	405	CLA	C1D-C2D	-2.26	1.40	1.45
33	d	404	CLA	C1D-C2D	-2.26	1.40	1.45
33	b	617	CLA	C1D-C2D	-2.26	1.40	1.45
33	b	608	CLA	C3D-C4D	-2.26	1.39	1.44
33	n	301	CLA	C3D-C4D	-2.26	1.39	1.44
33	0	310	CLA	C1D-C2D	-2.26	1.40	1.45
33	6	302	CLA	C3D-C4D	-2.25	1.39	1.44
33	N	304	CLA	C3D-C4D	-2.25	1.39	1.44
33	9	305	CLA	C3D-C4D	-2.25	1.39	1.44
33	a	405	CLA	C1D-C2D	-2.25	1.40	1.45
33	D	404	CLA	C1D-C2D	-2.25	1.40	1.45
33	4	302	CLA	C1D-C2D	-2.25	1.40	1.45
33	c	505	CLA	C1D-C2D	-2.25	1.40	1.45
33	4	301	CLA	C3D-C4D	-2.25	1.39	1.44
33	B	608	CLA	C1D-C2D	-2.25	1.40	1.45
33	A	408	CLA	C3D-C4D	-2.25	1.39	1.44
33	3	305	CLA	C3D-C4D	-2.25	1.39	1.44
33	5	308	CLA	C3D-C4D	-2.25	1.39	1.44
33	C	509	CLA	C3D-C4D	-2.25	1.39	1.44
33	d	404	CLA	C3D-C4D	-2.25	1.39	1.44
33	5	310	CLA	C1D-C2D	-2.25	1.40	1.45
33	b	612	CLA	C3D-C4D	-2.25	1.39	1.44
33	4	307	CLA	C3D-C4D	-2.25	1.39	1.44
33	B	608	CLA	C3D-C4D	-2.25	1.39	1.44
33	c	510	CLA	C3D-C4D	-2.25	1.39	1.44
33	C	505	CLA	C1D-C2D	-2.24	1.40	1.45
33	C	510	CLA	C3D-C4D	-2.24	1.39	1.44
33	0	302	CLA	C1D-C2D	-2.24	1.40	1.45
33	9	308	CLA	C1D-C2D	-2.24	1.40	1.45
33	B	618	CLA	C1D-C2D	-2.24	1.40	1.45
33	B	611	CLA	C3D-C4D	-2.24	1.39	1.44
33	6	304	CLA	C1D-C2D	-2.24	1.40	1.45
33	b	606	CLA	C1D-C2D	-2.24	1.40	1.45
33	C	510	CLA	C1D-C2D	-2.24	1.40	1.45
37	b	623	LHG	O7-C5	-2.24	1.41	1.46
33	5	306	CLA	C3D-C4D	-2.24	1.39	1.44
33	c	510	CLA	C1D-C2D	-2.24	1.40	1.45
33	7	308	CLA	C3D-C4D	-2.24	1.39	1.44
33	n	304	CLA	C1D-C2D	-2.24	1.40	1.45
33	3	305	CLA	C1D-C2D	-2.24	1.40	1.45
33	g	308	CLA	C3D-C4D	-2.24	1.39	1.44
33	B	615	CLA	C3D-C4D	-2.24	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	3	308	CLA	C1D-C2D	-2.24	1.40	1.45
33	b	615	CLA	C3D-C4D	-2.23	1.39	1.44
36	D	407	PL9	C6-C1	-2.23	1.44	1.48
33	D	404	CLA	C3D-C4D	-2.23	1.39	1.44
36	d	407	PL9	C6-C1	-2.23	1.44	1.48
33	b	618	CLA	C3D-C4D	-2.23	1.39	1.44
33	1	308	CLA	C3D-C4D	-2.23	1.39	1.44
33	7	305	CLA	C3D-C4D	-2.23	1.39	1.44
33	b	613	CLA	C3D-C4D	-2.23	1.39	1.44
33	9	305	CLA	C1D-C2D	-2.23	1.40	1.45
33	n	301	CLA	C1D-C2D	-2.23	1.40	1.45
37	B	623	LHG	O7-C5	-2.23	1.41	1.46
33	1	304	CLA	C3D-C4D	-2.23	1.39	1.44
33	D	405	CLA	C1D-C2D	-2.23	1.40	1.45
33	8	302	CLA	C3D-C4D	-2.23	1.39	1.44
33	c	507	CLA	C3D-C4D	-2.23	1.39	1.44
33	7	308	CLA	C1D-C2D	-2.22	1.40	1.45
33	C	507	CLA	C3D-C4D	-2.22	1.39	1.44
33	A	406	CLA	C3D-C4D	-2.22	1.39	1.44
33	a	408	CLA	C3D-C4D	-2.22	1.39	1.44
33	0	307	CLA	C3D-C4D	-2.22	1.39	1.44
33	g	303	CLA	C3D-C4D	-2.22	1.39	1.44
33	5	303	CLA	C3D-C4D	-2.22	1.39	1.44
33	7	302	CLA	C1D-C2D	-2.22	1.40	1.45
33	2	302	CLA	C3D-C4D	-2.22	1.39	1.44
33	9	312	CLA	C1D-C2D	-2.22	1.40	1.45
33	7	304	CLA	C3D-C4D	-2.22	1.39	1.44
33	8	308	CLA	C3D-C4D	-2.22	1.39	1.44
33	c	503	CLA	C3D-C4D	-2.22	1.39	1.44
33	b	605	CLA	C3D-C4D	-2.22	1.39	1.44
33	c	509	CLA	C3D-C4D	-2.22	1.39	1.44
33	3	308	CLA	C3D-C4D	-2.22	1.39	1.44
33	B	613	CLA	C3D-C4D	-2.22	1.39	1.44
33	8	307	CLA	C3D-C4D	-2.22	1.39	1.44
33	C	502	CLA	C3D-C4D	-2.22	1.39	1.44
33	n	302	CLA	C3D-C4D	-2.22	1.39	1.44
33	6	307	CLA	C1D-C2D	-2.22	1.41	1.45
33	p	304	CLA	C1D-C2D	-2.22	1.41	1.45
33	b	614	CLA	C3D-C4D	-2.22	1.39	1.44
33	g	306	CLA	C3D-C4D	-2.22	1.39	1.44
33	N	302	CLA	C3D-C4D	-2.21	1.39	1.44
33	5	301	CLA	C1D-C2D	-2.21	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	612	CLA	C3D-C4D	-2.21	1.39	1.44
33	5	302	CLA	C3D-C4D	-2.21	1.39	1.44
33	1	303	CLA	C3D-C4D	-2.21	1.39	1.44
33	7	307	CLA	C1D-C2D	-2.21	1.41	1.45
33	C	505	CLA	C3D-C4D	-2.21	1.39	1.44
33	c	505	CLA	C3D-C4D	-2.21	1.39	1.44
33	5	308	CLA	C1D-C2D	-2.21	1.41	1.45
33	2	307	CLA	C3D-C4D	-2.21	1.39	1.44
33	g	304	CLA	C1D-C2D	-2.21	1.41	1.45
33	b	606	CLA	C1C-C2C	2.21	1.48	1.44
33	a	406	CLA	C3D-C4D	-2.21	1.39	1.44
33	3	310	CLA	C1D-C2D	-2.21	1.41	1.45
33	C	512	CLA	C1D-C2D	-2.21	1.41	1.45
33	3	304	CLA	C3D-C4D	-2.21	1.39	1.44
33	7	303	CLA	C3D-C4D	-2.21	1.39	1.44
33	9	308	CLA	C3D-C4D	-2.21	1.39	1.44
33	9	314	CLA	C3D-C4D	-2.21	1.39	1.44
33	g	302	CLA	C3D-C4D	-2.21	1.39	1.44
33	B	606	CLA	C1C-C2C	2.21	1.48	1.44
33	1	302	CLA	C1D-C2D	-2.21	1.41	1.45
33	N	301	CLA	C1D-C2D	-2.21	1.41	1.45
33	c	507	CLA	C1D-C2D	-2.21	1.41	1.45
33	9	310	CLA	C1D-C2D	-2.20	1.41	1.45
33	3	309	CLA	C3D-C4D	-2.20	1.39	1.44
33	B	602	CLA	C1D-C2D	-2.20	1.41	1.45
33	C	513	CLA	C3D-C4D	-2.20	1.39	1.44
33	7	304	CLA	C1D-C2D	-2.20	1.41	1.45
33	c	502	CLA	C3D-C4D	-2.20	1.39	1.44
33	c	512	CLA	C1D-C2D	-2.20	1.41	1.45
33	2	301	CLA	C3D-C4D	-2.20	1.39	1.44
33	D	405	CLA	C3D-C4D	-2.20	1.39	1.44
33	g	301	CLA	C3D-C4D	-2.20	1.39	1.44
33	C	506	CLA	C3D-C4D	-2.20	1.39	1.44
33	B	605	CLA	C3D-C4D	-2.20	1.39	1.44
33	B	614	CLA	C3D-C4D	-2.20	1.39	1.44
33	c	514	CLA	C3D-C4D	-2.19	1.39	1.44
44	F	101	HEM	C3C-C4C	-2.19	1.42	1.46
33	C	503	CLA	C3D-C4D	-2.19	1.39	1.44
33	d	405	CLA	C3D-C4D	-2.19	1.39	1.44
33	9	310	CLA	C3D-C4D	-2.19	1.39	1.44
33	c	506	CLA	C3D-C4D	-2.19	1.39	1.44
33	3	310	CLA	C3D-C4D	-2.19	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	7	302	CLA	C3D-C4D	-2.19	1.39	1.44
33	c	508	CLA	C3D-C4D	-2.19	1.39	1.44
33	B	609	CLA	C3D-C4D	-2.19	1.39	1.44
33	d	405	CLA	C1D-C2D	-2.19	1.41	1.45
33	g	308	CLA	C1D-C2D	-2.19	1.41	1.45
33	C	514	CLA	C3D-C4D	-2.19	1.39	1.44
33	A	408	CLA	C1D-C2D	-2.19	1.41	1.45
33	0	308	CLA	C1D-C2D	-2.19	1.41	1.45
33	p	307	CLA	C1D-C2D	-2.19	1.41	1.45
33	8	301	CLA	C3D-C4D	-2.18	1.39	1.44
33	b	607	CLA	C3D-C4D	-2.18	1.39	1.44
33	p	304	CLA	C3D-C4D	-2.18	1.39	1.44
33	6	304	CLA	C3D-C4D	-2.18	1.39	1.44
33	8	301	CLA	C1D-C2D	-2.18	1.41	1.45
33	1	307	CLA	C3D-C4D	-2.18	1.39	1.44
33	2	304	CLA	C1D-C2D	-2.18	1.41	1.45
33	g	301	CLA	C1D-C2D	-2.18	1.41	1.45
33	b	609	CLA	C3D-C4D	-2.18	1.39	1.44
33	1	304	CLA	C1D-C2D	-2.18	1.41	1.45
33	5	301	CLA	C3D-C4D	-2.18	1.39	1.44
33	b	602	CLA	C1D-C2D	-2.18	1.41	1.45
33	1	307	CLA	C1D-C2D	-2.18	1.41	1.45
33	4	303	CLA	C1D-C2D	-2.18	1.41	1.45
33	c	504	CLA	C3D-C4D	-2.18	1.39	1.44
33	2	310	CLA	C3D-C4D	-2.18	1.39	1.44
33	c	513	CLA	C3D-C4D	-2.18	1.39	1.44
33	9	309	CLA	C1D-C2D	-2.18	1.41	1.45
33	2	303	CLA	C1D-C2D	-2.18	1.41	1.45
33	8	303	CLA	C1D-C2D	-2.18	1.41	1.45
33	C	507	CLA	C1D-C2D	-2.17	1.41	1.45
33	1	302	CLA	C3D-C4D	-2.17	1.39	1.44
33	1	309	CLA	C3D-C4D	-2.17	1.39	1.44
33	A	405	CLA	C3D-C4D	-2.17	1.39	1.44
33	9	309	CLA	C3D-C4D	-2.17	1.39	1.44
33	7	309	CLA	C3D-C4D	-2.17	1.39	1.44
33	a	405	CLA	C3D-C4D	-2.17	1.39	1.44
33	7	306	CLA	C3D-C4D	-2.17	1.39	1.44
33	B	617	CLA	C3D-C4D	-2.17	1.39	1.44
33	9	313	CLA	C3D-C4D	-2.17	1.39	1.44
33	C	508	CLA	C3D-C4D	-2.17	1.39	1.44
33	7	307	CLA	C3D-C4D	-2.17	1.39	1.44
33	3	309	CLA	C1D-C2D	-2.16	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	8	310	CLA	C3D-C4D	-2.16	1.39	1.44
33	a	406	CLA	C1D-C2D	-2.16	1.41	1.45
33	1	306	CLA	C3D-C4D	-2.16	1.39	1.44
33	0	303	CLA	C1D-C2D	-2.16	1.41	1.45
33	3	313	CLA	C3D-C4D	-2.16	1.39	1.44
33	1	301	CLA	C1D-C2D	-2.16	1.41	1.45
33	N	303	CLA	C1D-C2D	-2.16	1.41	1.45
33	B	602	CLA	C3D-C4D	-2.16	1.39	1.44
33	3	312	CLA	C1D-C2D	-2.16	1.41	1.45
33	3	314	CLA	C3D-C4D	-2.16	1.39	1.44
37	9	322	LHG	O7-C5	-2.16	1.41	1.46
37	3	322	LHG	O7-C5	-2.16	1.41	1.46
33	b	610	CLA	C3D-C4D	-2.15	1.39	1.44
33	7	301	CLA	C1D-C2D	-2.15	1.41	1.45
33	8	304	CLA	C1D-C2D	-2.15	1.41	1.45
33	B	607	CLA	C3D-C4D	-2.15	1.39	1.44
33	A	406	CLA	C1D-C2D	-2.15	1.41	1.45
33	a	408	CLA	C1D-C2D	-2.15	1.41	1.45
33	N	302	CLA	C1D-C2D	-2.15	1.41	1.45
33	5	302	CLA	C1D-C2D	-2.15	1.41	1.45
33	2	301	CLA	C1D-C2D	-2.14	1.41	1.45
33	n	302	CLA	C1D-C2D	-2.14	1.41	1.45
33	9	306	CLA	C3D-C4D	-2.14	1.39	1.44
33	b	617	CLA	C3D-C4D	-2.14	1.39	1.44
33	A	412	CLA	C1D-C2D	-2.14	1.41	1.45
33	3	307	CLA	C3D-C4D	-2.14	1.39	1.44
33	g	303	CLA	C1D-C2D	-2.14	1.41	1.45
33	4	303	CLA	C3D-C4D	-2.14	1.39	1.44
33	5	317	CLA	C1D-C2D	-2.14	1.41	1.45
33	n	306	CLA	C1D-C2D	-2.14	1.41	1.45
37	D	401	LHG	O7-C5	-2.13	1.41	1.46
33	2	302	CLA	C1D-C2D	-2.13	1.41	1.45
33	b	602	CLA	C3D-C4D	-2.13	1.39	1.44
43	h	101	DGD	O2G-C2G	-2.13	1.41	1.46
33	N	304	CLA	C1D-C2D	-2.13	1.41	1.45
33	5	311	CLA	C1D-C2D	-2.13	1.41	1.45
33	g	317	CLA	C1D-C2D	-2.13	1.41	1.45
33	3	315	CLA	C3D-C4D	-2.13	1.39	1.44
33	3	306	CLA	C3D-C4D	-2.13	1.39	1.44
33	N	307	CLA	C1D-C2D	-2.13	1.41	1.45
33	g	310	CLA	C3D-C4D	-2.13	1.39	1.44
33	B	610	CLA	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	8	302	CLA	C1D-C2D	-2.13	1.41	1.45
33	C	504	CLA	C3D-C4D	-2.13	1.39	1.44
33	0	303	CLA	C3D-C4D	-2.12	1.39	1.44
44	V	201	HEM	FE-NB	2.12	2.01	1.94
33	3	303	CLA	C1D-C2D	-2.12	1.41	1.45
33	5	303	CLA	C1D-C2D	-2.12	1.41	1.45
33	g	317	CLA	C3D-C4D	-2.12	1.39	1.44
33	g	311	CLA	C3D-C4D	-2.12	1.39	1.44
33	n	303	CLA	C1D-C2D	-2.12	1.41	1.45
37	A	411	LHG	O7-C5	-2.12	1.41	1.46
33	g	311	CLA	C1D-C2D	-2.12	1.41	1.45
33	5	311	CLA	C3D-C4D	-2.12	1.39	1.44
44	v	201	HEM	FE-NB	2.12	2.01	1.94
33	n	306	CLA	C3D-C4D	-2.12	1.39	1.44
33	B	616	CLA	C3D-C4D	-2.11	1.39	1.44
33	b	616	CLA	C3D-C4D	-2.11	1.39	1.44
33	5	310	CLA	C3D-C4D	-2.11	1.39	1.44
33	9	307	CLA	C3D-C4D	-2.11	1.39	1.44
33	g	302	CLA	C1D-C2D	-2.11	1.41	1.45
44	F	101	HEM	C1D-ND	-2.11	1.34	1.38
33	N	307	CLA	C3D-C4D	-2.11	1.39	1.44
37	d	401	LHG	O7-C5	-2.11	1.41	1.46
33	8	310	CLA	C1D-C2D	-2.11	1.41	1.45
33	5	317	CLA	C3D-C4D	-2.11	1.39	1.44
43	H	101	DGD	O2G-C2G	-2.11	1.41	1.46
33	9	315	CLA	C3D-C4D	-2.11	1.39	1.44
33	a	412	CLA	C1D-C2D	-2.11	1.41	1.45
43	C	518	DGD	O2G-C2G	-2.10	1.41	1.46
33	9	303	CLA	C1D-C2D	-2.10	1.41	1.45
33	9	306	CLA	C1D-C2D	-2.10	1.41	1.45
33	n	304	CLA	C3D-C4D	-2.10	1.39	1.44
43	c	518	DGD	O2G-C2G	-2.09	1.41	1.46
33	c	512	CLA	C3D-C4D	-2.09	1.39	1.44
37	9	322	LHG	P-O6	2.09	1.67	1.59
37	a	411	LHG	O7-C5	-2.09	1.41	1.46
37	3	322	LHG	P-O6	2.09	1.67	1.59
33	N	305	CLA	C3D-C4D	-2.09	1.39	1.44
33	3	306	CLA	C1D-C2D	-2.09	1.41	1.45
33	2	310	CLA	C1D-C2D	-2.08	1.41	1.45
36	d	407	PL9	C52-C5	-2.08	1.46	1.50
43	c	519	DGD	O6D-C5D	-2.08	1.39	1.44
43	C	519	DGD	O6D-C5D	-2.07	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	607	CLA	C1D-C2D	-2.07	1.41	1.45
33	B	607	CLA	C1D-C2D	-2.07	1.41	1.45
36	D	407	PL9	C52-C5	-2.06	1.46	1.50
42	C	520	LMG	O7-C8	-2.06	1.41	1.46
33	C	512	CLA	C3D-C4D	-2.04	1.39	1.44
37	9	302	LHG	O7-C5	-2.04	1.41	1.46
42	c	520	LMG	O7-C8	-2.04	1.41	1.46
36	d	407	PL9	C7-C3	-2.02	1.49	1.51
44	F	101	HEM	C1A-C2A	-2.01	1.40	1.44
37	3	302	LHG	O7-C5	-2.01	1.41	1.46
33	5	303	CLA	C1C-C2C	2.01	1.48	1.44
37	9	321	LHG	O7-C5	-2.01	1.41	1.46

All (2237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	p	302	CLA	C4A-NA-C1A	-8.29	102.98	106.71
33	6	302	CLA	C4A-NA-C1A	-8.28	102.98	106.71
33	2	302	CLA	C4A-NA-C1A	-8.27	102.99	106.71
33	0	310	CLA	C4A-NA-C1A	-8.25	103.00	106.71
33	8	302	CLA	C4A-NA-C1A	-8.23	103.01	106.71
33	8	303	CLA	C4A-NA-C1A	-8.23	103.01	106.71
33	4	309	CLA	C4A-NA-C1A	-8.18	103.03	106.71
33	2	303	CLA	C4A-NA-C1A	-8.11	103.06	106.71
33	1	301	CLA	C4A-NA-C1A	-7.92	103.15	106.71
33	9	306	CLA	C4A-NA-C1A	-7.79	103.20	106.71
33	7	301	CLA	C4A-NA-C1A	-7.77	103.22	106.71
33	1	307	CLA	C4A-NA-C1A	-7.75	103.22	106.71
33	7	307	CLA	C4A-NA-C1A	-7.73	103.23	106.71
33	3	306	CLA	C4A-NA-C1A	-7.72	103.24	106.71
33	0	311	CLA	C4A-NA-C1A	-7.70	103.24	106.71
33	4	310	CLA	C4A-NA-C1A	-7.70	103.24	106.71
33	n	303	CLA	C4A-NA-C1A	-7.70	103.24	106.71
33	d	404	CLA	C4A-NA-C1A	-7.59	103.30	106.71
33	N	304	CLA	C4A-NA-C1A	-7.55	103.31	106.71
33	D	404	CLA	C4A-NA-C1A	-7.55	103.31	106.71
33	B	615	CLA	C4A-NA-C1A	-7.44	103.36	106.71
33	b	615	CLA	C4A-NA-C1A	-7.44	103.36	106.71
33	5	310	CLA	C4A-NA-C1A	-7.41	103.37	106.71
33	g	310	CLA	C4A-NA-C1A	-7.41	103.38	106.71
33	9	307	CLA	C4A-NA-C1A	-7.38	103.39	106.71
33	3	309	CLA	C4A-NA-C1A	-7.36	103.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	306	CLA	C4A-NA-C1A	-7.35	103.40	106.71
33	9	314	CLA	C4A-NA-C1A	-7.35	103.40	106.71
33	3	307	CLA	C4A-NA-C1A	-7.34	103.41	106.71
33	2	306	CLA	C4A-NA-C1A	-7.31	103.42	106.71
33	3	314	CLA	C4A-NA-C1A	-7.30	103.42	106.71
33	p	303	CLA	C4A-NA-C1A	-7.22	103.46	106.71
33	7	302	CLA	C4A-NA-C1A	-7.21	103.47	106.71
33	1	302	CLA	C4A-NA-C1A	-7.21	103.47	106.71
33	2	310	CLA	C4A-NA-C1A	-7.19	103.47	106.71
33	9	309	CLA	C4A-NA-C1A	-7.19	103.47	106.71
33	g	308	CLA	C4A-NA-C1A	-7.19	103.47	106.71
33	5	304	CLA	C4A-NA-C1A	-7.18	103.48	106.71
33	8	310	CLA	C4A-NA-C1A	-7.16	103.49	106.71
33	5	308	CLA	C4A-NA-C1A	-7.14	103.50	106.71
33	6	303	CLA	C4A-NA-C1A	-7.13	103.50	106.71
33	g	304	CLA	C4A-NA-C1A	-7.12	103.50	106.71
33	2	301	CLA	C4A-NA-C1A	-7.07	103.53	106.71
33	p	309	CLA	C4A-NA-C1A	-7.00	103.56	106.71
33	6	309	CLA	C4A-NA-C1A	-7.00	103.56	106.71
33	6	308	CLA	C4A-NA-C1A	-6.97	103.57	106.71
33	p	308	CLA	C4A-NA-C1A	-6.96	103.58	106.71
33	8	301	CLA	C4A-NA-C1A	-6.95	103.58	106.71
33	B	618	CLA	C4A-NA-C1A	-6.91	103.60	106.71
33	b	618	CLA	C4A-NA-C1A	-6.85	103.63	106.71
33	n	301	CLA	C4A-NA-C1A	-6.82	103.64	106.71
33	B	611	CLA	C4A-NA-C1A	-6.81	103.65	106.71
33	g	302	CLA	C4A-NA-C1A	-6.77	103.66	106.71
33	5	302	CLA	C4A-NA-C1A	-6.75	103.67	106.71
33	b	611	CLA	C4A-NA-C1A	-6.74	103.67	106.71
33	N	301	CLA	C4A-NA-C1A	-6.70	103.69	106.71
33	n	302	CLA	C4A-NA-C1A	-6.69	103.70	106.71
33	N	302	CLA	C4A-NA-C1A	-6.68	103.70	106.71
33	5	311	CLA	C4A-NA-C1A	-6.68	103.70	106.71
33	g	303	CLA	C4A-NA-C1A	-6.67	103.71	106.71
33	B	609	CLA	C4A-NA-C1A	-6.66	103.71	106.71
33	0	309	CLA	C1D-ND-C4D	-6.64	101.62	106.33
33	g	311	CLA	C4A-NA-C1A	-6.63	103.72	106.71
33	4	308	CLA	C1D-ND-C4D	-6.62	101.63	106.33
33	5	303	CLA	C4A-NA-C1A	-6.58	103.75	106.71
33	b	609	CLA	C4A-NA-C1A	-6.54	103.77	106.71
33	g	306	CLA	C4A-NA-C1A	-6.49	103.79	106.71
33	8	304	CLA	C1D-ND-C4D	-6.47	101.74	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	5	306	CLA	C4A-NA-C1A	-6.47	103.80	106.71
33	b	603	CLA	C4A-NA-C1A	-6.46	103.80	106.71
33	4	301	CLA	C4A-NA-C1A	-6.44	103.81	106.71
33	2	304	CLA	C1D-ND-C4D	-6.44	101.76	106.33
33	8	303	CLA	C1D-ND-C4D	-6.41	101.78	106.33
33	0	301	CLA	C4A-NA-C1A	-6.41	103.83	106.71
33	B	603	CLA	C4A-NA-C1A	-6.40	103.83	106.71
33	6	307	CLA	C1D-ND-C4D	-6.40	101.79	106.33
33	2	303	CLA	C1D-ND-C4D	-6.39	101.80	106.33
33	p	307	CLA	C1D-ND-C4D	-6.36	101.82	106.33
33	0	302	CLA	C1D-ND-C4D	-6.32	101.84	106.33
33	4	302	CLA	C1D-ND-C4D	-6.32	101.85	106.33
33	g	307	CLA	C1D-ND-C4D	-6.31	101.85	106.33
33	5	303	CLA	C1D-ND-C4D	-6.31	101.86	106.33
33	B	606	CLA	C1D-ND-C4D	-6.30	101.86	106.33
33	b	606	CLA	C1D-ND-C4D	-6.28	101.87	106.33
33	0	302	CLA	C4A-NA-C1A	-6.28	103.88	106.71
33	4	304	CLA	C4A-NA-C1A	-6.28	103.88	106.71
33	5	307	CLA	C1D-ND-C4D	-6.28	101.88	106.33
33	1	308	CLA	C1D-ND-C4D	-6.27	101.88	106.33
33	0	304	CLA	C4A-NA-C1A	-6.26	103.89	106.71
33	b	612	CLA	C1D-ND-C4D	-6.26	101.89	106.33
33	8	305	CLA	C4A-NA-C1A	-6.26	103.89	106.71
33	g	303	CLA	C1D-ND-C4D	-6.26	101.89	106.33
33	4	302	CLA	C4A-NA-C1A	-6.25	103.89	106.71
33	2	305	CLA	C4A-NA-C1A	-6.25	103.90	106.71
33	6	319	CLA	C4A-NA-C1A	-6.25	103.90	106.71
33	p	304	CLA	C1D-ND-C4D	-6.25	101.90	106.33
33	p	319	CLA	C4A-NA-C1A	-6.24	103.90	106.71
33	p	312	CLA	C1D-ND-C4D	-6.24	101.90	106.33
33	7	306	CLA	C4A-NA-C1A	-6.23	103.90	106.71
33	6	304	CLA	C1D-ND-C4D	-6.23	101.91	106.33
33	B	612	CLA	C1D-ND-C4D	-6.23	101.91	106.33
33	A	408	CLA	C1D-ND-C4D	-6.23	101.91	106.33
33	C	504	CLA	C1D-ND-C4D	-6.22	101.92	106.33
33	b	604	CLA	C1D-ND-C4D	-6.22	101.92	106.33
33	4	307	CLA	C1D-ND-C4D	-6.21	101.93	106.33
33	0	307	CLA	C1D-ND-C4D	-6.20	101.93	106.33
33	N	306	CLA	C1D-ND-C4D	-6.20	101.93	106.33
33	4	303	CLA	C4A-NA-C1A	-6.20	103.92	106.71
33	N	307	CLA	C1D-ND-C4D	-6.19	101.94	106.33
33	0	303	CLA	C4A-NA-C1A	-6.19	103.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	5	317	CLA	C4A-NA-C1A	-6.19	103.92	106.71
33	6	307	CLA	C4A-NA-C1A	-6.19	103.92	106.71
33	0	311	CLA	C1D-ND-C4D	-6.19	101.94	106.33
33	g	311	CLA	C1D-ND-C4D	-6.19	101.94	106.33
33	a	408	CLA	C1D-ND-C4D	-6.18	101.94	106.33
33	6	312	CLA	C1D-ND-C4D	-6.18	101.94	106.33
33	c	504	CLA	C1D-ND-C4D	-6.18	101.95	106.33
33	A	406	CLA	C1D-ND-C4D	-6.17	101.95	106.33
33	3	312	CLA	C4A-NA-C1A	-6.17	103.93	106.71
33	4	310	CLA	C1D-ND-C4D	-6.17	101.95	106.33
33	5	311	CLA	C1D-ND-C4D	-6.17	101.95	106.33
33	c	507	CLA	C1D-ND-C4D	-6.16	101.96	106.33
33	p	307	CLA	C4A-NA-C1A	-6.16	103.94	106.71
33	n	305	CLA	C1D-ND-C4D	-6.16	101.96	106.33
33	a	406	CLA	C1D-ND-C4D	-6.16	101.96	106.33
33	1	304	CLA	C1D-ND-C4D	-6.15	101.96	106.33
33	5	301	CLA	C1D-ND-C4D	-6.15	101.97	106.33
33	B	604	CLA	C1D-ND-C4D	-6.15	101.97	106.33
33	c	509	CLA	C1D-ND-C4D	-6.15	101.97	106.33
33	d	405	CLA	C1D-ND-C4D	-6.15	101.97	106.33
33	g	301	CLA	C1D-ND-C4D	-6.14	101.97	106.33
33	7	308	CLA	C1D-ND-C4D	-6.14	101.97	106.33
33	D	405	CLA	C1D-ND-C4D	-6.14	101.97	106.33
33	g	302	CLA	C1D-ND-C4D	-6.14	101.97	106.33
33	n	306	CLA	C1D-ND-C4D	-6.14	101.98	106.33
33	9	305	CLA	C1D-ND-C4D	-6.13	101.98	106.33
33	A	412	CLA	C1D-ND-C4D	-6.13	101.98	106.33
33	g	317	CLA	C4A-NA-C1A	-6.13	103.95	106.71
33	3	305	CLA	C1D-ND-C4D	-6.13	101.98	106.33
33	b	611	CLA	C1D-ND-C4D	-6.13	101.98	106.33
33	C	509	CLA	C1D-ND-C4D	-6.12	101.98	106.33
33	1	306	CLA	C4A-NA-C1A	-6.12	103.95	106.71
33	B	617	CLA	C1D-ND-C4D	-6.12	101.99	106.33
33	5	302	CLA	C1D-ND-C4D	-6.11	101.99	106.33
33	b	617	CLA	C1D-ND-C4D	-6.11	101.99	106.33
33	9	312	CLA	C4A-NA-C1A	-6.11	103.96	106.71
33	B	604	CLA	C4A-NA-C1A	-6.11	103.96	106.71
33	7	304	CLA	C1D-ND-C4D	-6.11	102.00	106.33
33	9	303	CLA	C4A-NA-C1A	-6.10	103.96	106.71
33	8	307	CLA	C4A-NA-C1A	-6.10	103.96	106.71
33	9	306	CLA	C1D-ND-C4D	-6.10	102.00	106.33
33	a	412	CLA	C1D-ND-C4D	-6.10	102.00	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	408	CLA	C4A-NA-C1A	-6.09	103.97	106.71
33	A	408	CLA	C4A-NA-C1A	-6.09	103.97	106.71
33	8	304	CLA	C4A-NA-C1A	-6.09	103.97	106.71
33	a	406	CLA	C4A-NA-C1A	-6.09	103.97	106.71
33	2	304	CLA	C4A-NA-C1A	-6.09	103.97	106.71
33	b	603	CLA	C1D-ND-C4D	-6.08	102.01	106.33
33	N	303	CLA	C1D-ND-C4D	-6.08	102.01	106.33
33	b	607	CLA	C1D-ND-C4D	-6.08	102.01	106.33
33	B	611	CLA	C1D-ND-C4D	-6.08	102.02	106.33
33	C	513	CLA	C4A-NA-C1A	-6.08	103.97	106.71
33	B	603	CLA	C1D-ND-C4D	-6.07	102.02	106.33
33	0	303	CLA	C1D-ND-C4D	-6.07	102.02	106.33
33	3	313	CLA	C1D-ND-C4D	-6.06	102.03	106.33
33	9	313	CLA	C1D-ND-C4D	-6.06	102.03	106.33
33	b	608	CLA	C1D-ND-C4D	-6.06	102.03	106.33
33	9	303	CLA	C1D-ND-C4D	-6.06	102.03	106.33
33	9	310	CLA	C1D-ND-C4D	-6.06	102.03	106.33
33	B	608	CLA	C1D-ND-C4D	-6.06	102.03	106.33
33	3	310	CLA	C1D-ND-C4D	-6.06	102.03	106.33
33	A	406	CLA	C4A-NA-C1A	-6.05	103.98	106.71
33	1	301	CLA	C1D-ND-C4D	-6.05	102.03	106.33
33	2	308	CLA	C1D-ND-C4D	-6.05	102.03	106.33
33	C	507	CLA	C1D-ND-C4D	-6.05	102.03	106.33
33	0	308	CLA	C1D-ND-C4D	-6.05	102.04	106.33
33	7	301	CLA	C1D-ND-C4D	-6.05	102.04	106.33
33	3	303	CLA	C1D-ND-C4D	-6.05	102.04	106.33
33	3	303	CLA	C4A-NA-C1A	-6.05	103.99	106.71
33	c	505	CLA	C1D-ND-C4D	-6.05	102.04	106.33
33	C	505	CLA	C1D-ND-C4D	-6.05	102.04	106.33
33	B	612	CLA	C4A-NA-C1A	-6.04	103.99	106.71
33	6	309	CLA	C1D-ND-C4D	-6.04	102.04	106.33
33	9	304	CLA	C1D-ND-C4D	-6.04	102.04	106.33
33	b	604	CLA	C4A-NA-C1A	-6.04	103.99	106.71
33	c	513	CLA	C4A-NA-C1A	-6.04	103.99	106.71
33	3	304	CLA	C1D-ND-C4D	-6.04	102.05	106.33
33	b	602	CLA	C1D-ND-C4D	-6.04	102.05	106.33
33	B	607	CLA	C1D-ND-C4D	-6.03	102.05	106.33
33	4	303	CLA	C1D-ND-C4D	-6.03	102.05	106.33
33	C	513	CLA	C1D-ND-C4D	-6.03	102.05	106.33
33	6	303	CLA	C1D-ND-C4D	-6.02	102.06	106.33
33	g	317	CLA	C1D-ND-C4D	-6.02	102.06	106.33
33	c	513	CLA	C1D-ND-C4D	-6.01	102.06	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	0	304	CLA	C1D-ND-C4D	-6.01	102.06	106.33
33	3	306	CLA	C1D-ND-C4D	-6.01	102.06	106.33
33	b	612	CLA	C4A-NA-C1A	-6.01	104.00	106.71
33	p	309	CLA	C1D-ND-C4D	-6.01	102.07	106.33
33	2	301	CLA	C1D-ND-C4D	-6.00	102.07	106.33
33	B	609	CLA	C1D-ND-C4D	-6.00	102.07	106.33
33	8	308	CLA	C1D-ND-C4D	-6.00	102.07	106.33
33	B	618	CLA	C1D-ND-C4D	-6.00	102.07	106.33
33	5	308	CLA	C1D-ND-C4D	-6.00	102.07	106.33
33	6	306	CLA	C1D-ND-C4D	-6.00	102.07	106.33
33	B	602	CLA	C1D-ND-C4D	-6.00	102.07	106.33
33	p	303	CLA	C1D-ND-C4D	-6.00	102.08	106.33
33	p	308	CLA	C1D-ND-C4D	-6.00	102.08	106.33
33	n	302	CLA	C1D-ND-C4D	-5.98	102.08	106.33
33	6	308	CLA	C1D-ND-C4D	-5.98	102.08	106.33
33	g	308	CLA	C1D-ND-C4D	-5.98	102.09	106.33
33	5	317	CLA	C1D-ND-C4D	-5.98	102.09	106.33
33	8	301	CLA	C1D-ND-C4D	-5.98	102.09	106.33
33	c	510	CLA	C4A-NA-C1A	-5.97	104.02	106.71
33	N	301	CLA	C1D-ND-C4D	-5.97	102.09	106.33
33	p	306	CLA	C1D-ND-C4D	-5.97	102.09	106.33
33	N	302	CLA	C1D-ND-C4D	-5.97	102.10	106.33
33	c	514	CLA	C1D-ND-C4D	-5.97	102.10	106.33
33	C	514	CLA	C1D-ND-C4D	-5.96	102.10	106.33
33	C	510	CLA	C4A-NA-C1A	-5.96	104.03	106.71
33	B	613	CLA	C4A-NA-C1A	-5.96	104.03	106.71
33	2	310	CLA	C1D-ND-C4D	-5.96	102.10	106.33
33	3	310	CLA	C4A-NA-C1A	-5.96	104.03	106.71
33	6	313	CLA	C4A-NA-C1A	-5.96	104.03	106.71
33	b	609	CLA	C1D-ND-C4D	-5.95	102.11	106.33
33	2	307	CLA	C4A-NA-C1A	-5.95	104.03	106.71
33	1	302	CLA	C1D-ND-C4D	-5.95	102.11	106.33
33	n	301	CLA	C1D-ND-C4D	-5.95	102.11	106.33
33	4	304	CLA	C1D-ND-C4D	-5.95	102.11	106.33
33	8	306	CLA	C1D-ND-C4D	-5.95	102.11	106.33
33	3	309	CLA	C1D-ND-C4D	-5.94	102.11	106.33
33	9	310	CLA	C4A-NA-C1A	-5.94	104.04	106.71
33	7	306	CLA	C1D-ND-C4D	-5.93	102.12	106.33
33	p	313	CLA	C4A-NA-C1A	-5.93	104.04	106.71
33	c	503	CLA	C4A-NA-C1A	-5.93	104.04	106.71
33	c	512	CLA	C1D-ND-C4D	-5.93	102.12	106.33
33	B	610	CLA	C4A-NA-C1A	-5.93	104.04	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	503	CLA	C4A-NA-C1A	-5.93	104.04	106.71
33	9	304	CLA	C4A-NA-C1A	-5.93	104.04	106.71
33	7	302	CLA	C1D-ND-C4D	-5.92	102.13	106.33
33	g	310	CLA	C1D-ND-C4D	-5.92	102.13	106.33
33	8	310	CLA	C1D-ND-C4D	-5.92	102.13	106.33
33	c	506	CLA	C1D-ND-C4D	-5.91	102.13	106.33
33	b	613	CLA	C1D-ND-C4D	-5.91	102.14	106.33
33	C	502	CLA	C1D-ND-C4D	-5.91	102.14	106.33
33	A	412	CLA	CHD-C1D-ND	-5.90	119.03	124.45
33	7	303	CLA	C1D-ND-C4D	-5.90	102.14	106.33
33	b	615	CLA	C1D-ND-C4D	-5.90	102.14	106.33
33	1	303	CLA	C1D-ND-C4D	-5.90	102.15	106.33
33	3	304	CLA	C4A-NA-C1A	-5.90	104.06	106.71
33	g	301	CLA	C4A-NA-C1A	-5.90	104.06	106.71
33	1	306	CLA	C1D-ND-C4D	-5.89	102.15	106.33
33	2	306	CLA	C1D-ND-C4D	-5.89	102.15	106.33
33	9	309	CLA	C1D-ND-C4D	-5.89	102.15	106.33
33	N	304	CLA	C1D-ND-C4D	-5.89	102.15	106.33
33	b	613	CLA	C4A-NA-C1A	-5.89	104.06	106.71
33	C	506	CLA	C1D-ND-C4D	-5.89	102.15	106.33
33	b	606	CLA	C4A-NA-C1A	-5.89	104.06	106.71
33	2	307	CLA	C1D-ND-C4D	-5.89	102.15	106.33
33	5	310	CLA	C1D-ND-C4D	-5.88	102.16	106.33
33	B	613	CLA	C1D-ND-C4D	-5.88	102.16	106.33
33	a	412	CLA	CHD-C1D-ND	-5.88	119.05	124.45
33	c	511	CLA	C1D-ND-C4D	-5.88	102.16	106.33
33	5	301	CLA	C4A-NA-C1A	-5.88	104.06	106.71
33	6	310	CLA	C4A-NA-C1A	-5.87	104.06	106.71
33	b	616	CLA	C1D-ND-C4D	-5.87	102.16	106.33
33	d	404	CLA	C1D-ND-C4D	-5.87	102.16	106.33
33	C	512	CLA	C1D-ND-C4D	-5.87	102.17	106.33
33	b	618	CLA	C1D-ND-C4D	-5.87	102.17	106.33
33	1	309	CLA	C1D-ND-C4D	-5.87	102.17	106.33
33	n	303	CLA	C1D-ND-C4D	-5.87	102.17	106.33
33	D	404	CLA	C1D-ND-C4D	-5.86	102.17	106.33
33	2	305	CLA	C1D-ND-C4D	-5.86	102.17	106.33
33	b	610	CLA	C4A-NA-C1A	-5.86	104.07	106.71
33	b	614	CLA	C4A-NA-C1A	-5.85	104.07	106.71
33	C	511	CLA	C1D-ND-C4D	-5.85	102.18	106.33
33	c	502	CLA	C1D-ND-C4D	-5.84	102.18	106.33
33	b	614	CLA	C1D-ND-C4D	-5.83	102.19	106.33
33	3	308	CLA	C1D-ND-C4D	-5.83	102.19	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	B	614	CLA	C1D-ND-C4D	-5.83	102.19	106.33
33	7	304	CLA	C4A-NA-C1A	-5.82	104.09	106.71
33	B	615	CLA	C1D-ND-C4D	-5.82	102.20	106.33
33	5	304	CLA	C1D-ND-C4D	-5.82	102.20	106.33
33	c	510	CLA	C1D-ND-C4D	-5.82	102.20	106.33
33	7	309	CLA	C1D-ND-C4D	-5.81	102.20	106.33
33	8	305	CLA	C1D-ND-C4D	-5.81	102.21	106.33
33	2	302	CLA	C1D-ND-C4D	-5.81	102.21	106.33
33	9	308	CLA	C1D-ND-C4D	-5.81	102.21	106.33
33	1	304	CLA	C4A-NA-C1A	-5.81	104.10	106.71
33	9	314	CLA	C1D-ND-C4D	-5.80	102.21	106.33
33	p	310	CLA	C4A-NA-C1A	-5.80	104.10	106.71
33	B	616	CLA	C1D-ND-C4D	-5.80	102.22	106.33
33	B	605	CLA	C1D-ND-C4D	-5.80	102.22	106.33
33	B	606	CLA	C4A-NA-C1A	-5.80	104.10	106.71
33	4	301	CLA	C1D-ND-C4D	-5.79	102.22	106.33
33	c	503	CLA	C1D-ND-C4D	-5.79	102.22	106.33
33	8	307	CLA	C1D-ND-C4D	-5.79	102.22	106.33
33	8	302	CLA	C1D-ND-C4D	-5.79	102.22	106.33
33	1	305	CLA	C1D-ND-C4D	-5.79	102.22	106.33
33	3	307	CLA	C1D-ND-C4D	-5.78	102.23	106.33
33	b	605	CLA	C1D-ND-C4D	-5.78	102.23	106.33
33	B	614	CLA	C4A-NA-C1A	-5.78	104.11	106.71
33	5	305	CLA	C1D-ND-C4D	-5.78	102.23	106.33
33	N	305	CLA	C1D-ND-C4D	-5.78	102.23	106.33
33	C	503	CLA	C1D-ND-C4D	-5.77	102.23	106.33
33	C	511	CLA	C4A-NA-C1A	-5.77	104.11	106.71
33	C	510	CLA	C1D-ND-C4D	-5.76	102.24	106.33
33	g	305	CLA	C1D-ND-C4D	-5.75	102.25	106.33
33	7	305	CLA	C1D-ND-C4D	-5.75	102.25	106.33
33	n	304	CLA	C1D-ND-C4D	-5.75	102.25	106.33
33	9	312	CLA	C1D-ND-C4D	-5.75	102.25	106.33
33	0	301	CLA	C1D-ND-C4D	-5.74	102.26	106.33
33	g	304	CLA	C1D-ND-C4D	-5.73	102.26	106.33
33	3	312	CLA	C1D-ND-C4D	-5.73	102.27	106.33
33	7	303	CLA	C4A-NA-C1A	-5.73	104.13	106.71
33	3	314	CLA	C1D-ND-C4D	-5.73	102.27	106.33
33	a	405	CLA	C1D-ND-C4D	-5.72	102.27	106.33
33	g	305	CLA	C4A-NA-C1A	-5.72	104.13	106.71
33	9	315	CLA	C1D-ND-C4D	-5.71	102.28	106.33
33	3	308	CLA	C4A-NA-C1A	-5.71	104.14	106.71
33	0	308	CLA	CHD-C1D-ND	-5.71	119.20	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	N	303	CLA	CHD-C1D-ND	-5.71	119.21	124.45
33	9	307	CLA	C1D-ND-C4D	-5.70	102.28	106.33
33	c	508	CLA	C1D-ND-C4D	-5.70	102.28	106.33
33	A	405	CLA	C4A-NA-C1A	-5.70	104.14	106.71
33	9	308	CLA	C4A-NA-C1A	-5.70	104.14	106.71
33	c	507	CLA	C4A-NA-C1A	-5.70	104.14	106.71
33	3	315	CLA	C1D-ND-C4D	-5.69	102.29	106.33
33	5	305	CLA	C4A-NA-C1A	-5.69	104.15	106.71
33	7	307	CLA	C1D-ND-C4D	-5.69	102.29	106.33
33	5	306	CLA	C1D-ND-C4D	-5.68	102.30	106.33
33	1	307	CLA	C1D-ND-C4D	-5.68	102.30	106.33
33	g	306	CLA	C1D-ND-C4D	-5.68	102.30	106.33
33	C	508	CLA	C1D-ND-C4D	-5.67	102.31	106.33
33	N	306	CLA	C4A-NA-C1A	-5.67	104.16	106.71
33	c	511	CLA	C4A-NA-C1A	-5.67	104.16	106.71
33	B	610	CLA	C1D-ND-C4D	-5.67	102.31	106.33
33	b	610	CLA	C1D-ND-C4D	-5.67	102.31	106.33
33	0	307	CLA	C4A-NA-C1A	-5.67	104.16	106.71
33	C	507	CLA	C4A-NA-C1A	-5.66	104.16	106.71
33	a	405	CLA	C4A-NA-C1A	-5.66	104.16	106.71
33	A	405	CLA	C1D-ND-C4D	-5.65	102.32	106.33
33	n	305	CLA	C4A-NA-C1A	-5.64	104.17	106.71
33	4	307	CLA	C4A-NA-C1A	-5.63	104.17	106.71
33	D	405	CLA	C4A-NA-C1A	-5.63	104.18	106.71
33	1	303	CLA	C4A-NA-C1A	-5.62	104.18	106.71
33	0	310	CLA	C1D-ND-C4D	-5.61	102.35	106.33
33	b	602	CLA	C4A-NA-C1A	-5.60	104.19	106.71
33	7	308	CLA	C4A-NA-C1A	-5.59	104.19	106.71
33	B	602	CLA	C4A-NA-C1A	-5.59	104.19	106.71
33	4	309	CLA	C1D-ND-C4D	-5.58	102.37	106.33
33	6	313	CLA	C1D-ND-C4D	-5.58	102.37	106.33
33	p	313	CLA	C1D-ND-C4D	-5.58	102.37	106.33
33	1	308	CLA	C4A-NA-C1A	-5.55	104.21	106.71
33	1	309	CLA	C4A-NA-C1A	-5.54	104.21	106.71
33	0	306	CLA	C1D-ND-C4D	-5.54	102.40	106.33
33	9	305	CLA	C4A-NA-C1A	-5.53	104.22	106.71
33	b	608	CLA	C4A-NA-C1A	-5.53	104.22	106.71
33	p	304	CLA	C4A-NA-C1A	-5.53	104.22	106.71
31	a	403	BCT	O2-C-O1	5.53	133.90	119.55
31	A	403	BCT	O2-C-O1	5.53	133.88	119.55
44	F	101	HEM	CHC-C4B-NB	5.52	130.41	124.42
33	4	306	CLA	C1D-ND-C4D	-5.51	102.42	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	6	304	CLA	C4A-NA-C1A	-5.51	104.23	106.71
33	d	405	CLA	C4A-NA-C1A	-5.51	104.23	106.71
33	3	305	CLA	C4A-NA-C1A	-5.49	104.24	106.71
33	7	309	CLA	C4A-NA-C1A	-5.48	104.24	106.71
33	p	306	CLA	C4A-NA-C1A	-5.47	104.25	106.71
33	B	608	CLA	C4A-NA-C1A	-5.47	104.25	106.71
33	6	302	CLA	C1D-ND-C4D	-5.46	102.45	106.33
33	6	306	CLA	C4A-NA-C1A	-5.46	104.25	106.71
33	p	302	CLA	C1D-ND-C4D	-5.44	102.47	106.33
33	0	302	CLA	CHD-C1D-ND	-5.44	119.46	124.45
33	p	305	CLA	C1D-ND-C4D	-5.43	102.48	106.33
33	4	302	CLA	CHD-C1D-ND	-5.43	119.46	124.45
33	p	310	CLA	C1D-ND-C4D	-5.42	102.48	106.33
33	p	319	CLA	C1D-ND-C4D	-5.42	102.48	106.33
33	6	305	CLA	C1D-ND-C4D	-5.42	102.49	106.33
33	N	305	CLA	C4A-NA-C1A	-5.41	104.27	106.71
33	N	303	CLA	CMA-C3A-C4A	-5.40	97.25	111.77
33	6	310	CLA	C1D-ND-C4D	-5.39	102.50	106.33
33	b	607	CLA	C4A-NA-C1A	-5.39	104.28	106.71
33	0	308	CLA	CMA-C3A-C4A	-5.39	97.28	111.77
33	6	319	CLA	C1D-ND-C4D	-5.38	102.51	106.33
33	n	306	CLA	C4A-NA-C1A	-5.37	104.29	106.71
33	n	304	CLA	C4A-NA-C1A	-5.35	104.30	106.71
33	B	607	CLA	C4A-NA-C1A	-5.35	104.30	106.71
33	N	307	CLA	C4A-NA-C1A	-5.32	104.31	106.71
33	p	303	CLA	CHD-C1D-ND	-5.28	119.61	124.45
33	0	310	CLA	CHD-C1D-ND	-5.25	119.63	124.45
33	6	303	CLA	CHD-C1D-ND	-5.25	119.63	124.45
38	p	311	KC2	C4D-C3D-CAD	5.25	110.96	107.42
33	4	309	CLA	CHD-C1D-ND	-5.25	119.63	124.45
33	9	313	CLA	C4A-NA-C1A	-5.24	104.35	106.71
38	6	311	KC2	C4D-C3D-CAD	5.22	110.94	107.42
38	0	305	KC2	C4D-C3D-CAD	5.22	110.94	107.42
33	C	505	CLA	C4A-NA-C1A	-5.22	104.36	106.71
38	4	305	KC2	C4D-C3D-CAD	5.21	110.93	107.42
33	6	307	CLA	CHD-C1D-ND	-5.21	119.67	124.45
33	c	505	CLA	C4A-NA-C1A	-5.20	104.37	106.71
33	p	307	CLA	CHD-C1D-ND	-5.19	119.68	124.45
33	N	303	CLA	C4A-NA-C1A	-5.19	104.37	106.71
33	0	308	CLA	C4A-NA-C1A	-5.18	104.38	106.71
39	5	314	II0	C03-C09-C13	-5.18	115.32	122.63
39	g	314	II0	C03-C09-C13	-5.16	115.35	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	307	CLA	CHD-C1D-ND	-5.15	119.72	124.45
33	B	617	CLA	C4A-NA-C1A	-5.13	104.40	106.71
33	B	607	CLA	CHD-C1D-ND	-5.13	119.74	124.45
33	0	307	CLA	CHD-C1D-ND	-5.12	119.75	124.45
33	C	514	CLA	C4A-NA-C1A	-5.12	104.40	106.71
33	b	607	CLA	CHD-C1D-ND	-5.12	119.75	124.45
33	3	313	CLA	C4A-NA-C1A	-5.12	104.41	106.71
33	A	412	CLA	C4A-NA-C1A	-5.11	104.41	106.71
33	7	302	CLA	CHD-C1D-ND	-5.11	119.76	124.45
33	c	509	CLA	C4A-NA-C1A	-5.11	104.41	106.71
33	a	406	CLA	CHD-C1D-ND	-5.11	119.76	124.45
33	C	509	CLA	C4A-NA-C1A	-5.10	104.41	106.71
33	1	302	CLA	CHD-C1D-ND	-5.10	119.77	124.45
33	B	618	CLA	CHD-C1D-ND	-5.10	119.77	124.45
33	c	514	CLA	C4A-NA-C1A	-5.10	104.41	106.71
33	b	617	CLA	C4A-NA-C1A	-5.09	104.42	106.71
33	2	310	CLA	CHD-C1D-ND	-5.08	119.78	124.45
33	A	406	CLA	CHD-C1D-ND	-5.08	119.78	124.45
33	5	307	CLA	CHD-C1D-ND	-5.08	119.78	124.45
33	9	306	CLA	CHD-C1D-ND	-5.08	119.79	124.45
33	4	301	CLA	CHD-C1D-ND	-5.08	119.79	124.45
33	p	308	CLA	CHD-C1D-ND	-5.08	119.79	124.45
33	n	302	CLA	CHD-C1D-ND	-5.07	119.79	124.45
33	6	308	CLA	CHD-C1D-ND	-5.07	119.80	124.45
33	a	412	CLA	C4A-NA-C1A	-5.07	104.43	106.71
33	2	302	CLA	CHD-C1D-ND	-5.05	119.81	124.45
33	N	302	CLA	CHD-C1D-ND	-5.05	119.81	124.45
33	8	310	CLA	CHD-C1D-ND	-5.05	119.82	124.45
33	g	307	CLA	CHD-C1D-ND	-5.04	119.82	124.45
33	0	301	CLA	CHD-C1D-ND	-5.03	119.83	124.45
33	3	306	CLA	CHD-C1D-ND	-5.03	119.83	124.45
33	5	305	CLA	CHD-C1D-ND	-5.02	119.84	124.45
33	8	302	CLA	CHD-C1D-ND	-5.02	119.84	124.45
33	3	303	CLA	CHD-C1D-ND	-5.02	119.84	124.45
33	b	616	CLA	C4A-NA-C1A	-5.02	104.45	106.71
33	4	306	CLA	C4A-NA-C1A	-5.01	104.45	106.71
33	b	618	CLA	CHD-C1D-ND	-5.01	119.85	124.45
33	C	502	CLA	C4A-NA-C1A	-5.00	104.46	106.71
33	g	305	CLA	CHD-C1D-ND	-5.00	119.86	124.45
33	N	307	CLA	CHD-C1D-ND	-5.00	119.86	124.45
33	g	317	CLA	CHD-C1D-ND	-4.99	119.86	124.45
33	0	306	CLA	C4A-NA-C1A	-4.99	104.46	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	0	311	CLA	CHD-C1D-ND	-4.98	119.87	124.45
33	9	303	CLA	CHD-C1D-ND	-4.98	119.88	124.45
33	c	502	CLA	C4A-NA-C1A	-4.98	104.47	106.71
33	8	303	CLA	CHD-C1D-ND	-4.98	119.88	124.45
33	6	306	CLA	CHD-C1D-ND	-4.98	119.88	124.45
33	n	306	CLA	CHD-C1D-ND	-4.97	119.89	124.45
33	p	319	CLA	CHD-C1D-ND	-4.97	119.89	124.45
33	B	606	CLA	CHD-C1D-ND	-4.97	119.89	124.45
33	5	317	CLA	CHD-C1D-ND	-4.97	119.89	124.45
33	4	310	CLA	CHD-C1D-ND	-4.96	119.89	124.45
33	p	309	CLA	CHD-C1D-ND	-4.96	119.89	124.45
33	2	303	CLA	CHD-C1D-ND	-4.96	119.90	124.45
33	B	616	CLA	C4A-NA-C1A	-4.96	104.48	106.71
33	6	319	CLA	CHD-C1D-ND	-4.95	119.90	124.45
33	6	309	CLA	CHD-C1D-ND	-4.95	119.90	124.45
33	p	306	CLA	CHD-C1D-ND	-4.94	119.92	124.45
33	8	304	CLA	CHD-C1D-ND	-4.93	119.92	124.45
33	b	606	CLA	CHD-C1D-ND	-4.92	119.93	124.45
33	g	303	CLA	CHD-C1D-ND	-4.92	119.93	124.45
33	5	303	CLA	CHD-C1D-ND	-4.92	119.94	124.45
38	1	310	KC2	C4D-C3D-CAD	4.91	110.73	107.42
33	8	308	CLA	C4A-NA-C1A	-4.91	104.50	106.71
33	2	304	CLA	CHD-C1D-ND	-4.91	119.94	124.45
33	0	304	CLA	CHD-C1D-ND	-4.90	119.95	124.45
33	6	313	CLA	CHD-C1D-ND	-4.90	119.95	124.45
33	C	506	CLA	C4A-NA-C1A	-4.90	104.50	106.71
33	9	315	CLA	C4A-NA-C1A	-4.89	104.51	106.71
33	c	506	CLA	C4A-NA-C1A	-4.89	104.51	106.71
33	4	306	CLA	CHD-C1D-ND	-4.89	119.96	124.45
38	7	310	KC2	C4D-C3D-CAD	4.89	110.72	107.42
33	p	313	CLA	CHD-C1D-ND	-4.88	119.97	124.45
33	4	304	CLA	CHD-C1D-ND	-4.88	119.97	124.45
33	0	306	CLA	CHD-C1D-ND	-4.87	119.98	124.45
33	9	309	CLA	CHD-C1D-ND	-4.87	119.98	124.45
33	c	507	CLA	CHD-C1D-ND	-4.87	119.98	124.45
33	a	405	CLA	CHD-C1D-ND	-4.87	119.98	124.45
33	3	309	CLA	CHD-C1D-ND	-4.87	119.98	124.45
33	c	504	CLA	C4A-NA-C1A	-4.87	104.52	106.71
33	9	312	CLA	CHD-C1D-ND	-4.86	119.99	124.45
33	A	405	CLA	CHD-C1D-ND	-4.86	119.99	124.45
33	7	305	CLA	C4A-NA-C1A	-4.84	104.53	106.71
33	1	305	CLA	C4A-NA-C1A	-4.84	104.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	3	312	CLA	CHD-C1D-ND	-4.83	120.01	124.45
33	8	306	CLA	CHD-C1D-ND	-4.83	120.01	124.45
33	1	304	CLA	CHD-C1D-ND	-4.83	120.02	124.45
33	2	308	CLA	C4A-NA-C1A	-4.83	104.53	106.71
33	7	304	CLA	CHD-C1D-ND	-4.82	120.02	124.45
33	5	307	CLA	C4A-NA-C1A	-4.82	104.54	106.71
33	B	605	CLA	C4A-NA-C1A	-4.82	104.54	106.71
33	g	307	CLA	C4A-NA-C1A	-4.81	104.54	106.71
33	C	504	CLA	C4A-NA-C1A	-4.81	104.54	106.71
38	9	311	KC2	C4D-C3D-CAD	4.81	110.66	107.42
33	N	304	CLA	CHD-C1D-ND	-4.81	120.03	124.45
33	3	315	CLA	C4A-NA-C1A	-4.81	104.55	106.71
33	n	303	CLA	CHD-C1D-ND	-4.80	120.04	124.45
33	b	615	CLA	CHD-C1D-ND	-4.79	120.05	124.45
38	3	311	KC2	C4D-C3D-CAD	4.79	110.65	107.42
33	C	507	CLA	CHD-C1D-ND	-4.77	120.07	124.45
33	5	302	CLA	CHD-C1D-ND	-4.77	120.07	124.45
33	b	605	CLA	C4A-NA-C1A	-4.77	104.56	106.71
33	N	301	CLA	CHD-C1D-ND	-4.77	120.07	124.45
33	2	306	CLA	CHD-C1D-ND	-4.77	120.07	124.45
33	7	307	CLA	CHD-C1D-ND	-4.77	120.07	124.45
33	p	312	CLA	CHD-C1D-ND	-4.77	120.07	124.45
33	6	310	CLA	CHD-C1D-ND	-4.75	120.08	124.45
33	n	301	CLA	CHD-C1D-ND	-4.75	120.09	124.45
33	p	310	CLA	CHD-C1D-ND	-4.75	120.09	124.45
38	5	309	KC2	C4D-C3D-CAD	4.75	110.62	107.42
38	g	309	KC2	C4D-C3D-CAD	4.75	110.62	107.42
33	c	505	CLA	CHD-C1D-ND	-4.75	120.09	124.45
33	g	302	CLA	CHD-C1D-ND	-4.75	120.09	124.45
33	g	311	CLA	CHD-C1D-ND	-4.75	120.09	124.45
33	B	615	CLA	CHD-C1D-ND	-4.74	120.09	124.45
33	C	505	CLA	CHD-C1D-ND	-4.74	120.10	124.45
33	5	311	CLA	CHD-C1D-ND	-4.74	120.10	124.45
33	6	312	CLA	CHD-C1D-ND	-4.74	120.10	124.45
33	1	307	CLA	CHD-C1D-ND	-4.73	120.10	124.45
33	8	301	CLA	CHD-C1D-ND	-4.72	120.11	124.45
33	2	301	CLA	CHD-C1D-ND	-4.71	120.12	124.45
33	A	408	CLA	CHD-C1D-ND	-4.71	120.12	124.45
33	C	512	CLA	CHD-C1D-ND	-4.71	120.13	124.45
33	b	603	CLA	CHD-C1D-ND	-4.71	120.13	124.45
33	C	508	CLA	C4A-NA-C1A	-4.70	104.59	106.71
33	c	512	CLA	CHD-C1D-ND	-4.70	120.14	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	9	308	CLA	CHD-C1D-ND	-4.70	120.14	124.45
33	B	614	CLA	CHD-C1D-ND	-4.70	120.14	124.45
33	3	308	CLA	CHD-C1D-ND	-4.69	120.14	124.45
33	c	510	CLA	CHD-C1D-ND	-4.69	120.14	124.45
33	a	408	CLA	CHD-C1D-ND	-4.69	120.14	124.45
33	6	305	CLA	C4A-NA-C1A	-4.69	104.60	106.71
33	C	510	CLA	CHD-C1D-ND	-4.68	120.15	124.45
33	6	304	CLA	CHD-C1D-ND	-4.67	120.16	124.45
33	1	306	CLA	CHD-C1D-ND	-4.67	120.16	124.45
33	7	306	CLA	CHD-C1D-ND	-4.67	120.16	124.45
33	p	304	CLA	CHD-C1D-ND	-4.67	120.16	124.45
33	p	305	CLA	C4A-NA-C1A	-4.67	104.61	106.71
33	D	404	CLA	CHD-C1D-ND	-4.67	120.16	124.45
33	5	304	CLA	CHD-C1D-ND	-4.66	120.17	124.45
33	c	508	CLA	C4A-NA-C1A	-4.66	104.61	106.71
33	B	609	CLA	CHD-C1D-ND	-4.66	120.17	124.45
33	d	404	CLA	CHD-C1D-ND	-4.66	120.17	124.45
33	B	603	CLA	CHD-C1D-ND	-4.65	120.19	124.45
33	C	502	CLA	CHD-C1D-ND	-4.64	120.19	124.45
33	B	611	CLA	CHD-C1D-ND	-4.63	120.20	124.45
33	b	614	CLA	CHD-C1D-ND	-4.63	120.20	124.45
33	b	609	CLA	CHD-C1D-ND	-4.63	120.20	124.45
33	b	602	CLA	CHD-C1D-ND	-4.63	120.20	124.45
33	c	504	CLA	CHD-C1D-ND	-4.62	120.20	124.45
33	2	305	CLA	CHD-C1D-ND	-4.62	120.21	124.45
33	8	305	CLA	CHD-C1D-ND	-4.62	120.21	124.45
33	1	301	CLA	CHD-C1D-ND	-4.62	120.21	124.45
33	3	307	CLA	CHD-C1D-ND	-4.62	120.21	124.45
33	B	602	CLA	CHD-C1D-ND	-4.62	120.21	124.45
33	b	611	CLA	CHD-C1D-ND	-4.61	120.21	124.45
33	9	314	CLA	CHD-C1D-ND	-4.61	120.22	124.45
33	C	504	CLA	CHD-C1D-ND	-4.61	120.22	124.45
33	4	303	CLA	CHD-C1D-ND	-4.61	120.22	124.45
33	5	310	CLA	CHD-C1D-ND	-4.61	120.22	124.45
33	0	303	CLA	CHD-C1D-ND	-4.61	120.22	124.45
33	b	608	CLA	CHD-C1D-ND	-4.61	120.22	124.45
33	p	305	CLA	CHD-C1D-ND	-4.61	120.22	124.45
33	g	310	CLA	CHD-C1D-ND	-4.60	120.22	124.45
33	3	314	CLA	CHD-C1D-ND	-4.60	120.23	124.45
33	5	308	CLA	CHD-C1D-ND	-4.60	120.23	124.45
33	B	608	CLA	CHD-C1D-ND	-4.60	120.23	124.45
33	d	405	CLA	CHD-C1D-ND	-4.60	120.23	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	1	308	CLA	CHD-C1D-ND	-4.59	120.23	124.45
33	g	304	CLA	CHD-C1D-ND	-4.59	120.23	124.45
33	D	405	CLA	CHD-C1D-ND	-4.59	120.24	124.45
33	7	301	CLA	CHD-C1D-ND	-4.58	120.24	124.45
33	6	305	CLA	CHD-C1D-ND	-4.58	120.24	124.45
33	c	502	CLA	CHD-C1D-ND	-4.58	120.24	124.45
33	9	307	CLA	CHD-C1D-ND	-4.58	120.25	124.45
33	g	308	CLA	CHD-C1D-ND	-4.58	120.25	124.45
33	6	312	CLA	C4A-NA-C1A	-4.57	104.65	106.71
33	1	305	CLA	CHD-C1D-ND	-4.56	120.26	124.45
33	7	305	CLA	CHD-C1D-ND	-4.56	120.27	124.45
33	B	612	CLA	CHD-C1D-ND	-4.55	120.27	124.45
33	g	306	CLA	CHD-C1D-ND	-4.55	120.27	124.45
33	7	308	CLA	CHD-C1D-ND	-4.54	120.28	124.45
33	3	304	CLA	CHD-C1D-ND	-4.54	120.28	124.45
33	5	306	CLA	CHD-C1D-ND	-4.54	120.28	124.45
33	N	305	CLA	CHD-C1D-ND	-4.53	120.29	124.45
33	3	305	CLA	CHD-C1D-ND	-4.53	120.30	124.45
33	b	612	CLA	CHD-C1D-ND	-4.52	120.30	124.45
33	9	315	CLA	CHD-C1D-ND	-4.52	120.30	124.45
33	9	304	CLA	CHD-C1D-ND	-4.52	120.30	124.45
33	1	303	CLA	CHD-C1D-ND	-4.50	120.32	124.45
33	n	304	CLA	CHD-C1D-ND	-4.49	120.32	124.45
33	p	312	CLA	C4A-NA-C1A	-4.49	104.69	106.71
33	7	303	CLA	CHD-C1D-ND	-4.49	120.33	124.45
33	c	506	CLA	CHD-C1D-ND	-4.49	120.33	124.45
33	6	302	CLA	CHD-C1D-ND	-4.49	120.33	124.45
33	9	305	CLA	CHD-C1D-ND	-4.49	120.33	124.45
33	0	309	CLA	CHD-C1D-ND	-4.49	120.33	124.45
38	2	309	KC2	C4D-C3D-CAD	4.48	110.44	107.42
33	4	308	CLA	CHD-C1D-ND	-4.48	120.34	124.45
33	3	315	CLA	CHD-C1D-ND	-4.48	120.34	124.45
38	8	309	KC2	C4D-C3D-CAD	4.46	110.43	107.42
33	p	302	CLA	CHD-C1D-ND	-4.46	120.36	124.45
33	B	617	CLA	CHD-C1D-ND	-4.44	120.38	124.45
33	C	506	CLA	CHD-C1D-ND	-4.44	120.38	124.45
33	C	513	CLA	CHD-C1D-ND	-4.44	120.38	124.45
33	3	313	CLA	CHD-C1D-ND	-4.43	120.38	124.45
33	c	514	CLA	CHD-C1D-ND	-4.42	120.39	124.45
33	b	617	CLA	CHD-C1D-ND	-4.42	120.39	124.45
33	C	514	CLA	CHD-C1D-ND	-4.42	120.39	124.45
33	N	306	CLA	CHD-C1D-ND	-4.42	120.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	c	509	CLA	CHD-C1D-ND	-4.42	120.39	124.45
38	0	305	KC2	C1D-ND-C4D	4.41	109.47	106.33
33	n	305	CLA	CHD-C1D-ND	-4.41	120.40	124.45
33	b	604	CLA	CHD-C1D-ND	-4.41	120.40	124.45
33	2	307	CLA	CHD-C1D-ND	-4.41	120.40	124.45
33	C	509	CLA	CHD-C1D-ND	-4.41	120.41	124.45
33	9	313	CLA	CHD-C1D-ND	-4.39	120.42	124.45
33	B	604	CLA	CHD-C1D-ND	-4.39	120.42	124.45
33	b	610	CLA	CHD-C1D-ND	-4.39	120.42	124.45
33	c	513	CLA	CHD-C1D-ND	-4.39	120.42	124.45
33	8	307	CLA	CHD-C1D-ND	-4.37	120.44	124.45
38	4	305	KC2	C1D-ND-C4D	4.36	109.44	106.33
33	5	301	CLA	CHD-C1D-ND	-4.36	120.45	124.45
38	6	311	KC2	C1D-ND-C4D	4.36	109.43	106.33
33	c	511	CLA	CHD-C1D-ND	-4.36	120.45	124.45
33	3	310	CLA	CHD-C1D-ND	-4.35	120.45	124.45
33	9	310	CLA	CHD-C1D-ND	-4.35	120.45	124.45
33	4	308	CLA	C4A-NA-C1A	-4.35	104.75	106.71
33	B	610	CLA	CHD-C1D-ND	-4.35	120.46	124.45
33	g	301	CLA	CHD-C1D-ND	-4.34	120.46	124.45
41	j	101	SQD	O7-S-C6	4.32	112.08	106.94
33	C	511	CLA	CHD-C1D-ND	-4.32	120.48	124.45
33	0	309	CLA	C4A-NA-C1A	-4.31	104.77	106.71
33	b	614	CLA	CHB-C1B-NB	-4.30	119.70	124.26
33	B	613	CLA	CHD-C1D-ND	-4.29	120.51	124.45
44	F	101	HEM	CHD-C1D-ND	4.29	129.08	124.42
41	J	101	SQD	O7-S-C6	4.28	112.03	106.94
36	D	407	PL9	C7-C8-C9	-4.28	119.67	126.79
33	1	309	CLA	CHD-C1D-ND	-4.28	120.52	124.45
33	b	613	CLA	CHD-C1D-ND	-4.28	120.53	124.45
37	b	623	LHG	O4-P-O5	4.27	133.37	112.24
37	B	623	LHG	O4-P-O5	4.27	133.35	112.24
38	p	311	KC2	C1D-ND-C4D	4.27	109.37	106.33
38	7	311	KC2	C4D-C3D-CAD	4.27	110.30	107.42
33	c	503	CLA	CHD-C1D-ND	-4.27	120.53	124.45
36	d	407	PL9	C7-C8-C9	-4.26	119.69	126.79
38	1	311	KC2	C4D-C3D-CAD	4.26	110.29	107.42
33	B	616	CLA	CHD-C1D-ND	-4.25	120.55	124.45
33	b	616	CLA	CHD-C1D-ND	-4.24	120.55	124.45
33	B	614	CLA	CHB-C1B-NB	-4.24	119.76	124.26
33	C	503	CLA	CHD-C1D-ND	-4.23	120.57	124.45
33	7	309	CLA	CHD-C1D-ND	-4.22	120.57	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	d	401	LHG	O4-P-O5	4.22	133.11	112.24
33	2	308	CLA	CHD-C1D-ND	-4.22	120.58	124.45
37	D	401	LHG	O4-P-O5	4.22	133.10	112.24
37	8	315	LHG	O4-P-O5	4.21	133.05	112.24
33	8	308	CLA	CHD-C1D-ND	-4.21	120.59	124.45
37	2	315	LHG	O4-P-O5	4.21	133.03	112.24
37	D	408	LHG	O4-P-O5	4.21	133.03	112.24
37	d	408	LHG	O4-P-O5	4.20	133.01	112.24
37	A	411	LHG	O4-P-O5	4.20	133.00	112.24
37	a	411	LHG	O4-P-O5	4.20	133.00	112.24
37	0	317	LHG	O4-P-O5	4.18	132.92	112.24
37	4	316	LHG	O4-P-O5	4.18	132.90	112.24
37	9	321	LHG	O4-P-O5	4.18	132.89	112.24
37	3	302	LHG	O4-P-O5	4.18	132.88	112.24
37	d	402	LHG	O4-P-O5	4.18	132.88	112.24
37	9	302	LHG	O4-P-O5	4.17	132.88	112.24
37	D	402	LHG	O4-P-O5	4.17	132.87	112.24
37	3	321	LHG	O4-P-O5	4.17	132.85	112.24
37	7	317	LHG	O4-P-O5	4.16	132.80	112.24
33	0	308	CLA	CHB-C1B-NB	-4.16	119.86	124.26
37	1	317	LHG	O4-P-O5	4.16	132.79	112.24
33	N	303	CLA	CHB-C1B-NB	-4.16	119.86	124.26
37	9	322	LHG	O4-P-O5	4.15	132.74	112.24
37	3	322	LHG	O4-P-O5	4.14	132.70	112.24
37	5	316	LHG	O4-P-O5	4.13	132.67	112.24
37	g	316	LHG	O4-P-O5	4.13	132.67	112.24
38	5	309	KC2	C1D-ND-C4D	4.09	109.24	106.33
43	C	518	DGD	O3G-C3G-C2G	-4.09	101.03	110.90
43	c	518	DGD	O3G-C3G-C2G	-4.09	101.04	110.90
38	g	309	KC2	C1D-ND-C4D	4.08	109.23	106.33
33	c	508	CLA	CHD-C1D-ND	-4.08	120.70	124.45
33	C	508	CLA	CHD-C1D-ND	-4.05	120.73	124.45
33	B	615	CLA	CHB-C1B-NB	-4.04	119.98	124.26
33	b	615	CLA	CHB-C1B-NB	-4.02	120.00	124.26
33	a	412	CLA	CHB-C1B-NB	-4.01	120.01	124.26
33	b	605	CLA	CHD-C1D-ND	-3.99	120.78	124.45
33	0	301	CLA	CHB-C1B-NB	-3.98	120.04	124.26
33	4	301	CLA	CHB-C1B-NB	-3.97	120.05	124.26
33	A	412	CLA	CHB-C1B-NB	-3.96	120.06	124.26
33	c	510	CLA	CHB-C1B-NB	-3.96	120.07	124.26
39	g	314	II0	C05-C07-C11	3.95	115.72	110.30
33	B	605	CLA	CHD-C1D-ND	-3.95	120.83	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	B	610	CLA	CHB-C1B-NB	-3.95	120.08	124.26
39	5	314	II0	C05-C07-C11	3.94	115.70	110.30
33	a	405	CLA	CHB-C1B-NB	-3.94	120.08	124.26
33	c	511	CLA	CHB-C1B-NB	-3.94	120.08	124.26
33	6	310	CLA	CHB-C1B-NB	-3.93	120.10	124.26
33	b	610	CLA	CHB-C1B-NB	-3.92	120.10	124.26
33	A	405	CLA	CHB-C1B-NB	-3.92	120.11	124.26
39	p	314	II0	C04-C10-C14	-3.92	117.10	122.63
39	6	314	II0	C04-C10-C14	-3.92	117.10	122.63
33	p	310	CLA	CHB-C1B-NB	-3.91	120.12	124.26
33	C	512	CLA	C4A-NA-C1A	-3.91	104.95	106.71
33	C	511	CLA	CHB-C1B-NB	-3.91	120.12	124.26
33	C	514	CLA	CHB-C1B-NB	-3.91	120.12	124.26
33	c	514	CLA	CHB-C1B-NB	-3.90	120.13	124.26
33	c	512	CLA	C4A-NA-C1A	-3.89	104.96	106.71
33	C	510	CLA	CHB-C1B-NB	-3.88	120.14	124.26
33	b	618	CLA	CHB-C1B-NB	-3.88	120.14	124.26
33	b	606	CLA	CHB-C1B-NB	-3.88	120.15	124.26
33	B	606	CLA	CHB-C1B-NB	-3.87	120.16	124.26
33	b	603	CLA	CHB-C1B-NB	-3.87	120.16	124.26
38	7	310	KC2	C1D-ND-C4D	3.86	109.08	106.33
33	A	412	CLA	C1-C2-C3	-3.85	119.38	126.04
33	A	408	CLA	CHB-C1B-NB	-3.85	120.18	124.26
33	B	603	CLA	CHB-C1B-NB	-3.84	120.19	124.26
33	a	408	CLA	CHB-C1B-NB	-3.84	120.19	124.26
33	4	306	CLA	CHB-C1B-NB	-3.84	120.19	124.26
33	0	306	CLA	CHB-C1B-NB	-3.84	120.19	124.26
33	a	412	CLA	C1-C2-C3	-3.83	119.43	126.04
33	g	317	CLA	CHB-C1B-NB	-3.83	120.21	124.26
33	5	317	CLA	CHB-C1B-NB	-3.82	120.21	124.26
33	C	507	CLA	CHB-C1B-NB	-3.82	120.21	124.26
33	B	618	CLA	CHB-C1B-NB	-3.81	120.22	124.26
33	g	306	CLA	CHB-C1B-NB	-3.81	120.22	124.26
33	7	305	CLA	CHB-C1B-NB	-3.80	120.23	124.26
33	1	305	CLA	CHB-C1B-NB	-3.79	120.24	124.26
33	c	507	CLA	CHB-C1B-NB	-3.79	120.25	124.26
33	b	611	CLA	CHB-C1B-NB	-3.79	120.25	124.26
33	5	306	CLA	CHB-C1B-NB	-3.79	120.25	124.26
44	F	101	HEM	C1B-NB-C4B	3.78	108.97	105.07
38	1	310	KC2	C1D-ND-C4D	3.78	109.02	106.33
33	g	303	CLA	CHC-C4B-NB	-3.77	120.26	124.26
33	n	306	CLA	CHB-C1B-NB	-3.77	120.26	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	5	303	CLA	CHC-C4B-NB	-3.77	120.27	124.26
33	N	307	CLA	CHB-C1B-NB	-3.76	120.27	124.26
33	7	306	CLA	CHB-C1B-NB	-3.76	120.28	124.26
41	l	101	SQD	O47-C7-C8	3.76	119.60	111.50
33	B	611	CLA	CHB-C1B-NB	-3.76	120.28	124.26
33	9	308	CLA	CHB-C1B-NB	-3.76	120.28	124.26
33	b	604	CLA	CHB-C1B-NB	-3.75	120.28	124.26
41	L	101	SQD	O47-C7-C8	3.75	119.59	111.50
33	B	604	CLA	CHB-C1B-NB	-3.75	120.29	124.26
33	1	306	CLA	CHB-C1B-NB	-3.74	120.29	124.26
33	6	304	CLA	CHB-C1B-NB	-3.74	120.30	124.26
33	3	308	CLA	CHB-C1B-NB	-3.73	120.30	124.26
33	n	305	CLA	CHB-C1B-NB	-3.73	120.31	124.26
33	g	302	CLA	CHB-C1B-NB	-3.73	120.31	124.26
33	5	302	CLA	CHB-C1B-NB	-3.72	120.32	124.26
33	6	306	CLA	CHB-C1B-NB	-3.72	120.32	124.26
33	n	304	CLA	CHB-C1B-NB	-3.71	120.33	124.26
34	A	407	PHO	C1-O2A-CGA	3.71	126.18	116.44
35	d	406	8CT	C30-C31-C32	-3.71	116.90	121.47
33	C	508	CLA	CHB-C1B-NB	-3.71	120.33	124.26
34	a	407	PHO	C1-O2A-CGA	3.71	126.18	116.44
44	F	101	HEM	CHA-C4D-ND	3.71	128.94	124.37
33	4	308	CLA	CHB-C1B-NB	-3.70	120.33	124.26
33	p	306	CLA	CHB-C1B-NB	-3.70	120.33	124.26
33	0	309	CLA	CHB-C1B-NB	-3.70	120.34	124.26
33	N	306	CLA	CHB-C1B-NB	-3.70	120.34	124.26
33	p	319	CLA	CHB-C1B-NB	-3.70	120.34	124.26
41	c	501	SQD	O47-C7-C8	3.70	119.47	111.50
33	N	305	CLA	CHB-C1B-NB	-3.70	120.34	124.26
41	C	501	SQD	O47-C7-C8	3.70	119.47	111.50
33	b	613	CLA	CHB-C1B-NB	-3.70	120.34	124.26
35	D	406	8CT	C30-C31-C32	-3.70	116.92	121.47
33	p	304	CLA	CHB-C1B-NB	-3.69	120.35	124.26
43	C	519	DGD	O3G-C3G-C2G	-3.69	102.00	110.90
33	N	304	CLA	CHB-C1B-NB	-3.69	120.35	124.26
33	c	508	CLA	CHB-C1B-NB	-3.69	120.35	124.26
33	6	319	CLA	CHB-C1B-NB	-3.69	120.35	124.26
43	c	519	DGD	O3G-C3G-C2G	-3.68	102.01	110.90
33	4	304	CLA	CHB-C1B-NB	-3.68	120.36	124.26
33	B	613	CLA	CHB-C1B-NB	-3.68	120.36	124.26
33	6	312	CLA	CHB-C1B-NB	-3.67	120.37	124.26
33	0	304	CLA	CHB-C1B-NB	-3.67	120.37	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	c	505	CLA	CHB-C1B-NB	-3.67	120.37	124.26
33	C	505	CLA	CHB-C1B-NB	-3.67	120.38	124.26
33	p	312	CLA	CHB-C1B-NB	-3.66	120.38	124.26
38	1	310	KC2	CHD-C1D-ND	-3.66	120.38	124.26
33	n	303	CLA	CHB-C1B-NB	-3.66	120.39	124.26
38	8	309	KC2	C1D-ND-C4D	3.65	108.93	106.33
33	8	306	CLA	CHB-C1B-NB	-3.65	120.39	124.26
38	0	305	KC2	CHD-C1D-ND	-3.65	120.39	124.26
38	4	305	KC2	CHD-C1D-ND	-3.64	120.41	124.26
33	9	309	CLA	CHB-C1B-NB	-3.63	120.41	124.26
33	B	618	CLA	CBD-CHA-C1A	3.63	132.78	128.50
38	7	310	KC2	CHD-C1D-ND	-3.63	120.41	124.26
33	7	303	CLA	CHB-C1B-NB	-3.63	120.41	124.26
33	2	306	CLA	CHB-C1B-NB	-3.63	120.42	124.26
33	9	304	CLA	CHB-C1B-NB	-3.63	120.42	124.26
44	F	101	HEM	CHB-C1B-NB	3.62	128.84	124.37
33	3	304	CLA	CHB-C1B-NB	-3.62	120.42	124.26
33	6	307	CLA	CHB-C1B-NB	-3.62	120.42	124.26
38	2	309	KC2	C1D-ND-C4D	3.62	108.91	106.33
33	B	605	CLA	CHB-C1B-NB	-3.62	120.43	124.26
33	b	605	CLA	CHB-C1B-NB	-3.62	120.43	124.26
33	7	308	CLA	CHB-C1B-NB	-3.61	120.43	124.26
33	2	308	CLA	CHB-C1B-NB	-3.61	120.44	124.26
33	8	301	CLA	CHB-C1B-NB	-3.61	120.44	124.26
33	9	314	CLA	CHB-C1B-NB	-3.60	120.44	124.26
33	1	308	CLA	CHB-C1B-NB	-3.60	120.45	124.26
33	p	305	CLA	CHB-C1B-NB	-3.60	120.45	124.26
33	8	307	CLA	CHB-C1B-NB	-3.60	120.45	124.26
33	g	308	CLA	CHB-C1B-NB	-3.60	120.45	124.26
33	3	309	CLA	CHB-C1B-NB	-3.59	120.45	124.26
38	9	311	KC2	CHD-C1D-ND	-3.59	120.45	124.26
33	8	308	CLA	CHB-C1B-NB	-3.59	120.46	124.26
33	b	617	CLA	CHB-C1B-NB	-3.59	120.46	124.26
33	0	311	CLA	CHB-C1B-NB	-3.59	120.46	124.26
38	3	311	KC2	CHD-C1D-ND	-3.59	120.46	124.26
33	p	307	CLA	CHB-C1B-NB	-3.58	120.46	124.26
33	B	617	CLA	CHB-C1B-NB	-3.58	120.47	124.26
33	6	305	CLA	CHB-C1B-NB	-3.58	120.47	124.26
33	4	310	CLA	CHB-C1B-NB	-3.57	120.47	124.26
33	5	310	CLA	CHB-C1B-NB	-3.57	120.48	124.26
33	C	513	CLA	CHB-C1B-NB	-3.57	120.48	124.26
33	b	618	CLA	CBD-CHA-C1A	3.57	132.70	128.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	5	308	CLA	CHB-C1B-NB	-3.56	120.48	124.26
38	1	311	KC2	C1D-ND-C4D	3.56	108.87	106.33
38	3	311	KC2	C1D-ND-C4D	3.56	108.87	106.33
33	c	513	CLA	CHB-C1B-NB	-3.56	120.49	124.26
33	2	301	CLA	CHB-C1B-NB	-3.56	120.49	124.26
33	1	303	CLA	CHB-C1B-NB	-3.56	120.49	124.26
33	b	608	CLA	CHB-C1B-NB	-3.56	120.49	124.26
33	0	307	CLA	CHB-C1B-NB	-3.56	120.49	124.26
33	7	309	CLA	CHB-C1B-NB	-3.55	120.49	124.26
33	C	512	CLA	CHB-C1B-NB	-3.55	120.50	124.26
38	7	311	KC2	C1D-ND-C4D	3.55	108.86	106.33
43	C	518	DGD	O5D-C6D-C5D	-3.55	102.47	109.05
33	5	307	CLA	CHB-C1B-NB	-3.55	120.50	124.26
33	a	406	CLA	CHB-C1B-NB	-3.55	120.50	124.26
33	A	406	CLA	CHB-C1B-NB	-3.55	120.50	124.26
33	2	307	CLA	CHB-C1B-NB	-3.55	120.50	124.26
33	c	502	CLA	CHB-C1B-NB	-3.54	120.51	124.26
33	g	310	CLA	CHB-C1B-NB	-3.54	120.51	124.26
43	c	518	DGD	O5D-C6D-C5D	-3.54	102.49	109.05
33	c	512	CLA	CHB-C1B-NB	-3.54	120.51	124.26
33	3	307	CLA	CHB-C1B-NB	-3.54	120.51	124.26
33	c	504	CLA	CHB-C1B-NB	-3.54	120.51	124.26
33	9	307	CLA	CHB-C1B-NB	-3.53	120.52	124.26
33	B	608	CLA	CHB-C1B-NB	-3.53	120.52	124.26
33	8	305	CLA	CHB-C1B-NB	-3.53	120.52	124.26
38	9	311	KC2	C1D-ND-C4D	3.53	108.84	106.33
33	C	502	CLA	CHB-C1B-NB	-3.53	120.52	124.26
33	3	306	CLA	CHB-C1B-NB	-3.53	120.52	124.26
33	d	405	CLA	CHB-C1B-NB	-3.53	120.52	124.26
38	7	311	KC2	CHD-C1D-ND	-3.53	120.52	124.26
33	5	305	CLA	CHB-C1B-NB	-3.53	120.52	124.26
33	9	306	CLA	CHB-C1B-NB	-3.53	120.52	124.26
33	b	616	CLA	CHB-C1B-NB	-3.53	120.53	124.26
38	1	311	KC2	CHD-C1D-ND	-3.52	120.53	124.26
33	1	309	CLA	CHB-C1B-NB	-3.52	120.53	124.26
33	9	315	CLA	CHB-C1B-NB	-3.52	120.53	124.26
33	3	314	CLA	CHB-C1B-NB	-3.52	120.53	124.26
39	5	313	II0	C18-C04-C06	3.52	124.84	109.05
33	g	307	CLA	CHB-C1B-NB	-3.52	120.53	124.26
33	4	307	CLA	CHB-C1B-NB	-3.51	120.54	124.26
33	2	305	CLA	CHB-C1B-NB	-3.51	120.54	124.26
36	a	410	PL9	C7-C3-C4	3.51	119.73	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	303	CLA	CHB-C1B-NB	-3.51	120.55	124.26
39	g	313	II0	C18-C04-C06	3.51	124.79	109.05
33	3	315	CLA	CHB-C1B-NB	-3.51	120.55	124.26
33	D	405	CLA	CHB-C1B-NB	-3.50	120.55	124.26
33	C	504	CLA	CHB-C1B-NB	-3.50	120.55	124.26
36	A	410	PL9	C7-C3-C4	3.50	119.72	116.88
33	g	317	CLA	CBD-CHA-C1A	3.49	132.62	128.50
33	g	305	CLA	CHB-C1B-NB	-3.49	120.56	124.26
33	4	302	CLA	CHB-C1B-NB	-3.49	120.56	124.26
33	B	607	CLA	CHB-C1B-NB	-3.49	120.56	124.26
33	b	607	CLA	CHB-C1B-NB	-3.49	120.56	124.26
33	9	305	CLA	CHB-C1B-NB	-3.49	120.56	124.26
33	0	303	CLA	CHB-C1B-NB	-3.49	120.56	124.26
33	B	616	CLA	CHB-C1B-NB	-3.49	120.56	124.26
33	8	310	CLA	CHB-C1B-NB	-3.48	120.57	124.26
33	g	304	CLA	CHB-C1B-NB	-3.48	120.57	124.26
33	c	509	CLA	CHB-C1B-NB	-3.48	120.57	124.26
33	0	302	CLA	CHB-C1B-NB	-3.48	120.57	124.26
33	b	612	CLA	CHB-C1B-NB	-3.47	120.58	124.26
33	n	301	CLA	CHB-C1B-NB	-3.46	120.59	124.26
38	5	309	KC2	CHD-C1D-ND	-3.46	120.59	124.26
33	C	506	CLA	CHB-C1B-NB	-3.46	120.59	124.26
38	g	309	KC2	CHD-C1D-ND	-3.46	120.59	124.26
33	5	317	CLA	CBD-CHA-C1A	3.46	132.58	128.50
33	3	313	CLA	CHB-C1B-NB	-3.46	120.60	124.26
33	C	509	CLA	CHB-C1B-NB	-3.46	120.60	124.26
41	J	101	SQD	O47-C7-C8	3.46	118.95	111.50
33	p	313	CLA	CHB-C1B-NB	-3.46	120.60	124.26
33	2	310	CLA	CHB-C1B-NB	-3.46	120.60	124.26
33	3	305	CLA	CHB-C1B-NB	-3.46	120.60	124.26
33	C	503	CLA	CHB-C1B-NB	-3.46	120.60	124.26
41	j	101	SQD	O47-C7-C8	3.46	118.95	111.50
33	N	301	CLA	CHB-C1B-NB	-3.45	120.60	124.26
33	c	506	CLA	CHB-C1B-NB	-3.45	120.60	124.26
33	6	313	CLA	CHB-C1B-NB	-3.45	120.61	124.26
33	5	304	CLA	CHB-C1B-NB	-3.44	120.61	124.26
33	p	302	CLA	CHB-C1B-NB	-3.44	120.61	124.26
33	B	609	CLA	CHB-C1B-NB	-3.44	120.61	124.26
33	B	612	CLA	CHB-C1B-NB	-3.44	120.62	124.26
33	2	304	CLA	CHB-C1B-NB	-3.43	120.63	124.26
33	5	301	CLA	CHB-C1B-NB	-3.43	120.63	124.26
33	5	305	CLA	C2C-C1C-NC	3.43	113.18	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	6	302	CLA	CHB-C1B-NB	-3.43	120.63	124.26
33	7	307	CLA	CHB-C1B-NB	-3.42	120.64	124.26
33	c	503	CLA	CHB-C1B-NB	-3.42	120.64	124.26
33	9	303	CLA	CHB-C1B-NB	-3.42	120.64	124.26
36	d	407	PL9	C8-C7-C3	3.42	121.64	111.98
33	1	307	CLA	CHB-C1B-NB	-3.42	120.64	124.26
38	8	309	KC2	CHD-C1D-ND	-3.41	120.64	124.26
33	8	303	CLA	CHB-C1B-NB	-3.41	120.65	124.26
33	9	312	CLA	CHB-C1B-NB	-3.41	120.65	124.26
33	b	609	CLA	CHB-C1B-NB	-3.41	120.65	124.26
33	9	313	CLA	CHB-C1B-NB	-3.41	120.65	124.26
33	g	301	CLA	CHB-C1B-NB	-3.40	120.66	124.26
33	3	312	CLA	CHC-C4B-NB	-3.40	120.66	124.26
33	8	304	CLA	CHB-C1B-NB	-3.40	120.66	124.26
36	D	407	PL9	C8-C7-C3	3.40	121.59	111.98
33	3	312	CLA	CHB-C1B-NB	-3.40	120.66	124.26
41	l	101	SQD	O7-S-C6	3.39	110.97	106.94
33	4	309	CLA	CHB-C1B-NB	-3.39	120.67	124.26
33	B	602	CLA	CHB-C1B-NB	-3.39	120.67	124.26
38	2	309	KC2	CHD-C1D-ND	-3.39	120.67	124.26
33	3	303	CLA	CHB-C1B-NB	-3.39	120.67	124.26
41	L	101	SQD	O7-S-C6	3.38	110.96	106.94
33	5	311	CLA	CHB-C1B-NB	-3.38	120.68	124.26
33	9	312	CLA	CHC-C4B-NB	-3.38	120.68	124.26
33	g	305	CLA	C2C-C1C-NC	3.38	113.14	109.97
33	8	302	CLA	CHB-C1B-NB	-3.37	120.69	124.26
33	g	311	CLA	CHB-C1B-NB	-3.36	120.70	124.26
33	2	303	CLA	CHB-C1B-NB	-3.36	120.70	124.26
33	b	602	CLA	CHB-C1B-NB	-3.35	120.71	124.26
33	8	303	CLA	C1-C2-C3	-3.35	120.25	126.04
33	0	310	CLA	CHB-C1B-NB	-3.35	120.71	124.26
41	C	501	SQD	O9-S-C6	3.35	110.92	106.94
33	2	303	CLA	C1-C2-C3	-3.34	120.26	126.04
41	c	501	SQD	O9-S-C6	3.34	110.91	106.94
42	d	410	LMG	O6-C1-O1	-3.34	102.07	109.97
33	n	302	CLA	CHB-C1B-NB	-3.34	120.72	124.26
41	j	101	SQD	C45-O47-C7	-3.34	109.58	117.79
33	2	302	CLA	CHB-C1B-NB	-3.33	120.73	124.26
41	J	101	SQD	C45-O47-C7	-3.33	109.60	117.79
33	6	309	CLA	CHB-C1B-NB	-3.33	120.73	124.26
33	7	301	CLA	CHB-C1B-NB	-3.32	120.74	124.26
33	1	301	CLA	CHB-C1B-NB	-3.32	120.74	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	6	303	CLA	CHB-C1B-NB	-3.32	120.74	124.26
42	D	410	LMG	O6-C1-O1	-3.32	102.11	109.97
33	6	308	CLA	CHB-C1B-NB	-3.32	120.74	124.26
33	p	309	CLA	CHB-C1B-NB	-3.32	120.74	124.26
33	p	303	CLA	CHB-C1B-NB	-3.32	120.75	124.26
33	3	310	CLA	CHB-C1B-NB	-3.32	120.75	124.26
43	H	101	DGD	O3G-C3G-C2G	-3.31	102.91	110.90
43	h	101	DGD	O3G-C3G-C2G	-3.31	102.92	110.90
33	N	302	CLA	CHB-C1B-NB	-3.30	120.76	124.26
43	c	519	DGD	O6D-C1D-O3G	-3.30	102.17	109.97
43	C	519	DGD	O6D-C1D-O3G	-3.30	102.17	109.97
33	p	308	CLA	CHB-C1B-NB	-3.29	120.77	124.26
33	9	310	CLA	CHB-C1B-NB	-3.28	120.78	124.26
33	1	302	CLA	CHB-C1B-NB	-3.28	120.78	124.26
33	7	302	CLA	CHB-C1B-NB	-3.28	120.79	124.26
43	c	521	DGD	O6D-C1D-O3G	-3.26	102.25	109.97
33	0	309	CLA	CHC-C4B-NB	-3.26	120.80	124.26
33	8	304	CLA	C3D-C4D-ND	3.26	115.52	110.24
41	B	601	SQD	O47-C7-C8	3.26	118.53	111.50
33	6	307	CLA	C3D-C4D-ND	3.26	115.50	110.24
41	b	601	SQD	O47-C7-C8	3.25	118.51	111.50
33	4	308	CLA	CHC-C4B-NB	-3.25	120.82	124.26
33	2	304	CLA	C3D-C4D-ND	3.25	115.49	110.24
33	4	308	CLA	C3D-C4D-ND	3.24	115.49	110.24
43	C	521	DGD	O6D-C1D-O3G	-3.24	102.30	109.97
33	p	307	CLA	C3D-C4D-ND	3.24	115.48	110.24
33	0	309	CLA	C3D-C4D-ND	3.24	115.48	110.24
33	d	404	CLA	CHB-C1B-NB	-3.22	120.84	124.26
33	a	412	CLA	CHC-C4B-NB	-3.22	120.84	124.26
33	1	304	CLA	CHB-C1B-NB	-3.22	120.85	124.26
33	8	303	CLA	C3D-C4D-ND	3.21	115.44	110.24
33	2	303	CLA	C3D-C4D-ND	3.21	115.44	110.24
39	8	312	II0	C04-C10-C14	-3.21	118.11	122.63
43	C	521	DGD	O3G-C3G-C2G	-3.20	103.19	110.90
33	A	412	CLA	CHC-C4B-NB	-3.19	120.88	124.26
33	p	313	CLA	C2C-C1C-NC	3.19	112.96	109.97
43	c	521	DGD	O3G-C3G-C2G	-3.19	103.20	110.90
33	N	303	CLA	CHB-C4A-NA	3.19	128.92	124.51
33	7	304	CLA	CHB-C1B-NB	-3.19	120.88	124.26
39	2	312	II0	C04-C10-C14	-3.18	118.14	122.63
33	D	404	CLA	CHB-C1B-NB	-3.18	120.89	124.26
33	4	310	CLA	C3D-C4D-ND	3.18	115.38	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	m	101	LMG	O1-C1-C2	-3.17	103.35	108.30
34	A	407	PHO	C2D-C1D-ND	-3.17	107.33	109.53
33	0	308	CLA	CHB-C4A-NA	3.17	128.90	124.51
33	0	311	CLA	C3D-C4D-ND	3.17	115.37	110.24
33	4	302	CLA	C3D-C4D-ND	3.17	115.36	110.24
33	8	303	CLA	O2A-C1-C2	3.16	116.95	108.64
34	A	407	PHO	C4D-CHA-CBD	3.16	109.95	108.52
33	g	303	CLA	C3D-C4D-ND	3.16	115.35	110.24
42	l	102	LMG	O1-C1-C2	-3.16	103.37	108.30
34	a	407	PHO	C4D-CHA-CBD	3.16	109.94	108.52
39	g	313	II0	C17-C04-C06	-3.16	94.88	109.05
33	2	303	CLA	O2A-C1-C2	3.15	116.93	108.64
39	5	313	II0	C17-C04-C06	-3.15	94.89	109.05
33	5	303	CLA	C3D-C4D-ND	3.15	115.33	110.24
37	A	411	LHG	O8-C23-C24	3.14	119.62	111.38
33	0	302	CLA	C3D-C4D-ND	3.14	115.32	110.24
34	a	407	PHO	C2D-C1D-ND	-3.14	107.36	109.53
37	a	411	LHG	O8-C23-C24	3.13	119.59	111.38
36	D	407	PL9	C12-C13-C14	-3.13	120.13	127.66
34	D	403	PHO	C2D-C1D-ND	-3.13	107.37	109.53
43	C	518	DGD	C6D-O5D-C1E	3.12	119.84	113.74
36	d	407	PL9	C12-C13-C14	-3.12	120.14	127.66
33	6	303	CLA	C3D-C4D-ND	3.12	115.29	110.24
43	c	518	DGD	C6D-O5D-C1E	3.12	119.83	113.74
33	6	313	CLA	C2C-C1C-NC	3.12	112.89	109.97
33	p	303	CLA	C3D-C4D-ND	3.12	115.28	110.24
33	A	412	CLA	C3D-C4D-ND	3.11	115.27	110.24
33	7	301	CLA	C3D-C4D-ND	3.11	115.26	110.24
33	1	301	CLA	C3D-C4D-ND	3.10	115.26	110.24
33	6	308	CLA	C3D-C4D-ND	3.10	115.25	110.24
33	p	308	CLA	C3D-C4D-ND	3.09	115.24	110.24
33	A	408	CLA	C3D-C4D-ND	3.09	115.23	110.24
34	d	403	PHO	C2D-C1D-ND	-3.08	107.40	109.53
33	a	412	CLA	C3D-C4D-ND	3.07	115.20	110.24
33	b	606	CLA	C3D-C4D-ND	3.06	115.19	110.24
33	4	309	CLA	CBD-CHA-C1A	3.06	132.10	128.50
33	a	408	CLA	C3D-C4D-ND	3.05	115.18	110.24
38	p	311	KC2	CHD-C1D-ND	-3.05	121.02	124.26
33	B	606	CLA	C3D-C4D-ND	3.05	115.18	110.24
33	N	307	CLA	C3D-C4D-ND	3.04	115.16	110.24
33	0	310	CLA	CBD-CHA-C1A	3.04	132.08	128.50
33	1	308	CLA	C3D-C4D-ND	3.04	115.15	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	g	307	CLA	C3D-C4D-ND	3.03	115.15	110.24
33	1	304	CLA	C3D-C4D-ND	3.03	115.13	110.24
33	n	306	CLA	C3D-C4D-ND	3.02	115.13	110.24
39	p	316	II0	C04-C10-C14	-3.02	118.37	122.63
39	6	316	II0	C04-C10-C14	-3.02	118.37	122.63
33	b	612	CLA	C1-C2-C3	-3.02	120.82	126.04
33	b	604	CLA	C3D-C4D-ND	3.02	115.12	110.24
33	N	306	CLA	C1-C2-C3	-3.02	120.82	126.04
33	7	304	CLA	C3D-C4D-ND	3.02	115.11	110.24
33	b	612	CLA	C3D-C4D-ND	3.01	115.11	110.24
38	6	311	KC2	CHD-C1D-ND	-3.01	121.07	124.26
33	n	305	CLA	C1-C2-C3	-3.01	120.84	126.04
33	5	307	CLA	C3D-C4D-ND	3.01	115.10	110.24
33	B	604	CLA	C3D-C4D-ND	3.01	115.10	110.24
33	9	306	CLA	C3D-C4D-ND	3.00	115.09	110.24
33	B	612	CLA	C3D-C4D-ND	3.00	115.09	110.24
33	4	307	CLA	C3D-C4D-ND	3.00	115.09	110.24
33	7	308	CLA	C3D-C4D-ND	3.00	115.09	110.24
33	p	312	CLA	C3D-C4D-ND	3.00	115.08	110.24
33	6	312	CLA	C2C-C1C-NC	2.99	112.78	109.97
44	F	101	HEM	C4C-NC-C1C	2.99	108.28	105.35
33	0	307	CLA	C3D-C4D-ND	2.99	115.07	110.24
33	3	308	CLA	CHC-C4B-NB	-2.99	121.09	124.26
33	B	612	CLA	C1-C2-C3	-2.99	120.87	126.04
33	p	306	CLA	C3D-C4D-ND	2.99	115.07	110.24
33	6	306	CLA	C3D-C4D-ND	2.98	115.07	110.24
33	c	509	CLA	C3D-C4D-ND	2.98	115.05	110.24
33	C	509	CLA	C3D-C4D-ND	2.97	115.05	110.24
33	3	306	CLA	C3D-C4D-ND	2.97	115.05	110.24
41	b	601	SQD	O9-S-C6	2.97	110.47	106.94
33	g	311	CLA	C3D-C4D-ND	2.97	115.04	110.24
33	6	312	CLA	C3D-C4D-ND	2.97	115.04	110.24
33	9	303	CLA	C3D-C4D-ND	2.97	115.04	110.24
33	5	305	CLA	C3D-C4D-ND	2.97	115.04	110.24
41	B	601	SQD	O9-S-C6	2.97	110.47	106.94
33	5	311	CLA	C3D-C4D-ND	2.97	115.04	110.24
33	B	603	CLA	C3D-C4D-ND	2.96	115.03	110.24
33	g	305	CLA	C3D-C4D-ND	2.96	115.03	110.24
33	p	312	CLA	C2C-C1C-NC	2.96	112.75	109.97
33	3	303	CLA	C3D-C4D-ND	2.96	115.03	110.24
33	2	301	CLA	C3D-C4D-ND	2.96	115.02	110.24
33	p	313	CLA	C3D-C4D-ND	2.96	115.02	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	507	CLA	C3D-C4D-ND	2.96	115.02	110.24
33	8	301	CLA	C3D-C4D-ND	2.96	115.02	110.24
33	g	302	CLA	C3D-C4D-ND	2.96	115.02	110.24
33	g	310	CLA	C3D-C4D-ND	2.95	115.01	110.24
33	4	309	CLA	C3D-C4D-ND	2.95	115.01	110.24
33	0	310	CLA	C3D-C4D-ND	2.95	115.01	110.24
33	7	302	CLA	C3D-C4D-ND	2.95	115.01	110.24
33	b	603	CLA	C3D-C4D-ND	2.95	115.00	110.24
33	5	310	CLA	C3D-C4D-ND	2.95	115.00	110.24
33	1	302	CLA	C3D-C4D-ND	2.95	115.00	110.24
33	A	412	CLA	C2C-C1C-NC	2.94	112.73	109.97
33	a	412	CLA	C2C-C1C-NC	2.94	112.73	109.97
33	3	309	CLA	C3D-C4D-ND	2.94	115.00	110.24
33	6	313	CLA	C3D-C4D-ND	2.94	115.00	110.24
33	9	308	CLA	CHC-C4B-NB	-2.94	121.14	124.26
33	9	305	CLA	C3D-C4D-ND	2.94	114.99	110.24
33	N	303	CLA	C3D-C4D-ND	2.94	114.99	110.24
33	5	302	CLA	C3D-C4D-ND	2.94	114.99	110.24
33	N	306	CLA	C3D-C4D-ND	2.94	114.99	110.24
33	c	504	CLA	C3D-C4D-ND	2.94	114.99	110.24
33	c	507	CLA	C3D-C4D-ND	2.94	114.99	110.24
33	c	511	CLA	C3D-C4D-ND	2.93	114.98	110.24
42	c	520	LMG	O6-C1-O1	-2.93	103.03	109.97
33	C	511	CLA	C3D-C4D-ND	2.93	114.98	110.24
33	D	405	CLA	C3D-C4D-ND	2.93	114.98	110.24
33	9	309	CLA	C3D-C4D-ND	2.93	114.98	110.24
33	g	301	CLA	C3D-C4D-ND	2.93	114.98	110.24
33	g	303	CLA	CHB-C1B-NB	-2.93	121.16	124.26
42	C	520	LMG	O6-C1-O1	-2.93	103.04	109.97
33	d	405	CLA	C3D-C4D-ND	2.93	114.97	110.24
33	0	308	CLA	C3D-C4D-ND	2.93	114.97	110.24
33	B	606	CLA	CMC-C2C-C1C	2.92	129.49	125.04
33	D	404	CLA	CHC-C4B-NB	-2.92	121.16	124.26
33	C	504	CLA	C3D-C4D-ND	2.92	114.96	110.24
33	5	301	CLA	C3D-C4D-ND	2.92	114.96	110.24
33	n	303	CLA	C3D-C4D-ND	2.92	114.96	110.24
33	b	606	CLA	CMC-C2C-C1C	2.92	129.48	125.04
37	D	408	LHG	O8-C23-C24	2.92	121.06	111.91
33	5	304	CLA	C3D-C4D-ND	2.92	114.95	110.24
33	p	304	CLA	C3D-C4D-ND	2.92	114.95	110.24
33	9	312	CLA	C3D-C4D-ND	2.91	114.95	110.24
33	n	305	CLA	C3D-C4D-ND	2.91	114.95	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	3	305	CLA	C3D-C4D-ND	2.91	114.95	110.24
33	5	303	CLA	CHB-C1B-NB	-2.91	121.17	124.26
44	F	101	HEM	CHD-C4C-NC	2.91	127.59	124.44
33	N	304	CLA	C3D-C4D-ND	2.91	114.95	110.24
33	d	404	CLA	C3D-C4D-ND	2.91	114.94	110.24
33	A	406	CLA	C3D-C4D-ND	2.91	114.94	110.24
33	9	313	CLA	C3D-C4D-ND	2.90	114.94	110.24
33	D	404	CLA	C3D-C4D-ND	2.90	114.94	110.24
33	g	308	CLA	C3D-C4D-ND	2.90	114.93	110.24
33	B	618	CLA	C3D-C4D-ND	2.90	114.93	110.24
33	3	312	CLA	C3D-C4D-ND	2.90	114.93	110.24
33	6	304	CLA	C3D-C4D-ND	2.90	114.93	110.24
33	2	302	CLA	C3D-C4D-ND	2.90	114.93	110.24
33	0	304	CLA	C3D-C4D-ND	2.90	114.92	110.24
33	g	304	CLA	C3D-C4D-ND	2.90	114.92	110.24
33	3	310	CLA	C3D-C4D-ND	2.89	114.92	110.24
33	3	313	CLA	C3D-C4D-ND	2.89	114.92	110.24
33	8	302	CLA	C3D-C4D-ND	2.89	114.92	110.24
33	B	609	CLA	C3D-C4D-ND	2.89	114.92	110.24
33	a	406	CLA	C3D-C4D-ND	2.89	114.92	110.24
33	c	513	CLA	C3D-C4D-ND	2.89	114.92	110.24
33	4	304	CLA	C3D-C4D-ND	2.89	114.91	110.24
33	5	308	CLA	C3D-C4D-ND	2.89	114.91	110.24
33	2	302	CLA	CBA-CAA-C2A	2.89	122.39	113.86
37	d	408	LHG	O8-C23-C24	2.89	120.97	111.91
33	b	602	CLA	C3D-C4D-ND	2.89	114.91	110.24
33	p	309	CLA	C3D-C4D-ND	2.89	114.91	110.24
33	8	302	CLA	CBA-CAA-C2A	2.89	122.39	113.86
33	9	310	CLA	C3D-C4D-ND	2.89	114.91	110.24
33	8	306	CLA	C3D-C4D-ND	2.89	114.91	110.24
33	7	305	CLA	C3D-C4D-ND	2.88	114.90	110.24
39	2	312	II0	C06-C08-C12	2.88	114.25	110.30
33	6	309	CLA	C3D-C4D-ND	2.88	114.90	110.24
33	9	308	CLA	C3D-C4D-ND	2.88	114.90	110.24
39	8	312	II0	C06-C08-C12	2.88	114.25	110.30
33	0	303	CLA	C3D-C4D-ND	2.88	114.90	110.24
33	C	513	CLA	C3D-C4D-ND	2.88	114.89	110.24
33	3	308	CLA	C3D-C4D-ND	2.88	114.89	110.24
33	p	310	CLA	C2C-C1C-NC	2.87	112.67	109.97
33	2	306	CLA	C3D-C4D-ND	2.87	114.89	110.24
33	2	308	CLA	C3D-C4D-ND	2.87	114.89	110.24
33	b	609	CLA	C3D-C4D-ND	2.87	114.88	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	1	305	CLA	C3D-C4D-ND	2.87	114.88	110.24
33	d	404	CLA	CHC-C4B-NB	-2.87	121.22	124.26
33	B	611	CLA	C3D-C4D-ND	2.87	114.88	110.24
33	g	317	CLA	C3D-C4D-ND	2.87	114.87	110.24
33	4	303	CLA	C3D-C4D-ND	2.86	114.86	110.24
33	B	608	CLA	C3D-C4D-ND	2.86	114.86	110.24
33	2	305	CLA	C3D-C4D-ND	2.86	114.86	110.24
33	b	618	CLA	C3D-C4D-ND	2.86	114.86	110.24
33	b	617	CLA	C3D-C4D-ND	2.86	114.86	110.24
33	b	611	CLA	C3D-C4D-ND	2.85	114.86	110.24
33	5	317	CLA	C3D-C4D-ND	2.85	114.85	110.24
33	8	305	CLA	C3D-C4D-ND	2.85	114.85	110.24
33	c	506	CLA	C3D-C4D-ND	2.85	114.85	110.24
33	B	602	CLA	C3D-C4D-ND	2.85	114.85	110.24
33	B	617	CLA	C3D-C4D-ND	2.85	114.85	110.24
33	C	505	CLA	C3D-C4D-ND	2.85	114.85	110.24
33	c	505	CLA	C3D-C4D-ND	2.84	114.84	110.24
33	b	607	CLA	C3D-C4D-ND	2.84	114.84	110.24
33	b	608	CLA	C3D-C4D-ND	2.84	114.84	110.24
33	C	506	CLA	C3D-C4D-ND	2.84	114.83	110.24
33	4	309	CLA	CHC-C4B-NB	-2.84	121.25	124.26
33	N	301	CLA	C3D-C4D-ND	2.84	114.83	110.24
33	6	310	CLA	C2C-C1C-NC	2.84	112.63	109.97
33	1	306	CLA	C3D-C4D-ND	2.84	114.83	110.24
42	w	101	LMG	O6-C1-O1	-2.84	103.26	109.97
33	3	315	CLA	CAA-C2A-C3A	-2.83	109.48	116.10
33	7	306	CLA	C3D-C4D-ND	2.83	114.82	110.24
33	8	308	CLA	C3D-C4D-ND	2.83	114.82	110.24
42	W	101	LMG	O6-C1-O1	-2.83	103.27	109.97
33	5	302	CLA	CAA-C2A-C3A	2.83	120.52	112.78
33	b	615	CLA	C3D-C4D-ND	2.83	114.81	110.24
33	C	514	CLA	C3D-C4D-ND	2.83	114.81	110.24
33	1	307	CLA	C3D-C4D-ND	2.82	114.81	110.24
33	4	306	CLA	CHC-C4B-NB	-2.82	121.27	124.26
33	0	306	CLA	CHC-C4B-NB	-2.82	121.27	124.26
33	9	315	CLA	CAA-C2A-C3A	-2.82	109.52	116.10
33	c	514	CLA	C3D-C4D-ND	2.81	114.79	110.24
33	g	302	CLA	CAA-C2A-C3A	2.81	120.48	112.78
33	0	310	CLA	CHC-C4B-NB	-2.81	121.28	124.26
33	B	607	CLA	C3D-C4D-ND	2.81	114.79	110.24
33	0	306	CLA	C3D-C4D-ND	2.81	114.78	110.24
33	B	615	CLA	C3D-C4D-ND	2.81	114.78	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	n	301	CLA	C3D-C4D-ND	2.80	114.77	110.24
34	a	407	PHO	C1C-C2C-C3C	-2.80	106.28	108.61
33	4	306	CLA	C3D-C4D-ND	2.80	114.77	110.24
38	2	309	KC2	C2A-C3A-C4A	2.80	108.56	106.49
33	3	307	CLA	C3D-C4D-ND	2.79	114.76	110.24
33	2	307	CLA	C3D-C4D-ND	2.79	114.75	110.24
34	A	407	PHO	C1C-C2C-C3C	-2.79	106.29	108.61
33	7	307	CLA	C3D-C4D-ND	2.79	114.75	110.24
33	n	302	CLA	C3D-C4D-ND	2.78	114.74	110.24
38	8	309	KC2	C2A-C3A-C4A	2.78	108.55	106.49
33	b	613	CLA	C3D-C4D-ND	2.77	114.72	110.24
33	N	302	CLA	C3D-C4D-ND	2.77	114.72	110.24
33	8	307	CLA	C3D-C4D-ND	2.77	114.72	110.24
33	C	510	CLA	C3D-C4D-ND	2.77	114.72	110.24
33	c	510	CLA	C3D-C4D-ND	2.77	114.71	110.24
37	B	623	LHG	C11-C10-C9	-2.76	100.39	114.42
33	4	301	CLA	C3D-C4D-ND	2.76	114.71	110.24
33	8	310	CLA	C3D-C4D-ND	2.76	114.71	110.24
33	9	307	CLA	C3D-C4D-ND	2.76	114.70	110.24
33	g	306	CLA	C3D-C4D-ND	2.76	114.70	110.24
33	g	302	CLA	CBA-CAA-C2A	2.76	122.01	113.86
33	N	307	CLA	C1-C2-C3	-2.76	122.29	126.75
33	p	308	CLA	CHC-C4B-NB	-2.76	121.33	124.26
33	2	310	CLA	C3D-C4D-ND	2.76	114.70	110.24
33	p	305	CLA	C2C-C1C-NC	2.76	112.56	109.97
33	6	305	CLA	C2C-C1C-NC	2.76	112.56	109.97
37	b	623	LHG	C11-C10-C9	-2.76	100.43	114.42
33	5	302	CLA	CBA-CAA-C2A	2.75	121.99	113.86
33	n	306	CLA	C1-C2-C3	-2.75	122.30	126.75
33	C	508	CLA	C2C-C1C-NC	2.75	112.55	109.97
43	H	101	DGD	O6D-C1D-O3G	-2.75	103.47	109.97
33	5	306	CLA	C3D-C4D-ND	2.75	114.68	110.24
33	9	304	CLA	C3D-C4D-ND	2.75	114.68	110.24
33	3	314	CLA	C3D-C4D-ND	2.74	114.68	110.24
33	6	302	CLA	C3D-C4D-ND	2.74	114.67	110.24
43	h	101	DGD	O6D-C1D-O3G	-2.74	103.49	109.97
33	0	301	CLA	C3D-C4D-ND	2.74	114.66	110.24
43	c	518	DGD	O6D-C1D-O3G	-2.73	103.50	109.97
33	B	613	CLA	C3D-C4D-ND	2.73	114.66	110.24
33	0	304	CLA	C2C-C1C-NC	2.72	112.52	109.97
33	9	314	CLA	C3D-C4D-ND	2.72	114.64	110.24
33	p	302	CLA	C3D-C4D-ND	2.72	114.64	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	c	508	CLA	C2C-C1C-NC	2.72	112.52	109.97
33	3	304	CLA	C3D-C4D-ND	2.72	114.64	110.24
43	C	518	DGD	O6D-C1D-O3G	-2.72	103.54	109.97
33	p	319	CLA	C2A-C3A-C4A	-2.72	98.32	101.78
33	6	319	CLA	C2A-C3A-C4A	-2.72	98.32	101.78
33	6	308	CLA	CHC-C4B-NB	-2.72	121.38	124.26
33	c	503	CLA	C3D-C4D-ND	2.71	114.62	110.24
33	C	503	CLA	C3D-C4D-ND	2.70	114.60	110.24
38	5	309	KC2	CHB-C1B-NB	2.70	126.93	124.45
33	4	304	CLA	C2C-C1C-NC	2.70	112.50	109.97
37	B	623	LHG	O8-C23-C24	2.69	120.36	111.91
33	7	303	CLA	C3D-C4D-ND	2.69	114.59	110.24
37	b	623	LHG	O8-C23-C24	2.69	120.36	111.91
33	C	502	CLA	C3D-C4D-ND	2.69	114.59	110.24
41	l	101	SQD	O48-C23-C24	2.69	120.35	111.91
33	c	502	CLA	C3D-C4D-ND	2.69	114.58	110.24
41	c	501	SQD	O7-S-C6	2.68	110.13	106.94
41	L	101	SQD	O48-C23-C24	2.68	120.33	111.91
38	0	305	KC2	CHB-C4A-NA	2.68	128.43	124.20
33	1	303	CLA	C3D-C4D-ND	2.68	114.57	110.24
37	2	315	LHG	O8-C23-C24	2.68	120.31	111.91
33	a	412	CLA	O2A-C1-C2	2.68	115.67	108.64
33	B	610	CLA	C3D-C4D-ND	2.68	114.56	110.24
41	C	501	SQD	O7-S-C6	2.67	110.12	106.94
33	B	605	CLA	C3D-C4D-ND	2.67	114.56	110.24
38	4	305	KC2	CHB-C4A-NA	2.67	128.41	124.20
39	4	313	II0	C05-C07-C11	-2.67	106.65	110.30
34	D	403	PHO	C1C-C2C-C3C	-2.67	106.39	108.61
33	b	610	CLA	C3D-C4D-ND	2.67	114.56	110.24
37	8	315	LHG	O8-C23-C24	2.67	120.28	111.91
33	A	412	CLA	O2A-C1-C2	2.67	115.64	108.64
39	8	312	II0	C05-C07-C11	-2.67	106.65	110.30
39	0	314	II0	C05-C07-C11	-2.67	106.66	110.30
37	9	322	LHG	O8-C23-C24	2.66	120.26	111.91
38	g	309	KC2	CHB-C1B-NB	2.66	126.90	124.45
33	6	305	CLA	C3D-C4D-ND	2.66	114.53	110.24
34	d	403	PHO	C1C-C2C-C3C	-2.65	106.40	108.61
33	b	605	CLA	C3D-C4D-ND	2.65	114.53	110.24
37	3	322	LHG	O8-C23-C24	2.65	120.22	111.91
33	p	305	CLA	C3D-C4D-ND	2.65	114.52	110.24
34	A	407	PHO	C2B-C1B-NB	-2.64	107.70	109.53
33	2	310	CLA	CHC-C4B-NB	-2.64	121.46	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	p	319	CLA	C3D-C4D-ND	2.64	114.50	110.24
33	9	307	CLA	CHC-C4B-NB	-2.63	121.47	124.26
33	5	305	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
33	g	305	CLA	CHC-C1C-C2C	-2.62	119.44	126.73
33	N	307	CLA	C2C-C1C-NC	2.62	112.43	109.97
33	1	309	CLA	C3D-C4D-ND	2.62	114.47	110.24
33	7	309	CLA	C3D-C4D-ND	2.62	114.47	110.24
38	4	305	KC2	CHB-C1B-NB	2.62	126.86	124.45
33	6	319	CLA	C3D-C4D-ND	2.62	114.47	110.24
43	c	521	DGD	CDB-CCB-CBB	-2.62	101.14	114.42
39	7	315	II0	C03-C09-C13	-2.62	118.94	122.63
44	F	101	HEM	CHD-C1D-C2D	-2.62	120.89	124.98
39	2	312	II0	C05-C07-C11	-2.62	106.72	110.30
33	n	306	CLA	C2C-C1C-NC	2.62	112.42	109.97
43	C	521	DGD	CDB-CCB-CBB	-2.61	101.16	114.42
33	n	304	CLA	C3D-C4D-ND	2.61	114.47	110.24
33	3	307	CLA	CHC-C4B-NB	-2.61	121.49	124.26
38	g	309	KC2	CHB-C4A-NA	2.61	128.32	124.20
33	N	305	CLA	C3D-C4D-ND	2.61	114.46	110.24
41	j	101	SQD	O48-C23-C24	2.61	120.09	111.91
38	5	309	KC2	CHB-C4A-NA	2.61	128.31	124.20
33	N	303	CLA	CHC-C4B-NB	-2.60	121.50	124.26
33	8	310	CLA	CHC-C4B-NB	-2.60	121.50	124.26
41	J	101	SQD	O48-C23-C24	2.60	120.07	111.91
39	1	315	II0	C03-C09-C13	-2.60	118.96	122.63
43	C	519	DGD	C1D-C2D-C3D	-2.60	104.58	110.00
43	c	519	DGD	C1D-C2D-C3D	-2.60	104.58	110.00
38	0	305	KC2	CHB-C1B-NB	2.59	126.84	124.45
37	9	302	LHG	O8-C23-C24	2.59	120.04	111.91
33	a	405	CLA	C3D-C4D-ND	2.59	114.42	110.24
33	7	302	CLA	CAA-C2A-C3A	2.59	119.86	112.78
38	p	311	KC2	CHB-C1B-NB	2.59	126.83	124.45
33	B	614	CLA	C3D-C4D-ND	2.58	114.41	110.24
34	a	407	PHO	C2B-C1B-NB	-2.58	107.75	109.53
33	0	308	CLA	CHC-C4B-NB	-2.58	121.53	124.26
33	b	614	CLA	C3D-C4D-ND	2.58	114.41	110.24
38	6	311	KC2	CHB-C1B-NB	2.58	126.82	124.45
33	1	302	CLA	CAA-C2A-C3A	2.57	119.82	112.78
37	3	302	LHG	O8-C23-C24	2.57	119.98	111.91
42	B	622	LMG	O6-C1-O1	-2.57	103.89	109.97
33	4	307	CLA	C1-C2-C3	-2.57	121.60	126.04
43	c	519	DGD	O5D-C6D-C5D	-2.57	104.30	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	3	315	CLA	C3D-C4D-ND	2.57	114.39	110.24
33	9	309	CLA	CHC-C4B-NB	-2.56	121.54	124.26
33	A	405	CLA	C3D-C4D-ND	2.56	114.38	110.24
33	9	315	CLA	C3D-C4D-ND	2.56	114.38	110.24
42	b	622	LMG	O6-C1-O1	-2.56	103.92	109.97
42	D	410	LMG	O6-C5-C4	2.55	114.33	109.69
33	A	412	CLA	CHD-C1D-C2D	2.55	130.83	125.48
43	C	519	DGD	O5D-C6D-C5D	-2.55	104.33	109.05
42	d	410	LMG	O6-C5-C4	2.55	114.32	109.69
33	4	310	CLA	C2C-C1C-NC	2.55	112.36	109.97
37	5	316	LHG	O8-C23-C24	2.55	119.90	111.91
33	4	303	CLA	O2A-C1-C2	2.54	115.32	108.64
33	3	309	CLA	CHC-C4B-NB	-2.54	121.57	124.26
33	a	412	CLA	CHD-C1D-C2D	2.54	130.81	125.48
33	0	307	CLA	C1-C2-C3	-2.54	121.65	126.04
33	0	311	CLA	C2C-C1C-NC	2.54	112.35	109.97
33	0	303	CLA	O2A-C1-C2	2.54	115.30	108.64
38	1	310	KC2	CHB-C1B-NB	2.53	126.78	124.45
37	b	623	LHG	C20-C19-C18	-2.53	101.56	114.42
33	8	302	CLA	CAA-C2A-C3A	2.53	119.70	112.78
37	g	316	LHG	O8-C23-C24	2.53	119.84	111.91
38	7	310	KC2	CHB-C1B-NB	2.53	126.78	124.45
33	5	310	CLA	CHC-C4B-NB	-2.53	121.58	124.26
37	B	623	LHG	C20-C19-C18	-2.53	101.60	114.42
33	2	302	CLA	CAA-C2A-C3A	2.53	119.69	112.78
33	4	301	CLA	CHC-C4B-NB	-2.52	121.58	124.26
42	t	101	LMG	O6-C1-O1	-2.52	104.00	109.97
33	p	310	CLA	C3D-C4D-ND	2.52	114.32	110.24
42	D	410	LMG	O1-C7-C8	-2.52	104.82	110.90
33	0	308	CLA	CHD-C1D-C2D	2.52	130.76	125.48
33	0	301	CLA	CHC-C4B-NB	-2.52	121.59	124.26
33	0	309	CLA	CHD-C4C-C3C	-2.52	121.14	124.84
42	d	410	LMG	O1-C7-C8	-2.51	104.83	110.90
33	4	308	CLA	CHD-C4C-C3C	-2.51	121.15	124.84
33	g	310	CLA	CHC-C4B-NB	-2.51	121.60	124.26
33	b	616	CLA	C3D-C4D-ND	2.51	114.30	110.24
33	2	306	CLA	CHC-C4B-NB	-2.51	121.60	124.26
33	6	310	CLA	C3D-C4D-ND	2.51	114.30	110.24
36	D	407	PL9	O1-C4-C3	-2.51	117.96	120.72
42	T	101	LMG	O6-C1-O1	-2.51	104.04	109.97
36	d	407	PL9	O1-C4-C3	-2.51	117.96	120.72
33	N	303	CLA	CHD-C1D-C2D	2.50	130.72	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	3	319	II0	C06-C08-C12	2.50	113.72	110.30
42	t	101	LMG	C3-C4-C5	-2.50	105.78	110.24
39	9	319	II0	C06-C08-C12	2.50	113.72	110.30
33	p	309	CLA	CAA-C2A-C1A	-2.49	106.64	112.14
33	B	616	CLA	C3D-C4D-ND	2.49	114.26	110.24
33	6	307	CLA	C2C-C1C-NC	2.49	112.30	109.97
33	b	618	CLA	C2C-C1C-NC	2.49	112.30	109.97
33	6	309	CLA	CAA-C2A-C1A	-2.49	106.64	112.14
33	B	609	CLA	CHC-C4B-NB	-2.48	121.63	124.26
33	p	312	CLA	CHC-C1C-C2C	-2.48	119.83	126.73
33	c	512	CLA	C3D-C4D-ND	2.48	114.25	110.24
33	A	405	CLA	CHC-C4B-NB	-2.48	121.63	124.26
33	6	312	CLA	CHC-C1C-C2C	-2.48	119.84	126.73
33	p	307	CLA	C2C-C1C-NC	2.48	112.29	109.97
33	C	502	CLA	C1-C2-C3	-2.48	121.76	126.04
33	c	507	CLA	C1-C2-C3	-2.48	121.76	126.04
33	2	302	CLA	C3A-C2A-C1A	-2.48	97.63	101.34
42	T	101	LMG	C3-C4-C5	-2.48	105.82	110.24
33	b	609	CLA	CHC-C4B-NB	-2.47	121.64	124.26
42	d	410	LMG	O1-C1-C2	-2.47	104.44	108.30
38	2	309	KC2	CHB-C1B-NB	2.47	126.73	124.45
33	C	507	CLA	C1-C2-C3	-2.47	121.77	126.04
33	c	505	CLA	CHC-C4B-NB	-2.47	121.64	124.26
33	a	405	CLA	CHC-C4B-NB	-2.46	121.65	124.26
33	c	502	CLA	C1-C2-C3	-2.46	121.78	126.04
33	0	308	CLA	C2A-C3A-C4A	2.46	105.84	101.87
37	3	322	LHG	C11-C10-C9	-2.46	101.94	114.42
33	N	303	CLA	C2A-C3A-C4A	2.46	105.84	101.87
33	B	616	CLA	C2C-C1C-NC	2.46	112.28	109.97
34	D	403	PHO	C2B-C1B-NB	-2.46	107.83	109.53
42	D	410	LMG	O1-C1-C2	-2.46	104.47	108.30
37	9	322	LHG	C11-C10-C9	-2.46	101.95	114.42
33	g	301	CLA	C2C-C1C-NC	2.46	112.27	109.97
33	C	512	CLA	C3D-C4D-ND	2.46	114.21	110.24
41	c	501	SQD	O48-C23-C24	2.46	119.61	111.91
33	8	306	CLA	CHC-C4B-NB	-2.45	121.66	124.26
33	C	505	CLA	CHC-C4B-NB	-2.45	121.66	124.26
33	p	309	CLA	C2C-C1C-NC	2.45	112.27	109.97
37	7	317	LHG	O8-C23-C24	2.45	119.59	111.91
33	8	302	CLA	C3A-C2A-C1A	-2.45	97.67	101.34
33	p	310	CLA	CAA-C2A-C3A	-2.45	110.39	116.10
36	D	407	PL9	O2-C1-C2	-2.45	116.18	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	B	618	CLA	C2C-C1C-NC	2.44	112.26	109.97
37	7	317	LHG	C11-C10-C9	-2.44	102.02	114.42
33	9	309	CLA	CBA-CAA-C2A	2.44	121.07	113.86
33	A	412	CLA	CHC-C1C-C2C	-2.44	119.95	126.73
41	C	501	SQD	O48-C23-C24	2.44	119.56	111.91
33	3	309	CLA	CBA-CAA-C2A	2.44	121.06	113.86
38	8	309	KC2	CHB-C1B-NB	2.44	126.69	124.45
36	d	407	PL9	O2-C1-C2	-2.44	116.20	121.78
33	6	310	CLA	CAA-C2A-C3A	-2.44	110.41	116.10
37	1	317	LHG	C11-C10-C9	-2.43	102.07	114.42
33	4	306	CLA	C2C-C1C-NC	2.43	112.25	109.97
37	1	317	LHG	O8-C23-C24	2.43	119.54	111.91
33	p	308	CLA	C2C-C1C-NC	2.43	112.25	109.97
38	4	305	KC2	CHC-C4B-NB	2.43	126.69	124.45
33	p	313	CLA	CHC-C1C-C2C	-2.43	119.98	126.73
33	a	412	CLA	CHC-C1C-C2C	-2.43	119.98	126.73
33	b	616	CLA	C2C-C1C-NC	2.43	112.25	109.97
33	B	618	CLA	CHC-C4B-NB	-2.43	121.69	124.26
37	D	402	LHG	O8-C23-C24	2.42	119.52	111.91
38	1	310	KC2	C4C-C3C-C2C	2.42	109.04	107.11
33	p	310	CLA	CHC-C1C-C2C	-2.42	120.01	126.73
33	6	313	CLA	CHC-C1C-C2C	-2.42	120.01	126.73
38	2	309	KC2	C3A-C4A-NA	-2.42	107.93	110.57
33	0	306	CLA	C2C-C1C-NC	2.42	112.24	109.97
33	0	310	CLA	CHA-C1A-NA	-2.42	120.97	126.41
33	6	310	CLA	CHC-C1C-C2C	-2.42	120.01	126.73
37	d	402	LHG	O8-C23-C24	2.42	119.49	111.91
34	d	403	PHO	C2B-C1B-NB	-2.42	107.86	109.53
42	t	101	LMG	O2-C2-C1	-2.41	104.19	110.05
38	0	305	KC2	CHC-C4B-NB	2.41	126.67	124.45
33	6	309	CLA	C2C-C1C-NC	2.41	112.23	109.97
33	B	617	CLA	CHC-C4B-NB	-2.41	121.71	124.26
33	6	303	CLA	C2C-C1C-NC	2.41	112.23	109.97
43	h	101	DGD	C1D-C2D-C3D	-2.41	104.99	110.00
33	5	301	CLA	C2C-C1C-NC	2.40	112.22	109.97
42	m	101	LMG	O1-C7-C8	-2.40	105.10	110.90
42	T	101	LMG	O2-C2-C1	-2.40	104.21	110.05
33	C	508	CLA	CHA-C1A-NA	-2.40	120.89	126.40
41	B	601	SQD	O8-S-C6	2.40	109.57	105.74
43	H	101	DGD	C1D-C2D-C3D	-2.40	105.00	110.00
33	4	309	CLA	CHA-C1A-NA	-2.40	121.01	126.41
33	b	617	CLA	CHC-C4B-NB	-2.40	121.72	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	p	317	II0	C05-C07-C11	2.40	113.59	110.30
38	8	309	KC2	C3A-C4A-NA	-2.40	107.95	110.57
42	l	102	LMG	O1-C7-C8	-2.40	105.12	110.90
33	p	303	CLA	C2C-C1C-NC	2.40	112.22	109.97
38	1	311	KC2	CHD-C4C-NC	2.40	127.84	124.20
39	6	301	II0	C03-C09-C13	-2.39	119.26	122.63
41	b	601	SQD	O8-S-C6	2.39	109.55	105.74
33	1	302	CLA	CHA-C1A-NA	-2.39	120.93	126.40
37	b	623	LHG	C18-C17-C16	-2.39	102.30	114.42
37	1	317	LHG	C20-C19-C18	-2.39	102.31	114.42
37	7	317	LHG	C20-C19-C18	-2.39	102.31	114.42
42	d	409	LMG	C1-C2-C3	-2.39	105.02	110.00
44	F	101	HEM	CHA-C4D-C3D	-2.39	120.85	125.33
33	c	508	CLA	CHA-C1A-NA	-2.38	120.94	126.40
33	p	304	CLA	CAA-C2A-C1A	-2.38	106.86	112.14
33	C	505	CLA	C11-C12-C13	2.38	123.62	115.92
33	7	302	CLA	CHA-C1A-NA	-2.38	120.94	126.40
39	3	316	II0	C06-C08-C12	2.38	113.57	110.30
40	8	314	IHT	C03-C11-C15	2.38	126.00	122.63
40	2	314	IHT	C03-C11-C15	2.38	126.00	122.63
38	7	310	KC2	C4C-C3C-C2C	2.38	109.00	107.11
33	6	308	CLA	C2C-C1C-NC	2.38	112.20	109.97
42	D	409	LMG	C1-C2-C3	-2.38	105.04	110.00
37	B	623	LHG	C18-C17-C16	-2.38	102.34	114.42
33	c	505	CLA	C11-C12-C13	2.38	123.61	115.92
33	N	304	CLA	CHC-C4B-NB	-2.38	121.74	124.26
39	p	301	II0	C03-C09-C13	-2.38	119.28	122.63
38	7	311	KC2	CHD-C4C-NC	2.38	127.81	124.20
33	1	308	CLA	CHC-C4B-NB	-2.38	121.74	124.26
33	6	304	CLA	CAA-C2A-C1A	-2.38	106.88	112.14
39	6	317	II0	C05-C07-C11	2.37	113.56	110.30
33	b	614	CLA	CHC-C4B-NB	-2.37	121.75	124.26
36	D	407	PL9	C40-C39-C41	2.37	119.25	115.27
33	p	306	CLA	C2C-C1C-NC	2.37	112.19	109.97
37	8	315	LHG	C11-C10-C9	-2.36	102.42	114.42
38	9	311	KC2	CHD-C4C-NC	2.36	127.79	124.20
37	2	315	LHG	C11-C10-C9	-2.36	102.43	114.42
39	9	316	II0	C06-C08-C12	2.36	113.54	110.30
38	p	311	KC2	CHC-C1C-NC	2.36	127.92	124.20
33	9	303	CLA	CBA-CAA-C2A	2.36	120.83	113.86
33	6	306	CLA	C2C-C1C-NC	2.36	112.18	109.97
36	a	410	PL9	O2-C1-C6	2.36	124.67	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	C	518	DGD	O6E-C5E-C4E	2.36	113.97	109.69
33	6	312	CLA	CAA-C2A-C1A	-2.36	105.99	111.81
33	n	303	CLA	CHC-C4B-NB	-2.36	121.76	124.26
43	h	101	DGD	C3G-C2G-C1G	-2.35	106.22	111.79
33	g	301	CLA	CAA-C2A-C1A	-2.35	106.93	112.14
36	a	410	PL9	O2-C1-C2	-2.35	116.39	121.78
33	b	616	CLA	CHA-C1A-NA	-2.35	121.02	126.40
36	d	407	PL9	C40-C39-C41	2.35	119.22	115.27
42	c	520	LMG	O3-C3-C2	-2.35	104.92	110.35
33	5	301	CLA	CAA-C2A-C1A	-2.35	106.94	112.14
33	3	303	CLA	CBA-CAA-C2A	2.35	120.80	113.86
36	A	410	PL9	O2-C1-C2	-2.35	116.40	121.78
33	6	319	CLA	C2C-C1C-NC	2.35	112.17	109.97
33	g	306	CLA	CHA-C1A-NA	-2.35	121.02	126.40
33	7	308	CLA	CHC-C4B-NB	-2.35	121.77	124.26
43	c	518	DGD	O6E-C5E-C4E	2.35	113.96	109.69
33	B	616	CLA	CHA-C1A-NA	-2.35	121.03	126.40
33	3	309	CLA	CHA-C1A-NA	-2.34	121.03	126.40
33	p	312	CLA	CAA-C2A-C1A	-2.34	106.02	111.81
33	1	307	CLA	CHC-C4B-NB	-2.34	121.78	124.26
33	7	307	CLA	CHC-C4B-NB	-2.34	121.78	124.26
33	4	302	CLA	CHD-C1D-C2D	2.34	130.39	125.48
33	c	508	CLA	C3D-C4D-ND	2.34	114.02	110.24
38	1	310	KC2	CHD-C4C-NC	2.34	127.75	124.20
33	4	309	CLA	CHD-C1D-C2D	2.34	130.39	125.48
33	8	302	CLA	CAA-C2A-C1A	-2.34	104.31	111.97
36	A	410	PL9	O2-C1-C6	2.34	124.64	120.59
33	0	303	CLA	C1-C2-C3	-2.34	122.97	126.75
33	2	302	CLA	CAA-C2A-C1A	-2.34	104.31	111.97
33	C	507	CLA	CHC-C4B-NB	-2.34	121.78	124.26
33	0	310	CLA	CHD-C1D-C2D	2.34	130.38	125.48
33	5	306	CLA	CHA-C1A-NA	-2.34	121.05	126.40
33	C	506	CLA	C1-C2-C3	-2.34	122.00	126.04
38	3	311	KC2	CHD-C4C-NC	2.34	127.75	124.20
42	m	101	LMG	O2-C2-C1	-2.33	104.37	110.05
33	4	303	CLA	C1-C2-C3	-2.33	122.97	126.75
38	7	310	KC2	CHD-C4C-NC	2.33	127.75	124.20
38	1	311	KC2	CHB-C1B-NB	2.33	126.60	124.45
41	j	101	SQD	O8-S-C6	2.33	109.46	105.74
42	b	624	LMG	O1-C7-C8	-2.33	105.27	110.90
33	p	313	CLA	CAA-C2A-C1A	-2.33	106.05	111.81
42	B	624	LMG	O1-C7-C8	-2.33	105.27	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	6	313	CLA	CAA-C2A-C1A	-2.33	106.05	111.81
43	H	101	DGD	C3G-C2G-C1G	-2.33	106.28	111.79
33	C	508	CLA	C3D-C4D-ND	2.33	114.01	110.24
42	t	101	LMG	O1-C7-C8	-2.33	105.28	110.90
33	p	319	CLA	C2C-C1C-NC	2.33	112.16	109.97
33	B	614	CLA	CHC-C4B-NB	-2.33	121.79	124.26
42	T	101	LMG	O1-C7-C8	-2.33	105.28	110.90
42	l	102	LMG	O2-C2-C1	-2.33	104.39	110.05
33	c	507	CLA	CHC-C4B-NB	-2.33	121.79	124.26
33	p	302	CLA	C3A-C2A-C1A	-2.33	97.70	101.64
41	J	101	SQD	O8-S-C6	2.33	109.45	105.74
33	g	306	CLA	CHC-C4B-NB	-2.33	121.79	124.26
38	6	311	KC2	CHC-C1C-NC	2.33	127.87	124.20
33	p	303	CLA	CHD-C1D-C2D	2.33	130.36	125.48
38	p	311	KC2	CHB-C4A-NA	2.33	127.87	124.20
42	C	520	LMG	O3-C3-C2	-2.32	104.97	110.35
42	m	101	LMG	O6-C5-C4	2.32	113.92	109.69
33	3	306	CLA	CHC-C4B-NB	-2.32	121.80	124.26
33	9	309	CLA	CHA-C1A-NA	-2.32	121.08	126.40
41	b	601	SQD	O48-C23-C24	2.32	119.19	111.91
42	D	410	LMG	O3-C3-C2	-2.32	104.98	110.35
33	C	510	CLA	CHB-C4A-NA	2.32	127.72	124.51
37	B	623	LHG	C27-C26-C25	-2.32	102.65	114.42
38	6	311	KC2	CHB-C4A-NA	2.32	127.86	124.20
33	0	302	CLA	CHD-C1D-C2D	2.32	130.34	125.48
33	6	303	CLA	CHD-C1D-C2D	2.32	130.34	125.48
33	p	302	CLA	CHC-C4B-NB	-2.32	121.80	124.26
36	D	407	PL9	C22-C23-C24	-2.32	122.08	127.66
34	D	403	PHO	C4D-CHA-CBD	2.32	109.56	108.52
34	d	403	PHO	C4D-CHA-CBD	2.32	109.56	108.52
36	a	410	PL9	C20-C19-C21	2.32	119.17	115.27
33	6	302	CLA	C3A-C2A-C1A	-2.32	97.72	101.64
41	B	601	SQD	O48-C23-C24	2.31	119.17	111.91
33	B	614	CLA	CHB-C4A-NA	2.31	127.71	124.51
38	0	305	KC2	CHD-C4C-NC	2.31	127.71	124.20
44	F	101	HEM	C1A-CHA-C4D	-2.31	120.85	126.34
36	A	410	PL9	C20-C19-C21	2.31	119.16	115.27
33	2	302	CLA	CHA-C1A-NA	-2.31	121.10	126.40
42	l	102	LMG	O6-C5-C4	2.31	113.89	109.69
33	N	306	CLA	CHC-C4B-NB	-2.31	121.81	124.26
33	b	614	CLA	CHB-C4A-NA	2.31	127.71	124.51
33	6	302	CLA	C2A-C3A-C4A	-2.31	98.84	101.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	d	407	PL9	C22-C23-C24	-2.31	122.10	127.66
33	g	302	CLA	CHA-C1A-NA	-2.31	121.11	126.40
33	c	506	CLA	C1-C2-C3	-2.31	122.05	126.04
42	d	410	LMG	O3-C3-C2	-2.31	105.01	110.35
39	7	314	II0	C03-C09-C13	2.31	125.89	122.63
33	8	302	CLA	CHA-C1A-NA	-2.31	121.11	126.40
38	7	311	KC2	CHB-C1B-NB	2.30	126.57	124.45
33	c	510	CLA	CHB-C4A-NA	2.30	127.70	124.51
37	b	623	LHG	C27-C26-C25	-2.30	102.74	114.42
43	C	518	DGD	C3G-C2G-C1G	-2.30	106.35	111.79
38	4	305	KC2	CHD-C4C-NC	2.30	127.69	124.20
33	5	307	CLA	C1-C2-C3	-2.30	122.07	126.04
33	9	306	CLA	CHC-C4B-NB	-2.30	121.83	124.26
33	n	305	CLA	CHC-C4B-NB	-2.30	121.83	124.26
33	p	306	CLA	CHC-C1C-C2C	-2.30	120.35	126.73
43	c	518	DGD	C3G-C2G-C1G	-2.29	106.36	111.79
33	2	310	CLA	CHA-C1A-NA	-2.29	121.14	126.40
33	0	310	CLA	C2A-C1A-CHA	2.29	126.27	122.71
43	c	521	DGD	C4E-C3E-C2E	-2.29	106.82	110.82
37	d	401	LHG	O8-C23-C24	2.29	119.10	111.91
38	7	311	KC2	C4B-C3B-C2B	2.29	108.63	106.75
33	6	306	CLA	CHC-C1C-C2C	-2.29	120.37	126.73
33	6	302	CLA	CHC-C4B-NB	-2.29	121.83	124.26
33	8	310	CLA	CHA-C1A-NA	-2.29	121.16	126.40
37	D	401	LHG	O8-C23-C24	2.29	119.08	111.91
33	B	611	CLA	CHC-C4B-NB	-2.29	121.84	124.26
42	B	622	LMG	O3-C3-C2	-2.29	105.06	110.35
36	d	407	PL9	O2-C1-C6	2.29	124.55	120.59
33	5	302	CLA	CHA-C1A-NA	-2.29	121.16	126.40
33	4	309	CLA	C2A-C1A-CHA	2.29	126.25	122.71
33	5	306	CLA	CHC-C4B-NB	-2.28	121.84	124.26
38	1	311	KC2	C4B-C3B-C2B	2.28	108.63	106.75
43	c	518	DGD	CBB-CAB-C9B	-2.28	102.84	114.42
43	C	518	DGD	CBB-CAB-C9B	-2.28	102.84	114.42
33	2	305	CLA	CHC-C4B-NB	-2.28	121.84	124.26
33	g	307	CLA	C1-C2-C3	-2.28	122.10	126.04
39	1	314	II0	C03-C09-C13	2.28	125.86	122.63
33	n	306	CLA	CHC-C1C-C2C	-2.28	120.39	126.73
33	p	302	CLA	C2A-C3A-C4A	-2.28	98.87	101.78
43	C	521	DGD	C4E-C3E-C2E	-2.28	106.84	110.82
42	W	101	LMG	O3-C3-C2	-2.28	105.08	110.35
33	N	307	CLA	CHC-C1C-C2C	-2.28	120.40	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	0	304	CLA	CHC-C1C-C2C	-2.28	120.40	126.73
39	1	315	II0	C05-C07-C11	2.28	113.42	110.30
33	B	603	CLA	C1-C2-C3	-2.28	122.11	126.04
33	b	615	CLA	CHC-C4B-NB	-2.28	121.85	124.26
39	4	314	II0	C05-C07-C11	-2.27	107.19	110.30
34	a	407	PHO	CMD-C2D-C3D	2.27	128.93	124.68
33	g	317	CLA	C2C-C1C-NC	2.27	112.10	109.97
39	0	315	II0	C05-C07-C11	-2.27	107.19	110.30
33	1	307	CLA	C3A-C2A-C1A	-2.27	97.94	101.34
42	t	101	LMG	C1-O6-C5	2.27	118.14	113.69
33	C	502	CLA	CHC-C4B-NB	-2.27	121.85	124.26
33	b	607	CLA	CHD-C1D-C2D	2.27	130.24	125.48
33	5	317	CLA	C2C-C1C-NC	2.27	112.10	109.97
33	4	301	CLA	C2C-C1C-NC	2.26	112.09	109.97
33	B	607	CLA	CHD-C1D-C2D	2.26	130.23	125.48
33	b	603	CLA	C1-C2-C3	-2.26	122.13	126.04
36	A	410	PL9	O1-C4-C3	-2.26	118.23	120.72
33	2	302	CLA	CHC-C4B-NB	-2.26	121.86	124.26
33	b	611	CLA	CHC-C4B-NB	-2.26	121.86	124.26
33	4	306	CLA	CHC-C1C-C2C	-2.26	120.45	126.73
33	4	304	CLA	CHC-C1C-C2C	-2.26	120.45	126.73
42	w	101	LMG	O3-C3-C2	-2.26	105.12	110.35
36	D	407	PL9	O2-C1-C6	2.26	124.50	120.59
33	0	306	CLA	CHC-C1C-C2C	-2.26	120.45	126.73
33	b	618	CLA	CHC-C1C-C2C	-2.26	120.45	126.73
33	6	307	CLA	CHD-C1D-C2D	2.26	130.21	125.48
33	p	304	CLA	CHC-C4B-NB	-2.26	121.87	124.26
42	b	622	LMG	O3-C3-C2	-2.26	105.14	110.35
33	p	308	CLA	CAA-C2A-C1A	-2.25	107.15	112.14
36	a	410	PL9	O1-C4-C3	-2.25	118.24	120.72
39	7	315	II0	C05-C07-C11	2.25	113.39	110.30
33	c	502	CLA	CHC-C4B-NB	-2.25	121.87	124.26
33	a	406	CLA	CHD-C1D-C2D	2.25	130.21	125.48
33	6	308	CLA	CAA-C2A-C1A	-2.25	107.15	112.14
33	p	302	CLA	CHA-C1A-NA	-2.25	121.24	126.40
33	4	309	CLA	C2A-C3A-C4A	-2.25	99.58	103.59
42	T	101	LMG	O6-C1-C2	2.25	115.12	110.35
33	8	305	CLA	CHC-C4B-NB	-2.25	121.87	124.26
33	6	302	CLA	CHA-C1A-NA	-2.25	121.24	126.40
33	0	310	CLA	C2A-C3A-C4A	-2.25	99.59	103.59
34	A	407	PHO	CMD-C2D-C3D	2.25	128.89	124.68
33	0	307	CLA	CMC-C2C-C1C	2.25	128.47	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	5	309	KC2	CHD-C4C-NC	2.25	127.62	124.20
42	b	624	LMG	O2-C2-C1	-2.25	104.58	110.05
33	p	307	CLA	CHD-C1D-C2D	2.25	130.20	125.48
34	D	403	PHO	CMD-C2D-C3D	2.25	128.89	124.68
33	A	406	CLA	CHD-C1D-C2D	2.25	130.20	125.48
33	4	307	CLA	CMC-C2C-C1C	2.25	128.46	125.04
33	6	319	CLA	CHA-C1A-NA	-2.25	121.25	126.40
33	5	307	CLA	CHC-C4B-NB	-2.25	121.88	124.26
42	d	410	LMG	O2-C2-C1	-2.24	104.59	110.05
33	p	319	CLA	CHA-C1A-NA	-2.24	121.26	126.40
33	0	301	CLA	C2C-C1C-NC	2.24	112.07	109.97
42	D	410	LMG	O2-C2-C1	-2.24	104.60	110.05
33	7	307	CLA	C3A-C2A-C1A	-2.24	97.98	101.34
33	a	405	CLA	CHA-C1A-NA	-2.24	121.26	126.40
42	C	520	LMG	C40-C39-C38	-2.24	103.05	114.42
33	A	405	CLA	CHA-C1A-NA	-2.24	121.27	126.40
38	9	311	KC2	CHB-C1B-NB	2.24	126.51	124.45
33	7	301	CLA	CHC-C4B-NB	-2.24	121.89	124.26
42	T	101	LMG	C1-O6-C5	2.24	118.08	113.69
33	3	308	CLA	CHA-C1A-NA	-2.24	121.27	126.40
33	1	301	CLA	CHC-C4B-NB	-2.24	121.89	124.26
33	7	302	CLA	CHC-C4B-NB	-2.24	121.89	124.26
38	p	311	KC2	CHC-C1C-C2C	-2.24	121.48	124.98
33	6	304	CLA	CHC-C4B-NB	-2.24	121.89	124.26
38	7	311	KC2	CHB-C4A-NA	2.24	127.73	124.20
42	B	624	LMG	O2-C2-C1	-2.24	104.61	110.05
33	g	307	CLA	CHC-C4B-NB	-2.24	121.89	124.26
42	c	520	LMG	C40-C39-C38	-2.24	103.08	114.42
38	8	309	KC2	CHC-C4B-NB	2.24	126.51	124.45
33	B	615	CLA	CHC-C4B-NB	-2.23	121.89	124.26
38	g	309	KC2	CHD-C4C-NC	2.23	127.59	124.20
42	c	520	LMG	O8-C28-O10	-2.23	117.95	123.59
33	6	308	CLA	CHD-C1D-C2D	2.23	130.17	125.48
33	3	306	CLA	CHD-C1D-C2D	2.23	130.16	125.48
34	d	403	PHO	CMD-C2D-C3D	2.23	128.85	124.68
38	8	309	KC2	CHD-C4C-NC	2.23	127.59	124.20
33	B	618	CLA	CHD-C1D-C2D	2.23	130.16	125.48
33	B	611	CLA	CHA-C1A-NA	-2.23	121.29	126.40
33	7	302	CLA	CHD-C1D-C2D	2.23	130.15	125.48
33	B	618	CLA	CHC-C1C-C2C	-2.23	120.54	126.73
33	9	306	CLA	CHD-C1D-C2D	2.23	130.15	125.48
42	t	101	LMG	O6-C1-C2	2.23	115.06	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	302	CLA	CHC-C4B-NB	-2.23	121.90	124.26
33	p	308	CLA	CHD-C1D-C2D	2.23	130.15	125.48
33	b	605	CLA	C2C-C1C-NC	2.23	112.06	109.97
39	9	319	II0	C05-C07-C11	-2.23	107.26	110.30
33	1	307	CLA	CHA-C1A-NA	-2.22	121.30	126.40
33	N	301	CLA	CHC-C4B-NB	-2.22	121.90	124.26
39	2	311	II0	C05-C07-C11	-2.22	107.26	110.30
33	p	309	CLA	CHD-C1D-C2D	2.22	130.14	125.48
33	g	317	CLA	CHC-C4B-NB	-2.22	121.90	124.26
39	3	319	II0	C05-C07-C11	-2.22	107.26	110.30
38	2	309	KC2	CHC-C4B-NB	2.22	126.50	124.45
33	2	302	CLA	CHD-C1D-C2D	2.22	130.14	125.48
33	9	308	CLA	CHA-C1A-NA	-2.22	121.31	126.40
33	9	309	CLA	CAA-C2A-C3A	2.22	118.86	112.78
33	n	302	CLA	CHD-C1D-C2D	2.22	130.14	125.48
33	1	302	CLA	CHD-C1D-C2D	2.22	130.14	125.48
33	3	309	CLA	CAA-C2A-C3A	2.22	118.86	112.78
33	g	317	CLA	CHD-C1D-C2D	2.22	130.14	125.48
38	6	311	KC2	CHC-C1C-C2C	-2.22	121.51	124.98
36	D	407	PL9	C36-C34-C33	-2.22	116.62	121.12
33	b	611	CLA	CHA-C1A-NA	-2.22	121.31	126.40
38	1	311	KC2	CHB-C4A-NA	2.22	127.70	124.20
33	7	302	CLA	CAA-C2A-C1A	-2.22	104.70	111.97
39	8	311	II0	C05-C07-C11	-2.22	107.27	110.30
38	2	309	KC2	CHD-C4C-NC	2.22	127.57	124.20
33	5	305	CLA	CHD-C1D-C2D	2.22	130.13	125.48
36	d	407	PL9	C36-C34-C33	-2.22	116.63	121.12
42	B	624	LMG	O3-C3-C2	-2.22	105.22	110.35
33	n	303	CLA	CHA-C1A-NA	-2.22	121.32	126.40
33	1	302	CLA	CBA-CAA-C2A	2.22	120.40	113.86
42	b	624	LMG	O3-C3-C2	-2.21	105.23	110.35
33	p	319	CLA	CHD-C1D-C2D	2.21	130.12	125.48
33	C	513	CLA	C1-C2-C3	-2.21	122.22	126.04
33	9	314	CLA	CHC-C4B-NB	-2.21	121.92	124.26
33	6	319	CLA	CHD-C1D-C2D	2.21	130.12	125.48
33	p	308	CLA	CHC-C1C-C2C	-2.21	120.59	126.73
43	c	521	DGD	O5D-C6D-C5D	-2.21	104.96	109.05
43	C	521	DGD	O5D-C6D-C5D	-2.21	104.96	109.05
39	6	316	II0	C05-C07-C11	-2.21	107.28	110.30
33	1	302	CLA	CAA-C2A-C1A	-2.21	104.74	111.97
33	B	614	CLA	C2C-C1C-NC	2.21	112.04	109.97
36	d	407	PL9	C11-C9-C8	-2.21	116.65	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	302	CLA	CHD-C1D-C2D	2.21	130.11	125.48
42	m	101	LMG	O3-C3-C2	-2.21	105.25	110.35
33	B	610	CLA	CHA-C1A-NA	-2.21	121.34	126.40
42	C	520	LMG	O8-C28-O10	-2.21	118.02	123.59
33	5	302	CLA	CHC-C4B-NB	-2.21	121.92	124.26
33	b	614	CLA	C2C-C1C-NC	2.21	112.04	109.97
33	5	317	CLA	CHD-C1D-C2D	2.21	130.11	125.48
33	1	302	CLA	CHC-C4B-NB	-2.21	121.92	124.26
33	5	317	CLA	CHC-C4B-NB	-2.21	121.92	124.26
33	g	305	CLA	CHD-C1D-C2D	2.21	130.11	125.48
33	0	308	CLA	C2C-C1C-NC	2.21	112.04	109.97
33	6	309	CLA	CHD-C1D-C2D	2.21	130.10	125.48
33	N	302	CLA	CHD-C1D-C2D	2.21	130.10	125.48
33	g	307	CLA	CAA-C2A-C1A	-2.20	104.75	111.97
33	a	405	CLA	CHB-C4A-NA	2.20	127.56	124.51
33	7	302	CLA	CBA-CAA-C2A	2.20	120.36	113.86
33	2	310	CLA	CHD-C1D-C2D	2.20	130.10	125.48
33	b	610	CLA	CHA-C1A-NA	-2.20	121.36	126.40
33	4	307	CLA	CHD-C1D-C2D	2.20	130.09	125.48
33	7	307	CLA	CHA-C1A-NA	-2.20	121.36	126.40
33	c	513	CLA	C1-C2-C3	-2.20	122.24	126.04
33	5	307	CLA	CAA-C2A-C1A	-2.20	104.77	111.97
33	N	303	CLA	CHC-C1C-C2C	-2.20	120.62	126.73
33	b	618	CLA	CHD-C1D-C2D	2.20	130.09	125.48
33	0	311	CLA	CHC-C1C-C2C	-2.20	120.63	126.73
33	0	308	CLA	CHC-C1C-C2C	-2.20	120.63	126.73
33	b	606	CLA	C1-C2-C3	-2.19	122.25	126.04
33	A	405	CLA	CHB-C4A-NA	2.19	127.55	124.51
33	8	310	CLA	CHD-C1D-C2D	2.19	130.08	125.48
33	5	302	CLA	CAA-C2A-C1A	-2.19	104.78	111.97
38	0	305	KC2	CHB-C4A-C3A	-2.19	121.55	124.98
33	N	304	CLA	CHA-C1A-NA	-2.19	121.38	126.40
38	3	311	KC2	CHB-C1B-NB	2.19	126.47	124.45
38	9	311	KC2	C4C-C3C-C2C	2.19	108.86	107.11
36	D	407	PL9	C11-C9-C8	-2.19	116.68	121.12
33	c	506	CLA	CBA-CAA-C2A	2.19	120.33	113.86
33	p	307	CLA	CHC-C1C-C2C	-2.19	120.64	126.73
33	0	311	CLA	CHD-C1D-C2D	2.19	130.07	125.48
33	6	307	CLA	CHC-C1C-C2C	-2.19	120.65	126.73
33	3	314	CLA	CHC-C4B-NB	-2.19	121.94	124.26
39	p	316	II0	C05-C07-C11	-2.19	107.31	110.30
33	B	605	CLA	C2C-C1C-NC	2.19	112.02	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	b	602	CLA	C2C-C1C-NC	2.19	112.02	109.97
33	g	302	CLA	CAA-C2A-C1A	-2.19	104.81	111.97
33	C	502	CLA	CBA-CAA-C2A	2.19	120.32	113.86
33	7	304	CLA	CHC-C4B-NB	-2.19	121.94	124.26
33	B	606	CLA	C1-C2-C3	-2.19	122.26	126.04
37	7	317	LHG	C18-C17-C16	-2.19	103.33	114.42
33	4	310	CLA	CHC-C1C-C2C	-2.19	120.66	126.73
42	l	102	LMG	O3-C3-C2	-2.19	105.30	110.35
33	4	301	CLA	CHC-C1C-C2C	-2.19	120.66	126.73
33	0	307	CLA	CHD-C1D-C2D	2.18	130.06	125.48
33	6	308	CLA	CHC-C1C-C2C	-2.18	120.66	126.73
33	C	506	CLA	CBA-CAA-C2A	2.18	120.31	113.86
33	c	502	CLA	CBA-CAA-C2A	2.18	120.31	113.86
33	p	309	CLA	CHA-C1A-NA	-2.18	121.40	126.40
37	1	317	LHG	C18-C17-C16	-2.18	103.34	114.42
37	2	315	LHG	C27-C26-C25	-2.18	103.34	114.42
38	3	311	KC2	C4C-C3C-C2C	2.18	108.85	107.11
43	c	521	DGD	CBB-CAB-C9B	-2.18	103.34	114.42
33	b	603	CLA	CHC-C4B-NB	-2.18	121.95	124.26
33	N	307	CLA	CHD-C1D-C2D	2.18	130.06	125.48
37	8	315	LHG	C27-C26-C25	-2.18	103.35	114.42
33	1	305	CLA	CHC-C4B-NB	-2.18	121.95	124.26
33	6	309	CLA	CHA-C1A-NA	-2.18	121.41	126.40
33	g	302	CLA	CHC-C4B-NB	-2.18	121.95	124.26
42	b	624	LMG	O6-C1-O1	-2.18	104.81	109.97
33	5	307	CLA	CHD-C1D-C2D	2.18	130.05	125.48
33	3	303	CLA	CHD-C1D-C2D	2.18	130.05	125.48
33	B	611	CLA	C2C-C1C-NC	2.18	112.01	109.97
33	6	305	CLA	CHC-C1C-C2C	-2.18	120.68	126.73
43	C	521	DGD	CBB-CAB-C9B	-2.18	103.37	114.42
33	N	303	CLA	C2C-C1C-NC	2.18	112.01	109.97
33	4	301	CLA	CHD-C1D-C2D	2.18	130.05	125.48
33	0	301	CLA	CHC-C1C-C2C	-2.18	120.68	126.73
42	t	101	LMG	O6-C5-C4	2.18	113.65	109.69
33	9	303	CLA	CHD-C1D-C2D	2.18	130.04	125.48
44	F	101	HEM	C4D-ND-C1D	2.17	107.32	105.07
33	n	306	CLA	CHD-C1D-C2D	2.17	130.04	125.48
33	g	308	CLA	CHC-C4B-NB	-2.17	121.96	124.26
33	p	305	CLA	CHC-C1C-C2C	-2.17	120.69	126.73
33	B	602	CLA	C2C-C1C-NC	2.17	112.01	109.97
33	4	301	CLA	CAA-C2A-C1A	-2.17	106.44	111.81
33	p	313	CLA	CHD-C1D-C2D	2.17	130.03	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	6	301	II0	C04-C10-C14	-2.17	119.57	122.63
42	B	624	LMG	O6-C1-O1	-2.17	104.83	109.97
33	4	310	CLA	CHD-C1D-C2D	2.17	130.03	125.48
33	0	301	CLA	CAA-C2A-C1A	-2.17	106.45	111.81
33	C	512	CLA	C2C-C1C-NC	2.17	112.00	109.97
33	9	308	CLA	CBA-CAA-C2A	2.17	120.27	113.86
33	5	308	CLA	CHC-C4B-NB	-2.17	121.96	124.26
38	4	305	KC2	CHB-C4A-C3A	-2.17	121.59	124.98
42	T	101	LMG	O6-C5-C4	2.17	113.63	109.69
33	6	306	CLA	CHD-C1D-C2D	2.17	130.03	125.48
33	6	313	CLA	CHD-C1D-C2D	2.17	130.02	125.48
33	g	302	CLA	CHB-C4A-NA	2.16	127.50	124.51
33	1	304	CLA	CHC-C4B-NB	-2.16	121.97	124.26
38	6	311	KC2	CHD-C4C-NC	2.16	127.49	124.20
34	a	407	PHO	O2A-C1-C2	-2.16	102.95	108.64
33	7	305	CLA	CHC-C4B-NB	-2.16	121.97	124.26
33	0	301	CLA	CHD-C1D-C2D	2.16	130.01	125.48
38	7	311	KC2	CHC-C4B-NB	2.16	126.44	124.45
33	3	308	CLA	CBA-CAA-C2A	2.16	120.24	113.86
33	b	611	CLA	CHB-C4A-NA	2.16	127.50	124.51
33	9	312	CLA	CHD-C1D-C2D	2.16	130.01	125.48
38	7	310	KC2	CHC-C4B-NB	2.16	126.44	124.45
41	l	101	SQD	O9-S-C6	2.16	109.50	106.94
33	b	614	CLA	CHA-C1A-NA	-2.16	121.46	126.40
33	B	611	CLA	CHB-C4A-NA	2.16	127.50	124.51
33	p	306	CLA	CHD-C1D-C2D	2.16	130.00	125.48
42	B	622	LMG	C1-C2-C3	-2.16	105.50	110.00
34	A	407	PHO	O2A-C1-C2	-2.16	102.97	108.64
33	5	302	CLA	CHB-C4A-NA	2.16	127.49	124.51
38	p	311	KC2	CHD-C4C-NC	2.16	127.47	124.20
33	B	614	CLA	CHA-C1A-NA	-2.16	121.46	126.40
33	n	301	CLA	CHC-C4B-NB	-2.15	121.98	124.26
37	3	322	LHG	C27-C26-C25	-2.15	103.49	114.42
33	B	610	CLA	C2C-C1C-NC	2.15	111.99	109.97
33	4	306	CLA	CHD-C1D-C2D	2.15	129.99	125.48
33	5	303	CLA	CHD-C1D-C2D	2.15	129.99	125.48
38	1	310	KC2	CHB-C4A-NA	2.15	127.59	124.20
39	3	317	II0	C05-C07-C11	-2.15	107.36	110.30
33	b	618	CLA	CHC-C4B-NB	-2.15	121.98	124.26
33	g	303	CLA	CHD-C1D-C2D	2.15	129.99	125.48
33	6	319	CLA	CHC-C1C-C2C	-2.15	120.76	126.73
33	g	307	CLA	CHD-C1D-C2D	2.15	129.99	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	303	CLA	CHD-C1D-C2D	2.15	129.99	125.48
37	9	322	LHG	C27-C26-C25	-2.15	103.52	114.42
33	c	512	CLA	C2C-C1C-NC	2.15	111.98	109.97
42	C	520	LMG	C38-C37-C36	-2.15	103.53	114.42
39	g	312	II0	C03-C05-C07	2.15	118.49	113.64
33	A	405	CLA	CHD-C1D-C2D	2.15	129.98	125.48
42	c	520	LMG	C38-C37-C36	-2.15	103.53	114.42
38	6	311	KC2	C2D-C1D-ND	-2.15	108.79	110.23
33	2	303	CLA	CHD-C1D-C2D	2.15	129.98	125.48
33	g	311	CLA	CHA-C1A-NA	-2.14	121.49	126.40
39	p	301	II0	C04-C10-C14	-2.14	119.61	122.63
38	1	311	KC2	CHC-C4B-NB	2.14	126.42	124.45
39	5	312	II0	C03-C05-C07	2.14	118.48	113.64
33	8	304	CLA	CHD-C1D-C2D	2.14	129.97	125.48
33	5	305	CLA	CBD-CHA-C1A	2.14	131.02	128.50
33	g	305	CLA	CBD-CHA-C1A	2.14	131.02	128.50
33	3	312	CLA	CHD-C1D-C2D	2.14	129.97	125.48
33	g	317	CLA	CHC-C1C-C2C	-2.14	120.79	126.73
33	n	303	CLA	CHD-C1D-C2D	2.14	129.97	125.48
33	b	611	CLA	C2C-C1C-NC	2.14	111.97	109.97
43	c	519	DGD	O3E-C3E-C2E	-2.14	105.41	110.35
41	L	101	SQD	O9-S-C6	2.14	109.48	106.94
42	b	622	LMG	C1-C2-C3	-2.14	105.55	110.00
33	0	307	CLA	C2C-C1C-NC	2.13	111.97	109.97
38	7	310	KC2	CHB-C4A-NA	2.13	127.57	124.20
33	p	319	CLA	CHC-C1C-C2C	-2.13	120.80	126.73
33	4	307	CLA	CHC-C4B-NB	-2.13	122.00	124.26
39	9	317	II0	C05-C07-C11	-2.13	107.38	110.30
33	a	405	CLA	CHD-C1D-C2D	2.13	129.95	125.48
33	5	311	CLA	CHA-C1A-NA	-2.13	121.52	126.40
33	9	309	CLA	CHD-C1D-C2D	2.13	129.95	125.48
33	0	306	CLA	CHD-C1D-C2D	2.13	129.95	125.48
37	d	402	LHG	C11-C10-C9	-2.13	103.61	114.42
33	2	306	CLA	CMC-C2C-C1C	2.13	128.28	125.04
38	9	311	KC2	CHB-C4A-NA	2.13	127.56	124.20
33	7	307	CLA	CHD-C1D-C2D	2.13	129.95	125.48
33	5	311	CLA	CHC-C4B-NB	-2.13	122.00	124.26
33	B	603	CLA	CHC-C4B-NB	-2.13	122.00	124.26
33	5	317	CLA	CHC-C1C-C2C	-2.13	120.82	126.73
44	F	101	HEM	CAA-CBA-CGA	-2.13	109.02	113.60
33	b	610	CLA	C2C-C1C-NC	2.13	111.97	109.97
33	9	305	CLA	CHC-C4B-NB	-2.13	122.00	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	2	304	CLA	CHD-C1D-C2D	2.13	129.94	125.48
37	D	402	LHG	C11-C10-C9	-2.13	103.62	114.42
43	C	519	DGD	O3E-C3E-C2E	-2.13	105.43	110.35
33	4	304	CLA	CHD-C1D-C2D	2.13	129.94	125.48
33	3	312	CLA	CHA-C1A-NA	-2.13	121.53	126.40
33	9	312	CLA	CHA-C1A-NA	-2.13	121.53	126.40
33	8	306	CLA	CMC-C2C-C1C	2.12	128.27	125.04
33	1	307	CLA	CHD-C1D-C2D	2.12	129.93	125.48
41	C	501	SQD	O6-C1-C2	2.12	111.61	108.30
37	7	317	LHG	C27-C26-C25	-2.12	103.66	114.42
36	a	410	PL9	C8-C7-C3	2.12	117.97	111.98
33	0	307	CLA	CHC-C4B-NB	-2.12	122.01	124.26
39	9	318	II0	C04-C10-C14	2.12	125.62	122.63
33	4	307	CLA	C2C-C1C-NC	2.12	111.96	109.97
42	t	101	LMG	O3-C3-C2	-2.12	105.45	110.35
33	6	306	CLA	CHB-C4A-NA	2.12	127.44	124.51
37	1	317	LHG	C27-C26-C25	-2.12	103.68	114.42
33	3	309	CLA	CHD-C1D-C2D	2.12	129.92	125.48
33	5	311	CLA	CBA-CAA-C2A	2.11	120.11	113.86
33	c	513	CLA	C2C-C1C-NC	2.11	111.95	109.97
33	0	304	CLA	CHD-C1D-C2D	2.11	129.91	125.48
33	g	311	CLA	CBA-CAA-C2A	2.11	120.10	113.86
33	6	310	CLA	CHA-C1A-NA	-2.11	121.56	126.40
33	g	311	CLA	CHC-C4B-NB	-2.11	122.02	124.26
37	D	401	LHG	C20-C19-C18	-2.11	103.71	114.42
36	A	410	PL9	C8-C7-C3	2.11	117.94	111.98
43	C	521	DGD	C5B-C4B-C3B	-2.11	103.71	114.42
33	2	307	CLA	CHC-C4B-NB	-2.11	122.02	124.26
41	c	501	SQD	O6-C1-C2	2.11	111.60	108.30
33	N	304	CLA	CHD-C1D-C2D	2.11	129.90	125.48
43	c	521	DGD	C5B-C4B-C3B	-2.11	103.72	114.42
37	d	401	LHG	C20-C19-C18	-2.11	103.72	114.42
33	b	607	CLA	CHC-C4B-NB	-2.11	122.03	124.26
42	T	101	LMG	O3-C3-C2	-2.11	105.48	110.35
36	D	407	PL9	C50-C49-C48	-2.11	116.56	122.65
36	d	407	PL9	C50-C49-C48	-2.11	116.56	122.65
33	b	609	CLA	C2C-C1C-NC	2.10	111.94	109.97
33	B	618	CLA	CHA-C1A-NA	-2.10	121.68	126.41
33	6	308	CLA	CHA-C1A-NA	-2.10	121.58	126.40
33	D	404	CLA	CHA-C1A-NA	-2.10	121.58	126.40
38	1	310	KC2	CHC-C4B-NB	2.10	126.39	124.45
33	C	512	CLA	CHD-C1D-C2D	2.10	129.89	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	5	302	CLA	CHD-C1D-C2D	2.10	129.89	125.48
33	6	302	CLA	CHD-C1D-C2D	2.10	129.88	125.48
33	d	404	CLA	CHA-C1A-NA	-2.10	121.59	126.40
33	A	412	CLA	CHB-C4A-NA	2.10	127.42	124.51
33	8	306	CLA	CHD-C1D-C2D	2.10	129.88	125.48
42	b	622	LMG	O2-C2-C1	-2.10	104.95	110.05
33	B	611	CLA	CHC-C1C-C2C	-2.10	120.90	126.73
44	F	101	HEM	CHA-C1A-NA	2.10	127.70	123.85
33	B	604	CLA	CHC-C4B-NB	-2.10	122.04	124.26
33	2	301	CLA	CHA-C1A-NA	-2.10	121.60	126.40
33	p	310	CLA	CHA-C1A-NA	-2.09	121.60	126.40
33	p	306	CLA	CHB-C4A-NA	2.09	127.41	124.51
33	b	604	CLA	CHC-C4B-NB	-2.09	122.04	124.26
33	9	315	CLA	CHA-C1A-NA	-2.09	121.60	126.40
42	B	622	LMG	O2-C2-C1	-2.09	104.96	110.05
33	B	616	CLA	CHC-C1C-C2C	-2.09	120.91	126.73
33	7	309	CLA	CHA-C1A-NA	-2.09	121.60	126.40
33	c	509	CLA	CHC-C4B-NB	-2.09	122.04	124.26
33	5	305	CLA	C3A-C4A-CHB	-2.09	118.50	124.01
33	g	302	CLA	CHD-C1D-C2D	2.09	129.87	125.48
33	p	308	CLA	CHA-C1A-NA	-2.09	121.61	126.40
33	c	514	CLA	C2C-C1C-NC	2.09	111.93	109.97
33	3	305	CLA	CHC-C4B-NB	-2.09	122.04	124.26
39	9	318	II0	C05-C07-C11	-2.09	107.44	110.30
33	b	616	CLA	CHC-C1C-C2C	-2.09	120.92	126.73
33	p	302	CLA	CHD-C1D-C2D	2.09	129.86	125.48
33	B	609	CLA	C2C-C1C-NC	2.09	111.93	109.97
43	c	518	DGD	C1D-C2D-C3D	-2.09	105.65	110.00
33	0	307	CLA	CHD-C4C-C3C	-2.09	121.77	124.84
37	D	401	LHG	C27-C26-C25	-2.09	103.83	114.42
44	F	101	HEM	C4C-CHD-C1D	-2.09	121.56	126.06
39	3	318	II0	C05-C07-C11	-2.09	107.45	110.30
38	p	311	KC2	C2D-C1D-ND	-2.09	108.83	110.23
33	n	305	CLA	C2C-C1C-NC	2.09	111.93	109.97
37	d	401	LHG	C27-C26-C25	-2.09	103.84	114.42
33	3	313	CLA	CAA-C2A-C1A	-2.09	106.66	111.81
33	8	306	CLA	CHA-C1A-NA	-2.08	121.62	126.40
33	a	412	CLA	CHB-C4A-NA	2.08	127.39	124.51
33	B	609	CLA	CHA-C1A-NA	-2.08	121.62	126.40
33	g	305	CLA	C3A-C4A-CHB	-2.08	118.52	124.01
33	3	315	CLA	CHA-C1A-NA	-2.08	121.63	126.40
33	b	618	CLA	CHA-C1A-NA	-2.08	121.72	126.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	b	603	CLA	CHD-C1D-C2D	2.08	129.85	125.48
33	8	301	CLA	CHA-C1A-NA	-2.08	121.63	126.40
33	C	510	CLA	CHD-C1D-C2D	2.08	129.85	125.48
37	9	302	LHG	C11-C10-C9	-2.08	103.86	114.42
33	6	310	CLA	CHD-C1D-C2D	2.08	129.85	125.48
37	3	302	LHG	C11-C10-C9	-2.08	103.86	114.42
33	1	309	CLA	CHA-C1A-NA	-2.08	121.63	126.40
33	B	614	CLA	CHD-C1D-C2D	2.08	129.84	125.48
38	3	311	KC2	CHB-C4A-NA	2.08	127.48	124.20
33	g	307	CLA	CHD-C4C-C3C	-2.08	121.78	124.84
42	C	520	LMG	O1-C1-C2	-2.08	105.06	108.30
33	2	306	CLA	CHD-C1D-C2D	2.08	129.84	125.48
33	6	303	CLA	CHC-C1C-C2C	-2.08	120.95	126.73
33	b	611	CLA	CHC-C1C-C2C	-2.08	120.95	126.73
43	C	518	DGD	C1D-C2D-C3D	-2.08	105.67	110.00
33	9	303	CLA	CHC-C4B-NB	-2.08	122.06	124.26
33	c	510	CLA	CHD-C1D-C2D	2.08	129.84	125.48
33	C	513	CLA	C2C-C1C-NC	2.08	111.92	109.97
42	l	102	LMG	O6-C1-O1	-2.08	105.06	109.97
42	m	101	LMG	O6-C1-O1	-2.08	105.06	109.97
44	F	101	HEM	CHB-C1B-C2B	-2.07	120.97	126.73
33	4	306	CLA	CHA-C1A-NA	-2.07	121.65	126.40
33	B	606	CLA	CHD-C1D-C2D	2.07	129.83	125.48
33	c	511	CLA	C2C-C1C-NC	2.07	111.92	109.97
33	0	306	CLA	CHB-C4A-NA	2.07	127.38	124.51
33	c	512	CLA	CHD-C1D-C2D	2.07	129.83	125.48
33	9	313	CLA	CAA-C2A-C1A	-2.07	106.69	111.81
33	8	307	CLA	CHC-C4B-NB	-2.07	122.06	124.26
33	2	306	CLA	CHA-C1A-NA	-2.07	121.65	126.40
33	5	307	CLA	CHD-C4C-C3C	-2.07	121.80	124.84
33	1	301	CLA	CHA-C1A-NA	-2.07	121.66	126.40
33	p	303	CLA	CHC-C1C-C2C	-2.07	120.98	126.73
43	h	101	DGD	CDB-CCB-CBB	-2.07	103.92	114.42
33	6	306	CLA	CHC-C4B-NB	-2.07	122.07	124.26
38	g	309	KC2	CHC-C4B-NB	2.07	126.35	124.45
39	3	318	II0	C04-C10-C14	2.07	125.55	122.63
42	c	520	LMG	O1-C1-C2	-2.07	105.08	108.30
33	8	301	CLA	CHD-C1D-C2D	2.07	129.81	125.48
33	p	310	CLA	CHD-C1D-C2D	2.07	129.81	125.48
33	9	304	CLA	CHA-C1A-NA	-2.07	121.67	126.40
33	b	609	CLA	CHA-C1A-NA	-2.07	121.67	126.40
33	N	301	CLA	CHD-C1D-C2D	2.07	129.81	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	5	309	KC2	CHC-C4B-NB	2.07	126.35	124.45
33	0	306	CLA	CHA-C1A-NA	-2.06	121.67	126.40
33	4	307	CLA	CHD-C4C-C3C	-2.06	121.81	124.84
33	p	306	CLA	CHC-C1C-NC	2.06	127.33	124.20
33	C	511	CLA	C2C-C1C-NC	2.06	111.91	109.97
33	b	606	CLA	CHD-C1D-C2D	2.06	129.81	125.48
33	B	609	CLA	CHD-C1D-C2D	2.06	129.81	125.48
33	4	302	CLA	C2C-C1C-NC	2.06	111.90	109.97
33	g	301	CLA	CHC-C1C-C2C	-2.06	121.00	126.73
43	H	101	DGD	CDB-CCB-CBB	-2.06	103.96	114.42
33	3	303	CLA	CHC-C4B-NB	-2.06	122.08	124.26
33	N	305	CLA	C2C-C1C-NC	2.06	111.90	109.97
33	9	307	CLA	CHA-C1A-NA	-2.06	121.68	126.40
33	9	314	CLA	CHA-C1A-NA	-2.06	121.68	126.40
33	5	311	CLA	CHD-C1D-C2D	2.06	129.80	125.48
33	7	304	CLA	CHD-C1D-C2D	2.06	129.80	125.48
33	8	305	CLA	CHD-C1D-C2D	2.06	129.80	125.48
33	9	306	CLA	CHA-C1A-NA	-2.06	121.69	126.40
33	n	302	CLA	CHA-C1A-NA	-2.06	121.69	126.40
33	B	603	CLA	CHD-C1D-C2D	2.06	129.79	125.48
33	2	308	CLA	CMC-C2C-C1C	2.06	128.17	125.04
33	C	512	CLA	CHA-C1A-NA	-2.06	121.69	126.40
33	c	512	CLA	CHA-C1A-NA	-2.06	121.69	126.40
33	p	306	CLA	CHC-C4B-NB	-2.06	122.08	124.26
39	g	312	II0	C15-C03-C05	-2.06	99.82	109.05
31	a	403	BCT	O3-C-O1	-2.06	114.21	119.55
33	b	609	CLA	CHD-C1D-C2D	2.06	129.79	125.48
42	B	622	LMG	C40-C39-C38	-2.05	103.99	114.42
39	5	312	II0	C15-C03-C05	-2.05	99.82	109.05
38	3	311	KC2	C4B-C3B-C2B	2.05	108.44	106.75
33	3	314	CLA	CHA-C1A-NA	-2.05	121.69	126.40
33	b	617	CLA	CHB-C4A-NA	2.05	127.35	124.51
33	4	306	CLA	CHB-C4A-NA	2.05	127.35	124.51
41	B	601	SQD	O7-S-C6	2.05	109.38	106.94
33	3	307	CLA	CHA-C1A-NA	-2.05	121.70	126.40
33	C	509	CLA	CHC-C4B-NB	-2.05	122.08	124.26
33	5	301	CLA	CHC-C1C-C2C	-2.05	121.03	126.73
33	6	306	CLA	CHC-C1C-NC	2.05	127.32	124.20
33	8	303	CLA	CHA-C1A-NA	-2.05	121.70	126.40
33	5	304	CLA	CHD-C1D-C2D	2.05	129.78	125.48
33	9	308	CLA	CHD-C1D-C2D	2.05	129.78	125.48
33	7	306	CLA	CHA-C1A-NA	-2.05	121.70	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	N	306	CLA	C2C-C1C-NC	2.05	111.89	109.97
33	1	304	CLA	CHD-C1D-C2D	2.05	129.78	125.48
33	2	301	CLA	CHD-C1D-C2D	2.05	129.78	125.48
31	A	403	BCT	O3-C-O1	-2.05	114.23	119.55
41	b	601	SQD	O7-S-C6	2.05	109.38	106.94
33	c	507	CLA	CHD-C1D-C2D	2.05	129.78	125.48
33	A	406	CLA	CHA-C1A-NA	-2.05	121.70	126.40
33	n	301	CLA	CHD-C1D-C2D	2.05	129.78	125.48
33	C	512	CLA	CHC-C4B-NB	-2.05	122.09	124.26
33	N	302	CLA	CHA-C1A-NA	-2.05	121.71	126.40
33	g	311	CLA	CHD-C1D-C2D	2.05	129.78	125.48
33	b	614	CLA	CHD-C1D-C2D	2.05	129.78	125.48
33	N	303	CLA	CHC-C1C-NC	2.05	127.31	124.20
33	5	304	CLA	CHA-C1A-NA	-2.05	121.71	126.40
33	b	602	CLA	CHD-C1D-C2D	2.05	129.77	125.48
33	a	406	CLA	CHC-C4B-NB	-2.05	122.09	124.26
33	C	507	CLA	CHD-C1D-C2D	2.05	129.77	125.48
33	n	304	CLA	C2C-C1C-NC	2.05	111.89	109.97
42	T	101	LMG	O1-C1-C2	-2.05	105.11	108.30
43	c	518	DGD	O3E-C3E-C2E	-2.05	105.62	110.35
33	g	308	CLA	CHA-C1A-NA	-2.04	121.72	126.40
39	6	315	II0	C05-C07-C11	-2.04	107.50	110.30
33	3	304	CLA	CHA-C1A-NA	-2.04	121.72	126.40
42	b	622	LMG	C40-C39-C38	-2.04	104.05	114.42
33	B	617	CLA	CHB-C4A-NA	2.04	127.34	124.51
33	0	310	CLA	CHC-C1C-C2C	-2.04	121.05	126.73
42	t	101	LMG	O1-C1-C2	-2.04	105.11	108.30
33	4	309	CLA	CHC-C1C-C2C	-2.04	121.06	126.73
33	6	310	CLA	CHC-C1C-NC	2.04	127.30	124.20
39	p	315	II0	C05-C07-C11	-2.04	107.51	110.30
33	c	503	CLA	C2C-C1C-NC	2.04	111.88	109.97
33	B	607	CLA	CHC-C4B-NB	-2.04	122.10	124.26
33	c	510	CLA	CHC-C4B-NB	-2.04	122.10	124.26
33	g	304	CLA	CHD-C1D-C2D	2.04	129.76	125.48
33	8	308	CLA	CMC-C2C-C1C	2.04	128.15	125.04
33	3	306	CLA	CHA-C1A-NA	-2.04	121.73	126.40
33	b	617	CLA	CHA-C1A-NA	-2.04	121.73	126.40
33	7	301	CLA	CHA-C1A-NA	-2.04	121.73	126.40
33	d	404	CLA	CHD-C1D-C2D	2.04	129.75	125.48
33	3	308	CLA	CHD-C1D-C2D	2.04	129.75	125.48
33	B	615	CLA	CHD-C1D-C2D	2.04	129.75	125.48
33	C	510	CLA	CHC-C4B-NB	-2.04	122.10	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	c	518	DGD	C3D-C4D-C5D	-2.04	106.61	110.24
43	C	518	DGD	O3E-C3E-C2E	-2.04	105.64	110.35
33	C	514	CLA	C2C-C1C-NC	2.04	111.88	109.97
33	0	302	CLA	C2C-C1C-NC	2.04	111.88	109.97
33	B	602	CLA	CHD-C1D-C2D	2.04	129.75	125.48
38	3	311	KC2	CHC-C4B-NB	2.03	126.32	124.45
33	3	314	CLA	CHD-C1D-C2D	2.03	129.75	125.48
33	C	505	CLA	CHD-C1D-C2D	2.03	129.75	125.48
33	b	615	CLA	CHD-C1D-C2D	2.03	129.74	125.48
43	c	518	DGD	O2D-C2D-C1D	-2.03	105.11	110.05
42	B	624	LMG	O6-C5-C4	2.03	113.38	109.69
44	F	101	HEM	C4A-CHB-C1B	-2.03	121.52	126.34
33	A	406	CLA	CHC-C4B-NB	-2.03	122.11	124.26
33	N	307	CLA	CHC-C4B-NB	-2.03	122.11	124.26
33	6	313	CLA	CHA-C1A-NA	-2.03	121.75	126.40
33	3	303	CLA	CHB-C4A-NA	2.03	127.32	124.51
33	B	617	CLA	CHA-C1A-NA	-2.03	121.75	126.40
33	2	305	CLA	CHB-C4A-NA	2.03	127.32	124.51
33	2	303	CLA	CHA-C1A-NA	-2.03	121.75	126.40
33	3	303	CLA	CHA-C1A-NA	-2.03	121.75	126.40
43	C	518	DGD	O2D-C2D-C1D	-2.03	105.12	110.05
33	9	304	CLA	C2C-C1C-NC	2.03	111.87	109.97
33	p	313	CLA	CHA-C1A-NA	-2.03	121.75	126.40
33	2	305	CLA	CHD-C1D-C2D	2.03	129.73	125.48
39	9	319	II0	C04-C10-C14	-2.03	119.77	122.63
33	C	503	CLA	C2C-C1C-NC	2.03	111.87	109.97
33	b	610	CLA	CMC-C2C-C1C	2.03	128.13	125.04
33	g	308	CLA	CHD-C1D-C2D	2.03	129.73	125.48
33	0	308	CLA	CHC-C1C-NC	2.03	127.28	124.20
33	5	308	CLA	CHA-C1A-NA	-2.03	121.76	126.40
33	9	303	CLA	CHA-C1A-NA	-2.03	121.76	126.40
33	g	304	CLA	CHA-C1A-NA	-2.03	121.76	126.40
33	a	406	CLA	CHA-C1A-NA	-2.03	121.76	126.40
33	A	408	CLA	CHD-C1D-C2D	2.02	129.73	125.48
33	D	404	CLA	CHD-C1D-C2D	2.02	129.73	125.48
33	C	508	CLA	CHC-C1C-C2C	-2.02	121.11	126.73
33	5	308	CLA	CHD-C1D-C2D	2.02	129.73	125.48
33	8	305	CLA	CHB-C4A-NA	2.02	127.31	124.51
33	N	304	CLA	C3A-C2A-C1A	-2.02	98.22	101.64
33	n	303	CLA	C3A-C2A-C1A	-2.02	98.22	101.64
33	5	310	CLA	CHA-C1A-NA	-2.02	121.76	126.40
33	9	303	CLA	CHB-C4A-NA	2.02	127.31	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	p	312	CLA	CHB-C4A-NA	2.02	127.31	124.51
33	4	302	CLA	CHC-C4B-NB	-2.02	122.11	124.26
33	1	301	CLA	CHD-C1D-C2D	2.02	129.72	125.48
33	p	310	CLA	CHC-C1C-NC	2.02	127.27	124.20
42	d	409	LMG	O6-C1-O1	-2.02	105.19	109.97
33	B	612	CLA	C2C-C1C-NC	2.02	111.87	109.97
43	C	518	DGD	C3D-C4D-C5D	-2.02	106.63	110.24
33	N	305	CLA	C1-C2-C3	-2.02	122.55	126.04
33	9	314	CLA	CHD-C1D-C2D	2.02	129.72	125.48
42	b	624	LMG	O6-C5-C4	2.02	113.36	109.69
33	c	505	CLA	CHD-C1D-C2D	2.02	129.72	125.48
33	B	611	CLA	CHD-C1D-C2D	2.02	129.72	125.48
33	C	503	CLA	CHC-C4B-NB	-2.02	122.12	124.26
33	N	305	CLA	CHD-C1D-C2D	2.02	129.71	125.48
33	n	306	CLA	CHC-C4B-NB	-2.02	122.12	124.26
33	g	302	CLA	CMC-C2C-C1C	2.02	128.11	125.04
33	d	405	CLA	C2C-C1C-NC	2.02	111.86	109.97
33	c	508	CLA	CHC-C1C-C2C	-2.02	121.13	126.73
38	p	311	KC2	CHC-C4B-NB	2.02	126.31	124.45
33	N	305	CLA	CHA-C1A-NA	-2.02	121.78	126.40
33	0	311	CLA	CHA-C1A-NA	-2.02	121.78	126.40
33	a	408	CLA	CHD-C1D-C2D	2.01	129.71	125.48
33	8	301	CLA	CHC-C4B-NB	-2.01	122.12	124.26
33	6	312	CLA	CHB-C4A-NA	2.01	127.30	124.51
43	c	521	DGD	CAB-C9B-C8B	-2.01	104.20	114.42
33	9	307	CLA	CHD-C1D-C2D	2.01	129.71	125.48
33	p	304	CLA	CHD-C1D-C2D	2.01	129.70	125.48
42	c	520	LMG	O2-C2-C1	-2.01	105.15	110.05
33	6	304	CLA	CHD-C1D-C2D	2.01	129.70	125.48
33	6	305	CLA	CHD-C1D-C2D	2.01	129.70	125.48
38	9	311	KC2	CHC-C4B-NB	2.01	126.30	124.45
33	c	503	CLA	CHC-C4B-NB	-2.01	122.13	124.26
33	5	310	CLA	CHD-C1D-C2D	2.01	129.70	125.48
42	C	520	LMG	O2-C2-C1	-2.01	105.16	110.05
38	6	311	KC2	CHC-C4B-NB	2.01	126.30	124.45
33	9	313	CLA	CHC-C4B-NB	-2.01	122.13	124.26
33	b	611	CLA	CHD-C1D-C2D	2.01	129.70	125.48
33	B	610	CLA	CMC-C2C-C1C	2.01	128.10	125.04
33	p	309	CLA	CHC-C1C-C2C	-2.01	121.14	126.73
33	B	614	CLA	CHC-C1C-C2C	-2.01	121.14	126.73
33	4	303	CLA	CHC-C4B-NB	-2.01	122.13	124.26
33	N	305	CLA	CHC-C4B-NB	-2.01	122.13	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	n	304	CLA	C1-C2-C3	-2.01	122.57	126.04
33	B	615	CLA	CMC-C2C-C1C	2.01	128.10	125.04
33	3	307	CLA	CHD-C1D-C2D	2.01	129.69	125.48
33	p	305	CLA	CHD-C1D-C2D	2.01	129.69	125.48
33	7	301	CLA	CHD-C1D-C2D	2.01	129.69	125.48
33	b	614	CLA	CHC-C1C-C2C	-2.01	121.15	126.73
33	2	304	CLA	CHC-C4B-NB	-2.01	122.13	124.26
33	n	304	CLA	CHD-C1D-C2D	2.01	129.69	125.48
33	5	302	CLA	CMC-C2C-C1C	2.01	128.10	125.04
42	D	409	LMG	O6-C1-O1	-2.01	105.22	109.97
38	4	305	KC2	C4C-C3C-C2C	2.01	108.71	107.11
33	g	310	CLA	CHA-C1A-NA	-2.01	121.80	126.40
33	g	310	CLA	CHD-C1D-C2D	2.01	129.69	125.48
33	6	303	CLA	CAA-C2A-C1A	-2.01	106.85	111.81
33	7	305	CLA	CHD-C1D-C2D	2.01	129.69	125.48
43	C	521	DGD	CAB-C9B-C8B	-2.01	104.24	114.42
33	1	306	CLA	CHA-C1A-NA	-2.01	121.81	126.40
33	0	311	CLA	C3A-C2A-C1A	-2.01	98.34	101.34
33	6	309	CLA	CHC-C1C-C2C	-2.01	121.16	126.73
33	8	304	CLA	CHC-C4B-NB	-2.00	122.14	124.26
33	C	511	CLA	CMC-C2C-C1C	2.00	128.09	125.04
33	B	602	CLA	CHC-C1C-C2C	-2.00	121.17	126.73
33	b	608	CLA	CHD-C1D-C2D	2.00	129.68	125.48
33	4	310	CLA	CHA-C1A-NA	-2.00	121.81	126.40
39	5	312	II0	C16-C03-C05	2.00	118.04	109.05
33	n	304	CLA	CHA-C1A-NA	-2.00	121.81	126.40
39	g	312	II0	C16-C03-C05	2.00	118.04	109.05

There are no chirality outliers.

All (2639) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	a	412	CLA	C1A-C2A-CAA-CBA
33	a	412	CLA	C3A-C2A-CAA-CBA
33	A	412	CLA	C1A-C2A-CAA-CBA
33	A	412	CLA	C3A-C2A-CAA-CBA
33	0	306	CLA	C2-C3-C5-C6
33	0	306	CLA	C4-C3-C5-C6
33	0	307	CLA	C4B-C3B-CAB-CBB
33	0	308	CLA	CHA-CBD-CGD-O1D
33	0	308	CLA	CHA-CBD-CGD-O2D
33	0	310	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	0	310	CLA	C4B-C3B-CAB-CBB
33	0	310	CLA	CHA-CBD-CGD-O1D
33	0	310	CLA	CHA-CBD-CGD-O2D
33	0	310	CLA	CAD-CBD-CGD-O1D
33	0	310	CLA	CAD-CBD-CGD-O2D
33	1	301	CLA	C2B-C3B-CAB-CBB
33	1	301	CLA	C4B-C3B-CAB-CBB
33	1	302	CLA	C3A-C2A-CAA-CBA
33	1	302	CLA	CHA-CBD-CGD-O1D
33	1	302	CLA	CHA-CBD-CGD-O2D
33	1	307	CLA	C1A-C2A-CAA-CBA
33	1	308	CLA	C2-C3-C5-C6
33	1	308	CLA	C4-C3-C5-C6
33	1	309	CLA	C2B-C3B-CAB-CBB
33	1	309	CLA	C4B-C3B-CAB-CBB
33	2	301	CLA	C2B-C3B-CAB-CBB
33	2	301	CLA	C4B-C3B-CAB-CBB
33	2	302	CLA	C1A-C2A-CAA-CBA
33	2	302	CLA	C3A-C2A-CAA-CBA
33	2	302	CLA	CHA-CBD-CGD-O1D
33	2	302	CLA	CHA-CBD-CGD-O2D
33	2	303	CLA	C2B-C3B-CAB-CBB
33	2	303	CLA	C4B-C3B-CAB-CBB
33	2	303	CLA	CAD-CBD-CGD-O1D
33	2	303	CLA	CAD-CBD-CGD-O2D
33	2	305	CLA	C2B-C3B-CAB-CBB
33	2	305	CLA	C4B-C3B-CAB-CBB
33	2	310	CLA	CHA-CBD-CGD-O1D
33	2	310	CLA	CHA-CBD-CGD-O2D
33	3	303	CLA	C1A-C2A-CAA-CBA
33	3	303	CLA	C3A-C2A-CAA-CBA
33	3	303	CLA	C2B-C3B-CAB-CBB
33	3	303	CLA	C4B-C3B-CAB-CBB
33	3	306	CLA	C2B-C3B-CAB-CBB
33	3	306	CLA	C4B-C3B-CAB-CBB
33	3	307	CLA	C1A-C2A-CAA-CBA
33	3	308	CLA	C1A-C2A-CAA-CBA
33	3	308	CLA	C3A-C2A-CAA-CBA
33	3	309	CLA	C1A-C2A-CAA-CBA
33	3	309	CLA	C3A-C2A-CAA-CBA
33	3	309	CLA	CHA-CBD-CGD-O1D
33	3	309	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
33	3	309	CLA	C2-C3-C5-C6
33	3	309	CLA	C4-C3-C5-C6
33	3	313	CLA	CHA-CBD-CGD-O1D
33	3	313	CLA	CHA-CBD-CGD-O2D
33	3	315	CLA	CHA-CBD-CGD-O1D
33	3	315	CLA	CHA-CBD-CGD-O2D
33	3	315	CLA	CAD-CBD-CGD-O1D
33	4	306	CLA	C2-C3-C5-C6
33	4	306	CLA	C4-C3-C5-C6
33	4	307	CLA	C4B-C3B-CAB-CBB
33	4	309	CLA	C2B-C3B-CAB-CBB
33	4	309	CLA	C4B-C3B-CAB-CBB
33	4	309	CLA	CHA-CBD-CGD-O1D
33	4	309	CLA	CHA-CBD-CGD-O2D
33	4	309	CLA	CAD-CBD-CGD-O1D
33	4	309	CLA	CAD-CBD-CGD-O2D
33	5	301	CLA	CHA-CBD-CGD-O1D
33	5	301	CLA	CHA-CBD-CGD-O2D
33	5	302	CLA	C3A-C2A-CAA-CBA
33	5	302	CLA	CHA-CBD-CGD-O1D
33	5	302	CLA	CHA-CBD-CGD-O2D
33	5	304	CLA	C2B-C3B-CAB-CBB
33	5	304	CLA	C4B-C3B-CAB-CBB
33	5	305	CLA	CBD-CGD-O2D-CED
33	6	306	CLA	C2B-C3B-CAB-CBB
33	6	306	CLA	C4B-C3B-CAB-CBB
33	6	306	CLA	CBD-CGD-O2D-CED
33	6	308	CLA	CBD-CGD-O2D-CED
33	6	309	CLA	C2B-C3B-CAB-CBB
33	6	309	CLA	C4B-C3B-CAB-CBB
33	6	310	CLA	C2B-C3B-CAB-CBB
33	6	310	CLA	C4B-C3B-CAB-CBB
33	6	312	CLA	CHA-CBD-CGD-O1D
33	6	312	CLA	CHA-CBD-CGD-O2D
33	6	319	CLA	CHA-CBD-CGD-O1D
33	6	319	CLA	CHA-CBD-CGD-O2D
33	6	319	CLA	CAD-CBD-CGD-O1D
33	6	319	CLA	CAD-CBD-CGD-O2D
33	6	319	CLA	CBD-CGD-O2D-CED
33	7	301	CLA	C2B-C3B-CAB-CBB
33	7	301	CLA	C4B-C3B-CAB-CBB
33	7	302	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	7	302	CLA	CHA-CBD-CGD-O1D
33	7	302	CLA	CHA-CBD-CGD-O2D
33	7	307	CLA	C1A-C2A-CAA-CBA
33	7	308	CLA	C2-C3-C5-C6
33	7	308	CLA	C4-C3-C5-C6
33	7	309	CLA	C2B-C3B-CAB-CBB
33	7	309	CLA	C4B-C3B-CAB-CBB
33	8	301	CLA	C2B-C3B-CAB-CBB
33	8	301	CLA	C4B-C3B-CAB-CBB
33	8	302	CLA	C1A-C2A-CAA-CBA
33	8	302	CLA	C3A-C2A-CAA-CBA
33	8	302	CLA	CHA-CBD-CGD-O1D
33	8	302	CLA	CHA-CBD-CGD-O2D
33	8	303	CLA	C2B-C3B-CAB-CBB
33	8	303	CLA	C4B-C3B-CAB-CBB
33	8	303	CLA	CAD-CBD-CGD-O1D
33	8	303	CLA	CAD-CBD-CGD-O2D
33	8	305	CLA	C2B-C3B-CAB-CBB
33	8	305	CLA	C4B-C3B-CAB-CBB
33	8	310	CLA	CHA-CBD-CGD-O1D
33	8	310	CLA	CHA-CBD-CGD-O2D
33	9	303	CLA	C1A-C2A-CAA-CBA
33	9	303	CLA	C3A-C2A-CAA-CBA
33	9	303	CLA	C2B-C3B-CAB-CBB
33	9	303	CLA	C4B-C3B-CAB-CBB
33	9	306	CLA	C2B-C3B-CAB-CBB
33	9	306	CLA	C4B-C3B-CAB-CBB
33	9	307	CLA	C1A-C2A-CAA-CBA
33	9	308	CLA	C1A-C2A-CAA-CBA
33	9	308	CLA	C3A-C2A-CAA-CBA
33	9	309	CLA	C1A-C2A-CAA-CBA
33	9	309	CLA	C3A-C2A-CAA-CBA
33	9	309	CLA	CHA-CBD-CGD-O1D
33	9	309	CLA	CHA-CBD-CGD-O2D
33	9	309	CLA	C2-C3-C5-C6
33	9	309	CLA	C4-C3-C5-C6
33	9	313	CLA	CHA-CBD-CGD-O1D
33	9	313	CLA	CHA-CBD-CGD-O2D
33	9	315	CLA	CHA-CBD-CGD-O1D
33	9	315	CLA	CHA-CBD-CGD-O2D
33	9	315	CLA	CAD-CBD-CGD-O1D
33	B	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
33	B	602	CLA	CHA-CBD-CGD-O2D
33	B	610	CLA	C2B-C3B-CAB-CBB
33	B	610	CLA	C4B-C3B-CAB-CBB
33	C	505	CLA	C2-C3-C5-C6
33	C	505	CLA	C4-C3-C5-C6
33	C	507	CLA	C11-C10-C8-C9
33	C	508	CLA	C2B-C3B-CAB-CBB
33	C	510	CLA	O2A-C1-C2-C3
33	N	301	CLA	CHA-CBD-CGD-O1D
33	N	301	CLA	CHA-CBD-CGD-O2D
33	N	302	CLA	C2B-C3B-CAB-CBB
33	N	302	CLA	C4B-C3B-CAB-CBB
33	N	303	CLA	CHA-CBD-CGD-O1D
33	N	303	CLA	CHA-CBD-CGD-O2D
33	b	602	CLA	CHA-CBD-CGD-O1D
33	b	602	CLA	CHA-CBD-CGD-O2D
33	b	610	CLA	C2B-C3B-CAB-CBB
33	b	610	CLA	C4B-C3B-CAB-CBB
33	b	618	CLA	CBD-CGD-O2D-CED
33	c	505	CLA	C2-C3-C5-C6
33	c	505	CLA	C4-C3-C5-C6
33	c	507	CLA	C11-C10-C8-C9
33	c	508	CLA	C2B-C3B-CAB-CBB
33	c	510	CLA	O2A-C1-C2-C3
33	g	301	CLA	CHA-CBD-CGD-O1D
33	g	301	CLA	CHA-CBD-CGD-O2D
33	g	302	CLA	C3A-C2A-CAA-CBA
33	g	302	CLA	CHA-CBD-CGD-O1D
33	g	302	CLA	CHA-CBD-CGD-O2D
33	g	304	CLA	C2B-C3B-CAB-CBB
33	g	304	CLA	C4B-C3B-CAB-CBB
33	g	305	CLA	CBD-CGD-O2D-CED
33	n	301	CLA	CHA-CBD-CGD-O1D
33	n	301	CLA	CHA-CBD-CGD-O2D
33	n	302	CLA	C2B-C3B-CAB-CBB
33	n	302	CLA	C4B-C3B-CAB-CBB
33	p	306	CLA	C2B-C3B-CAB-CBB
33	p	306	CLA	C4B-C3B-CAB-CBB
33	p	306	CLA	CBD-CGD-O2D-CED
33	p	308	CLA	CBD-CGD-O2D-CED
33	p	309	CLA	C2B-C3B-CAB-CBB
33	p	309	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	p	310	CLA	C2B-C3B-CAB-CBB
33	p	310	CLA	C4B-C3B-CAB-CBB
33	p	312	CLA	CHA-CBD-CGD-O1D
33	p	312	CLA	CHA-CBD-CGD-O2D
33	p	319	CLA	CHA-CBD-CGD-O1D
33	p	319	CLA	CHA-CBD-CGD-O2D
33	p	319	CLA	CAD-CBD-CGD-O1D
33	p	319	CLA	CAD-CBD-CGD-O2D
33	p	319	CLA	CBD-CGD-O2D-CED
34	a	407	PHO	CBA-CGA-O2A-C1
34	a	407	PHO	O1A-CGA-O2A-C1
34	A	407	PHO	CBA-CGA-O2A-C1
34	A	407	PHO	O1A-CGA-O2A-C1
35	a	409	8CT	C28-C29-C30-C31
35	a	409	8CT	C28-C29-C30-C35
35	A	409	8CT	C28-C29-C30-C31
35	A	409	8CT	C28-C29-C30-C35
35	0	312	8CT	C21-C23-C24-C25
35	0	312	8CT	C28-C29-C30-C31
35	0	312	8CT	C28-C29-C30-C35
35	1	312	8CT	C03-C10-C11-C12
35	1	312	8CT	C13-C14-C15-C16
35	1	312	8CT	C28-C29-C30-C35
35	4	311	8CT	C21-C23-C24-C25
35	4	311	8CT	C28-C29-C30-C31
35	4	311	8CT	C28-C29-C30-C35
35	7	312	8CT	C03-C10-C11-C12
35	7	312	8CT	C13-C14-C15-C16
35	7	312	8CT	C28-C29-C30-C35
35	B	619	8CT	C21-C23-C24-C25
35	B	620	8CT	C18-C19-C20-C21
35	B	620	8CT	C27-C26-C28-C29
35	B	620	8CT	C28-C29-C30-C31
35	B	620	8CT	C28-C29-C30-C35
35	C	515	8CT	C03-C10-C11-C12
35	C	515	8CT	C28-C29-C30-C31
35	C	515	8CT	C28-C29-C30-C35
35	C	516	8CT	C03-C10-C11-C12
35	C	516	8CT	C13-C14-C15-C16
35	C	517	8CT	C28-C29-C30-C31
35	D	406	8CT	C03-C10-C11-C12
35	D	406	8CT	C21-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
35	D	406	8CT	C23-C24-C25-C26
35	D	406	8CT	C28-C29-C30-C31
35	D	406	8CT	C28-C29-C30-C35
35	H	102	8CT	C03-C10-C11-C12
35	H	102	8CT	C21-C23-C24-C25
35	Y	101	8CT	C03-C10-C11-C12
35	Y	101	8CT	C25-C26-C28-C29
35	Y	101	8CT	C27-C26-C28-C29
35	b	619	8CT	C21-C23-C24-C25
35	b	620	8CT	C18-C19-C20-C21
35	b	620	8CT	C25-C26-C28-C29
35	b	620	8CT	C27-C26-C28-C29
35	b	620	8CT	C28-C29-C30-C31
35	b	620	8CT	C28-C29-C30-C35
35	c	515	8CT	C03-C10-C11-C12
35	c	515	8CT	C28-C29-C30-C31
35	c	515	8CT	C28-C29-C30-C35
35	c	516	8CT	C03-C10-C11-C12
35	c	516	8CT	C13-C14-C15-C16
35	c	517	8CT	C28-C29-C30-C31
35	d	406	8CT	C03-C10-C11-C12
35	d	406	8CT	C21-C23-C24-C25
35	d	406	8CT	C23-C24-C25-C26
35	d	406	8CT	C28-C29-C30-C31
35	d	406	8CT	C28-C29-C30-C35
35	h	102	8CT	C03-C10-C11-C12
35	h	102	8CT	C21-C23-C24-C25
35	y	101	8CT	C03-C10-C11-C12
35	y	101	8CT	C25-C26-C28-C29
35	y	101	8CT	C27-C26-C28-C29
36	a	410	PL9	C12-C13-C14-C15
36	A	410	PL9	C12-C13-C14-C15
36	D	407	PL9	C37-C38-C39-C40
36	D	407	PL9	C42-C43-C44-C45
36	d	407	PL9	C37-C38-C39-C40
36	d	407	PL9	C42-C43-C44-C45
37	0	317	LHG	C3-O3-P-O4
37	0	317	LHG	C3-O3-P-O5
37	0	317	LHG	C3-O3-P-O6
37	1	317	LHG	C3-O3-P-O4
37	2	315	LHG	O1-C1-C2-C3
37	2	315	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
37	2	315	LHG	C4-O6-P-O5
37	2	315	LHG	C8-C7-O7-C5
37	3	302	LHG	C1-C2-C3-O3
37	3	321	LHG	C3-O3-P-O4
37	3	321	LHG	C3-O3-P-O6
37	4	316	LHG	C3-O3-P-O4
37	4	316	LHG	C3-O3-P-O5
37	4	316	LHG	C3-O3-P-O6
37	5	316	LHG	C4-O6-P-O5
37	5	316	LHG	C4-C5-C6-O8
37	7	317	LHG	C3-O3-P-O4
37	8	315	LHG	O1-C1-C2-C3
37	8	315	LHG	C2-C3-O3-P
37	8	315	LHG	C4-O6-P-O5
37	8	315	LHG	C8-C7-O7-C5
37	9	302	LHG	C1-C2-C3-O3
37	9	321	LHG	C3-O3-P-O4
37	9	321	LHG	C3-O3-P-O6
37	B	623	LHG	O1-C1-C2-C3
37	D	401	LHG	C8-C7-O7-C5
37	D	402	LHG	C4-O6-P-O5
37	D	402	LHG	O7-C5-C6-O8
37	D	408	LHG	C3-O3-P-O4
37	D	408	LHG	C3-O3-P-O6
37	D	408	LHG	C4-O6-P-O3
37	D	408	LHG	C4-O6-P-O5
37	b	623	LHG	O1-C1-C2-C3
37	d	401	LHG	C8-C7-O7-C5
37	d	402	LHG	C4-O6-P-O5
37	d	402	LHG	O7-C5-C6-O8
37	d	408	LHG	C3-O3-P-O4
37	d	408	LHG	C3-O3-P-O6
37	d	408	LHG	C4-O6-P-O3
37	d	408	LHG	C4-O6-P-O5
37	g	316	LHG	C4-O6-P-O5
37	g	316	LHG	C4-C5-C6-O8
38	0	305	KC2	C2C-C3C-CAC-CBC
38	0	305	KC2	CAA-CBA-CGA-O1A
38	0	305	KC2	CAA-CBA-CGA-O2A
38	0	305	KC2	CBD-CGD-O2D-CED
38	1	310	KC2	C2B-C3B-CAB-CBB
38	1	310	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
38	1	311	KC2	C1A-C2A-CAA-CBA
38	1	311	KC2	C3A-C2A-CAA-CBA
38	2	309	KC2	C1A-C2A-CAA-CBA
38	2	309	KC2	C3A-C2A-CAA-CBA
38	2	309	KC2	C4C-C3C-CAC-CBC
38	2	309	KC2	CHA-CBD-CGD-O1D
38	2	309	KC2	CHA-CBD-CGD-O2D
38	3	311	KC2	C1A-C2A-CAA-CBA
38	3	311	KC2	CHA-CBD-CGD-O1D
38	3	311	KC2	CHA-CBD-CGD-O2D
38	4	305	KC2	C2C-C3C-CAC-CBC
38	4	305	KC2	CAA-CBA-CGA-O1A
38	4	305	KC2	CAA-CBA-CGA-O2A
38	4	305	KC2	CBD-CGD-O2D-CED
38	5	309	KC2	C1A-C2A-CAA-CBA
38	5	309	KC2	C3A-C2A-CAA-CBA
38	6	311	KC2	C1A-C2A-CAA-CBA
38	6	311	KC2	C3A-C2A-CAA-CBA
38	7	310	KC2	C2B-C3B-CAB-CBB
38	7	310	KC2	C2C-C3C-CAC-CBC
38	7	311	KC2	C1A-C2A-CAA-CBA
38	7	311	KC2	C3A-C2A-CAA-CBA
38	8	309	KC2	C1A-C2A-CAA-CBA
38	8	309	KC2	C3A-C2A-CAA-CBA
38	8	309	KC2	C4C-C3C-CAC-CBC
38	8	309	KC2	CHA-CBD-CGD-O1D
38	8	309	KC2	CHA-CBD-CGD-O2D
38	9	311	KC2	C1A-C2A-CAA-CBA
38	9	311	KC2	CHA-CBD-CGD-O1D
38	9	311	KC2	CHA-CBD-CGD-O2D
38	g	309	KC2	C1A-C2A-CAA-CBA
38	g	309	KC2	C3A-C2A-CAA-CBA
38	p	311	KC2	C1A-C2A-CAA-CBA
38	p	311	KC2	C3A-C2A-CAA-CBA
39	0	316	II0	C31-C33-C35-C39
39	1	313	II0	C09-C21-C23-C25
39	3	316	II0	C31-C33-C35-C39
39	4	315	II0	C31-C33-C35-C39
39	6	317	II0	C10-C22-C24-C26
39	7	313	II0	C09-C21-C23-C25
39	9	316	II0	C31-C33-C35-C39
39	p	317	II0	C10-C22-C24-C26

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Mol	Chain	Res	Type	Atoms
40	3	320	IHT	C18-C22-C23-C25
40	3	320	IHT	C18-C22-C23-C27
40	3	320	IHT	C31-C34-C35-C39
40	9	320	IHT	C18-C22-C23-C25
40	9	320	IHT	C18-C22-C23-C27
40	9	320	IHT	C31-C34-C35-C39
41	B	601	SQD	O5-C1-O6-C44
41	C	501	SQD	C5-C6-S-O7
41	C	501	SQD	C5-C6-S-O8
41	C	501	SQD	C5-C6-S-O9
41	J	101	SQD	O6-C44-C45-O47
41	J	101	SQD	C8-C7-O47-C45
41	J	101	SQD	C5-C6-S-O8
41	L	101	SQD	O5-C5-C6-S
41	L	101	SQD	C5-C6-S-O7
41	L	101	SQD	C5-C6-S-O8
41	L	101	SQD	C5-C6-S-O9
41	b	601	SQD	O5-C1-O6-C44
41	c	501	SQD	C5-C6-S-O7
41	c	501	SQD	C5-C6-S-O8
41	c	501	SQD	C5-C6-S-O9
41	j	101	SQD	O6-C44-C45-O47
41	j	101	SQD	C8-C7-O47-C45
41	j	101	SQD	C5-C6-S-O8
41	l	101	SQD	O5-C5-C6-S
41	l	101	SQD	C5-C6-S-O7
41	l	101	SQD	C5-C6-S-O8
41	l	101	SQD	C5-C6-S-O9
42	C	520	LMG	C2-C1-O1-C7
42	C	520	LMG	O6-C1-O1-C7
42	C	520	LMG	C11-C10-O7-C8
42	D	410	LMG	C2-C1-O1-C7
42	D	410	LMG	O6-C1-O1-C7
42	T	101	LMG	C11-C10-O7-C8
42	W	101	LMG	C2-C1-O1-C7
42	W	101	LMG	O6-C1-O1-C7
42	W	101	LMG	O7-C8-C9-O8
42	c	520	LMG	C2-C1-O1-C7
42	c	520	LMG	O6-C1-O1-C7
42	c	520	LMG	C11-C10-O7-C8
42	d	410	LMG	C2-C1-O1-C7
42	d	410	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
42	l	102	LMG	O6-C1-O1-C7
42	l	102	LMG	O9-C10-O7-C8
42	l	102	LMG	C11-C10-O7-C8
42	m	101	LMG	O6-C1-O1-C7
42	m	101	LMG	O9-C10-O7-C8
42	m	101	LMG	C11-C10-O7-C8
42	t	101	LMG	C11-C10-O7-C8
42	w	101	LMG	C2-C1-O1-C7
42	w	101	LMG	O6-C1-O1-C7
42	w	101	LMG	O7-C8-C9-O8
43	C	519	DGD	C2E-C1E-O5D-C6D
43	C	519	DGD	O6E-C1E-O5D-C6D
43	C	521	DGD	C2A-C1A-O1G-C1G
43	C	521	DGD	O1A-C1A-O1G-C1G
43	c	519	DGD	C2E-C1E-O5D-C6D
43	c	519	DGD	O6E-C1E-O5D-C6D
43	c	521	DGD	C2A-C1A-O1G-C1G
43	c	521	DGD	O1A-C1A-O1G-C1G
44	F	101	HEM	C2B-C3B-CAB-CBB
44	F	101	HEM	C4B-C3B-CAB-CBB
44	F	101	HEM	C2C-C3C-CAC-CBC
44	F	101	HEM	C4C-C3C-CAC-CBC
38	0	305	KC2	O1D-CGD-O2D-CED
38	4	305	KC2	O1D-CGD-O2D-CED
33	0	310	CLA	O1D-CGD-O2D-CED
33	4	309	CLA	O1D-CGD-O2D-CED
33	6	306	CLA	O1D-CGD-O2D-CED
33	6	308	CLA	O1D-CGD-O2D-CED
33	p	306	CLA	O1D-CGD-O2D-CED
33	p	308	CLA	O1D-CGD-O2D-CED
33	0	308	CLA	CBD-CGD-O2D-CED
33	0	309	CLA	CBD-CGD-O2D-CED
33	0	310	CLA	CBD-CGD-O2D-CED
33	4	308	CLA	CBD-CGD-O2D-CED
33	4	309	CLA	CBD-CGD-O2D-CED
33	6	303	CLA	CBD-CGD-O2D-CED
33	6	310	CLA	CBD-CGD-O2D-CED
33	N	303	CLA	CBD-CGD-O2D-CED
33	p	303	CLA	CBD-CGD-O2D-CED
33	p	310	CLA	CBD-CGD-O2D-CED
38	5	309	KC2	CBD-CGD-O2D-CED
38	g	309	KC2	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
42	B	622	LMG	O10-C28-O8-C9
42	b	622	LMG	O10-C28-O8-C9
33	0	309	CLA	C2C-C3C-CAC-CBC
33	4	308	CLA	C2C-C3C-CAC-CBC
33	5	305	CLA	O1D-CGD-O2D-CED
33	6	310	CLA	O1D-CGD-O2D-CED
33	6	319	CLA	O1D-CGD-O2D-CED
33	b	618	CLA	O1D-CGD-O2D-CED
33	g	305	CLA	O1D-CGD-O2D-CED
33	p	310	CLA	O1D-CGD-O2D-CED
33	p	319	CLA	O1D-CGD-O2D-CED
38	5	309	KC2	O1D-CGD-O2D-CED
38	g	309	KC2	O1D-CGD-O2D-CED
33	0	309	CLA	C4C-C3C-CAC-CBC
33	2	303	CLA	C2C-C3C-CAC-CBC
33	2	303	CLA	C4C-C3C-CAC-CBC
33	4	308	CLA	C4C-C3C-CAC-CBC
33	8	303	CLA	C4C-C3C-CAC-CBC
33	0	309	CLA	O1D-CGD-O2D-CED
33	4	308	CLA	O1D-CGD-O2D-CED
33	0	301	CLA	CBD-CGD-O2D-CED
33	0	304	CLA	CBD-CGD-O2D-CED
33	0	306	CLA	CBD-CGD-O2D-CED
33	4	301	CLA	CBD-CGD-O2D-CED
33	4	304	CLA	CBD-CGD-O2D-CED
33	4	306	CLA	CBD-CGD-O2D-CED
33	5	311	CLA	CBD-CGD-O2D-CED
33	g	311	CLA	CBD-CGD-O2D-CED
33	8	303	CLA	C2C-C3C-CAC-CBC
37	1	317	LHG	O10-C23-O8-C6
37	3	322	LHG	O10-C23-O8-C6
37	5	316	LHG	O10-C23-O8-C6
37	7	317	LHG	O10-C23-O8-C6
37	9	322	LHG	O10-C23-O8-C6
37	g	316	LHG	O10-C23-O8-C6
41	B	601	SQD	O10-C23-O48-C46
41	b	601	SQD	O10-C23-O48-C46
42	B	624	LMG	O10-C28-O8-C9
42	b	624	LMG	O10-C28-O8-C9
37	2	315	LHG	O9-C7-O7-C5
37	8	315	LHG	O9-C7-O7-C5
37	D	401	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
37	d	401	LHG	O9-C7-O7-C5
41	J	101	SQD	O49-C7-O47-C45
41	j	101	SQD	O49-C7-O47-C45
42	D	410	LMG	O9-C10-O7-C8
42	T	101	LMG	O9-C10-O7-C8
42	d	410	LMG	O9-C10-O7-C8
42	t	101	LMG	O9-C10-O7-C8
33	5	303	CLA	C3-C5-C6-C7
33	B	607	CLA	C3-C5-C6-C7
33	C	507	CLA	C3-C5-C6-C7
33	b	607	CLA	C3-C5-C6-C7
33	c	507	CLA	C3-C5-C6-C7
33	g	303	CLA	C3-C5-C6-C7
37	1	317	LHG	C24-C23-O8-C6
37	3	322	LHG	C24-C23-O8-C6
37	7	317	LHG	C24-C23-O8-C6
37	9	322	LHG	C24-C23-O8-C6
41	B	601	SQD	C24-C23-O48-C46
41	b	601	SQD	C24-C23-O48-C46
42	B	624	LMG	C29-C28-O8-C9
42	C	520	LMG	C29-C28-O8-C9
42	b	624	LMG	C29-C28-O8-C9
42	c	520	LMG	C29-C28-O8-C9
37	D	408	LHG	C8-C7-O7-C5
37	d	408	LHG	C8-C7-O7-C5
42	D	410	LMG	C11-C10-O7-C8
42	d	410	LMG	C11-C10-O7-C8
33	0	308	CLA	O1D-CGD-O2D-CED
38	3	311	KC2	CAA-CBA-CGA-O1A
38	3	311	KC2	CAA-CBA-CGA-O2A
38	9	311	KC2	CAA-CBA-CGA-O1A
38	9	311	KC2	CAA-CBA-CGA-O2A
33	N	301	CLA	C4-C3-C5-C6
33	n	301	CLA	C4-C3-C5-C6
33	N	301	CLA	C2-C3-C5-C6
33	n	301	CLA	C2-C3-C5-C6
33	0	309	CLA	C2A-CAA-CBA-CGA
33	2	302	CLA	C2A-CAA-CBA-CGA
33	4	308	CLA	C2A-CAA-CBA-CGA
33	5	304	CLA	C2A-CAA-CBA-CGA
33	8	302	CLA	C2A-CAA-CBA-CGA
33	B	607	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
33	N	305	CLA	C2A-CAA-CBA-CGA
33	b	607	CLA	C2A-CAA-CBA-CGA
33	g	304	CLA	C2A-CAA-CBA-CGA
33	n	304	CLA	C2A-CAA-CBA-CGA
33	6	303	CLA	O1D-CGD-O2D-CED
33	N	303	CLA	O1D-CGD-O2D-CED
33	p	303	CLA	O1D-CGD-O2D-CED
33	2	306	CLA	C3-C5-C6-C7
33	8	306	CLA	C3-C5-C6-C7
33	2	303	CLA	CBA-CGA-O2A-C1
33	8	303	CLA	CBA-CGA-O2A-C1
37	5	316	LHG	C24-C23-O8-C6
37	g	316	LHG	C24-C23-O8-C6
41	J	101	SQD	C24-C23-O48-C46
41	j	101	SQD	C24-C23-O48-C46
43	C	521	DGD	C4D-C5D-C6D-O5D
43	c	521	DGD	C4D-C5D-C6D-O5D
36	D	407	PL9	C7-C8-C9-C11
36	d	407	PL9	C7-C8-C9-C11
42	B	622	LMG	C4-C5-C6-O5
42	C	520	LMG	C4-C5-C6-O5
42	b	622	LMG	C4-C5-C6-O5
42	c	520	LMG	C4-C5-C6-O5
43	C	519	DGD	C4E-C5E-C6E-O5E
43	c	519	DGD	C4E-C5E-C6E-O5E
35	H	102	8CT	C18-C19-C20-C21
35	h	102	8CT	C18-C19-C20-C21
33	0	307	CLA	CBD-CGD-O2D-CED
33	4	307	CLA	CBD-CGD-O2D-CED
33	B	618	CLA	CBD-CGD-O2D-CED
37	5	316	LHG	O2-C2-C3-O3
37	D	401	LHG	O2-C2-C3-O3
37	D	402	LHG	O2-C2-C3-O3
37	d	401	LHG	O2-C2-C3-O3
37	d	402	LHG	O2-C2-C3-O3
37	g	316	LHG	O2-C2-C3-O3
34	a	407	PHO	C3-C5-C6-C7
34	A	407	PHO	C3-C5-C6-C7
34	D	403	PHO	C3-C5-C6-C7
34	d	403	PHO	C3-C5-C6-C7
33	2	303	CLA	O1A-CGA-O2A-C1
33	8	303	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	5	316	LHG	O7-C5-C6-O8
37	g	316	LHG	O7-C5-C6-O8
37	1	317	LHG	C8-C7-O7-C5
37	7	317	LHG	C8-C7-O7-C5
33	6	313	CLA	CBD-CGD-O2D-CED
33	p	313	CLA	CBD-CGD-O2D-CED
43	C	518	DGD	C4E-C5E-C6E-O5E
43	c	518	DGD	C4E-C5E-C6E-O5E
33	6	308	CLA	C2C-C3C-CAC-CBC
33	p	308	CLA	C2C-C3C-CAC-CBC
42	W	101	LMG	C17-C18-C19-C20
42	w	101	LMG	C17-C18-C19-C20
43	C	518	DGD	O6E-C5E-C6E-O5E
43	c	518	DGD	O6E-C5E-C6E-O5E
42	B	622	LMG	C29-C28-O8-C9
42	b	622	LMG	C29-C28-O8-C9
41	J	101	SQD	O10-C23-O48-C46
41	j	101	SQD	O10-C23-O48-C46
33	2	303	CLA	C3-C5-C6-C7
33	8	303	CLA	C3-C5-C6-C7
37	3	322	LHG	C29-C30-C31-C32
37	9	322	LHG	C29-C30-C31-C32
33	1	305	CLA	C4-C3-C5-C6
33	2	305	CLA	C4-C3-C5-C6
33	7	305	CLA	C4-C3-C5-C6
33	8	305	CLA	C4-C3-C5-C6
33	B	604	CLA	C4-C3-C5-C6
33	B	614	CLA	C4-C3-C5-C6
33	b	604	CLA	C4-C3-C5-C6
33	b	614	CLA	C4-C3-C5-C6
33	1	305	CLA	C2-C3-C5-C6
33	2	305	CLA	C2-C3-C5-C6
33	7	305	CLA	C2-C3-C5-C6
33	8	305	CLA	C2-C3-C5-C6
33	B	604	CLA	C2-C3-C5-C6
33	B	614	CLA	C2-C3-C5-C6
33	b	604	CLA	C2-C3-C5-C6
33	b	614	CLA	C2-C3-C5-C6
33	N	307	CLA	C2A-CAA-CBA-CGA
33	n	306	CLA	C2A-CAA-CBA-CGA
37	1	317	LHG	C31-C32-C33-C34
37	7	317	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
42	C	520	LMG	O6-C5-C6-O5
42	W	101	LMG	O6-C5-C6-O5
42	c	520	LMG	O6-C5-C6-O5
42	w	101	LMG	O6-C5-C6-O5
33	0	303	CLA	CBA-CGA-O2A-C1
33	0	308	CLA	CBA-CGA-O2A-C1
33	4	303	CLA	CBA-CGA-O2A-C1
33	N	303	CLA	CBA-CGA-O2A-C1
33	0	304	CLA	O1D-CGD-O2D-CED
33	4	304	CLA	O1D-CGD-O2D-CED
38	1	310	KC2	CAA-CBA-CGA-O1A
38	1	310	KC2	CAA-CBA-CGA-O2A
38	7	310	KC2	CAA-CBA-CGA-O1A
38	7	310	KC2	CAA-CBA-CGA-O2A
36	D	407	PL9	C47-C48-C49-C51
36	d	407	PL9	C47-C48-C49-C51
33	0	301	CLA	O1D-CGD-O2D-CED
33	4	301	CLA	O1D-CGD-O2D-CED
43	c	519	DGD	O6E-C5E-C6E-O5E
37	1	317	LHG	O9-C7-O7-C5
37	7	317	LHG	O9-C7-O7-C5
42	C	520	LMG	O9-C10-O7-C8
42	c	520	LMG	O9-C10-O7-C8
33	0	307	CLA	CBA-CGA-O2A-C1
33	4	307	CLA	CBA-CGA-O2A-C1
37	D	401	LHG	C24-C23-O8-C6
37	d	401	LHG	C24-C23-O8-C6
42	B	622	LMG	O6-C5-C6-O5
42	b	622	LMG	O6-C5-C6-O5
43	C	519	DGD	O6E-C5E-C6E-O5E
42	W	101	LMG	C10-C11-C12-C13
42	w	101	LMG	C10-C11-C12-C13
33	0	307	CLA	O1A-CGA-O2A-C1
33	4	307	CLA	O1A-CGA-O2A-C1
33	2	307	CLA	C11-C10-C8-C9
33	8	307	CLA	C11-C10-C8-C9
34	a	407	PHO	C14-C13-C15-C16
34	A	407	PHO	C14-C13-C15-C16
33	2	304	CLA	C8-C10-C11-C12
39	2	313	II0	C31-C33-C35-C37
39	3	316	II0	C31-C33-C35-C37
39	8	313	II0	C31-C33-C35-C37

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Mol	Chain	Res	Type	Atoms
39	9	316	II0	C31-C33-C35-C37
35	B	620	8CT	C25-C26-C28-C29
40	3	320	IHT	C31-C34-C35-C38
40	9	320	IHT	C31-C34-C35-C38
42	W	101	LMG	C4-C5-C6-O5
42	w	101	LMG	C4-C5-C6-O5
37	3	302	LHG	C23-C24-C25-C26
37	9	302	LHG	C23-C24-C25-C26
37	D	401	LHG	C7-C8-C9-C10
37	d	401	LHG	C7-C8-C9-C10
33	8	304	CLA	C8-C10-C11-C12
33	0	306	CLA	O1D-CGD-O2D-CED
33	4	306	CLA	O1D-CGD-O2D-CED
42	D	410	LMG	C29-C28-O8-C9
42	d	410	LMG	C29-C28-O8-C9
33	1	305	CLA	C5-C6-C7-C8
33	C	505	CLA	C10-C11-C12-C13
33	C	506	CLA	C5-C6-C7-C8
33	C	508	CLA	C13-C15-C16-C17
33	D	405	CLA	C10-C11-C12-C13
33	c	505	CLA	C10-C11-C12-C13
33	c	506	CLA	C5-C6-C7-C8
33	c	508	CLA	C13-C15-C16-C17
33	d	405	CLA	C10-C11-C12-C13
37	3	322	LHG	C7-C8-C9-C10
37	9	322	LHG	C7-C8-C9-C10
33	0	302	CLA	CBD-CGD-O2D-CED
33	4	302	CLA	CBD-CGD-O2D-CED
33	2	302	CLA	C5-C6-C7-C8
33	7	305	CLA	C5-C6-C7-C8
33	8	302	CLA	C5-C6-C7-C8
33	C	507	CLA	C5-C6-C7-C8
33	c	507	CLA	C5-C6-C7-C8
43	C	521	DGD	CAA-CBA-CCA-CDA
43	c	521	DGD	CAA-CBA-CCA-CDA
37	2	315	LHG	C7-C8-C9-C10
37	8	315	LHG	C7-C8-C9-C10
42	C	520	LMG	C28-C29-C30-C31
42	c	520	LMG	C28-C29-C30-C31
43	C	519	DGD	C1B-C2B-C3B-C4B
43	C	521	DGD	C1A-C2A-C3A-C4A
43	c	519	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
43	c	521	DGD	C1A-C2A-C3A-C4A
33	2	302	CLA	CBA-CGA-O2A-C1
33	8	302	CLA	CBA-CGA-O2A-C1
37	2	315	LHG	C24-C23-O8-C6
37	8	315	LHG	C24-C23-O8-C6
41	L	101	SQD	C17-C18-C19-C20
41	l	101	SQD	C17-C18-C19-C20
43	C	521	DGD	O6D-C5D-C6D-O5D
43	c	521	DGD	O6D-C5D-C6D-O5D
42	W	101	LMG	O10-C28-O8-C9
42	w	101	LMG	O10-C28-O8-C9
37	D	408	LHG	C7-C8-C9-C10
37	d	408	LHG	C7-C8-C9-C10
42	B	624	LMG	C28-C29-C30-C31
42	D	410	LMG	C10-C11-C12-C13
42	b	624	LMG	C28-C29-C30-C31
42	d	410	LMG	C10-C11-C12-C13
41	B	601	SQD	C8-C7-O47-C45
41	b	601	SQD	C8-C7-O47-C45
35	B	621	8CT	C18-C19-C20-C21
35	H	102	8CT	C16-C17-C18-C19
35	b	621	8CT	C18-C19-C20-C21
35	h	102	8CT	C16-C17-C18-C19
33	5	311	CLA	O1D-CGD-O2D-CED
33	g	311	CLA	O1D-CGD-O2D-CED
33	B	604	CLA	C15-C16-C17-C18
33	b	604	CLA	C15-C16-C17-C18
42	C	520	LMG	O10-C28-O8-C9
42	c	520	LMG	O10-C28-O8-C9
36	a	410	PL9	C9-C11-C12-C13
36	A	410	PL9	C9-C11-C12-C13
41	B	601	SQD	C7-C8-C9-C10
41	b	601	SQD	C7-C8-C9-C10
35	a	409	8CT	C21-C23-C24-C25
35	A	409	8CT	C21-C23-C24-C25
35	0	312	8CT	C13-C14-C15-C16
35	1	312	8CT	C21-C23-C24-C25
35	4	311	8CT	C13-C14-C15-C16
35	7	312	8CT	C21-C23-C24-C25
35	B	620	8CT	C13-C14-C15-C16
35	B	620	8CT	C21-C23-C24-C25
35	B	621	8CT	C21-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
35	C	515	8CT	C13-C14-C15-C16
35	C	516	8CT	C21-C23-C24-C25
35	C	517	8CT	C13-C14-C15-C16
35	C	517	8CT	C21-C23-C24-C25
35	H	102	8CT	C13-C14-C15-C16
35	Y	101	8CT	C21-C23-C24-C25
35	b	620	8CT	C13-C14-C15-C16
35	b	620	8CT	C21-C23-C24-C25
35	b	621	8CT	C21-C23-C24-C25
35	c	515	8CT	C13-C14-C15-C16
35	c	516	8CT	C21-C23-C24-C25
35	c	517	8CT	C13-C14-C15-C16
35	c	517	8CT	C21-C23-C24-C25
35	h	102	8CT	C13-C14-C15-C16
35	y	101	8CT	C21-C23-C24-C25
43	C	521	DGD	O6E-C5E-C6E-O5E
43	c	521	DGD	O6E-C5E-C6E-O5E
37	2	315	LHG	O2-C2-C3-O3
37	8	315	LHG	O2-C2-C3-O3
37	B	623	LHG	O2-C2-C3-O3
37	b	623	LHG	O2-C2-C3-O3
33	C	506	CLA	C10-C11-C12-C13
33	C	512	CLA	C8-C10-C11-C12
33	c	506	CLA	C10-C11-C12-C13
33	c	512	CLA	C8-C10-C11-C12
33	0	308	CLA	O1A-CGA-O2A-C1
33	4	303	CLA	O1A-CGA-O2A-C1
33	N	303	CLA	O1A-CGA-O2A-C1
33	C	511	CLA	C13-C15-C16-C17
33	N	302	CLA	C15-C16-C17-C18
33	c	511	CLA	C13-C15-C16-C17
33	n	302	CLA	C15-C16-C17-C18
33	0	303	CLA	O1A-CGA-O2A-C1
33	1	302	CLA	C8-C10-C11-C12
33	7	302	CLA	C8-C10-C11-C12
37	2	315	LHG	C3-O3-P-O6
37	2	315	LHG	C4-O6-P-O3
37	8	315	LHG	C3-O3-P-O6
37	8	315	LHG	C4-O6-P-O3
37	1	317	LHG	C7-C8-C9-C10
37	7	317	LHG	C7-C8-C9-C10
33	1	302	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	7	302	CLA	C3-C5-C6-C7
33	B	605	CLA	C3-C5-C6-C7
33	b	605	CLA	C3-C5-C6-C7
33	a	412	CLA	CBA-CGA-O2A-C1
33	A	412	CLA	CBA-CGA-O2A-C1
33	0	309	CLA	CBA-CGA-O2A-C1
33	4	308	CLA	CBA-CGA-O2A-C1
37	2	315	LHG	C1-C2-C3-O3
37	5	316	LHG	C1-C2-C3-O3
37	8	315	LHG	C1-C2-C3-O3
37	B	623	LHG	C1-C2-C3-O3
37	D	401	LHG	C1-C2-C3-O3
37	b	623	LHG	C1-C2-C3-O3
37	d	401	LHG	C1-C2-C3-O3
37	g	316	LHG	C1-C2-C3-O3
37	D	408	LHG	O9-C7-O7-C5
37	d	408	LHG	O9-C7-O7-C5
41	B	601	SQD	O49-C7-O47-C45
41	b	601	SQD	O49-C7-O47-C45
36	D	407	PL9	C47-C48-C49-C50
36	d	407	PL9	C47-C48-C49-C50
42	W	101	LMG	C29-C28-O8-C9
42	w	101	LMG	C29-C28-O8-C9
33	C	511	CLA	C5-C6-C7-C8
33	c	511	CLA	C5-C6-C7-C8
33	6	308	CLA	C4C-C3C-CAC-CBC
33	p	308	CLA	C4C-C3C-CAC-CBC
37	3	322	LHG	C11-C12-C13-C14
37	9	322	LHG	C11-C12-C13-C14
37	B	623	LHG	C9-C10-C11-C12
37	B	623	LHG	C10-C11-C12-C13
37	D	402	LHG	C15-C16-C17-C18
37	D	402	LHG	C27-C28-C29-C30
37	b	623	LHG	C9-C10-C11-C12
37	b	623	LHG	C10-C11-C12-C13
37	d	402	LHG	C15-C16-C17-C18
37	d	402	LHG	C27-C28-C29-C30
42	W	101	LMG	C33-C34-C35-C36
42	W	101	LMG	C35-C36-C37-C38
42	w	101	LMG	C33-C34-C35-C36
42	w	101	LMG	C35-C36-C37-C38
43	C	519	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
43	C	519	DGD	C7B-C8B-C9B-CAB
43	C	519	DGD	C9B-CAB-CBB-CCB
43	C	521	DGD	C6A-C7A-C8A-C9A
43	c	519	DGD	C5B-C6B-C7B-C8B
43	c	519	DGD	C7B-C8B-C9B-CAB
43	c	519	DGD	C9B-CAB-CBB-CCB
43	c	521	DGD	C6A-C7A-C8A-C9A
37	2	315	LHG	C12-C13-C14-C15
37	3	302	LHG	C29-C30-C31-C32
37	7	317	LHG	C27-C28-C29-C30
37	9	302	LHG	C29-C30-C31-C32
37	B	623	LHG	C31-C32-C33-C34
37	D	401	LHG	C11-C12-C13-C14
37	b	623	LHG	C31-C32-C33-C34
42	B	622	LMG	C16-C17-C18-C19
42	T	101	LMG	C16-C17-C18-C19
42	W	101	LMG	C16-C17-C18-C19
42	b	622	LMG	C16-C17-C18-C19
42	t	101	LMG	C16-C17-C18-C19
42	w	101	LMG	C16-C17-C18-C19
42	T	101	LMG	C7-C8-O7-C10
42	t	101	LMG	C7-C8-O7-C10
37	1	317	LHG	C27-C28-C29-C30
37	8	315	LHG	C12-C13-C14-C15
37	d	401	LHG	C11-C12-C13-C14
42	T	101	LMG	C11-C12-C13-C14
42	t	101	LMG	C11-C12-C13-C14
37	1	317	LHG	C11-C12-C13-C14
37	7	317	LHG	C11-C12-C13-C14
42	D	409	LMG	C34-C35-C36-C37
42	d	409	LMG	C34-C35-C36-C37
43	C	519	DGD	C6A-C7A-C8A-C9A
43	c	519	DGD	C6A-C7A-C8A-C9A
33	N	302	CLA	C5-C6-C7-C8
33	n	302	CLA	C5-C6-C7-C8
37	3	302	LHG	O2-C2-C3-O3
37	9	302	LHG	O2-C2-C3-O3
44	F	101	HEM	C2A-CAA-CBA-CGA
33	6	306	CLA	C2C-C3C-CAC-CBC
33	p	306	CLA	C2C-C3C-CAC-CBC
37	2	315	LHG	C11-C12-C13-C14
37	2	315	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
37	D	408	LHG	C16-C17-C18-C19
37	d	408	LHG	C16-C17-C18-C19
42	D	409	LMG	C20-C21-C22-C23
42	d	409	LMG	C20-C21-C22-C23
41	B	601	SQD	C2-C1-O6-C44
41	J	101	SQD	C2-C1-O6-C44
41	b	601	SQD	C2-C1-O6-C44
41	j	101	SQD	C2-C1-O6-C44
37	8	315	LHG	C11-C12-C13-C14
37	8	315	LHG	C29-C30-C31-C32
37	9	322	LHG	C24-C25-C26-C27
42	D	409	LMG	C18-C19-C20-C21
42	d	409	LMG	C18-C19-C20-C21
33	0	309	CLA	O1A-CGA-O2A-C1
33	4	308	CLA	O1A-CGA-O2A-C1
33	B	616	CLA	C16-C17-C18-C20
33	b	616	CLA	C16-C17-C18-C20
33	B	618	CLA	O1D-CGD-O2D-CED
36	D	407	PL9	C7-C8-C9-C10
36	d	407	PL9	C7-C8-C9-C10
37	3	322	LHG	C9-C10-C11-C12
37	3	322	LHG	C24-C25-C26-C27
37	9	322	LHG	C9-C10-C11-C12
42	C	520	LMG	C36-C37-C38-C39
43	c	518	DGD	C5B-C6B-C7B-C8B
34	a	407	PHO	C2-C3-C5-C6
34	A	407	PHO	C2-C3-C5-C6
33	B	606	CLA	C6-C7-C8-C9
33	b	606	CLA	C6-C7-C8-C9
33	0	307	CLA	O1D-CGD-O2D-CED
33	4	307	CLA	O1D-CGD-O2D-CED
43	C	521	DGD	C1B-C2B-C3B-C4B
43	c	521	DGD	C1B-C2B-C3B-C4B
42	C	520	LMG	C33-C34-C35-C36
42	D	410	LMG	C11-C12-C13-C14
42	W	101	LMG	C14-C15-C16-C17
42	c	520	LMG	C33-C34-C35-C36
42	c	520	LMG	C36-C37-C38-C39
42	d	410	LMG	C11-C12-C13-C14
42	w	101	LMG	C14-C15-C16-C17
43	C	518	DGD	C5B-C6B-C7B-C8B
33	0	308	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
33	N	303	CLA	C2A-CAA-CBA-CGA
43	C	519	DGD	CBB-CCB-CDB-CEB
43	c	519	DGD	CBB-CCB-CDB-CEB
37	3	321	LHG	O1-C1-C2-C3
37	9	321	LHG	O1-C1-C2-C3
37	D	408	LHG	O1-C1-C2-C3
37	d	408	LHG	O1-C1-C2-C3
39	2	313	II0	C31-C33-C35-C39
39	8	313	II0	C31-C33-C35-C39
33	C	505	CLA	C3-C5-C6-C7
33	c	505	CLA	C3-C5-C6-C7
37	0	317	LHG	O9-C7-O7-C5
37	4	316	LHG	O9-C7-O7-C5
37	2	315	LHG	C30-C31-C32-C33
37	D	408	LHG	C14-C15-C16-C17
37	d	408	LHG	C14-C15-C16-C17
37	8	315	LHG	C30-C31-C32-C33
37	B	623	LHG	C27-C28-C29-C30
37	b	623	LHG	C27-C28-C29-C30
41	J	101	SQD	C10-C11-C12-C13
41	j	101	SQD	C10-C11-C12-C13
42	C	520	LMG	C37-C38-C39-C40
42	c	520	LMG	C37-C38-C39-C40
33	0	303	CLA	C4B-C3B-CAB-CBB
33	1	302	CLA	C4B-C3B-CAB-CBB
33	2	302	CLA	C4B-C3B-CAB-CBB
33	2	307	CLA	C4B-C3B-CAB-CBB
33	4	303	CLA	C4B-C3B-CAB-CBB
33	5	301	CLA	C4B-C3B-CAB-CBB
33	5	306	CLA	C4B-C3B-CAB-CBB
33	5	307	CLA	C4B-C3B-CAB-CBB
33	5	317	CLA	C4B-C3B-CAB-CBB
33	7	302	CLA	C4B-C3B-CAB-CBB
33	8	302	CLA	C4B-C3B-CAB-CBB
33	8	307	CLA	C4B-C3B-CAB-CBB
33	B	616	CLA	C4B-C3B-CAB-CBB
33	C	504	CLA	C4B-C3B-CAB-CBB
33	C	508	CLA	C4B-C3B-CAB-CBB
33	b	616	CLA	C4B-C3B-CAB-CBB
33	c	504	CLA	C4B-C3B-CAB-CBB
33	c	508	CLA	C4B-C3B-CAB-CBB
33	g	301	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	g	306	CLA	C4B-C3B-CAB-CBB
33	g	307	CLA	C4B-C3B-CAB-CBB
33	g	317	CLA	C4B-C3B-CAB-CBB
33	0	307	CLA	C6-C7-C8-C10
33	4	307	CLA	C6-C7-C8-C10
33	5	307	CLA	C6-C7-C8-C9
33	g	307	CLA	C6-C7-C8-C9
33	C	504	CLA	C8-C10-C11-C12
33	c	504	CLA	C8-C10-C11-C12
37	D	408	LHG	C27-C28-C29-C30
37	d	408	LHG	C27-C28-C29-C30
42	B	622	LMG	C18-C19-C20-C21
42	B	624	LMG	C17-C18-C19-C20
42	b	622	LMG	C18-C19-C20-C21
42	b	624	LMG	C17-C18-C19-C20
37	2	315	LHG	C27-C28-C29-C30
41	C	501	SQD	C11-C12-C13-C14
41	c	501	SQD	C11-C12-C13-C14
42	C	520	LMG	C32-C33-C34-C35
42	c	520	LMG	C12-C13-C14-C15
42	c	520	LMG	C32-C33-C34-C35
43	C	519	DGD	C4A-C5A-C6A-C7A
43	C	521	DGD	C6B-C7B-C8B-C9B
43	c	519	DGD	C4A-C5A-C6A-C7A
43	c	521	DGD	C6B-C7B-C8B-C9B
33	2	302	CLA	O1A-CGA-O2A-C1
37	8	315	LHG	C27-C28-C29-C30
37	D	408	LHG	C18-C19-C20-C21
37	d	408	LHG	C18-C19-C20-C21
42	C	520	LMG	C12-C13-C14-C15
43	C	519	DGD	C9A-CAA-CBA-CCA
43	c	519	DGD	C9A-CAA-CBA-CCA
42	W	101	LMG	C19-C20-C21-C22
42	w	101	LMG	C19-C20-C21-C22
33	2	303	CLA	C3A-C2A-CAA-CBA
33	8	303	CLA	C3A-C2A-CAA-CBA
35	B	620	8CT	C16-C17-C18-C19
35	b	620	8CT	C16-C17-C18-C19
33	8	302	CLA	O1A-CGA-O2A-C1
33	5	307	CLA	C6-C7-C8-C10
33	g	307	CLA	C6-C7-C8-C10
37	2	315	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
37	8	315	LHG	C4-C5-C6-O8
43	H	101	DGD	C9B-CAB-CBB-CCB
43	h	101	DGD	C9B-CAB-CBB-CCB
33	B	603	CLA	O2A-C1-C2-C3
33	b	603	CLA	O2A-C1-C2-C3
33	p	310	CLA	C2C-C3C-CAC-CBC
36	D	407	PL9	C30-C29-C31-C32
36	d	407	PL9	C30-C29-C31-C32
33	3	303	CLA	C2-C3-C5-C6
33	9	303	CLA	C2-C3-C5-C6
38	1	311	KC2	CAA-CBA-CGA-O1A
42	W	101	LMG	C11-C10-O7-C8
42	w	101	LMG	C11-C10-O7-C8
33	6	310	CLA	C2C-C3C-CAC-CBC
33	B	611	CLA	C2A-CAA-CBA-CGA
37	2	315	LHG	O1-C1-C2-O2
37	8	315	LHG	O1-C1-C2-O2
41	L	101	SQD	C26-C27-C28-C29
41	l	101	SQD	C26-C27-C28-C29
37	a	411	LHG	C7-C8-C9-C10
37	A	411	LHG	C7-C8-C9-C10
33	0	303	CLA	C2B-C3B-CAB-CBB
33	0	307	CLA	C2B-C3B-CAB-CBB
33	1	302	CLA	C2B-C3B-CAB-CBB
33	2	302	CLA	C2B-C3B-CAB-CBB
33	2	307	CLA	C2B-C3B-CAB-CBB
33	4	303	CLA	C2B-C3B-CAB-CBB
33	4	307	CLA	C2B-C3B-CAB-CBB
33	5	301	CLA	C2B-C3B-CAB-CBB
33	5	306	CLA	C2B-C3B-CAB-CBB
33	5	307	CLA	C2B-C3B-CAB-CBB
33	5	317	CLA	C2B-C3B-CAB-CBB
33	7	302	CLA	C2B-C3B-CAB-CBB
33	8	302	CLA	C2B-C3B-CAB-CBB
33	8	307	CLA	C2B-C3B-CAB-CBB
33	B	616	CLA	C2B-C3B-CAB-CBB
33	C	504	CLA	C2B-C3B-CAB-CBB
33	b	616	CLA	C2B-C3B-CAB-CBB
33	c	504	CLA	C2B-C3B-CAB-CBB
33	g	301	CLA	C2B-C3B-CAB-CBB
33	g	306	CLA	C2B-C3B-CAB-CBB
33	g	307	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	g	317	CLA	C2B-C3B-CAB-CBB
33	B	616	CLA	C10-C11-C12-C13
33	b	616	CLA	C10-C11-C12-C13
43	C	521	DGD	C5B-C6B-C7B-C8B
43	c	521	DGD	C5B-C6B-C7B-C8B
33	2	302	CLA	C3-C5-C6-C7
33	8	302	CLA	C3-C5-C6-C7
33	B	610	CLA	C5-C6-C7-C8
33	b	610	CLA	C5-C6-C7-C8
42	W	101	LMG	O9-C10-O7-C8
42	w	101	LMG	O9-C10-O7-C8
38	7	311	KC2	CAA-CBA-CGA-O1A
33	0	303	CLA	C2-C1-O2A-CGA
33	2	303	CLA	C2-C1-O2A-CGA
33	4	303	CLA	C2-C1-O2A-CGA
33	8	303	CLA	C2-C1-O2A-CGA
42	T	101	LMG	C18-C19-C20-C21
42	t	101	LMG	C18-C19-C20-C21
37	2	315	LHG	C5-C4-O6-P
37	8	315	LHG	C5-C4-O6-P
43	C	521	DGD	C9B-CAB-CBB-CCB
43	C	521	DGD	CCB-CDB-CEB-CFB
43	c	521	DGD	C9B-CAB-CBB-CCB
43	c	521	DGD	CCB-CDB-CEB-CFB
33	0	307	CLA	C6-C7-C8-C9
33	4	307	CLA	C6-C7-C8-C9
33	a	405	CLA	C3-C5-C6-C7
33	A	405	CLA	C3-C5-C6-C7
35	C	515	8CT	C02-C03-C10-C11
35	c	515	8CT	C02-C03-C10-C11
40	3	320	IHT	C10-C07-C18-C22
40	6	318	IHT	C02-C07-C18-C22
40	6	318	IHT	C10-C07-C18-C22
40	9	320	IHT	C10-C07-C18-C22
40	p	318	IHT	C02-C07-C18-C22
40	p	318	IHT	C10-C07-C18-C22
42	D	410	LMG	O6-C5-C6-O5
42	d	410	LMG	O6-C5-C6-O5
43	C	521	DGD	C2A-C3A-C4A-C5A
43	c	521	DGD	C2A-C3A-C4A-C5A
42	b	624	LMG	C14-C15-C16-C17
33	a	412	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	A	412	CLA	O1A-CGA-O2A-C1
42	B	624	LMG	C14-C15-C16-C17
33	B	606	CLA	C15-C16-C17-C18
33	D	405	CLA	C15-C16-C17-C18
33	b	606	CLA	C15-C16-C17-C18
33	d	405	CLA	C15-C16-C17-C18
38	1	311	KC2	CAA-CBA-CGA-O2A
38	7	311	KC2	CAA-CBA-CGA-O2A
37	B	623	LHG	C32-C33-C34-C35
37	b	623	LHG	C32-C33-C34-C35
33	3	303	CLA	C4-C3-C5-C6
33	9	303	CLA	C4-C3-C5-C6
34	a	407	PHO	C4-C3-C5-C6
34	A	407	PHO	C4-C3-C5-C6
36	D	407	PL9	C15-C14-C16-C17
36	d	407	PL9	C15-C14-C16-C17
33	1	307	CLA	C11-C10-C8-C7
33	7	307	CLA	C11-C10-C8-C7
33	B	605	CLA	C11-C10-C8-C7
33	b	605	CLA	C11-C10-C8-C7
36	D	407	PL9	C13-C14-C16-C17
36	D	407	PL9	C28-C29-C31-C32
36	d	407	PL9	C13-C14-C16-C17
36	d	407	PL9	C28-C29-C31-C32
35	C	516	8CT	C16-C17-C18-C19
35	D	406	8CT	C16-C17-C18-C19
35	c	516	8CT	C16-C17-C18-C19
35	d	406	8CT	C16-C17-C18-C19
43	C	519	DGD	O1B-C1B-O2G-C2G
43	c	519	DGD	O1B-C1B-O2G-C2G
37	D	402	LHG	C23-C24-C25-C26
37	d	402	LHG	C23-C24-C25-C26
33	C	513	CLA	CBA-CGA-O2A-C1
33	c	513	CLA	CBA-CGA-O2A-C1
37	D	402	LHG	C32-C33-C34-C35
37	d	402	LHG	C32-C33-C34-C35
33	5	302	CLA	C2A-CAA-CBA-CGA
33	b	611	CLA	C2A-CAA-CBA-CGA
33	g	302	CLA	C2A-CAA-CBA-CGA
33	6	313	CLA	O1D-CGD-O2D-CED
33	p	313	CLA	O1D-CGD-O2D-CED
41	L	101	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
41	l	101	SQD	C23-C24-C25-C26
42	B	622	LMG	C28-C29-C30-C31
42	b	622	LMG	C28-C29-C30-C31
33	c	504	CLA	C15-C16-C17-C18
37	1	317	LHG	C11-C10-C9-C8
37	1	317	LHG	C18-C19-C20-C21
37	7	317	LHG	C11-C10-C9-C8
37	7	317	LHG	C18-C19-C20-C21
38	1	311	KC2	C2C-C3C-CAC-CBC
38	2	309	KC2	C2B-C3B-CAB-CBB
38	2	309	KC2	C2C-C3C-CAC-CBC
38	3	311	KC2	C2C-C3C-CAC-CBC
38	7	311	KC2	C2C-C3C-CAC-CBC
38	8	309	KC2	C2B-C3B-CAB-CBB
38	8	309	KC2	C2C-C3C-CAC-CBC
38	9	311	KC2	C2C-C3C-CAC-CBC
41	J	101	SQD	O5-C1-O6-C44
41	j	101	SQD	O5-C1-O6-C44
33	C	504	CLA	C15-C16-C17-C18
37	0	317	LHG	C8-C7-O7-C5
37	3	302	LHG	C8-C7-O7-C5
37	4	316	LHG	C8-C7-O7-C5
37	9	302	LHG	C8-C7-O7-C5
41	C	501	SQD	C8-C7-O47-C45
41	c	501	SQD	C8-C7-O47-C45
38	0	305	KC2	C4C-C3C-CAC-CBC
38	1	310	KC2	C4B-C3B-CAB-CBB
38	1	310	KC2	C4C-C3C-CAC-CBC
38	1	311	KC2	C4C-C3C-CAC-CBC
38	2	309	KC2	C4B-C3B-CAB-CBB
38	3	311	KC2	C4C-C3C-CAC-CBC
38	4	305	KC2	C4C-C3C-CAC-CBC
38	7	310	KC2	C4B-C3B-CAB-CBB
38	7	310	KC2	C4C-C3C-CAC-CBC
38	7	311	KC2	C4C-C3C-CAC-CBC
38	8	309	KC2	C4B-C3B-CAB-CBB
38	9	311	KC2	C4C-C3C-CAC-CBC
33	1	307	CLA	C15-C16-C17-C18
33	7	307	CLA	C15-C16-C17-C18
33	B	612	CLA	C13-C15-C16-C17
33	b	612	CLA	C13-C15-C16-C17
43	C	521	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
43	c	521	DGD	O1B-C1B-O2G-C2G
43	H	101	DGD	O6E-C5E-C6E-O5E
43	h	101	DGD	O6E-C5E-C6E-O5E
42	C	520	LMG	C18-C19-C20-C21
42	c	520	LMG	C18-C19-C20-C21
36	D	407	PL9	C45-C44-C46-C47
36	d	407	PL9	C45-C44-C46-C47
37	2	315	LHG	C23-C24-C25-C26
37	8	315	LHG	C23-C24-C25-C26
39	0	314	II0	C10-C22-C24-C26
39	1	315	II0	C09-C21-C23-C25
39	1	315	II0	C10-C22-C24-C26
39	2	313	II0	C10-C22-C24-C26
39	3	318	II0	C10-C22-C24-C26
39	4	313	II0	C10-C22-C24-C26
39	5	312	II0	C10-C22-C24-C26
39	6	315	II0	C09-C21-C23-C25
39	6	315	II0	C10-C22-C24-C26
39	7	315	II0	C09-C21-C23-C25
39	7	315	II0	C10-C22-C24-C26
39	8	313	II0	C10-C22-C24-C26
39	9	318	II0	C10-C22-C24-C26
39	g	312	II0	C10-C22-C24-C26
39	p	315	II0	C09-C21-C23-C25
39	p	315	II0	C10-C22-C24-C26
33	9	310	CLA	C2C-C3C-CAC-CBC
33	a	412	CLA	C11-C12-C13-C14
33	A	412	CLA	C11-C12-C13-C14
33	B	605	CLA	C11-C10-C8-C9
33	C	511	CLA	C11-C12-C13-C14
33	b	605	CLA	C11-C10-C8-C9
33	c	511	CLA	C11-C12-C13-C14
41	L	101	SQD	C15-C16-C17-C18
41	l	101	SQD	C15-C16-C17-C18
42	D	410	LMG	C14-C15-C16-C17
42	d	410	LMG	C14-C15-C16-C17
33	3	305	CLA	C3-C5-C6-C7
33	9	305	CLA	C3-C5-C6-C7
33	3	310	CLA	C2C-C3C-CAC-CBC
37	B	623	LHG	C29-C30-C31-C32
37	b	623	LHG	C29-C30-C31-C32
33	0	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	0	306	CLA	C1A-C2A-CAA-CBA
33	1	302	CLA	C1A-C2A-CAA-CBA
33	1	308	CLA	C1A-C2A-CAA-CBA
33	2	301	CLA	C1A-C2A-CAA-CBA
33	2	303	CLA	C1A-C2A-CAA-CBA
33	2	307	CLA	C1A-C2A-CAA-CBA
33	4	304	CLA	C1A-C2A-CAA-CBA
33	4	306	CLA	C1A-C2A-CAA-CBA
33	5	302	CLA	C1A-C2A-CAA-CBA
33	5	311	CLA	C1A-C2A-CAA-CBA
33	7	302	CLA	C1A-C2A-CAA-CBA
33	7	308	CLA	C1A-C2A-CAA-CBA
33	8	301	CLA	C1A-C2A-CAA-CBA
33	8	303	CLA	C1A-C2A-CAA-CBA
33	8	307	CLA	C1A-C2A-CAA-CBA
33	B	612	CLA	C1A-C2A-CAA-CBA
33	C	509	CLA	C1A-C2A-CAA-CBA
33	b	612	CLA	C1A-C2A-CAA-CBA
33	c	509	CLA	C1A-C2A-CAA-CBA
33	g	302	CLA	C1A-C2A-CAA-CBA
33	g	311	CLA	C1A-C2A-CAA-CBA
42	W	101	LMG	C31-C32-C33-C34
42	w	101	LMG	C31-C32-C33-C34
35	D	406	8CT	C18-C19-C20-C21
35	d	406	8CT	C18-C19-C20-C21
37	1	317	LHG	C3-O3-P-O6
37	7	317	LHG	C3-O3-P-O6
37	B	623	LHG	C4-O6-P-O3
37	b	623	LHG	C4-O6-P-O3
33	0	311	CLA	CBD-CGD-O2D-CED
33	4	310	CLA	CBD-CGD-O2D-CED
42	D	409	LMG	C16-C17-C18-C19
42	d	409	LMG	C16-C17-C18-C19
33	2	304	CLA	C5-C6-C7-C8
33	8	304	CLA	C5-C6-C7-C8
37	B	623	LHG	O6-C4-C5-C6
37	b	623	LHG	O6-C4-C5-C6
33	B	616	CLA	C16-C17-C18-C19
33	b	616	CLA	C16-C17-C18-C19
41	j	101	SQD	C11-C10-C9-C8
42	W	101	LMG	C29-C30-C31-C32
42	w	101	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
37	3	321	LHG	C24-C23-O8-C6
37	9	321	LHG	C24-C23-O8-C6
41	J	101	SQD	C11-C10-C9-C8
42	B	622	LMG	C31-C32-C33-C34
42	b	622	LMG	C31-C32-C33-C34
33	C	512	CLA	CBA-CGA-O2A-C1
33	c	512	CLA	CBA-CGA-O2A-C1
42	T	101	LMG	C20-C21-C22-C23
42	b	624	LMG	C11-C12-C13-C14
42	t	101	LMG	C20-C21-C22-C23
42	B	624	LMG	C11-C12-C13-C14
42	b	624	LMG	C13-C14-C15-C16
43	H	101	DGD	O1A-C1A-O1G-C1G
43	h	101	DGD	O1A-C1A-O1G-C1G
37	2	315	LHG	C14-C15-C16-C17
37	8	315	LHG	C14-C15-C16-C17
37	D	402	LHG	C24-C25-C26-C27
37	d	402	LHG	C24-C25-C26-C27
42	B	624	LMG	C13-C14-C15-C16
33	N	301	CLA	C16-C17-C18-C20
33	n	301	CLA	C16-C17-C18-C20
37	3	321	LHG	C4-C5-C6-O8
37	9	321	LHG	C4-C5-C6-O8
42	C	520	LMG	C7-C8-C9-O8
42	W	101	LMG	C15-C16-C17-C18
42	c	520	LMG	C7-C8-C9-O8
42	w	101	LMG	C15-C16-C17-C18
43	C	519	DGD	C2G-C3G-O3G-C1D
43	c	519	DGD	C2G-C3G-O3G-C1D
42	T	101	LMG	O6-C5-C6-O5
42	t	101	LMG	O6-C5-C6-O5
37	d	401	LHG	C27-C28-C29-C30
37	D	408	LHG	O1-C1-C2-O2
37	d	408	LHG	O1-C1-C2-O2
33	0	308	CLA	C2C-C3C-CAC-CBC
33	N	303	CLA	C2C-C3C-CAC-CBC
37	2	315	LHG	C11-C10-C9-C8
37	8	315	LHG	C11-C10-C9-C8
37	D	401	LHG	C27-C28-C29-C30
37	1	317	LHG	C33-C34-C35-C36
42	D	409	LMG	O6-C5-C6-O5
42	d	409	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
33	1	304	CLA	C4-C3-C5-C6
37	7	317	LHG	C33-C34-C35-C36
38	2	309	KC2	C2A-CAA-CBA-CGA
38	8	309	KC2	C2A-CAA-CBA-CGA
33	N	301	CLA	CBA-CGA-O2A-C1
33	n	301	CLA	CBA-CGA-O2A-C1
37	B	623	LHG	C28-C29-C30-C31
37	D	401	LHG	C19-C20-C21-C22
37	b	623	LHG	C28-C29-C30-C31
33	0	302	CLA	O1D-CGD-O2D-CED
37	d	401	LHG	C19-C20-C21-C22
42	W	101	LMG	C36-C37-C38-C39
42	w	101	LMG	C36-C37-C38-C39
43	C	518	DGD	C6A-C7A-C8A-C9A
43	c	518	DGD	C6A-C7A-C8A-C9A
33	4	302	CLA	O1D-CGD-O2D-CED
33	B	614	CLA	C3-C5-C6-C7
33	0	308	CLA	C4C-C3C-CAC-CBC
33	N	303	CLA	C4C-C3C-CAC-CBC
42	B	624	LMG	C30-C31-C32-C33
42	B	624	LMG	C31-C32-C33-C34
42	C	520	LMG	C31-C32-C33-C34
42	b	624	LMG	C30-C31-C32-C33
42	c	520	LMG	C31-C32-C33-C34
43	H	101	DGD	CCB-CDB-CEB-CFB
43	h	101	DGD	CCB-CDB-CEB-CFB
33	1	308	CLA	CBA-CGA-O2A-C1
33	7	308	CLA	CBA-CGA-O2A-C1
42	b	624	LMG	C31-C32-C33-C34
37	2	315	LHG	O10-C23-O8-C6
37	8	315	LHG	O10-C23-O8-C6
37	B	623	LHG	O10-C23-O8-C6
37	b	623	LHG	O10-C23-O8-C6
43	C	519	DGD	C1A-C2A-C3A-C4A
43	c	519	DGD	C1A-C2A-C3A-C4A
42	l	102	LMG	C2-C1-O1-C7
42	m	101	LMG	C2-C1-O1-C7
42	B	622	LMG	C33-C34-C35-C36
42	b	622	LMG	C33-C34-C35-C36
42	D	410	LMG	O10-C28-O8-C9
42	d	410	LMG	O10-C28-O8-C9
37	3	302	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	9	302	LHG	C9-C10-C11-C12
43	H	101	DGD	C6A-C7A-C8A-C9A
43	H	101	DGD	C9A-CAA-CBA-CCA
43	h	101	DGD	C6A-C7A-C8A-C9A
33	2	303	CLA	C4-C3-C5-C6
33	7	304	CLA	C4-C3-C5-C6
33	8	303	CLA	C4-C3-C5-C6
43	h	101	DGD	C9A-CAA-CBA-CCA
33	1	304	CLA	C2-C3-C5-C6
33	1	305	CLA	C11-C10-C8-C7
33	7	304	CLA	C2-C3-C5-C6
33	7	305	CLA	C11-C10-C8-C7
43	H	101	DGD	O2G-C1B-C2B-C3B
33	1	307	CLA	C11-C10-C8-C9
33	7	307	CLA	C11-C10-C8-C9
37	D	401	LHG	C29-C30-C31-C32
37	d	401	LHG	C29-C30-C31-C32
33	N	305	CLA	CBA-CGA-O2A-C1
33	n	304	CLA	CBA-CGA-O2A-C1
37	a	411	LHG	C24-C23-O8-C6
37	A	411	LHG	C24-C23-O8-C6
42	B	622	LMG	C29-C30-C31-C32
33	b	614	CLA	C3-C5-C6-C7
41	C	501	SQD	O49-C7-O47-C45
41	c	501	SQD	O49-C7-O47-C45
33	6	306	CLA	C4C-C3C-CAC-CBC
33	p	306	CLA	C4C-C3C-CAC-CBC
42	b	622	LMG	C29-C30-C31-C32
37	D	401	LHG	C12-C13-C14-C15
37	d	401	LHG	C12-C13-C14-C15
43	h	101	DGD	O2G-C1B-C2B-C3B
33	a	406	CLA	C4B-C3B-CAB-CBB
33	A	406	CLA	C4B-C3B-CAB-CBB
33	0	304	CLA	C4B-C3B-CAB-CBB
33	1	306	CLA	C4B-C3B-CAB-CBB
33	2	306	CLA	C4B-C3B-CAB-CBB
33	4	304	CLA	C4B-C3B-CAB-CBB
33	5	308	CLA	C4B-C3B-CAB-CBB
33	6	302	CLA	C4B-C3B-CAB-CBB
33	6	304	CLA	C4B-C3B-CAB-CBB
33	7	306	CLA	C4B-C3B-CAB-CBB
33	8	306	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	B	606	CLA	C4B-C3B-CAB-CBB
33	B	607	CLA	C4B-C3B-CAB-CBB
33	N	307	CLA	C4B-C3B-CAB-CBB
33	b	606	CLA	C4B-C3B-CAB-CBB
33	b	607	CLA	C4B-C3B-CAB-CBB
33	g	308	CLA	C4B-C3B-CAB-CBB
33	n	306	CLA	C4B-C3B-CAB-CBB
33	p	302	CLA	C4B-C3B-CAB-CBB
33	p	304	CLA	C4B-C3B-CAB-CBB
37	a	411	LHG	O6-C4-C5-C6
37	A	411	LHG	O6-C4-C5-C6
37	D	408	LHG	O6-C4-C5-C6
37	d	408	LHG	O6-C4-C5-C6
37	3	322	LHG	C32-C33-C34-C35
37	9	322	LHG	C32-C33-C34-C35
37	B	623	LHG	C14-C15-C16-C17
37	3	322	LHG	C23-C24-C25-C26
37	9	322	LHG	C23-C24-C25-C26
37	B	623	LHG	C23-C24-C25-C26
37	b	623	LHG	C23-C24-C25-C26
42	B	624	LMG	C10-C11-C12-C13
42	b	624	LMG	C10-C11-C12-C13
37	b	623	LHG	C14-C15-C16-C17
42	B	622	LMG	C38-C39-C40-C41
42	b	622	LMG	C38-C39-C40-C41
43	C	518	DGD	C4A-C5A-C6A-C7A
43	c	518	DGD	C4A-C5A-C6A-C7A
42	C	520	LMG	C34-C35-C36-C37
33	B	610	CLA	C4-C3-C5-C6
33	b	610	CLA	C4-C3-C5-C6
33	B	608	CLA	C2-C3-C5-C6
33	b	608	CLA	C2-C3-C5-C6
36	D	407	PL9	C43-C44-C46-C47
36	d	407	PL9	C43-C44-C46-C47
37	B	623	LHG	C24-C25-C26-C27
42	c	520	LMG	C34-C35-C36-C37
37	1	317	LHG	C13-C14-C15-C16
37	7	317	LHG	C13-C14-C15-C16
37	b	623	LHG	C24-C25-C26-C27
33	3	307	CLA	C3A-C2A-CAA-CBA
33	9	307	CLA	C3A-C2A-CAA-CBA
37	3	322	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
37	9	322	LHG	C30-C31-C32-C33
44	F	101	HEM	C3D-CAD-CBD-CGD
37	B	623	LHG	C18-C19-C20-C21
37	b	623	LHG	C18-C19-C20-C21
35	C	517	8CT	C28-C29-C30-C35
35	Y	101	8CT	C28-C29-C30-C35
35	c	517	8CT	C28-C29-C30-C35
35	y	101	8CT	C28-C29-C30-C35
41	J	101	SQD	O6-C44-C45-C46
41	j	101	SQD	O6-C44-C45-C46
42	B	622	LMG	C7-C8-C9-O8
42	W	101	LMG	C7-C8-C9-O8
42	b	622	LMG	C7-C8-C9-O8
42	w	101	LMG	C7-C8-C9-O8
43	H	101	DGD	C4B-C5B-C6B-C7B
43	h	101	DGD	C4B-C5B-C6B-C7B
43	C	521	DGD	C4E-C5E-C6E-O5E
43	c	521	DGD	C4E-C5E-C6E-O5E
37	3	321	LHG	C11-C10-C9-C8
37	9	321	LHG	C11-C10-C9-C8
42	D	410	LMG	C22-C23-C24-C25
42	d	410	LMG	C22-C23-C24-C25
43	C	521	DGD	CBB-CCB-CDB-CEB
43	c	521	DGD	CBB-CCB-CDB-CEB
33	d	405	CLA	C13-C15-C16-C17
41	L	101	SQD	C9-C10-C11-C12
41	l	101	SQD	C9-C10-C11-C12
41	L	101	SQD	C35-C36-C37-C38
33	D	405	CLA	C13-C15-C16-C17
33	B	608	CLA	C4-C3-C5-C6
33	b	608	CLA	C4-C3-C5-C6
37	D	401	LHG	C16-C17-C18-C19
37	D	402	LHG	C30-C31-C32-C33
37	d	402	LHG	C30-C31-C32-C33
41	l	101	SQD	C35-C36-C37-C38
33	C	507	CLA	C10-C11-C12-C13
33	C	514	CLA	C5-C6-C7-C8
33	c	507	CLA	C10-C11-C12-C13
37	3	322	LHG	C4-O6-P-O3
37	9	322	LHG	C4-O6-P-O3
37	d	401	LHG	C16-C17-C18-C19
33	A	412	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
37	D	401	LHG	O1-C1-C2-O2
37	d	401	LHG	O1-C1-C2-O2
33	c	514	CLA	C5-C6-C7-C8
37	d	402	LHG	C12-C13-C14-C15
42	b	624	LMG	C20-C21-C22-C23
33	N	301	CLA	C16-C17-C18-C19
33	n	301	CLA	C16-C17-C18-C19
37	D	402	LHG	C12-C13-C14-C15
42	B	624	LMG	C20-C21-C22-C23
33	a	406	CLA	C2B-C3B-CAB-CBB
33	A	406	CLA	C2B-C3B-CAB-CBB
33	0	304	CLA	C2B-C3B-CAB-CBB
33	1	306	CLA	C2B-C3B-CAB-CBB
33	4	304	CLA	C2B-C3B-CAB-CBB
33	5	308	CLA	C2B-C3B-CAB-CBB
33	6	302	CLA	C2B-C3B-CAB-CBB
33	7	306	CLA	C2B-C3B-CAB-CBB
33	B	607	CLA	C2B-C3B-CAB-CBB
33	C	505	CLA	C2B-C3B-CAB-CBB
33	N	307	CLA	C2B-C3B-CAB-CBB
33	b	607	CLA	C2B-C3B-CAB-CBB
33	c	505	CLA	C2B-C3B-CAB-CBB
33	g	308	CLA	C2B-C3B-CAB-CBB
33	n	306	CLA	C2B-C3B-CAB-CBB
33	p	302	CLA	C2B-C3B-CAB-CBB
41	J	101	SQD	C26-C27-C28-C29
42	B	622	LMG	C19-C20-C21-C22
42	b	622	LMG	C19-C20-C21-C22
33	a	412	CLA	C3-C5-C6-C7
33	B	608	CLA	C3-C5-C6-C7
33	b	608	CLA	C3-C5-C6-C7
41	j	101	SQD	C26-C27-C28-C29
37	3	302	LHG	O7-C5-C6-O8
37	9	302	LHG	O7-C5-C6-O8
41	L	101	SQD	O6-C44-C45-O47
41	l	101	SQD	O6-C44-C45-O47
42	W	101	LMG	O1-C7-C8-O7
42	w	101	LMG	O1-C7-C8-O7
40	3	320	IHT	C26-C29-C31-C34
40	9	320	IHT	C26-C29-C31-C34
37	D	402	LHG	C1-C2-C3-O3
37	d	402	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	0	306	CLA	C2-C1-O2A-CGA
33	4	306	CLA	C2-C1-O2A-CGA
33	D	404	CLA	C2-C1-O2A-CGA
33	d	404	CLA	C2-C1-O2A-CGA
34	D	403	PHO	C2-C1-O2A-CGA
34	d	403	PHO	C2-C1-O2A-CGA
33	2	303	CLA	C2-C3-C5-C6
33	8	303	CLA	C2-C3-C5-C6
33	B	610	CLA	C2-C3-C5-C6
33	b	610	CLA	C2-C3-C5-C6
42	C	520	LMG	C20-C21-C22-C23
42	c	520	LMG	C20-C21-C22-C23
33	1	305	CLA	C11-C10-C8-C9
33	7	305	CLA	C11-C10-C8-C9
33	B	605	CLA	C6-C7-C8-C9
33	C	508	CLA	C14-C13-C15-C16
33	b	605	CLA	C6-C7-C8-C9
33	c	508	CLA	C14-C13-C15-C16
37	3	302	LHG	C11-C12-C13-C14
37	9	302	LHG	C11-C12-C13-C14
41	J	101	SQD	C28-C29-C30-C31
41	j	101	SQD	C28-C29-C30-C31
35	C	515	8CT	C04-C03-C10-C11
35	c	515	8CT	C04-C03-C10-C11
43	C	518	DGD	CDB-CEB-CFB-CGB
33	N	301	CLA	CAA-CBA-CGA-O2A
33	n	301	CLA	CAA-CBA-CGA-O2A
43	C	519	DGD	CBA-CCA-CDA-CEA
43	c	518	DGD	CDB-CEB-CFB-CGB
43	c	519	DGD	CBA-CCA-CDA-CEA
33	5	301	CLA	C1A-C2A-CAA-CBA
33	g	301	CLA	C1A-C2A-CAA-CBA
33	B	607	CLA	C10-C11-C12-C13
33	b	607	CLA	C10-C11-C12-C13
42	B	622	LMG	C37-C38-C39-C40
42	B	624	LMG	C32-C33-C34-C35
42	b	624	LMG	C32-C33-C34-C35
33	B	613	CLA	C16-C17-C18-C20
33	C	514	CLA	C16-C17-C18-C19
33	b	613	CLA	C16-C17-C18-C20
33	c	514	CLA	C16-C17-C18-C19
33	6	310	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
42	b	622	LMG	C40-C41-C42-C43
33	p	310	CLA	C4C-C3C-CAC-CBC
42	B	622	LMG	C13-C14-C15-C16
42	B	622	LMG	C40-C41-C42-C43
42	C	520	LMG	C17-C18-C19-C20
42	b	622	LMG	C13-C14-C15-C16
42	b	622	LMG	C37-C38-C39-C40
42	c	520	LMG	C17-C18-C19-C20
37	D	401	LHG	C15-C16-C17-C18
37	d	401	LHG	C15-C16-C17-C18
37	D	402	LHG	O6-C4-C5-C6
37	d	402	LHG	O6-C4-C5-C6
33	2	306	CLA	C6-C7-C8-C10
33	2	307	CLA	C11-C10-C8-C7
33	8	306	CLA	C6-C7-C8-C10
33	8	307	CLA	C11-C10-C8-C7
33	B	605	CLA	C6-C7-C8-C10
33	C	505	CLA	C11-C10-C8-C7
33	C	508	CLA	C12-C13-C15-C16
33	b	605	CLA	C6-C7-C8-C10
33	c	505	CLA	C11-C10-C8-C7
33	c	508	CLA	C12-C13-C15-C16
34	D	403	PHO	C6-C7-C8-C10
34	d	403	PHO	C6-C7-C8-C10
33	C	513	CLA	O1A-CGA-O2A-C1
33	c	513	CLA	O1A-CGA-O2A-C1
42	d	409	LMG	C31-C32-C33-C34
33	A	405	CLA	C13-C15-C16-C17
35	B	621	8CT	C16-C17-C18-C19
35	C	515	8CT	C18-C19-C20-C21
35	b	621	8CT	C16-C17-C18-C19
35	c	515	8CT	C18-C19-C20-C21
34	a	407	PHO	C16-C17-C18-C19
34	A	407	PHO	C16-C17-C18-C19
42	D	409	LMG	C31-C32-C33-C34
42	t	101	LMG	C31-C32-C33-C34
33	a	405	CLA	C13-C15-C16-C17
42	T	101	LMG	C31-C32-C33-C34
43	C	518	DGD	C7B-C8B-C9B-CAB
43	c	518	DGD	C7B-C8B-C9B-CAB
37	D	402	LHG	C24-C23-O8-C6
41	C	501	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
41	c	501	SQD	O47-C7-C8-C9
42	D	409	LMG	C19-C20-C21-C22
42	D	410	LMG	C13-C14-C15-C16
42	d	409	LMG	C19-C20-C21-C22
42	d	410	LMG	C13-C14-C15-C16
33	1	308	CLA	CAD-CBD-CGD-O2D
33	2	301	CLA	CAD-CBD-CGD-O2D
33	3	306	CLA	CAD-CBD-CGD-O2D
33	5	308	CLA	CAD-CBD-CGD-O2D
33	5	317	CLA	CAD-CBD-CGD-O2D
33	7	308	CLA	CAD-CBD-CGD-O2D
33	8	301	CLA	CAD-CBD-CGD-O2D
33	9	306	CLA	CAD-CBD-CGD-O2D
33	B	613	CLA	CAD-CBD-CGD-O2D
33	B	614	CLA	CAD-CBD-CGD-O2D
33	B	617	CLA	CAD-CBD-CGD-O2D
33	C	510	CLA	CAD-CBD-CGD-O2D
33	D	405	CLA	CAD-CBD-CGD-O2D
33	N	304	CLA	CAD-CBD-CGD-O2D
33	N	307	CLA	CAD-CBD-CGD-O2D
33	b	613	CLA	CAD-CBD-CGD-O2D
33	b	614	CLA	CAD-CBD-CGD-O2D
33	b	617	CLA	CAD-CBD-CGD-O2D
33	c	510	CLA	CAD-CBD-CGD-O2D
33	d	405	CLA	CAD-CBD-CGD-O2D
33	g	308	CLA	CAD-CBD-CGD-O2D
33	g	317	CLA	CAD-CBD-CGD-O2D
33	n	303	CLA	CAD-CBD-CGD-O2D
33	n	306	CLA	CAD-CBD-CGD-O2D
34	a	407	PHO	CAD-CBD-CGD-O2D
34	A	407	PHO	CAD-CBD-CGD-O2D
37	1	317	LHG	C6-C5-O7-C7
37	7	317	LHG	C6-C5-O7-C7
38	0	305	KC2	C2B-C3B-CAB-CBB
38	1	310	KC2	CAD-CBD-CGD-O2D
38	4	305	KC2	C2B-C3B-CAB-CBB
38	6	311	KC2	CAD-CBD-CGD-O2D
38	7	310	KC2	CAD-CBD-CGD-O2D
38	p	311	KC2	CAD-CBD-CGD-O2D
37	B	623	LHG	C15-C16-C17-C18
37	B	623	LHG	C34-C35-C36-C37
37	b	623	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
42	l	102	LMG	C31-C32-C33-C34
42	m	101	LMG	C31-C32-C33-C34
33	B	609	CLA	C15-C16-C17-C18
33	b	609	CLA	C15-C16-C17-C18
37	b	623	LHG	C15-C16-C17-C18
33	B	602	CLA	CBA-CGA-O2A-C1
37	d	402	LHG	C24-C23-O8-C6
36	D	407	PL9	C29-C31-C32-C33
36	d	407	PL9	C29-C31-C32-C33
33	N	301	CLA	O1A-CGA-O2A-C1
33	n	301	CLA	O1A-CGA-O2A-C1
37	a	411	LHG	O6-C4-C5-O7
37	A	411	LHG	O6-C4-C5-O7
37	D	402	LHG	O6-C4-C5-O7
37	D	408	LHG	O6-C4-C5-O7
37	d	402	LHG	O6-C4-C5-O7
37	d	408	LHG	O6-C4-C5-O7
33	C	510	CLA	C10-C11-C12-C13
33	c	510	CLA	C10-C11-C12-C13
42	C	520	LMG	C35-C36-C37-C38
33	b	602	CLA	CBA-CGA-O2A-C1
42	c	520	LMG	C35-C36-C37-C38
33	3	305	CLA	C4C-C3C-CAC-CBC
33	9	305	CLA	C4C-C3C-CAC-CBC
33	4	310	CLA	O1D-CGD-O2D-CED
33	3	303	CLA	CHA-CBD-CGD-O2D
33	3	307	CLA	CHA-CBD-CGD-O1D
33	3	307	CLA	CHA-CBD-CGD-O2D
33	5	311	CLA	CHA-CBD-CGD-O1D
33	5	311	CLA	CHA-CBD-CGD-O2D
33	9	303	CLA	CHA-CBD-CGD-O2D
33	9	307	CLA	CHA-CBD-CGD-O1D
33	9	307	CLA	CHA-CBD-CGD-O2D
33	B	605	CLA	CHA-CBD-CGD-O1D
33	B	608	CLA	CHA-CBD-CGD-O1D
33	B	608	CLA	CHA-CBD-CGD-O2D
33	C	503	CLA	CHA-CBD-CGD-O1D
33	C	505	CLA	CHA-CBD-CGD-O1D
33	C	508	CLA	CHA-CBD-CGD-O1D
33	C	508	CLA	CHA-CBD-CGD-O2D
33	b	605	CLA	CHA-CBD-CGD-O1D
33	b	608	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
33	b	608	CLA	CHA-CBD-CGD-O2D
33	c	503	CLA	CHA-CBD-CGD-O1D
33	c	505	CLA	CHA-CBD-CGD-O1D
33	c	508	CLA	CHA-CBD-CGD-O1D
33	c	508	CLA	CHA-CBD-CGD-O2D
33	g	311	CLA	CHA-CBD-CGD-O1D
33	g	311	CLA	CHA-CBD-CGD-O2D
37	D	402	LHG	C17-C18-C19-C20
33	1	308	CLA	O1A-CGA-O2A-C1
33	7	308	CLA	O1A-CGA-O2A-C1
33	C	512	CLA	O1A-CGA-O2A-C1
33	N	305	CLA	O1A-CGA-O2A-C1
33	c	512	CLA	O1A-CGA-O2A-C1
33	n	304	CLA	O1A-CGA-O2A-C1
37	D	401	LHG	O10-C23-O8-C6
37	d	401	LHG	O10-C23-O8-C6
37	d	402	LHG	C17-C18-C19-C20
43	H	101	DGD	CBB-CCB-CDB-CEB
43	h	101	DGD	CBB-CCB-CDB-CEB
33	0	311	CLA	O1D-CGD-O2D-CED
37	3	321	LHG	O7-C5-C6-O8
37	9	321	LHG	O7-C5-C6-O8
42	B	624	LMG	O1-C7-C8-O7
42	b	624	LMG	O1-C7-C8-O7
37	3	321	LHG	O1-C1-C2-O2
37	9	321	LHG	O1-C1-C2-O2
37	B	623	LHG	O1-C1-C2-O2
37	b	623	LHG	O1-C1-C2-O2
43	c	521	DGD	C8A-C9A-CAA-CBA
33	1	304	CLA	C5-C6-C7-C8
33	7	304	CLA	C5-C6-C7-C8
43	C	521	DGD	C2B-C1B-O2G-C2G
33	C	507	CLA	C4-C3-C5-C6
33	c	507	CLA	C4-C3-C5-C6
43	C	519	DGD	C8B-C9B-CAB-CBB
43	C	521	DGD	C8A-C9A-CAA-CBA
43	c	518	DGD	O1A-C1A-O1G-C1G
33	C	507	CLA	C2-C3-C5-C6
33	c	507	CLA	C2-C3-C5-C6
39	0	313	II0	C09-C21-C23-C25
39	0	313	II0	C10-C22-C24-C26
39	0	314	II0	C09-C21-C23-C25

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Mol	Chain	Res	Type	Atoms
39	0	315	II0	C10-C22-C24-C26
39	1	314	II0	C10-C22-C24-C26
39	1	316	II0	C09-C21-C23-C25
39	1	316	II0	C10-C22-C24-C26
39	2	312	II0	C09-C21-C23-C25
39	2	313	II0	C09-C21-C23-C25
39	4	312	II0	C09-C21-C23-C25
39	4	312	II0	C10-C22-C24-C26
39	4	313	II0	C09-C21-C23-C25
39	4	314	II0	C10-C22-C24-C26
39	7	314	II0	C10-C22-C24-C26
39	7	316	II0	C10-C22-C24-C26
39	8	313	II0	C09-C21-C23-C25
33	C	505	CLA	C11-C10-C8-C9
33	c	505	CLA	C11-C10-C8-C9
34	D	403	PHO	C6-C7-C8-C9
34	d	403	PHO	C6-C7-C8-C9
43	c	519	DGD	C8B-C9B-CAB-CBB
43	C	518	DGD	O1A-C1A-O1G-C1G
39	0	316	II0	C31-C33-C35-C37
39	4	315	II0	C31-C33-C35-C37
33	C	512	CLA	C3-C5-C6-C7
33	c	512	CLA	C3-C5-C6-C7
33	B	602	CLA	C1A-C2A-CAA-CBA
33	b	602	CLA	C1A-C2A-CAA-CBA
42	D	409	LMG	C10-C11-C12-C13
42	d	409	LMG	C10-C11-C12-C13
33	B	613	CLA	C16-C17-C18-C19
33	D	405	CLA	C16-C17-C18-C20
33	b	613	CLA	C16-C17-C18-C19
33	d	405	CLA	C16-C17-C18-C20
33	B	610	CLA	C15-C16-C17-C18
33	b	610	CLA	C15-C16-C17-C18
43	c	521	DGD	C2B-C1B-O2G-C2G
41	L	101	SQD	C24-C25-C26-C27
42	w	101	LMG	C32-C33-C34-C35
36	D	407	PL9	C27-C28-C29-C31
36	d	407	PL9	C27-C28-C29-C31
41	l	101	SQD	C24-C25-C26-C27
42	W	101	LMG	C32-C33-C34-C35
43	C	518	DGD	C3A-C4A-C5A-C6A
35	B	619	8CT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
35	B	620	8CT	C23-C24-C25-C26
35	Y	101	8CT	C23-C24-C25-C26
35	b	619	8CT	C12-C13-C14-C15
35	b	620	8CT	C23-C24-C25-C26
35	y	101	8CT	C23-C24-C25-C26
37	3	302	LHG	C3-O3-P-O6
37	3	302	LHG	C4-O6-P-O3
37	9	302	LHG	C3-O3-P-O6
37	9	302	LHG	C4-O6-P-O3
43	c	518	DGD	C3A-C4A-C5A-C6A
33	0	307	CLA	C4-C3-C5-C6
33	4	307	CLA	C4-C3-C5-C6
42	D	409	LMG	C15-C16-C17-C18
42	d	409	LMG	C15-C16-C17-C18
33	1	307	CLA	C4B-C3B-CAB-CBB
33	3	310	CLA	C4B-C3B-CAB-CBB
33	3	314	CLA	C4B-C3B-CAB-CBB
33	7	307	CLA	C4B-C3B-CAB-CBB
33	9	310	CLA	C4B-C3B-CAB-CBB
33	9	314	CLA	C4B-C3B-CAB-CBB
33	B	602	CLA	C4B-C3B-CAB-CBB
33	B	611	CLA	C4B-C3B-CAB-CBB
33	C	502	CLA	C4B-C3B-CAB-CBB
33	N	306	CLA	C4B-C3B-CAB-CBB
33	b	602	CLA	C4B-C3B-CAB-CBB
33	b	611	CLA	C4B-C3B-CAB-CBB
33	c	502	CLA	C4B-C3B-CAB-CBB
33	n	305	CLA	C4B-C3B-CAB-CBB
36	a	410	PL9	C3-C7-C8-C9
36	A	410	PL9	C3-C7-C8-C9
37	2	315	LHG	C3-O3-P-O5
37	3	302	LHG	C3-O3-P-O4
37	3	322	LHG	C4-O6-P-O5
37	8	315	LHG	C3-O3-P-O5
37	9	302	LHG	C3-O3-P-O4
37	9	322	LHG	C4-O6-P-O5
37	B	623	LHG	C4-O6-P-O5
37	b	623	LHG	C4-O6-P-O5
33	b	607	CLA	C16-C17-C18-C20
42	T	101	LMG	C30-C31-C32-C33
42	t	101	LMG	C30-C31-C32-C33
37	3	302	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
37	9	302	LHG	O6-C4-C5-C6
42	D	409	LMG	C14-C15-C16-C17
42	d	409	LMG	C14-C15-C16-C17
33	B	607	CLA	C16-C17-C18-C20
37	3	322	LHG	C31-C32-C33-C34
37	9	322	LHG	C31-C32-C33-C34
33	0	301	CLA	CAD-CBD-CGD-O1D
33	0	304	CLA	CAD-CBD-CGD-O1D
33	4	301	CLA	CAD-CBD-CGD-O1D
33	4	304	CLA	CAD-CBD-CGD-O1D
33	6	305	CLA	CAD-CBD-CGD-O1D
33	6	310	CLA	CAD-CBD-CGD-O1D
33	B	602	CLA	CAD-CBD-CGD-O1D
33	B	605	CLA	CAD-CBD-CGD-O1D
33	B	608	CLA	CAD-CBD-CGD-O1D
33	C	502	CLA	CAD-CBD-CGD-O1D
33	C	503	CLA	CAD-CBD-CGD-O1D
33	C	505	CLA	CAD-CBD-CGD-O1D
33	C	506	CLA	CAD-CBD-CGD-O1D
33	b	602	CLA	CAD-CBD-CGD-O1D
33	b	605	CLA	CAD-CBD-CGD-O1D
33	b	608	CLA	CAD-CBD-CGD-O1D
33	c	502	CLA	CAD-CBD-CGD-O1D
33	c	503	CLA	CAD-CBD-CGD-O1D
33	c	505	CLA	CAD-CBD-CGD-O1D
33	c	506	CLA	CAD-CBD-CGD-O1D
33	p	305	CLA	CAD-CBD-CGD-O1D
33	p	310	CLA	CAD-CBD-CGD-O1D
41	B	601	SQD	O5-C5-C6-S
41	J	101	SQD	C5-C6-S-O7
41	J	101	SQD	C5-C6-S-O9
41	b	601	SQD	O5-C5-C6-S
41	j	101	SQD	C5-C6-S-O7
41	j	101	SQD	C5-C6-S-O9
37	D	408	LHG	C29-C30-C31-C32
37	d	408	LHG	C29-C30-C31-C32
42	D	409	LMG	C33-C34-C35-C36
42	d	409	LMG	C33-C34-C35-C36
42	l	102	LMG	C28-C29-C30-C31
42	m	101	LMG	C28-C29-C30-C31
37	2	315	LHG	C33-C34-C35-C36
37	8	315	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
33	2	304	CLA	C6-C7-C8-C10
33	8	304	CLA	C6-C7-C8-C10
33	C	509	CLA	C11-C10-C8-C7
33	c	509	CLA	C11-C10-C8-C7
35	1	312	8CT	C28-C29-C30-C31
35	7	312	8CT	C28-C29-C30-C31
35	B	621	8CT	C28-C29-C30-C31
35	Y	101	8CT	C28-C29-C30-C31
35	b	621	8CT	C28-C29-C30-C31
35	y	101	8CT	C28-C29-C30-C31
37	2	315	LHG	O6-C4-C5-O7
37	3	302	LHG	O6-C4-C5-O7
37	8	315	LHG	O6-C4-C5-O7
37	9	302	LHG	O6-C4-C5-O7
37	D	401	LHG	O6-C4-C5-O7
37	d	401	LHG	O6-C4-C5-O7
43	c	519	DGD	CAB-CBB-CCB-CDB
43	C	519	DGD	CAB-CBB-CCB-CDB
44	V	201	HEM	C2D-C3D-CAD-CBD
44	v	201	HEM	C2D-C3D-CAD-CBD
33	1	301	CLA	C2A-CAA-CBA-CGA
33	7	301	CLA	C2A-CAA-CBA-CGA
33	1	306	CLA	C3-C5-C6-C7
33	7	306	CLA	C3-C5-C6-C7
37	D	402	LHG	C4-C5-C6-O8
37	d	402	LHG	C4-C5-C6-O8
41	L	101	SQD	O6-C44-C45-C46
41	l	101	SQD	O6-C44-C45-C46
42	T	101	LMG	C21-C22-C23-C24
42	W	101	LMG	O1-C7-C8-C9
42	t	101	LMG	C21-C22-C23-C24
42	w	101	LMG	O1-C7-C8-C9
37	2	315	LHG	O7-C5-C6-O8
37	8	315	LHG	O7-C5-C6-O8
42	B	622	LMG	O7-C8-C9-O8
42	C	520	LMG	O7-C8-C9-O8
42	b	622	LMG	O7-C8-C9-O8
42	c	520	LMG	O7-C8-C9-O8
37	9	302	LHG	C24-C25-C26-C27
37	3	302	LHG	C24-C25-C26-C27
33	D	405	CLA	C16-C17-C18-C19
33	d	405	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
33	N	302	CLA	C10-C11-C12-C13
33	3	310	CLA	C4C-C3C-CAC-CBC
33	9	310	CLA	C4C-C3C-CAC-CBC
42	b	624	LMG	C16-C17-C18-C19
33	1	305	CLA	C10-C11-C12-C13
33	7	305	CLA	C10-C11-C12-C13
33	n	302	CLA	C10-C11-C12-C13
33	B	607	CLA	C4-C3-C5-C6
33	b	607	CLA	C4-C3-C5-C6
33	B	605	CLA	CBA-CGA-O2A-C1
33	b	605	CLA	CBA-CGA-O2A-C1
37	B	623	LHG	C24-C23-O8-C6
37	b	623	LHG	C24-C23-O8-C6
37	d	401	LHG	C14-C15-C16-C17
37	D	401	LHG	C14-C15-C16-C17
41	L	101	SQD	C32-C33-C34-C35
42	B	624	LMG	C16-C17-C18-C19
33	p	305	CLA	CBD-CGD-O2D-CED
33	C	514	CLA	C16-C17-C18-C20
41	l	101	SQD	C32-C33-C34-C35
36	D	407	PL9	C39-C41-C42-C43
36	d	407	PL9	C39-C41-C42-C43
43	C	521	DGD	CDB-CEB-CFB-CGB
43	c	521	DGD	CDB-CEB-CFB-CGB
33	6	305	CLA	CBD-CGD-O2D-CED
33	c	514	CLA	C16-C17-C18-C20
39	2	313	II0	C32-C34-C36-C40
39	6	317	II0	C32-C34-C36-C40
39	8	313	II0	C32-C34-C36-C40
39	p	317	II0	C32-C34-C36-C40
33	1	307	CLA	C2B-C3B-CAB-CBB
33	2	306	CLA	C2B-C3B-CAB-CBB
33	3	310	CLA	C2B-C3B-CAB-CBB
33	3	314	CLA	C2B-C3B-CAB-CBB
33	6	304	CLA	C2B-C3B-CAB-CBB
33	7	307	CLA	C2B-C3B-CAB-CBB
33	8	306	CLA	C2B-C3B-CAB-CBB
33	9	310	CLA	C2B-C3B-CAB-CBB
33	9	314	CLA	C2B-C3B-CAB-CBB
33	B	606	CLA	C2B-C3B-CAB-CBB
33	B	613	CLA	C2B-C3B-CAB-CBB
33	C	503	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	C	513	CLA	C2B-C3B-CAB-CBB
33	b	606	CLA	C2B-C3B-CAB-CBB
33	b	613	CLA	C2B-C3B-CAB-CBB
33	c	503	CLA	C2B-C3B-CAB-CBB
33	c	513	CLA	C2B-C3B-CAB-CBB
33	p	304	CLA	C2B-C3B-CAB-CBB
42	T	101	LMG	C22-C23-C24-C25
42	t	101	LMG	C22-C23-C24-C25
33	B	607	CLA	C8-C10-C11-C12
33	B	616	CLA	C15-C16-C17-C18
33	b	607	CLA	C8-C10-C11-C12
33	b	616	CLA	C15-C16-C17-C18
33	a	406	CLA	C1-C2-C3-C4
33	A	406	CLA	C1-C2-C3-C4
33	g	301	CLA	C2C-C3C-CAC-CBC
33	a	408	CLA	C3-C5-C6-C7
33	A	408	CLA	C3-C5-C6-C7
37	2	315	LHG	C6-C5-O7-C7
37	8	315	LHG	C6-C5-O7-C7
41	L	101	SQD	C44-C45-O47-C7
41	l	101	SQD	C44-C45-O47-C7
33	3	305	CLA	C2A-CAA-CBA-CGA
33	9	305	CLA	C2A-CAA-CBA-CGA
37	D	401	LHG	C11-C10-C9-C8
37	d	401	LHG	C11-C10-C9-C8
33	2	305	CLA	C2-C1-O2A-CGA
33	8	305	CLA	C2-C1-O2A-CGA
33	5	301	CLA	C2C-C3C-CAC-CBC
37	D	402	LHG	C9-C10-C11-C12
37	d	402	LHG	C9-C10-C11-C12
37	8	315	LHG	C13-C14-C15-C16
37	2	315	LHG	C13-C14-C15-C16
37	B	623	LHG	O6-C4-C5-O7
37	b	623	LHG	O6-C4-C5-O7
34	d	403	PHO	C16-C17-C18-C20
35	D	406	8CT	C04-C03-C10-C11
35	d	406	8CT	C04-C03-C10-C11
42	B	624	LMG	C29-C30-C31-C32
42	b	624	LMG	C29-C30-C31-C32
33	0	306	CLA	C6-C7-C8-C10
33	4	306	CLA	C6-C7-C8-C10
41	B	601	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
41	J	101	SQD	O47-C45-C46-O48
41	b	601	SQD	O6-C44-C45-O47
41	j	101	SQD	O47-C45-C46-O48
33	5	307	CLA	CBD-CGD-O2D-CED
37	a	411	LHG	C3-O3-P-O6
37	A	411	LHG	C3-O3-P-O6
37	3	322	LHG	C3-O3-P-O6
37	5	316	LHG	C4-O6-P-O3
37	9	322	LHG	C3-O3-P-O6
37	D	402	LHG	C4-O6-P-O3
37	d	402	LHG	C4-O6-P-O3
37	g	316	LHG	C4-O6-P-O3
34	D	403	PHO	C16-C17-C18-C20
41	B	601	SQD	O6-C44-C45-C46
41	b	601	SQD	O6-C44-C45-C46
42	B	624	LMG	O1-C7-C8-C9
42	b	624	LMG	O1-C7-C8-C9
33	g	307	CLA	CBD-CGD-O2D-CED
33	2	306	CLA	C6-C7-C8-C9
33	8	306	CLA	C6-C7-C8-C9
35	H	102	8CT	C12-C13-C14-C15
35	H	102	8CT	C23-C24-C25-C26
35	h	102	8CT	C12-C13-C14-C15
35	h	102	8CT	C23-C24-C25-C26
33	C	507	CLA	C16-C17-C18-C19
33	B	613	CLA	C13-C15-C16-C17
33	b	613	CLA	C13-C15-C16-C17
41	B	601	SQD	C24-C25-C26-C27
42	B	622	LMG	C11-C12-C13-C14
42	b	622	LMG	C11-C12-C13-C14
41	b	601	SQD	C24-C25-C26-C27
37	3	322	LHG	O1-C1-C2-C3
37	9	322	LHG	O1-C1-C2-C3
42	D	409	LMG	C12-C13-C14-C15
42	d	409	LMG	C12-C13-C14-C15
33	0	310	CLA	C4C-C3C-CAC-CBC
33	4	309	CLA	C4C-C3C-CAC-CBC
33	B	607	CLA	C16-C17-C18-C19
33	b	607	CLA	C16-C17-C18-C19
33	c	507	CLA	C16-C17-C18-C19
33	B	617	CLA	CBA-CGA-O2A-C1
33	b	617	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	N	302	CLA	C2C-C3C-CAC-CBC
33	n	302	CLA	C2C-C3C-CAC-CBC
35	B	621	8CT	C03-C10-C11-C12
35	b	621	8CT	C03-C10-C11-C12
33	C	505	CLA	C4B-C3B-CAB-CBB
33	C	513	CLA	C4B-C3B-CAB-CBB
33	c	505	CLA	C4B-C3B-CAB-CBB
33	c	513	CLA	C4B-C3B-CAB-CBB
35	C	515	8CT	C16-C17-C18-C19
35	C	517	8CT	C16-C17-C18-C19
35	c	515	8CT	C16-C17-C18-C19
35	c	517	8CT	C16-C17-C18-C19
37	3	321	LHG	O6-C4-C5-C6
37	9	321	LHG	O6-C4-C5-C6
42	W	101	LMG	C13-C14-C15-C16
42	w	101	LMG	C13-C14-C15-C16
33	0	311	CLA	CAA-CBA-CGA-O1A
33	4	310	CLA	CAA-CBA-CGA-O1A
37	3	321	LHG	O6-C4-C5-O7
37	9	321	LHG	O6-C4-C5-O7
37	2	315	LHG	C32-C33-C34-C35
37	8	315	LHG	C32-C33-C34-C35
42	B	622	LMG	C14-C15-C16-C17
35	B	621	8CT	C13-C14-C15-C16
35	b	621	8CT	C13-C14-C15-C16
33	c	505	CLA	C15-C16-C17-C18
42	D	410	LMG	C35-C36-C37-C38
42	b	622	LMG	C14-C15-C16-C17
42	d	410	LMG	C35-C36-C37-C38
33	C	505	CLA	C15-C16-C17-C18
33	N	306	CLA	C2-C3-C5-C6
33	n	305	CLA	C2-C3-C5-C6
42	B	622	LMG	C36-C37-C38-C39
42	b	622	LMG	C36-C37-C38-C39
33	a	405	CLA	C15-C16-C17-C18
33	A	405	CLA	C15-C16-C17-C18
33	c	508	CLA	C16-C17-C18-C20
42	b	622	LMG	C12-C13-C14-C15
42	B	622	LMG	C12-C13-C14-C15
37	2	315	LHG	C28-C29-C30-C31
37	8	315	LHG	C28-C29-C30-C31
33	0	308	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	1	307	CLA	C3A-C2A-CAA-CBA
33	7	307	CLA	C3A-C2A-CAA-CBA
33	D	405	CLA	C3A-C2A-CAA-CBA
33	N	303	CLA	C3A-C2A-CAA-CBA
33	d	405	CLA	C3A-C2A-CAA-CBA
33	1	301	CLA	CAA-CBA-CGA-O1A
33	2	302	CLA	C6-C7-C8-C9
33	8	302	CLA	C6-C7-C8-C9
43	C	521	DGD	C7B-C8B-C9B-CAB
33	B	605	CLA	C8-C10-C11-C12
42	m	101	LMG	C14-C15-C16-C17
43	C	519	DGD	C3A-C4A-C5A-C6A
43	c	519	DGD	C3A-C4A-C5A-C6A
43	c	521	DGD	C7B-C8B-C9B-CAB
33	7	301	CLA	CAA-CBA-CGA-O1A
42	l	102	LMG	C14-C15-C16-C17
36	d	407	PL9	C12-C11-C9-C8
39	3	301	II0	C10-C22-C24-C26
39	3	319	II0	C09-C21-C23-C25
39	3	319	II0	C10-C22-C24-C26
39	5	313	II0	C09-C21-C23-C25
39	7	316	II0	C09-C21-C23-C25
39	8	312	II0	C09-C21-C23-C25
39	9	301	II0	C10-C22-C24-C26
39	9	319	II0	C09-C21-C23-C25
39	9	319	II0	C10-C22-C24-C26
39	g	313	II0	C09-C21-C23-C25
33	C	505	CLA	C11-C12-C13-C14
33	N	301	CLA	C6-C7-C8-C9
33	c	505	CLA	C11-C12-C13-C14
33	n	301	CLA	C6-C7-C8-C9
33	C	508	CLA	C16-C17-C18-C20
43	C	518	DGD	CAB-CBB-CCB-CDB
43	c	518	DGD	CAB-CBB-CCB-CDB
37	3	322	LHG	C8-C7-O7-C5
35	B	621	8CT	C28-C29-C30-C35
35	b	621	8CT	C28-C29-C30-C35
33	p	309	CLA	CBD-CGD-O2D-CED
33	0	303	CLA	C2A-CAA-CBA-CGA
33	2	303	CLA	C2A-CAA-CBA-CGA
33	4	303	CLA	C2A-CAA-CBA-CGA
33	8	303	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
33	b	605	CLA	C8-C10-C11-C12
37	D	401	LHG	C28-C29-C30-C31
37	d	401	LHG	C28-C29-C30-C31
33	B	610	CLA	C16-C17-C18-C20
33	0	306	CLA	O2A-C1-C2-C3
33	4	306	CLA	O2A-C1-C2-C3
33	C	513	CLA	O2A-C1-C2-C3
33	c	513	CLA	O2A-C1-C2-C3
43	C	519	DGD	O6D-C1D-O3G-C3G
43	c	519	DGD	O6D-C1D-O3G-C3G
41	J	101	SQD	C29-C30-C31-C32
41	j	101	SQD	C29-C30-C31-C32
42	l	102	LMG	C30-C31-C32-C33
42	m	101	LMG	C30-C31-C32-C33
33	3	305	CLA	C2C-C3C-CAC-CBC
37	7	317	LHG	C34-C35-C36-C37
37	D	408	LHG	C30-C31-C32-C33
37	d	408	LHG	C30-C31-C32-C33
33	0	307	CLA	C1A-C2A-CAA-CBA
33	4	307	CLA	C1A-C2A-CAA-CBA
33	5	303	CLA	C1A-C2A-CAA-CBA
33	g	303	CLA	C1A-C2A-CAA-CBA
37	1	317	LHG	C34-C35-C36-C37
42	D	410	LMG	C18-C19-C20-C21
42	d	410	LMG	C18-C19-C20-C21
33	b	610	CLA	C16-C17-C18-C20
33	C	511	CLA	C11-C10-C8-C7
33	C	512	CLA	C12-C13-C15-C16
33	c	511	CLA	C11-C10-C8-C7
33	c	512	CLA	C12-C13-C15-C16
36	D	407	PL9	C12-C11-C9-C8
33	B	605	CLA	O1A-CGA-O2A-C1
33	b	605	CLA	O1A-CGA-O2A-C1
33	5	304	CLA	CAA-CBA-CGA-O1A
33	g	304	CLA	CAA-CBA-CGA-O1A
37	9	302	LHG	C32-C33-C34-C35
42	t	101	LMG	C13-C14-C15-C16
33	9	305	CLA	C2C-C3C-CAC-CBC
37	3	302	LHG	C32-C33-C34-C35
42	T	101	LMG	C13-C14-C15-C16
37	d	401	LHG	C23-C24-C25-C26
33	4	309	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
33	0	310	CLA	C2C-C3C-CAC-CBC
33	2	301	CLA	CAA-CBA-CGA-O1A
33	8	301	CLA	CAA-CBA-CGA-O1A
42	C	520	LMG	C11-C12-C13-C14
37	2	315	LHG	O6-C4-C5-C6
37	8	315	LHG	O6-C4-C5-C6
42	c	520	LMG	C11-C12-C13-C14
33	6	309	CLA	CBD-CGD-O2D-CED
37	9	322	LHG	C8-C7-O7-C5
33	2	301	CLA	CAA-CBA-CGA-O2A
33	8	301	CLA	CAA-CBA-CGA-O2A
37	D	401	LHG	C23-C24-C25-C26
33	C	506	CLA	C2-C3-C5-C6
33	c	506	CLA	C2-C3-C5-C6
33	3	315	CLA	C2B-C3B-CAB-CBB
33	5	311	CLA	C2B-C3B-CAB-CBB
33	6	319	CLA	C2B-C3B-CAB-CBB
33	9	315	CLA	C2B-C3B-CAB-CBB
33	B	602	CLA	C2B-C3B-CAB-CBB
33	C	502	CLA	C2B-C3B-CAB-CBB
33	N	306	CLA	C2B-C3B-CAB-CBB
33	b	602	CLA	C2B-C3B-CAB-CBB
33	c	502	CLA	C2B-C3B-CAB-CBB
33	g	311	CLA	C2B-C3B-CAB-CBB
33	n	305	CLA	C2B-C3B-CAB-CBB
33	7	301	CLA	CAA-CBA-CGA-O2A
37	D	402	LHG	O10-C23-O8-C6
37	d	402	LHG	O10-C23-O8-C6
37	3	321	LHG	O9-C7-O7-C5
37	9	321	LHG	O9-C7-O7-C5
33	1	301	CLA	CAA-CBA-CGA-O2A
33	0	311	CLA	CAA-CBA-CGA-O2A
35	b	619	8CT	C03-C10-C11-C12
33	a	412	CLA	C8-C10-C11-C12
33	1	306	CLA	C5-C6-C7-C8
37	D	401	LHG	C9-C10-C11-C12
37	d	401	LHG	C9-C10-C11-C12
37	d	408	LHG	C10-C11-C12-C13
33	A	412	CLA	C8-C10-C11-C12
33	7	306	CLA	C5-C6-C7-C8
33	C	507	CLA	C13-C15-C16-C17
33	c	507	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	4	310	CLA	CAA-CBA-CGA-O2A
37	D	408	LHG	C10-C11-C12-C13
33	N	302	CLA	C4-C3-C5-C6
34	D	403	PHO	C4-C3-C5-C6
34	d	403	PHO	C4-C3-C5-C6
33	5	302	CLA	C2-C1-O2A-CGA
33	g	302	CLA	C2-C1-O2A-CGA
33	B	607	CLA	C2-C3-C5-C6
33	b	607	CLA	C2-C3-C5-C6
42	T	101	LMG	C15-C16-C17-C18
33	5	304	CLA	CAA-CBA-CGA-O2A
33	6	306	CLA	CAA-CBA-CGA-O1A
33	g	304	CLA	CAA-CBA-CGA-O2A
33	p	306	CLA	CAA-CBA-CGA-O1A
33	B	607	CLA	C14-C13-C15-C16
33	b	607	CLA	C14-C13-C15-C16
42	t	101	LMG	C15-C16-C17-C18
33	5	303	CLA	C2A-CAA-CBA-CGA
33	g	303	CLA	C2A-CAA-CBA-CGA
33	a	406	CLA	O2A-C1-C2-C3
33	A	406	CLA	O2A-C1-C2-C3
33	N	301	CLA	CAA-CBA-CGA-O1A
33	n	301	CLA	CAA-CBA-CGA-O1A
33	B	602	CLA	O1A-CGA-O2A-C1
33	b	602	CLA	O1A-CGA-O2A-C1
35	B	621	8CT	C04-C03-C10-C11
35	D	406	8CT	C02-C03-C10-C11
35	b	621	8CT	C04-C03-C10-C11
35	d	406	8CT	C02-C03-C10-C11
40	3	320	IHT	C02-C07-C18-C22
40	9	320	IHT	C02-C07-C18-C22
33	n	301	CLA	C15-C16-C17-C18
42	m	101	LMG	C29-C30-C31-C32
33	b	615	CLA	CAA-CBA-CGA-O2A
33	N	301	CLA	C15-C16-C17-C18
37	0	317	LHG	O1-C1-C2-C3
37	4	316	LHG	O1-C1-C2-C3
37	D	401	LHG	O1-C1-C2-C3
37	d	401	LHG	O1-C1-C2-C3
37	D	401	LHG	C30-C31-C32-C33
35	C	516	8CT	C23-C24-C25-C26
35	c	516	8CT	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
43	h	101	DGD	C2A-C1A-O1G-C1G
37	d	401	LHG	C30-C31-C32-C33
42	l	102	LMG	C29-C30-C31-C32
33	n	302	CLA	C4-C3-C5-C6
33	6	308	CLA	C1A-C2A-CAA-CBA
33	p	308	CLA	C1A-C2A-CAA-CBA
33	B	615	CLA	CAA-CBA-CGA-O2A
43	c	518	DGD	O1B-C1B-O2G-C2G
43	C	518	DGD	C5D-C6D-O5D-C1E
43	C	519	DGD	C5D-C6D-O5D-C1E
43	c	519	DGD	C5D-C6D-O5D-C1E
33	B	612	CLA	C15-C16-C17-C18
33	b	612	CLA	C15-C16-C17-C18
43	H	101	DGD	C2A-C1A-O1G-C1G
44	F	101	HEM	CAD-CBD-CGD-O2D
33	c	503	CLA	C16-C17-C18-C19
33	g	307	CLA	O1D-CGD-O2D-CED
33	5	307	CLA	O1D-CGD-O2D-CED
44	F	101	HEM	CAD-CBD-CGD-O1D
37	2	315	LHG	C34-C35-C36-C37
37	8	315	LHG	C34-C35-C36-C37
33	p	309	CLA	O1D-CGD-O2D-CED
33	3	304	CLA	C4B-C3B-CAB-CBB
33	3	315	CLA	C4B-C3B-CAB-CBB
33	5	311	CLA	C4B-C3B-CAB-CBB
33	6	312	CLA	C4B-C3B-CAB-CBB
33	6	319	CLA	C4B-C3B-CAB-CBB
33	9	304	CLA	C4B-C3B-CAB-CBB
33	9	315	CLA	C4B-C3B-CAB-CBB
33	B	603	CLA	C4B-C3B-CAB-CBB
33	B	608	CLA	C4B-C3B-CAB-CBB
33	B	613	CLA	C4B-C3B-CAB-CBB
33	C	503	CLA	C4B-C3B-CAB-CBB
33	b	603	CLA	C4B-C3B-CAB-CBB
33	b	608	CLA	C4B-C3B-CAB-CBB
33	b	613	CLA	C4B-C3B-CAB-CBB
33	c	503	CLA	C4B-C3B-CAB-CBB
33	g	311	CLA	C4B-C3B-CAB-CBB
33	p	312	CLA	C4B-C3B-CAB-CBB
33	p	319	CLA	C4B-C3B-CAB-CBB
33	C	503	CLA	C16-C17-C18-C19
33	C	513	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
33	c	513	CLA	C4-C3-C5-C6
36	a	410	PL9	C12-C11-C9-C10
36	A	410	PL9	C12-C11-C9-C10
36	D	407	PL9	C35-C34-C36-C37
36	d	407	PL9	C35-C34-C36-C37
33	0	307	CLA	C2-C3-C5-C6
33	4	307	CLA	C2-C3-C5-C6
33	C	512	CLA	C6-C7-C8-C10
33	c	512	CLA	C6-C7-C8-C10
37	0	317	LHG	O1-C1-C2-O2
37	4	316	LHG	O1-C1-C2-O2
35	Y	101	8CT	C12-C13-C14-C15
35	y	101	8CT	C12-C13-C14-C15
37	a	411	LHG	O7-C7-C8-C9
37	A	411	LHG	O7-C7-C8-C9
37	1	317	LHG	O7-C5-C6-O8
37	7	317	LHG	O7-C5-C6-O8
43	C	518	DGD	O1B-C1B-O2G-C2G
37	B	623	LHG	C19-C20-C21-C22
37	b	623	LHG	C19-C20-C21-C22
33	3	307	CLA	CAA-CBA-CGA-O2A
33	9	307	CLA	CAA-CBA-CGA-O2A
42	D	410	LMG	C32-C33-C34-C35
33	6	309	CLA	O1D-CGD-O2D-CED
42	d	410	LMG	C32-C33-C34-C35
33	0	309	CLA	CAA-CBA-CGA-O2A
33	c	511	CLA	CAA-CBA-CGA-O2A
37	D	408	LHG	O8-C23-C24-C25
37	d	408	LHG	O8-C23-C24-C25
42	D	409	LMG	O9-C10-O7-C8
42	d	409	LMG	O9-C10-O7-C8
33	5	311	CLA	CAA-CBA-CGA-O2A
33	g	311	CLA	CAA-CBA-CGA-O2A
33	C	513	CLA	C2-C3-C5-C6
33	c	513	CLA	C2-C3-C5-C6
33	4	308	CLA	CAA-CBA-CGA-O2A
33	C	511	CLA	CAA-CBA-CGA-O2A
33	C	509	CLA	C11-C10-C8-C9
33	c	509	CLA	C11-C10-C8-C9
33	N	307	CLA	CAA-CBA-CGA-O2A
33	n	306	CLA	CAA-CBA-CGA-O2A
37	2	315	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
37	8	315	LHG	O8-C23-C24-C25
37	B	623	LHG	O8-C23-C24-C25
37	b	623	LHG	O8-C23-C24-C25
33	0	311	CLA	CAD-CBD-CGD-O2D
33	3	315	CLA	CAD-CBD-CGD-O2D
33	4	310	CLA	CAD-CBD-CGD-O2D
33	6	307	CLA	CAD-CBD-CGD-O2D
33	9	315	CLA	CAD-CBD-CGD-O2D
33	B	610	CLA	CAD-CBD-CGD-O2D
33	B	611	CLA	CAD-CBD-CGD-O2D
33	C	507	CLA	CAD-CBD-CGD-O2D
33	C	511	CLA	CAD-CBD-CGD-O2D
33	C	513	CLA	CAD-CBD-CGD-O2D
33	b	610	CLA	CAD-CBD-CGD-O2D
33	b	611	CLA	CAD-CBD-CGD-O2D
33	c	507	CLA	CAD-CBD-CGD-O2D
33	c	511	CLA	CAD-CBD-CGD-O2D
33	c	513	CLA	CAD-CBD-CGD-O2D
33	p	307	CLA	CAD-CBD-CGD-O2D
37	2	315	LHG	C4-C5-O7-C7
37	8	315	LHG	C4-C5-O7-C7
38	0	305	KC2	CAD-CBD-CGD-O2D
38	4	305	KC2	CAD-CBD-CGD-O2D
42	D	410	LMG	C16-C17-C18-C19
33	4	307	CLA	C3-C5-C6-C7
42	W	101	LMG	C18-C19-C20-C21
42	d	410	LMG	C16-C17-C18-C19
42	w	101	LMG	C18-C19-C20-C21
33	B	605	CLA	C5-C6-C7-C8
33	b	605	CLA	C5-C6-C7-C8
33	N	302	CLA	C2-C1-O2A-CGA
33	n	302	CLA	C2-C1-O2A-CGA
33	2	305	CLA	CAA-CBA-CGA-O2A
33	8	305	CLA	CAA-CBA-CGA-O2A
35	B	619	8CT	C03-C10-C11-C12
35	C	517	8CT	C03-C10-C11-C12
35	c	517	8CT	C03-C10-C11-C12
43	H	101	DGD	C6B-C7B-C8B-C9B
43	h	101	DGD	C6B-C7B-C8B-C9B
33	a	412	CLA	C4-C3-C5-C6
33	A	412	CLA	C4-C3-C5-C6
33	0	307	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
39	3	316	II0	C32-C34-C36-C40
39	9	316	II0	C32-C34-C36-C40
37	1	317	LHG	C4-C5-C6-O8
37	3	302	LHG	C4-C5-C6-O8
37	7	317	LHG	C4-C5-C6-O8
37	9	302	LHG	C4-C5-C6-O8
41	J	101	SQD	C44-C45-C46-O48
41	j	101	SQD	C44-C45-C46-O48
43	H	101	DGD	C1G-C2G-C3G-O3G
43	h	101	DGD	C1G-C2G-C3G-O3G
37	3	322	LHG	O9-C7-O7-C5
33	b	611	CLA	CAA-CBA-CGA-O2A
43	C	518	DGD	O2G-C1B-C2B-C3B
43	c	518	DGD	O2G-C1B-C2B-C3B
33	B	615	CLA	CAA-CBA-CGA-O1A
33	b	615	CLA	CAA-CBA-CGA-O1A
33	a	405	CLA	O2A-C1-C2-C3
33	A	405	CLA	O2A-C1-C2-C3
33	2	307	CLA	O2A-C1-C2-C3
33	8	307	CLA	O2A-C1-C2-C3
33	B	605	CLA	O2A-C1-C2-C3
33	B	614	CLA	O2A-C1-C2-C3
33	D	405	CLA	O2A-C1-C2-C3
33	b	605	CLA	O2A-C1-C2-C3
33	b	614	CLA	O2A-C1-C2-C3
33	d	405	CLA	O2A-C1-C2-C3
42	C	520	LMG	C40-C41-C42-C43
38	0	305	KC2	C4B-C3B-CAB-CBB
38	4	305	KC2	C4B-C3B-CAB-CBB
42	c	520	LMG	C40-C41-C42-C43
37	g	316	LHG	C23-C24-C25-C26
33	B	611	CLA	CAA-CBA-CGA-O2A
41	J	101	SQD	O48-C23-C24-C25
41	j	101	SQD	O48-C23-C24-C25
33	3	307	CLA	CAA-CBA-CGA-O1A
33	9	307	CLA	CAA-CBA-CGA-O1A
33	g	311	CLA	CAA-CBA-CGA-O1A
33	C	507	CLA	C16-C17-C18-C20
33	c	507	CLA	C16-C17-C18-C20
43	C	519	DGD	CCA-CDA-CEA-CFA
43	c	519	DGD	CCA-CDA-CEA-CFA
37	5	316	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
37	9	322	LHG	O9-C7-O7-C5
33	a	406	CLA	CHA-CBD-CGD-O1D
33	a	406	CLA	CHA-CBD-CGD-O2D
33	A	406	CLA	CHA-CBD-CGD-O1D
33	A	406	CLA	CHA-CBD-CGD-O2D
33	1	303	CLA	CHA-CBD-CGD-O1D
33	1	303	CLA	CHA-CBD-CGD-O2D
33	1	306	CLA	CHA-CBD-CGD-O1D
33	1	306	CLA	CHA-CBD-CGD-O2D
33	3	303	CLA	CHA-CBD-CGD-O1D
33	5	307	CLA	CHA-CBD-CGD-O1D
33	5	307	CLA	CHA-CBD-CGD-O2D
33	6	304	CLA	CHA-CBD-CGD-O1D
33	6	304	CLA	CHA-CBD-CGD-O2D
33	6	305	CLA	CHA-CBD-CGD-O1D
33	6	305	CLA	CHA-CBD-CGD-O2D
33	6	313	CLA	CHA-CBD-CGD-O1D
33	6	313	CLA	CHA-CBD-CGD-O2D
33	7	303	CLA	CHA-CBD-CGD-O1D
33	7	303	CLA	CHA-CBD-CGD-O2D
33	7	306	CLA	CHA-CBD-CGD-O1D
33	7	306	CLA	CHA-CBD-CGD-O2D
33	9	303	CLA	CHA-CBD-CGD-O1D
33	B	603	CLA	CHA-CBD-CGD-O1D
33	B	603	CLA	CHA-CBD-CGD-O2D
33	B	605	CLA	CHA-CBD-CGD-O2D
33	B	617	CLA	CHA-CBD-CGD-O1D
33	C	503	CLA	CHA-CBD-CGD-O2D
33	C	505	CLA	CHA-CBD-CGD-O2D
33	C	506	CLA	CHA-CBD-CGD-O1D
33	C	506	CLA	CHA-CBD-CGD-O2D
33	b	603	CLA	CHA-CBD-CGD-O1D
33	b	603	CLA	CHA-CBD-CGD-O2D
33	b	605	CLA	CHA-CBD-CGD-O2D
33	b	617	CLA	CHA-CBD-CGD-O1D
33	c	503	CLA	CHA-CBD-CGD-O2D
33	c	505	CLA	CHA-CBD-CGD-O2D
33	c	506	CLA	CHA-CBD-CGD-O1D
33	c	506	CLA	CHA-CBD-CGD-O2D
33	g	307	CLA	CHA-CBD-CGD-O1D
33	g	307	CLA	CHA-CBD-CGD-O2D
33	p	304	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
33	p	304	CLA	CHA-CBD-CGD-O2D
33	p	305	CLA	CHA-CBD-CGD-O1D
33	p	305	CLA	CHA-CBD-CGD-O2D
33	p	313	CLA	CHA-CBD-CGD-O1D
33	p	313	CLA	CHA-CBD-CGD-O2D
33	B	613	CLA	C10-C11-C12-C13
33	5	311	CLA	CAA-CBA-CGA-O1A
37	g	316	LHG	O8-C23-C24-C25
33	B	613	CLA	CBA-CGA-O2A-C1
37	D	401	LHG	O6-C4-C5-C6
37	d	401	LHG	O6-C4-C5-C6
33	b	613	CLA	C10-C11-C12-C13
33	C	502	CLA	CAA-CBA-CGA-O2A
33	N	305	CLA	CAA-CBA-CGA-O2A
33	c	502	CLA	CAA-CBA-CGA-O2A
33	n	304	CLA	CAA-CBA-CGA-O2A
37	5	316	LHG	O8-C23-C24-C25
42	C	520	LMG	O8-C28-C29-C30
37	B	623	LHG	O7-C5-C6-O8
37	b	623	LHG	O7-C5-C6-O8
33	b	611	CLA	C8-C10-C11-C12
33	6	306	CLA	CAA-CBA-CGA-O2A
33	B	611	CLA	C8-C10-C11-C12
37	D	401	LHG	O8-C23-C24-C25
37	d	401	LHG	O8-C23-C24-C25
41	l	101	SQD	O48-C23-C24-C25
42	c	520	LMG	O8-C28-C29-C30
33	C	503	CLA	C2A-CAA-CBA-CGA
33	c	503	CLA	C2A-CAA-CBA-CGA
33	p	306	CLA	CAA-CBA-CGA-O2A
34	a	407	PHO	CHA-CBD-CGD-O1D
34	A	407	PHO	CHA-CBD-CGD-O1D
33	b	613	CLA	CBA-CGA-O2A-C1
42	D	409	LMG	C29-C28-O8-C9
42	d	409	LMG	C29-C28-O8-C9
42	D	409	LMG	C30-C31-C32-C33
33	5	302	CLA	CAA-CBA-CGA-O2A
33	5	307	CLA	CAA-CBA-CGA-O2A
33	g	302	CLA	CAA-CBA-CGA-O2A
33	g	307	CLA	CAA-CBA-CGA-O2A
41	L	101	SQD	O48-C23-C24-C25
42	D	409	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
42	d	409	LMG	O7-C10-C11-C12
42	d	409	LMG	C30-C31-C32-C33
33	4	306	CLA	C6-C7-C8-C9
33	B	610	CLA	C16-C17-C18-C19
33	b	610	CLA	C16-C17-C18-C19
34	a	407	PHO	C16-C17-C18-C20
34	A	407	PHO	C16-C17-C18-C20
36	a	410	PL9	C4-C3-C7-C8
36	A	410	PL9	C4-C3-C7-C8
36	D	407	PL9	C4-C3-C7-C8
36	d	407	PL9	C4-C3-C7-C8
39	4	315	II0	C10-C22-C24-C26
39	5	312	II0	C09-C21-C23-C25
33	5	301	CLA	C4C-C3C-CAC-CBC
33	g	301	CLA	C4C-C3C-CAC-CBC
33	2	304	CLA	C6-C7-C8-C9
33	8	304	CLA	C6-C7-C8-C9
33	B	603	CLA	C2B-C3B-CAB-CBB
33	b	603	CLA	C2B-C3B-CAB-CBB
33	p	319	CLA	C2B-C3B-CAB-CBB
37	3	322	LHG	C12-C13-C14-C15
37	9	322	LHG	C12-C13-C14-C15
33	2	305	CLA	CBA-CGA-O2A-C1
33	8	305	CLA	CBA-CGA-O2A-C1
33	3	312	CLA	CAA-CBA-CGA-O2A
33	9	312	CLA	CAA-CBA-CGA-O2A
33	0	306	CLA	C6-C7-C8-C9
33	C	503	CLA	C16-C17-C18-C20
33	c	503	CLA	C16-C17-C18-C20
33	7	302	CLA	C16-C17-C18-C19
33	2	304	CLA	C2A-CAA-CBA-CGA
33	3	307	CLA	C2A-CAA-CBA-CGA
33	8	304	CLA	C2A-CAA-CBA-CGA
33	9	307	CLA	C2A-CAA-CBA-CGA
33	C	511	CLA	CAA-CBA-CGA-O1A
33	c	511	CLA	CAA-CBA-CGA-O1A
33	1	302	CLA	C16-C17-C18-C19
41	L	101	SQD	C10-C11-C12-C13
41	l	101	SQD	C10-C11-C12-C13
43	c	519	DGD	O1B-C1B-C2B-C3B
37	1	317	LHG	C17-C18-C19-C20
37	7	317	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	B	606	CLA	C13-C15-C16-C17
33	b	606	CLA	C13-C15-C16-C17
33	0	309	CLA	C1A-C2A-CAA-CBA
33	4	308	CLA	C1A-C2A-CAA-CBA
33	B	605	CLA	C1A-C2A-CAA-CBA
33	D	405	CLA	C1A-C2A-CAA-CBA
33	b	605	CLA	C1A-C2A-CAA-CBA
33	d	405	CLA	C1A-C2A-CAA-CBA
33	N	303	CLA	C2-C1-O2A-CGA
42	t	101	LMG	O9-C10-C11-C12
43	C	519	DGD	O1B-C1B-C2B-C3B
33	7	306	CLA	C10-C11-C12-C13
33	0	308	CLA	C2-C1-O2A-CGA
33	N	305	CLA	CAA-CBA-CGA-O1A
33	n	304	CLA	CAA-CBA-CGA-O1A
41	C	501	SQD	O49-C7-C8-C9
41	c	501	SQD	O49-C7-C8-C9
42	T	101	LMG	O9-C10-C11-C12
42	C	520	LMG	C29-C30-C31-C32
42	c	520	LMG	C29-C30-C31-C32
41	c	501	SQD	C15-C16-C17-C18
43	C	521	DGD	CAB-CBB-CCB-CDB
43	c	521	DGD	CAB-CBB-CCB-CDB
33	2	308	CLA	C6-C7-C8-C10
33	8	308	CLA	C6-C7-C8-C10
33	4	308	CLA	CAA-CBA-CGA-O1A
33	C	502	CLA	CAA-CBA-CGA-O1A
33	N	307	CLA	CAA-CBA-CGA-O1A
33	c	502	CLA	CAA-CBA-CGA-O1A
33	n	306	CLA	CAA-CBA-CGA-O1A
33	1	306	CLA	C10-C11-C12-C13
41	C	501	SQD	C15-C16-C17-C18
33	0	309	CLA	CAA-CBA-CGA-O1A
33	5	302	CLA	CAA-CBA-CGA-O1A
42	D	409	LMG	O9-C10-C11-C12
42	d	409	LMG	O9-C10-C11-C12
33	2	310	CLA	C4B-C3B-CAB-CBB
33	3	307	CLA	C4B-C3B-CAB-CBB
33	8	310	CLA	C4B-C3B-CAB-CBB
33	9	307	CLA	C4B-C3B-CAB-CBB
33	B	617	CLA	C4B-C3B-CAB-CBB
33	b	617	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
37	1	317	LHG	C3-O3-P-O5
37	3	302	LHG	C4-O6-P-O4
37	3	322	LHG	C3-O3-P-O5
37	7	317	LHG	C3-O3-P-O5
37	9	302	LHG	C4-O6-P-O4
37	9	322	LHG	C3-O3-P-O5
37	D	408	LHG	C4-O6-P-O4
33	B	611	CLA	CAA-CBA-CGA-O1A
33	b	611	CLA	CAA-CBA-CGA-O1A
33	g	302	CLA	CAA-CBA-CGA-O1A
41	J	101	SQD	O10-C23-C24-C25
41	j	101	SQD	O10-C23-C24-C25
37	1	317	LHG	C15-C16-C17-C18
37	7	317	LHG	C15-C16-C17-C18
42	C	520	LMG	C39-C40-C41-C42
42	c	520	LMG	C39-C40-C41-C42
44	V	201	HEM	CAD-CBD-CGD-O2D
44	v	201	HEM	CAD-CBD-CGD-O2D
33	B	610	CLA	C13-C15-C16-C17
33	b	610	CLA	C13-C15-C16-C17
37	9	321	LHG	O9-C7-C8-C9
37	B	623	LHG	O10-C23-C24-C25
37	d	408	LHG	O10-C23-C24-C25
37	D	408	LHG	O10-C23-C24-C25
37	b	623	LHG	O10-C23-C24-C25
37	3	302	LHG	C13-C14-C15-C16
37	3	321	LHG	O9-C7-C8-C9
33	C	506	CLA	C4-C3-C5-C6
33	N	306	CLA	C4-C3-C5-C6
33	c	506	CLA	C4-C3-C5-C6
33	n	305	CLA	C4-C3-C5-C6
37	9	302	LHG	C13-C14-C15-C16
33	0	302	CLA	CAD-CBD-CGD-O1D
33	0	303	CLA	CAD-CBD-CGD-O1D
33	1	306	CLA	CAD-CBD-CGD-O1D
33	4	302	CLA	CAD-CBD-CGD-O1D
33	4	303	CLA	CAD-CBD-CGD-O1D
33	7	306	CLA	CAD-CBD-CGD-O1D
33	B	615	CLA	CAD-CBD-CGD-O1D
33	b	615	CLA	CAD-CBD-CGD-O1D
41	L	101	SQD	O10-C23-C24-C25
41	l	101	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
33	a	408	CLA	C6-C7-C8-C9
33	A	408	CLA	C6-C7-C8-C9
33	B	603	CLA	C11-C12-C13-C14
33	B	609	CLA	C11-C12-C13-C14
33	B	613	CLA	C11-C10-C8-C9
33	C	511	CLA	C11-C10-C8-C9
33	C	512	CLA	C6-C7-C8-C9
33	b	603	CLA	C11-C12-C13-C14
33	b	609	CLA	C11-C12-C13-C14
33	b	613	CLA	C11-C10-C8-C9
33	c	511	CLA	C11-C10-C8-C9
33	c	512	CLA	C6-C7-C8-C9
33	2	307	CLA	C8-C10-C11-C12
33	B	616	CLA	C13-C15-C16-C17
33	b	616	CLA	C13-C15-C16-C17
33	1	304	CLA	C2A-CAA-CBA-CGA
33	7	304	CLA	C2A-CAA-CBA-CGA
33	C	503	CLA	CAA-CBA-CGA-O2A
33	b	614	CLA	CAA-CBA-CGA-O2A
33	8	307	CLA	C8-C10-C11-C12
33	B	614	CLA	C10-C11-C12-C13
33	b	614	CLA	C10-C11-C12-C13
42	C	520	LMG	C30-C31-C32-C33
33	3	312	CLA	C3-C5-C6-C7
33	9	312	CLA	C3-C5-C6-C7
42	d	410	LMG	O10-C28-C29-C30
33	0	309	CLA	C3A-C2A-CAA-CBA
33	4	308	CLA	C3A-C2A-CAA-CBA
33	B	613	CLA	C11-C10-C8-C7
33	B	615	CLA	C3A-C2A-CAA-CBA
33	C	514	CLA	C6-C7-C8-C10
33	b	613	CLA	C11-C10-C8-C7
33	b	615	CLA	C3A-C2A-CAA-CBA
33	c	514	CLA	C6-C7-C8-C10
33	5	307	CLA	CAA-CBA-CGA-O1A
33	g	307	CLA	CAA-CBA-CGA-O1A
42	D	410	LMG	O10-C28-C29-C30
33	a	406	CLA	CAA-CBA-CGA-O2A
33	A	406	CLA	CAA-CBA-CGA-O2A
33	7	303	CLA	CAA-CBA-CGA-O2A
33	B	614	CLA	CAA-CBA-CGA-O2A
33	c	503	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
42	c	520	LMG	C30-C31-C32-C33
33	a	406	CLA	CAA-CBA-CGA-O1A
33	A	406	CLA	CAA-CBA-CGA-O1A
37	3	302	LHG	O10-C23-C24-C25
35	B	620	8CT	C12-C13-C14-C15
35	b	620	8CT	C12-C13-C14-C15
33	1	303	CLA	CAA-CBA-CGA-O2A
37	3	321	LHG	O7-C7-C8-C9
37	9	321	LHG	O7-C7-C8-C9
43	h	101	DGD	C5B-C6B-C7B-C8B
43	C	521	DGD	O6D-C1D-O3G-C3G
43	c	521	DGD	O6D-C1D-O3G-C3G
33	1	305	CLA	C8-C10-C11-C12
33	7	305	CLA	C8-C10-C11-C12
43	H	101	DGD	C5B-C6B-C7B-C8B
37	9	302	LHG	O10-C23-C24-C25
33	C	509	CLA	C8-C10-C11-C12
33	c	509	CLA	C8-C10-C11-C12
37	B	623	LHG	O7-C7-C8-C9
37	b	623	LHG	O7-C7-C8-C9
44	v	201	HEM	CAD-CBD-CGD-O1D
33	B	614	CLA	CAA-CBA-CGA-O1A
33	C	503	CLA	CAA-CBA-CGA-O1A
41	L	101	SQD	O47-C7-C8-C9
44	V	201	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

199 monomers are involved in 639 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	5	314	II0	2	0
41	L	101	SQD	2	0
33	B	611	CLA	3	0
33	p	306	CLA	2	0
38	0	305	KC2	4	0
39	7	313	II0	2	0
33	0	311	CLA	3	0
33	N	303	CLA	24	0
33	A	412	CLA	16	0
33	0	308	CLA	5	0
33	B	618	CLA	2	0
33	b	611	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	6	306	CLA	2	0
33	p	309	CLA	4	0
33	c	511	CLA	1	0
33	B	610	CLA	1	0
37	d	402	LHG	1	0
34	a	407	PHO	4	0
33	5	310	CLA	7	0
34	A	407	PHO	5	0
33	5	305	CLA	6	0
39	1	316	II0	1	0
33	4	302	CLA	4	0
39	3	317	II0	2	0
33	C	514	CLA	3	0
33	B	606	CLA	1	0
33	6	308	CLA	8	0
33	C	507	CLA	2	0
33	0	302	CLA	7	0
42	d	409	LMG	2	0
39	4	312	II0	11	0
33	4	310	CLA	3	0
33	6	303	CLA	1	0
33	a	406	CLA	1	0
33	0	304	CLA	6	0
33	b	605	CLA	2	0
33	5	302	CLA	3	0
39	8	312	II0	1	0
37	D	402	LHG	1	0
33	A	406	CLA	1	0
33	5	317	CLA	4	0
37	D	401	LHG	1	0
38	p	311	KC2	1	0
43	c	521	DGD	12	0
33	c	507	CLA	2	0
33	N	307	CLA	1	0
40	p	318	IHT	8	0
33	B	615	CLA	1	0
33	g	317	CLA	4	0
37	D	408	LHG	2	0
33	g	310	CLA	7	0
41	b	601	SQD	1	0
39	0	313	II0	9	0
33	p	310	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	310	CLA	6	0
33	4	306	CLA	6	0
41	B	601	SQD	1	0
33	p	305	CLA	7	0
40	6	318	IHT	5	0
33	2	303	CLA	1	0
33	B	603	CLA	2	0
33	d	404	CLA	1	0
37	3	322	LHG	1	0
35	C	516	8CT	1	0
39	g	314	II0	3	0
33	C	505	CLA	2	0
39	p	315	II0	3	0
35	0	312	8CT	1	0
37	1	317	LHG	2	0
33	4	309	CLA	6	0
44	v	201	HEM	2	0
39	0	316	II0	5	0
33	c	512	CLA	2	0
37	7	317	LHG	2	0
35	c	516	8CT	1	0
39	6	315	II0	1	0
39	2	313	II0	3	0
39	0	315	II0	1	0
33	g	305	CLA	6	0
33	0	307	CLA	1	0
37	2	315	LHG	2	0
39	5	313	II0	6	0
33	4	301	CLA	1	0
33	7	305	CLA	4	0
33	c	510	CLA	2	0
35	4	311	8CT	1	0
44	V	201	HEM	2	0
43	h	101	DGD	16	0
33	B	613	CLA	1	0
43	C	521	DGD	10	0
37	b	623	LHG	10	0
42	B	622	LMG	1	0
43	c	519	DGD	4	0
33	p	308	CLA	9	0
36	d	407	PL9	5	0
33	9	309	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	p	307	CLA	2	0
33	g	302	CLA	3	0
33	5	307	CLA	11	0
33	6	307	CLA	2	0
33	C	512	CLA	2	0
41	l	101	SQD	2	0
33	c	505	CLA	2	0
33	p	319	CLA	8	0
33	6	310	CLA	2	0
33	b	607	CLA	1	0
33	6	305	CLA	9	0
33	C	510	CLA	2	0
33	D	404	CLA	1	0
42	w	101	LMG	1	0
39	0	314	II0	6	0
39	5	312	II0	6	0
33	B	607	CLA	1	0
33	9	306	CLA	5	0
37	a	411	LHG	7	0
37	A	411	LHG	8	0
39	p	316	II0	2	0
33	p	303	CLA	2	0
33	4	308	CLA	4	0
39	6	316	II0	2	0
39	p	314	II0	9	0
41	J	101	SQD	1	0
44	F	101	HEM	3	0
33	8	303	CLA	1	0
33	g	311	CLA	2	0
33	a	405	CLA	2	0
37	B	623	LHG	10	0
42	d	410	LMG	1	0
33	n	306	CLA	1	0
31	A	403	BCT	1	0
39	p	301	II0	1	0
39	6	314	II0	13	0
33	0	306	CLA	6	0
33	2	305	CLA	1	0
42	c	520	LMG	4	0
33	b	615	CLA	1	0
33	g	307	CLA	14	0
37	9	322	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	b	616	CLA	1	0
43	C	519	DGD	4	0
34	d	403	PHO	1	0
33	A	405	CLA	2	0
33	5	303	CLA	1	0
33	6	309	CLA	5	0
33	1	305	CLA	4	0
33	p	313	CLA	9	0
33	6	313	CLA	10	0
33	6	319	CLA	8	0
33	b	603	CLA	3	0
33	g	304	CLA	2	0
39	1	313	II0	2	0
33	b	613	CLA	1	0
43	H	101	DGD	20	0
34	D	403	PHO	1	0
37	8	315	LHG	2	0
33	8	305	CLA	1	0
36	D	407	PL9	6	0
33	0	309	CLA	4	0
39	4	313	II0	2	0
37	d	408	LHG	2	0
42	C	520	LMG	4	0
39	8	313	II0	3	0
37	3	302	LHG	1	0
33	p	312	CLA	3	0
37	d	401	LHG	2	0
41	j	101	SQD	1	0
42	D	409	LMG	2	0
39	g	313	II0	6	0
33	1	308	CLA	1	0
33	5	311	CLA	1	0
33	C	511	CLA	1	0
33	4	304	CLA	7	0
42	b	622	LMG	1	0
33	6	312	CLA	6	0
42	T	101	LMG	7	0
33	a	412	CLA	15	0
42	t	101	LMG	7	0
33	c	514	CLA	3	0
33	0	301	CLA	1	0
33	B	605	CLA	2	0

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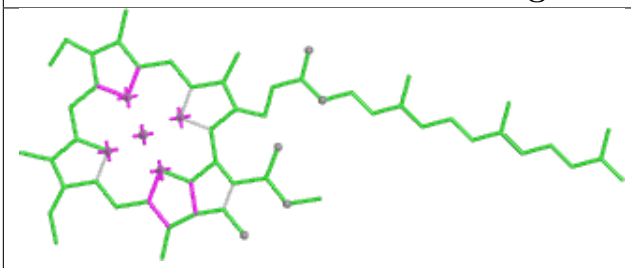
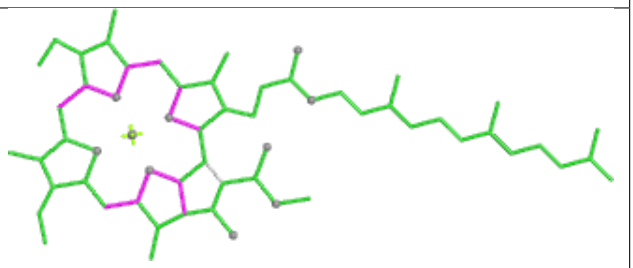
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	g	303	CLA	1	0
39	p	317	II0	4	0
44	f	101	HEM	3	0
39	9	317	II0	2	0
33	b	606	CLA	1	0
42	D	410	LMG	2	0
39	2	312	II0	1	0
33	b	614	CLA	2	0
39	6	317	II0	5	0
33	B	616	CLA	1	0
38	6	311	KC2	1	0
37	9	302	LHG	1	0
33	b	610	CLA	1	0
33	p	302	CLA	1	0
33	7	308	CLA	1	0
39	g	312	II0	6	0
42	W	101	LMG	1	0
33	4	307	CLA	1	0
39	7	316	II0	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.

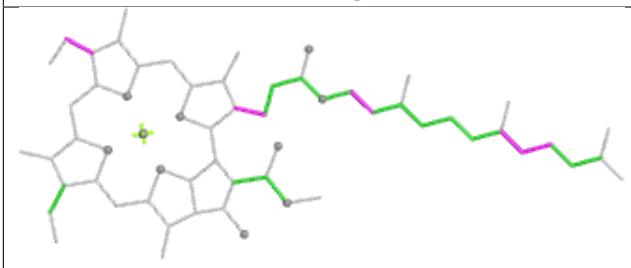
Ligand CLA 8 307



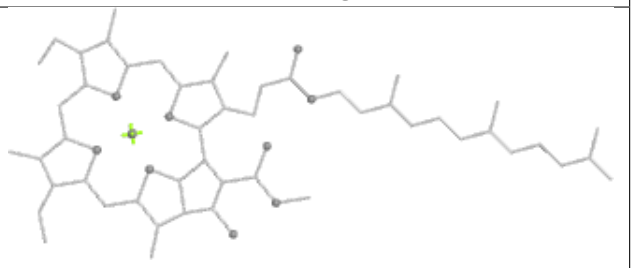
Bond lengths



Bond angles

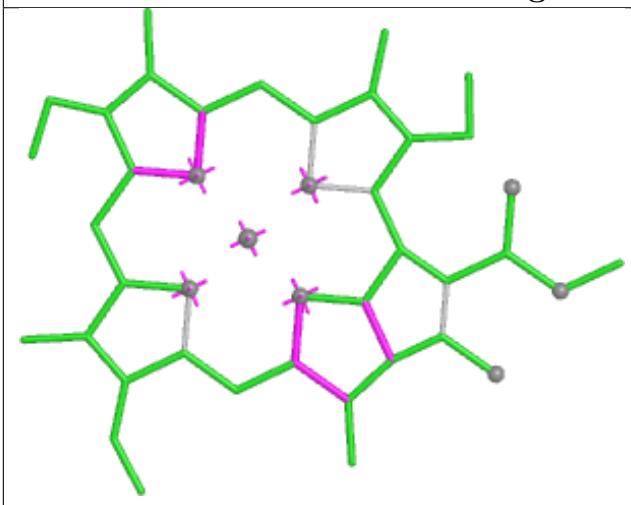


Torsions

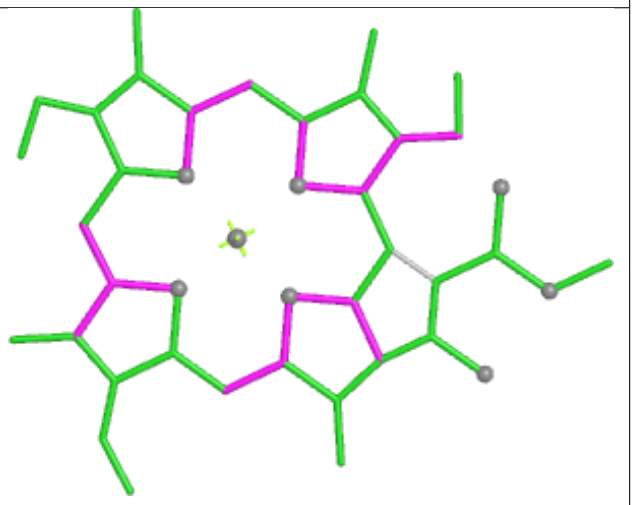


Rings

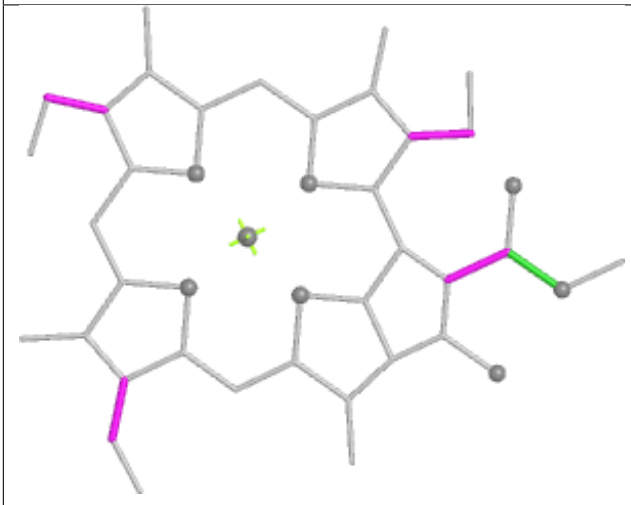
Ligand CLA 5 301



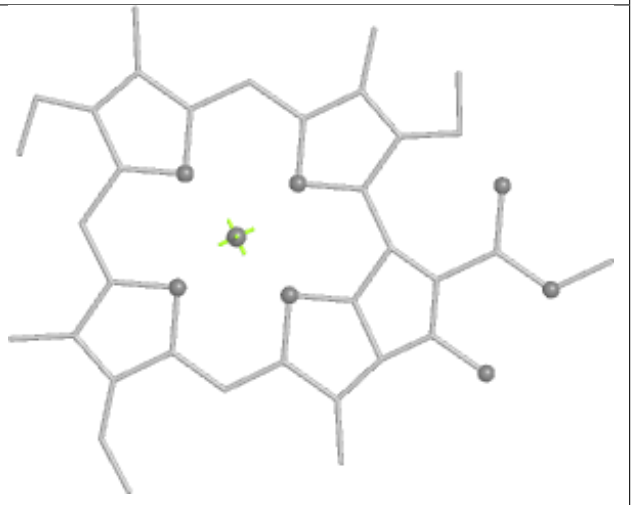
Bond lengths



Bond angles

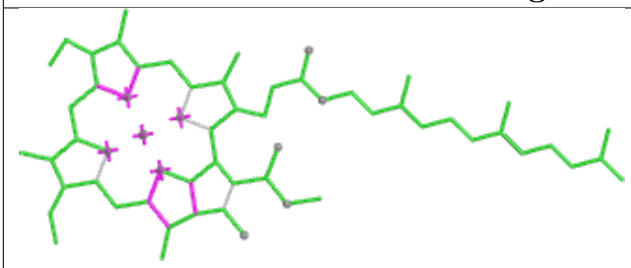


Torsions

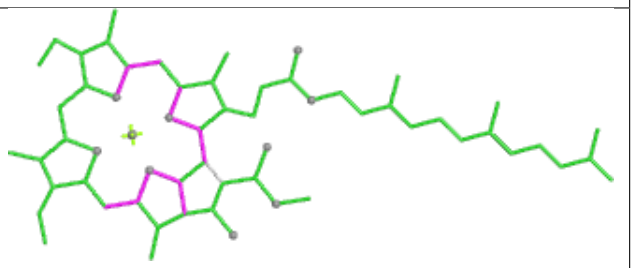


Rings

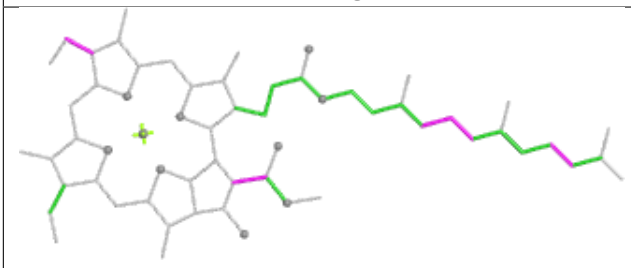
Ligand CLA 7 306



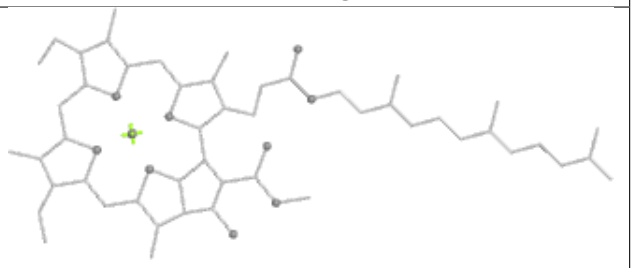
Bond lengths



Bond angles

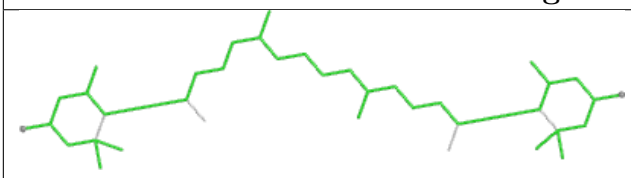


Torsions



Rings

Ligand II0 5 314



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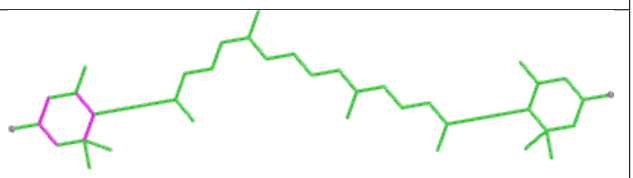

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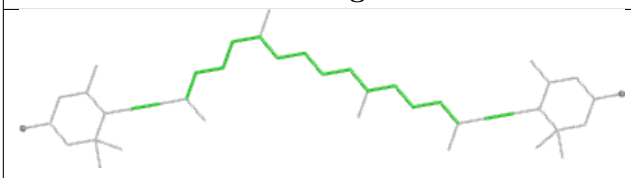

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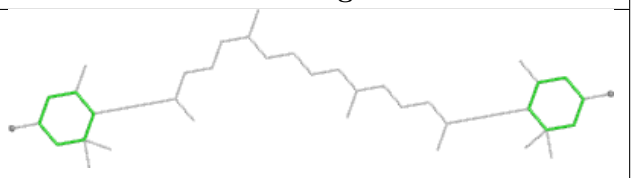
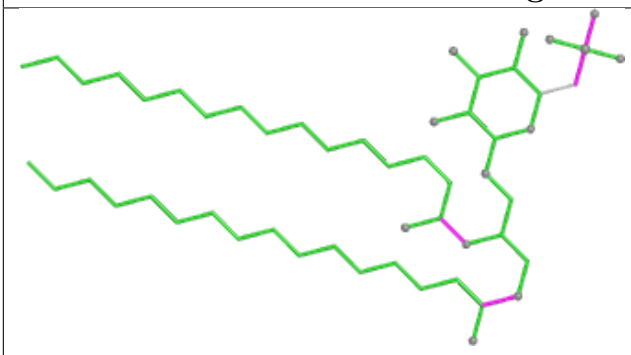


Rings

Ligand SQD L 101



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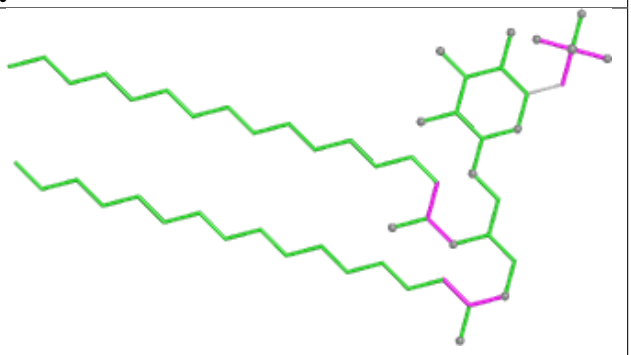

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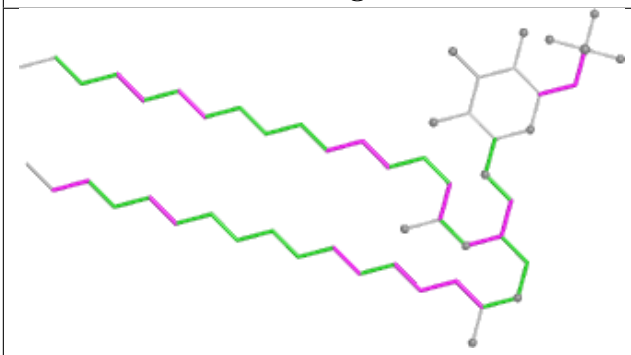

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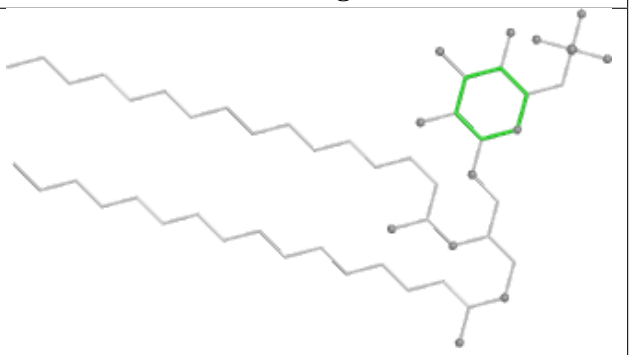
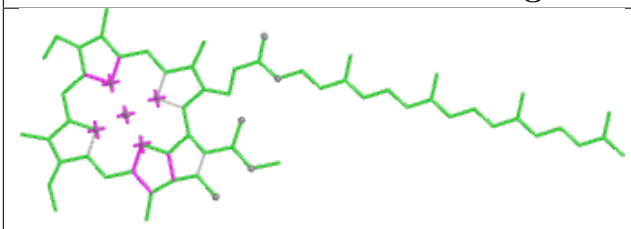


Rings

Ligand CLA B 611



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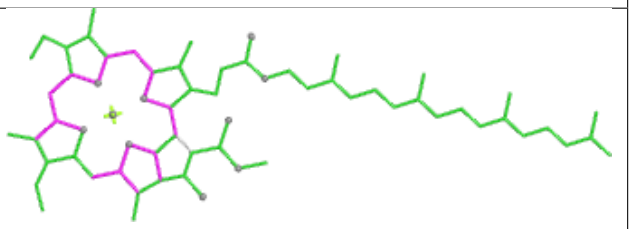

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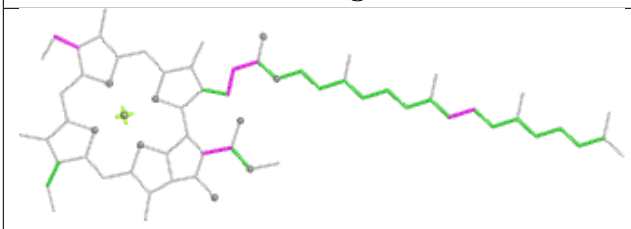

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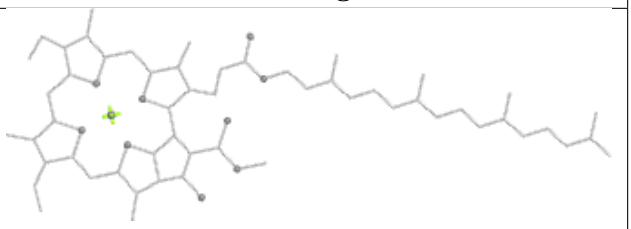
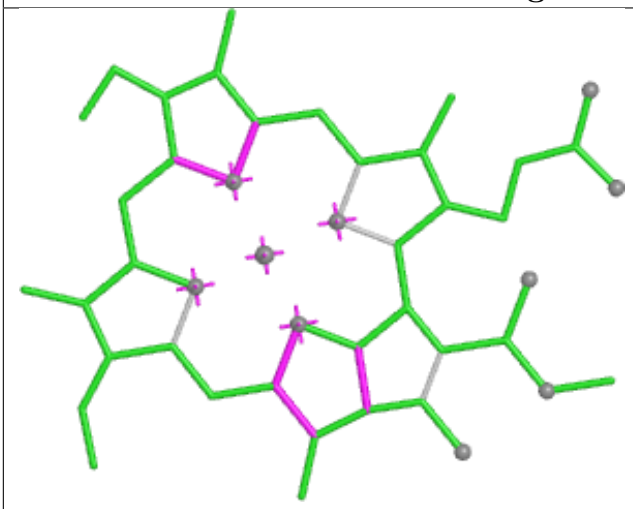


Rings

Ligand CLA p 306



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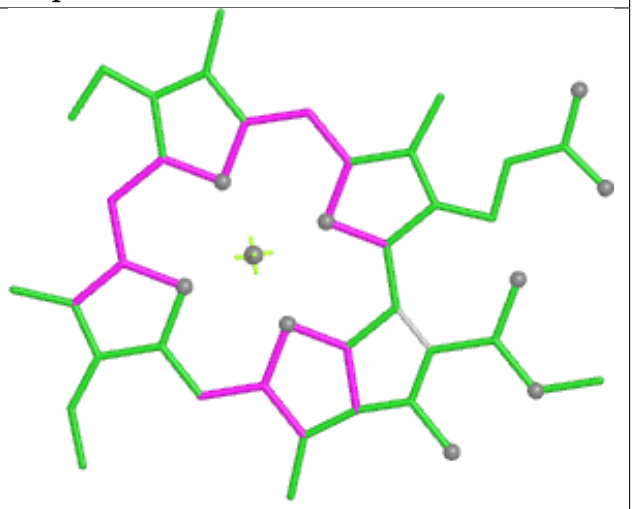

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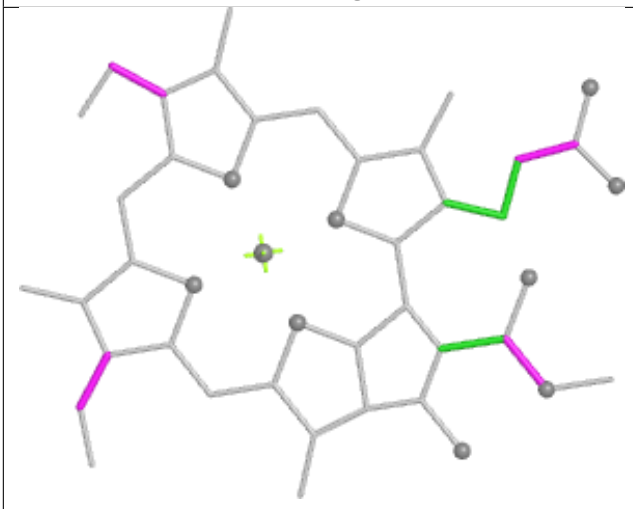
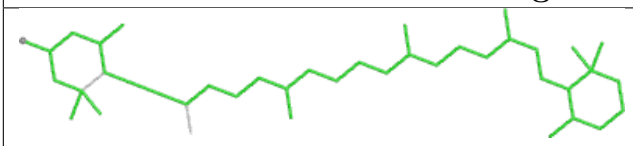


Torsions

Rings

Ligand IHT 8 314



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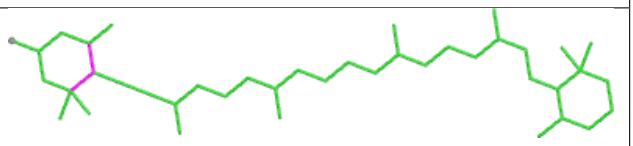

Bond angles

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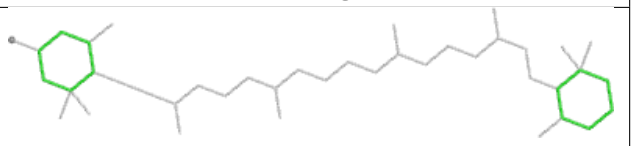
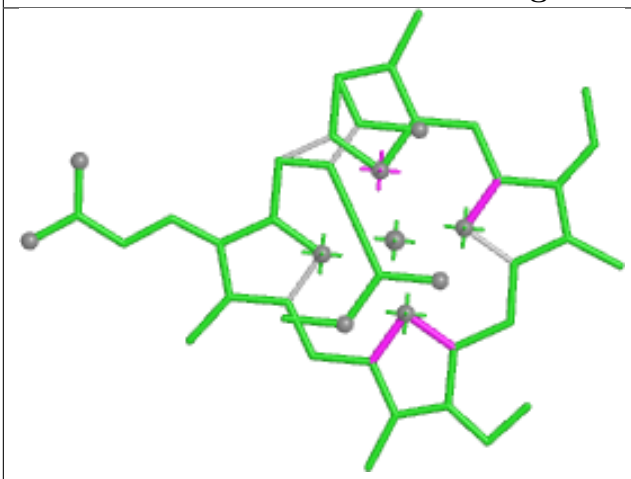


Rings

Ligand KC2 0 305



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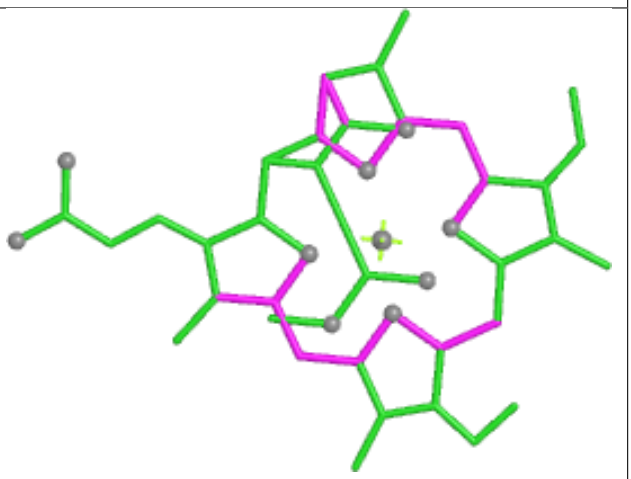

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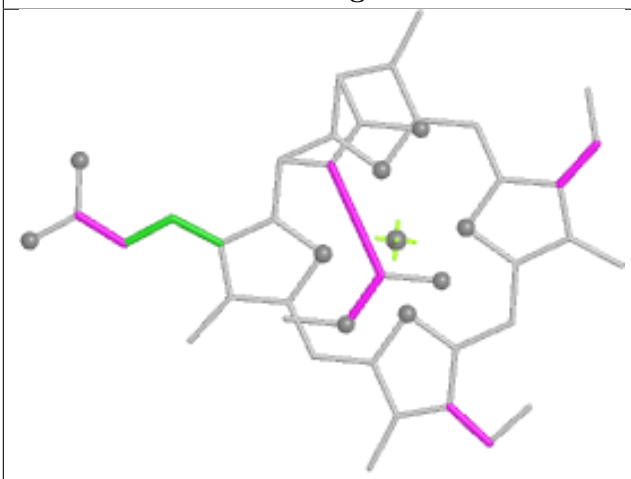

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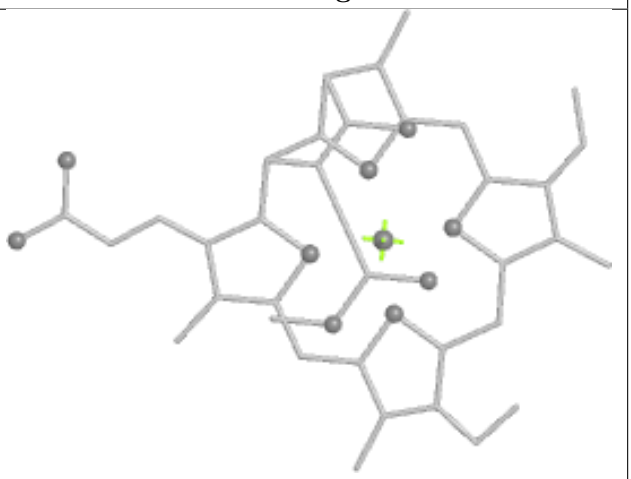
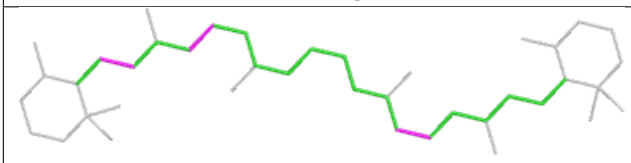


Rings

Ligand 8CT b 619

Bond lengths

Bond angles



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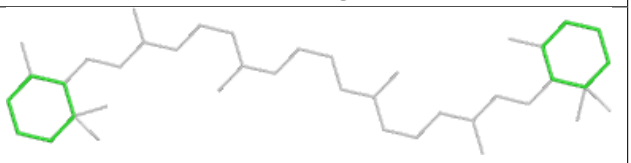
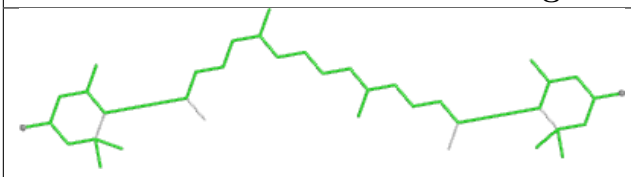


Rings

Ligand II0 7 313



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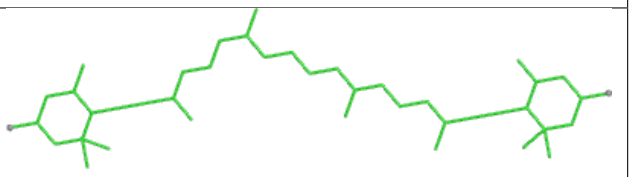

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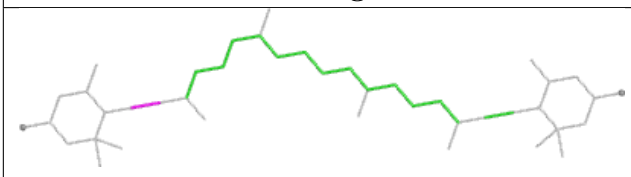

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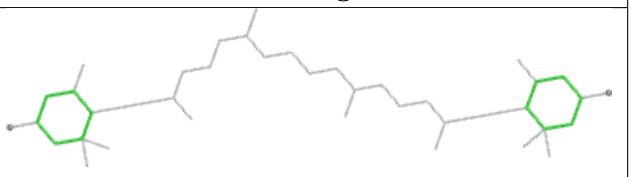

Rings

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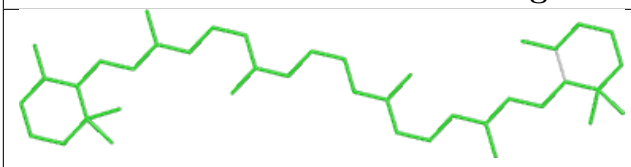

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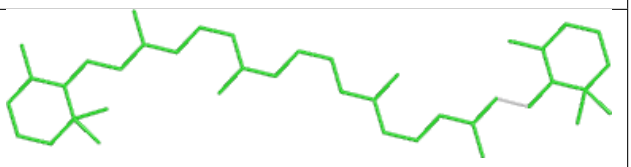

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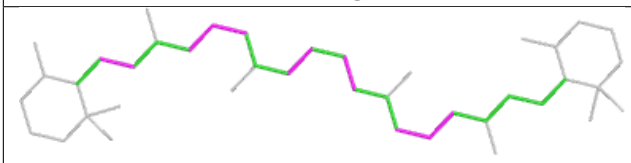

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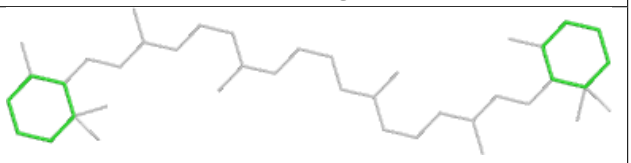
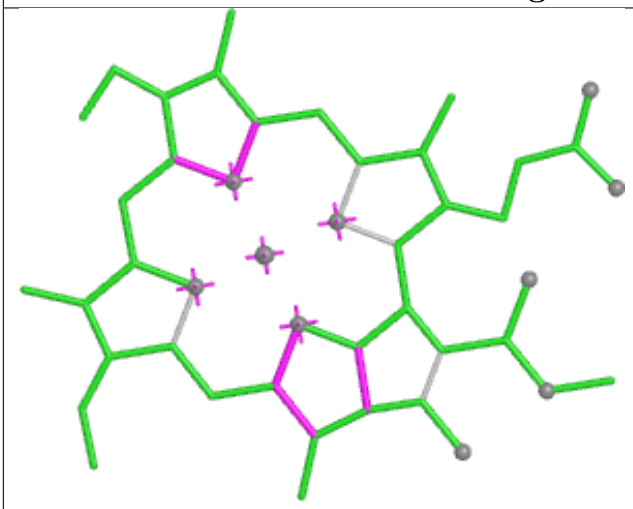


Rings

Ligand CLA g 306



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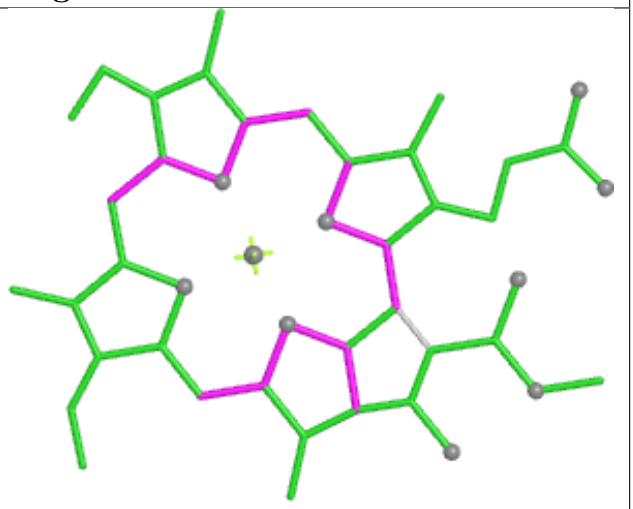

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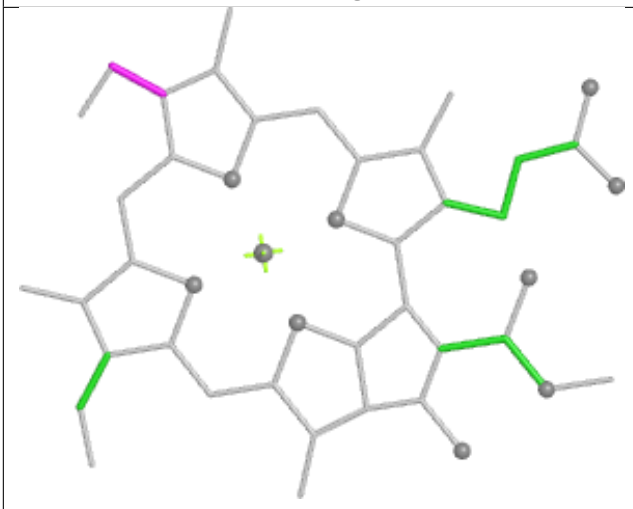

Torsions

Rings

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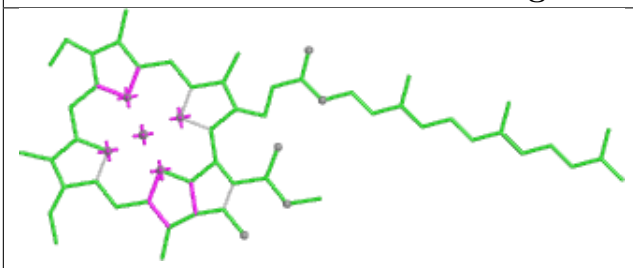

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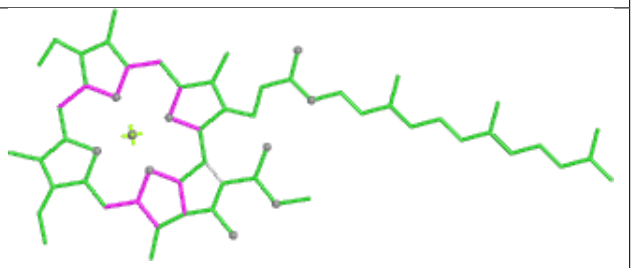

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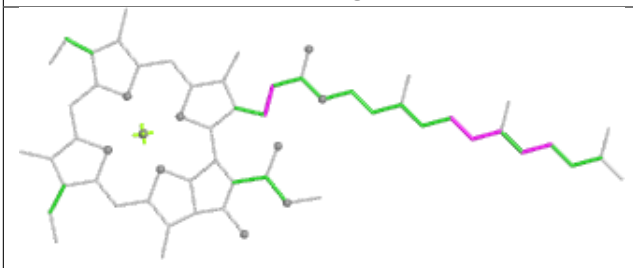

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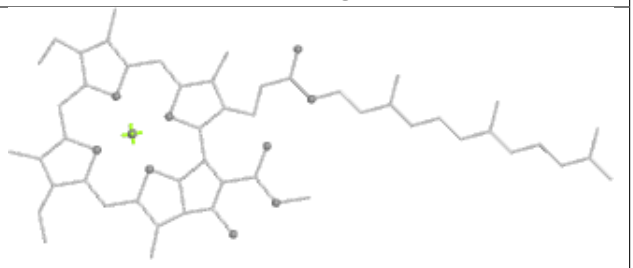

Rings

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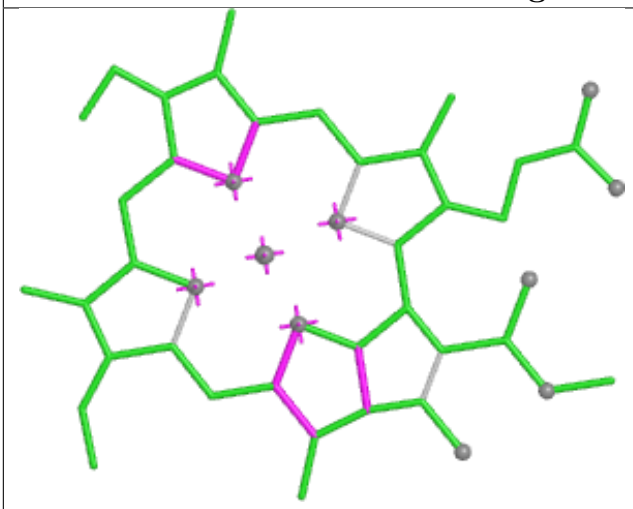

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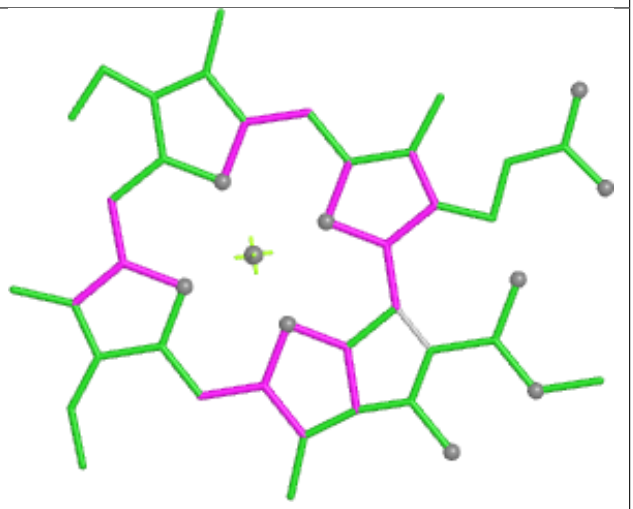

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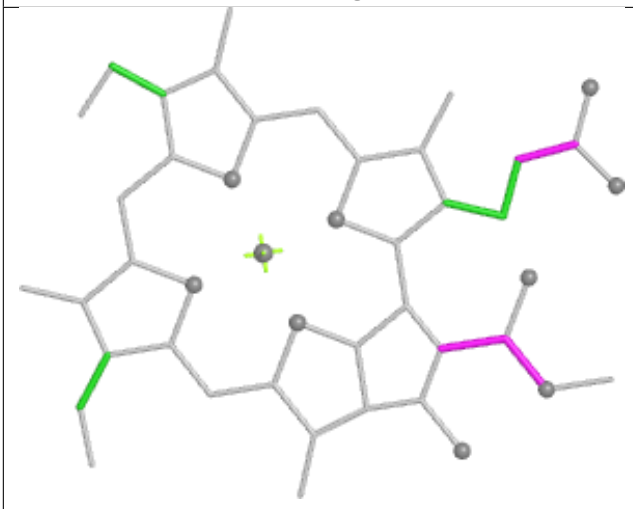
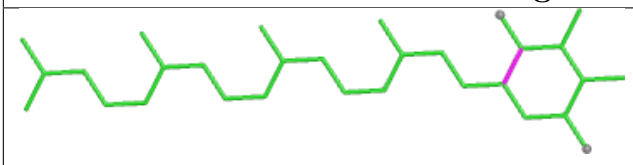


Torsions

Rings

Ligand PL9 a 410



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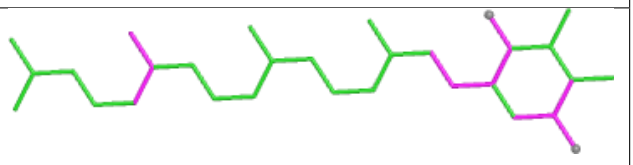
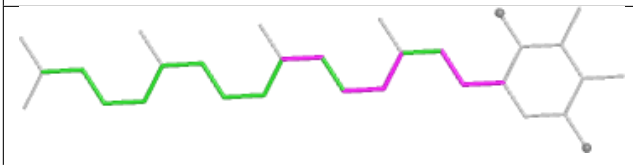


Bond angles



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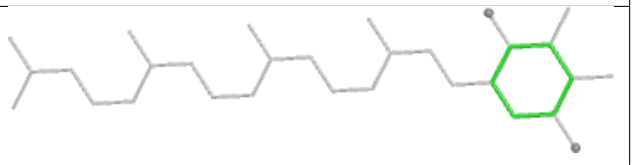
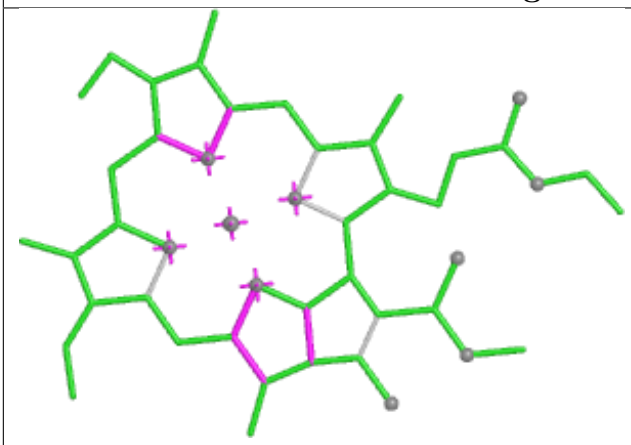


Rings

Ligand CLA N 303



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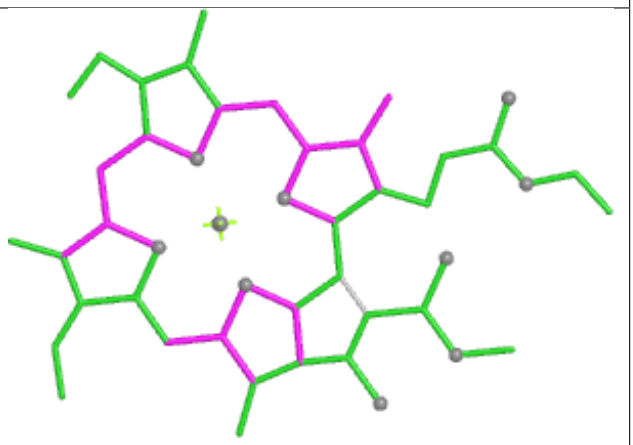
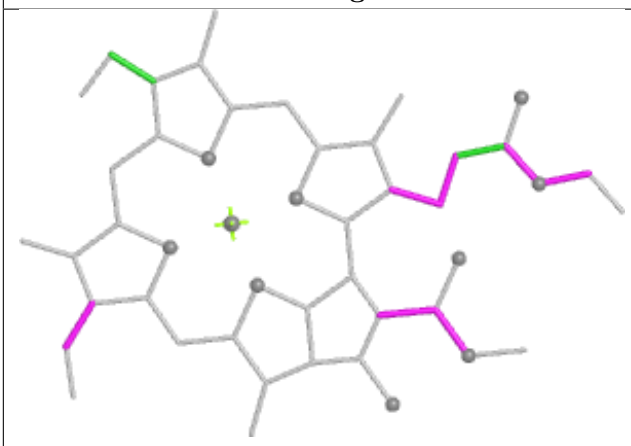


Bond angles



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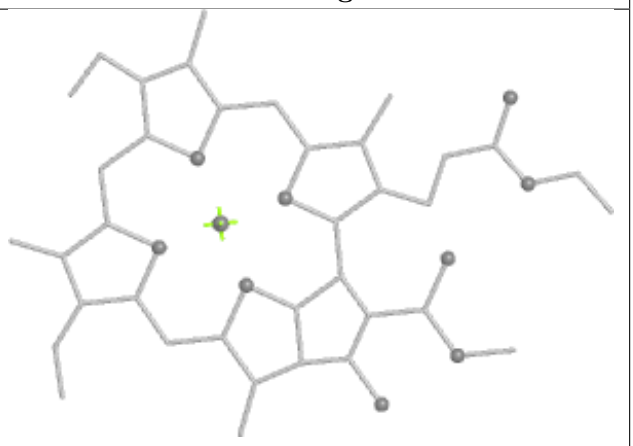
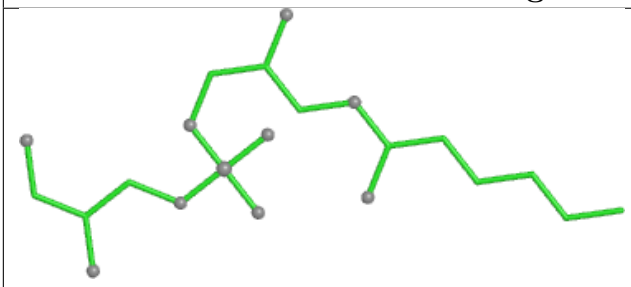


Rings

Ligand LHG 5 316



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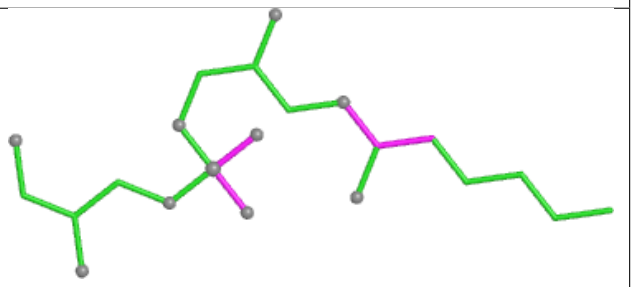
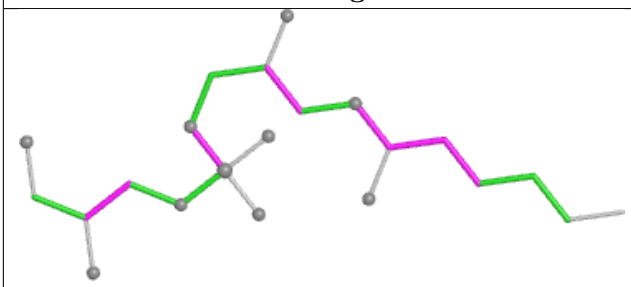
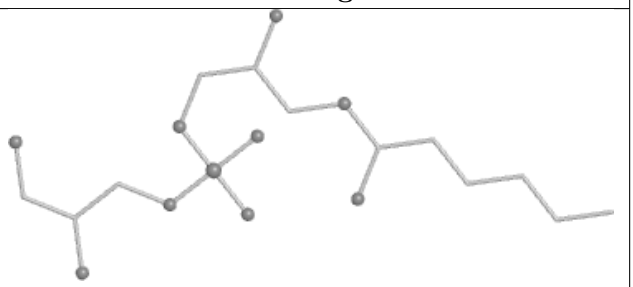


Bond angles

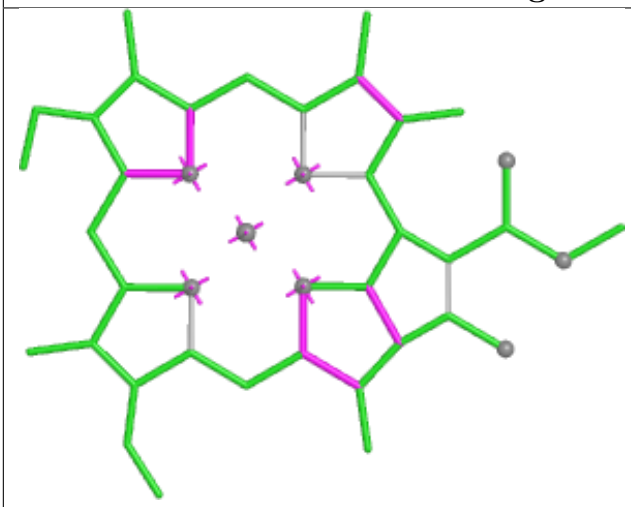


Torsions



Rings

Ligand CLA 9 314



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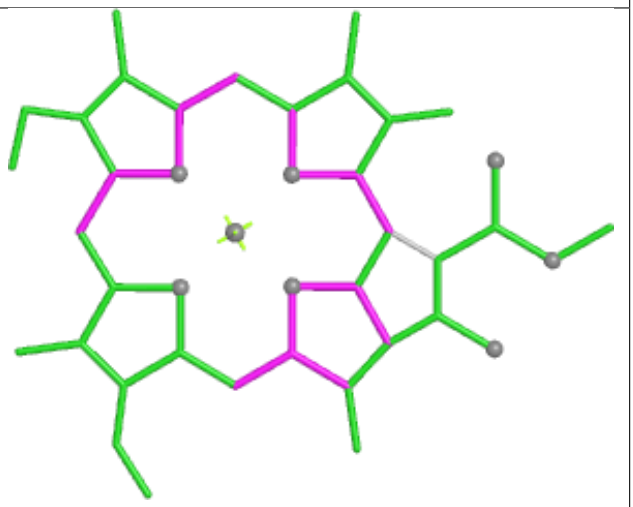
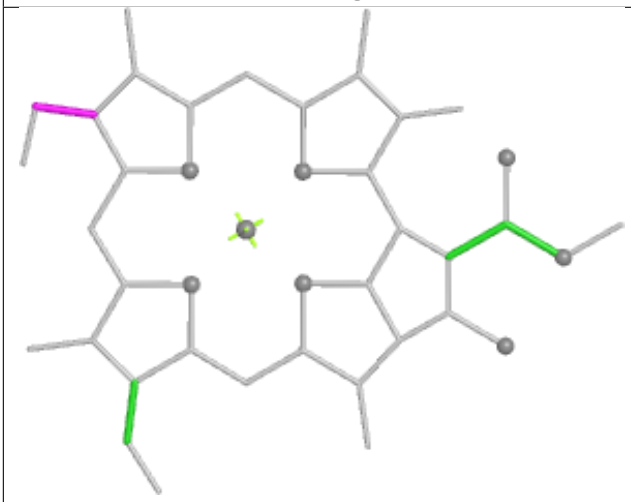
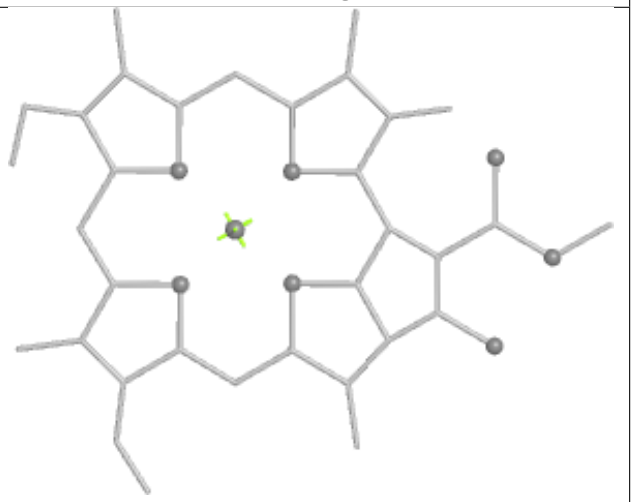


Bond angles

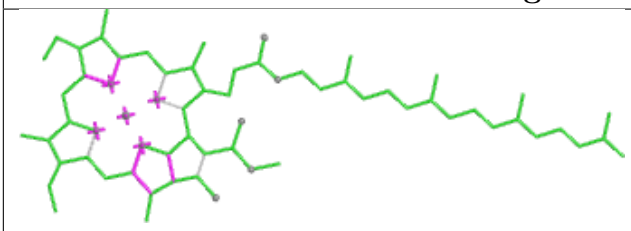


Torsions



Rings

Ligand CLA A 412



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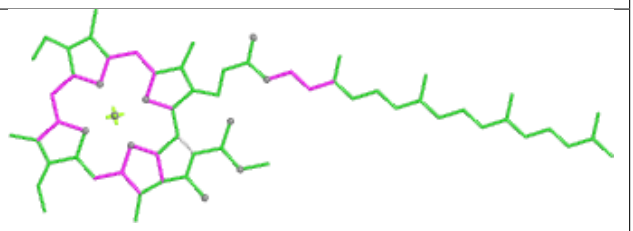

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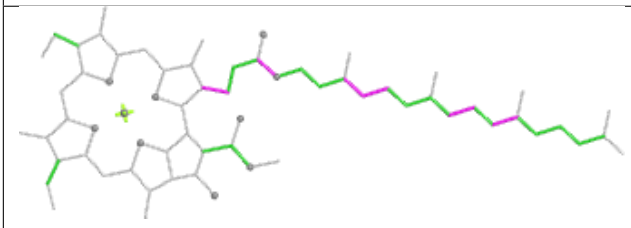

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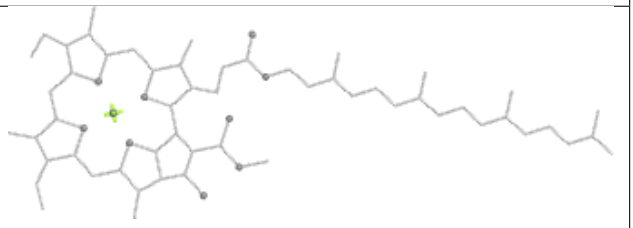
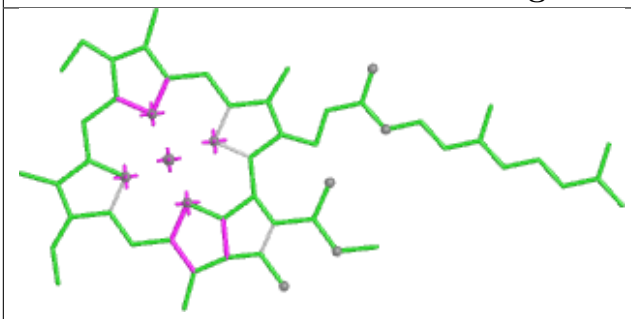


Rings

Ligand CLA 1 304



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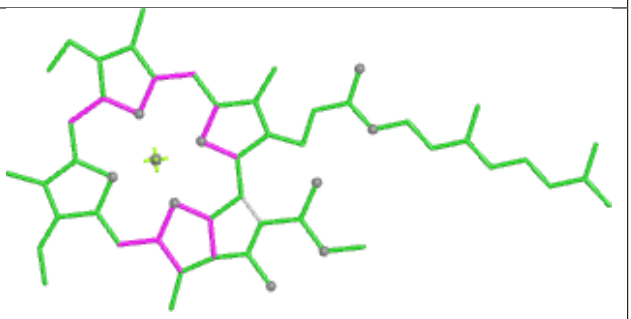

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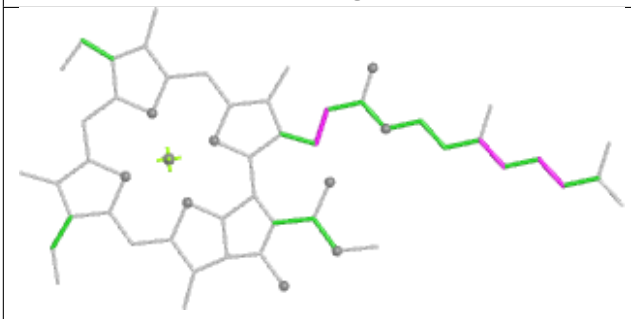

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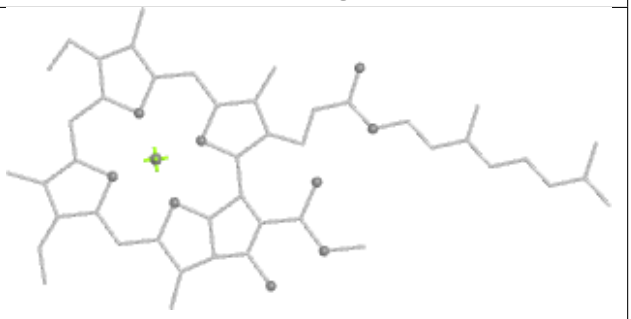
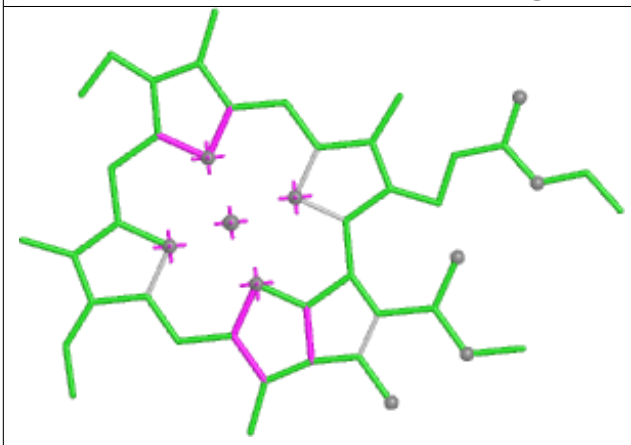


Rings

Ligand CLA 0 308



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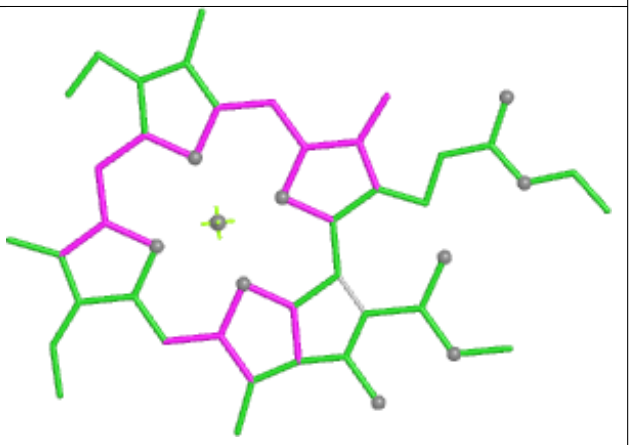

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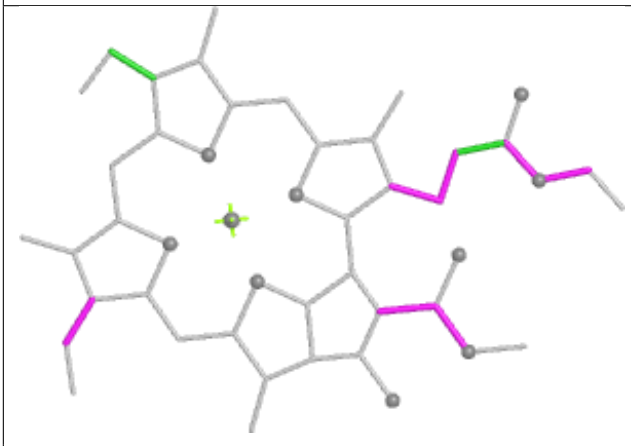

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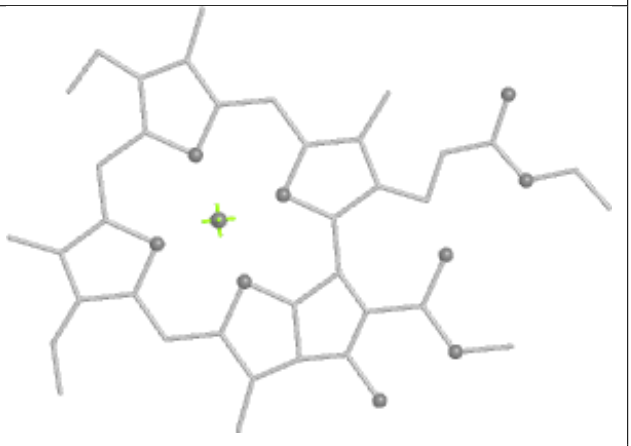
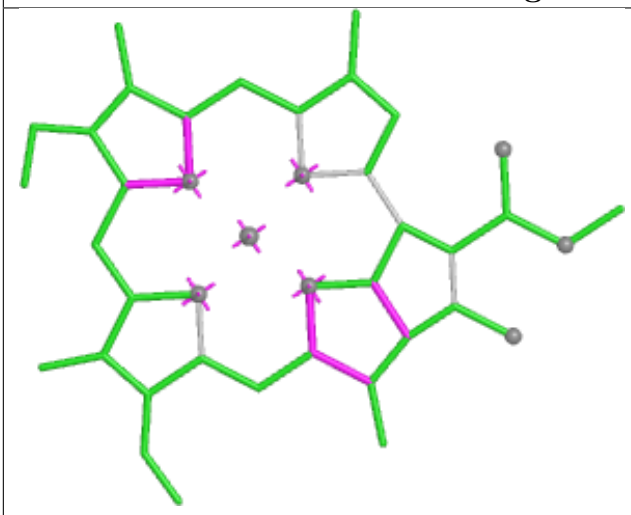


Rings

Ligand CLA B 618



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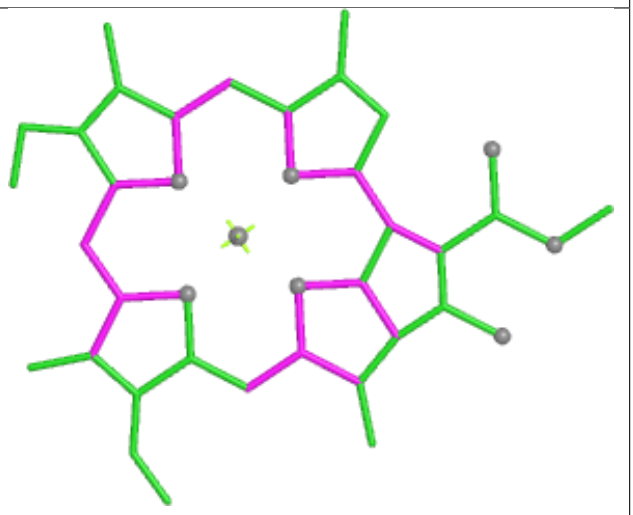

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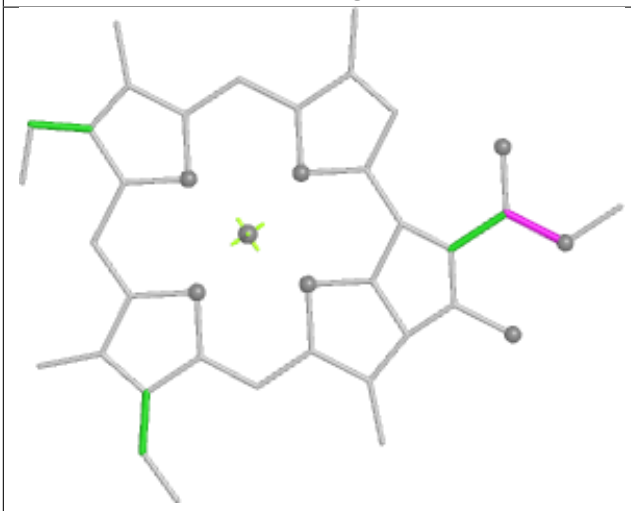

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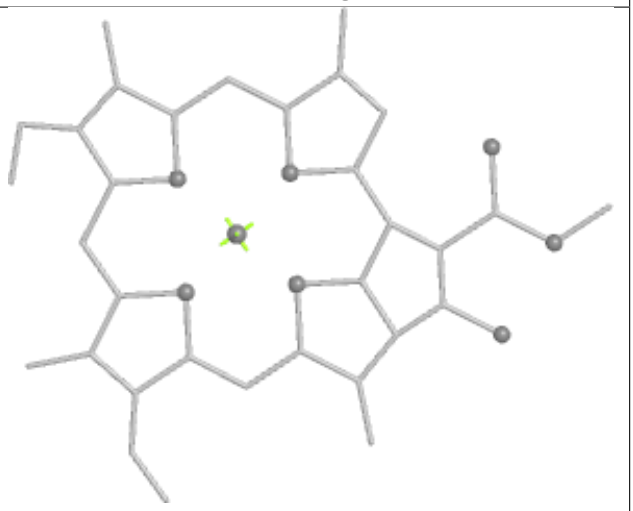
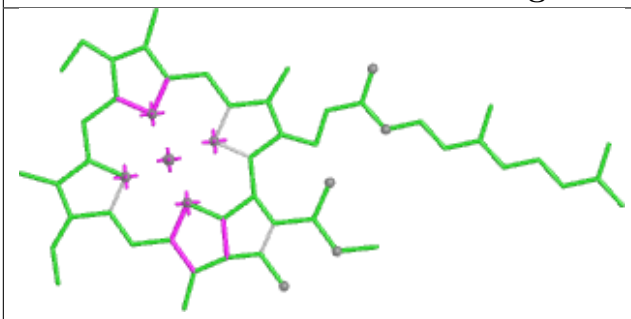


Rings

Ligand CLA 3 305



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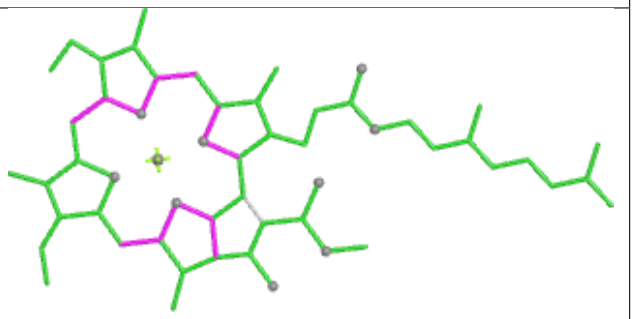
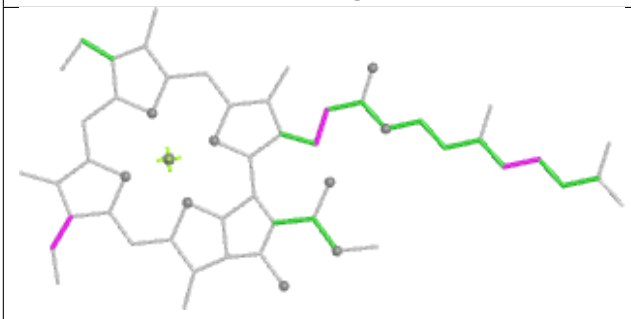


Bond angles



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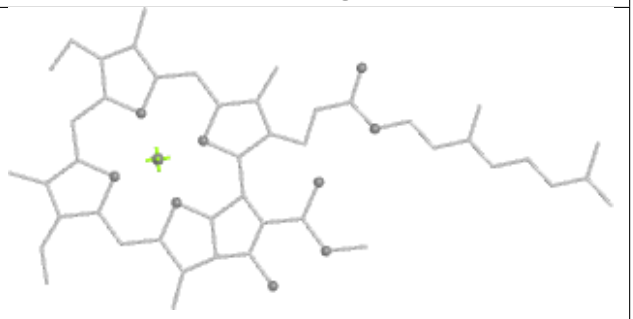
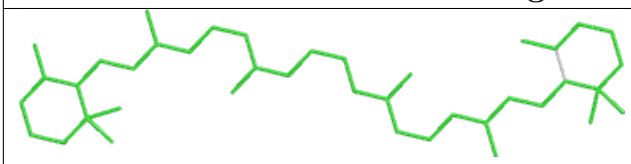


Rings

Ligand 8CT B 620



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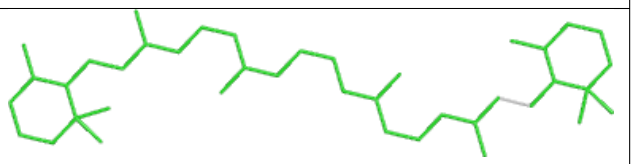

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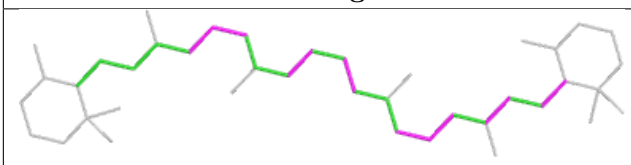

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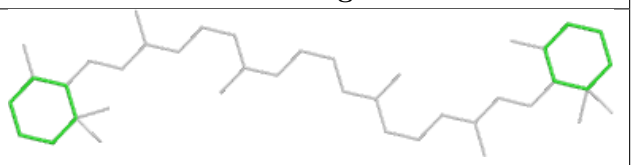

Rings

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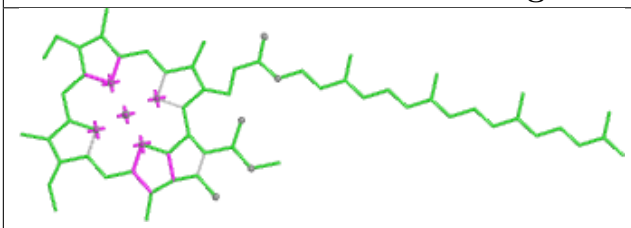

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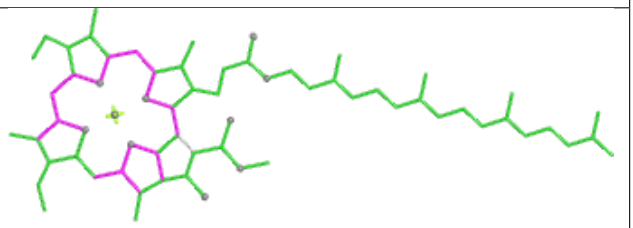

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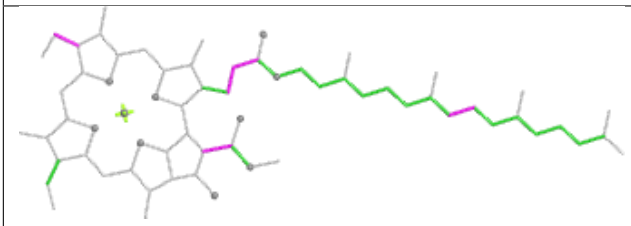

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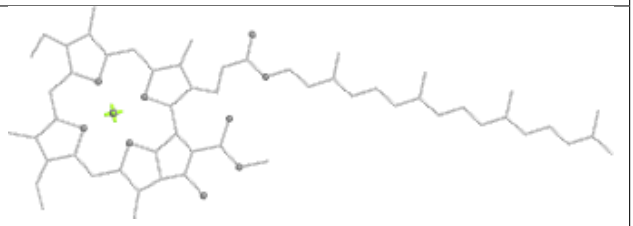
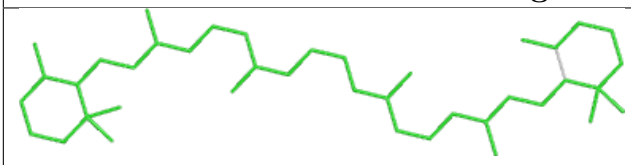


Rings

Ligand 8CT y 101



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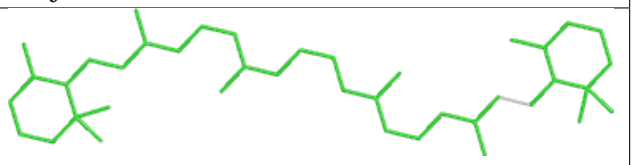
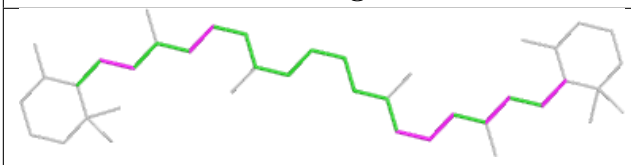


Bond angles



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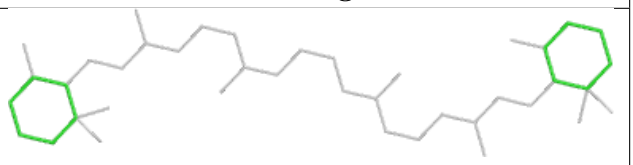
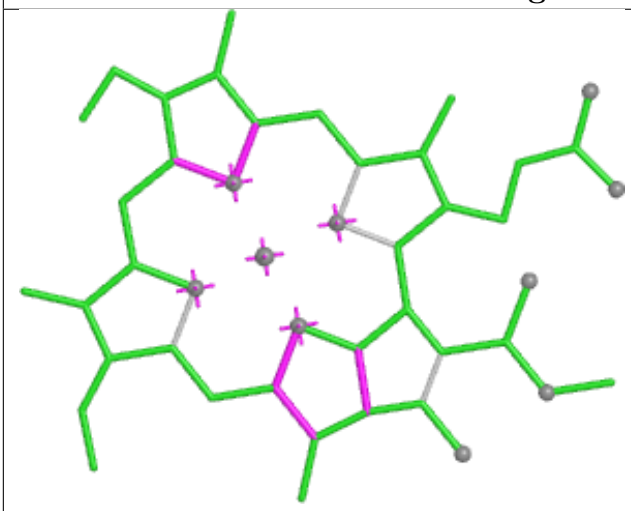


Rings

Ligand CLA 6 306



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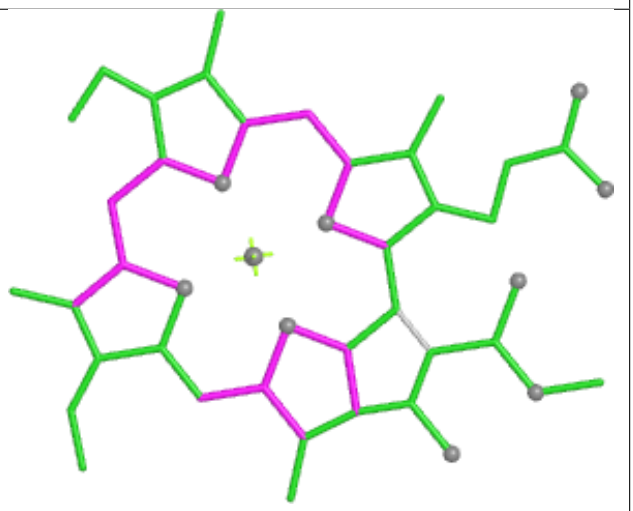

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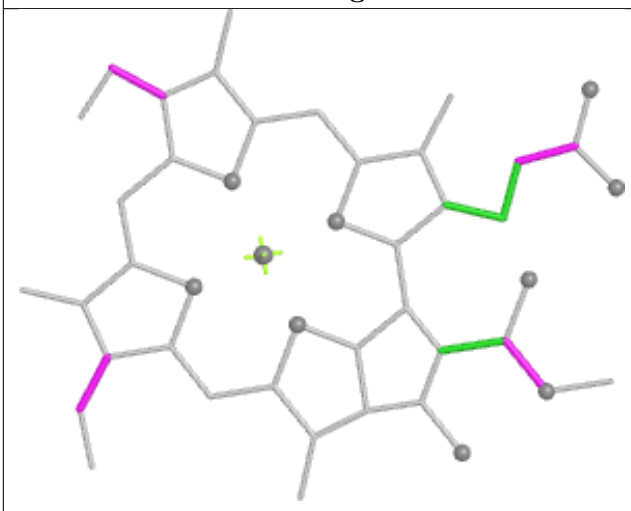

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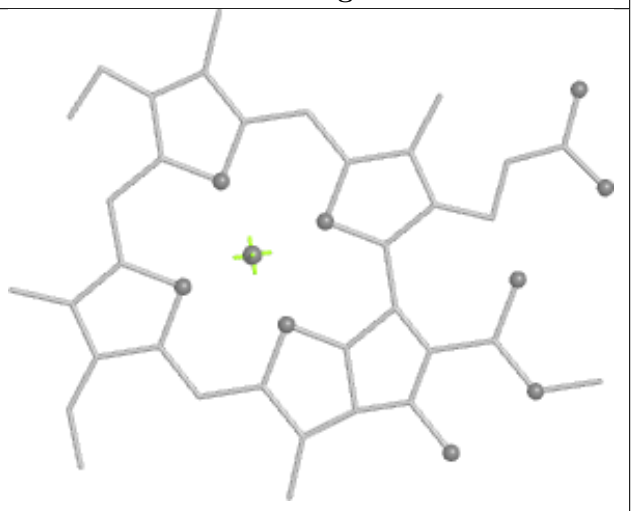
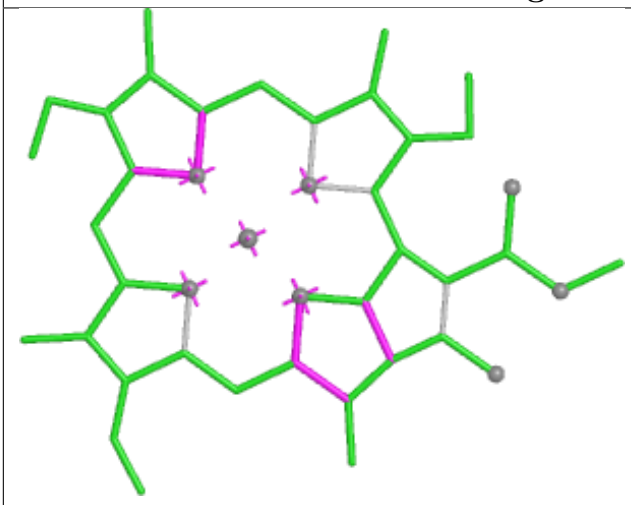


Rings

Ligand CLA p 309



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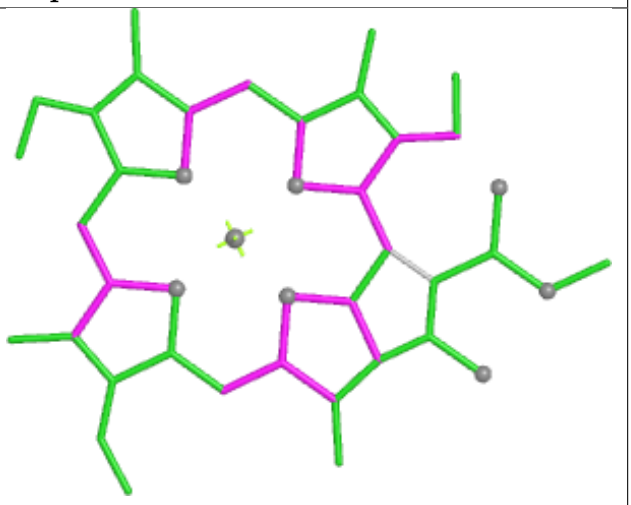

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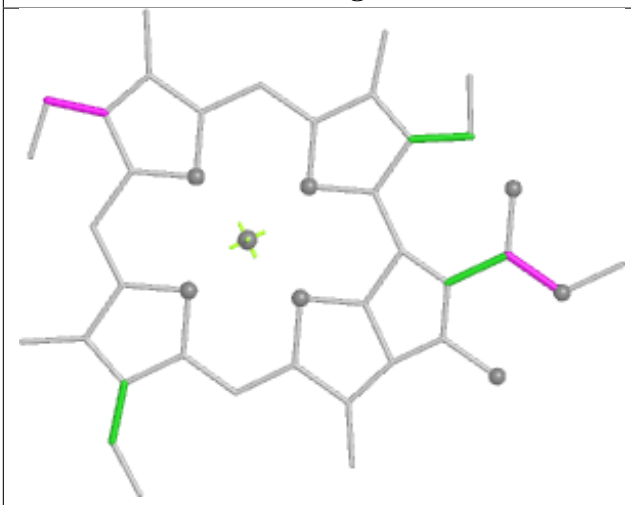
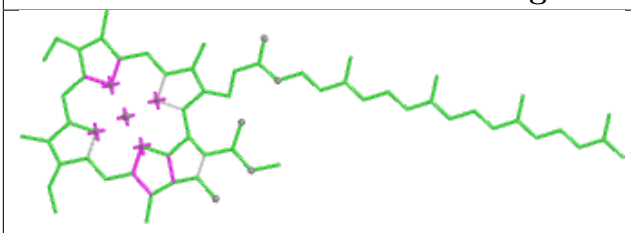


Torsions

Rings

Ligand CLA c 511



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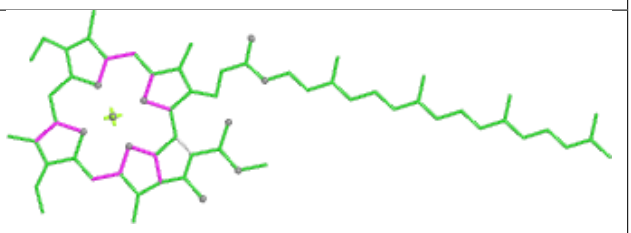
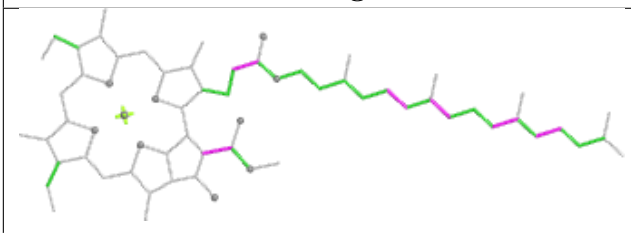


Bond angles



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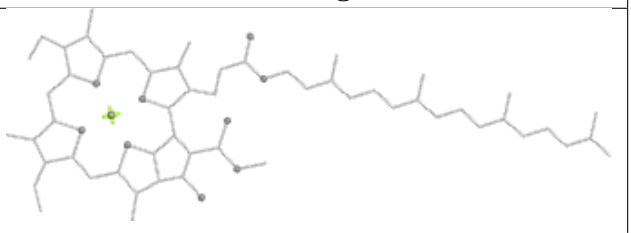
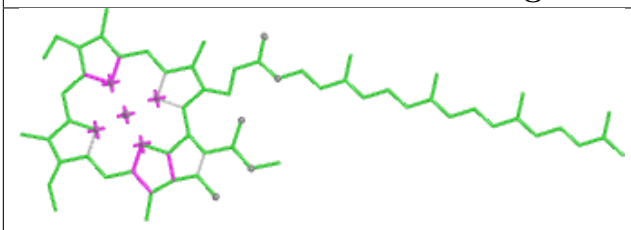


Rings

Ligand CLA B 610



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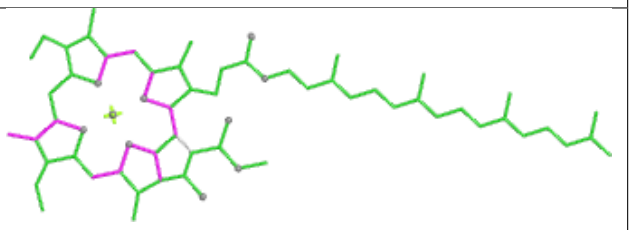
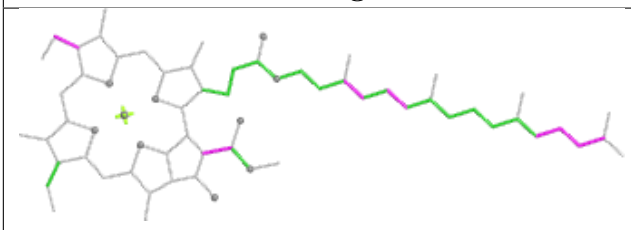


Bond angles



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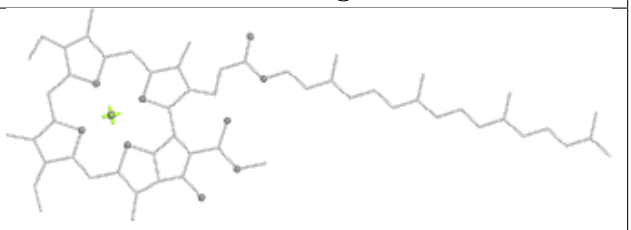
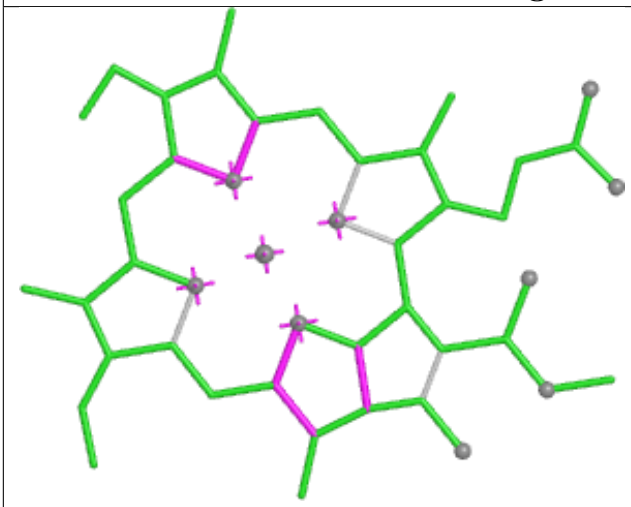


Rings

Ligand CLA 3 307



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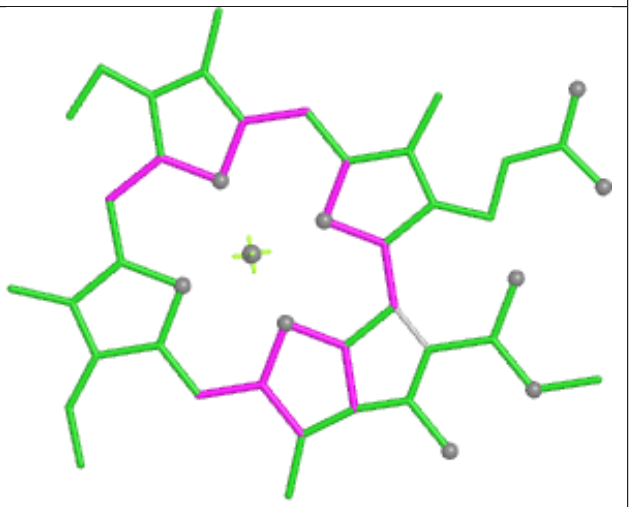

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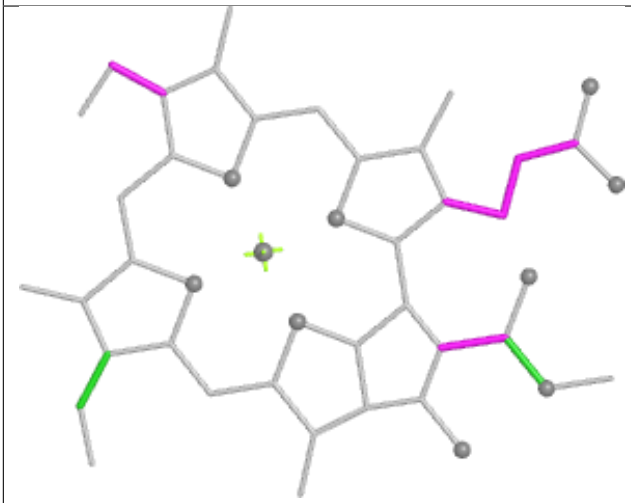

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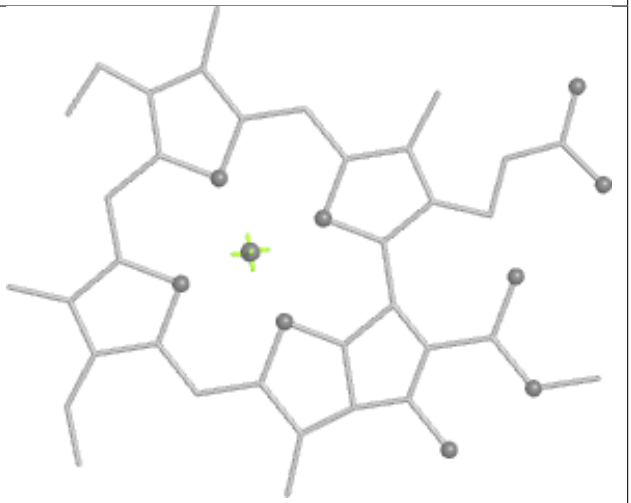
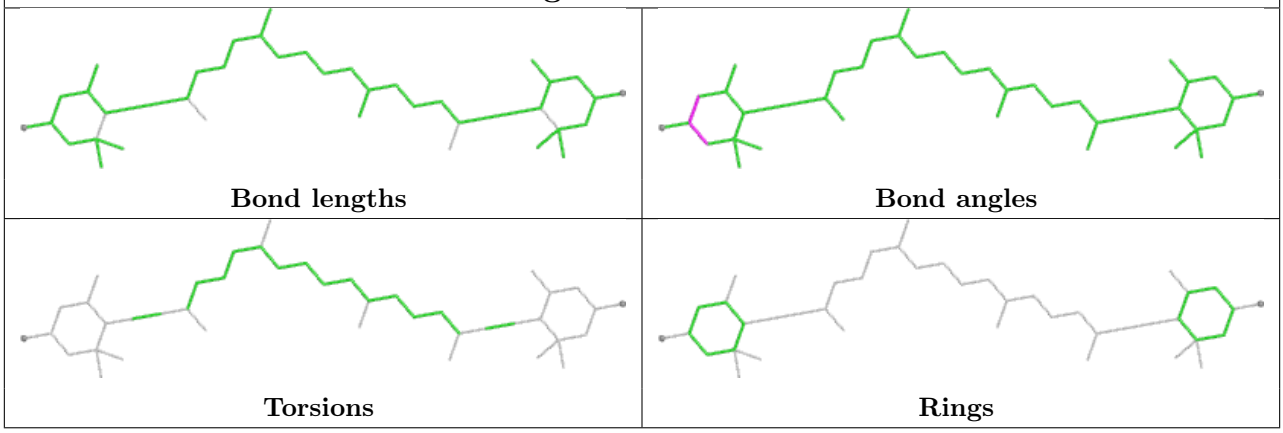
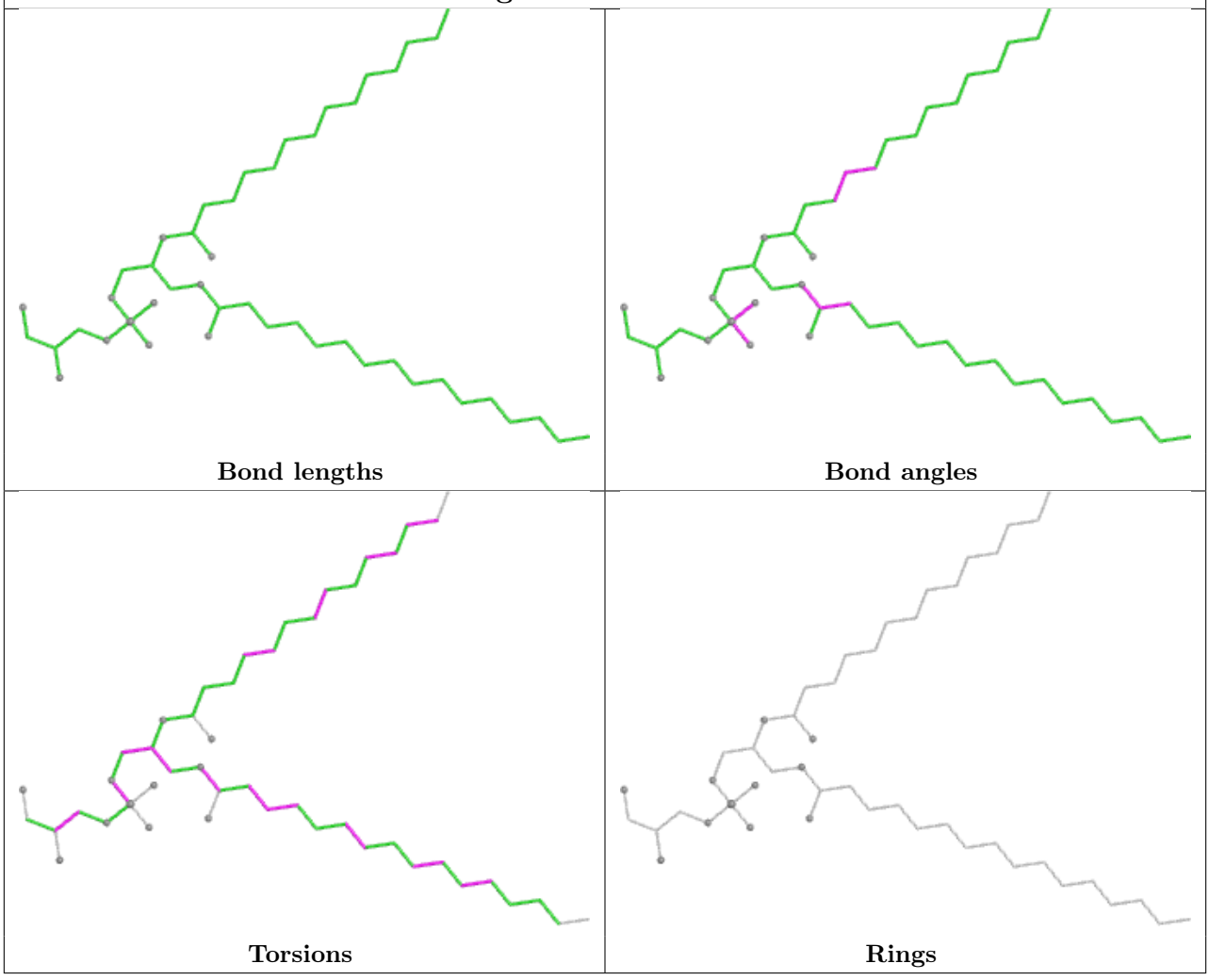


Rings

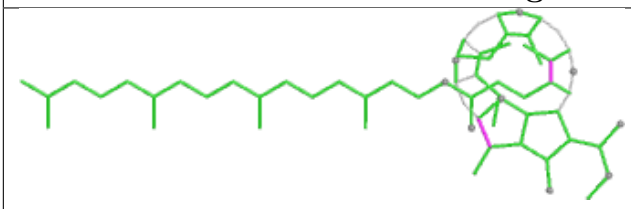
Ligand II0 8 311



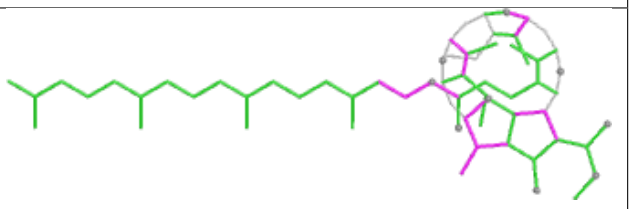
Ligand LHG d 402



Ligand PHO a 407



Bond lengths



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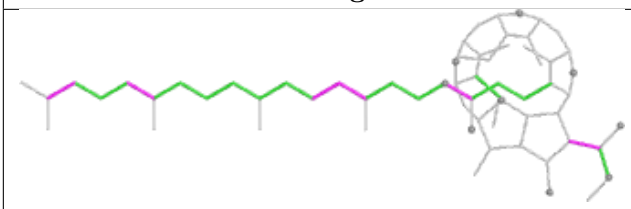
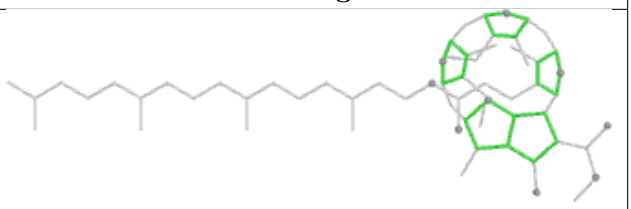
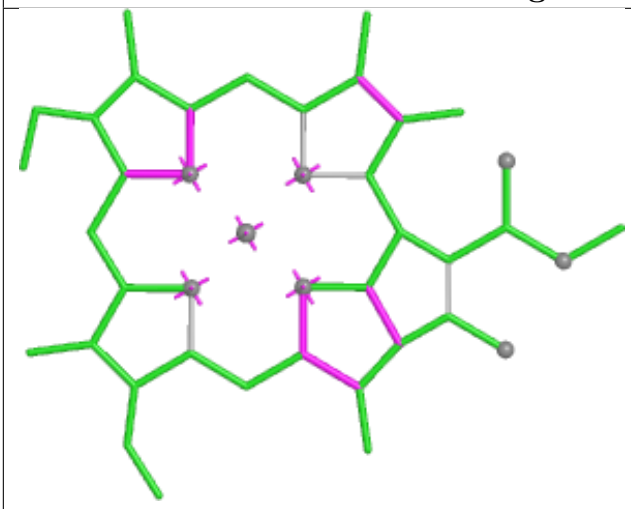


Torsions



Rings

Ligand CLA 5 310



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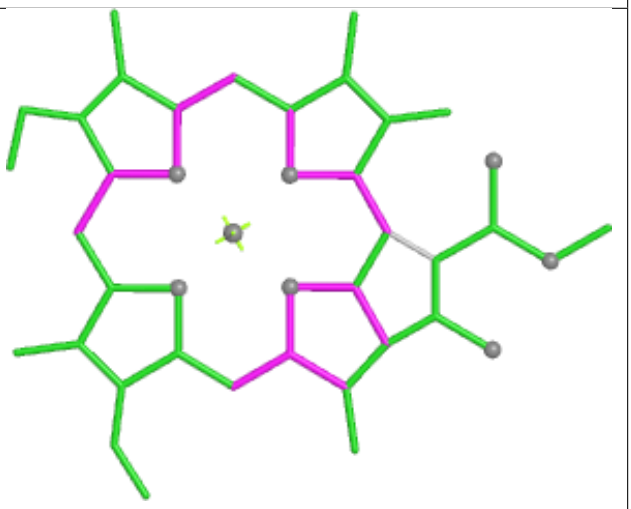

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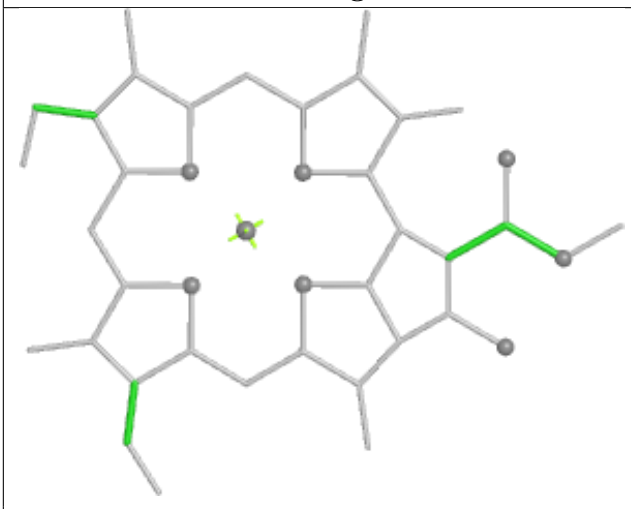

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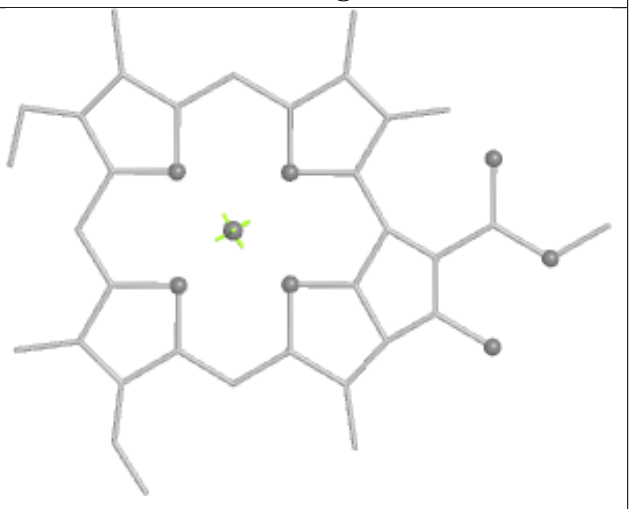
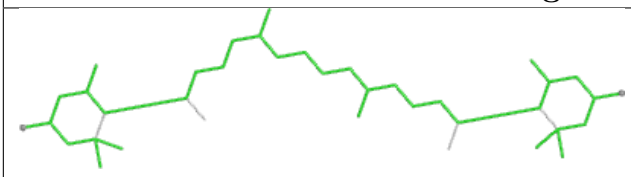


Rings

Ligand II0 7 315



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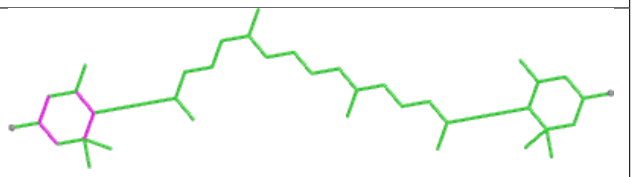

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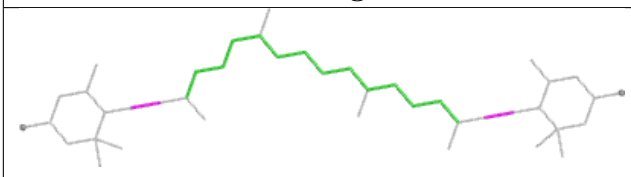

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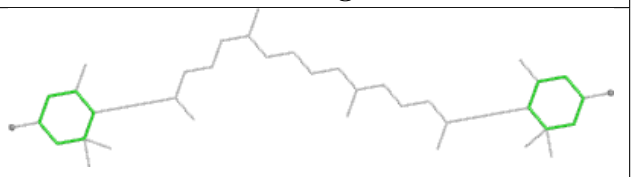
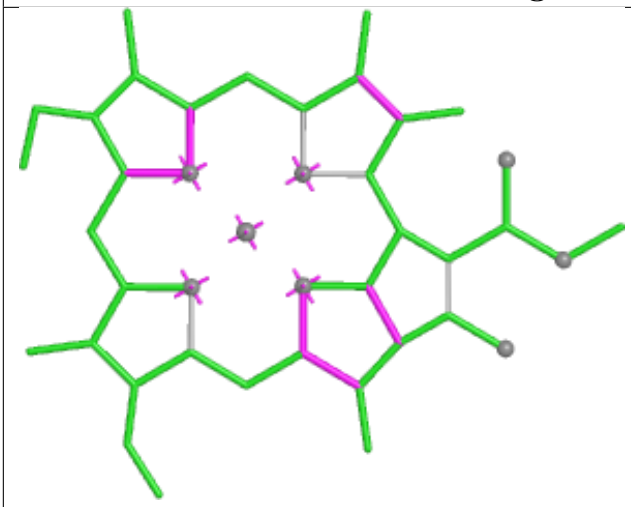


Rings

Ligand CLA 3 306



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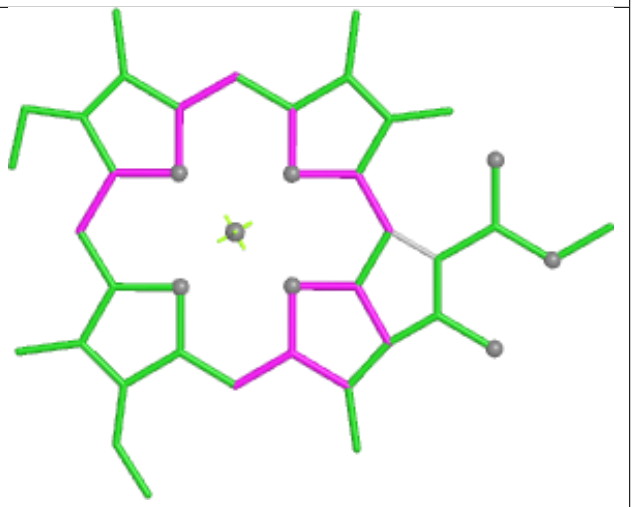

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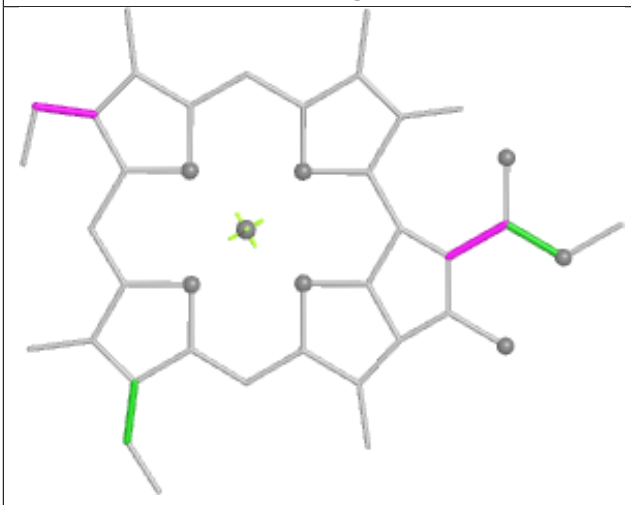

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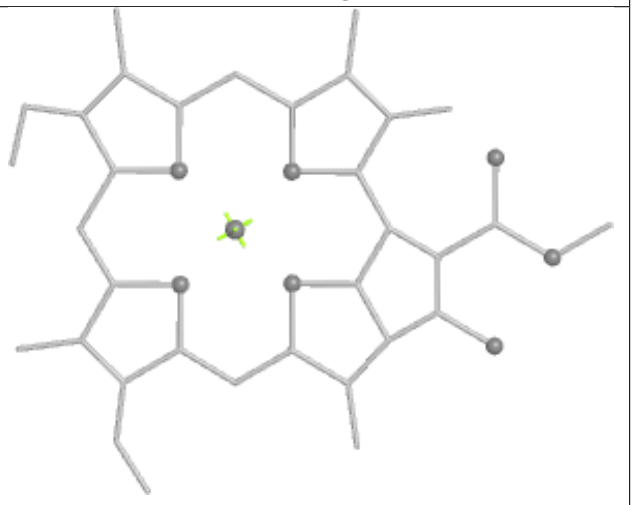

Rings

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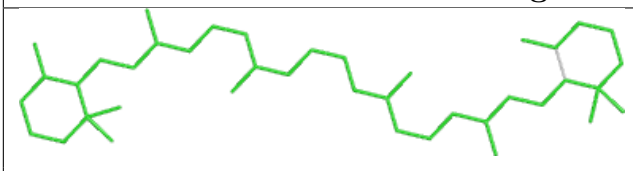

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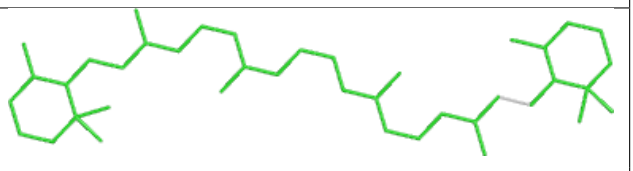

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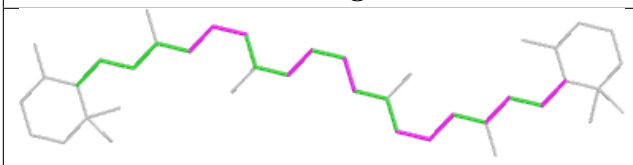

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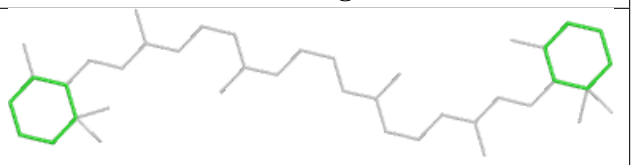
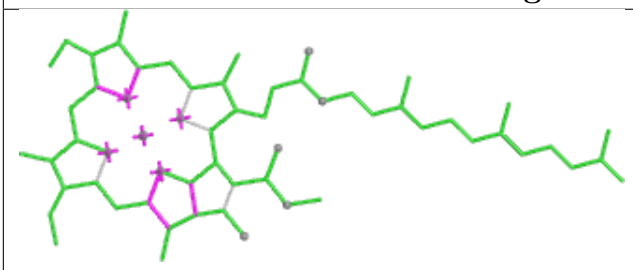


Rings

Ligand CLA A 408



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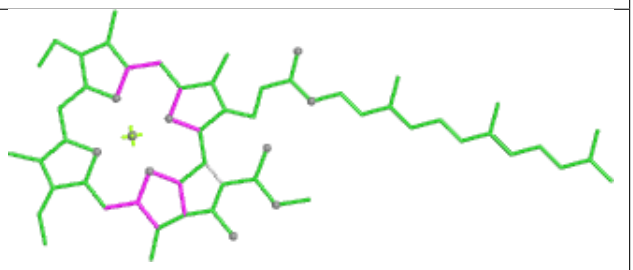

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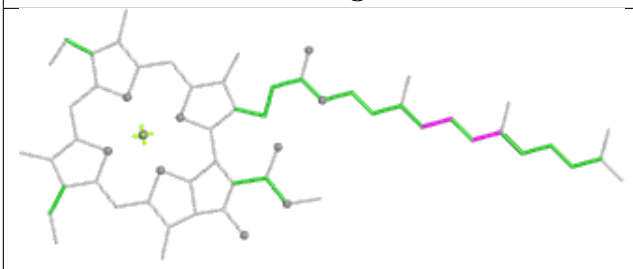

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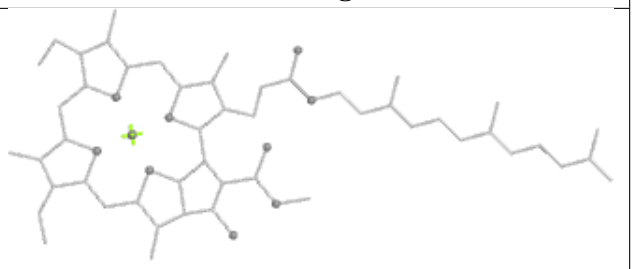

Rings

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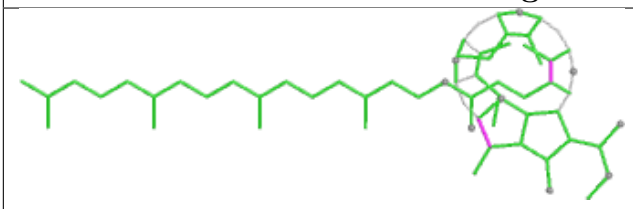

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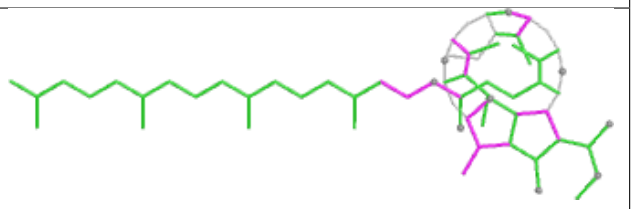

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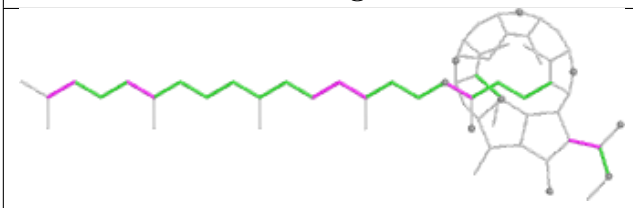

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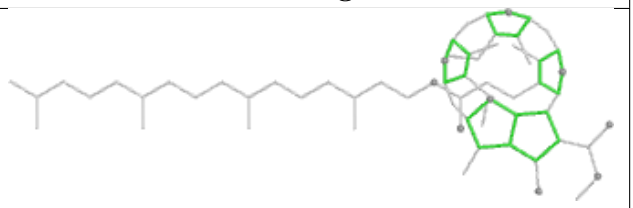

Rings

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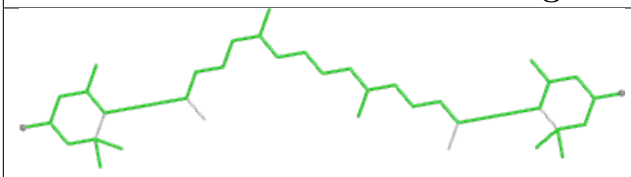

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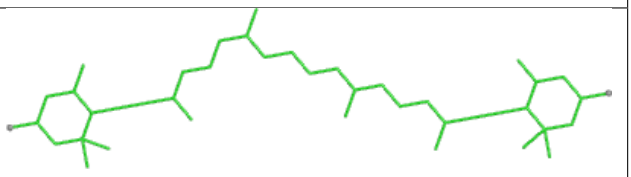

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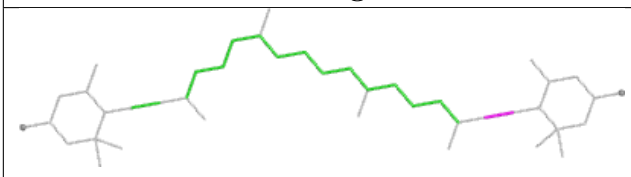

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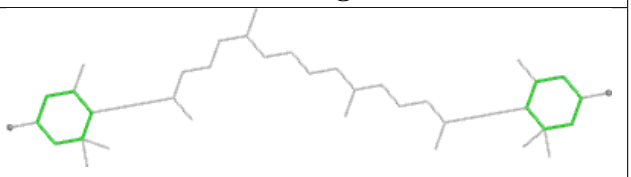
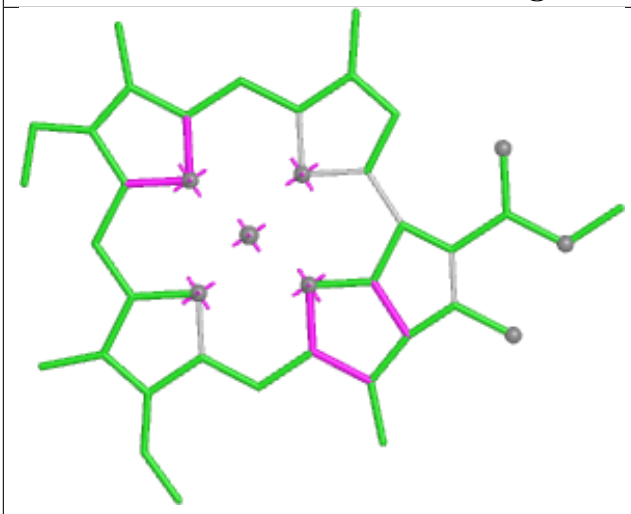


Rings

Ligand CLA 5 305



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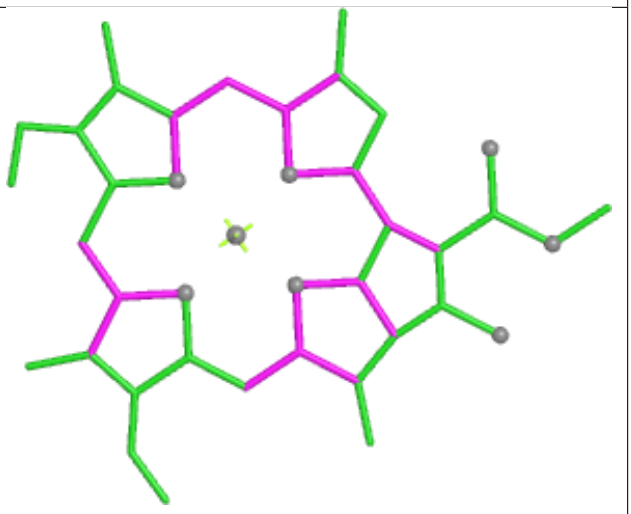

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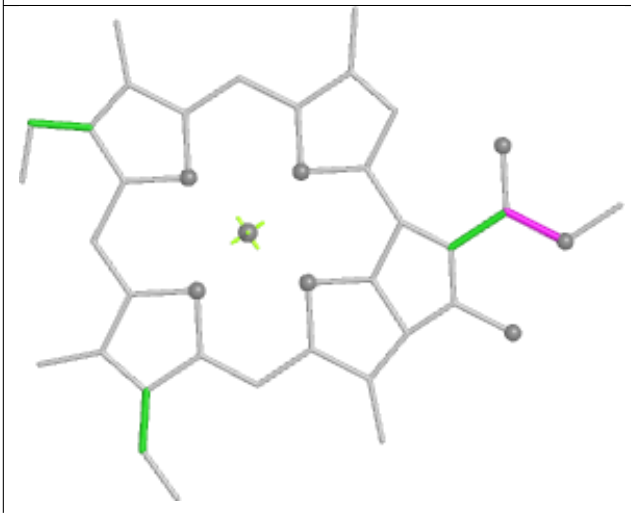

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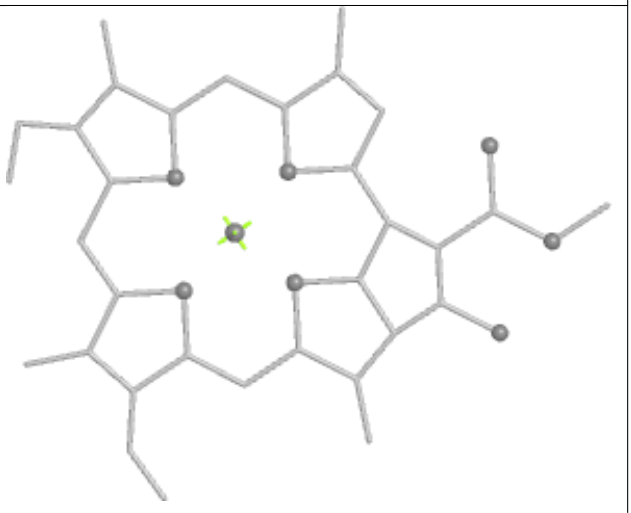

Rings

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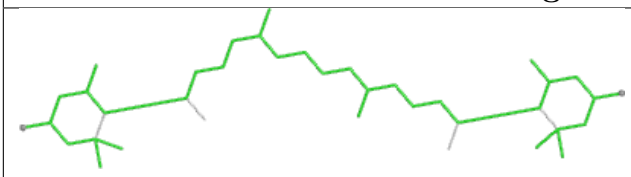

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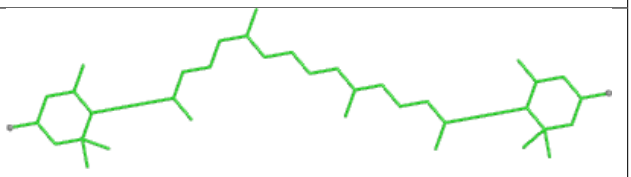

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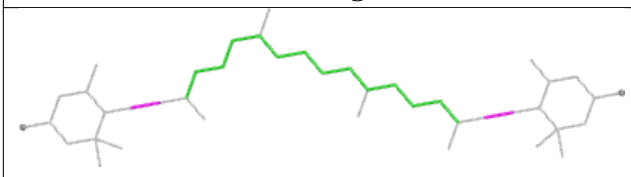

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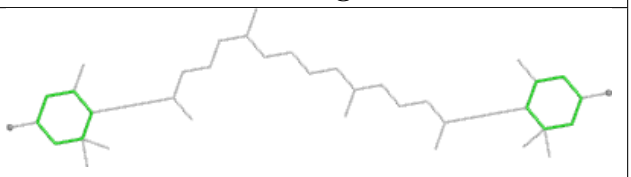
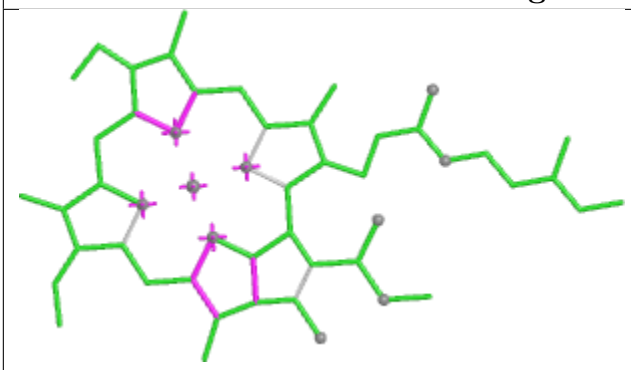


Rings

Ligand CLA 4 302



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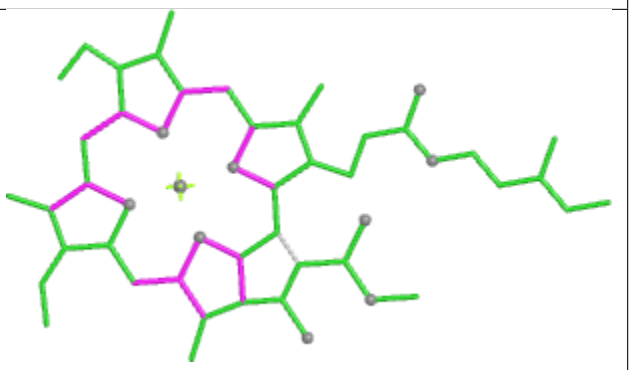

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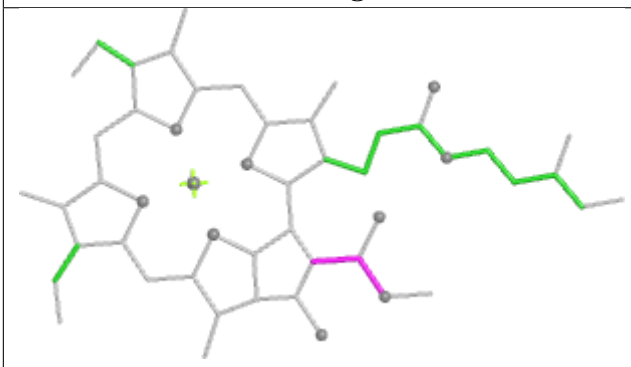

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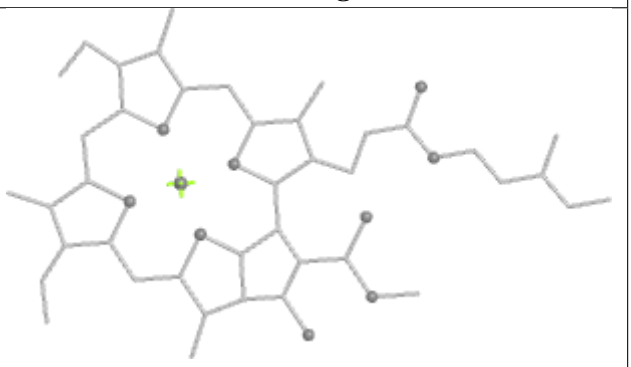
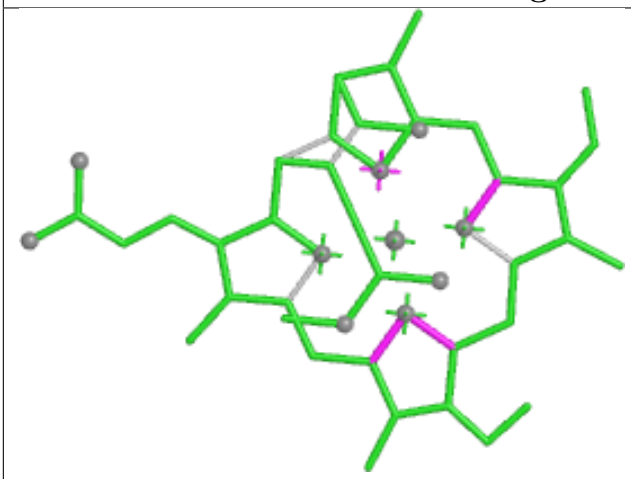


Rings

Ligand KC2 8 309



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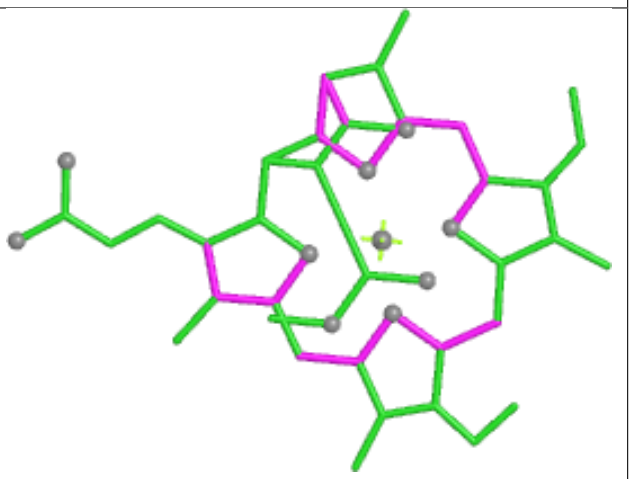

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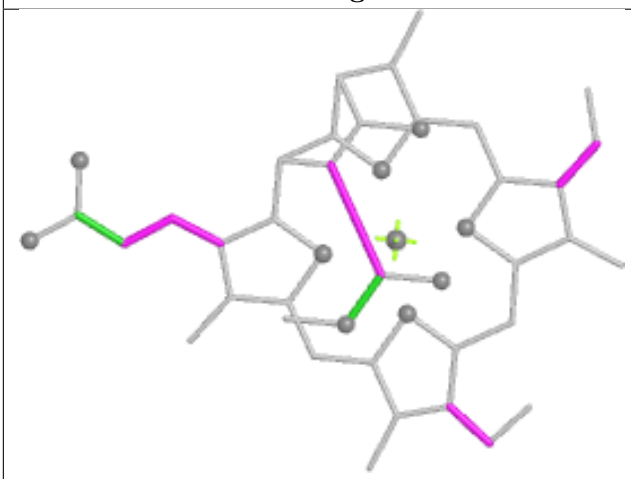

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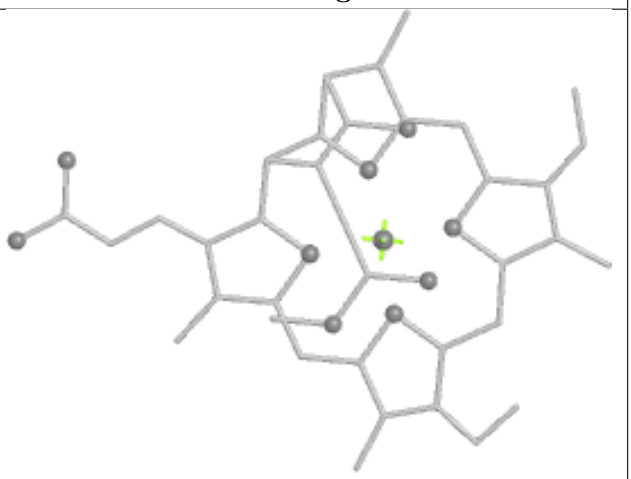
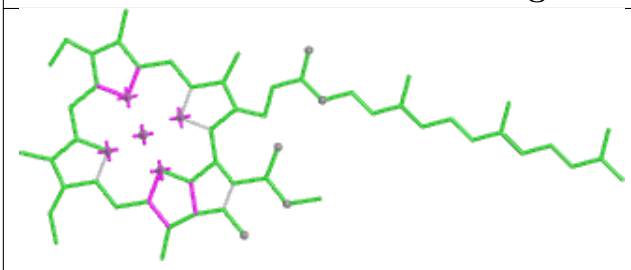


Rings

Ligand CLA 1 306



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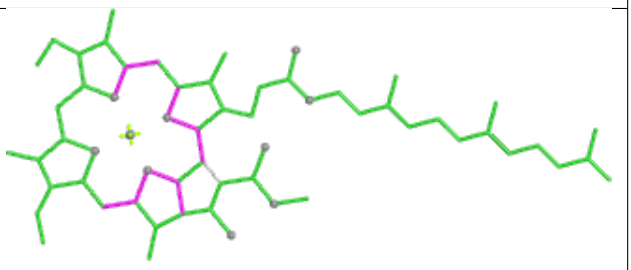

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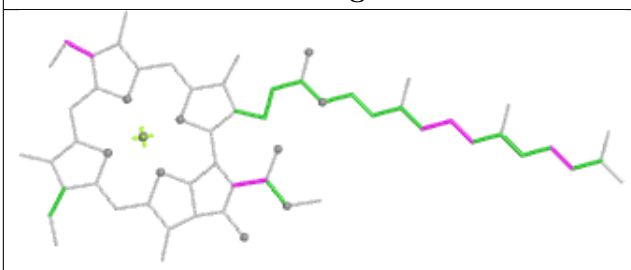

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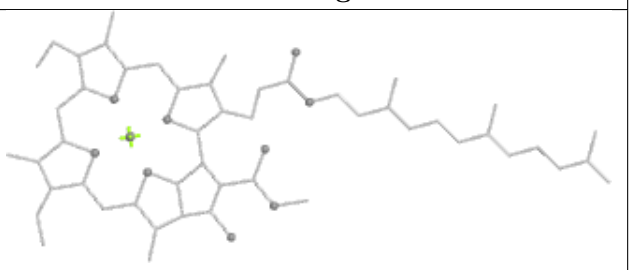
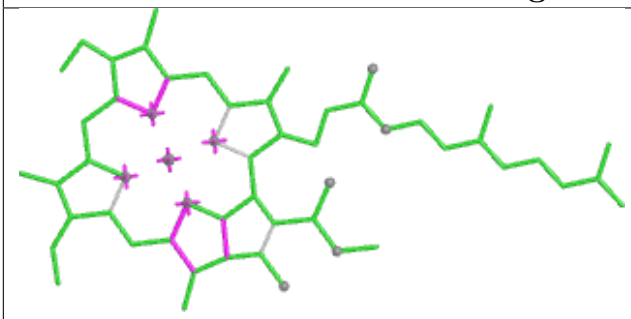


Rings

Ligand CLA 7 304



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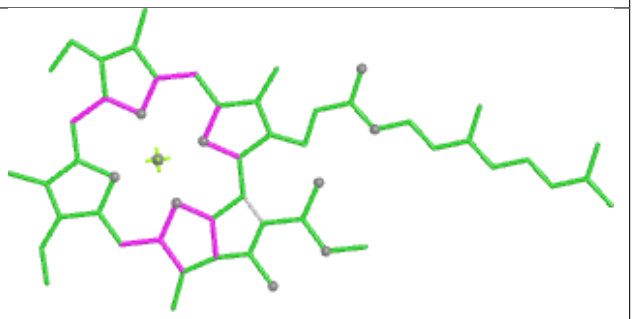
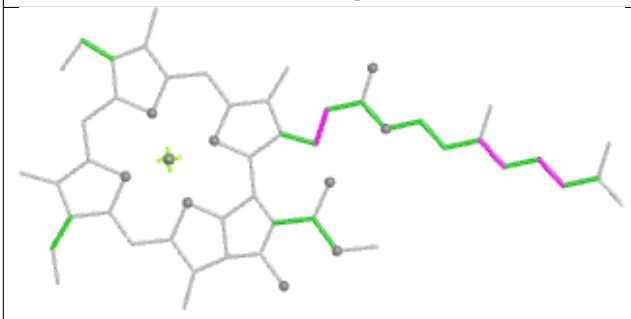
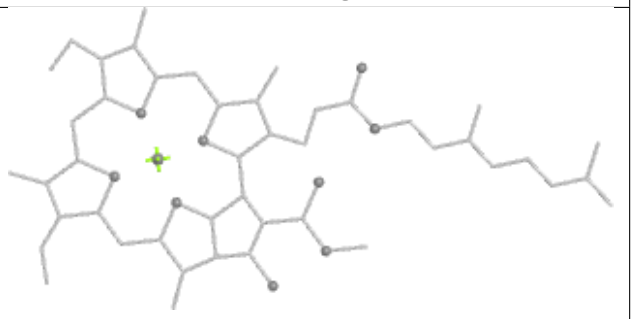


Bond angles

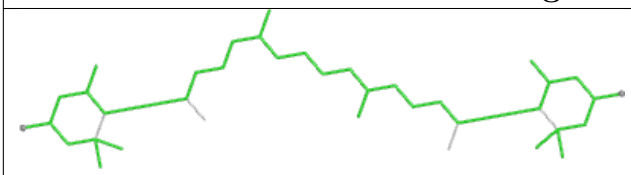


Torsions



Rings

Ligand II0 3 317



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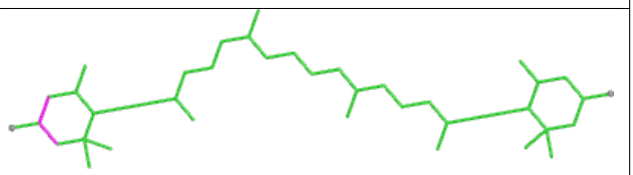

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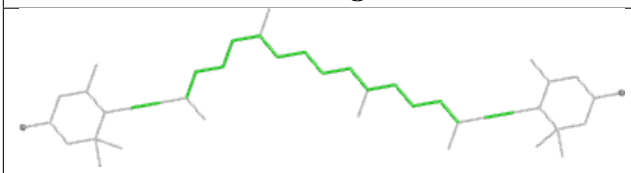

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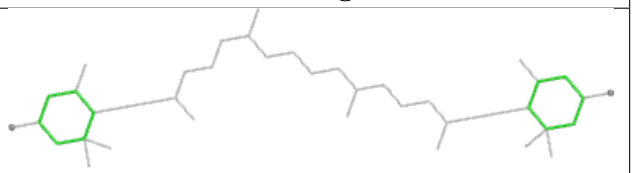
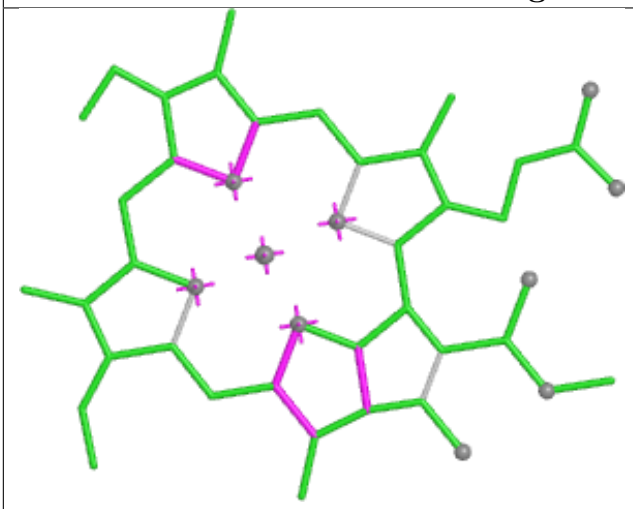


Rings

Ligand CLA 7 301



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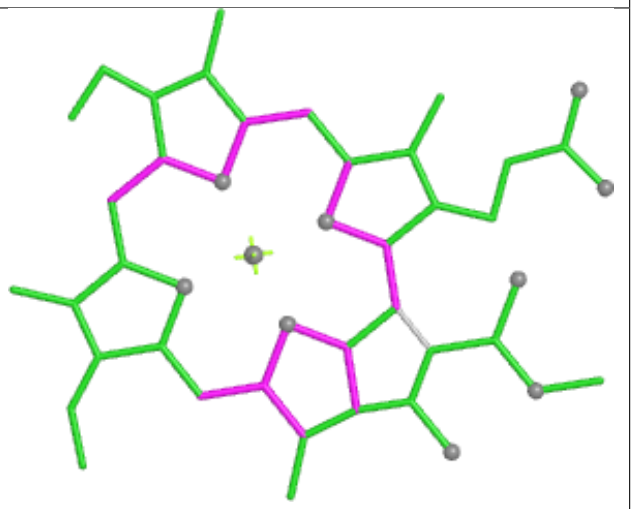

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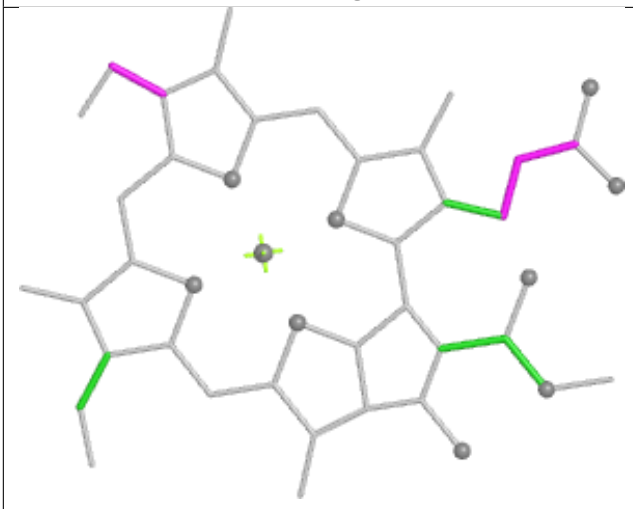
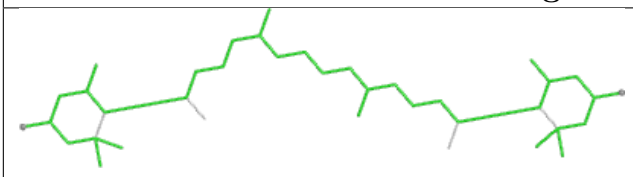


Torsions

Rings

Ligand II0 4 314



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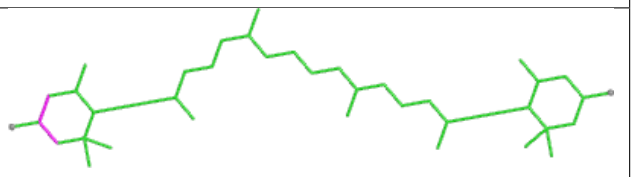

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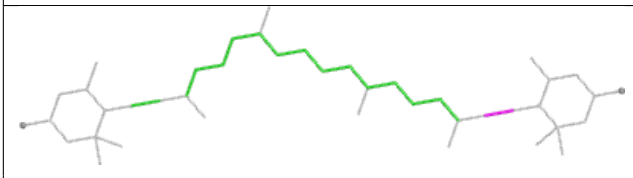

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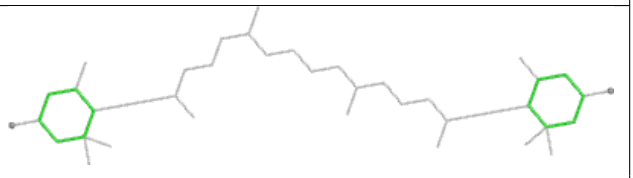
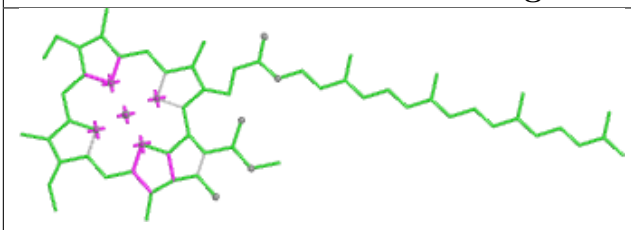


Rings

Ligand CLA C 514



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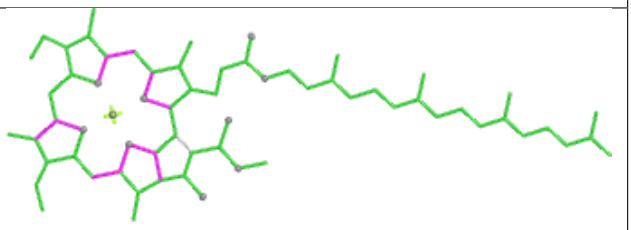

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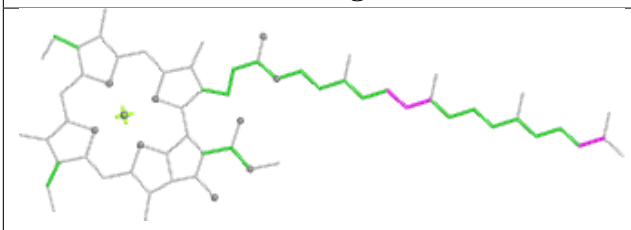

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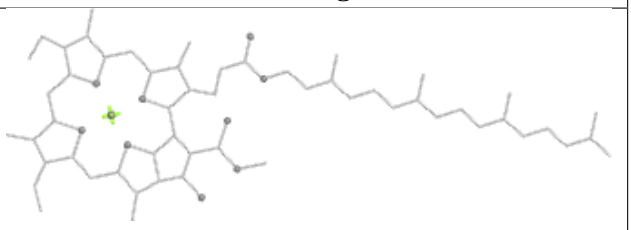

Rings

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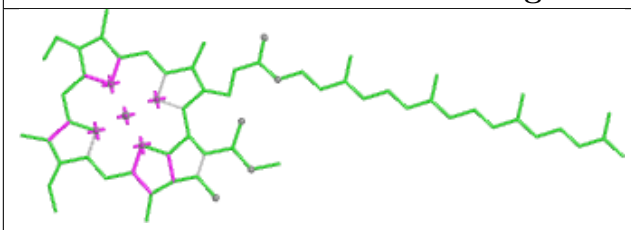

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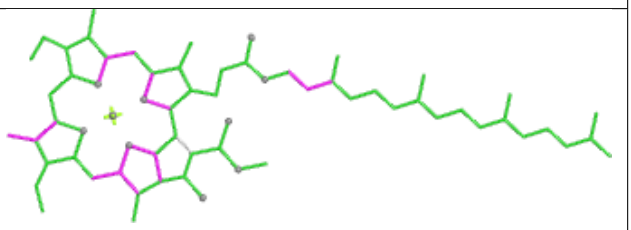

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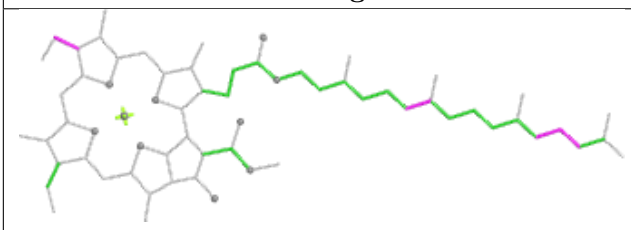

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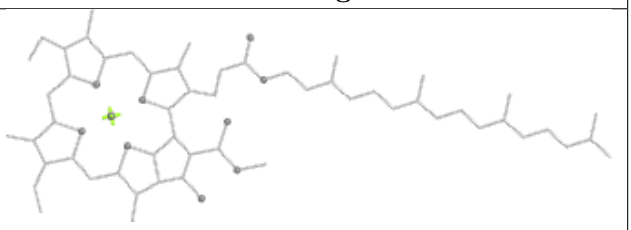

Rings

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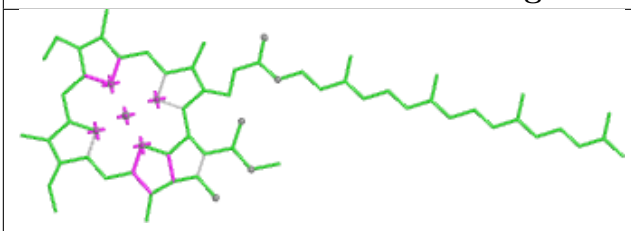

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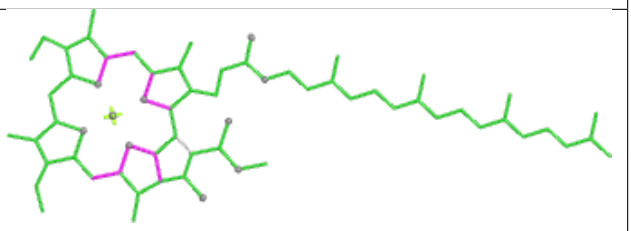

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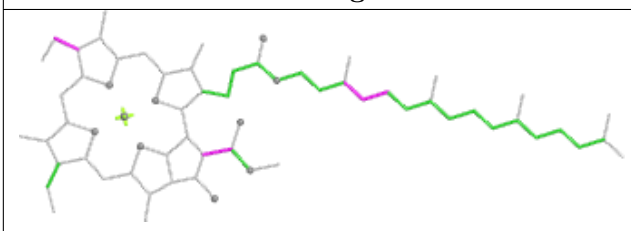

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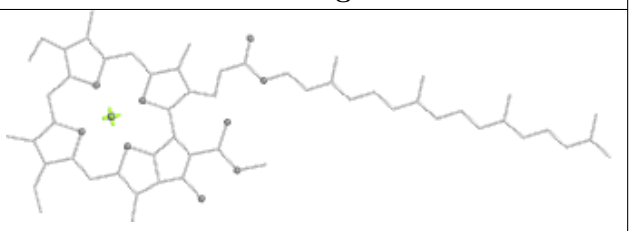
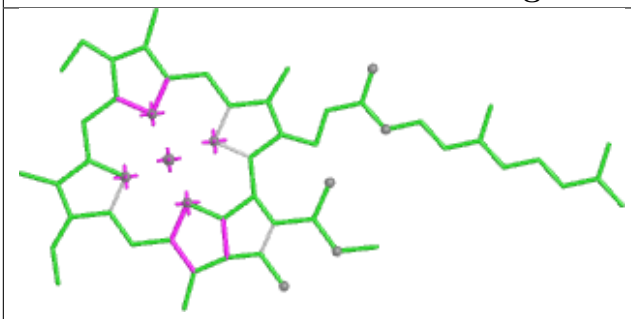


Rings

Ligand CLA N 305



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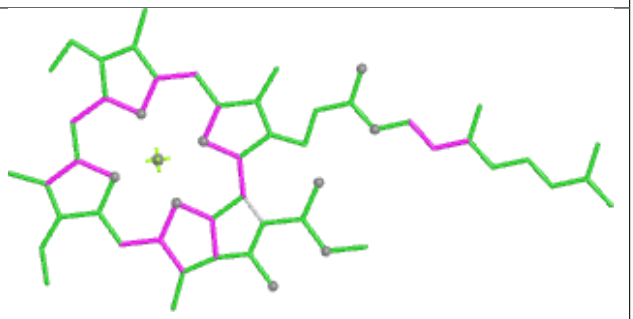

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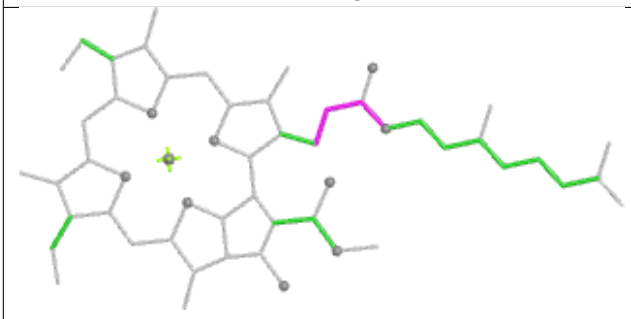

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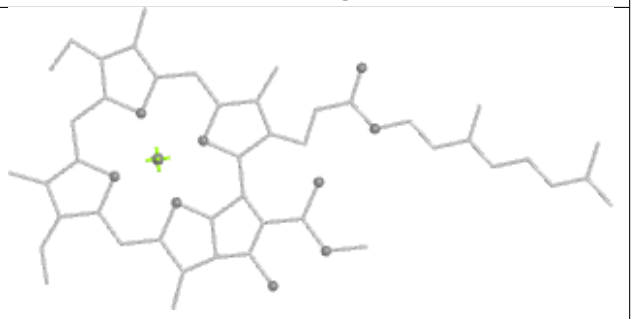
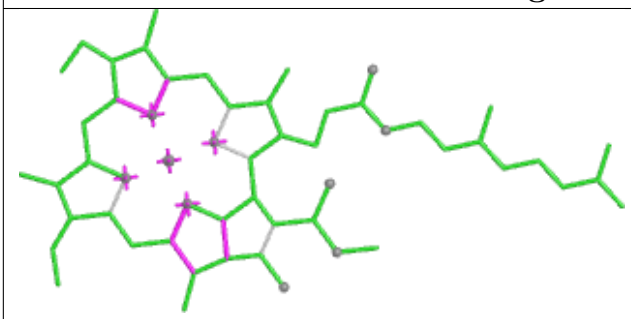


Rings

Ligand CLA 8 308



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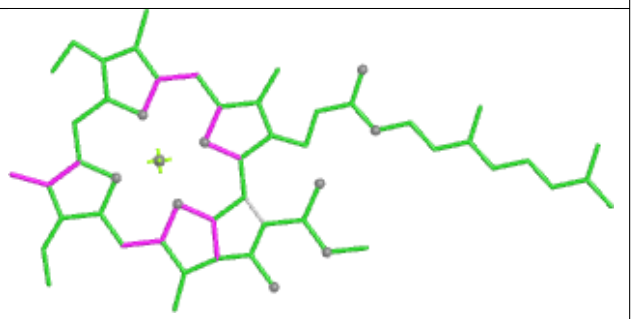

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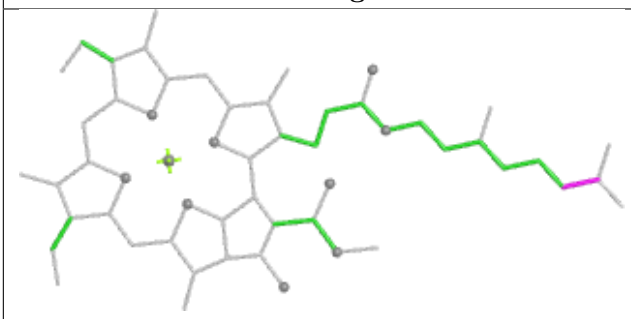

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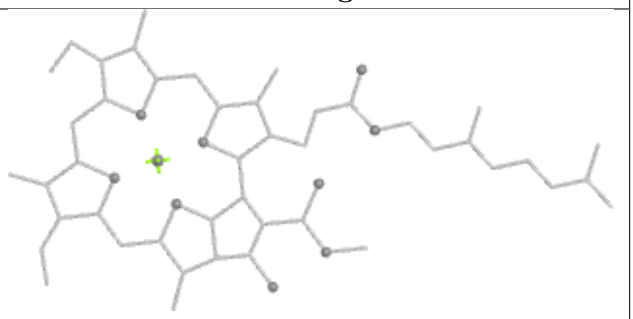
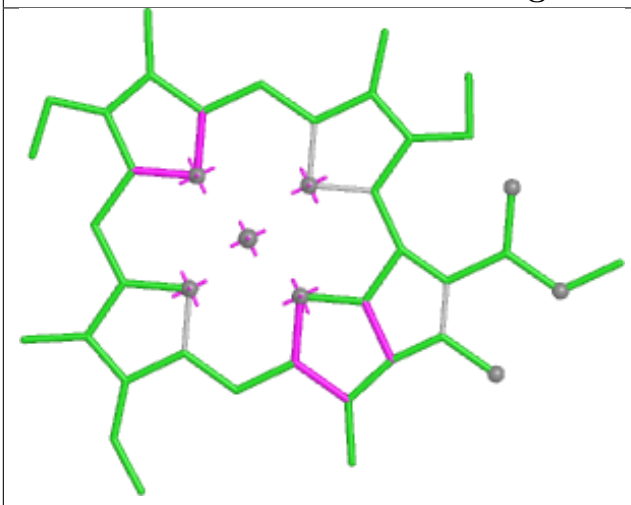


Rings

Ligand CLA 6 308



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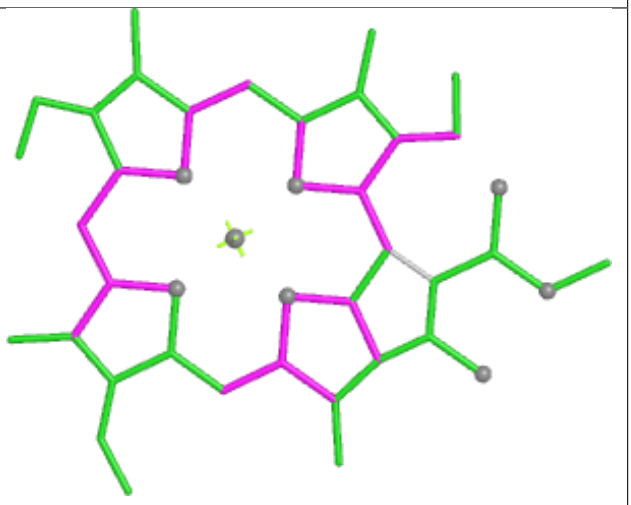

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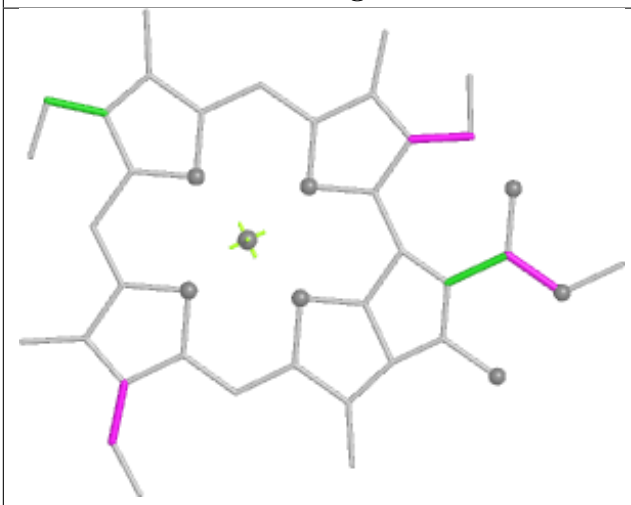
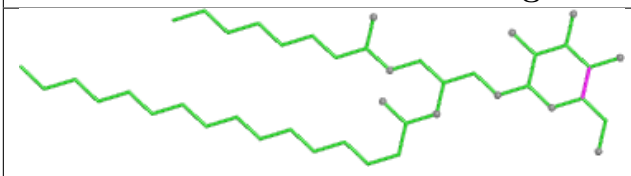


Torsions

Rings

Ligand LMG b 624



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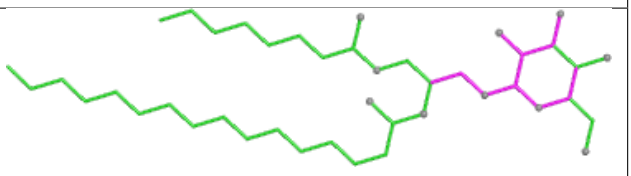

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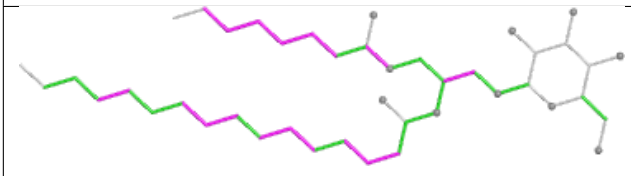

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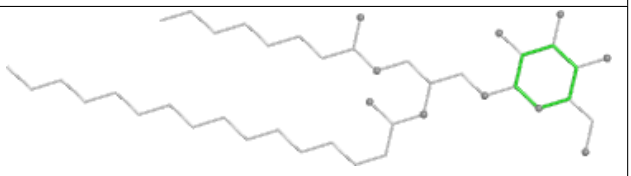
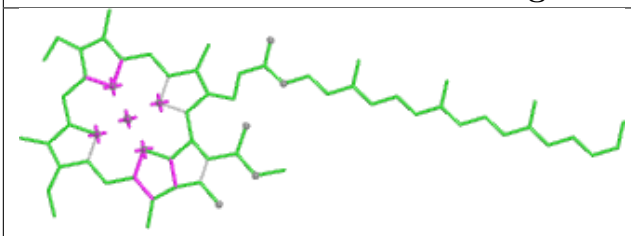


Rings

Ligand CLA 7 302



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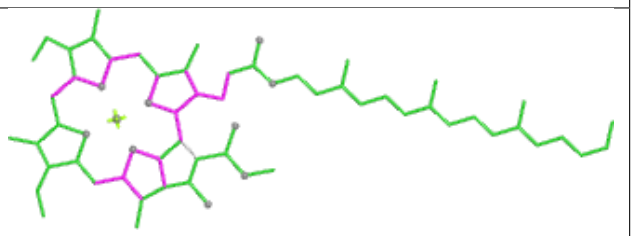

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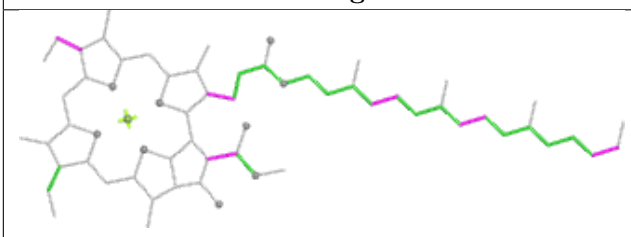

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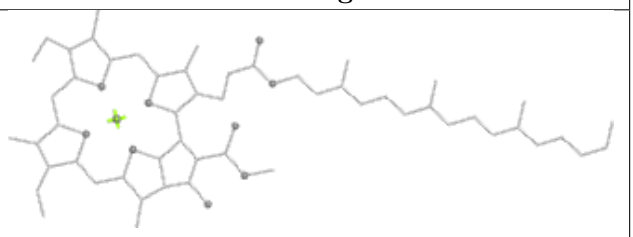
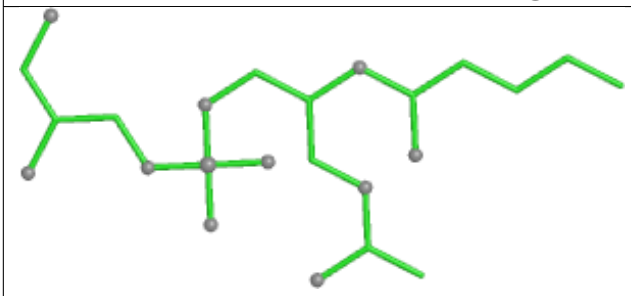


Rings

Ligand LHG 3 321



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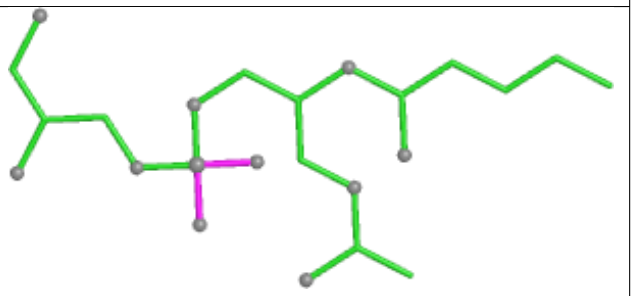

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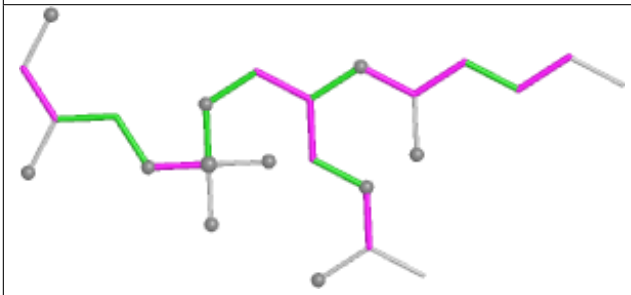

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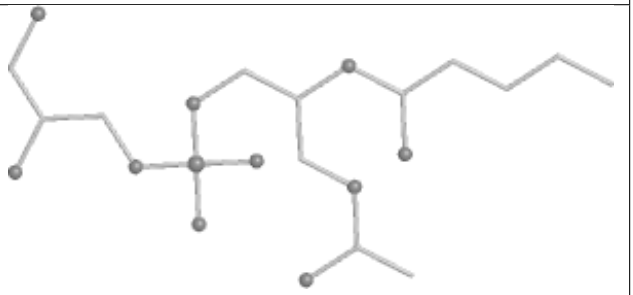
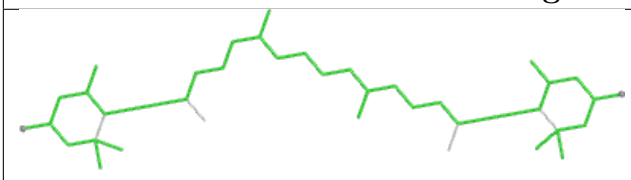


Rings

Ligand II0 1 314



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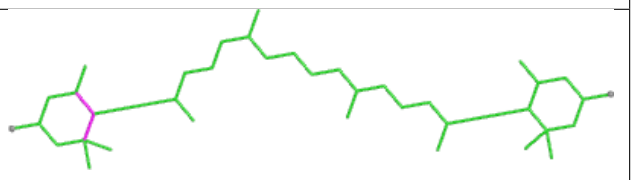

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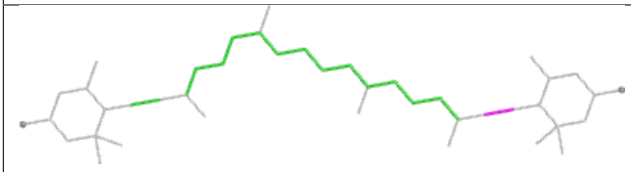

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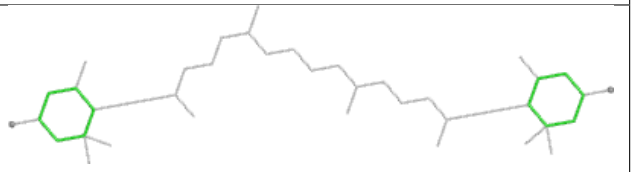
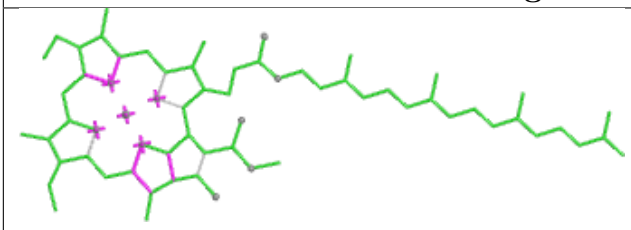


Rings

Ligand CLA C 507



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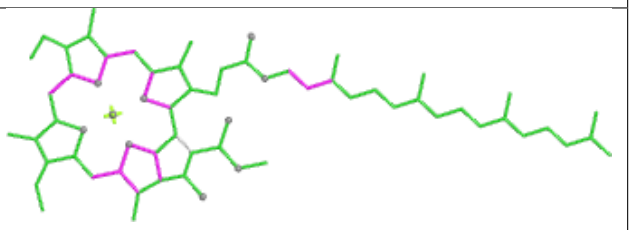
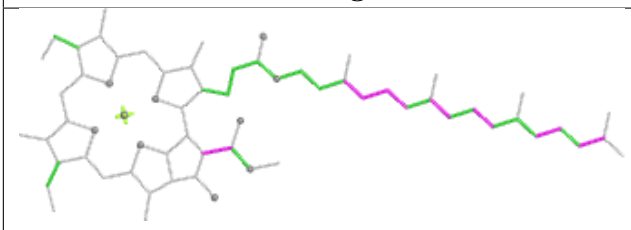


Bond angles



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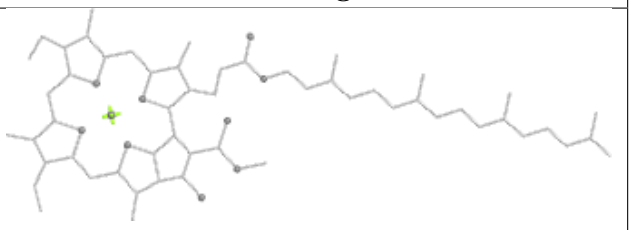
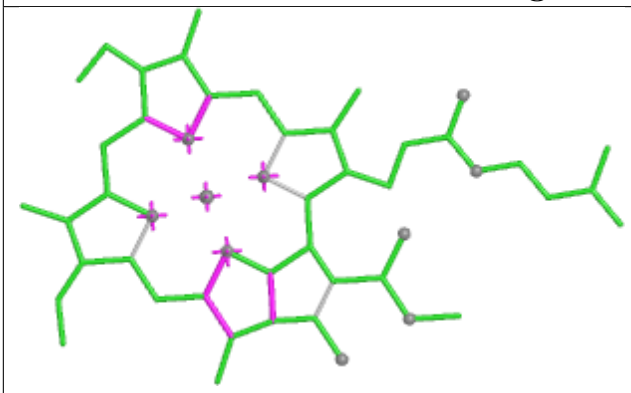


Rings

Ligand CLA 4 303



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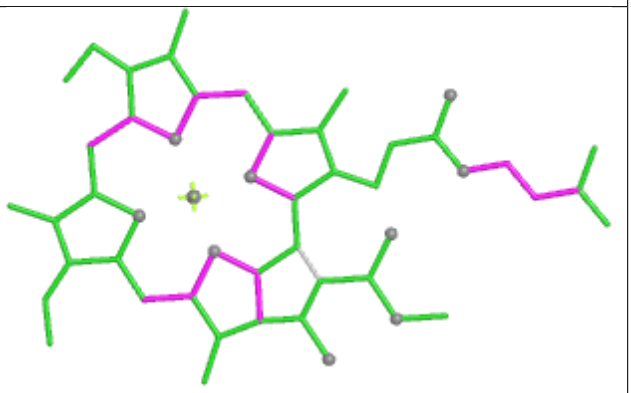

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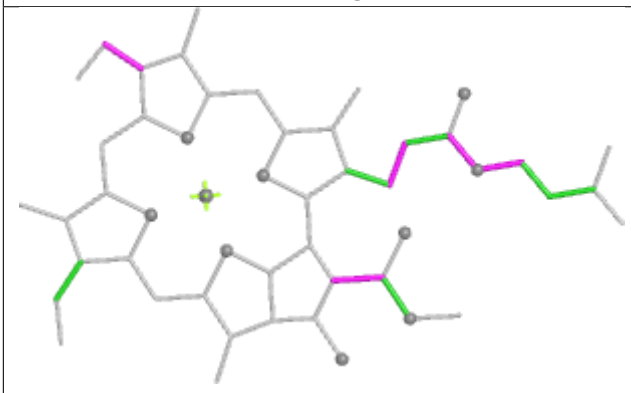
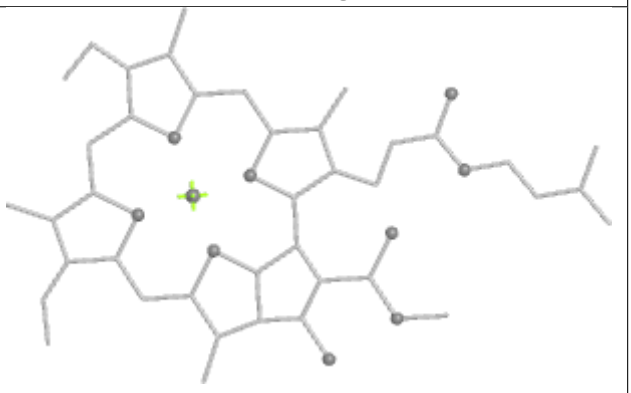
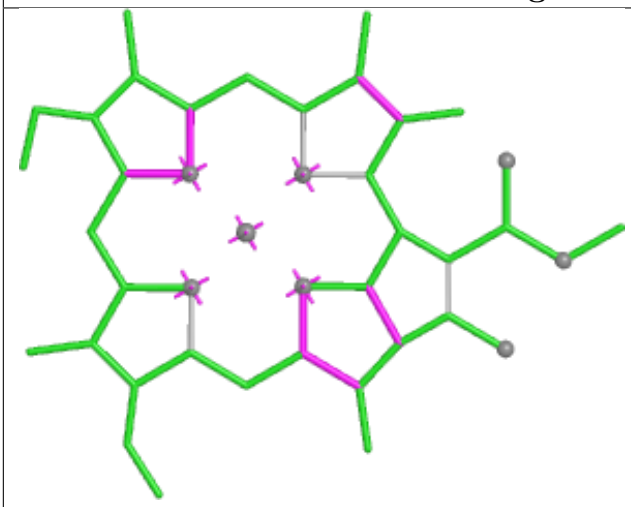


Torsions



Rings

Ligand CLA 3 310



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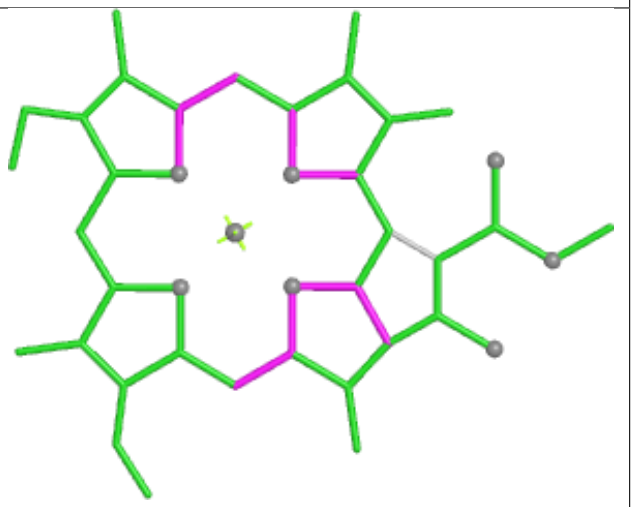

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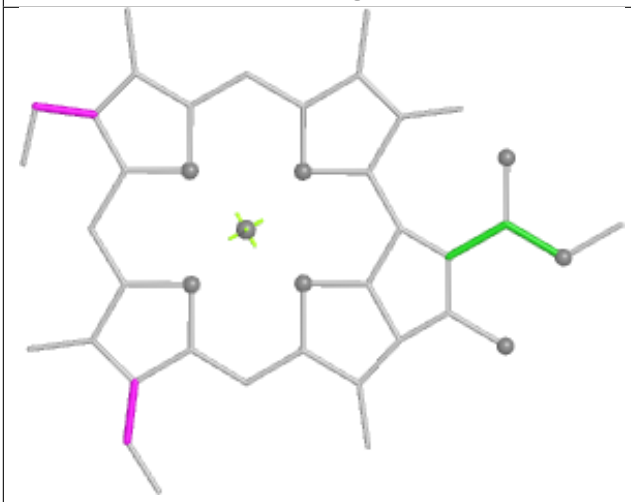

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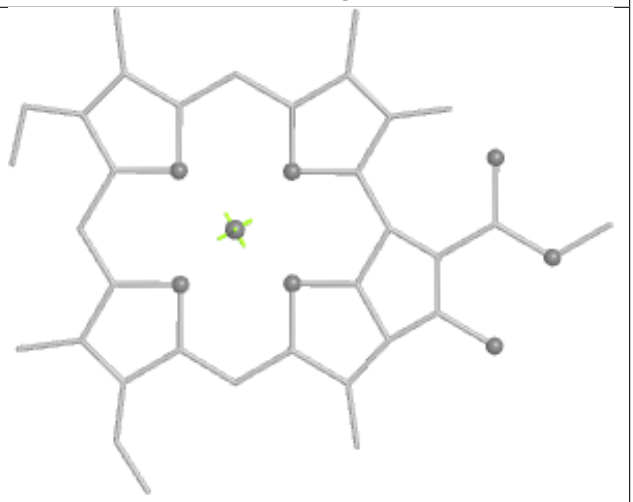
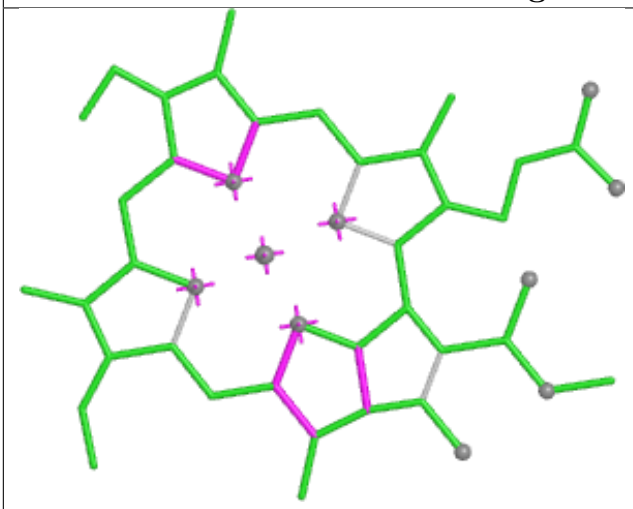


Rings

Ligand CLA 5 306



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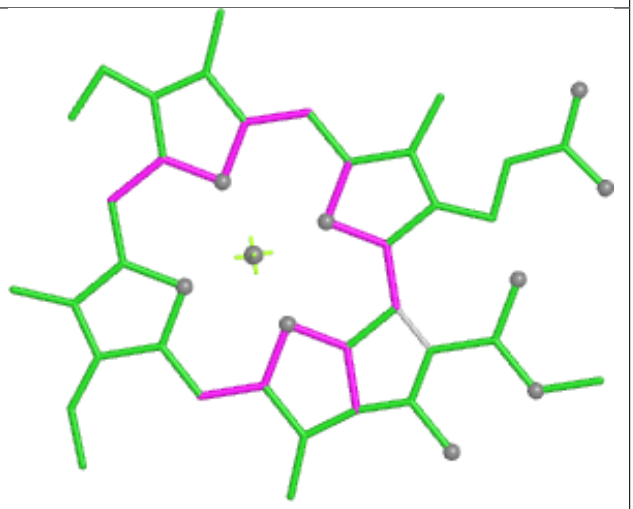

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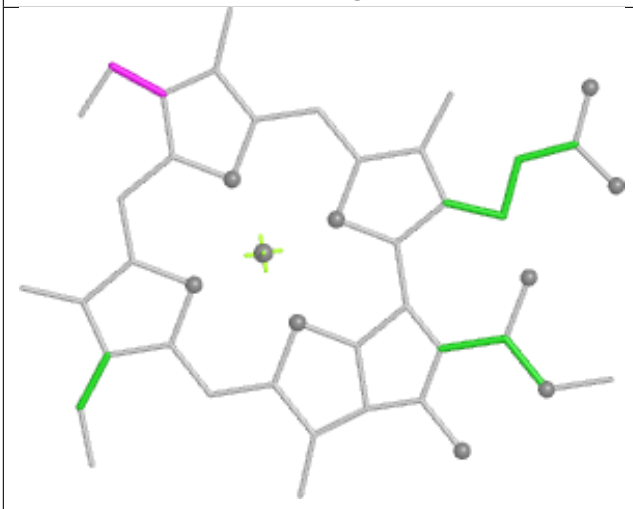
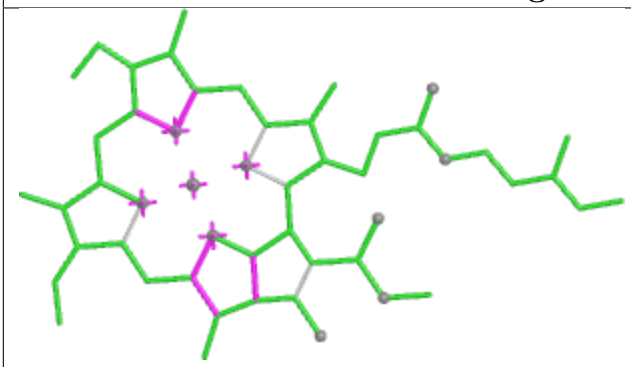


Torsions

Rings

Ligand CLA 0 302



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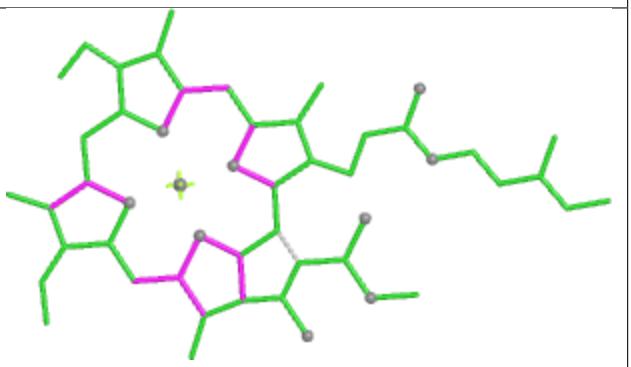

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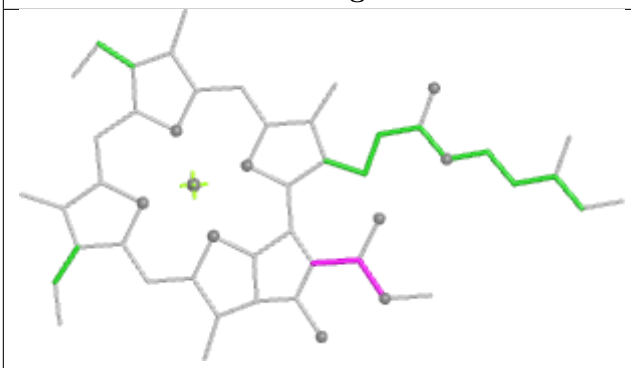

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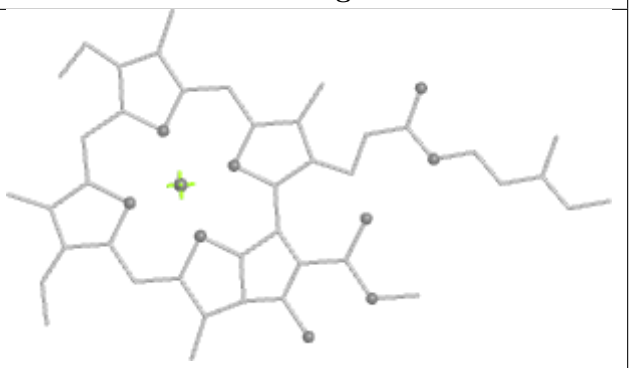
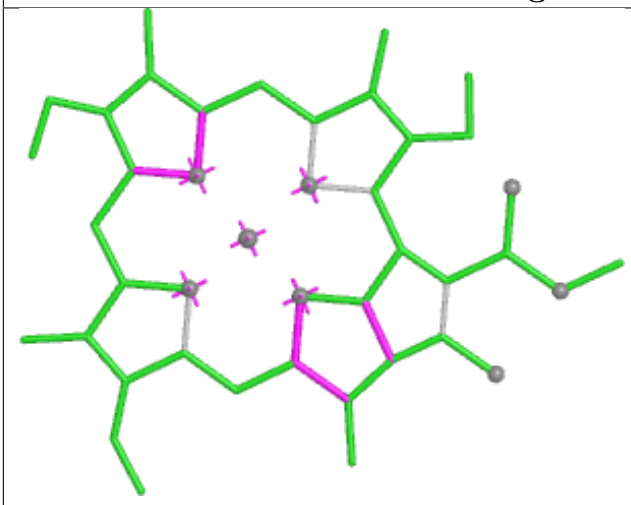


Rings

Ligand CLA g 301



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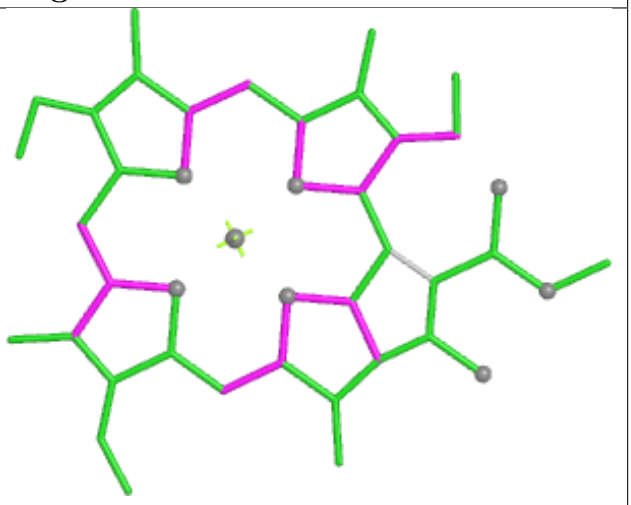

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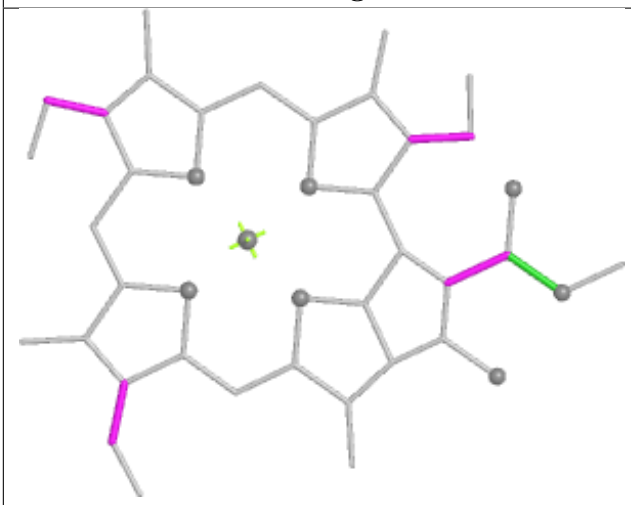
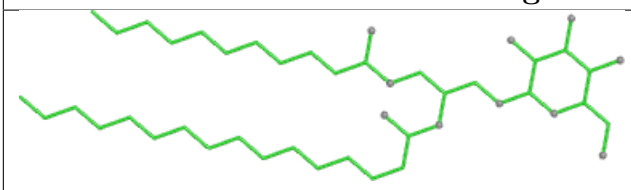


Torsions

Rings

Ligand LMG d 409



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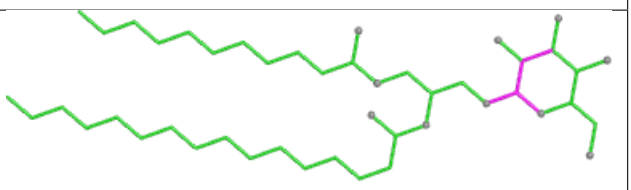

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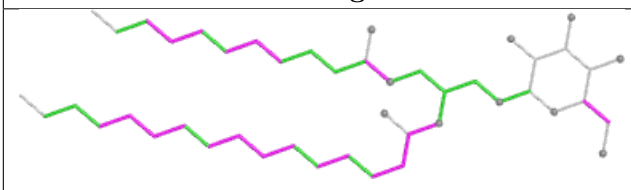

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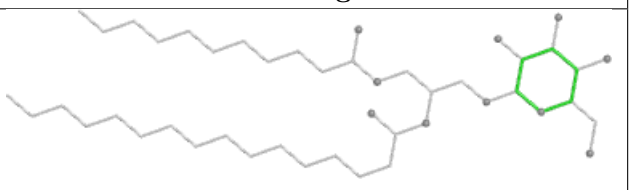
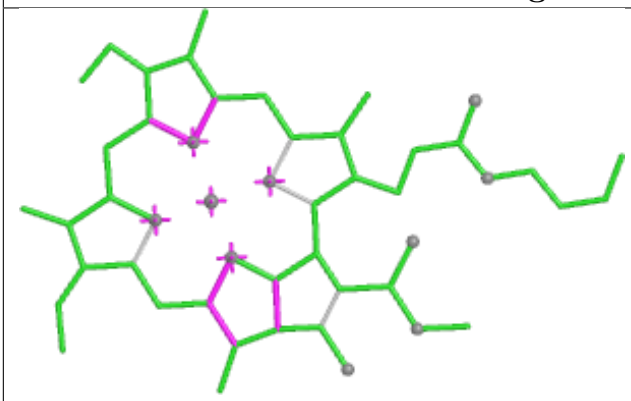


Rings

Ligand CLA 3 308



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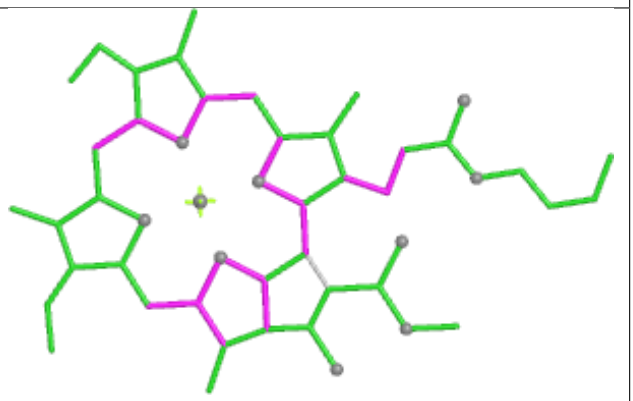

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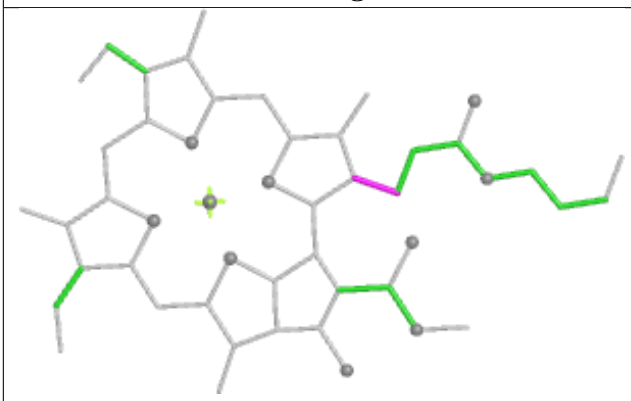

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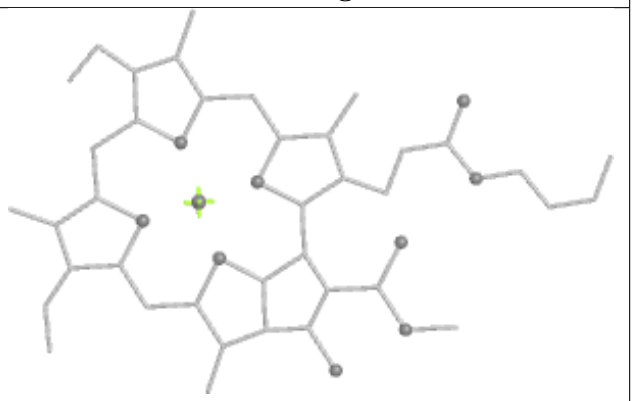
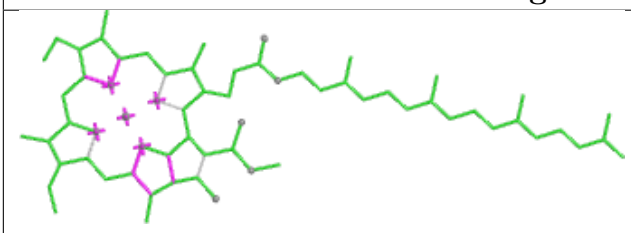


Rings

Ligand CLA c 506



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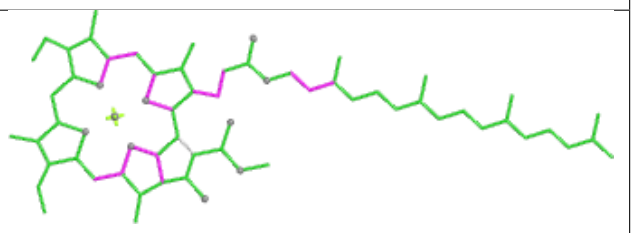

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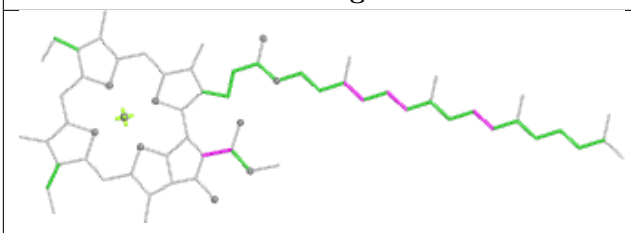

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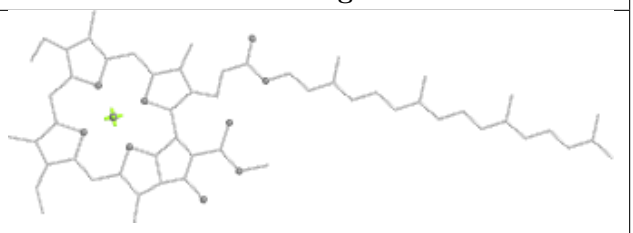
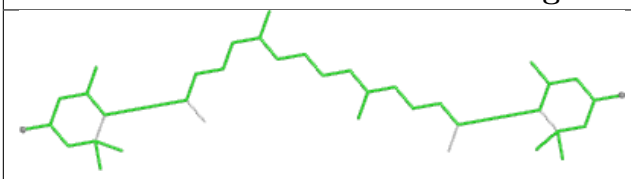


Rings

Ligand II0 4 312



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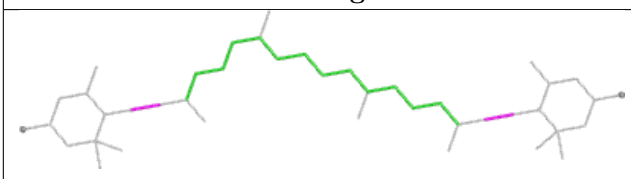

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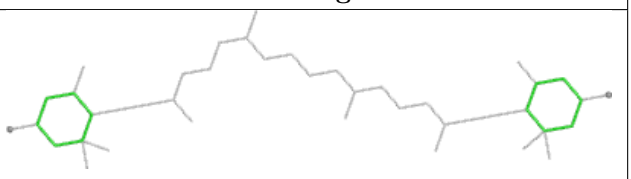
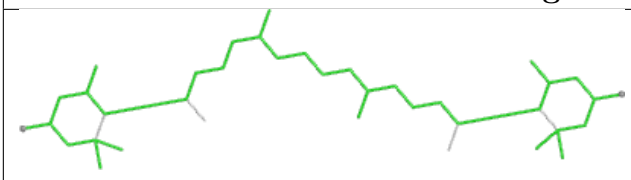


Rings

Ligand II0 3 316



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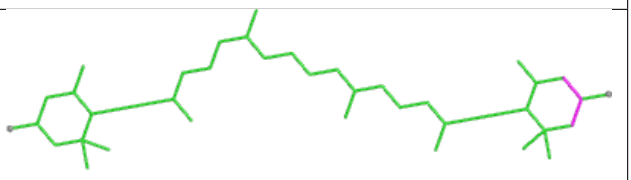

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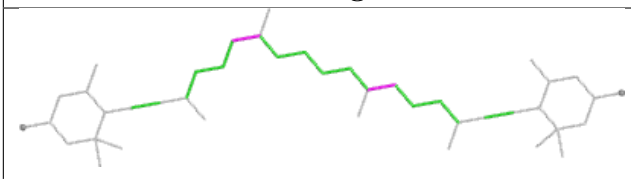

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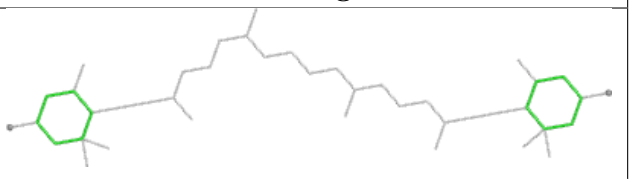
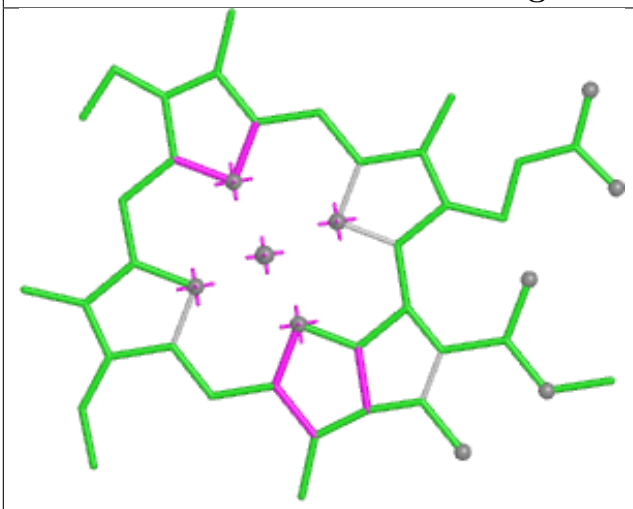


Rings

Ligand CLA 4 310



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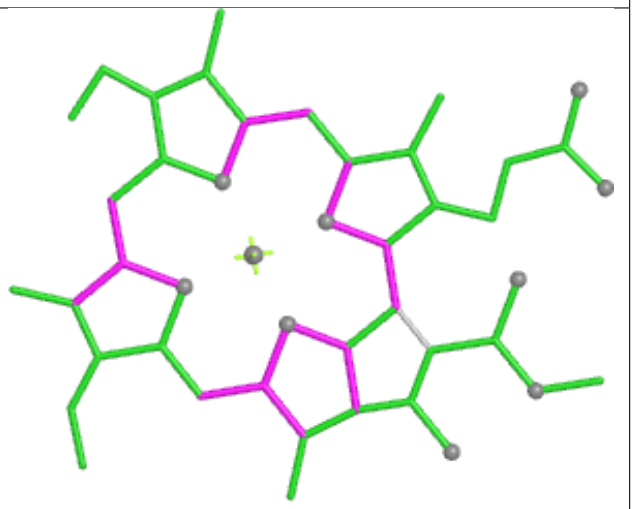

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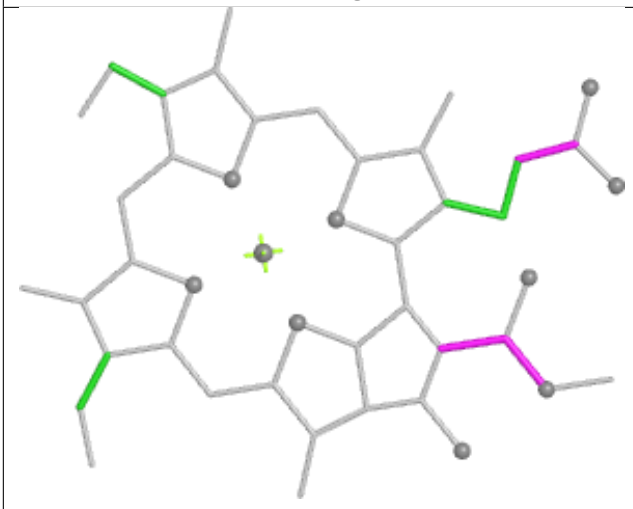
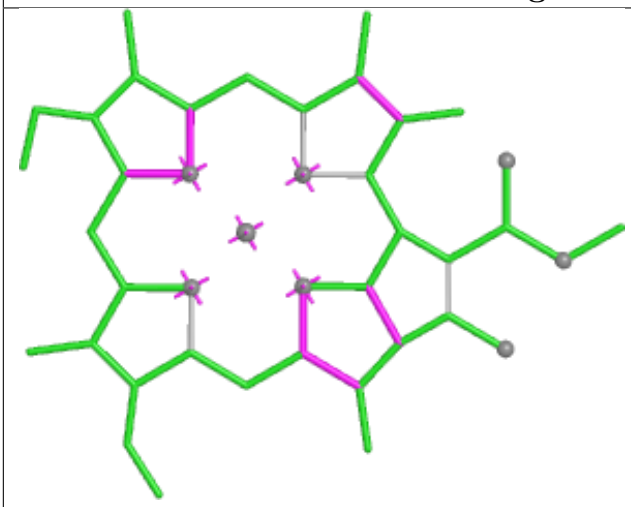


Torsions

Rings

Ligand CLA 6 303



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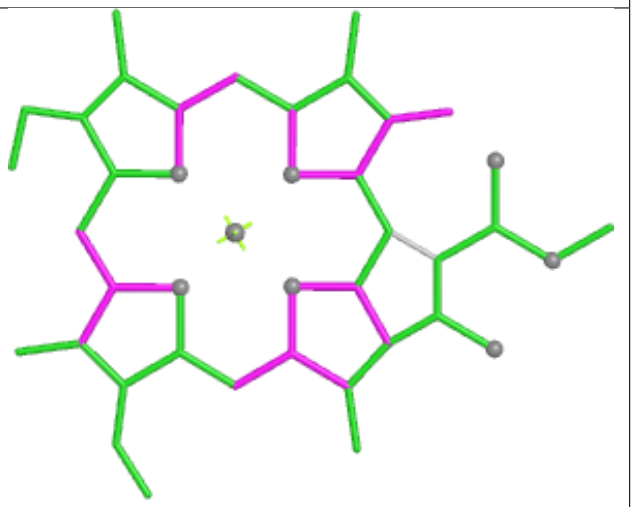

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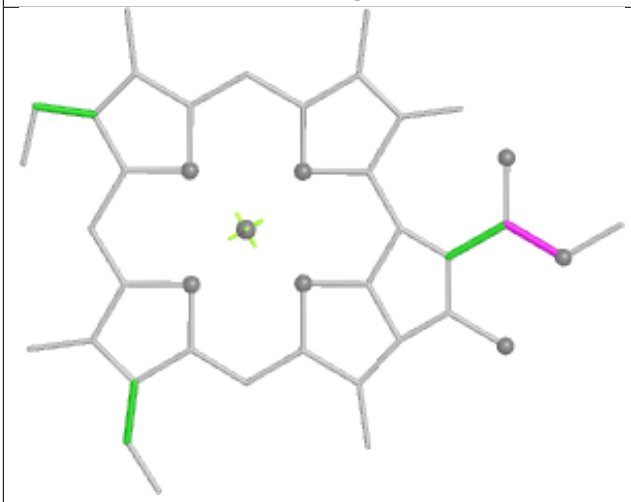

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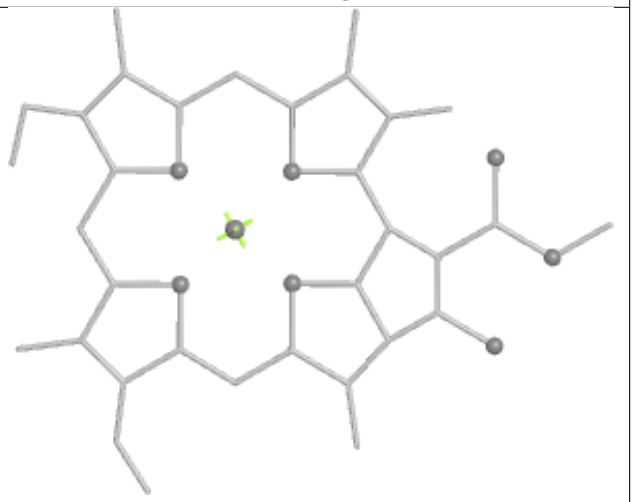
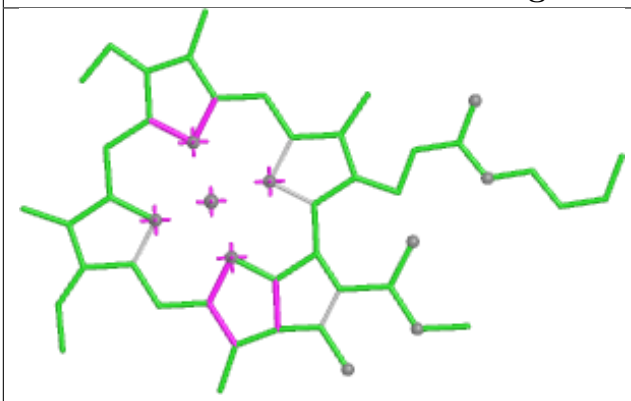


Rings

Ligand CLA a 406



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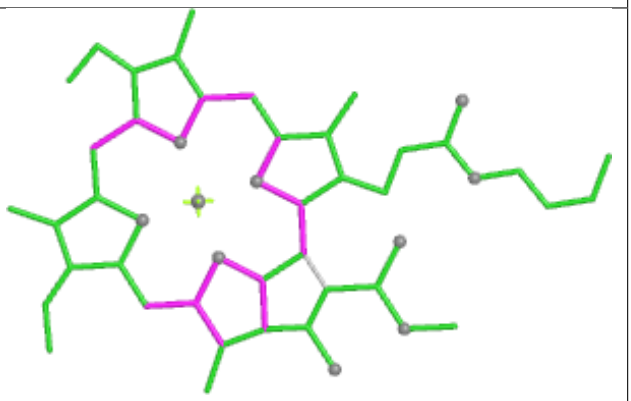

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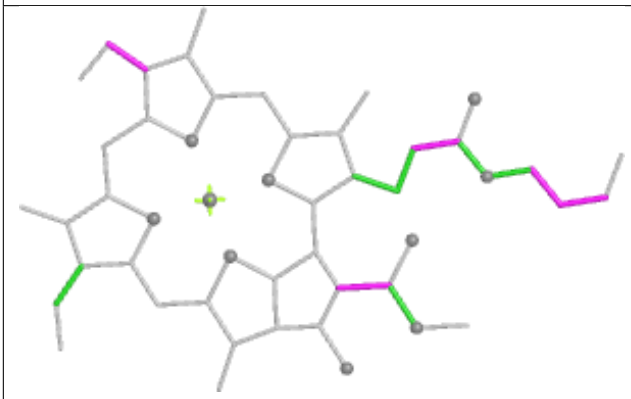

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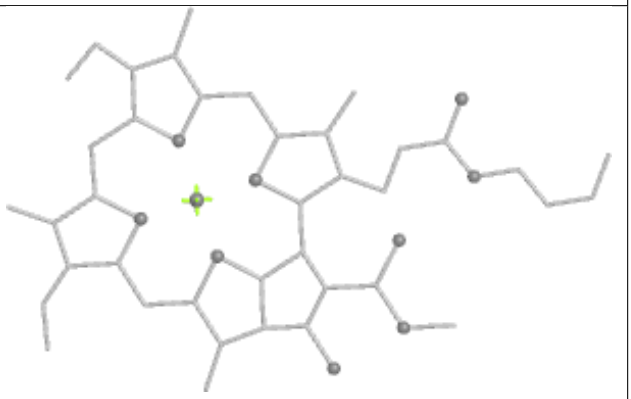
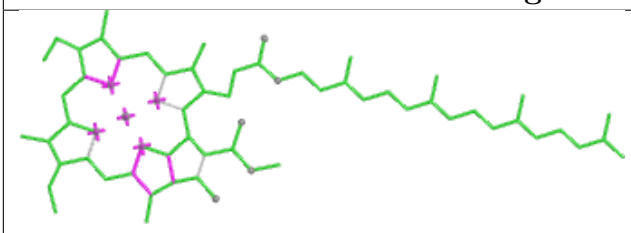


Rings

Ligand CLA B 614



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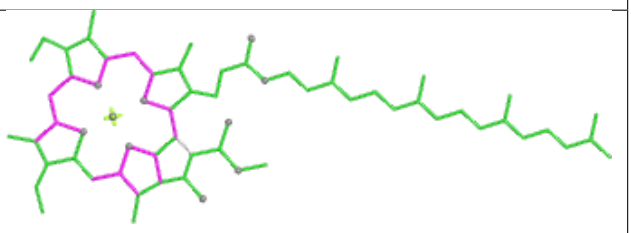
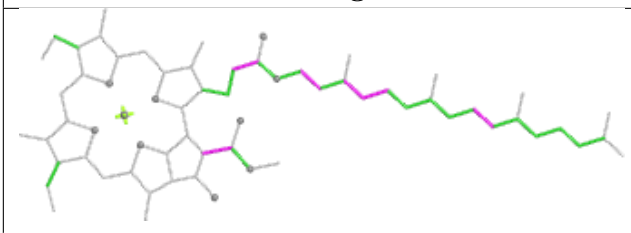


Bond angles



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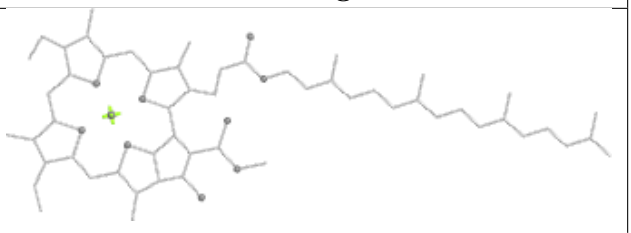
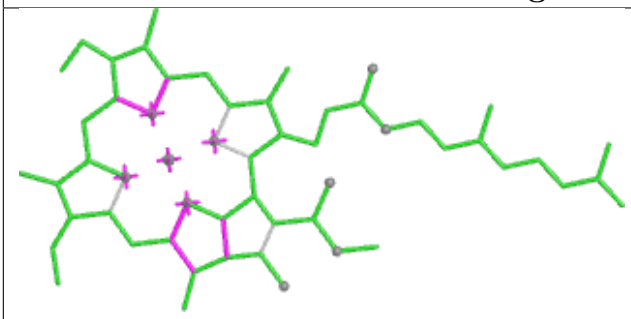


Rings

Ligand CLA 9 303



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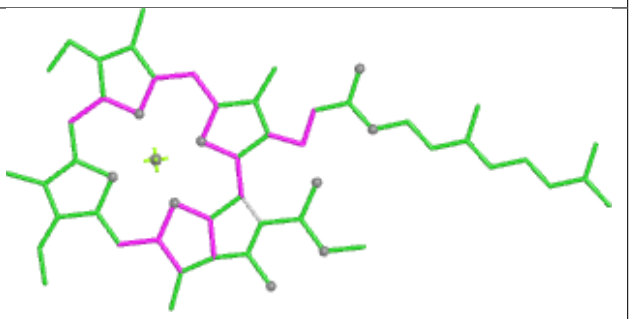

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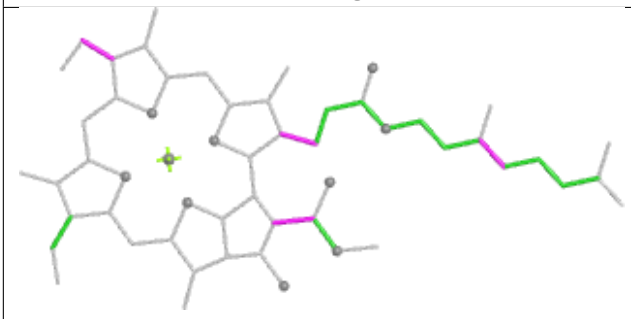

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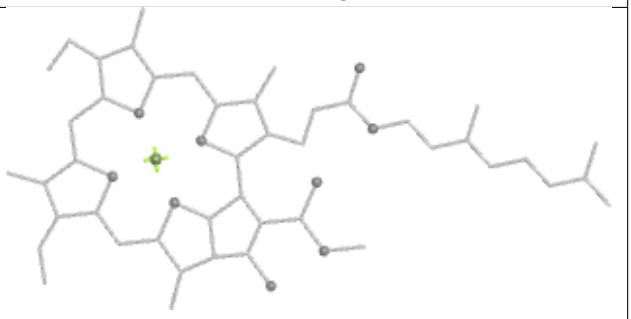
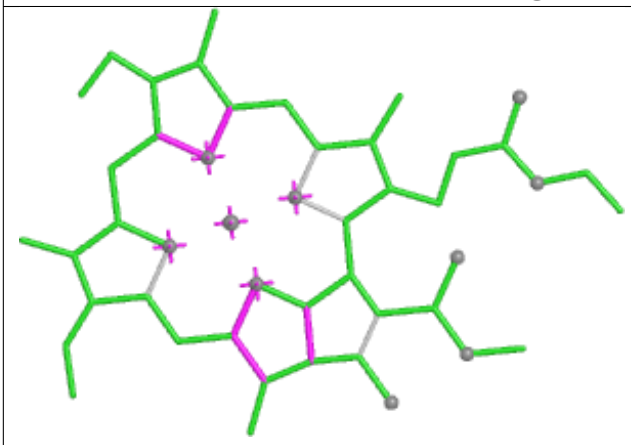
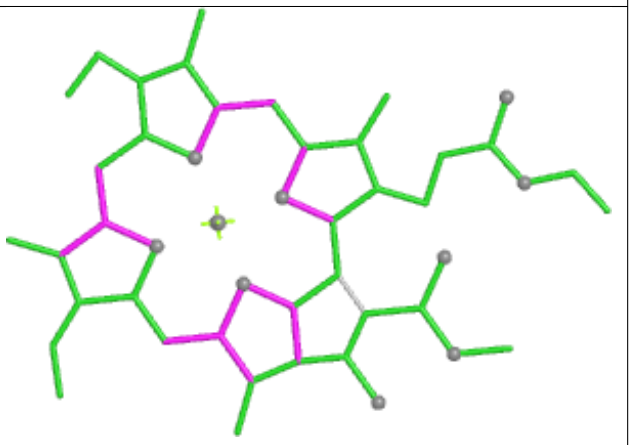


Rings

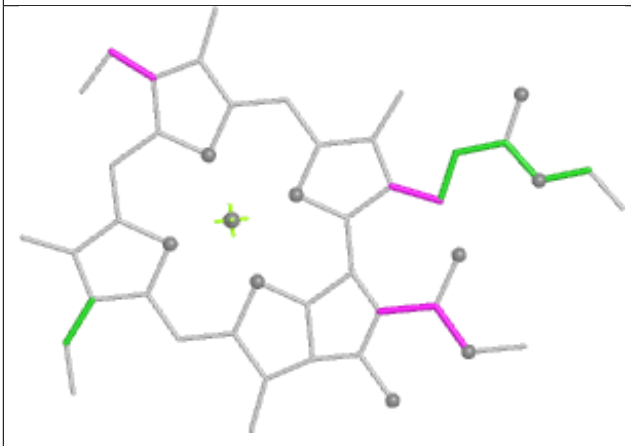
Ligand CLA 0 304



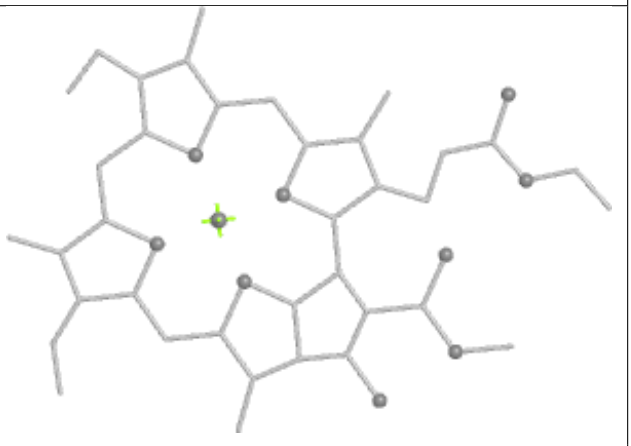
Bond lengths



Bond angles

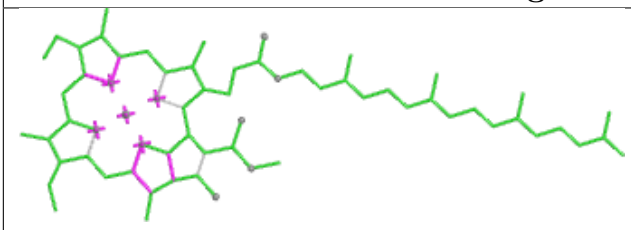


Torsions



Rings

Ligand CLA b 605



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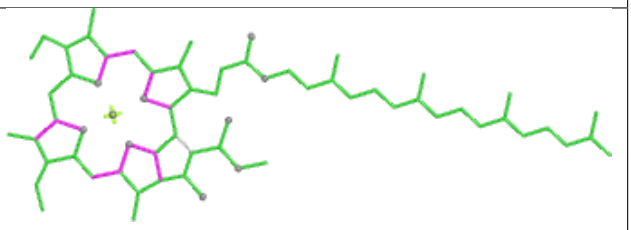
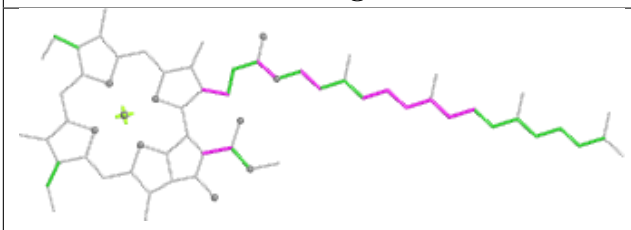


Bond angles



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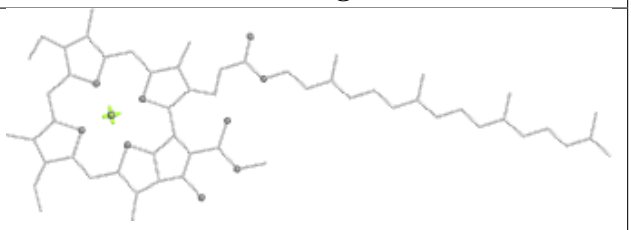
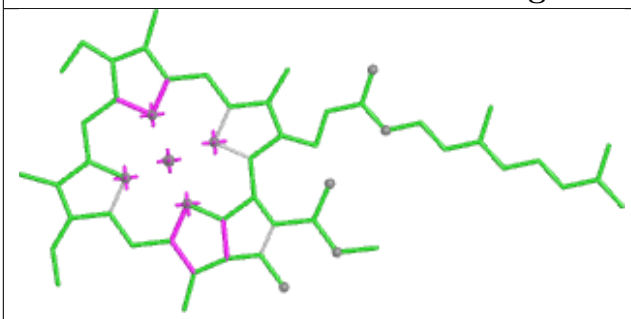


Rings

Ligand CLA 5 302



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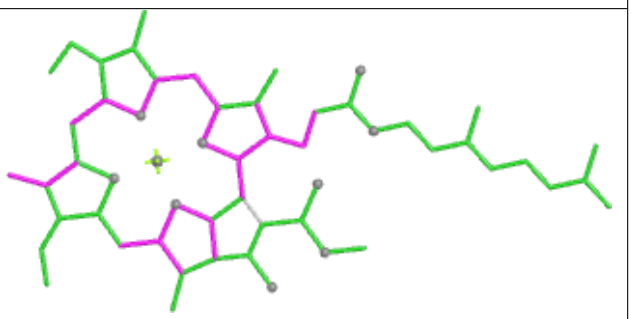

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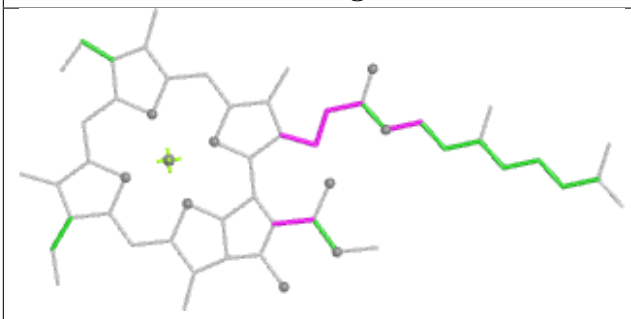

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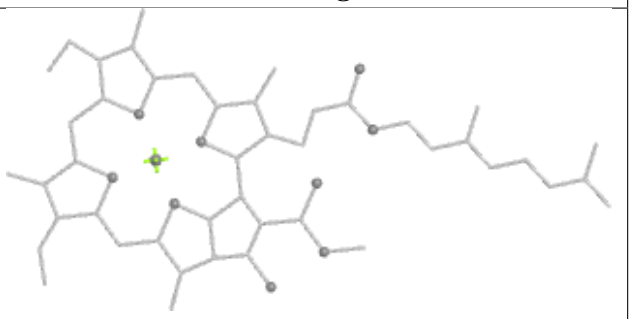
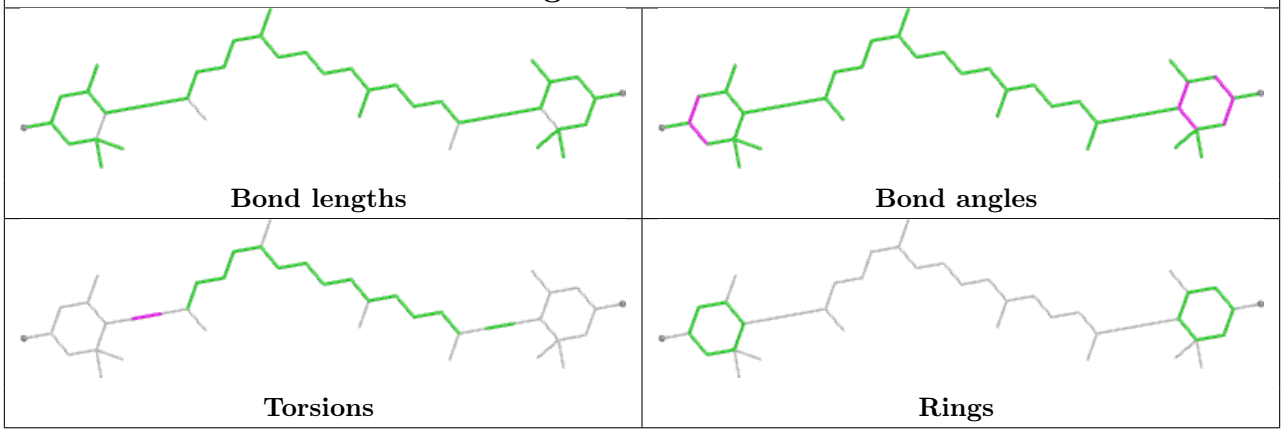
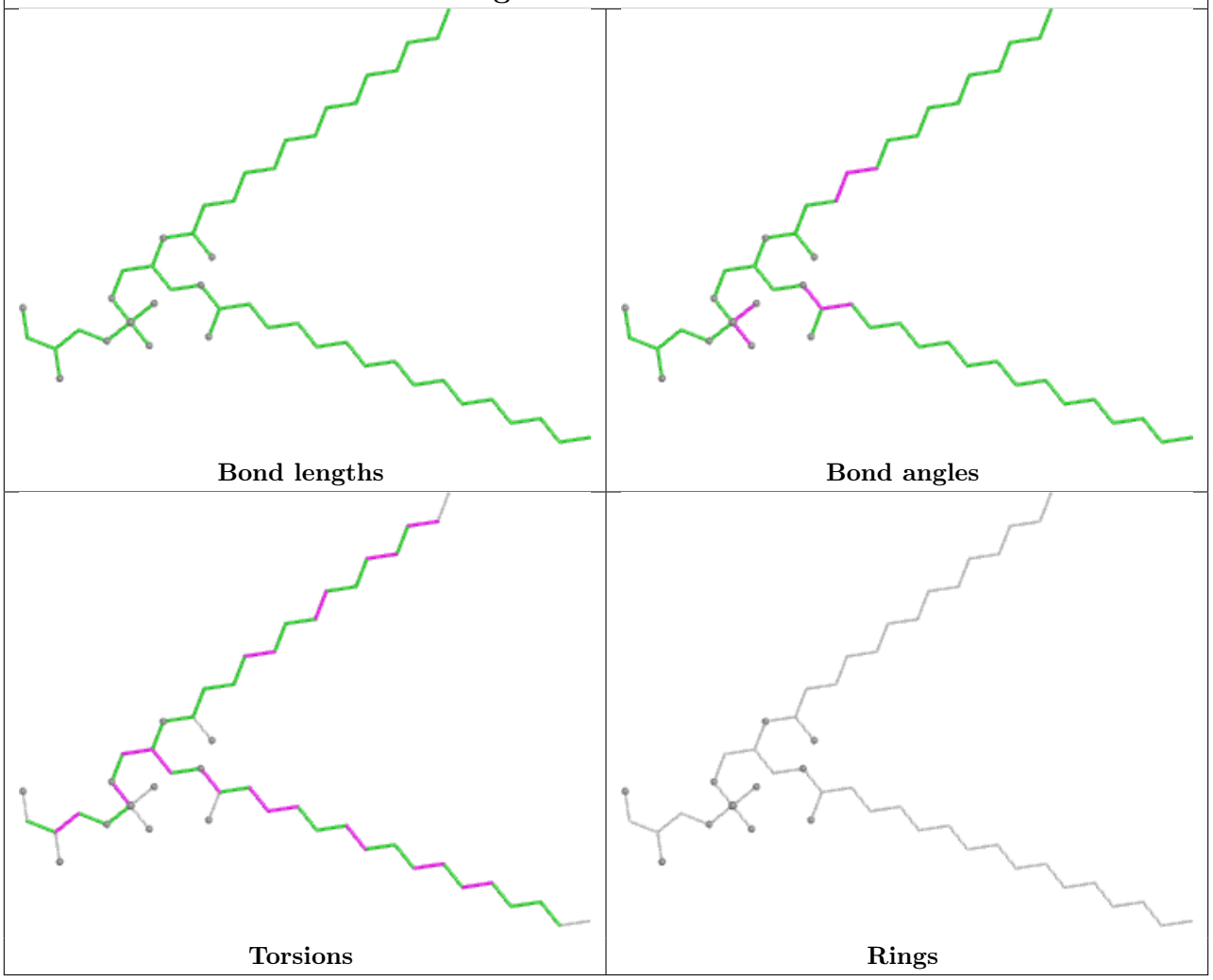


Rings

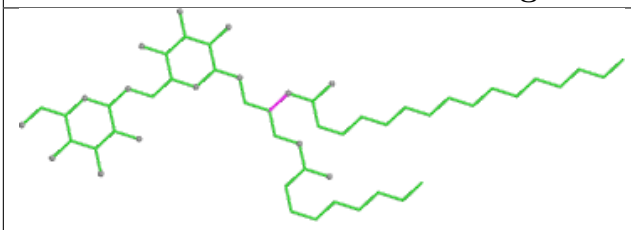
Ligand II0 8 312



Ligand LHG D 402



Ligand DGD C 518



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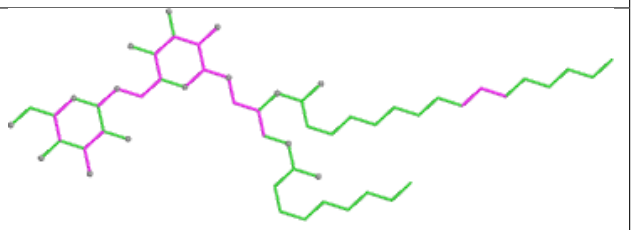
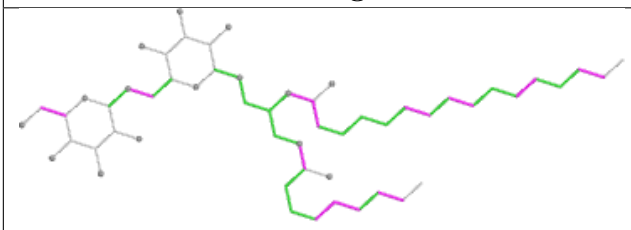


Bond angles



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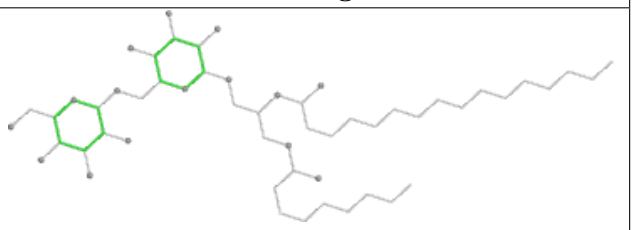
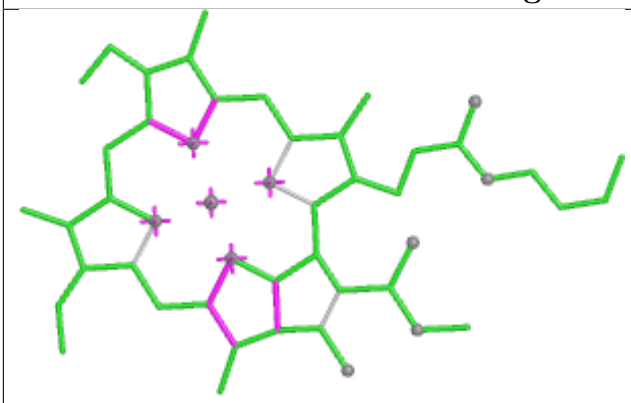


Rings

Ligand CLA A 406



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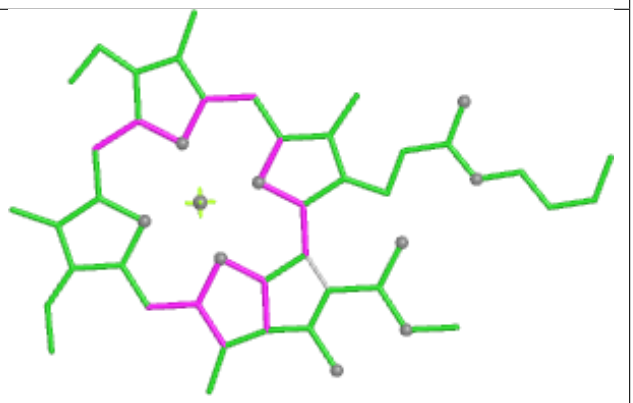
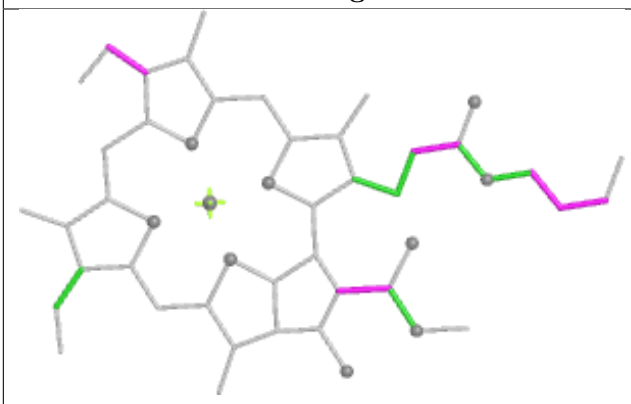


Bond angles



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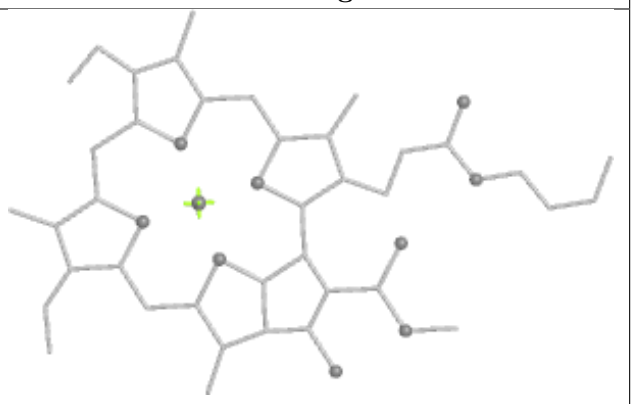
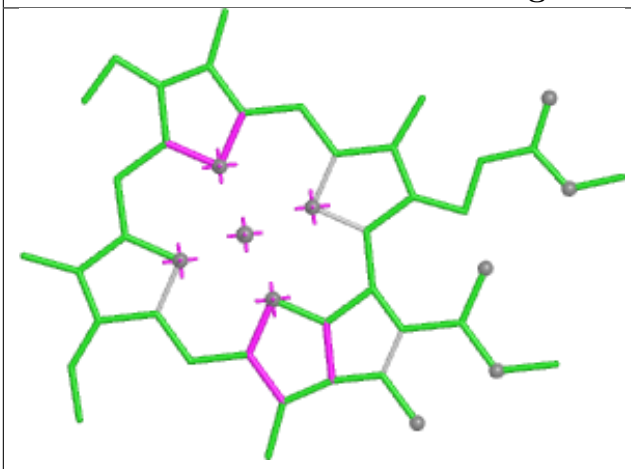


Rings

Ligand CLA 2 310



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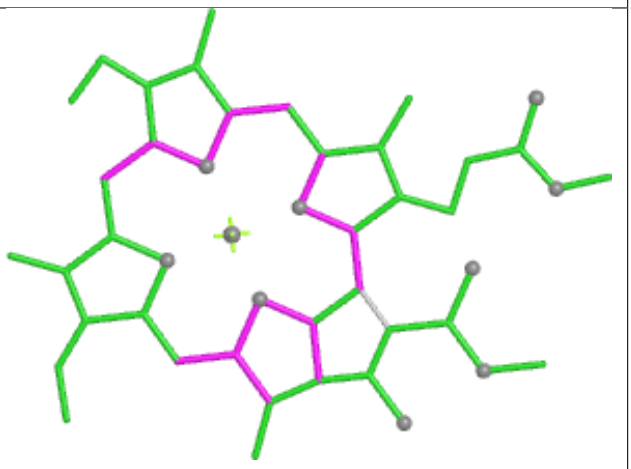
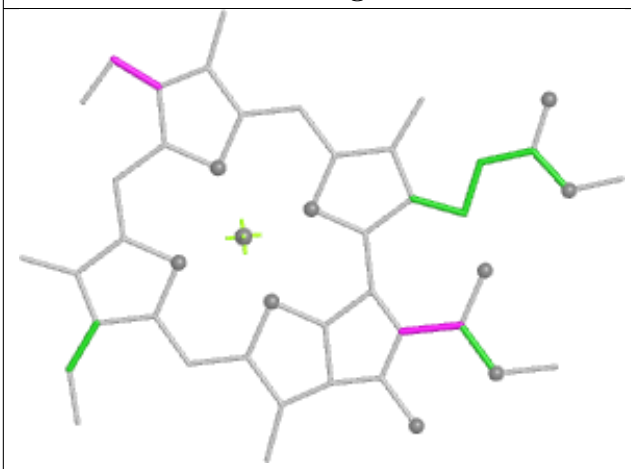


Bond angles



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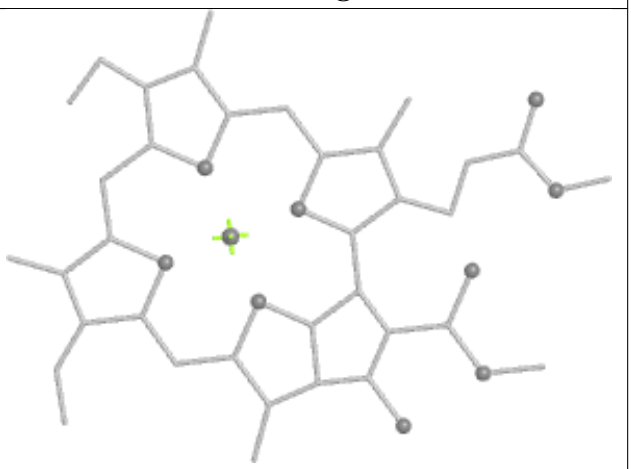
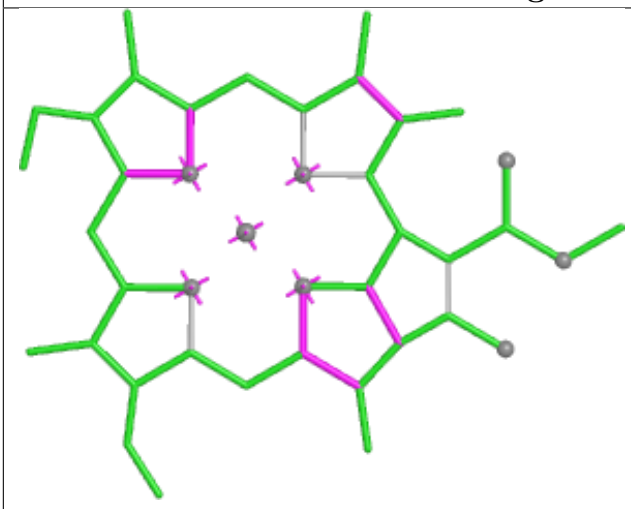


Rings

Ligand CLA n 303



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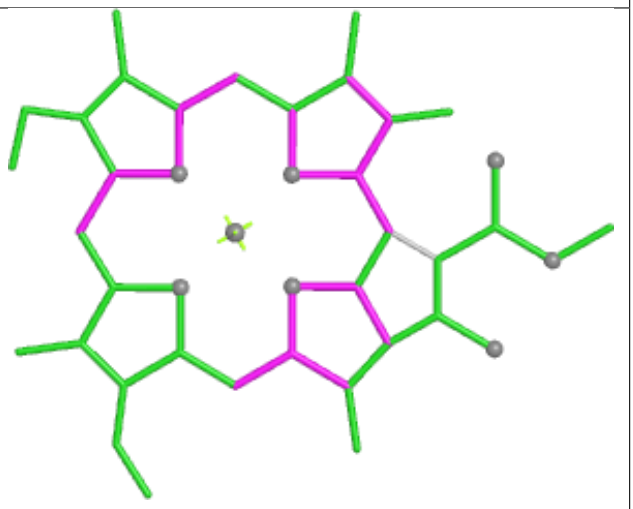
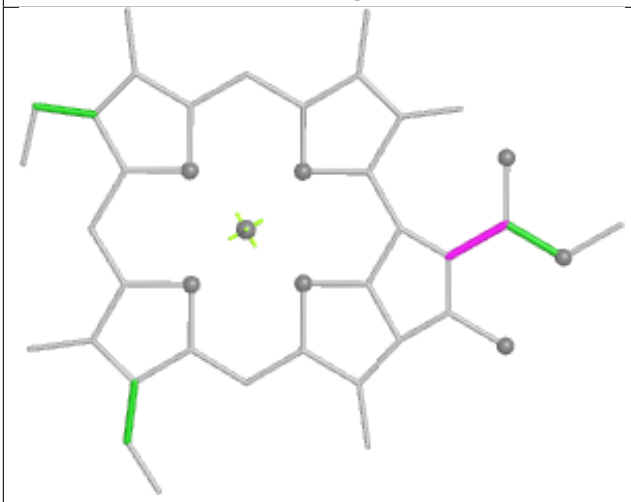


Bond angles



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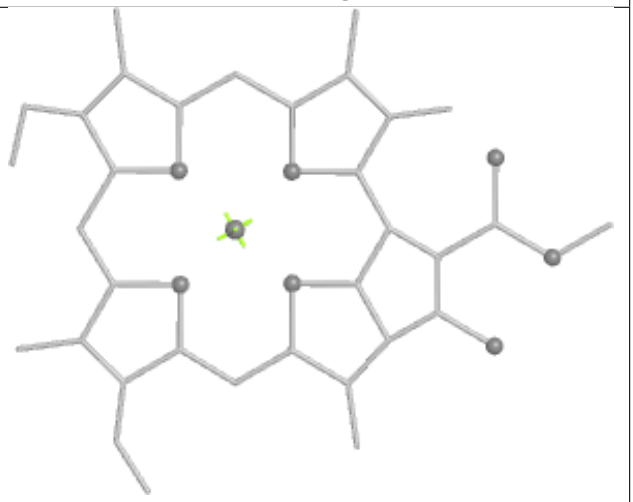
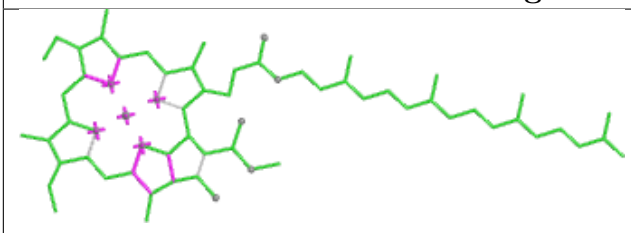


Rings

Ligand CLA C 504



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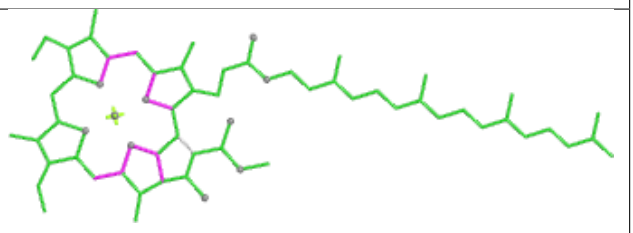
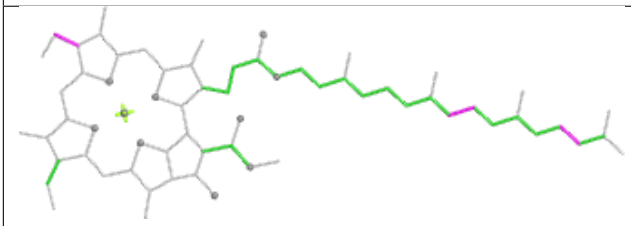


Bond angles



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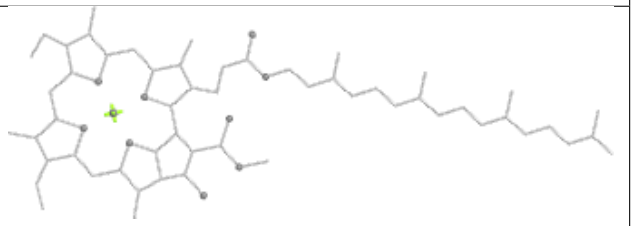
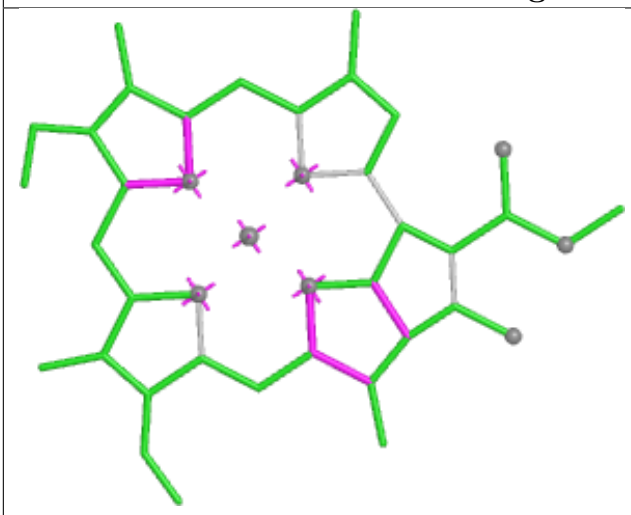


Rings

Ligand CLA 5 317



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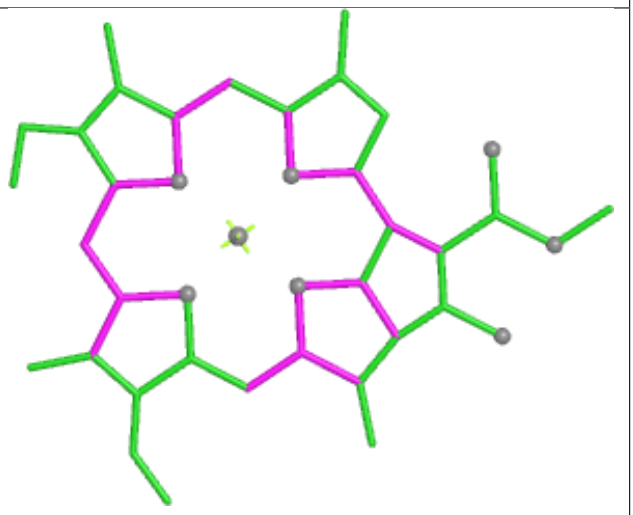

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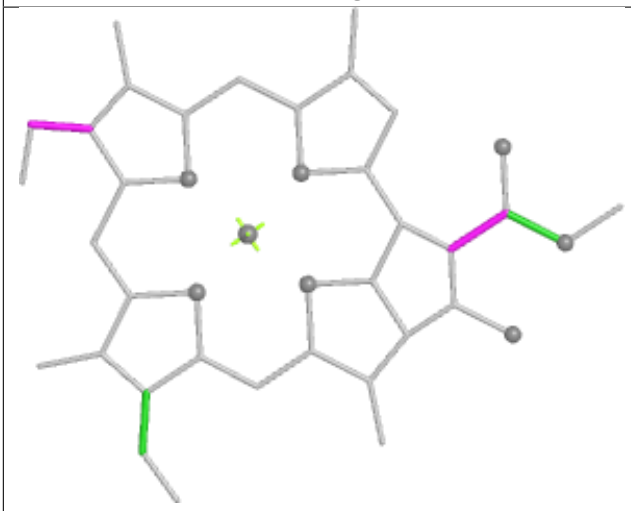

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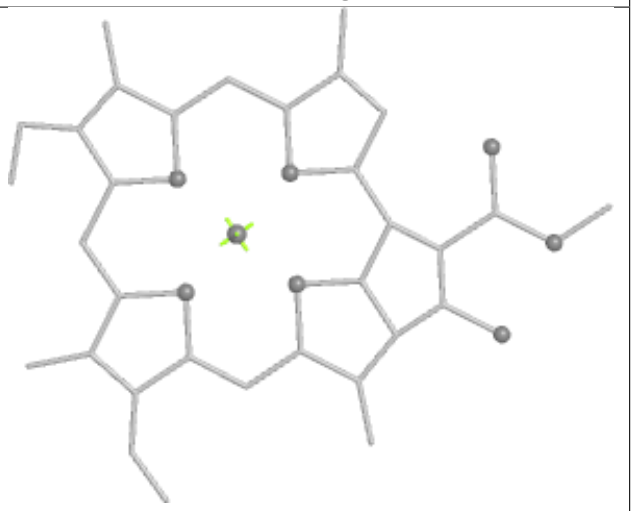
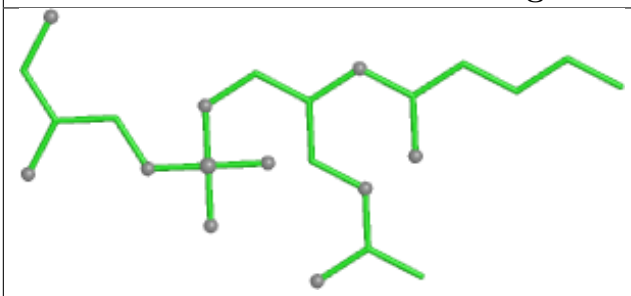


Rings

Ligand LHG 0 317



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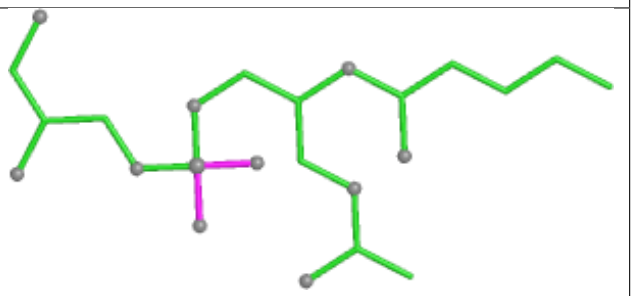

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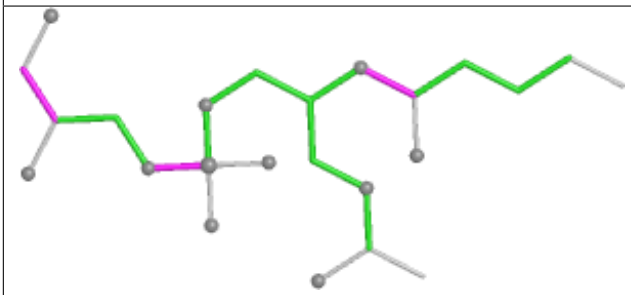

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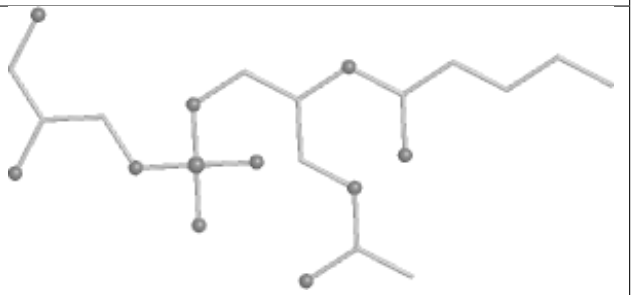
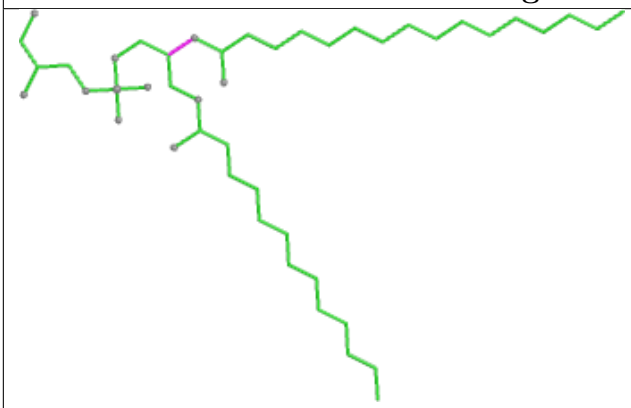


Rings

Ligand LHG D 401



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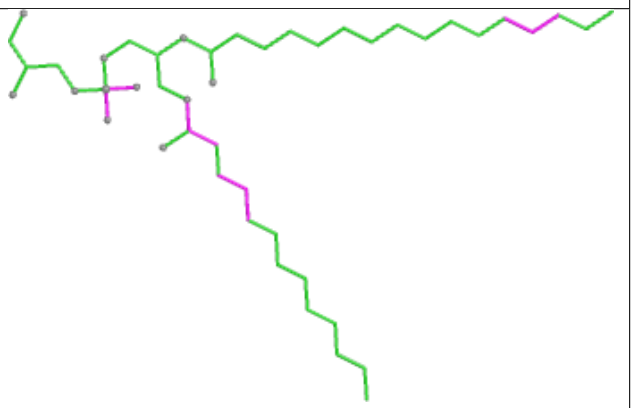
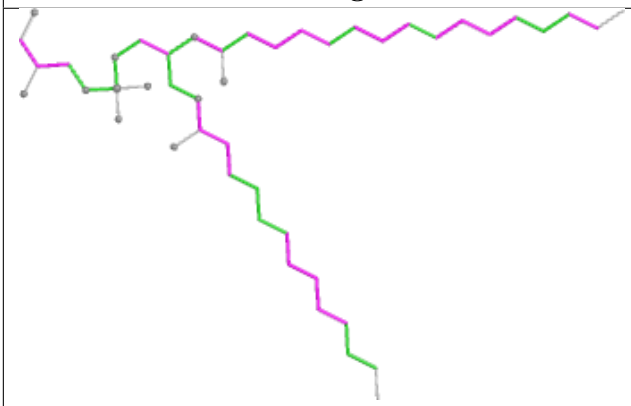


Bond angles



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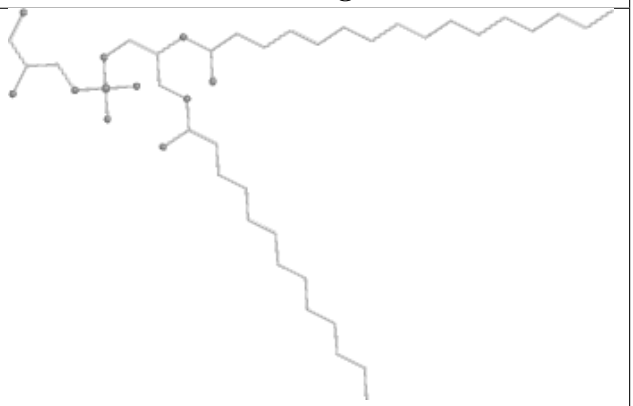
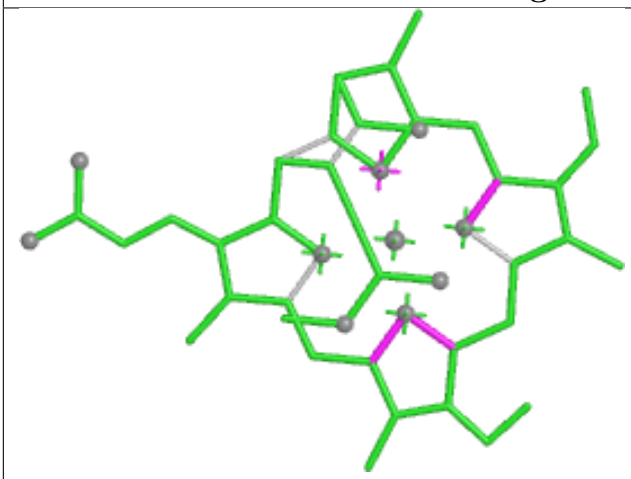


Rings

Ligand KC2 7 311



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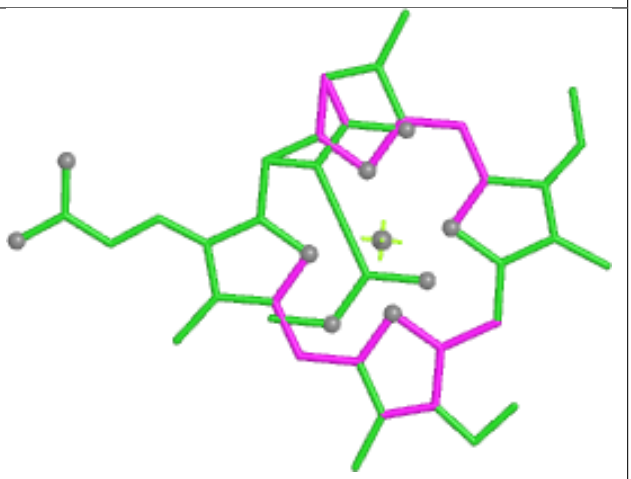
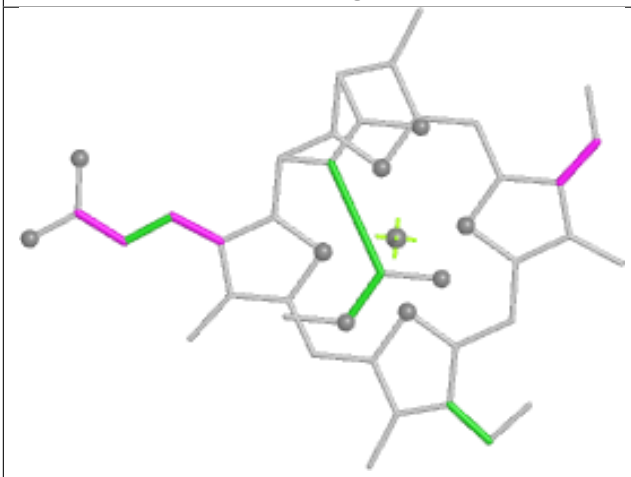


Bond angles



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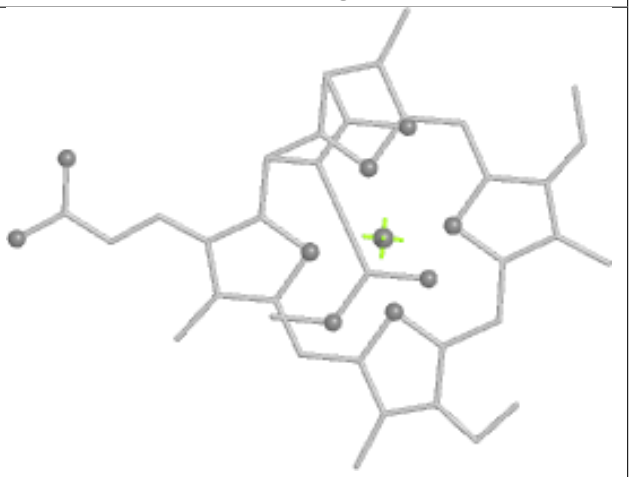
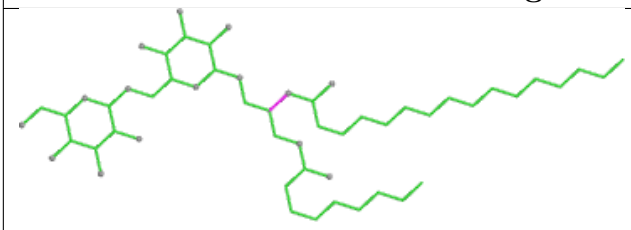


Rings

Ligand DGD c 518



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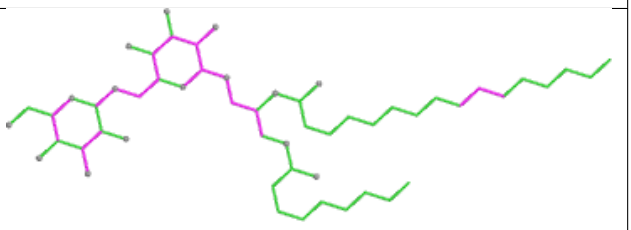
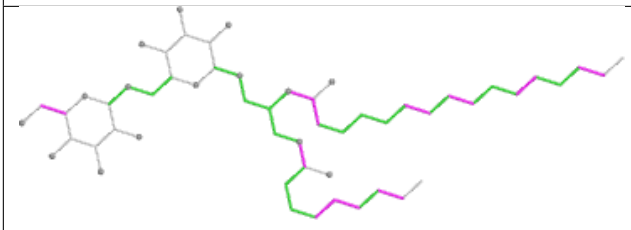
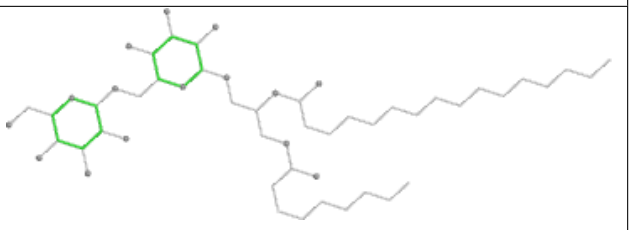


Bond angles

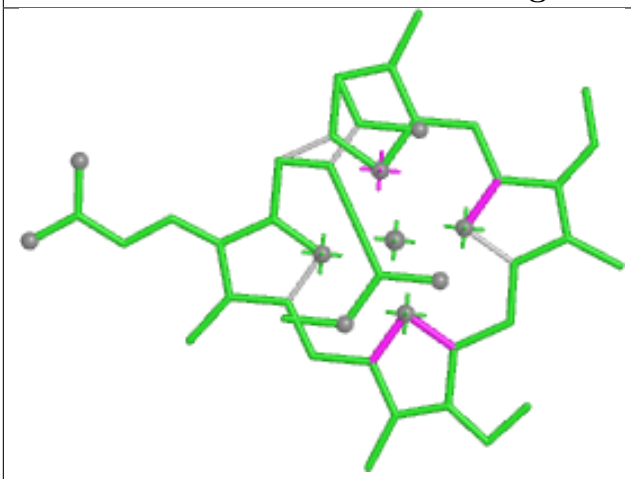


Torsions



Rings

Ligand KC2 p 311



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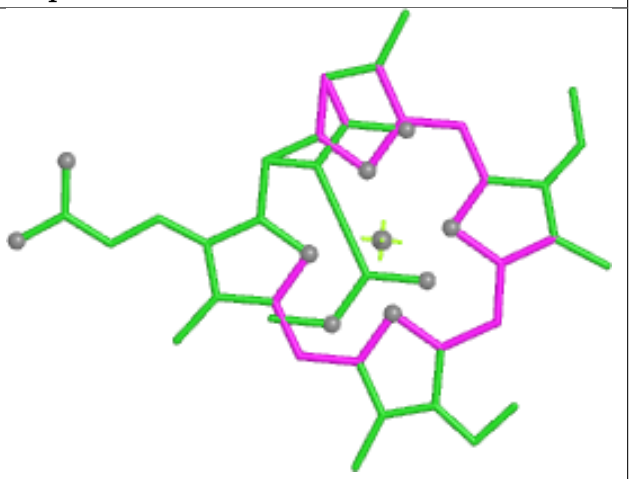
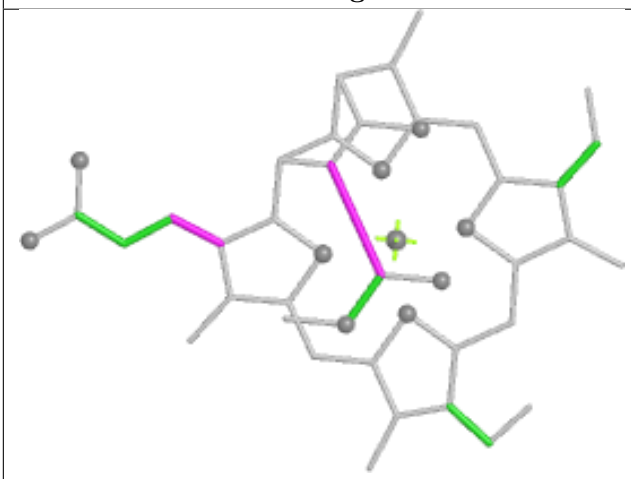
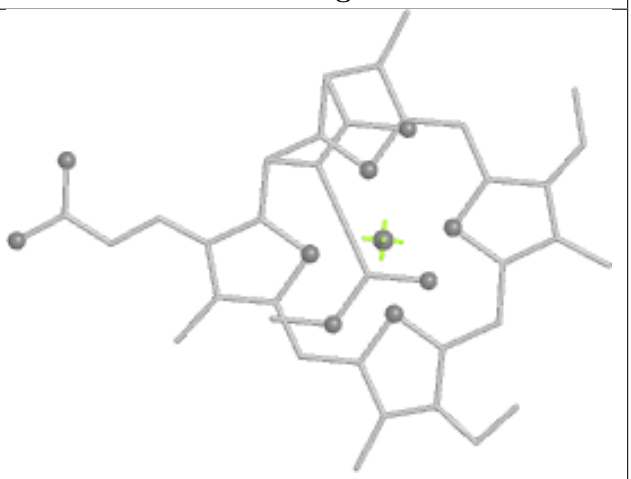


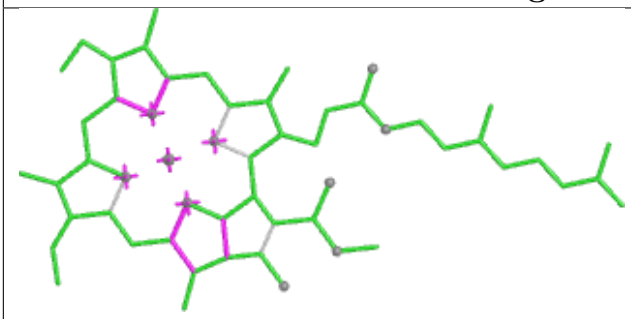
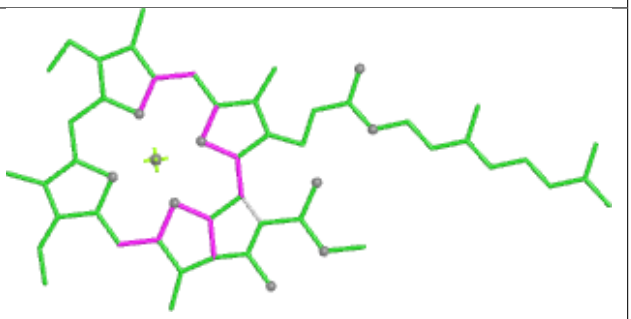
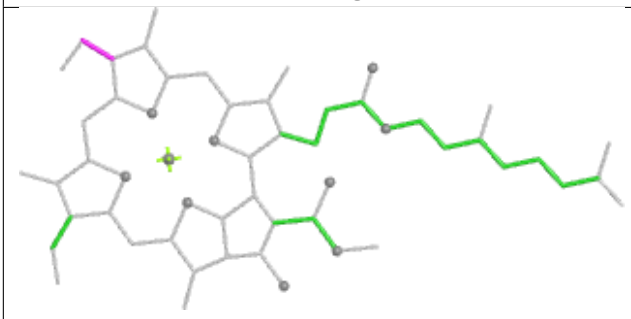
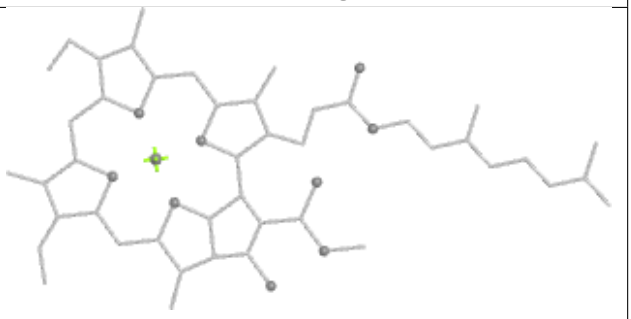
Bond angles

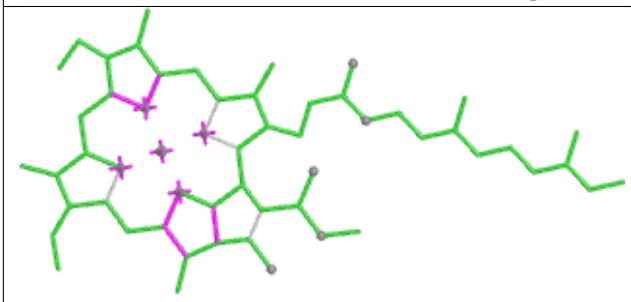
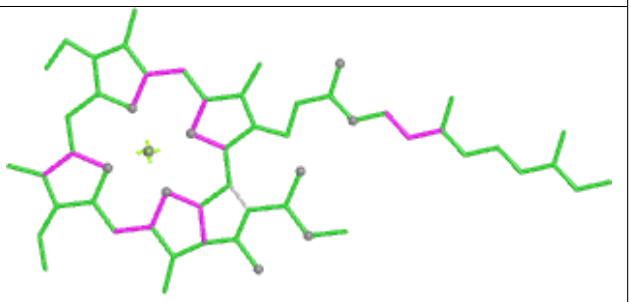
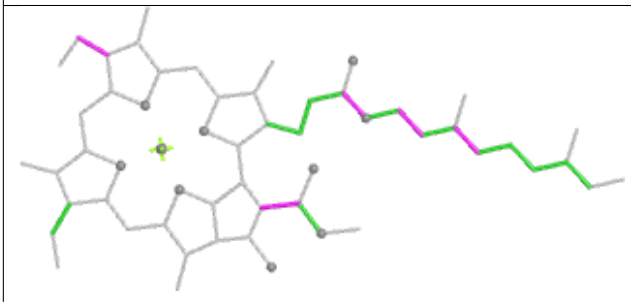
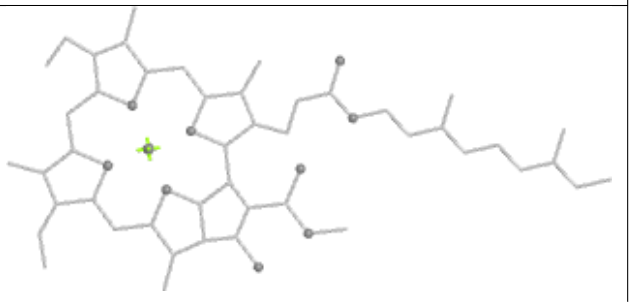


Torsions

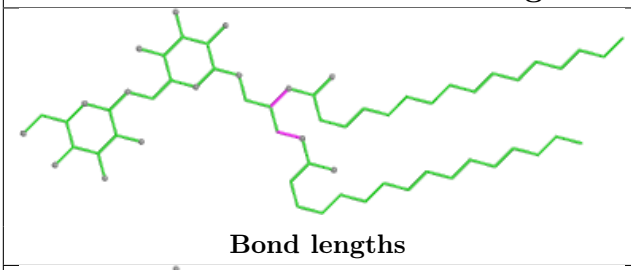


Rings

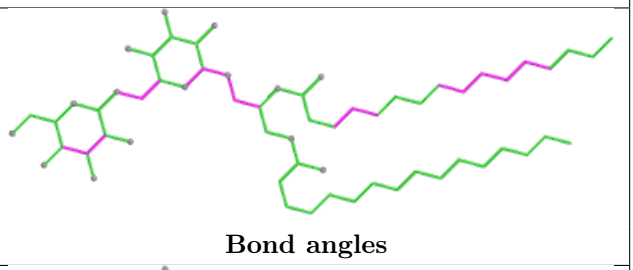
Ligand CLA 1 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

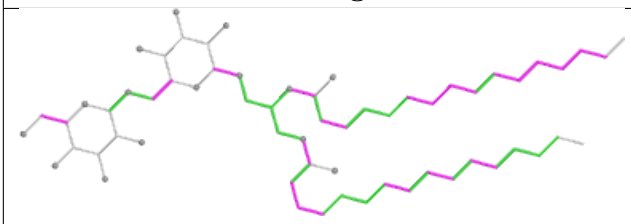
Ligand DGD c 521



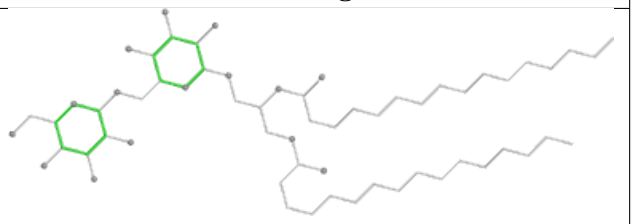
Bond lengths



Bond angles

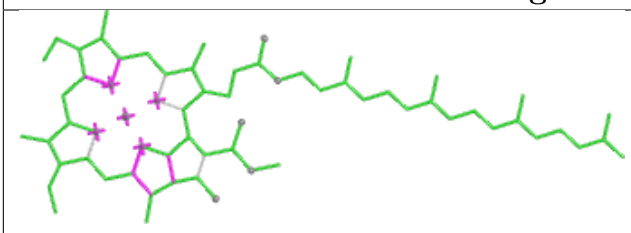


Torsions



Rings

Ligand CLA c 507



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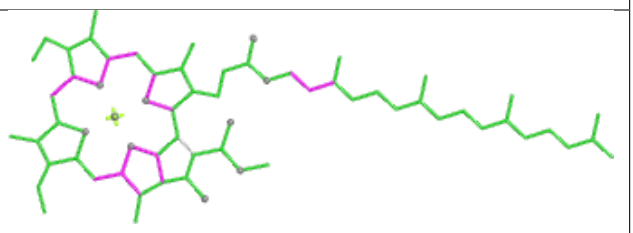
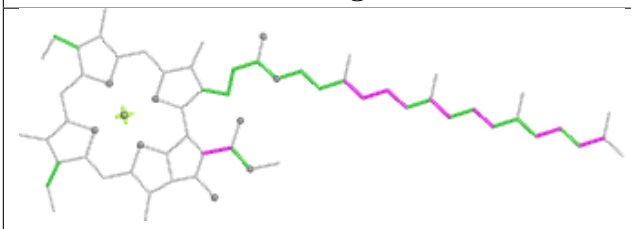


Bond angles



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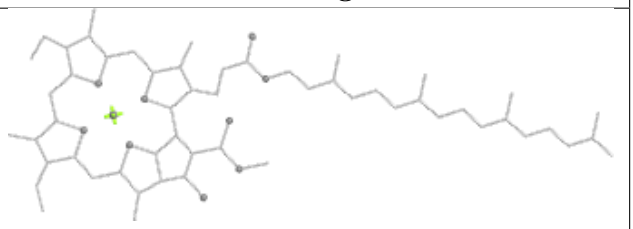
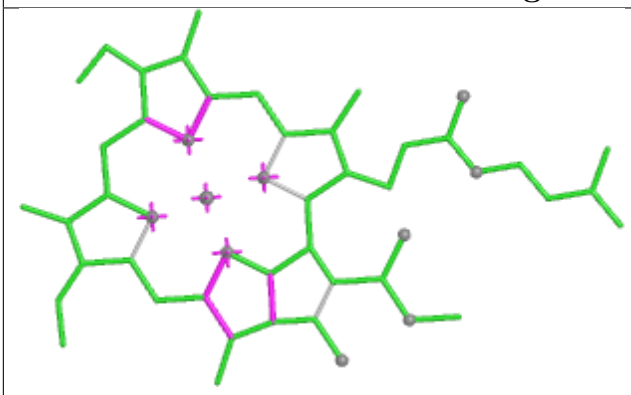


Rings

Ligand CLA N 307



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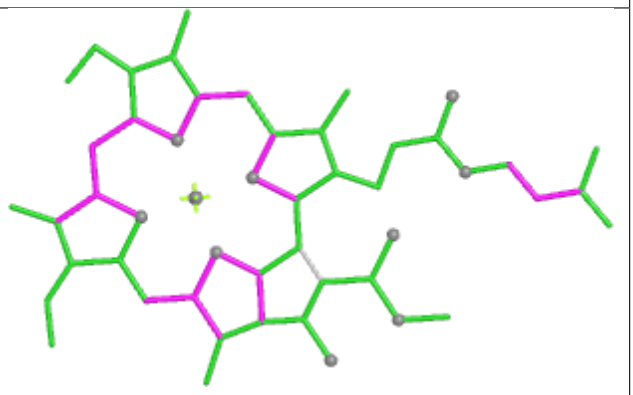
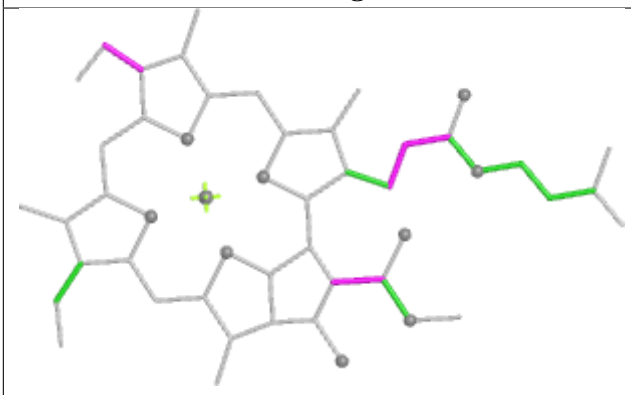


Bond angles



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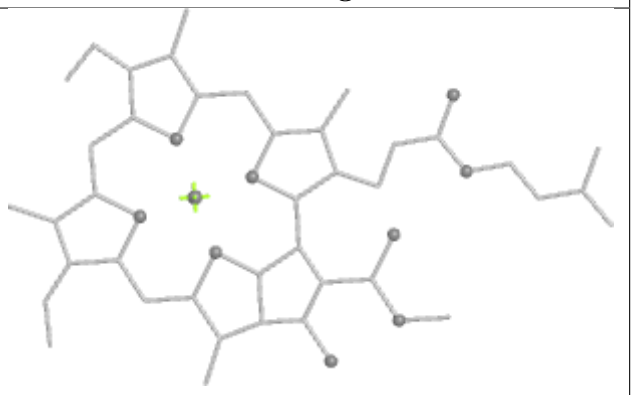
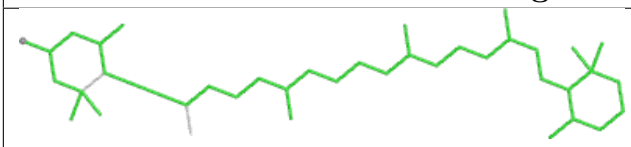


Rings

Ligand IHT p 318



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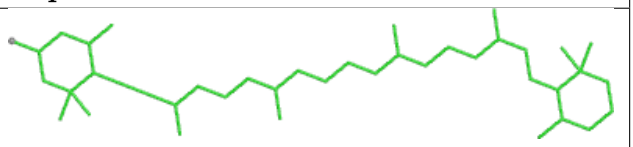
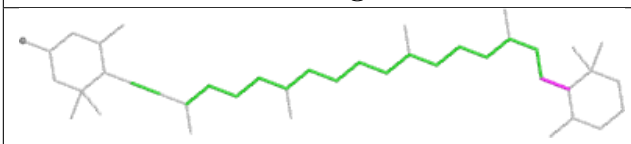


Bond angles



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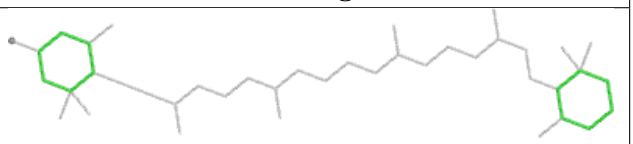
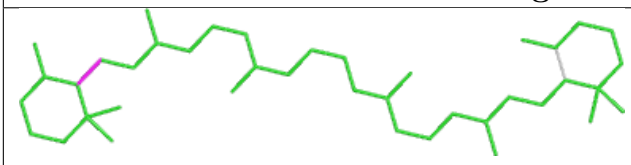


Rings

Ligand 8CT c 515



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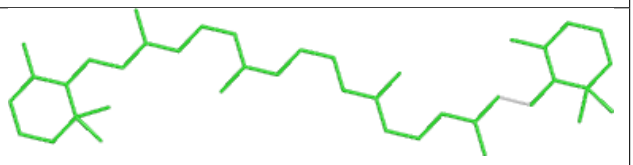
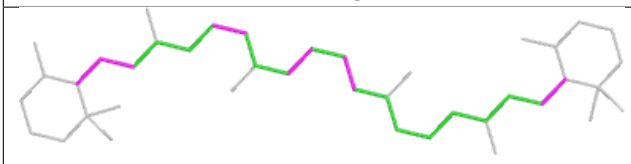


Bond angles



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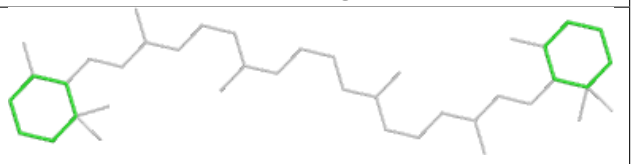
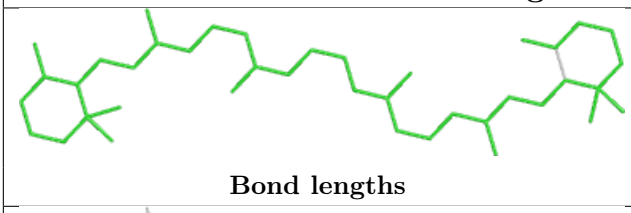


Rings

Ligand 8CT Y 101



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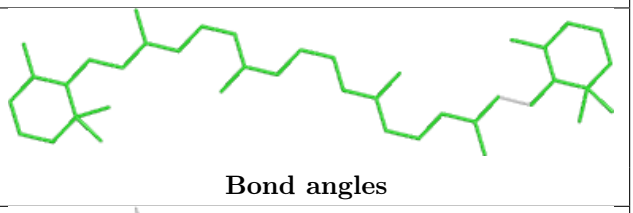
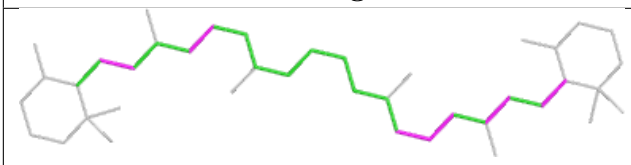


Bond angles



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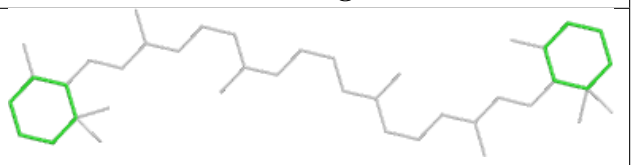
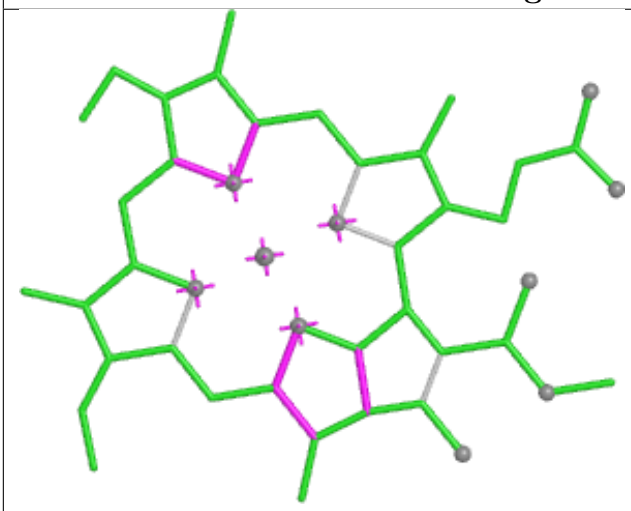


Rings

Ligand CLA B 615



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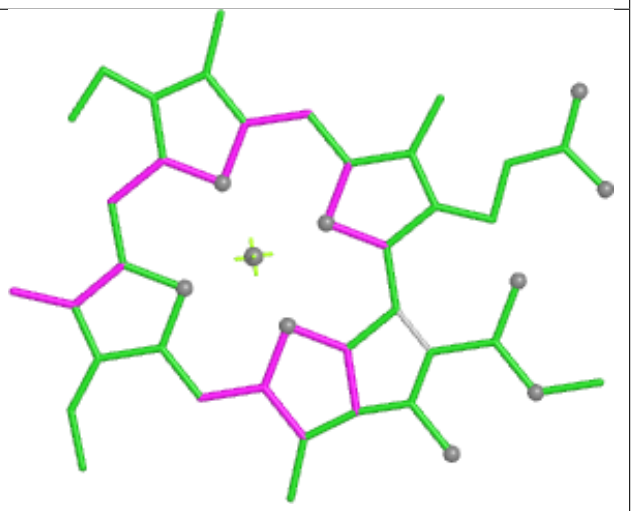
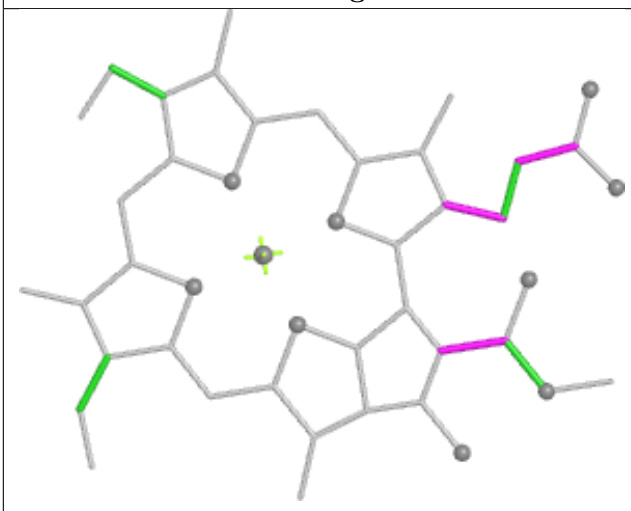


Bond angles



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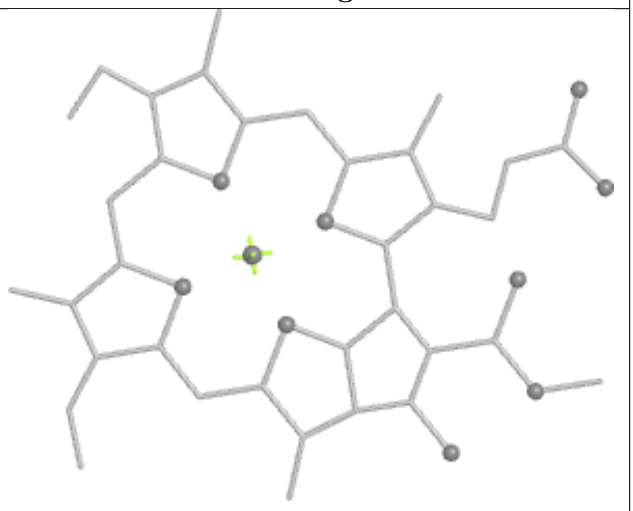
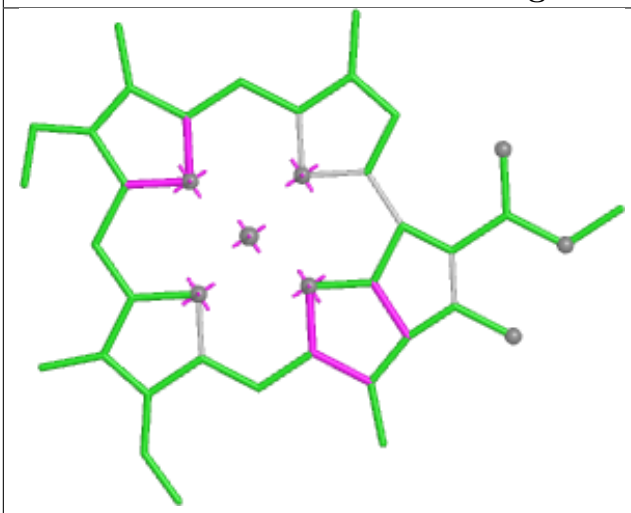


Rings

Ligand CLA g 317



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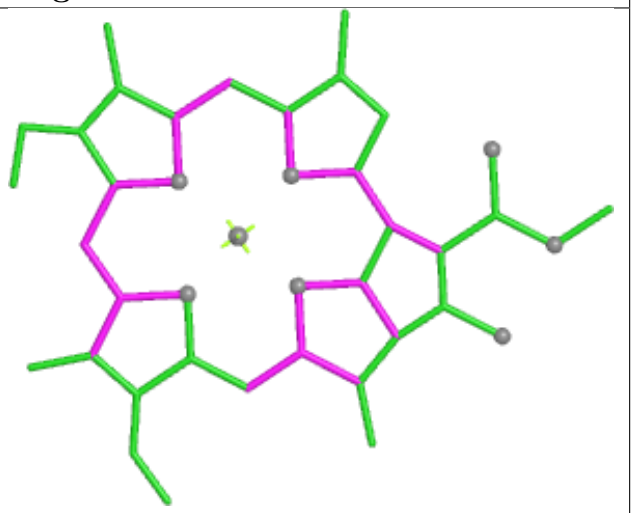
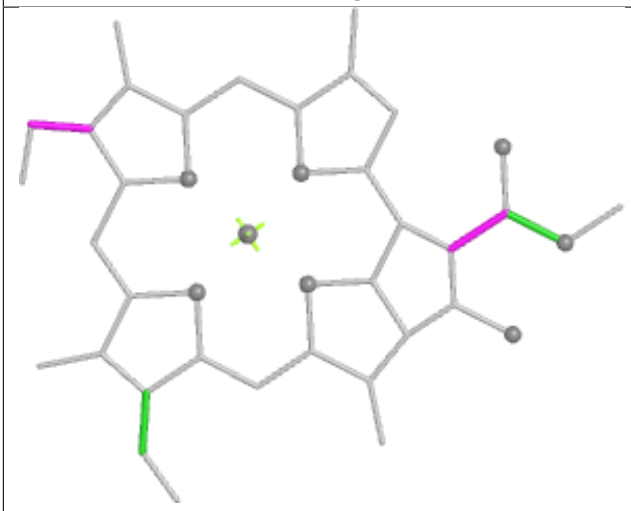


Bond angles



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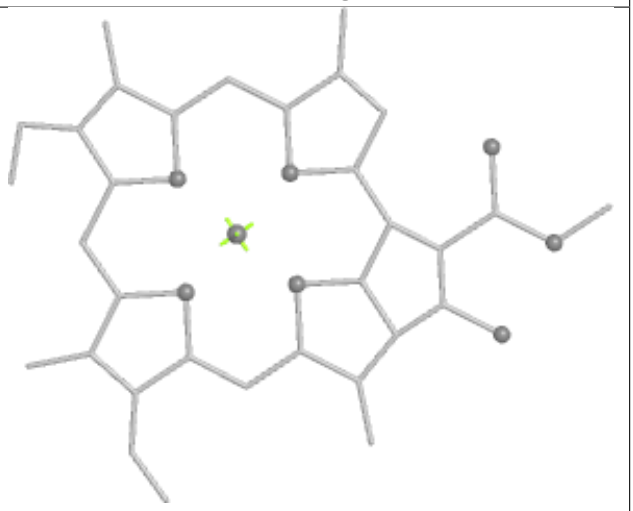
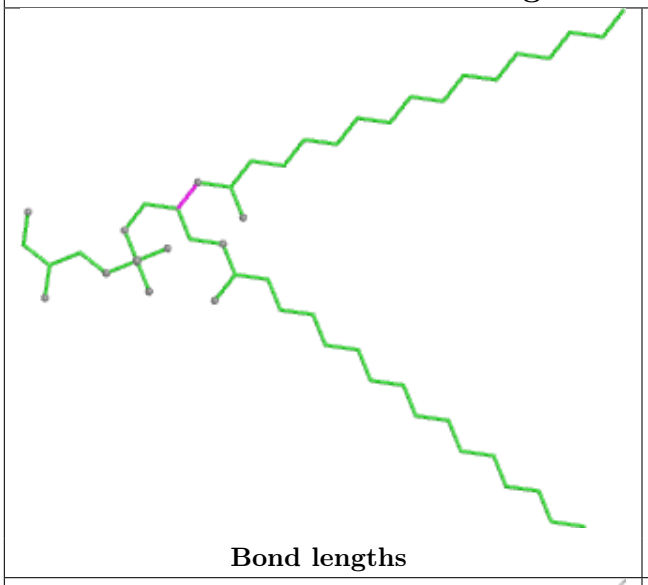


Rings

Ligand LHG D 408



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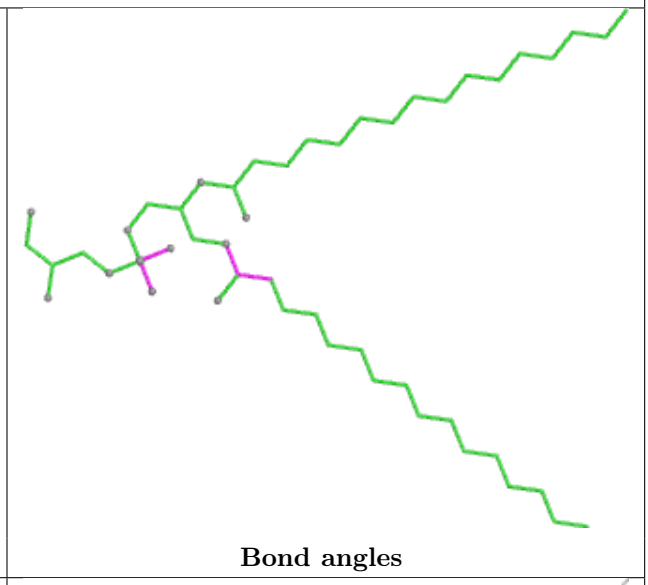
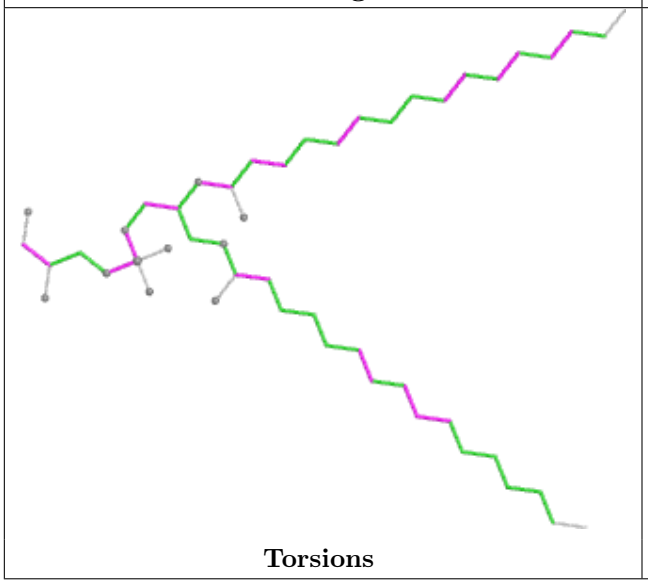
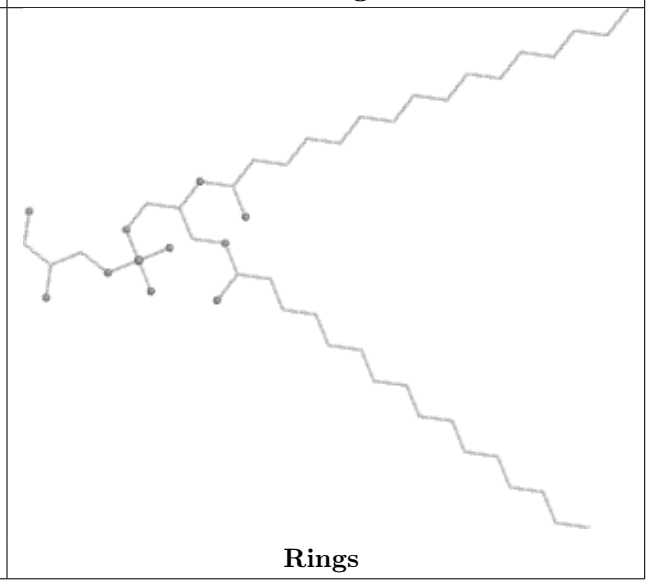


Bond angles

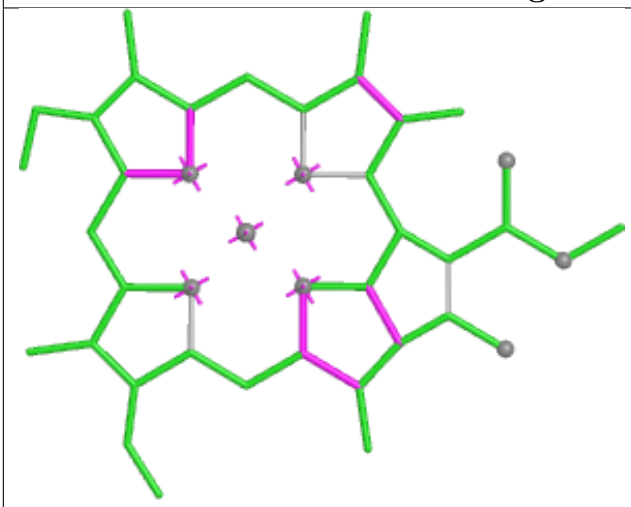


Torsions



Rings

Ligand CLA g 310



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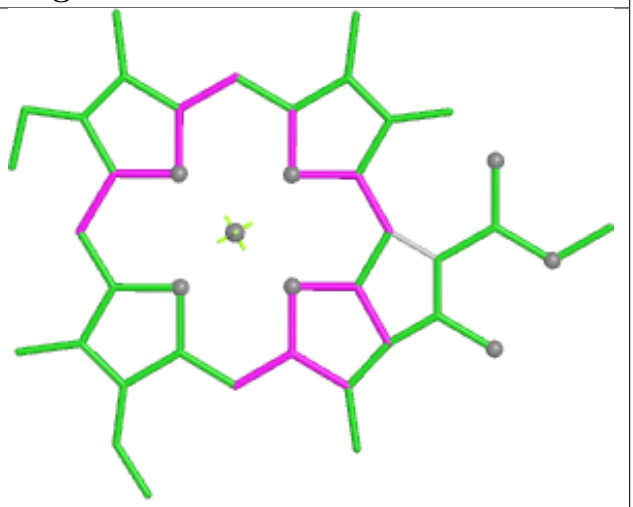
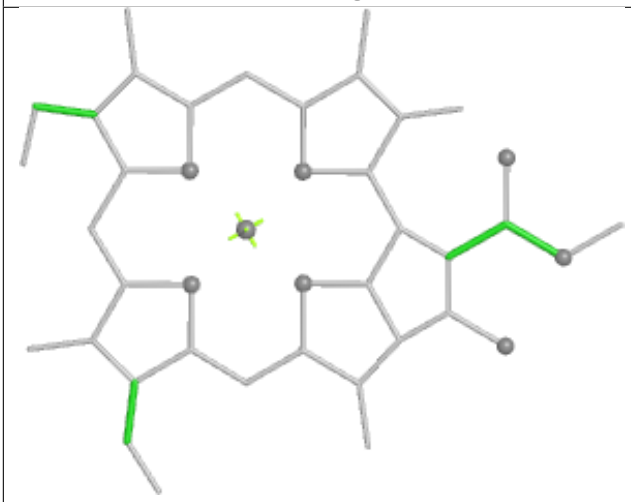


Bond angles



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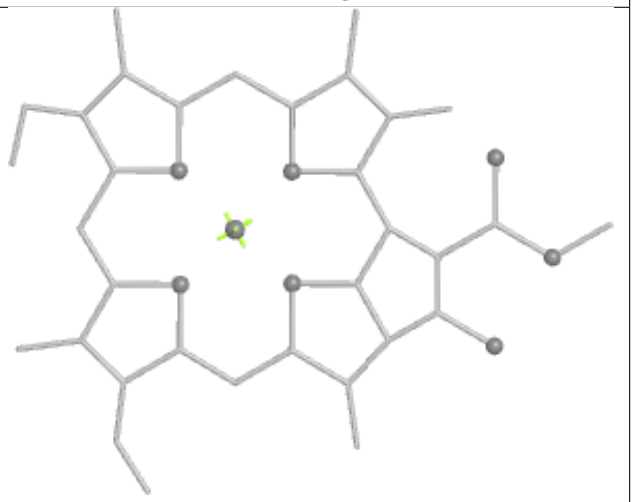
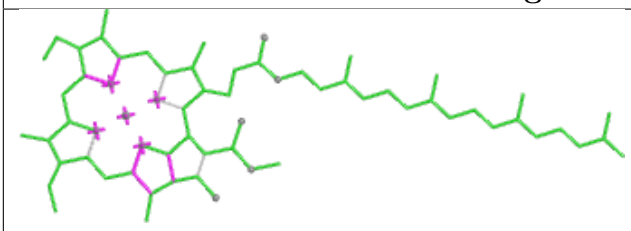


Rings

Ligand CLA B 612



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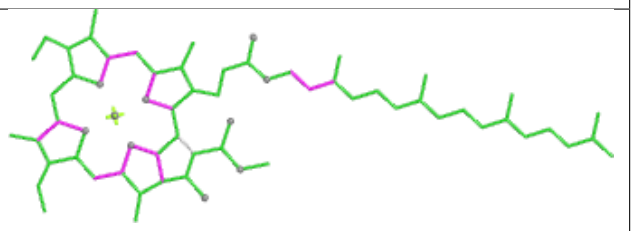
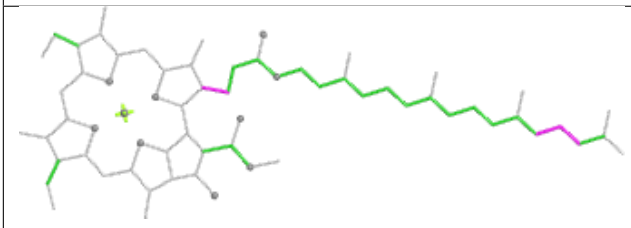
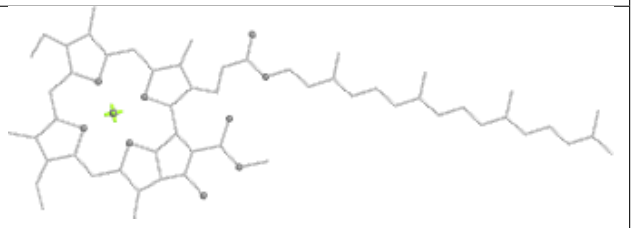


Bond angles

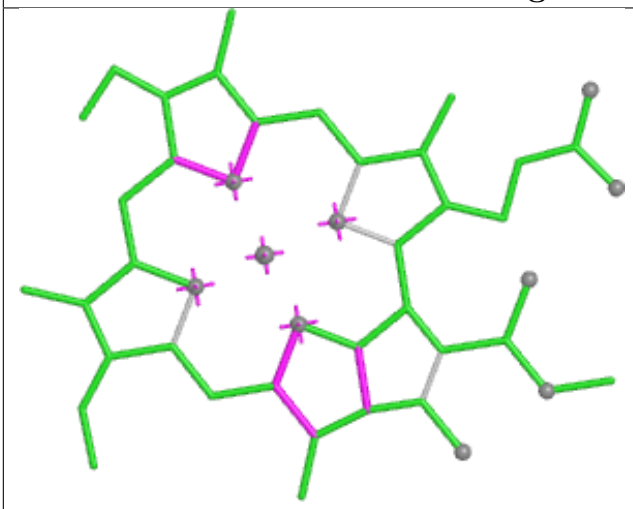


Torsions

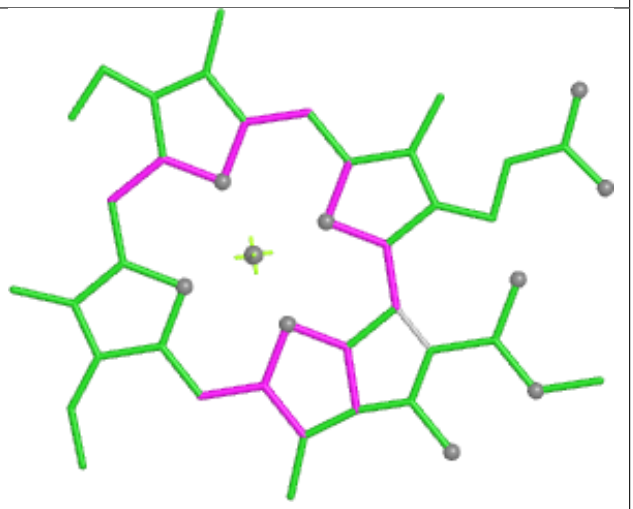


Rings

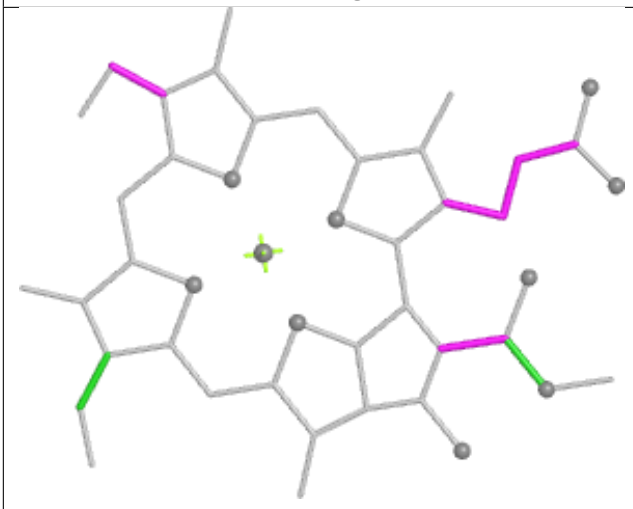
Ligand CLA 9 307



Bond lengths



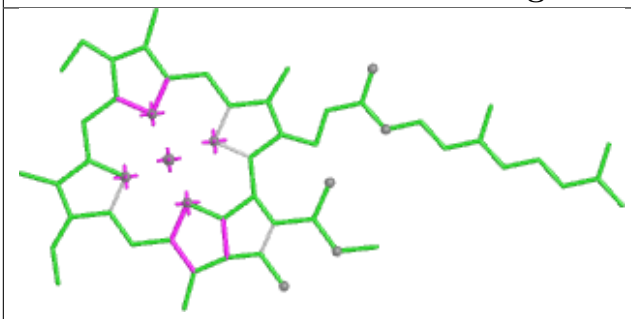
Bond angles



Torsions

Rings

Ligand CLA n 305



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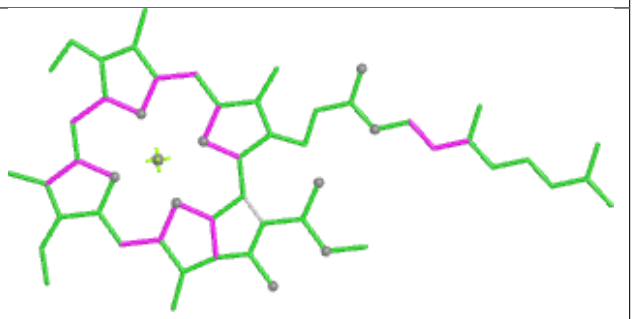

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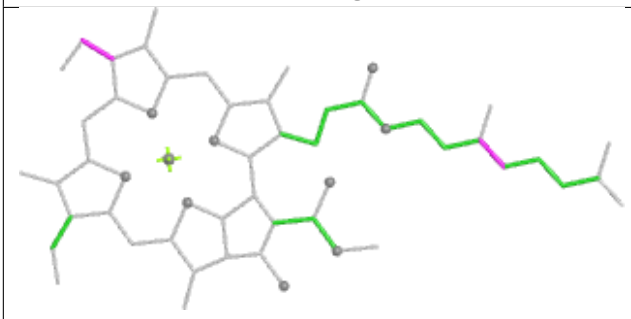

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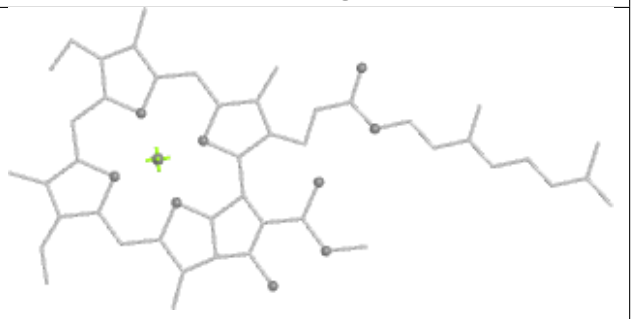
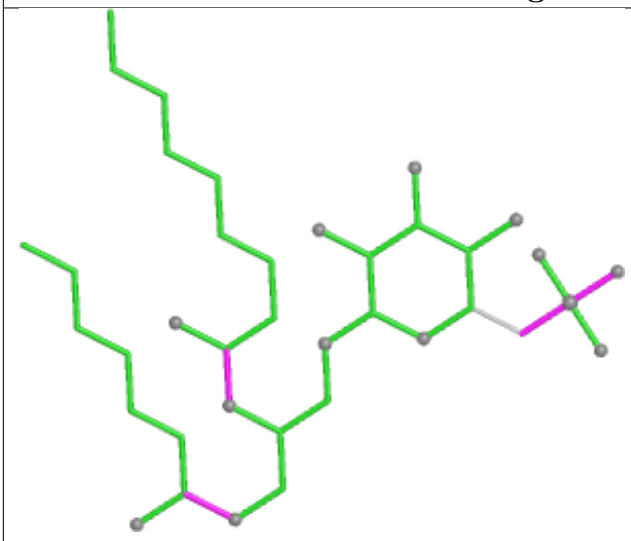


Rings

Ligand SQD b 601



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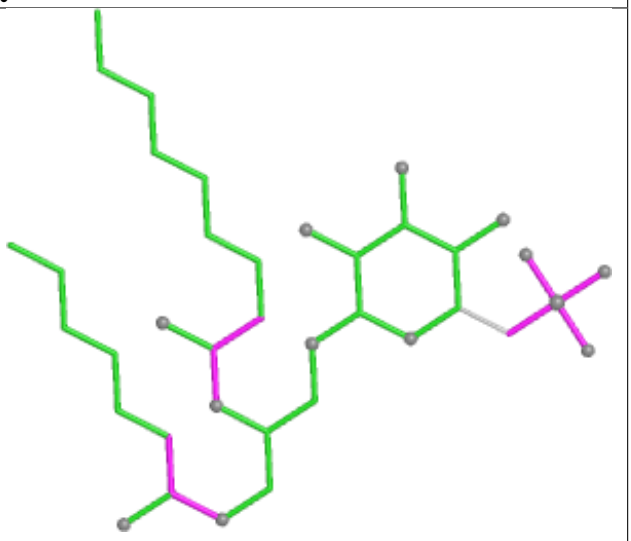

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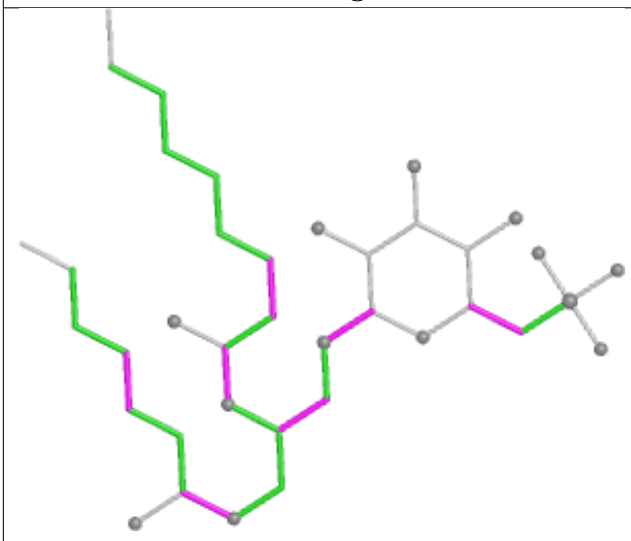

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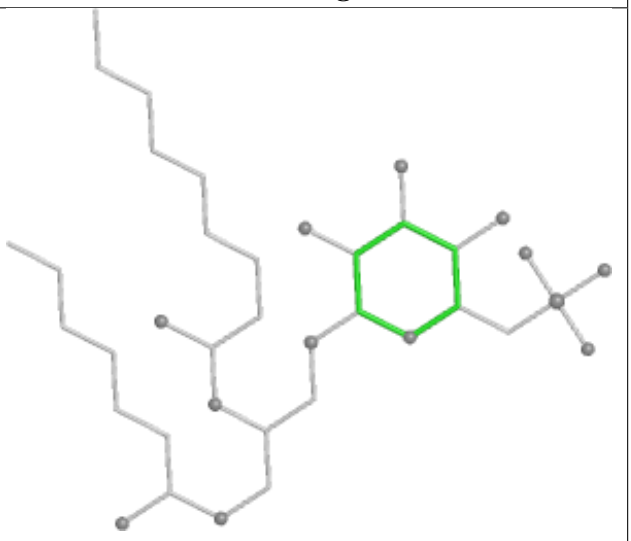
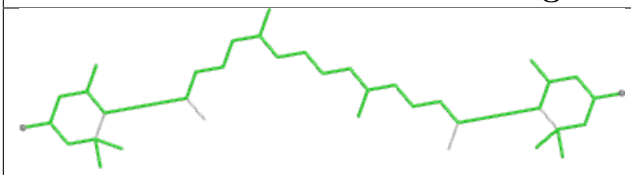


Rings

Ligand II0 9 319



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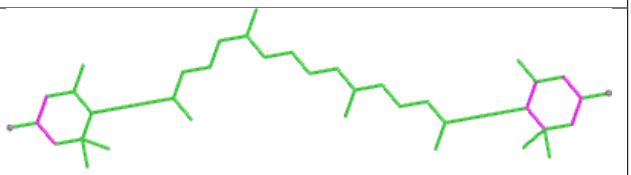

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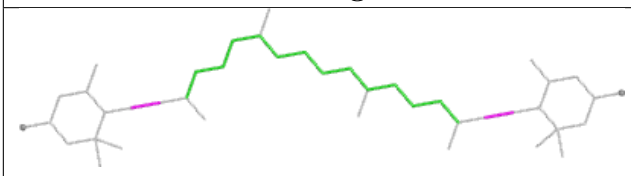

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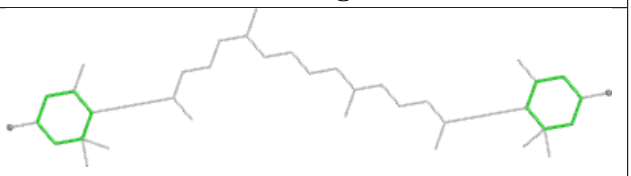
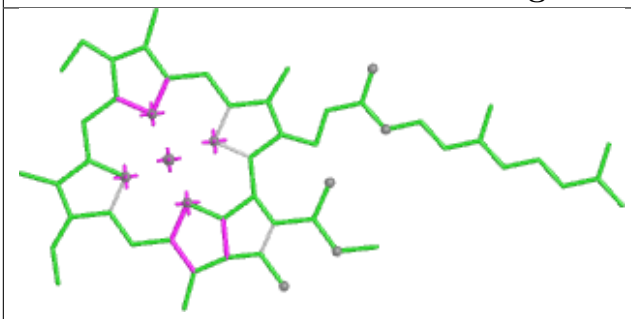


Rings

Ligand CLA 3 309



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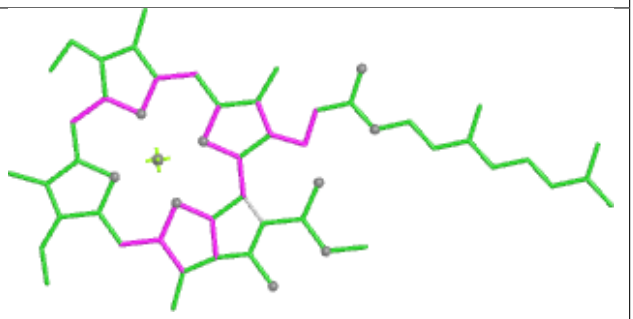

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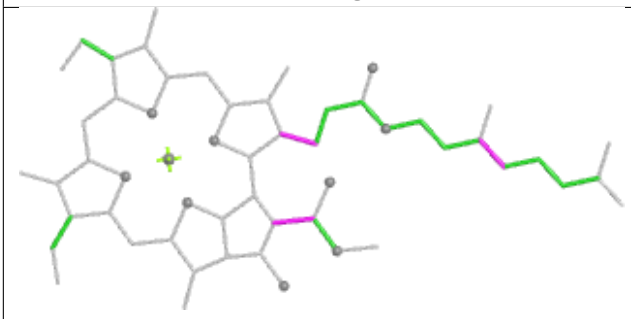

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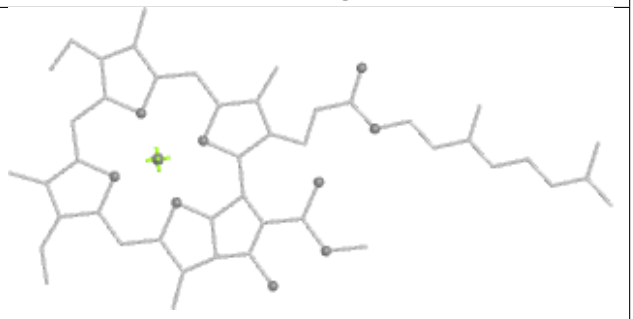
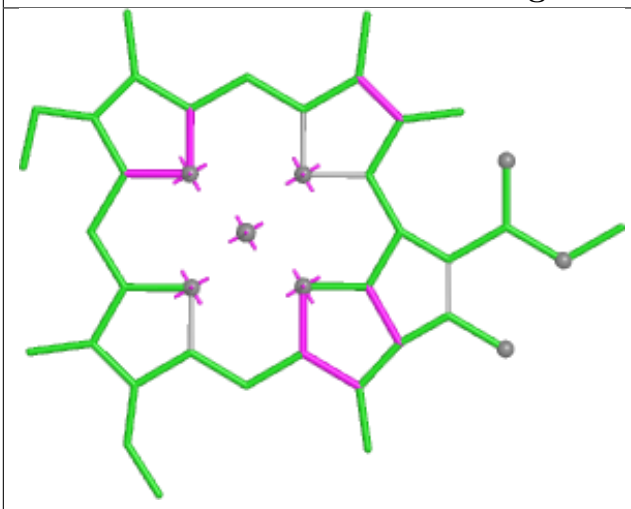


Rings

Ligand CLA 6 302



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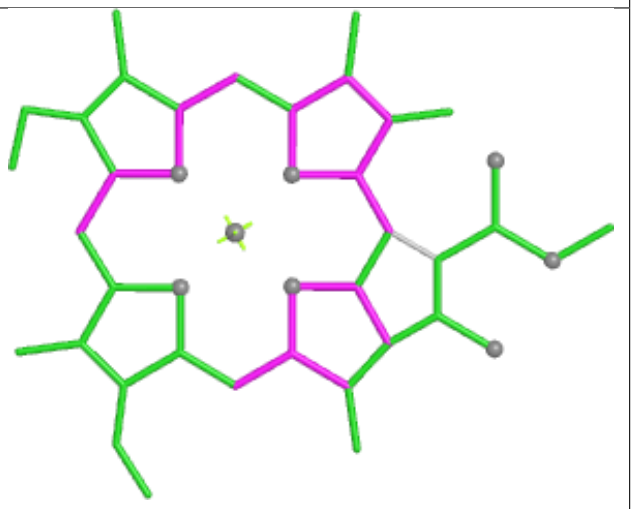

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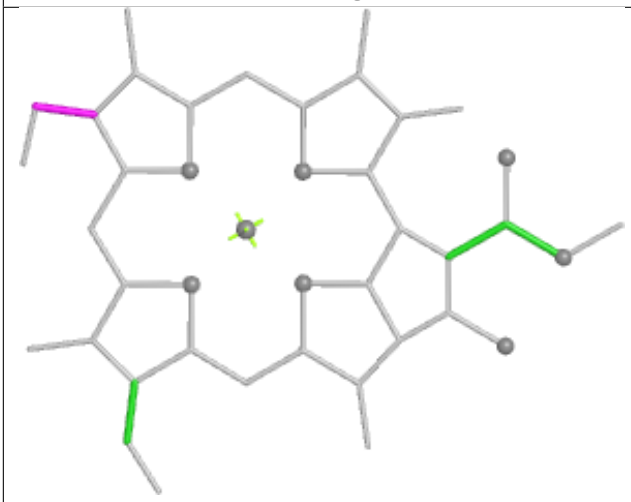

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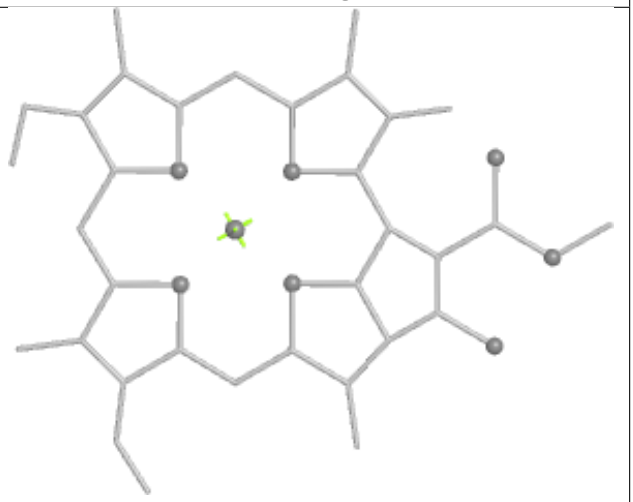
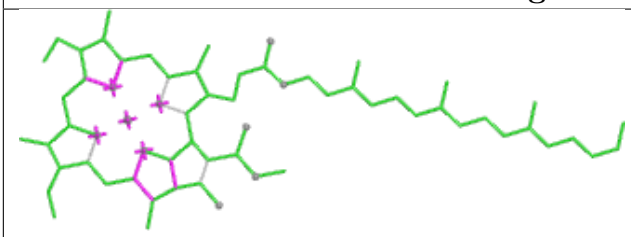


Rings

Ligand CLA 1 302



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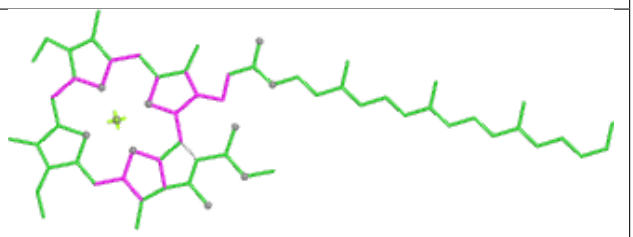

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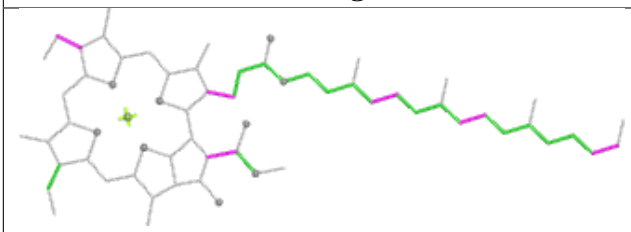

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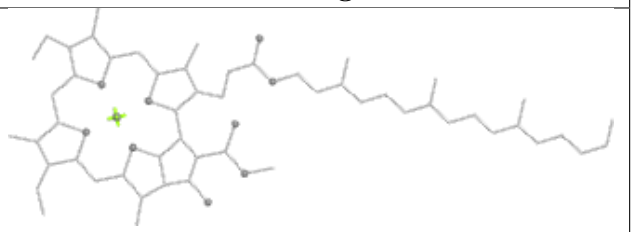
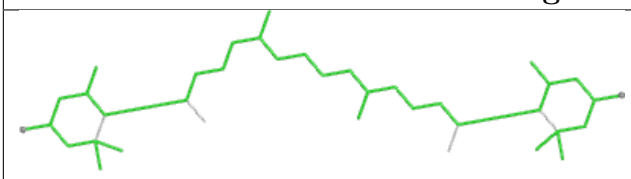


Rings

Ligand II0 0 313



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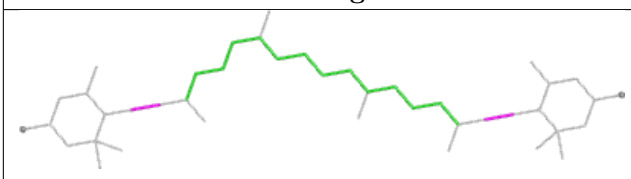

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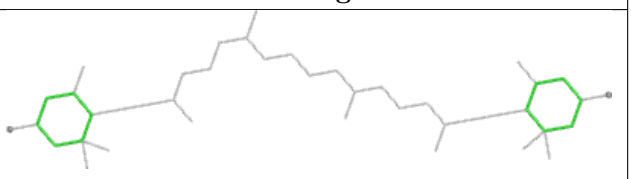
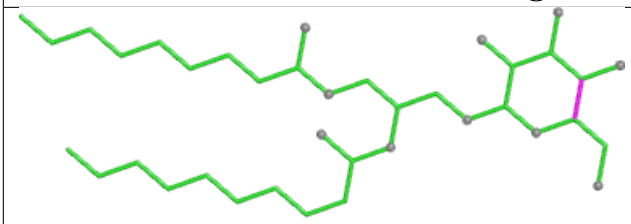


Rings

Ligand LMG l 102



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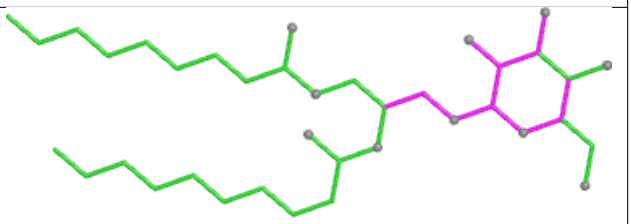

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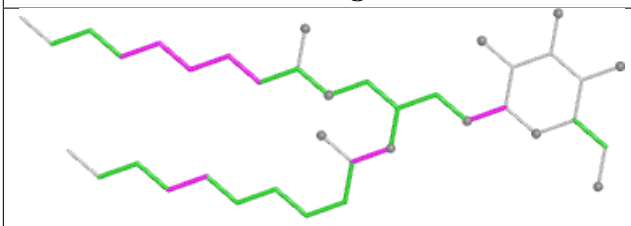

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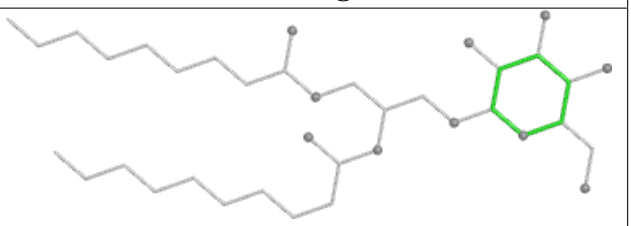
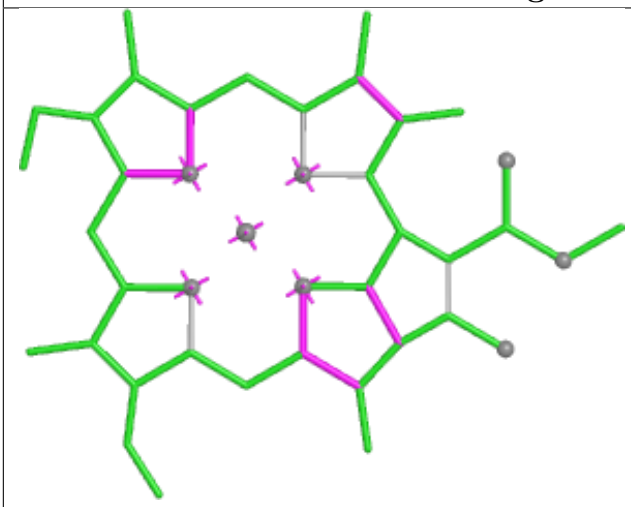


Rings

Ligand CLA p 310



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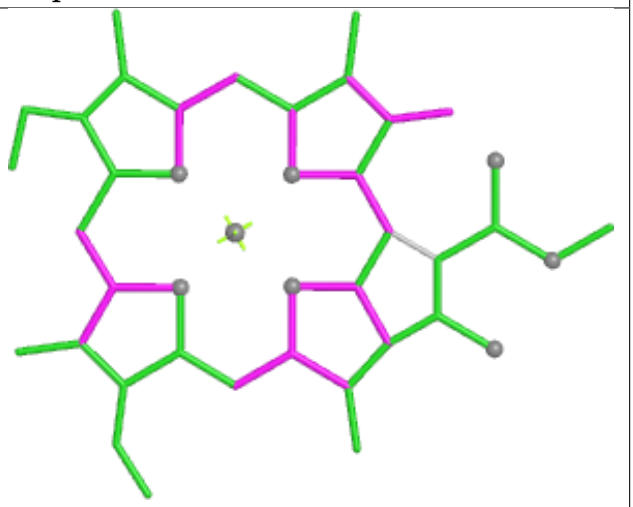

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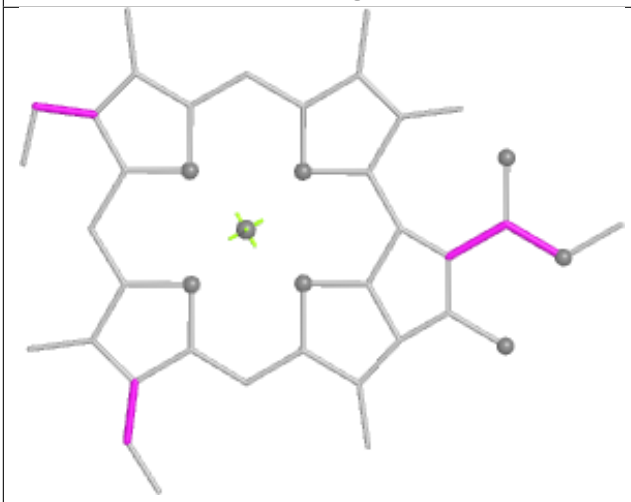

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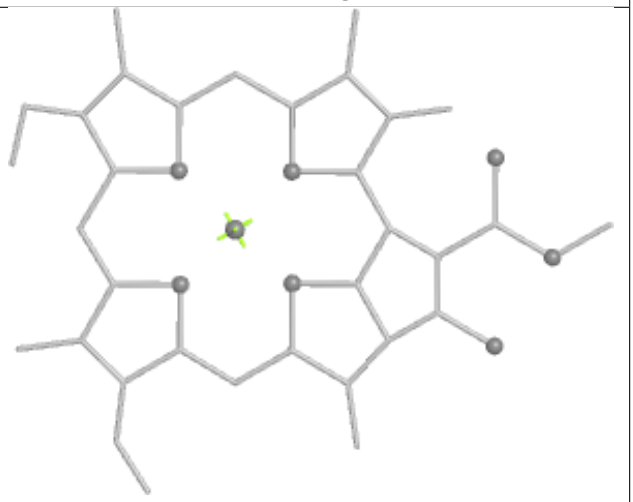
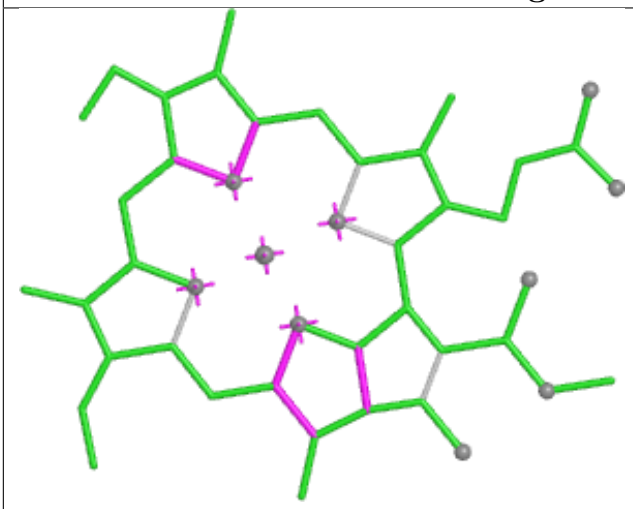


Rings

Ligand CLA 8 301



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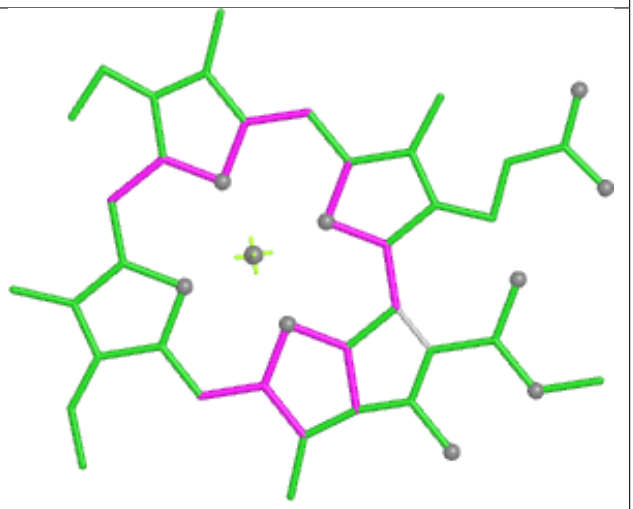

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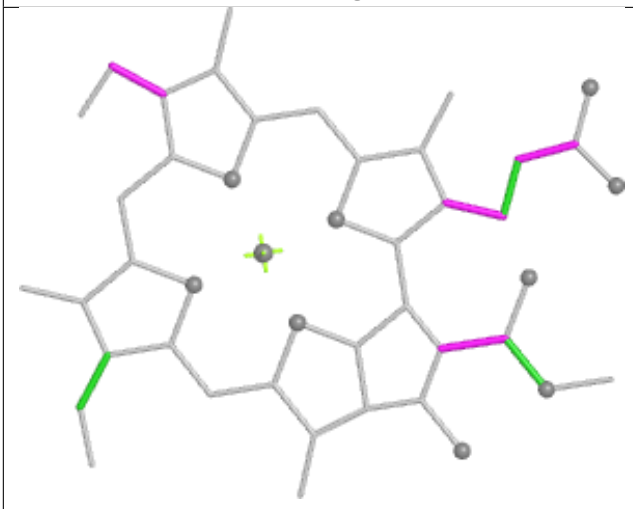
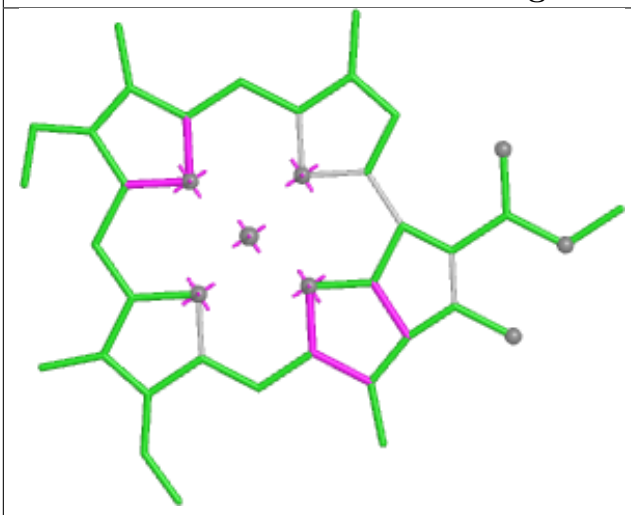


Torsions

Rings

Ligand CLA 0 310



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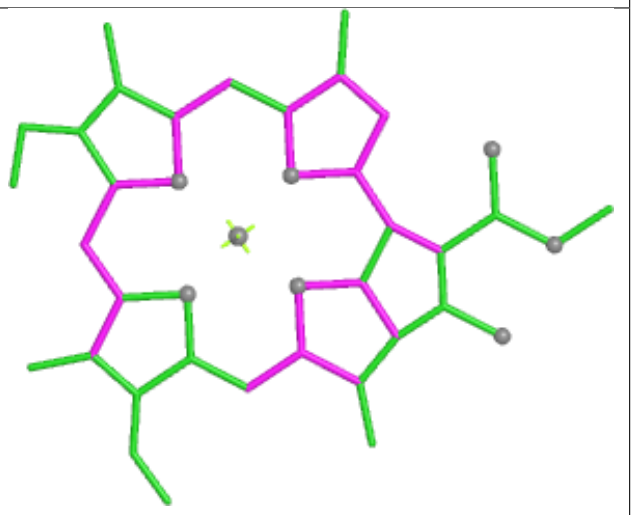

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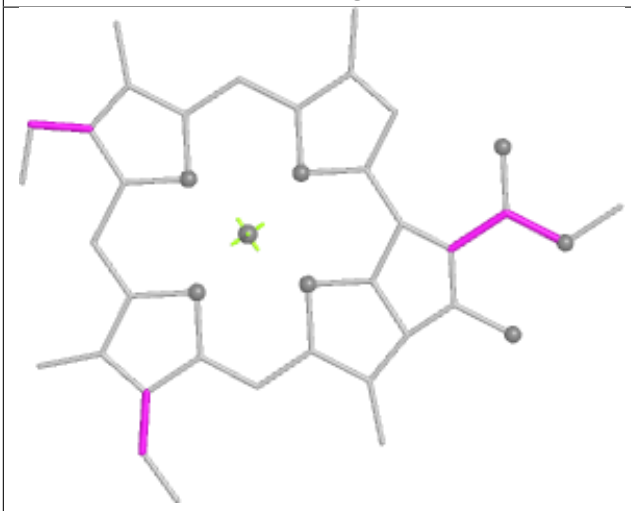

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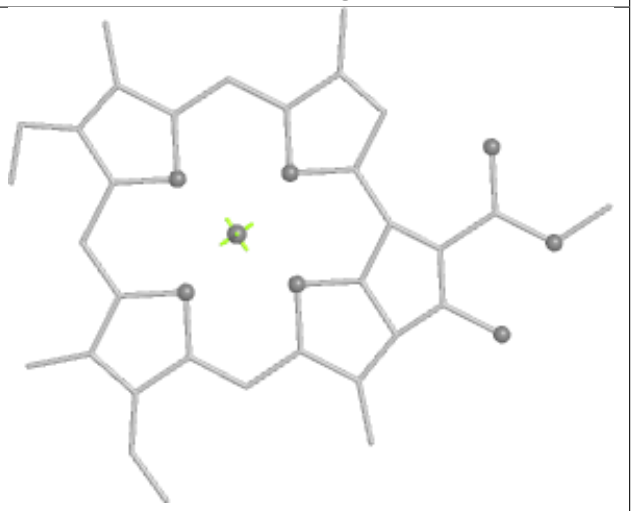
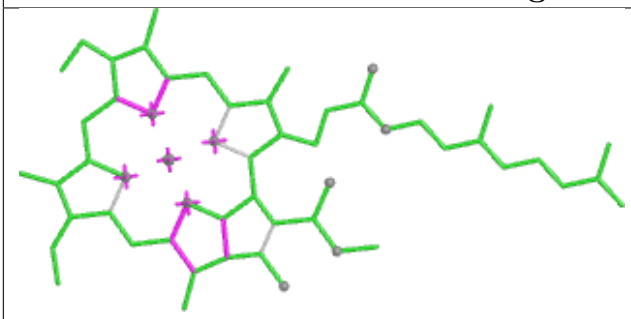


Rings

Ligand CLA 4 306



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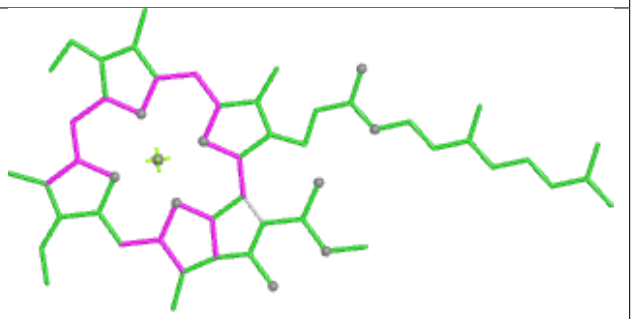

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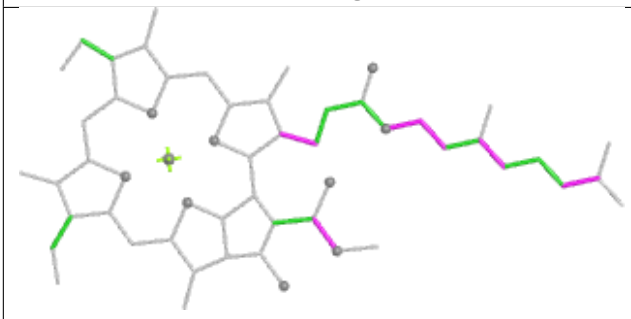

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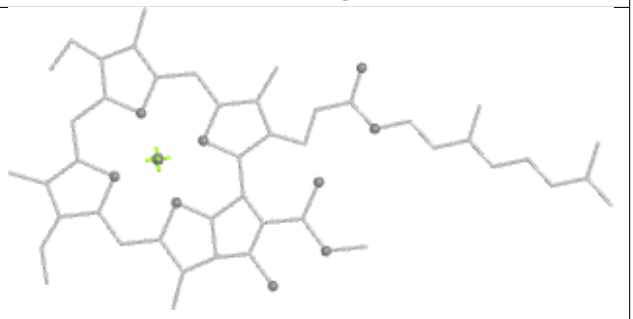
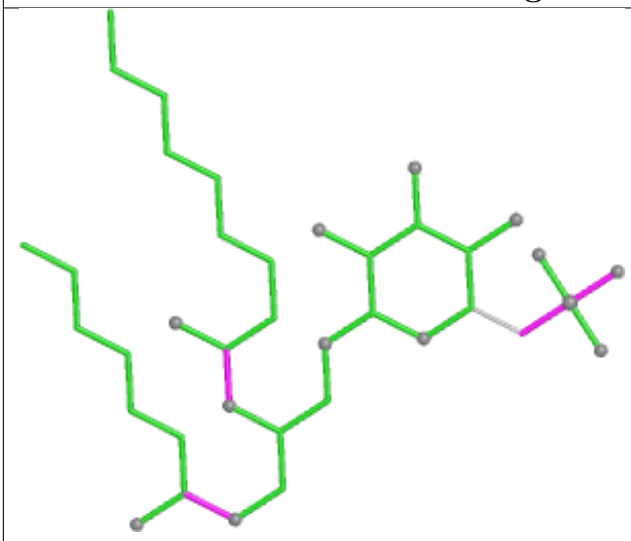


Rings

Ligand SQD B 601



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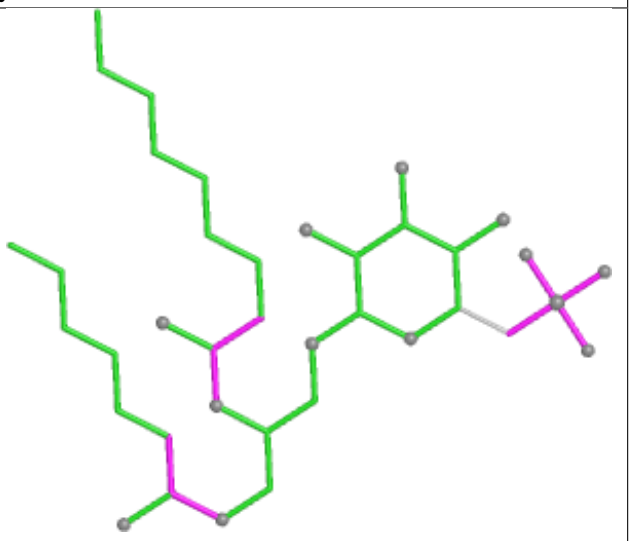

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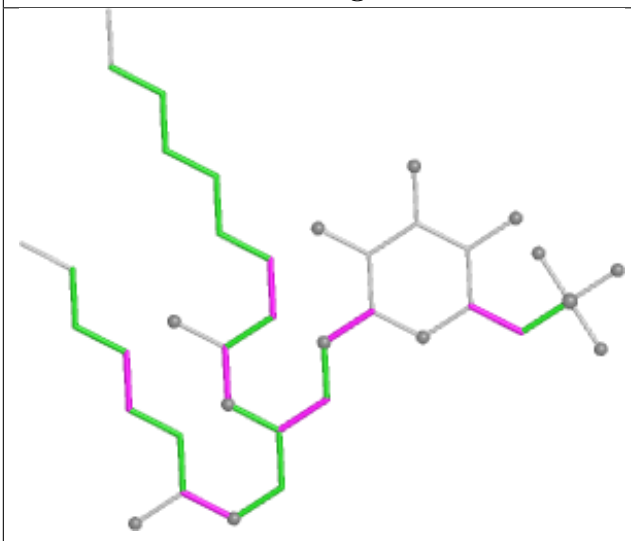

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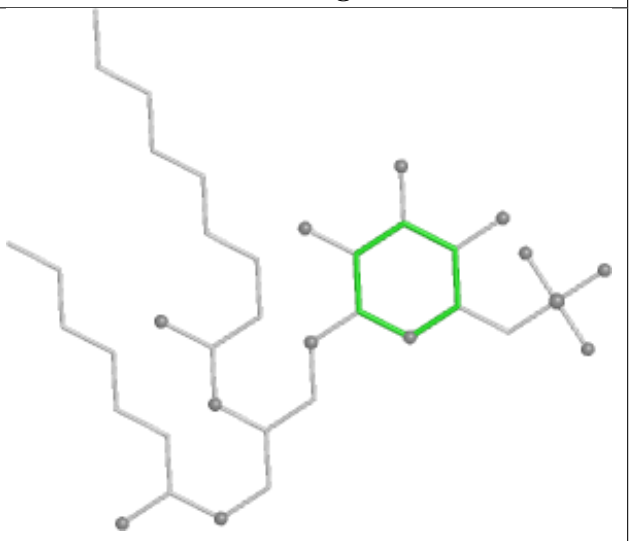
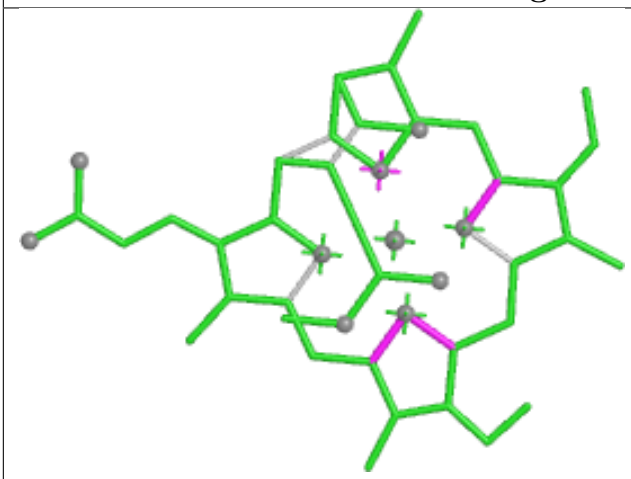


Rings

Ligand KC2 4 305



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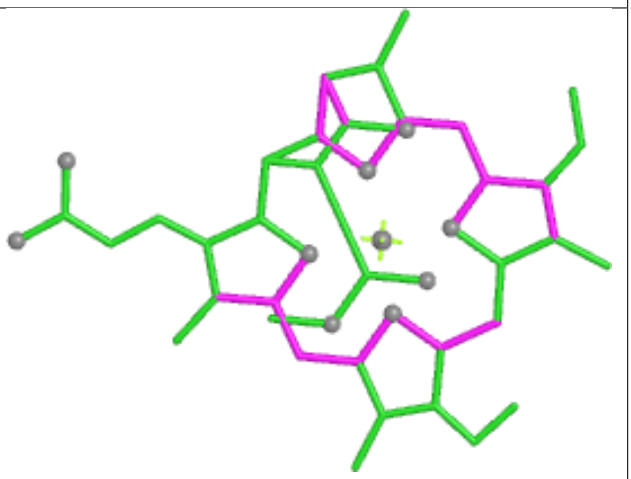
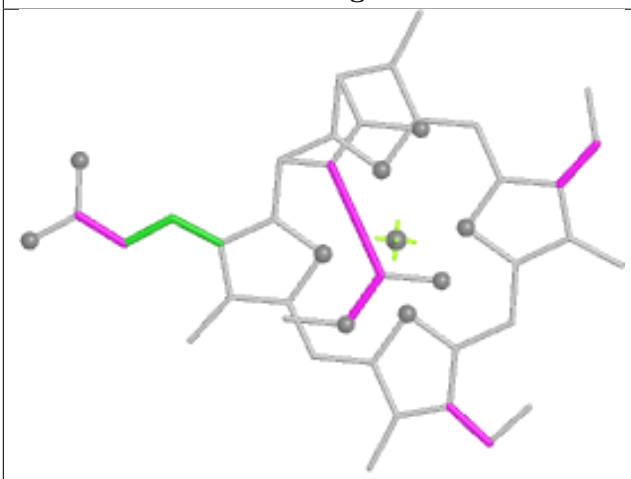


Bond angles



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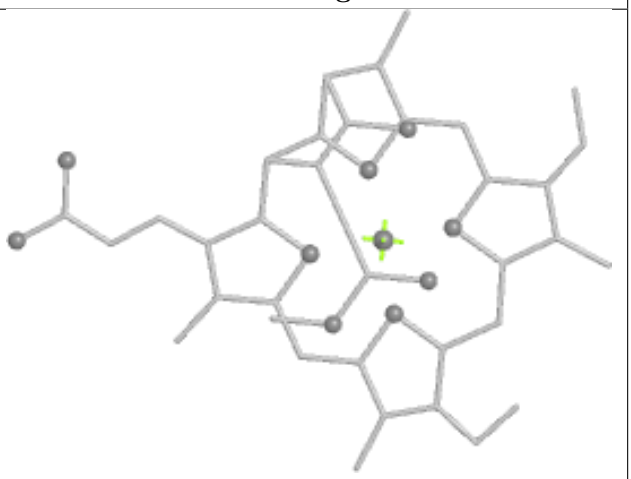
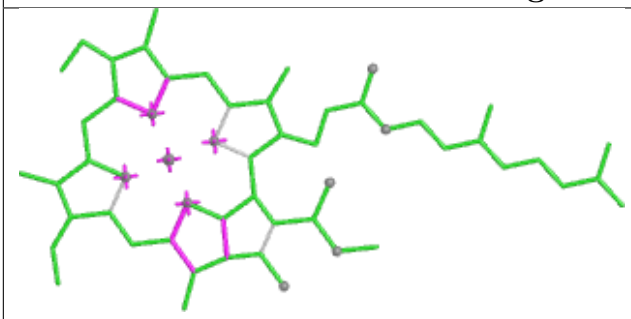
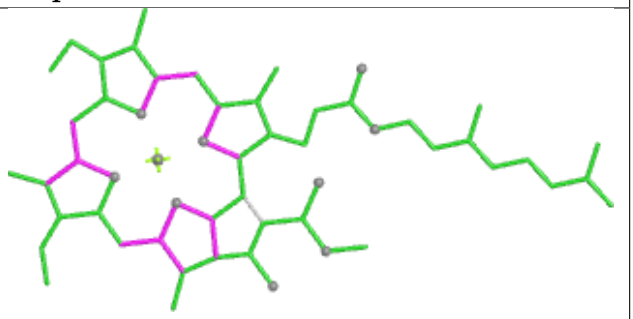


Rings

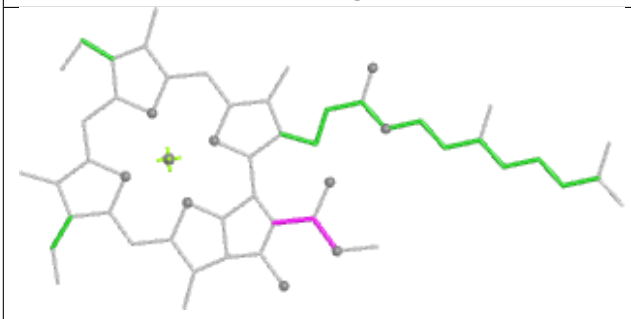
Ligand CLA p 305



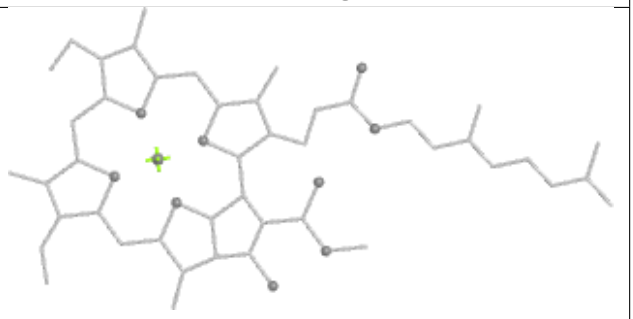
Bond lengths



Bond angles

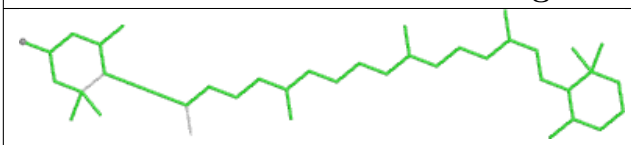


Torsions



Rings

Ligand IHT 6 318



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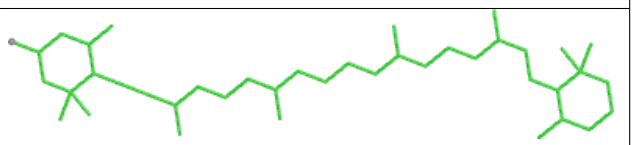

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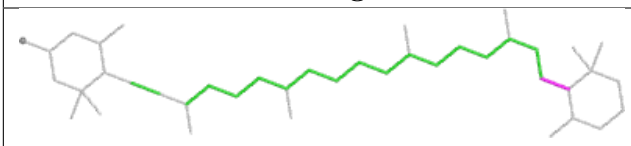

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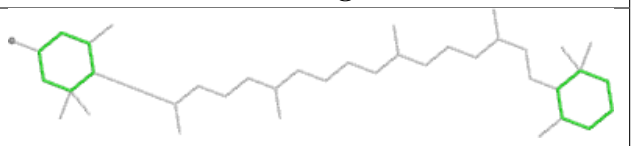
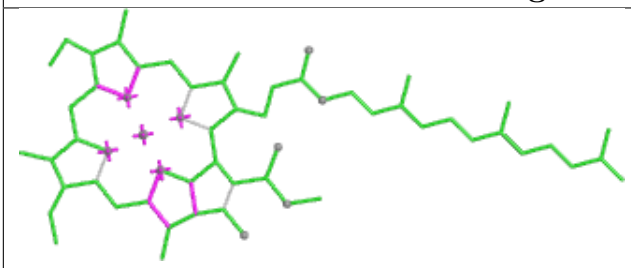


Rings

Ligand CLA 8 306



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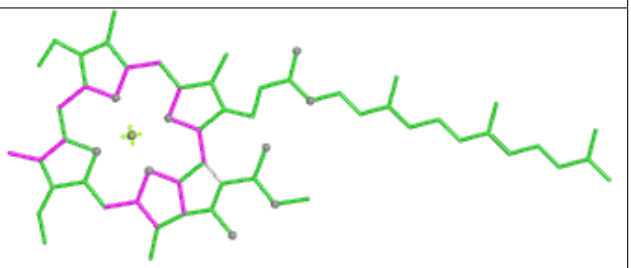

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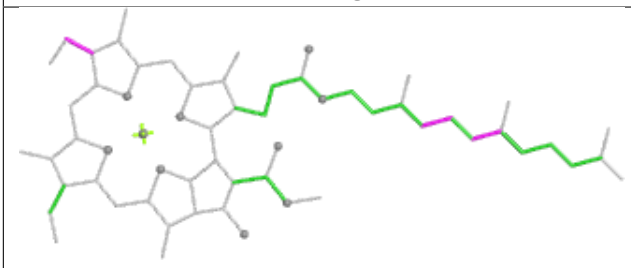

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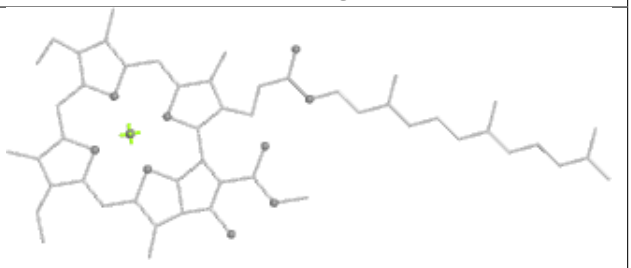
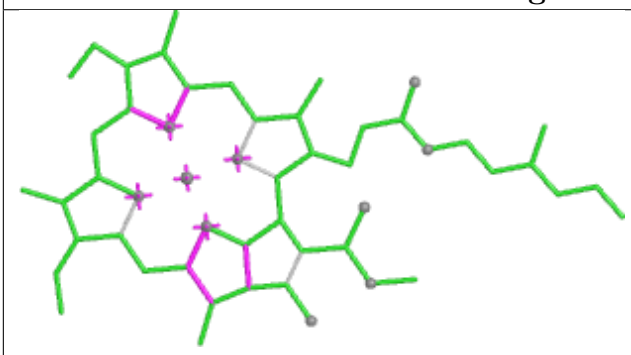


Rings

Ligand CLA 2 303



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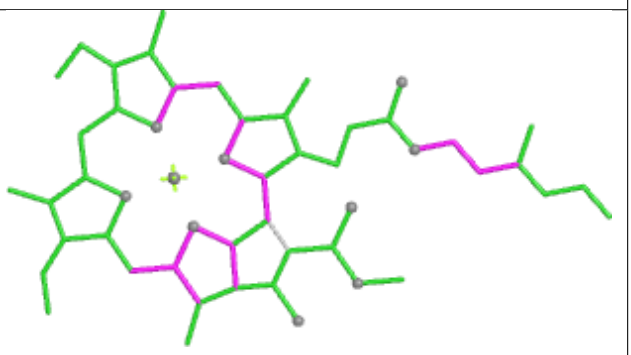
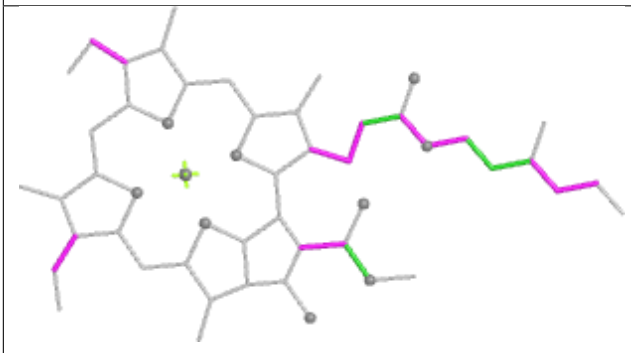


Bond angles



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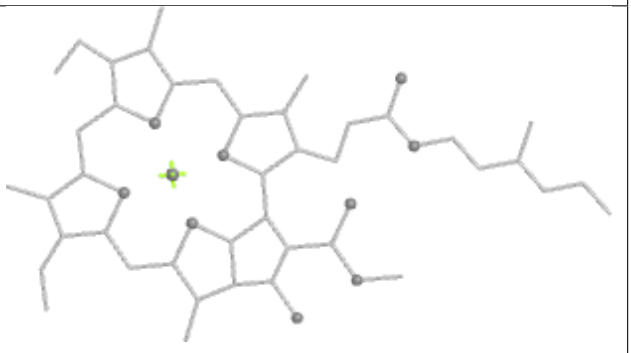
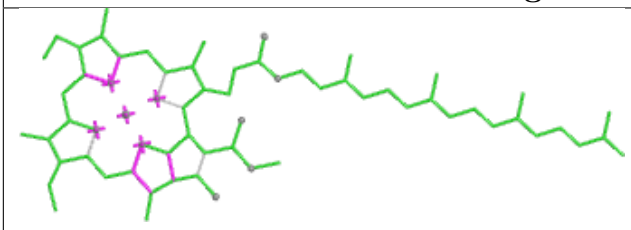
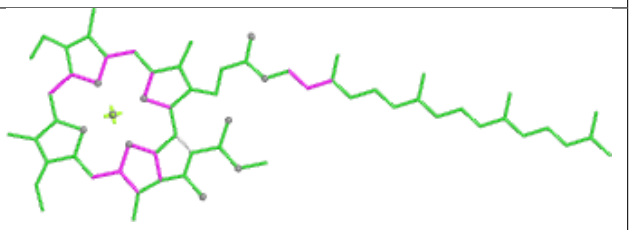
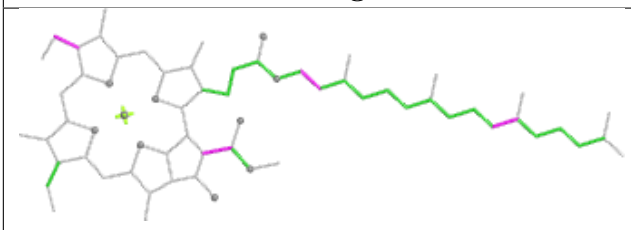
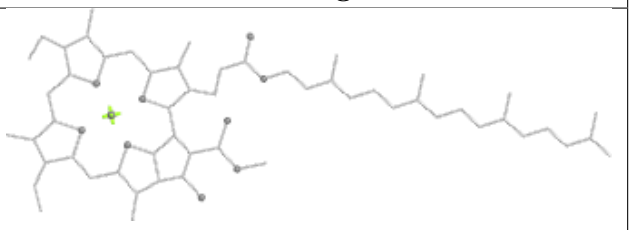
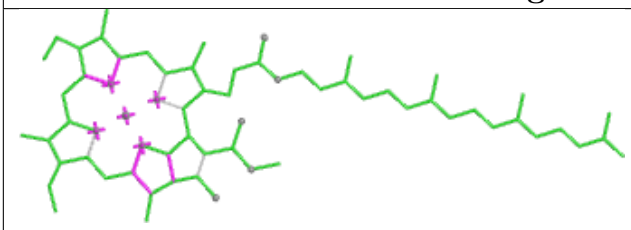
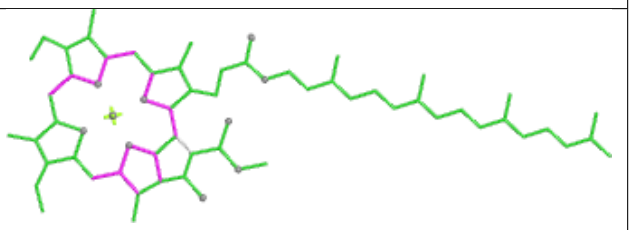
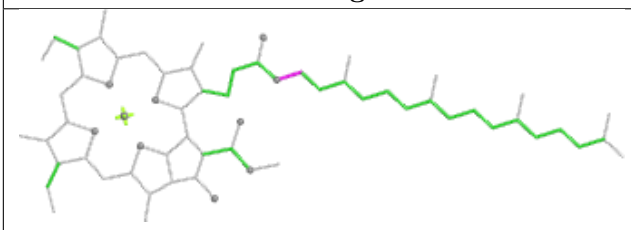
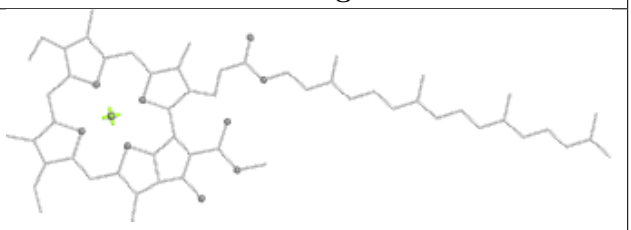
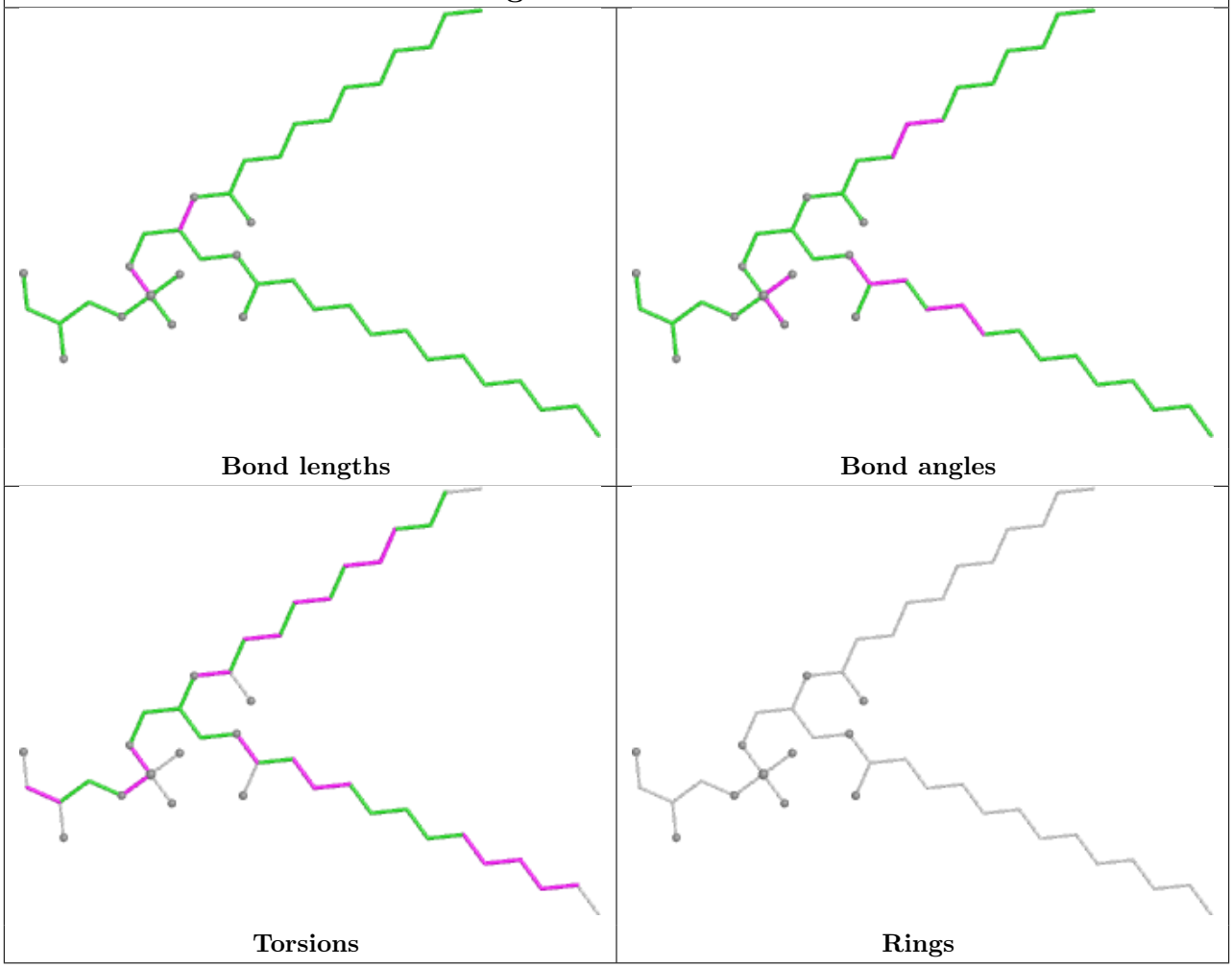


Rings

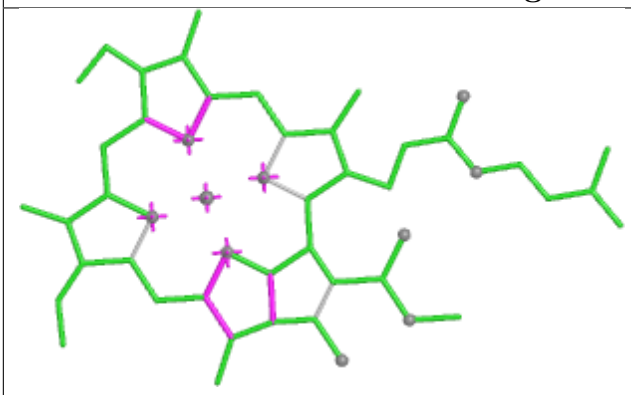
Ligand CLA B 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

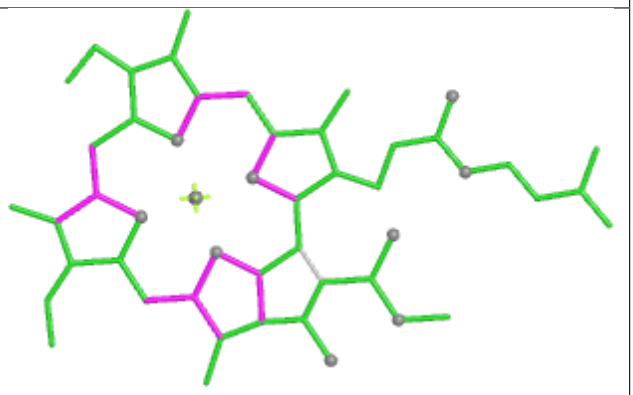
Ligand LHG 3 322



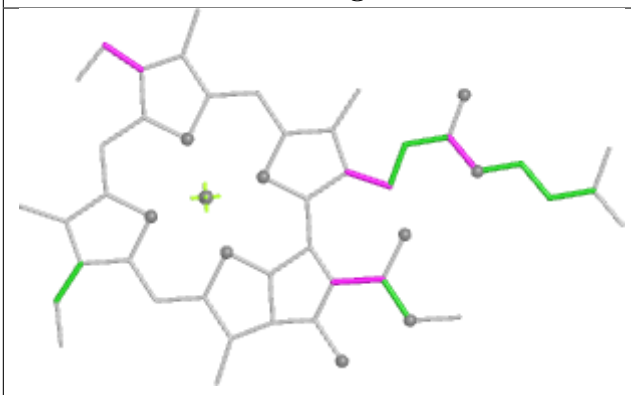
Ligand CLA B 602



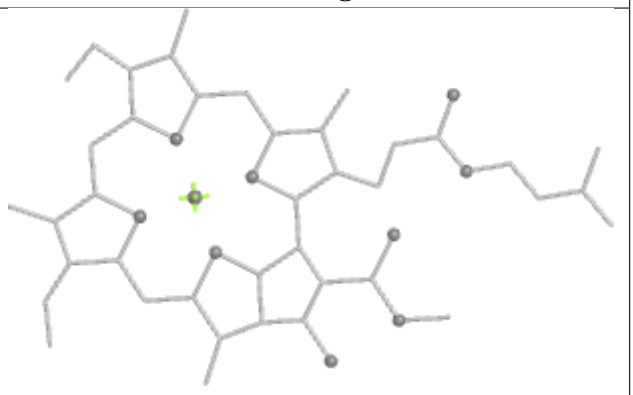
Bond lengths



Bond angles

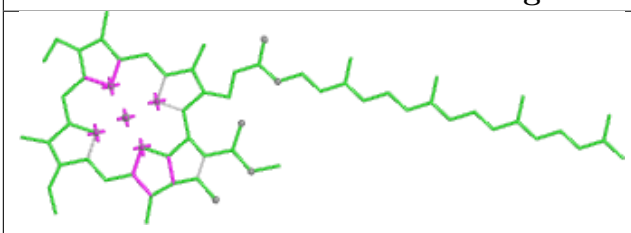


Torsions



Rings

Ligand CLA D 405



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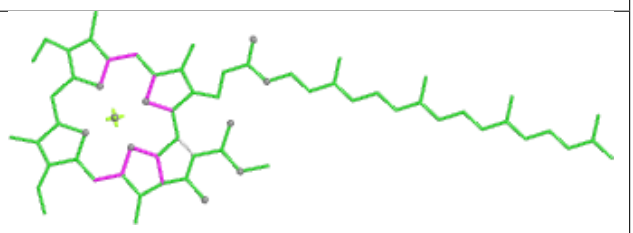
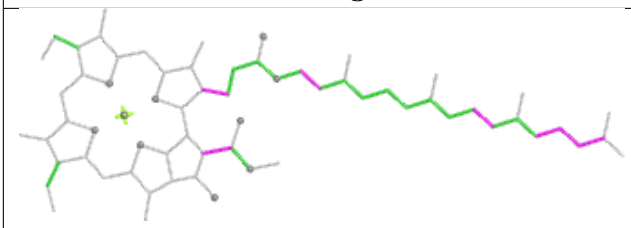


Bond angles



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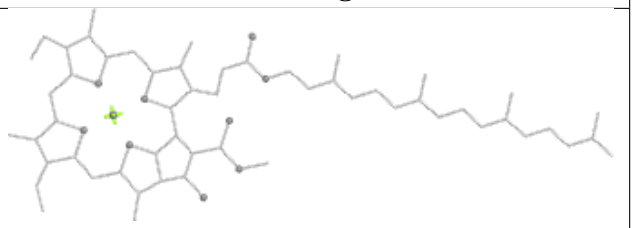
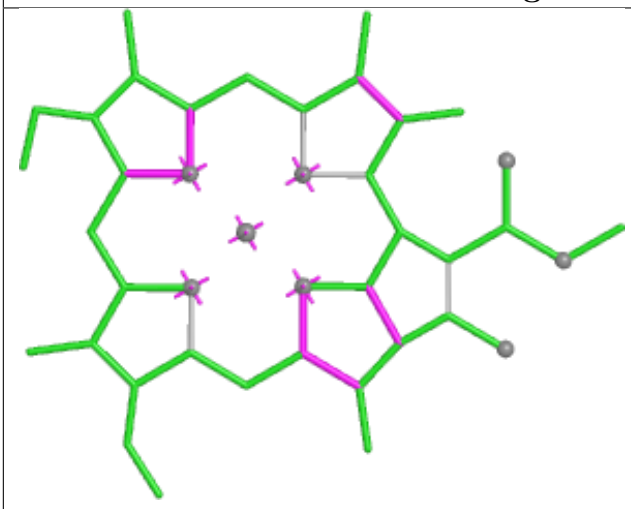


Rings

Ligand CLA N 304



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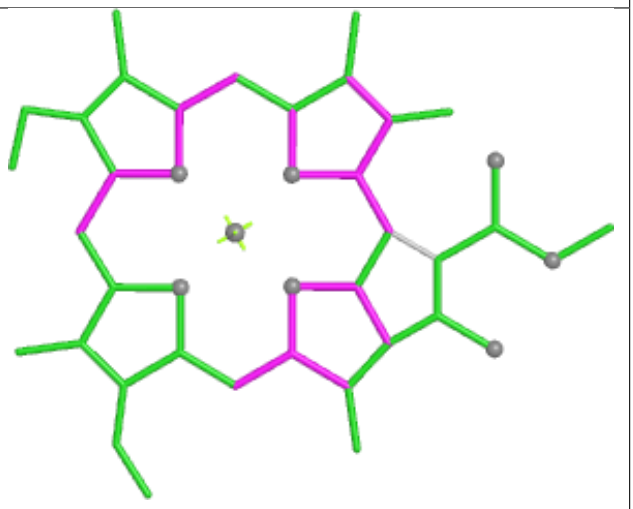
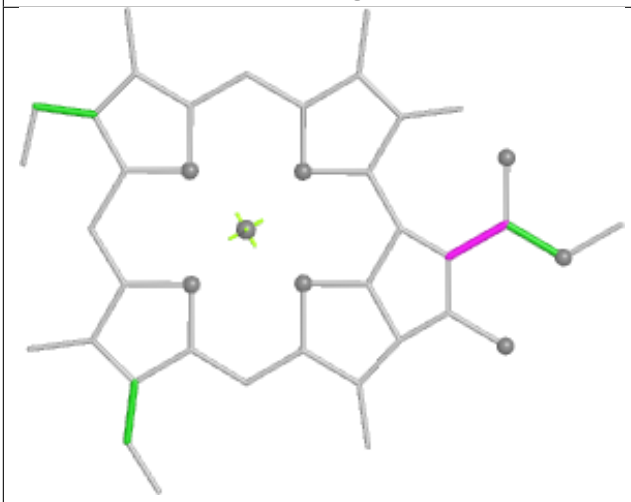


Bond angles



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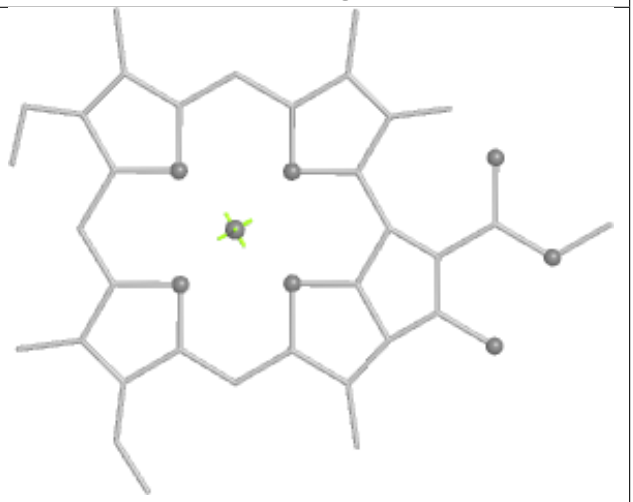
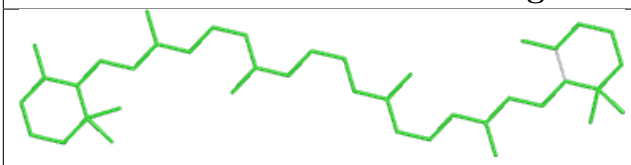


Rings

Ligand 8CT C 516



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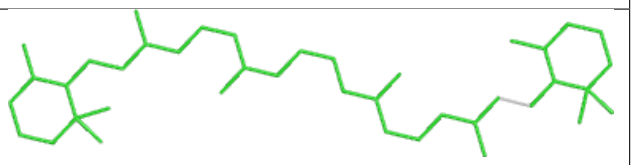
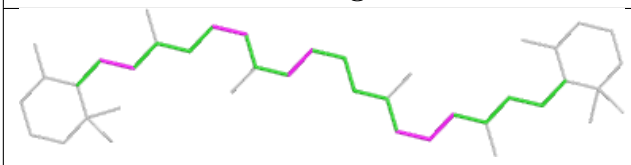


Bond angles



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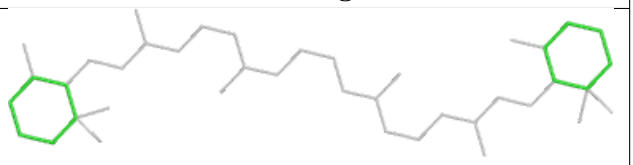
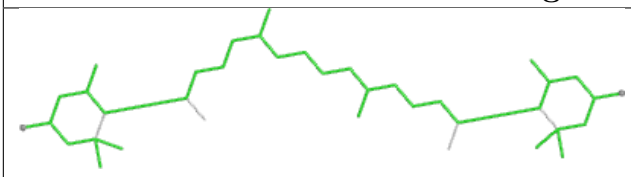


Rings

Ligand II0 g 314



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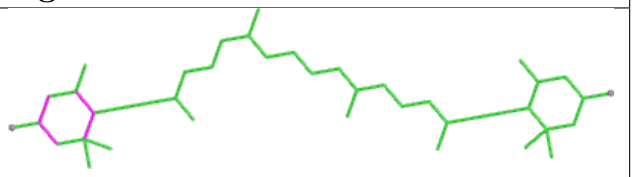
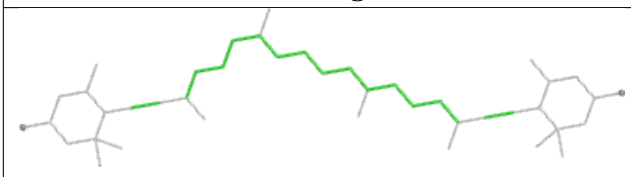


Bond angles



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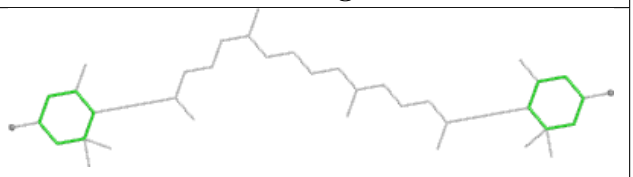
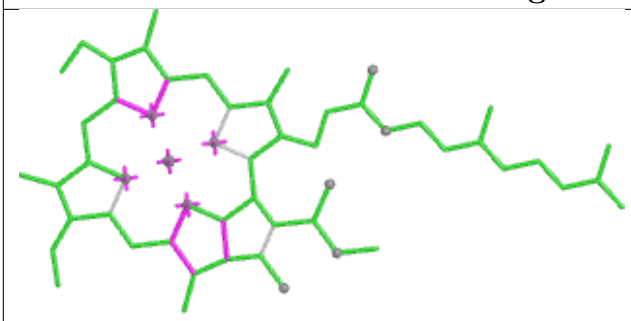


Rings

Ligand CLA 8 302



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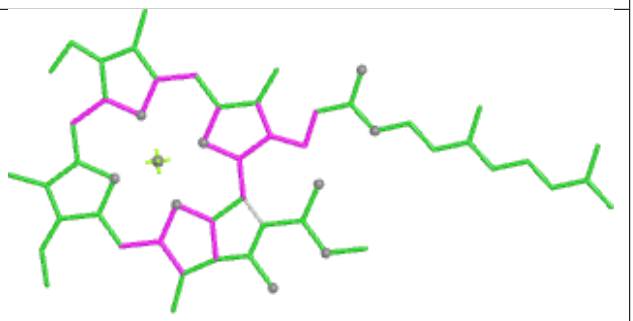
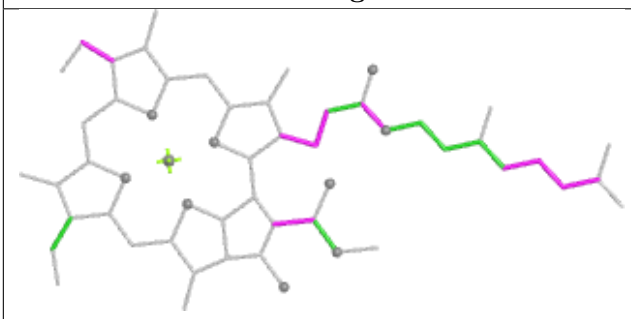
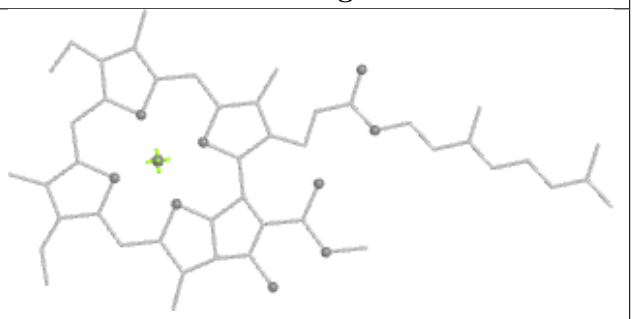


Bond angles

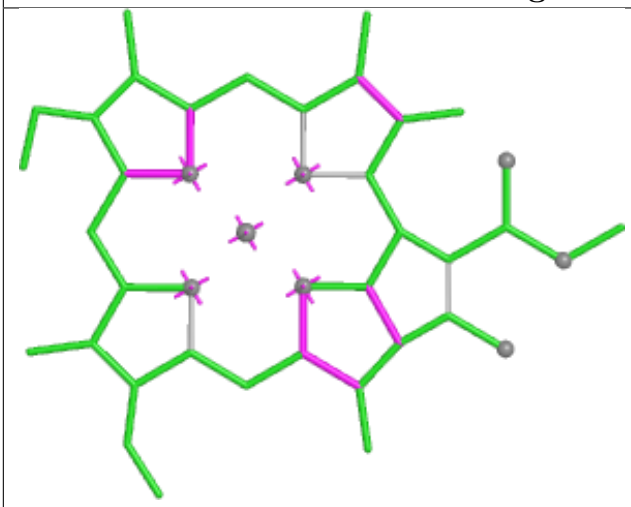


Torsions



Rings

Ligand CLA g 308



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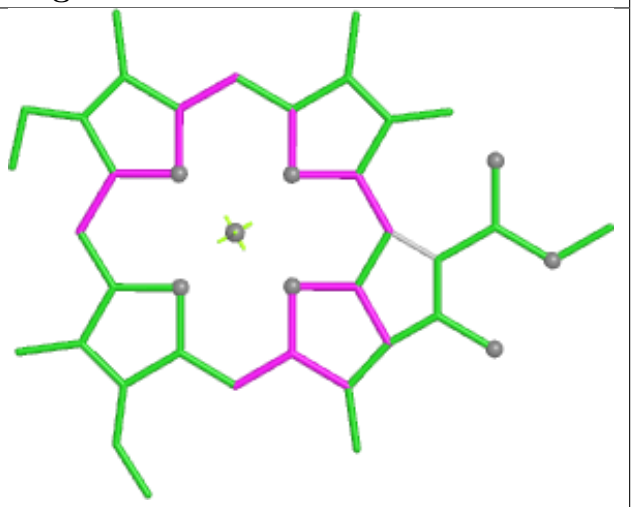
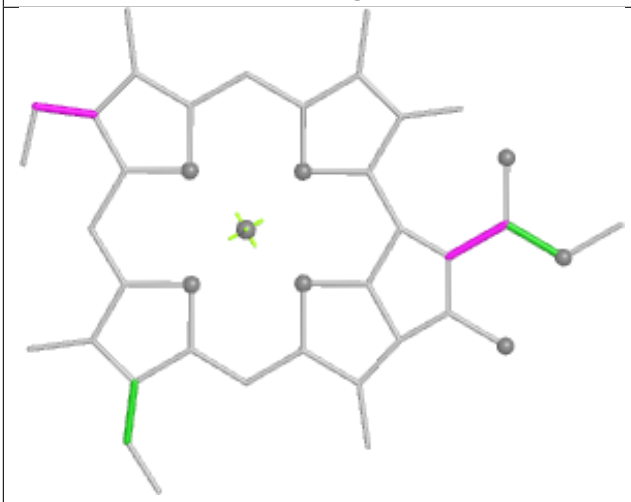


Bond angles



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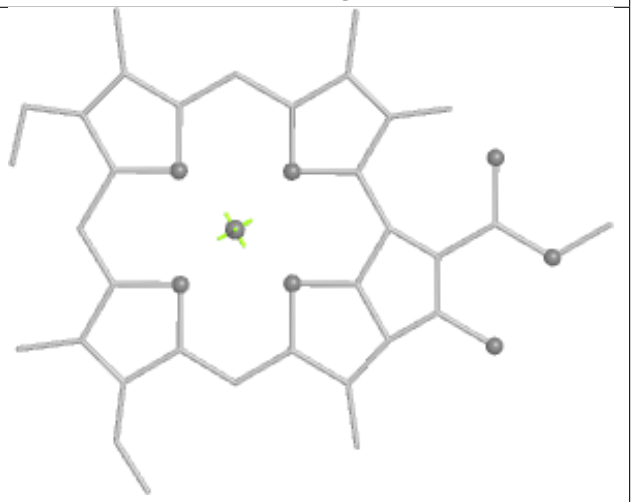
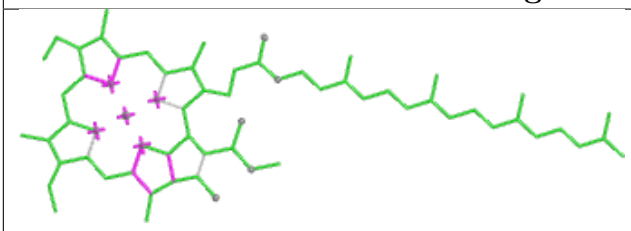


Rings

Ligand CLA C 505



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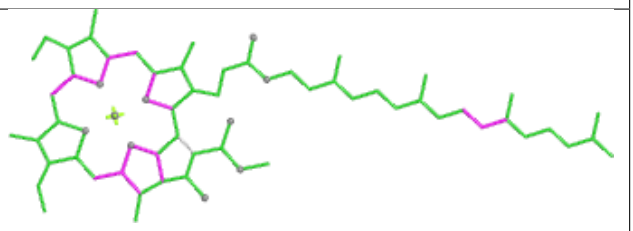
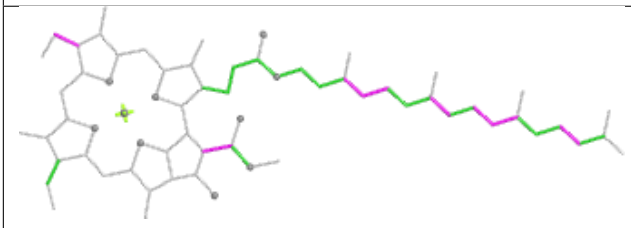
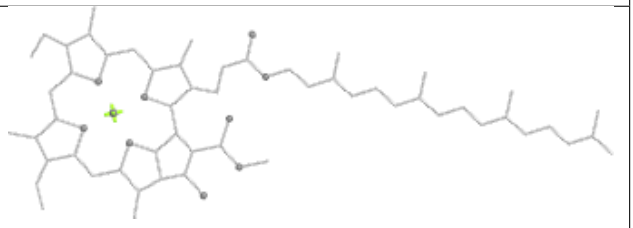


Bond angles

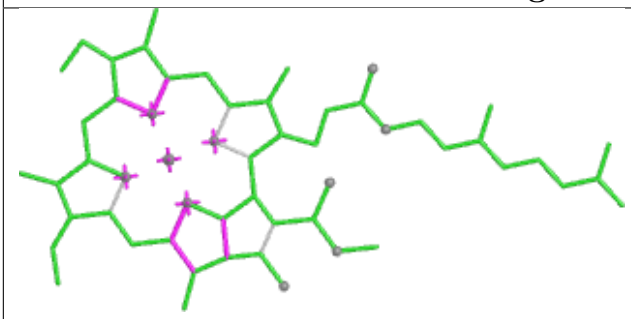


Torsions



Rings

Ligand CLA 3 312



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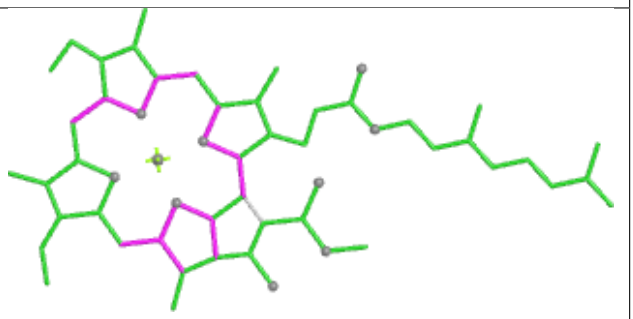

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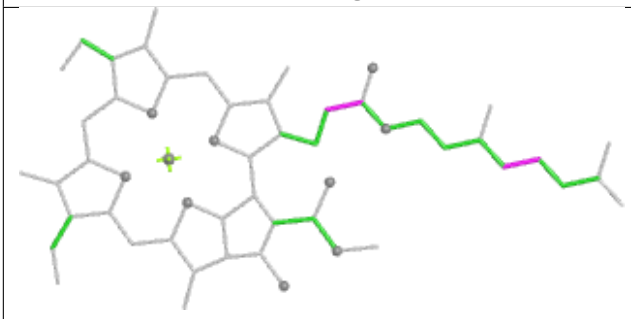
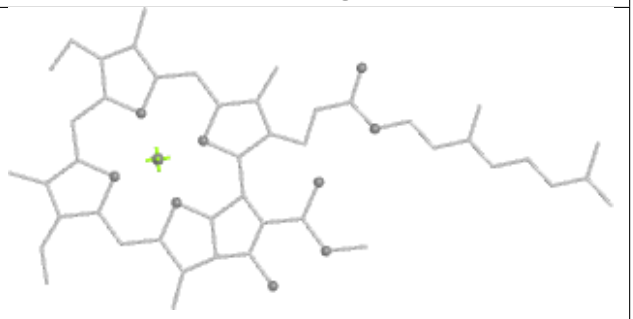
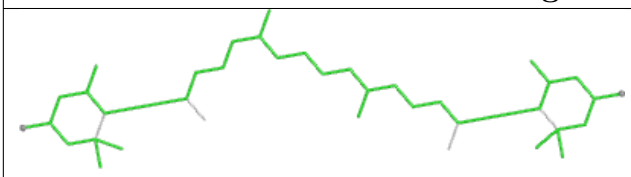


Torsions



Rings

Ligand II0 p 315



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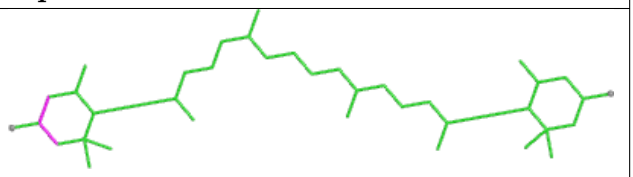

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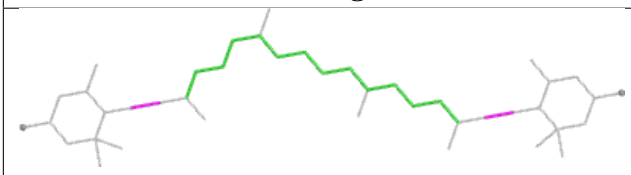

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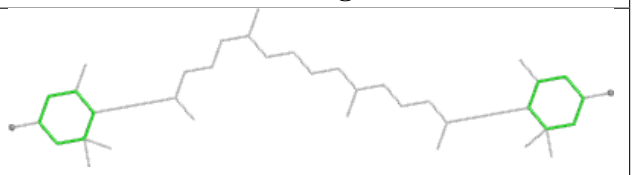
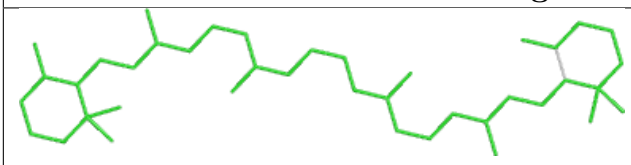


Rings

Ligand 8CT 0 312



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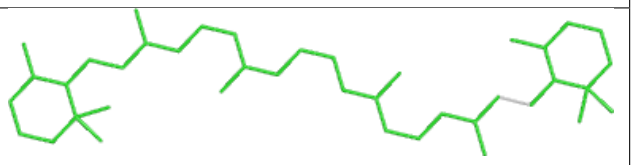

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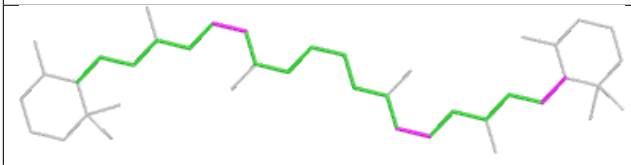

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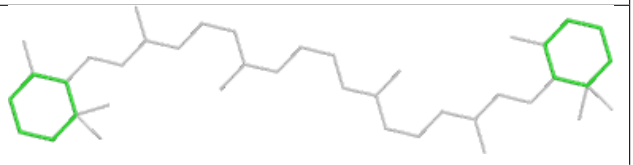
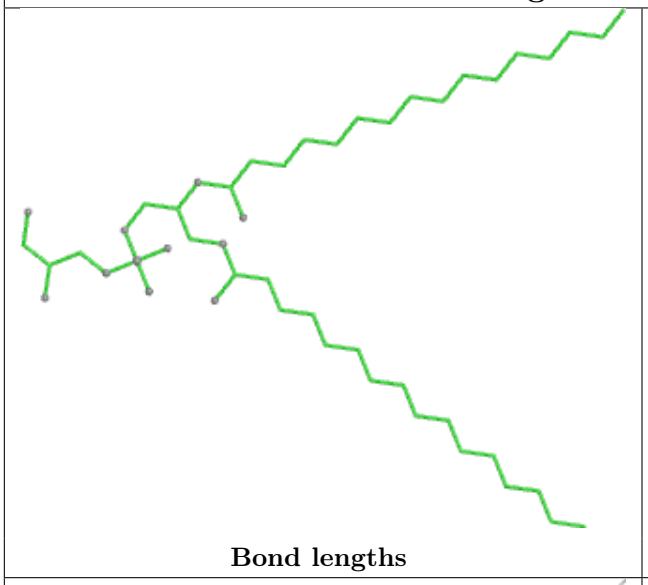


Rings

Ligand LHG 1 317



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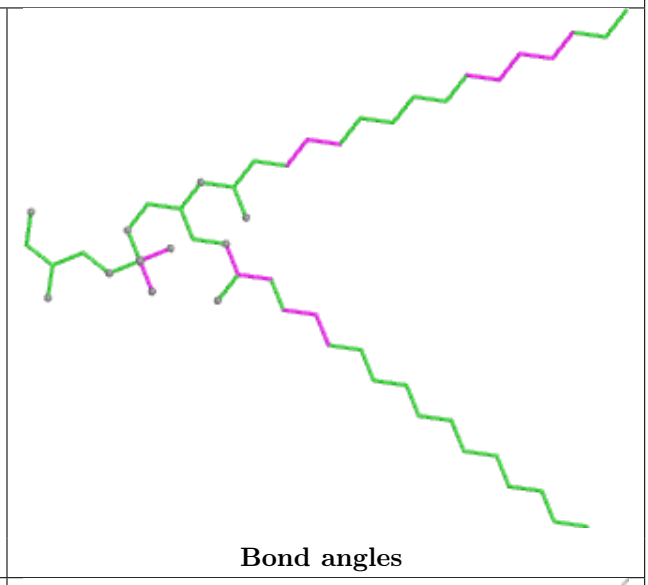

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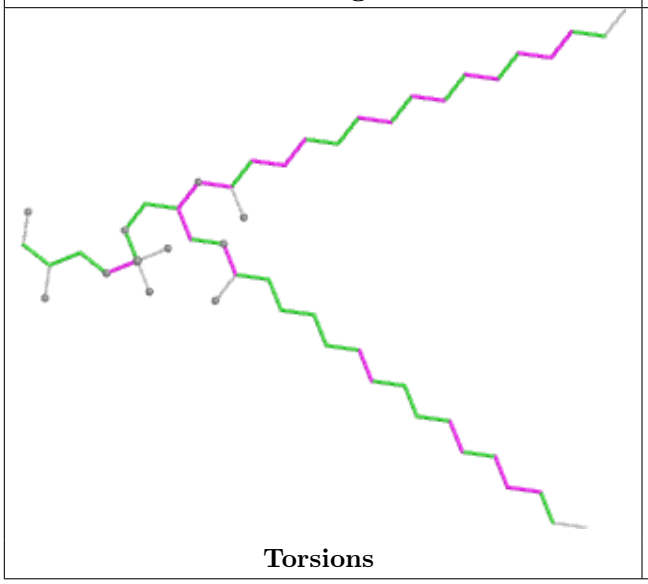

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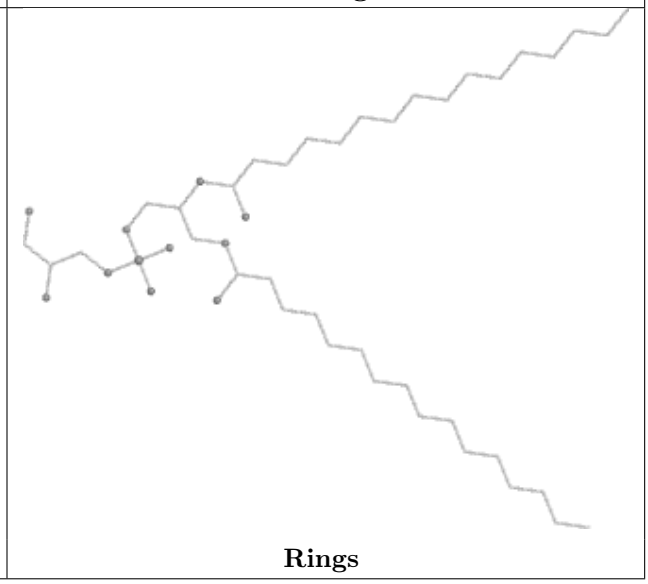
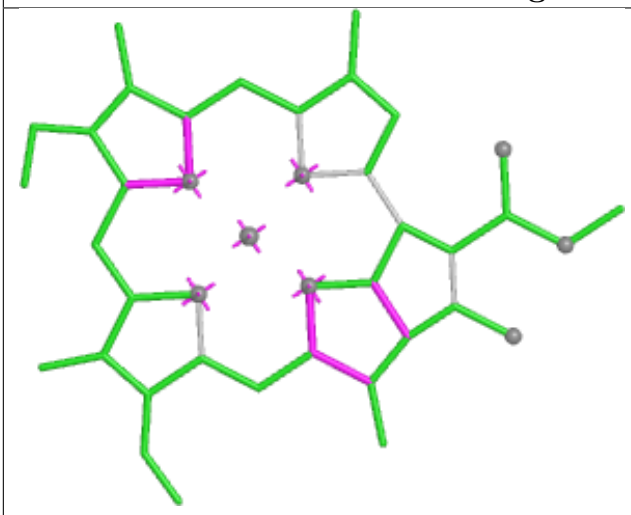


Rings

Ligand CLA 4 309



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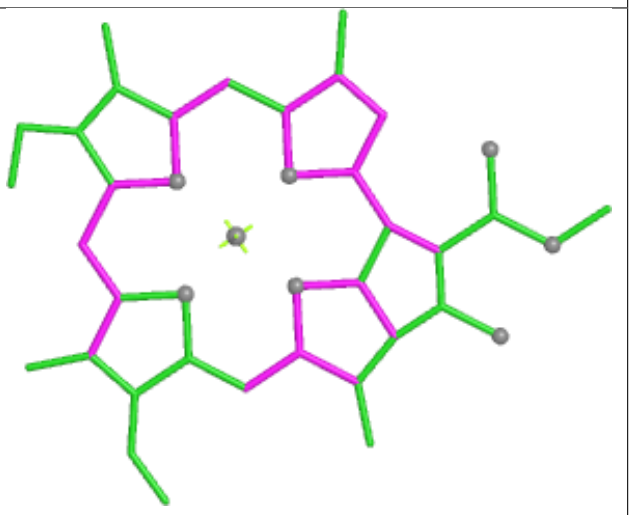

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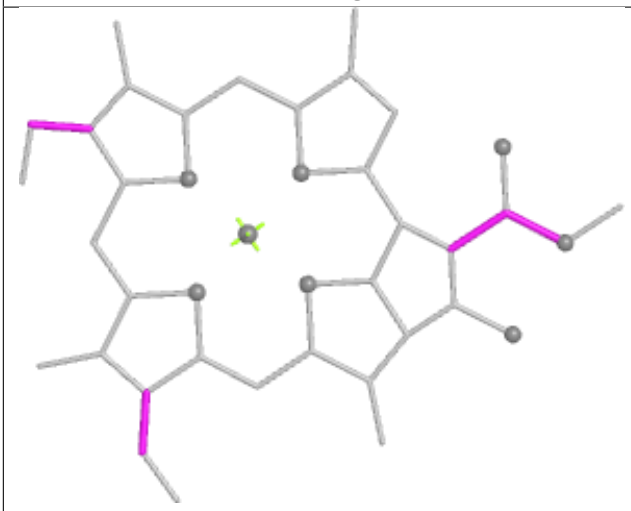

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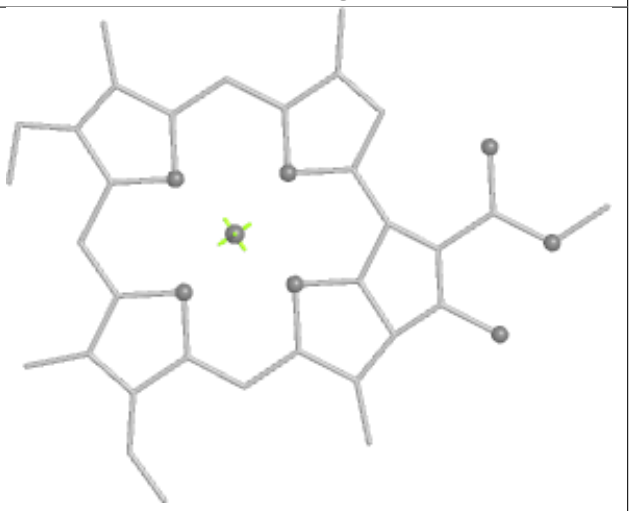
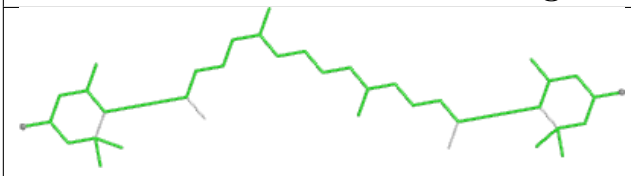


Rings

Ligand II0 9 301



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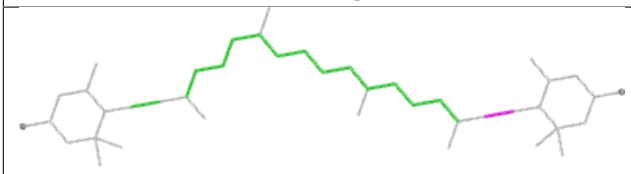

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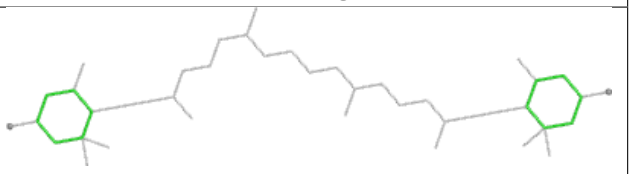
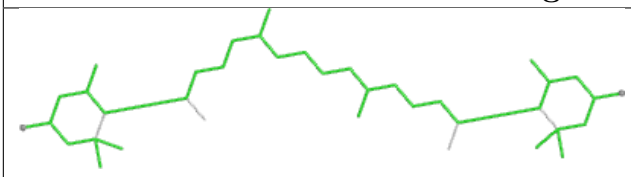


Rings

Ligand II0 7 314



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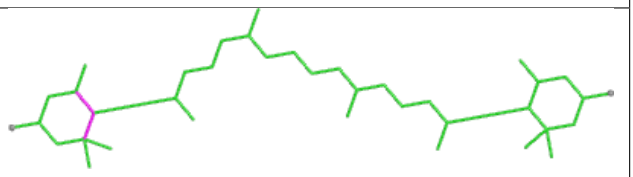

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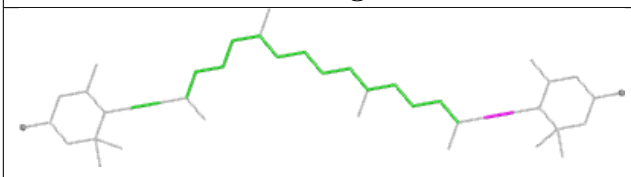

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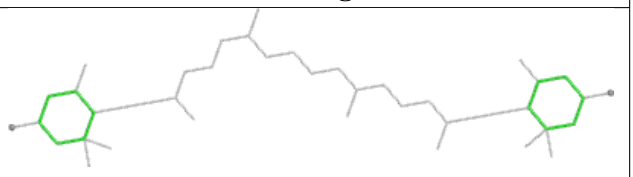
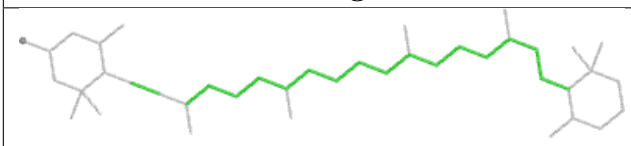


Rings

Ligand IHT 2 314

Bond lengths

Bond angles



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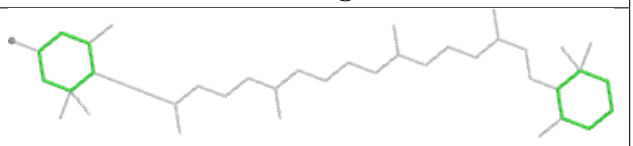
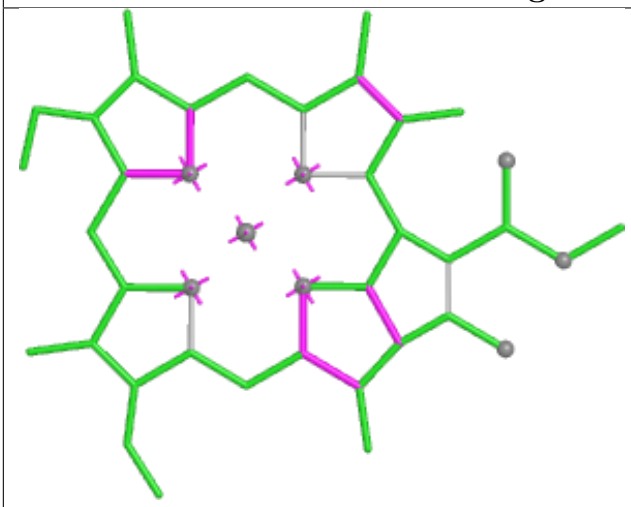


Rings

Ligand CLA 9 310



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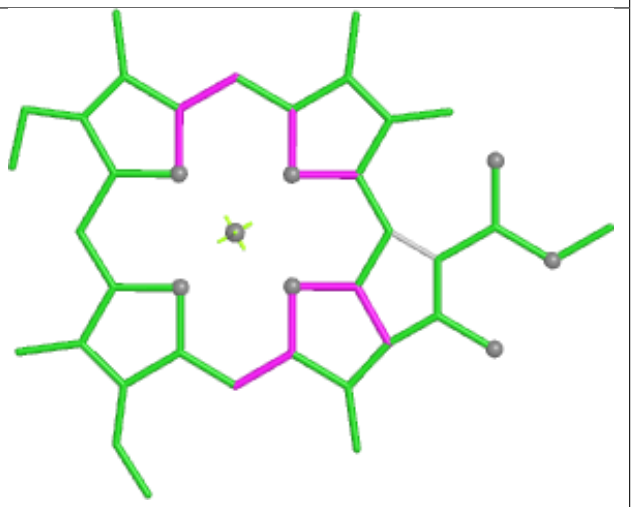

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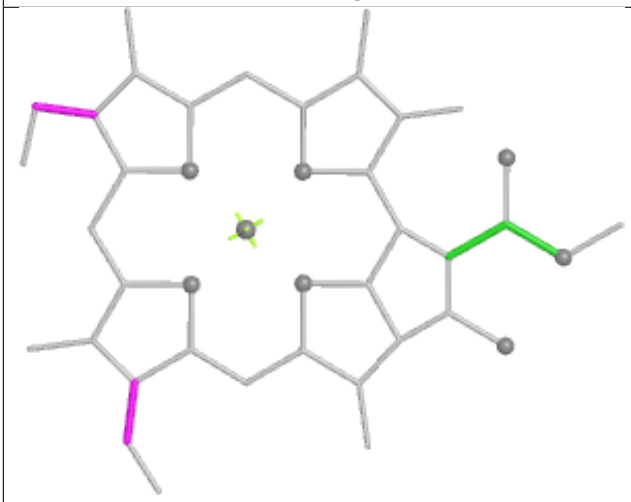

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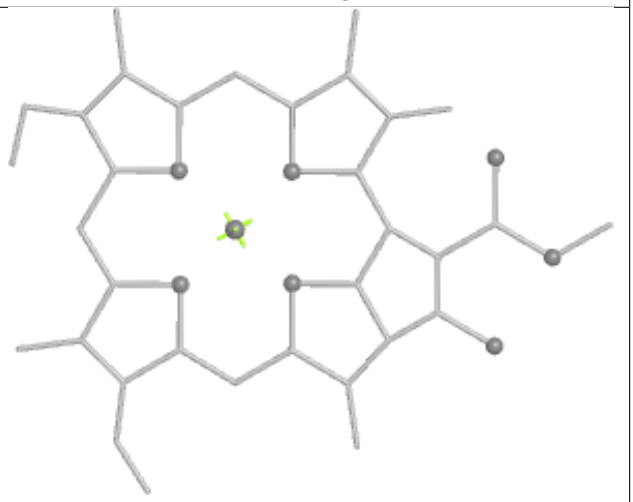
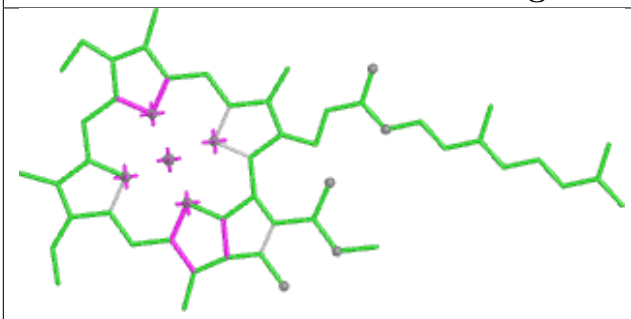


Rings

Ligand CLA 3 303



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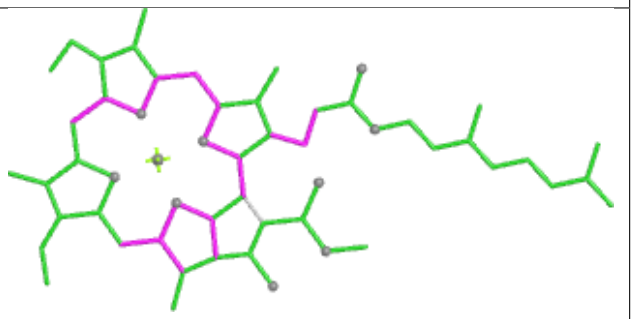

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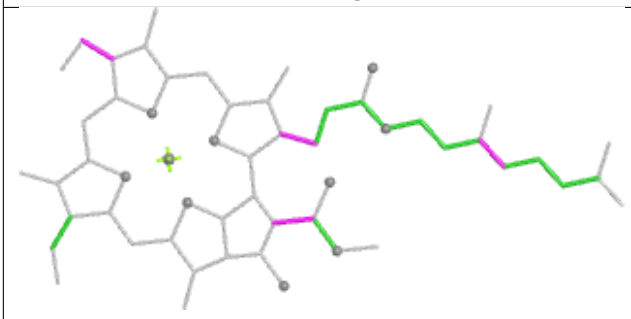

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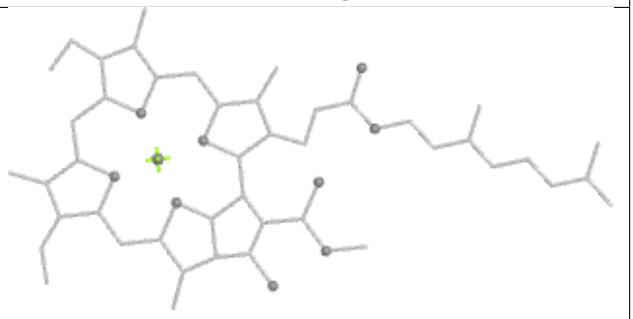
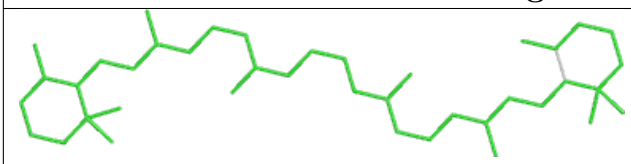


Rings

Ligand 8CT A 409



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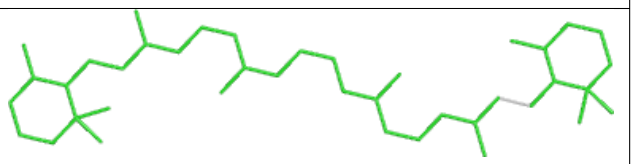

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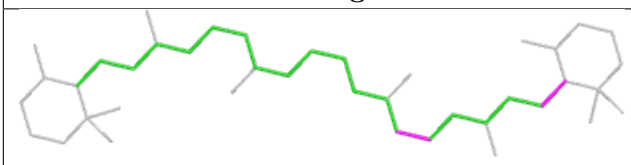

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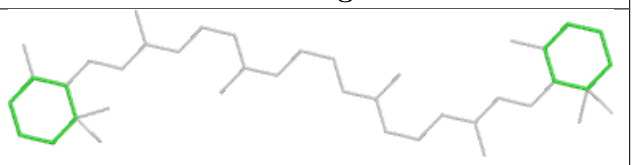
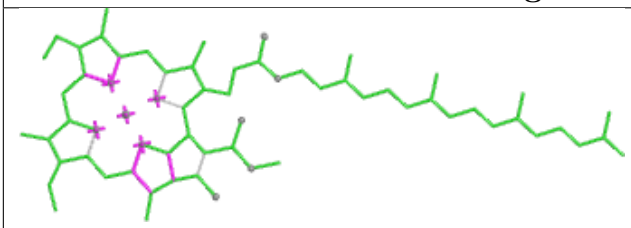


Rings

Ligand CLA B 609



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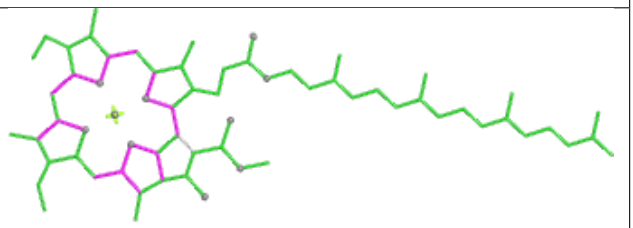

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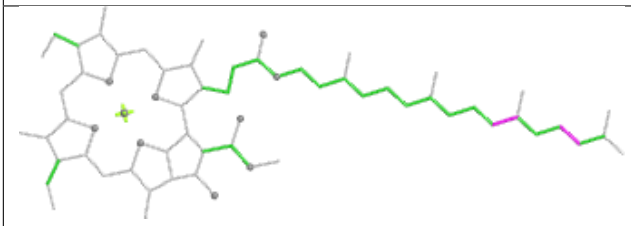

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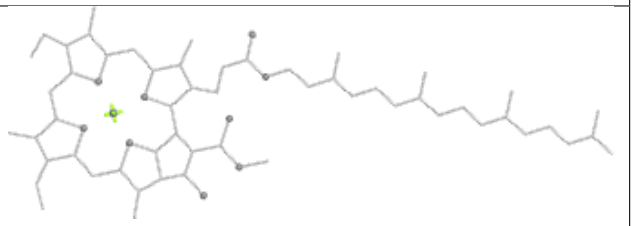
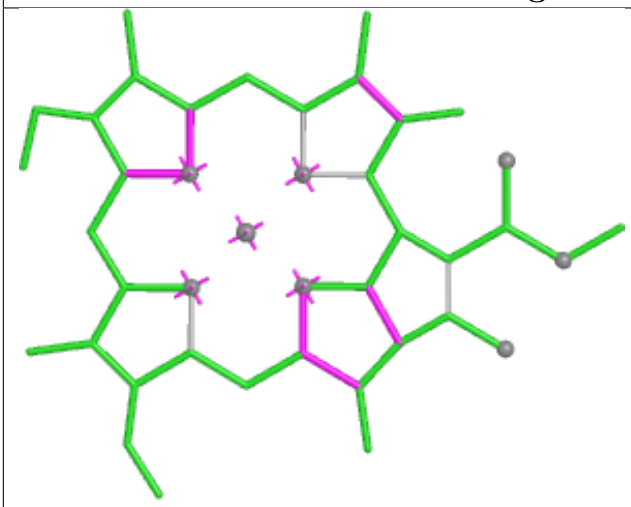


Rings

Ligand CLA 3 315



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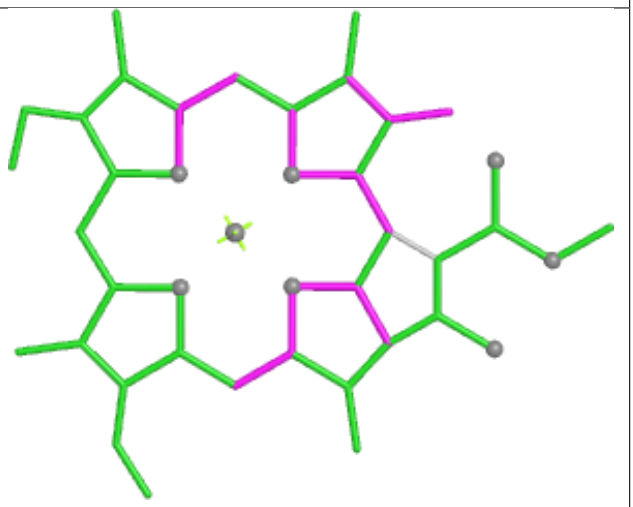
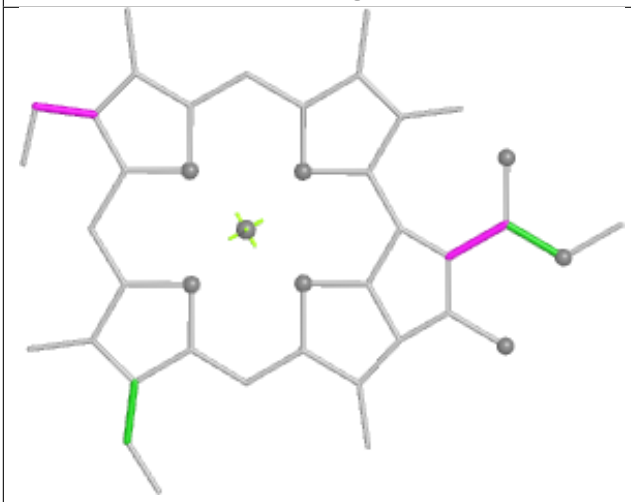
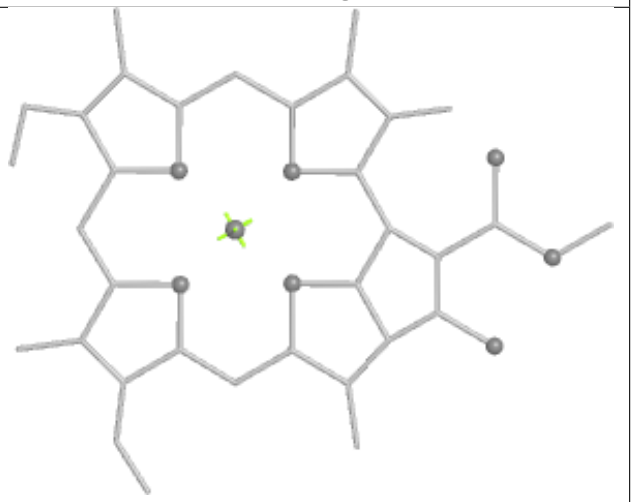


Bond angles

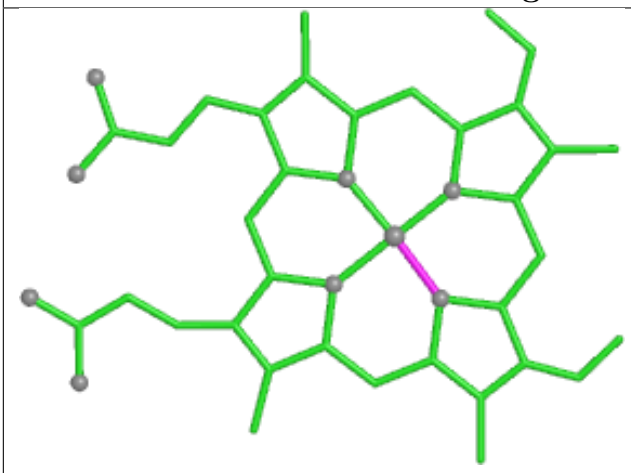


Torsions



Rings

Ligand HEM v 201



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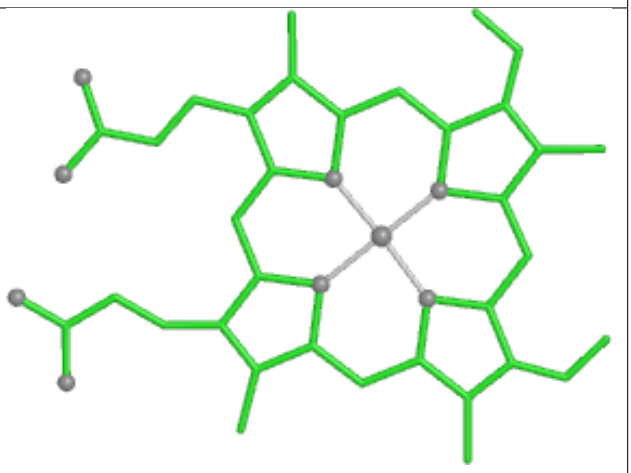
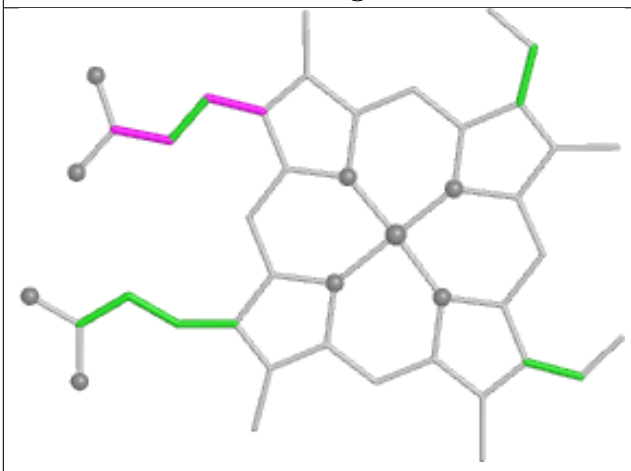


Bond angles



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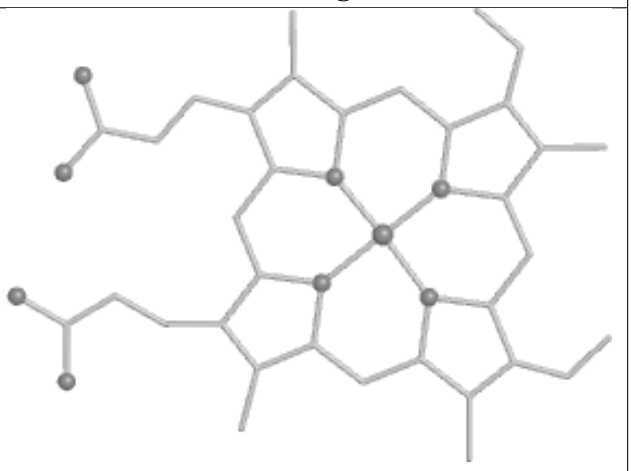
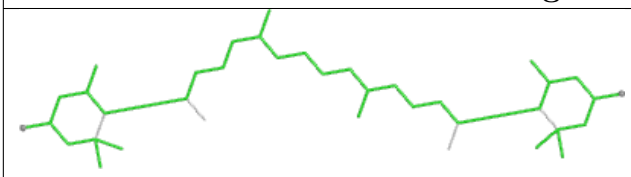


Rings

Ligand II0 0 316



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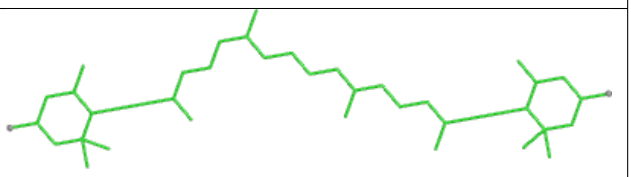
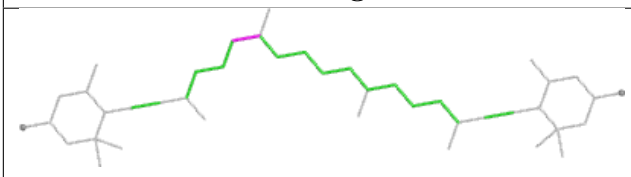
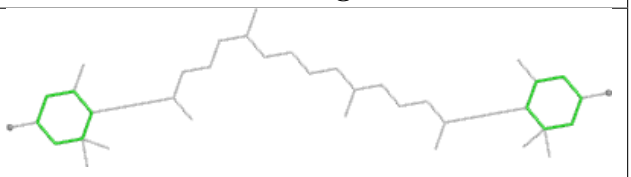


Bond angles

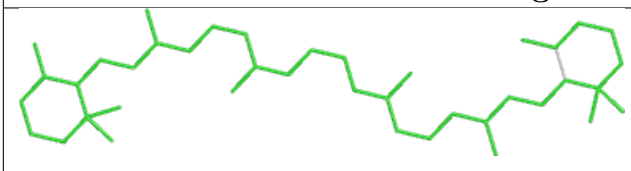


Torsions

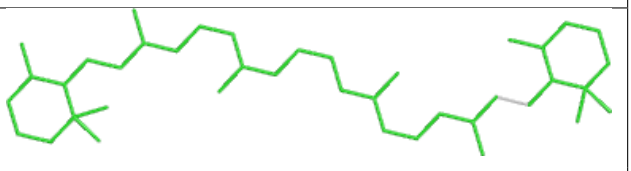


Rings

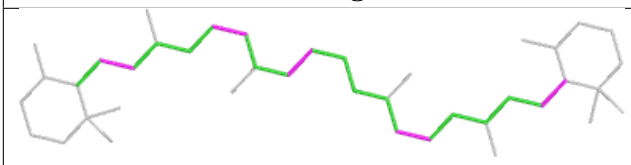
Ligand 8CT c 517



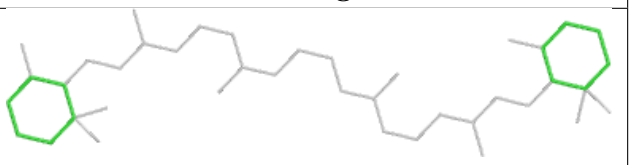
Bond lengths



Bond angles

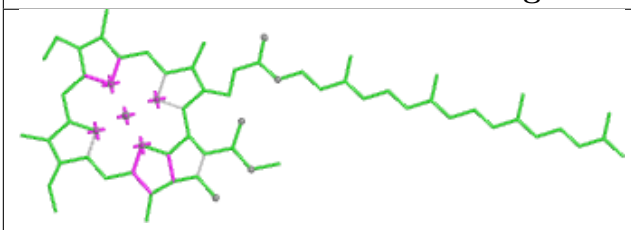


Torsions



Rings

Ligand CLA N 302



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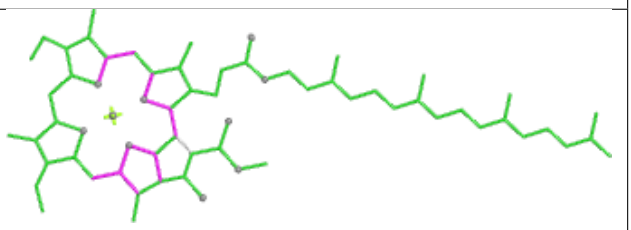

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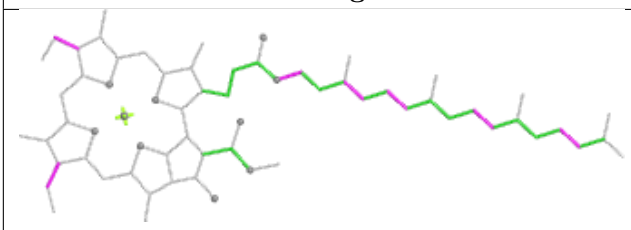
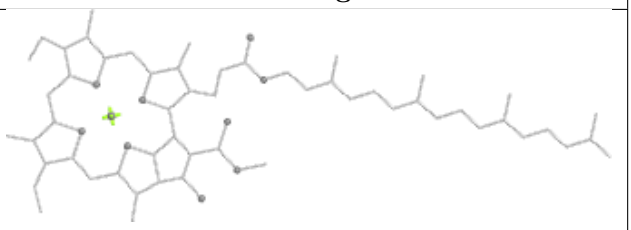
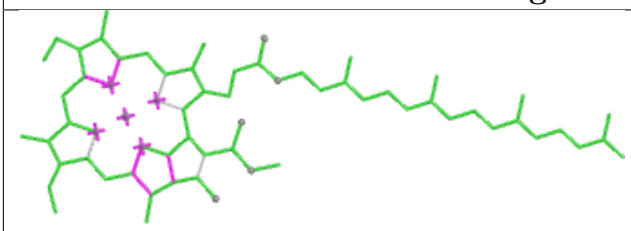


Torsions



Rings

Ligand CLA c 512



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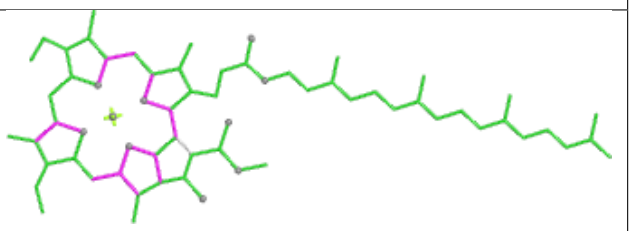

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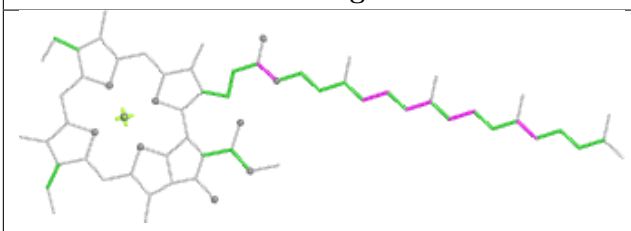

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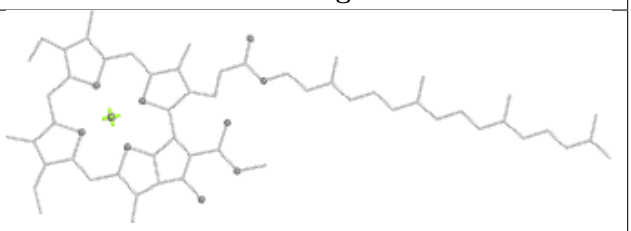
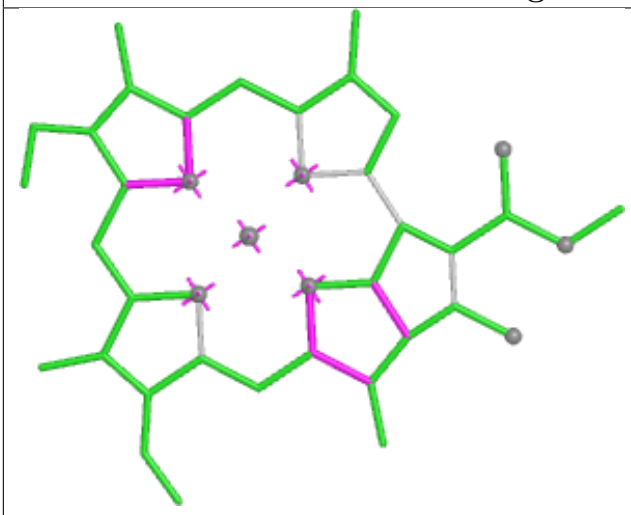


Rings

Ligand CLA b 618



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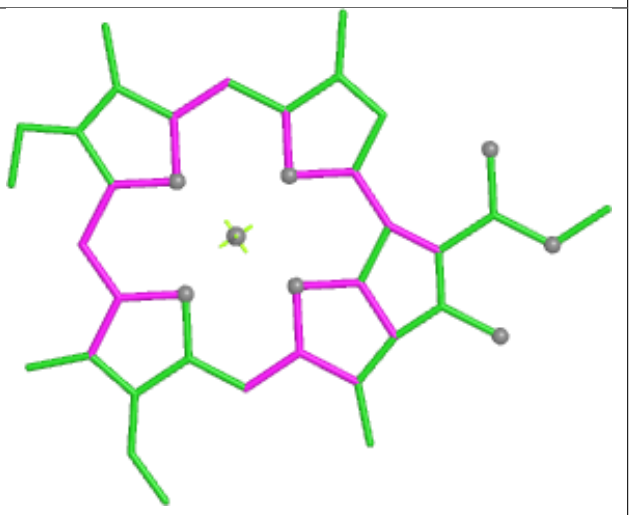
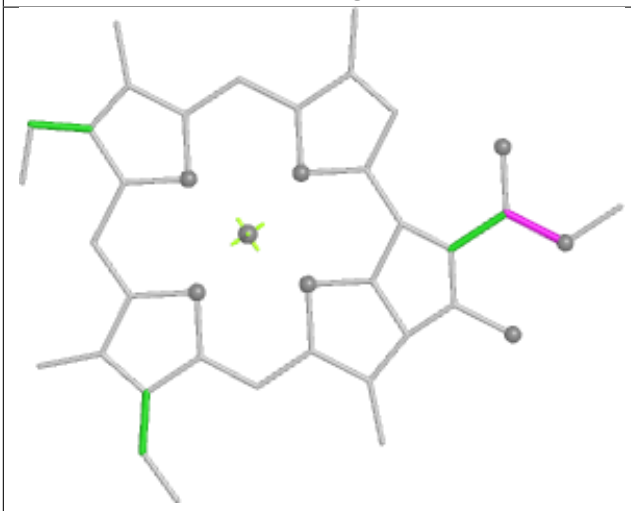


Bond angles



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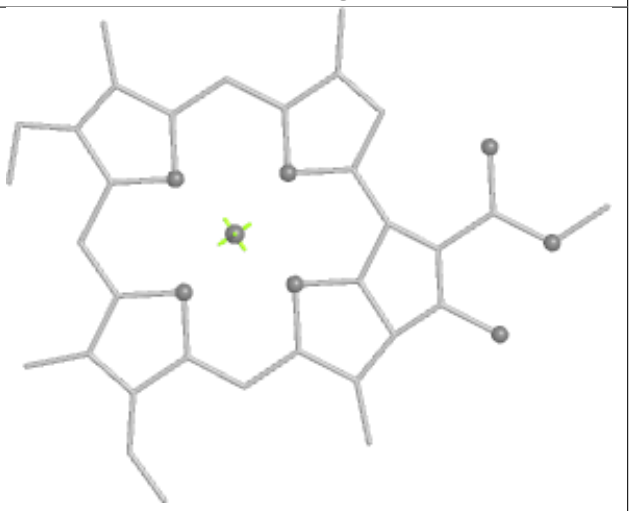
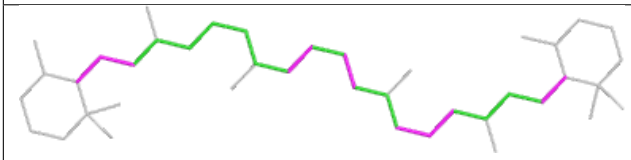


Rings

Ligand 8CT D 406

Bond lengths

Bond angles



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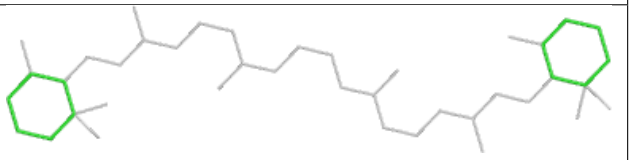
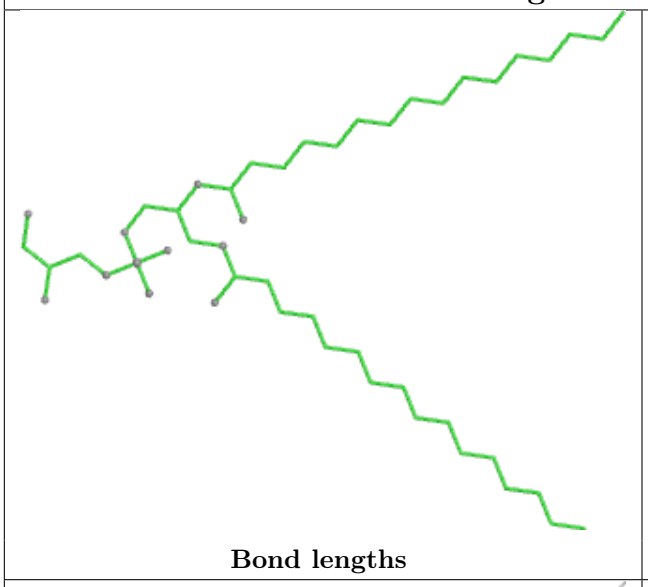


Rings

Ligand LHG 7 317



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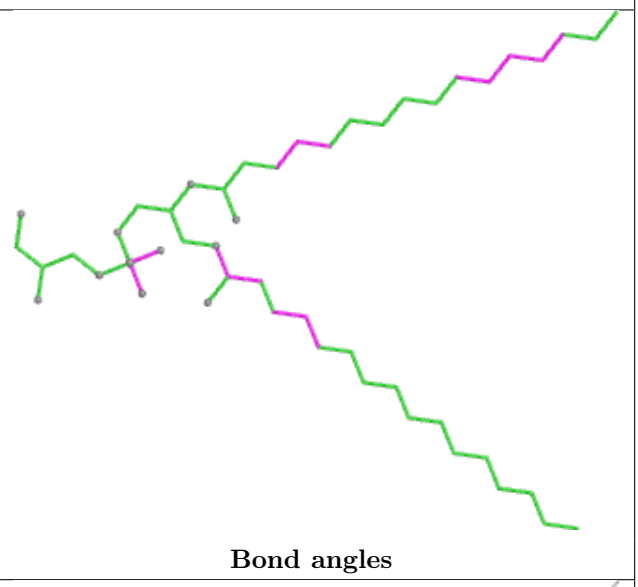
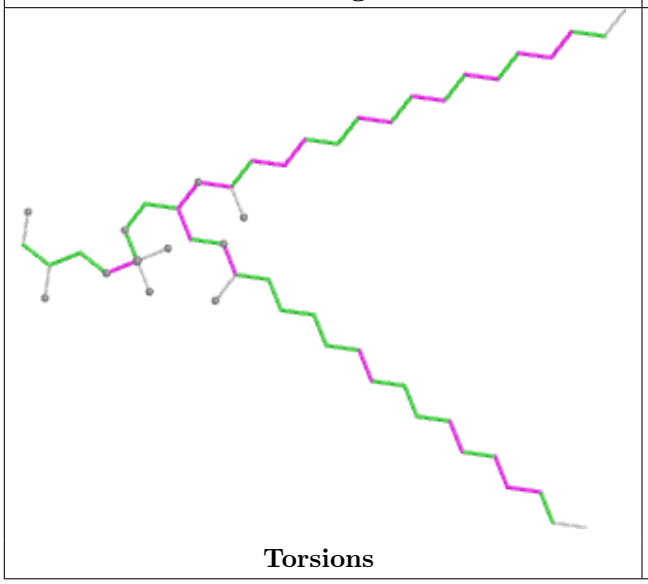


Bond angles



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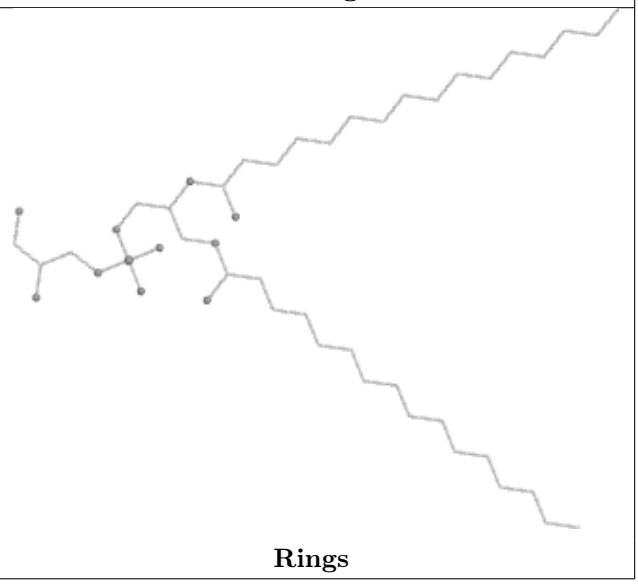
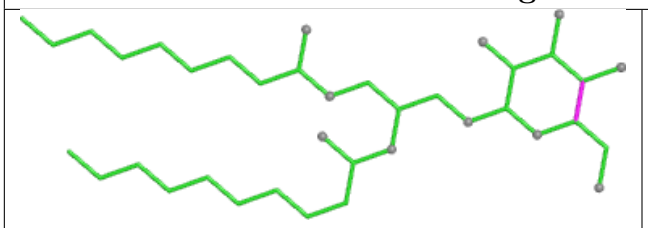


Rings

Ligand LMG m 101



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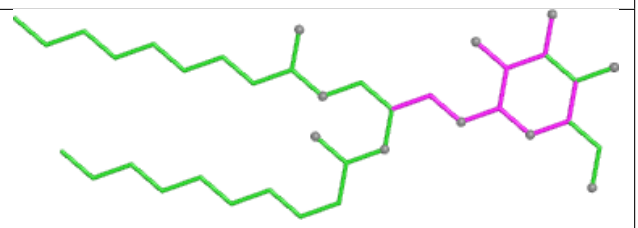
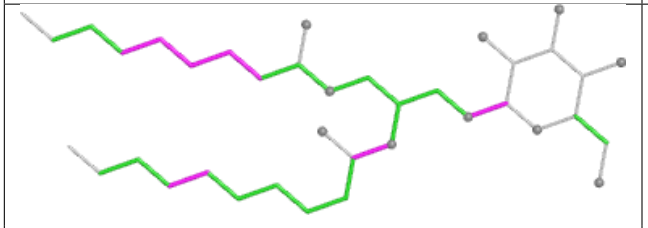


Bond angles



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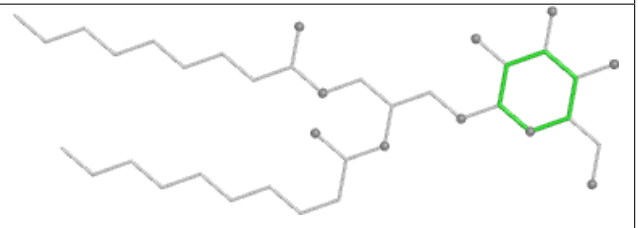
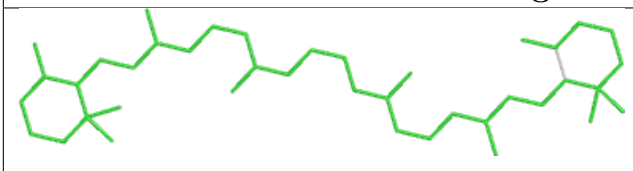


Rings

Ligand 8CT c 516



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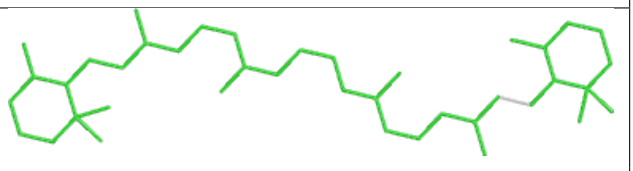
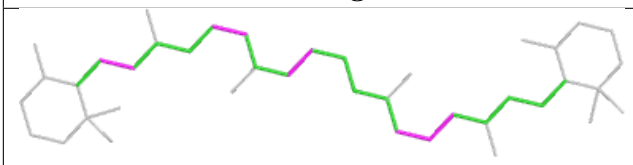


Bond angles



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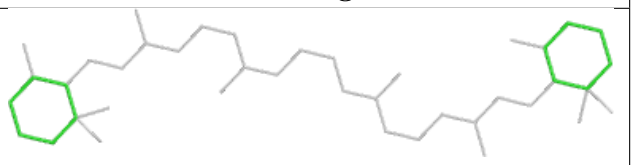
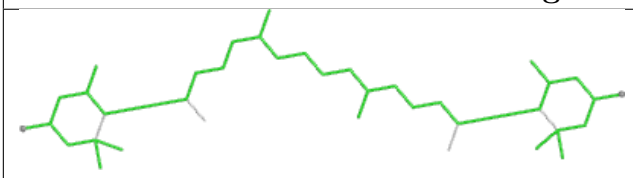


Rings

Ligand II0 6 315



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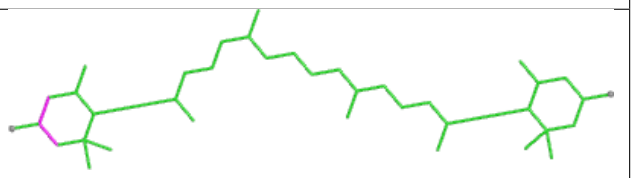

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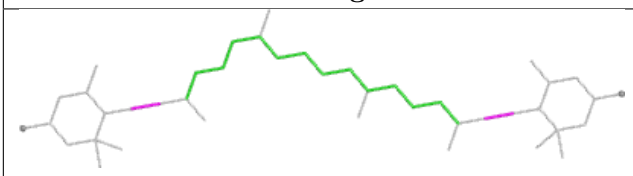

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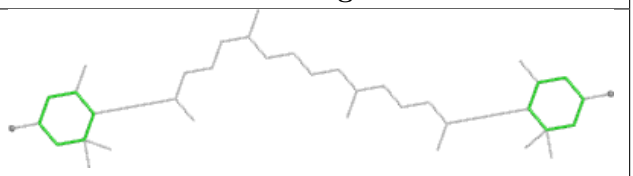
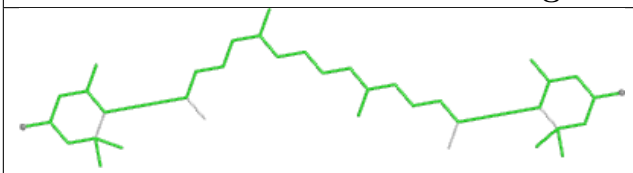


Rings

Ligand II0 2 313



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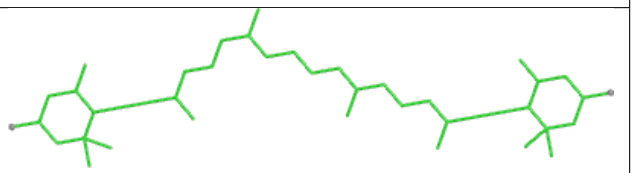
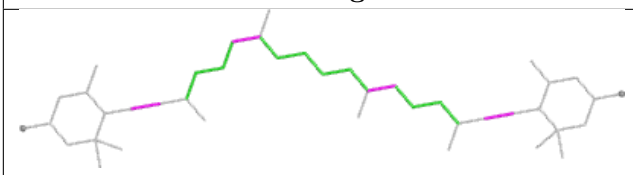


Bond angles



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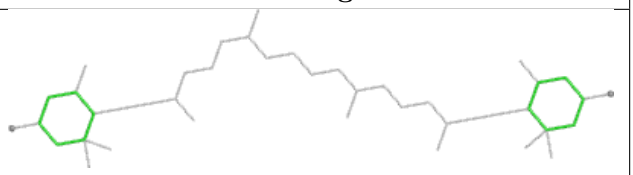
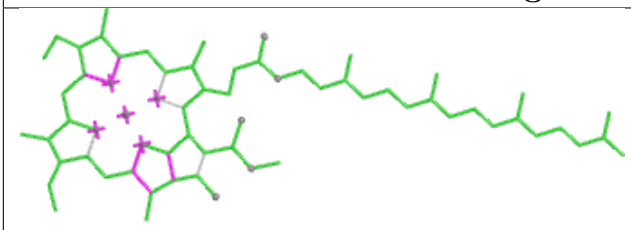


Rings

Ligand CLA C 508



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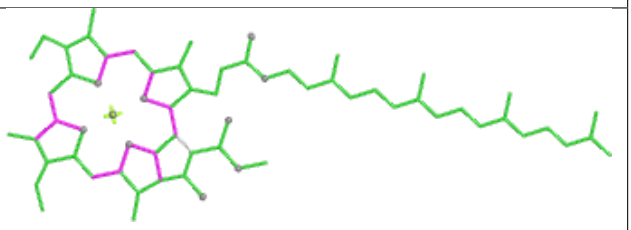
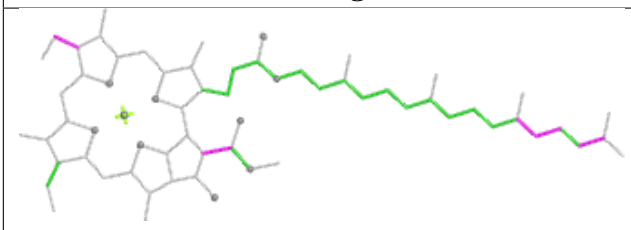


Bond angles



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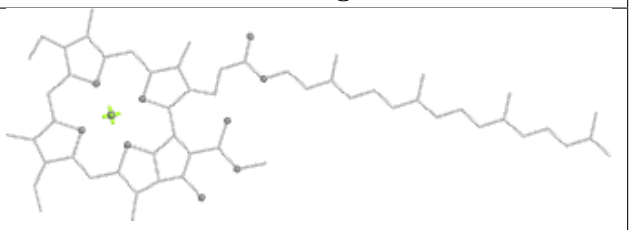
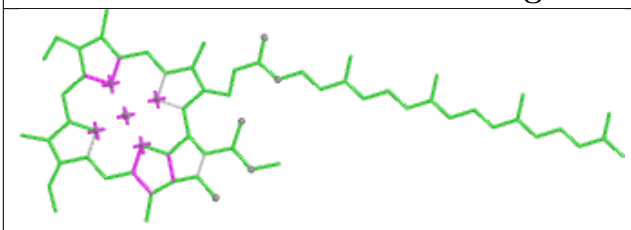


Rings

Ligand CLA C 506



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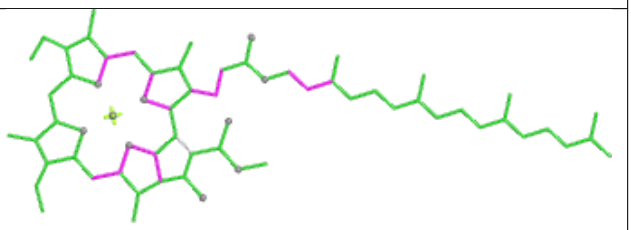
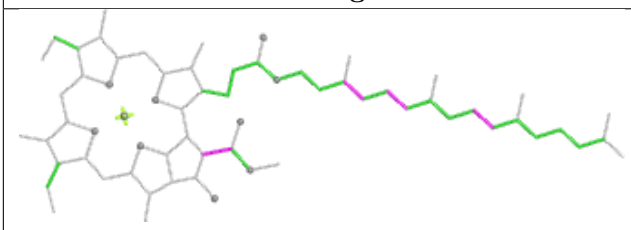
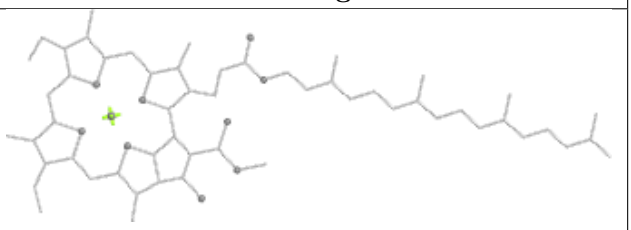


Bond angles

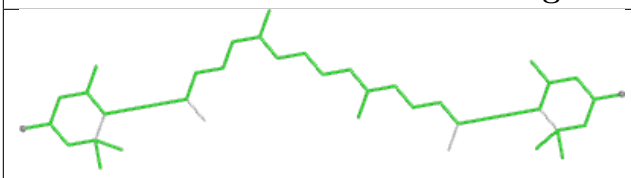


Torsions



Rings

Ligand II0 0 315



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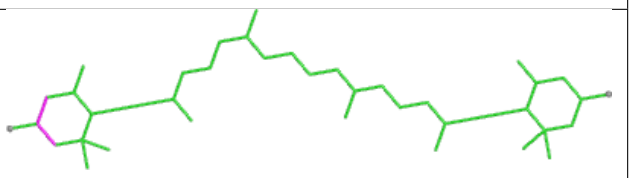
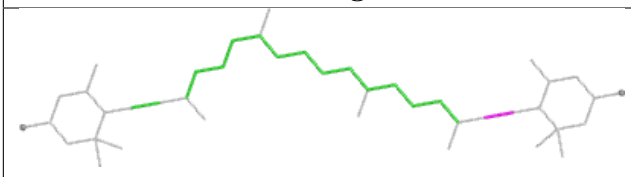


Bond angles



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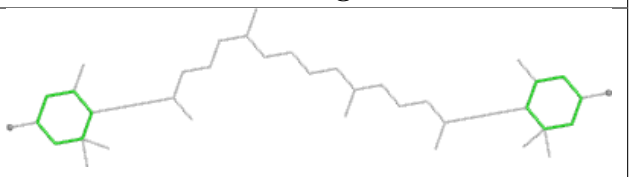
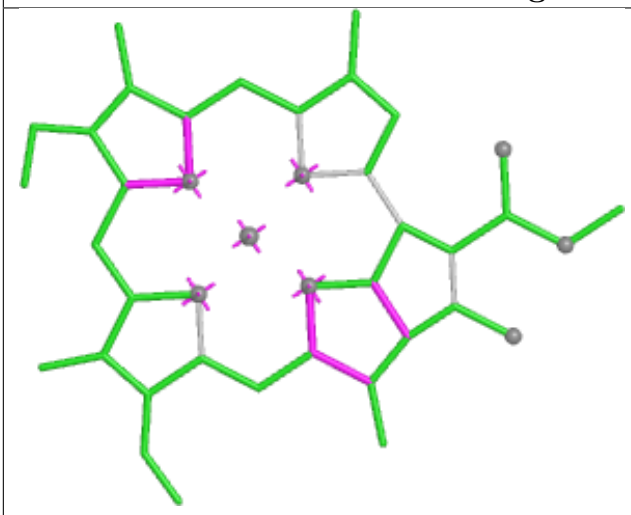
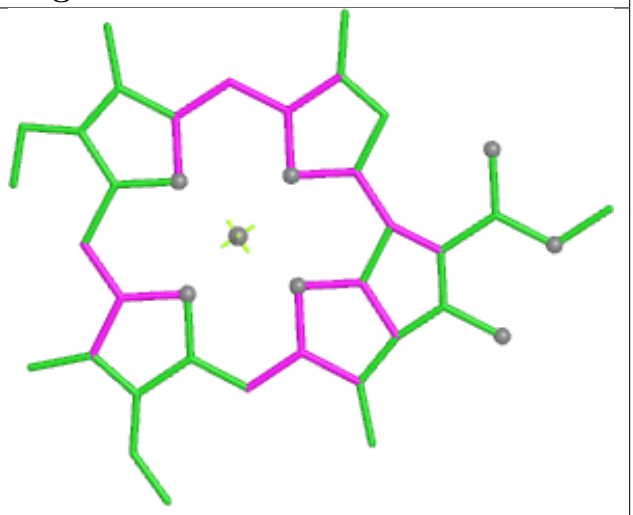


Rings

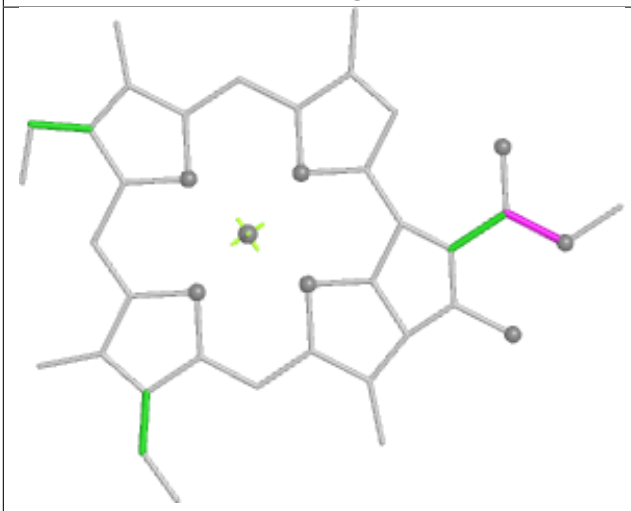
Ligand CLA g 305



Bond lengths



Bond angles



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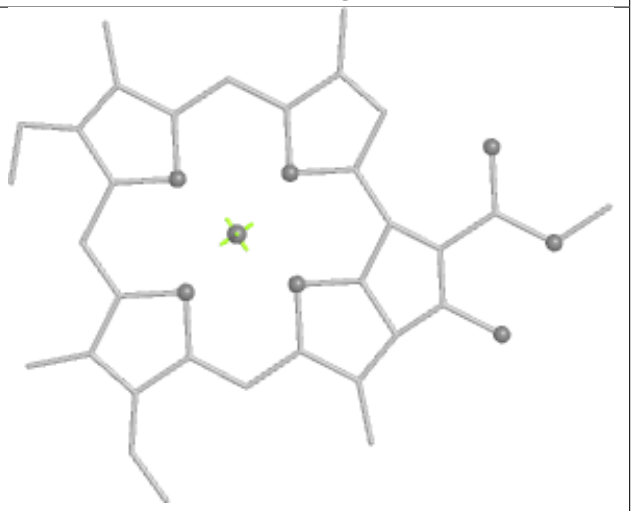
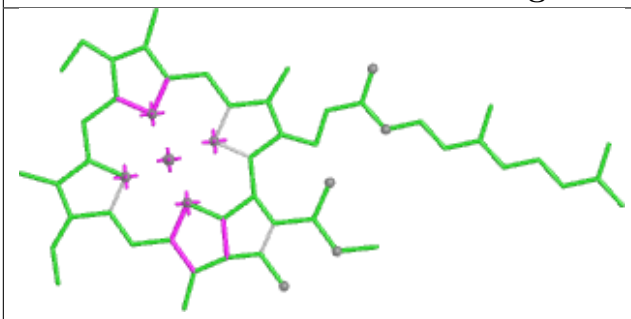
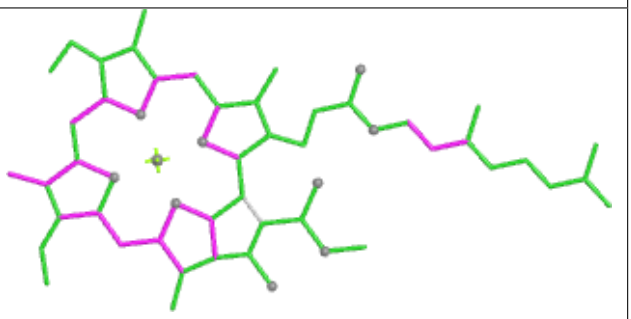
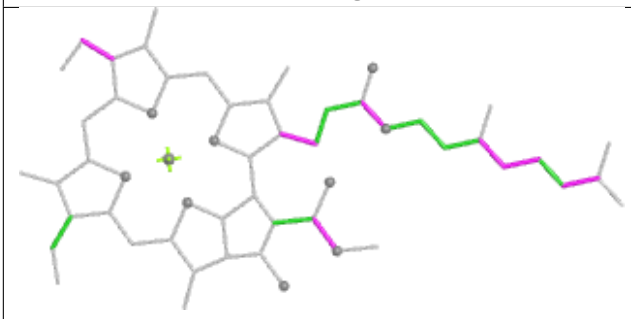
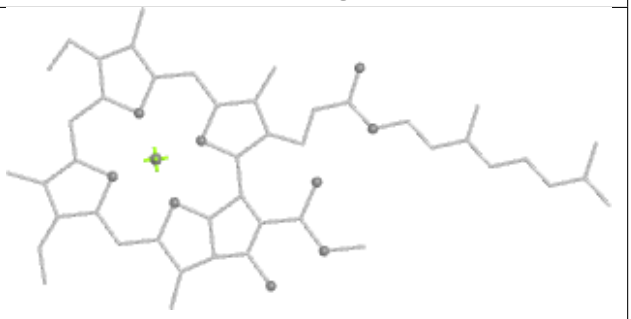
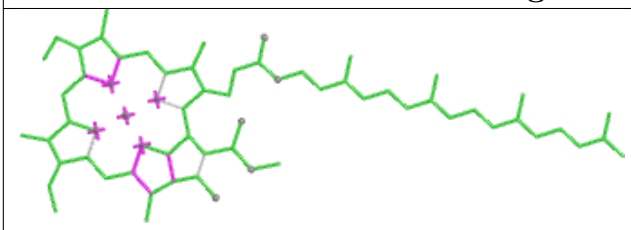
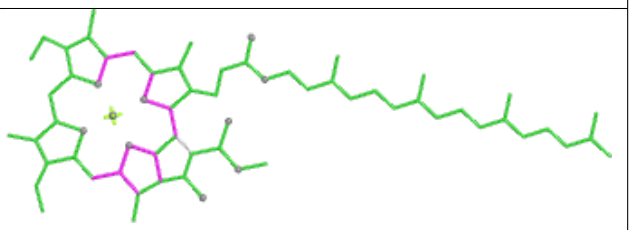
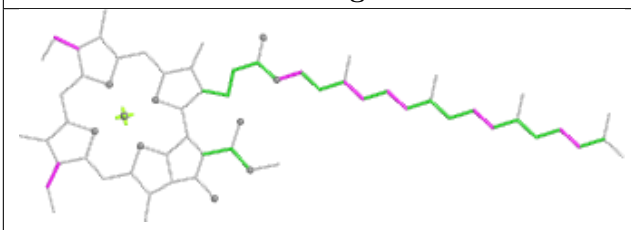
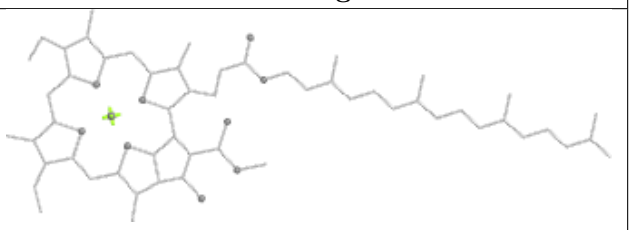
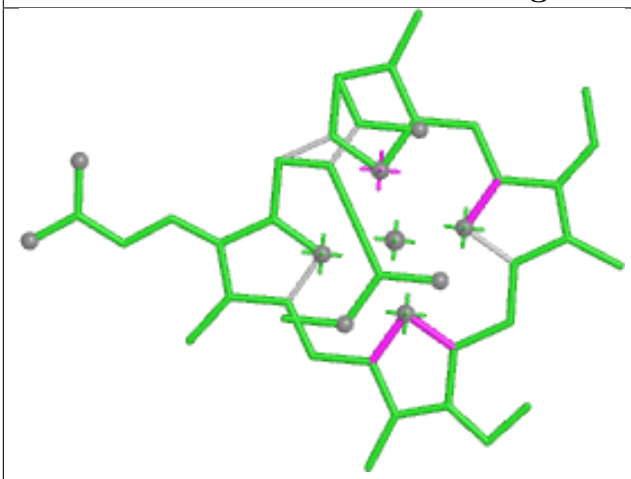


Rings

Ligand CLA 0 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA n 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand KC2 5 309



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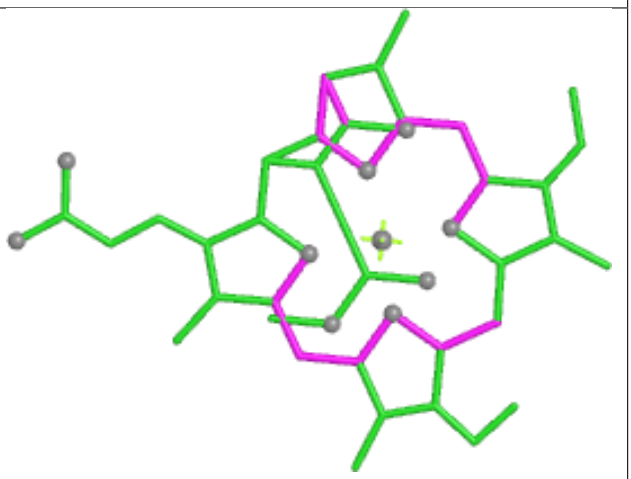
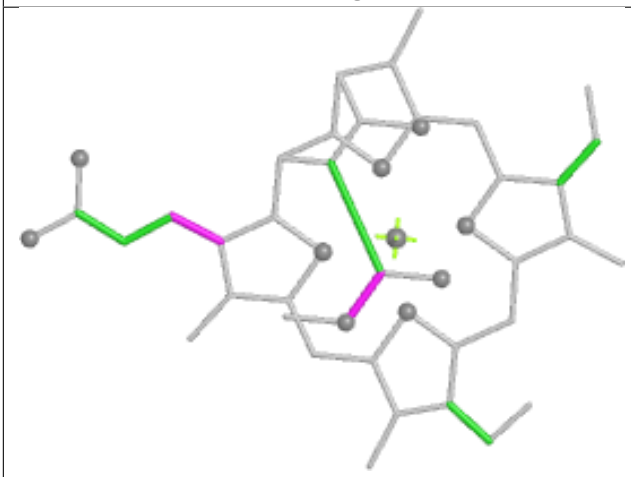
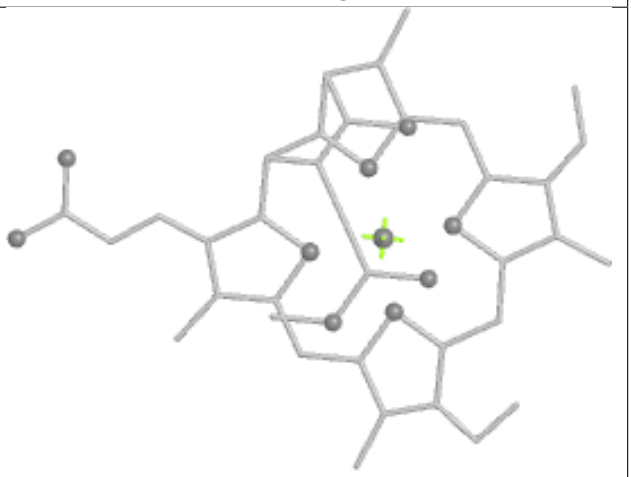


Bond angles

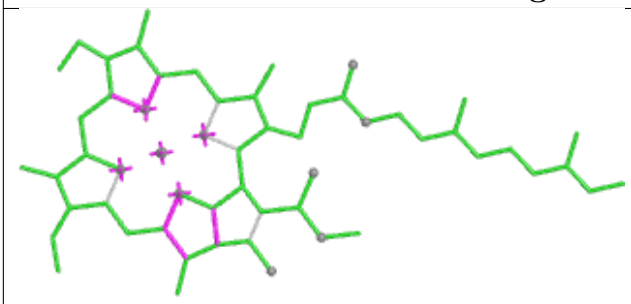


Torsions



Rings

Ligand CLA c 513



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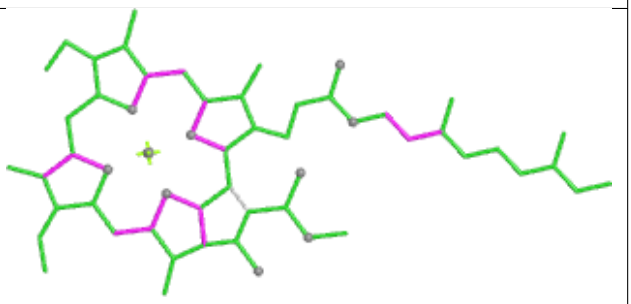

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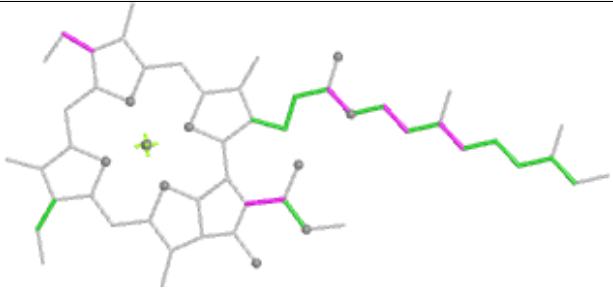
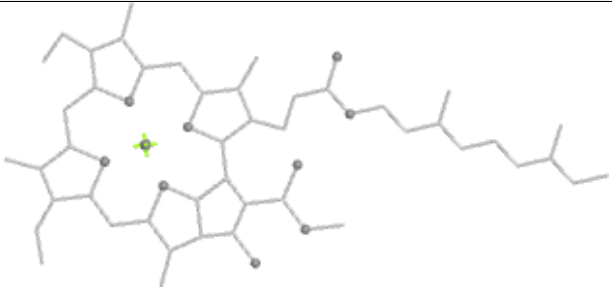
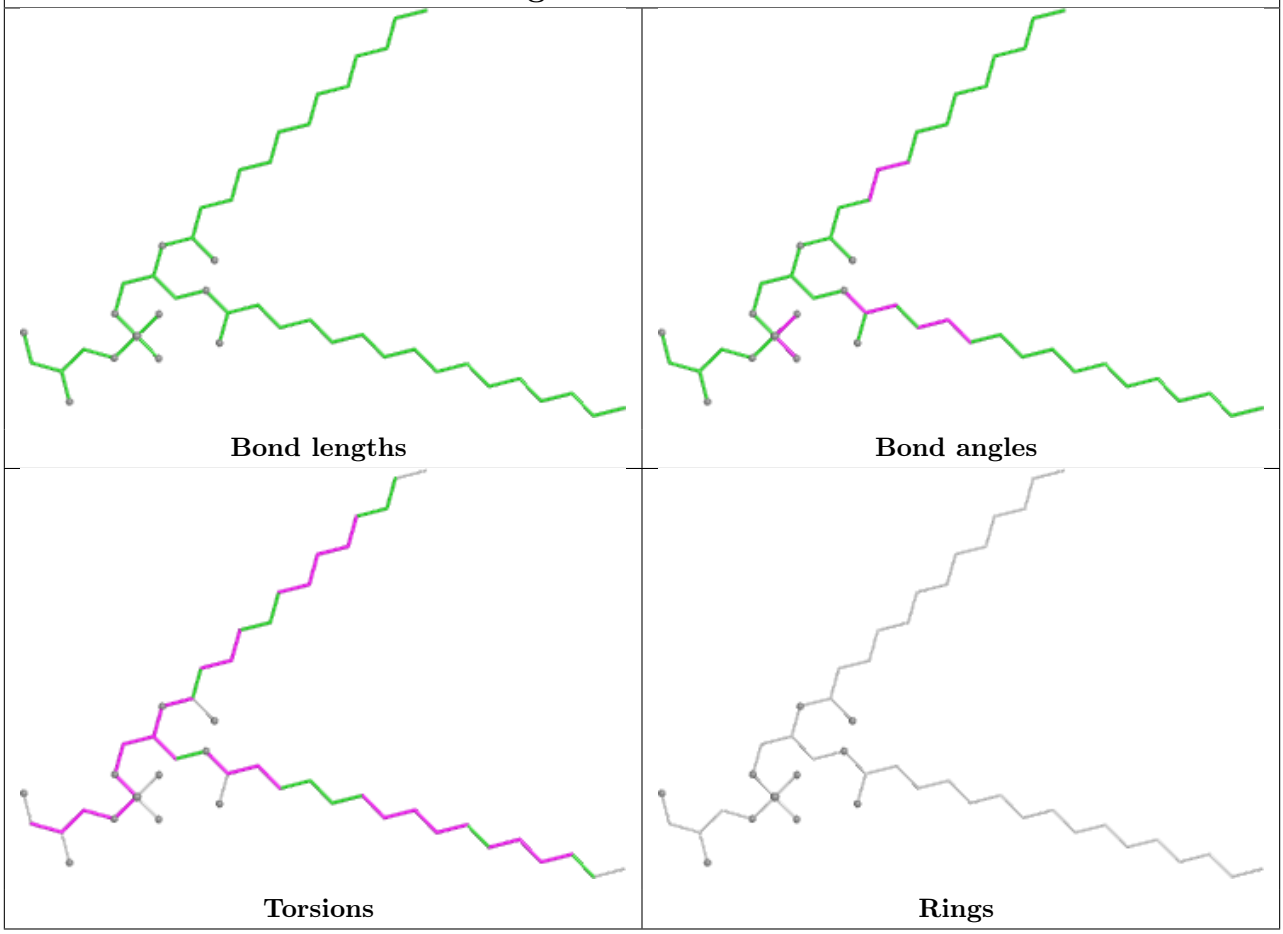


Torsions



Rings

Ligand LHG 2 315



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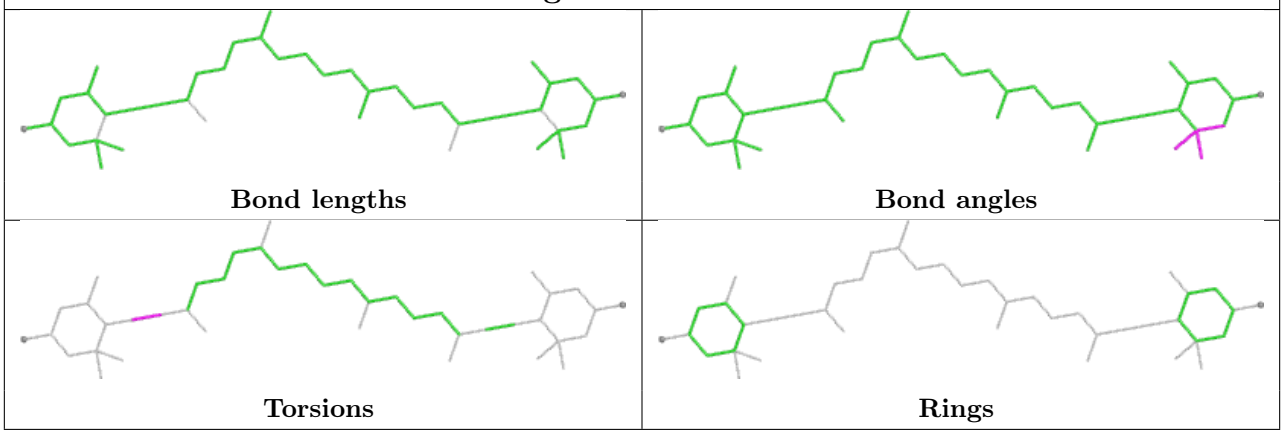
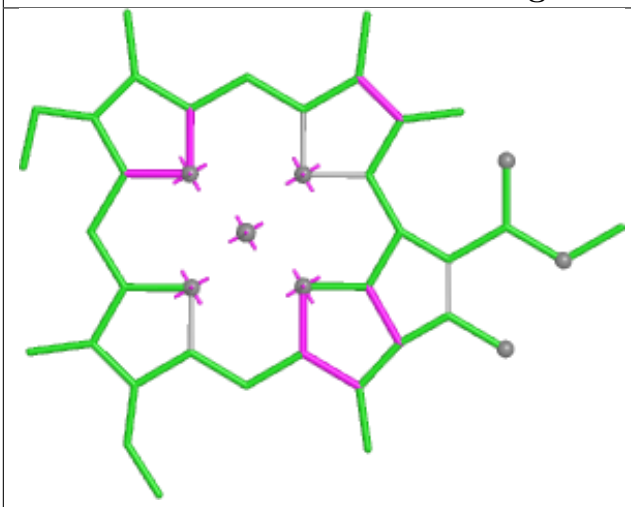


Ligand CLA 4 301



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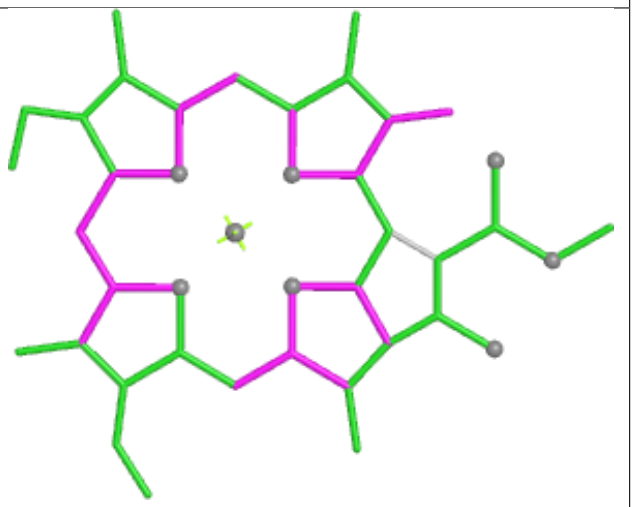

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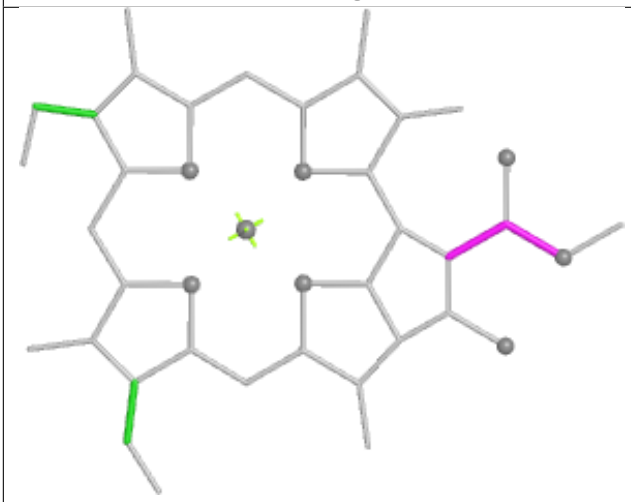

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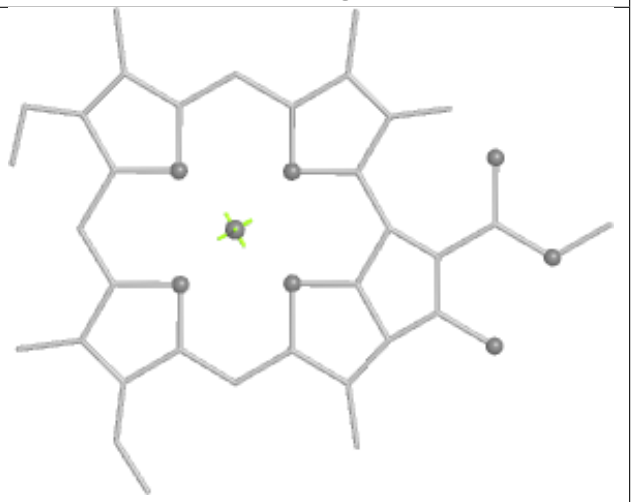
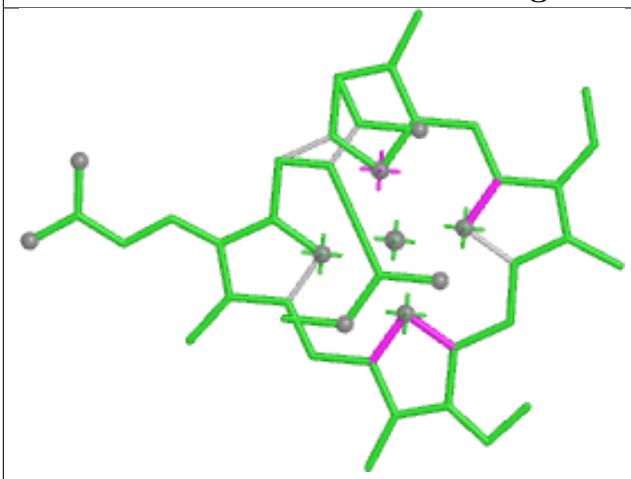


Rings

Ligand KC2 3 311



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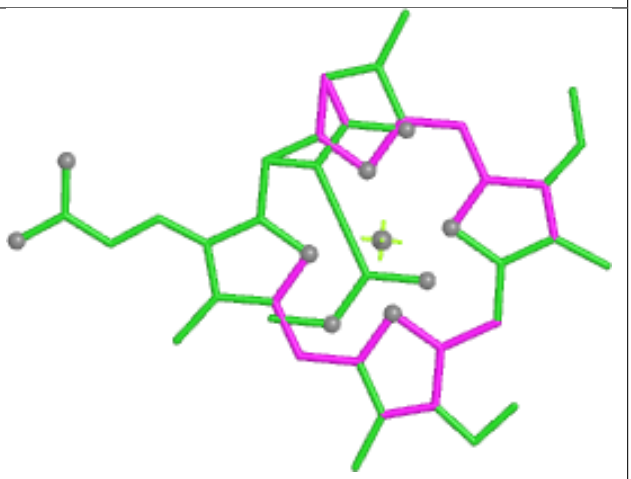
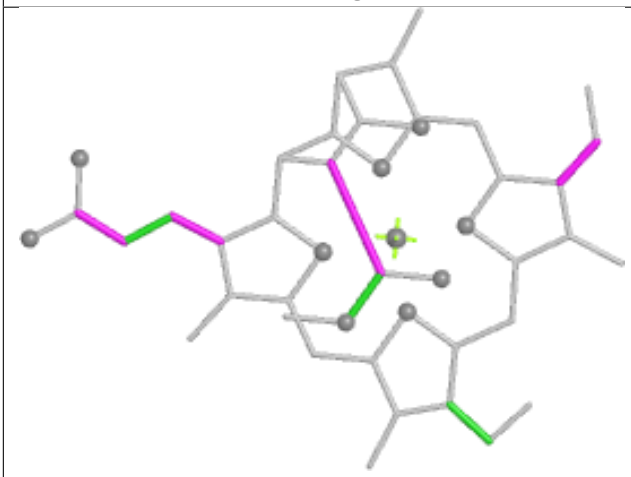


Bond angles



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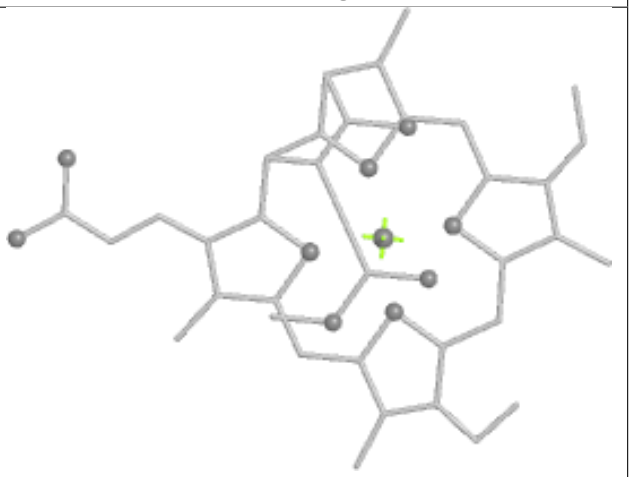
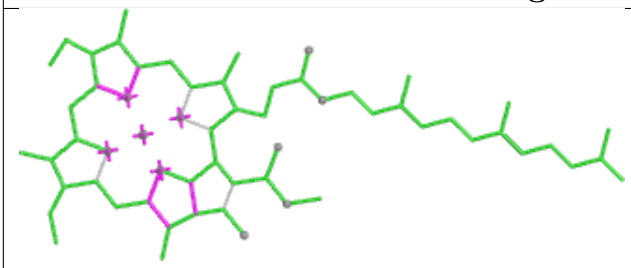


Rings

Ligand CLA 7 305



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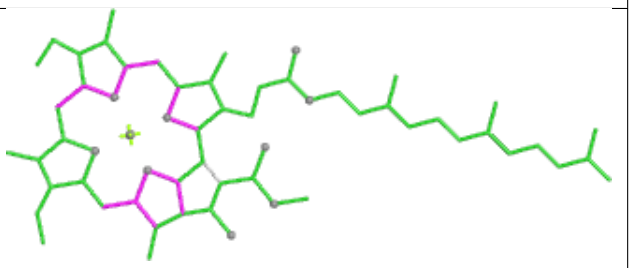

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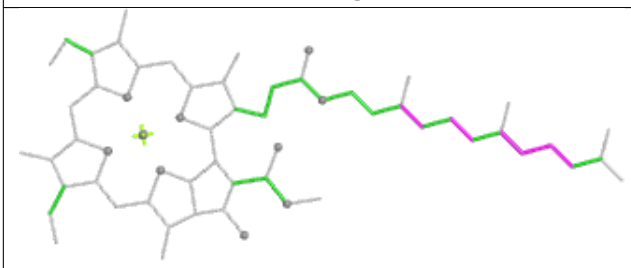

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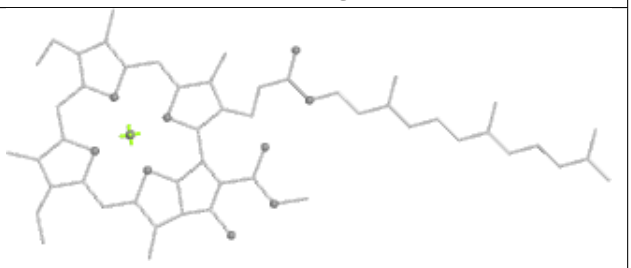
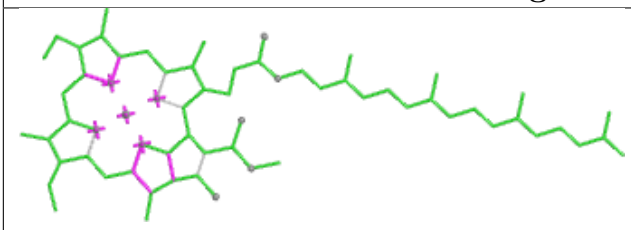


Rings

Ligand CLA c 510



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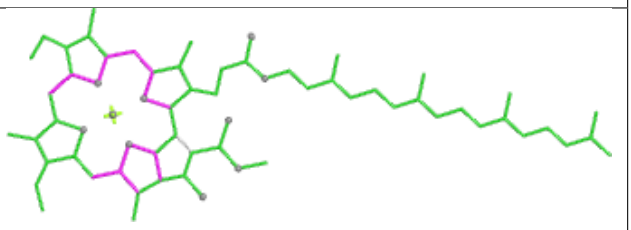
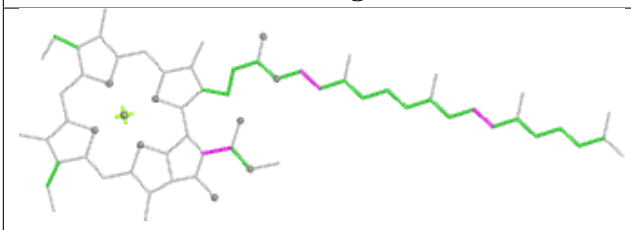


Bond angles



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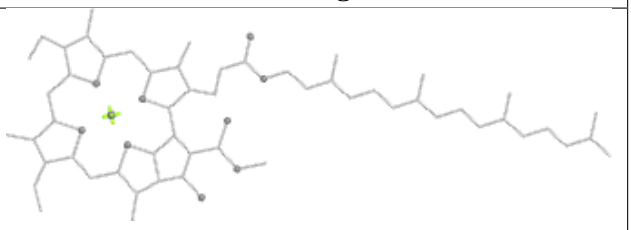
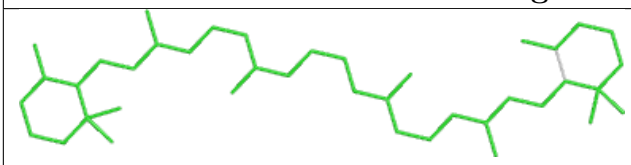


Rings

Ligand 8CT 4 311



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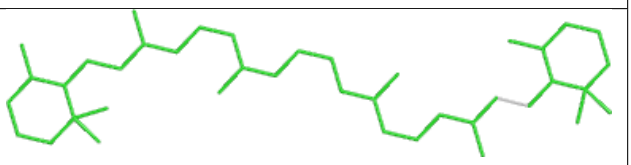
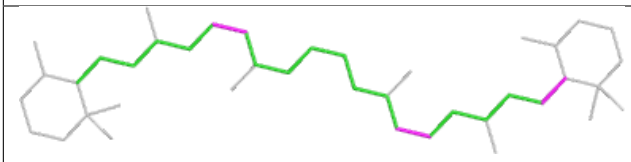
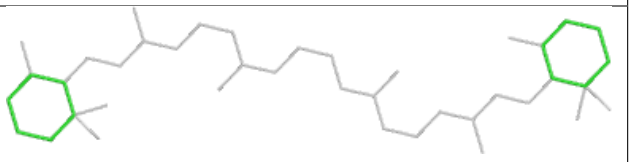


Bond angles

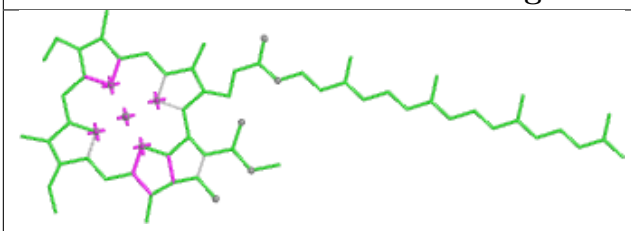


Torsions



Rings

Ligand CLA B 604



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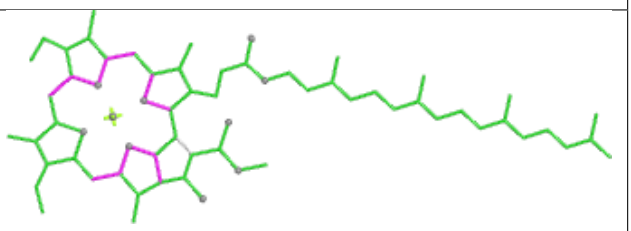
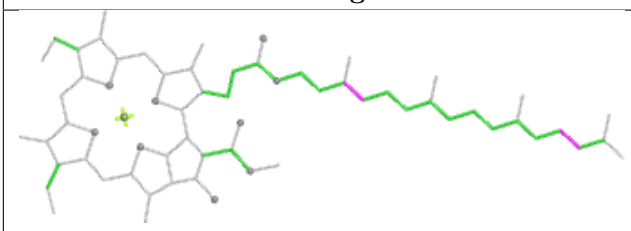
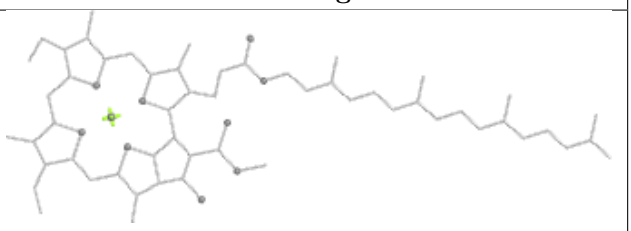


Bond angles

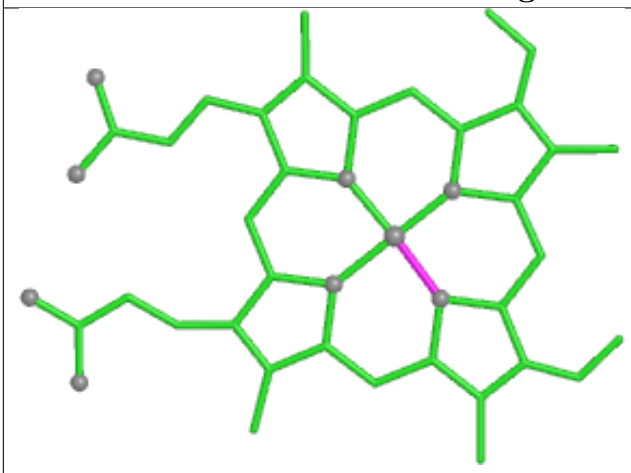


Torsions



Rings

Ligand HEM V 201



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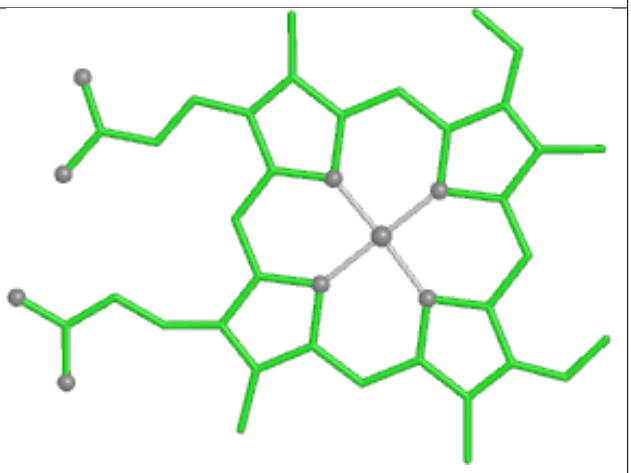

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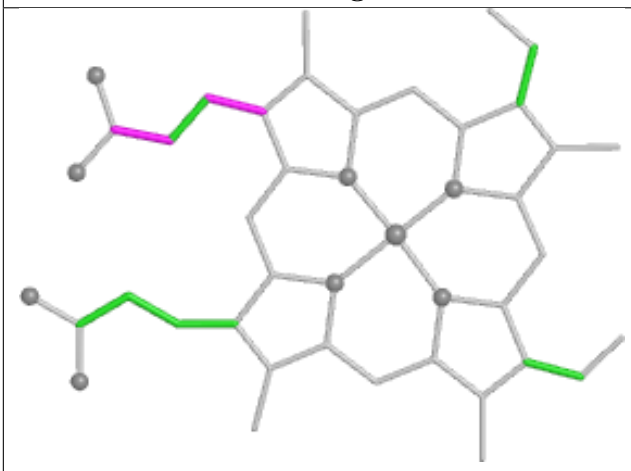

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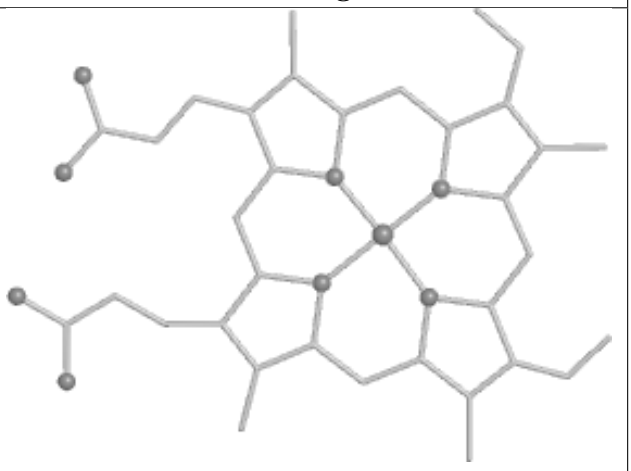
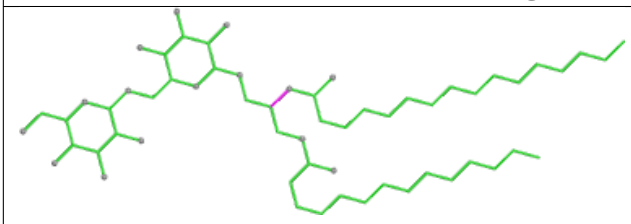


Rings

Ligand DGD h 101



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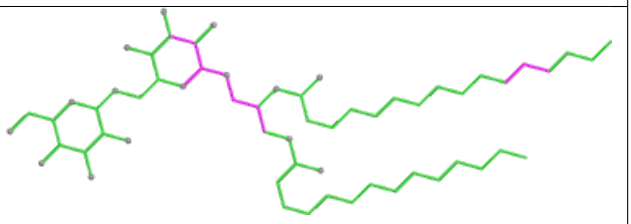
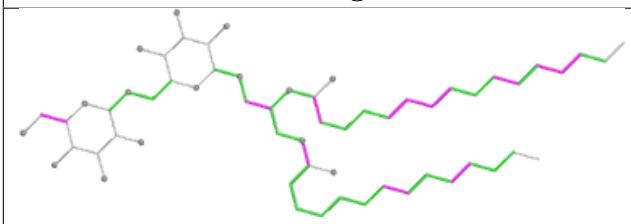


Bond angles



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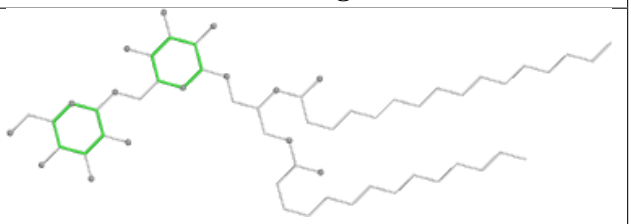
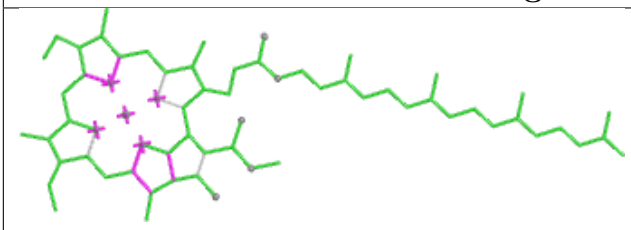
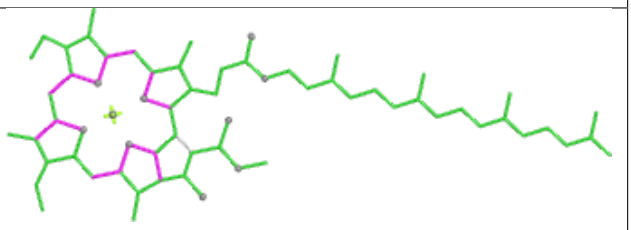


Rings

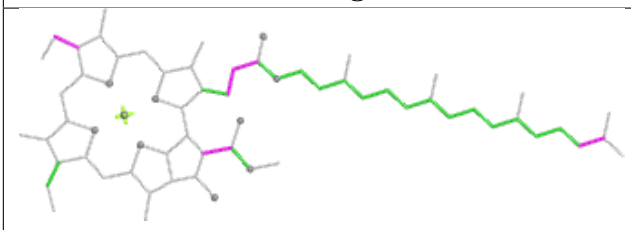
Ligand CLA C 503



Bond lengths



Bond angles



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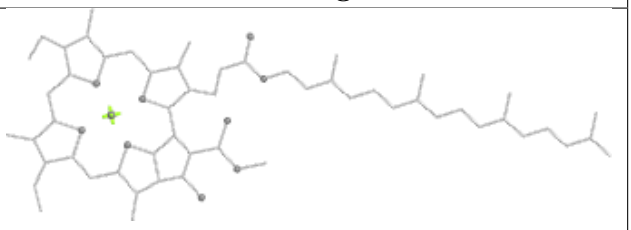
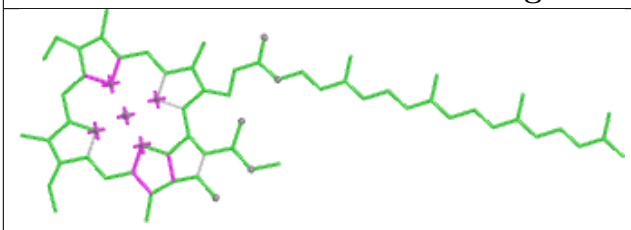
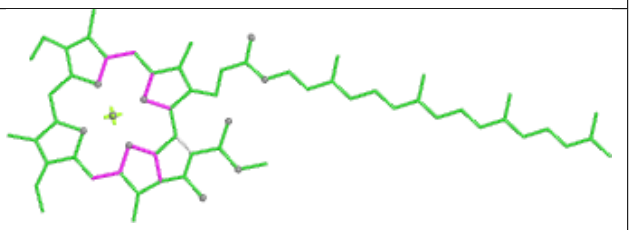


Rings

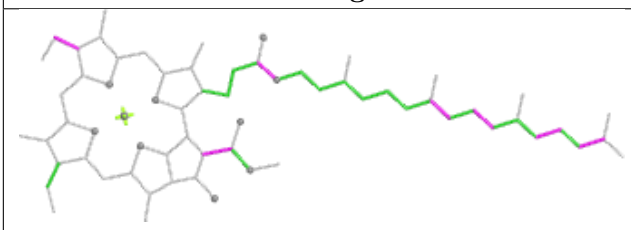
Ligand CLA B 613



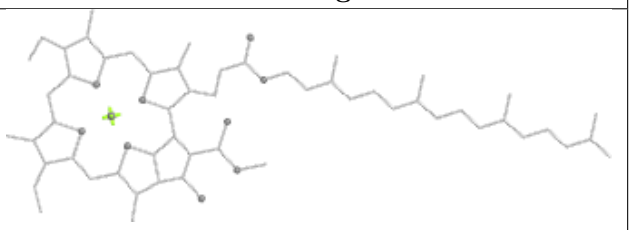
Bond lengths



Bond angles

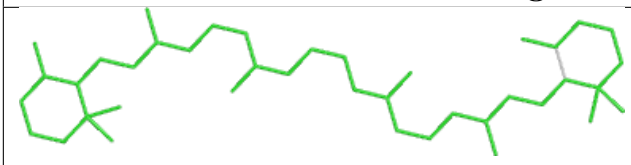


Torsions



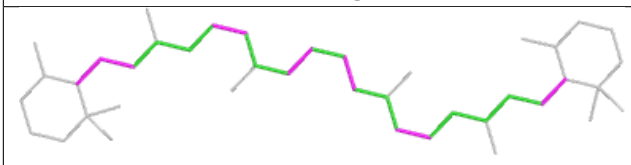
Rings

Ligand 8CT B 621

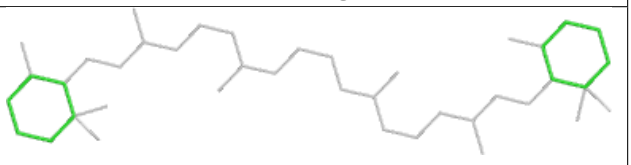


Bond lengths

Bond angles

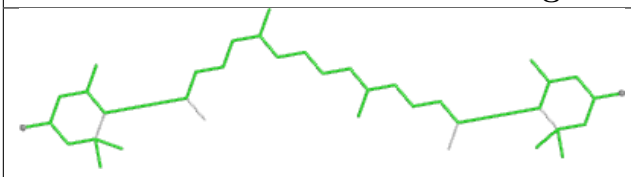


Torsions



Rings

Ligand II0 3 319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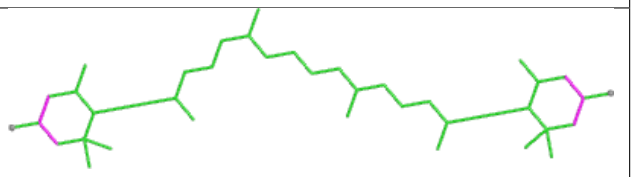
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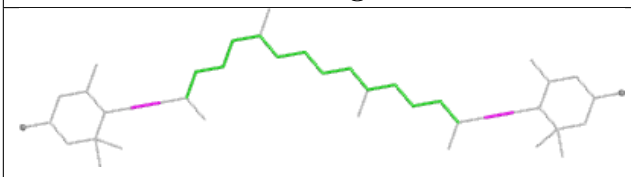
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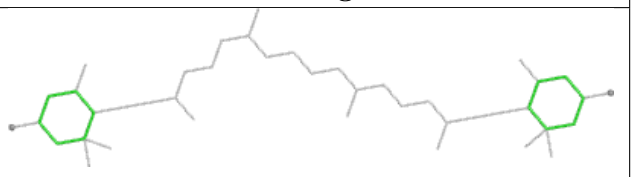
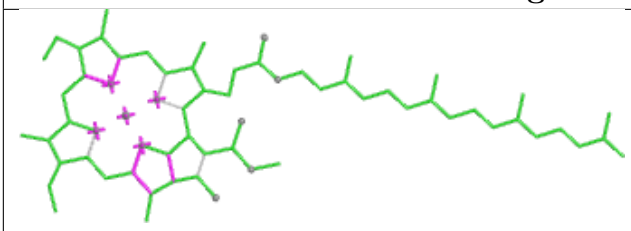

Rings

Ligand CLA b 612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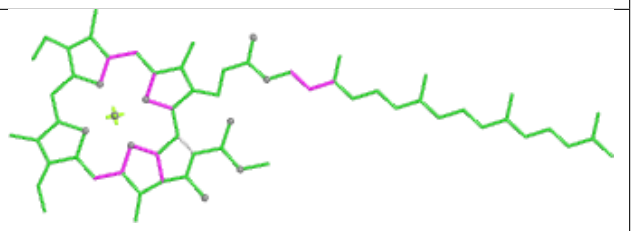
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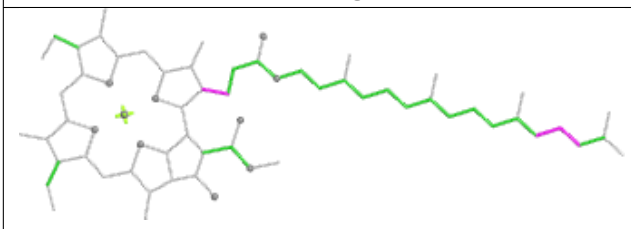
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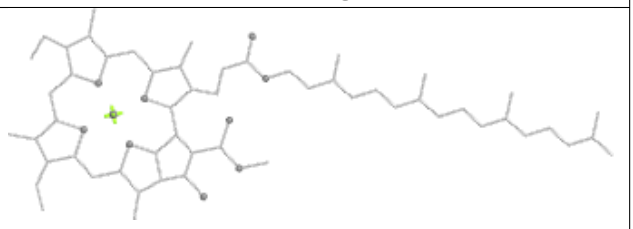
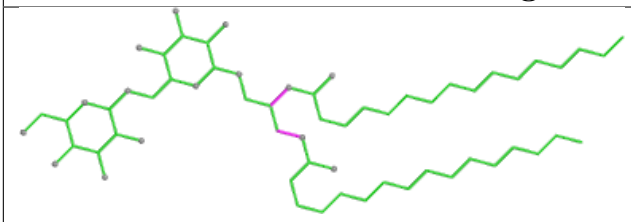

Rings

Ligand DGD C 521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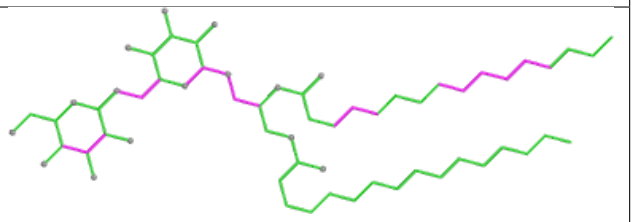
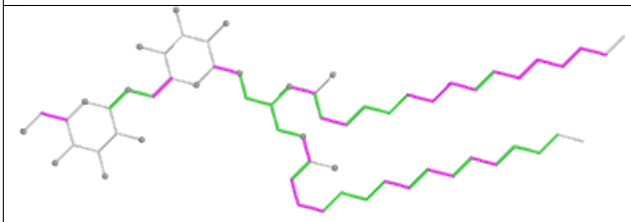

Bond angles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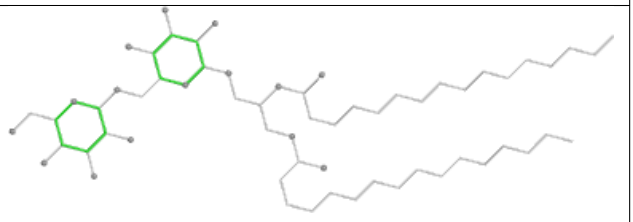
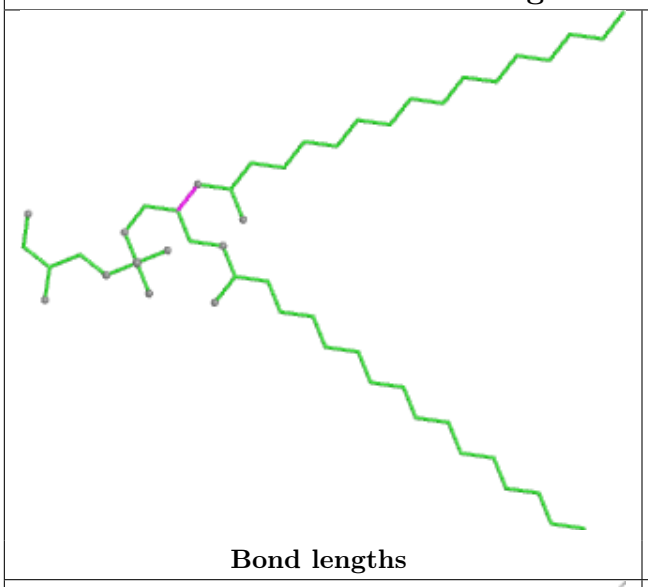

Rings

Ligand LHG b 623



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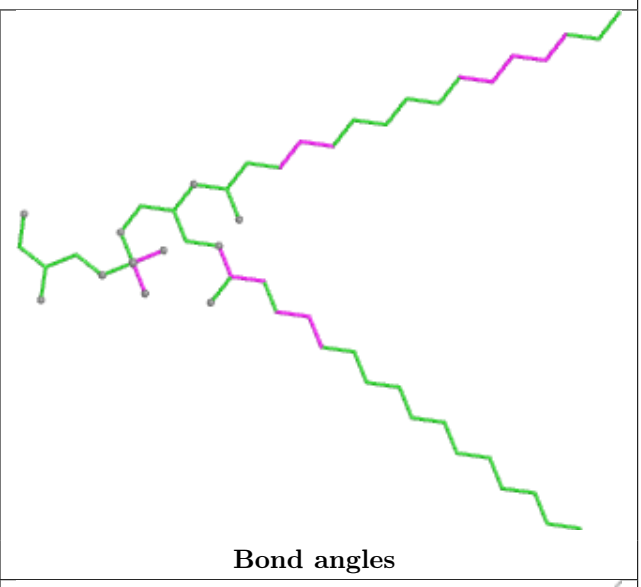
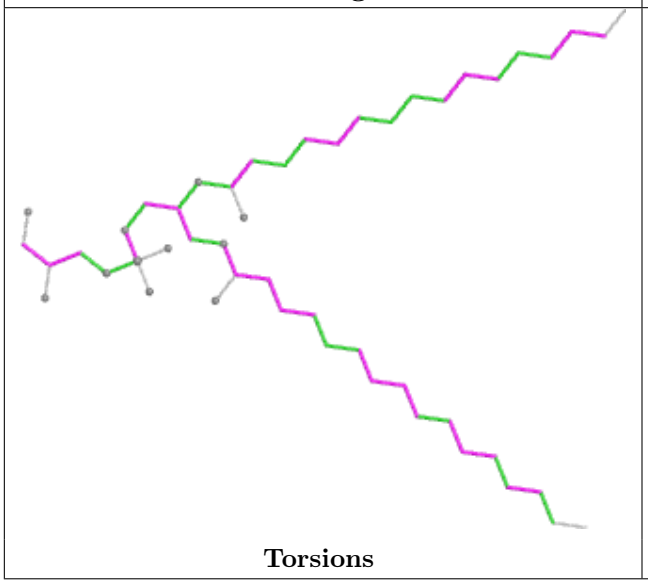


Bond angles



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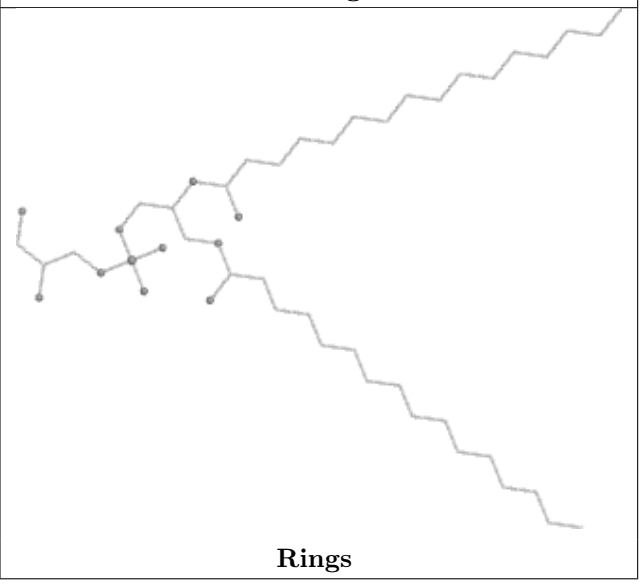
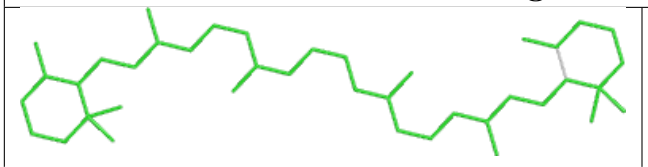


Rings

Ligand 8CT H 102



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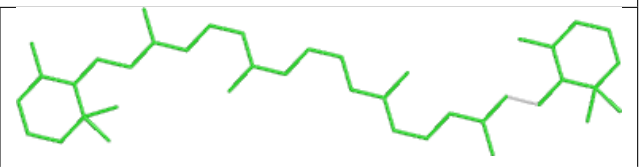
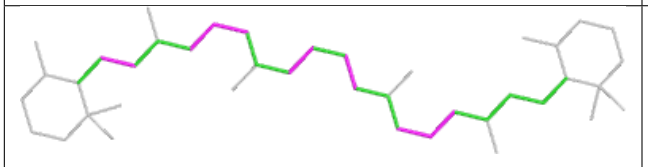


Bond angles



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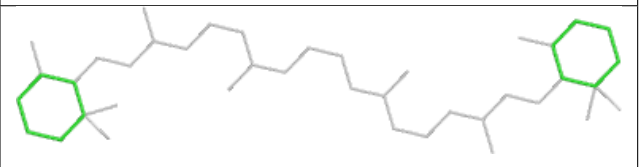
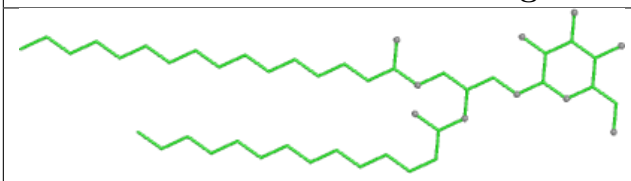


Rings

Ligand LMG B 622



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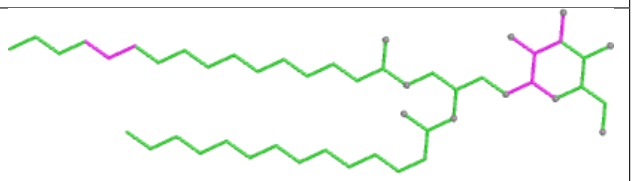

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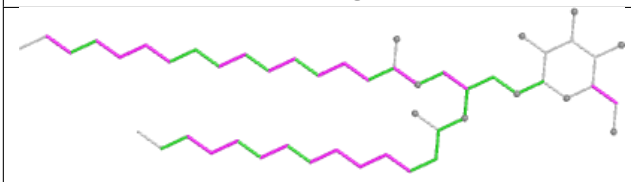

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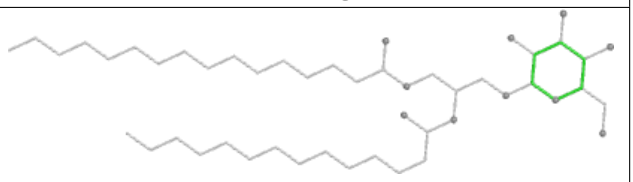
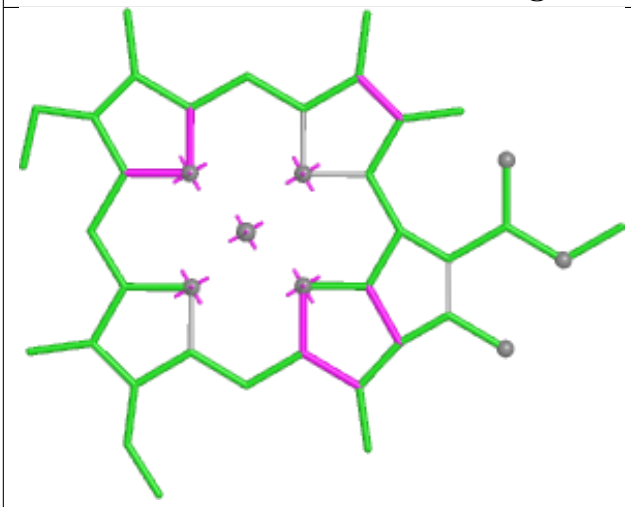


Rings

Ligand CLA 3 314



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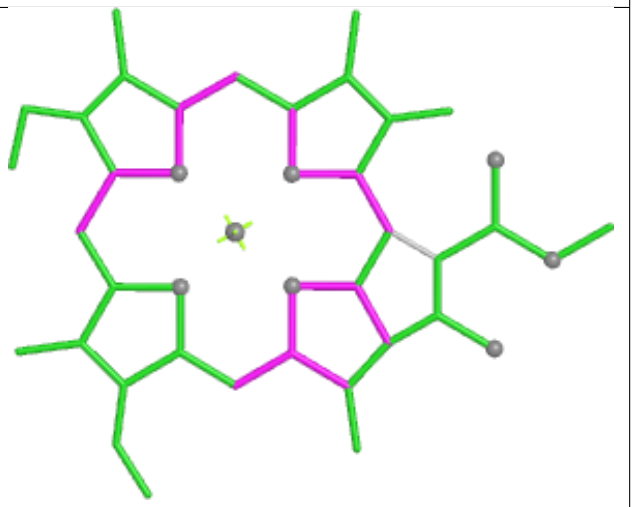
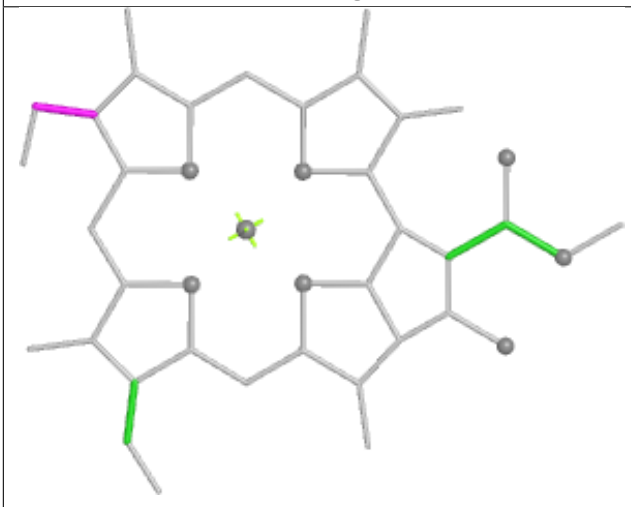


Bond angles



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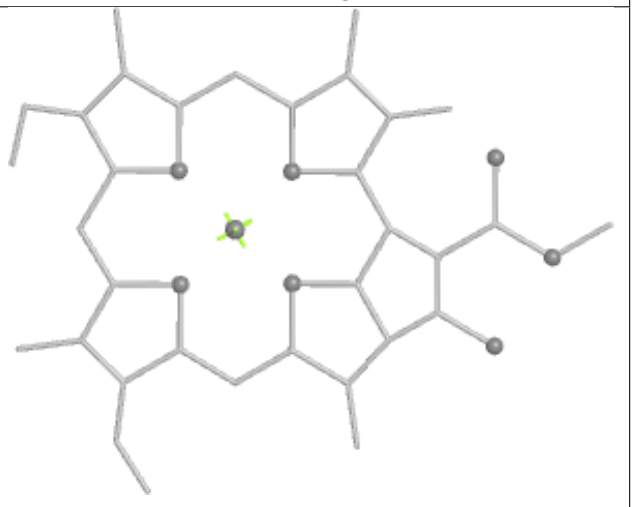
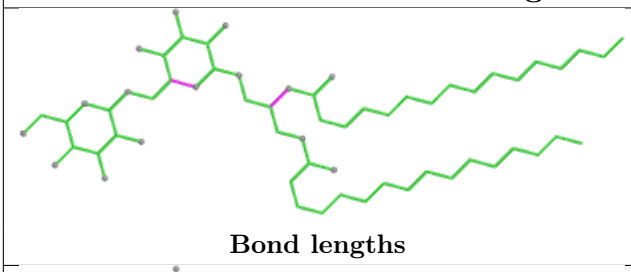


Rings

Ligand DGD c 519



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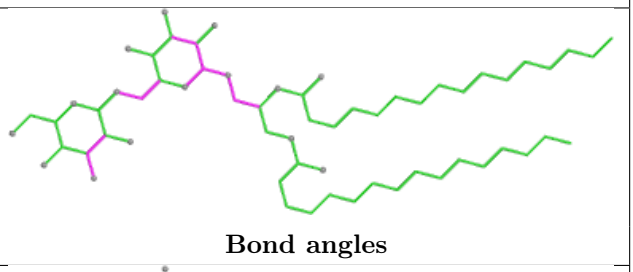
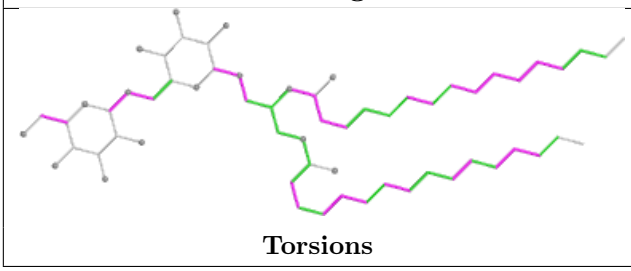


Bond angles



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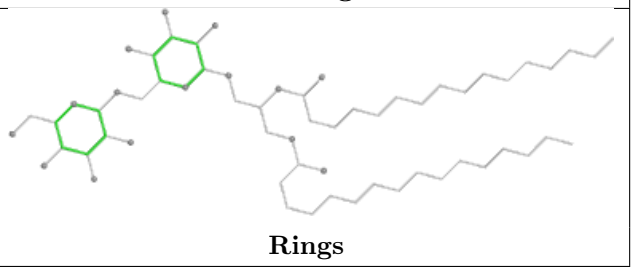
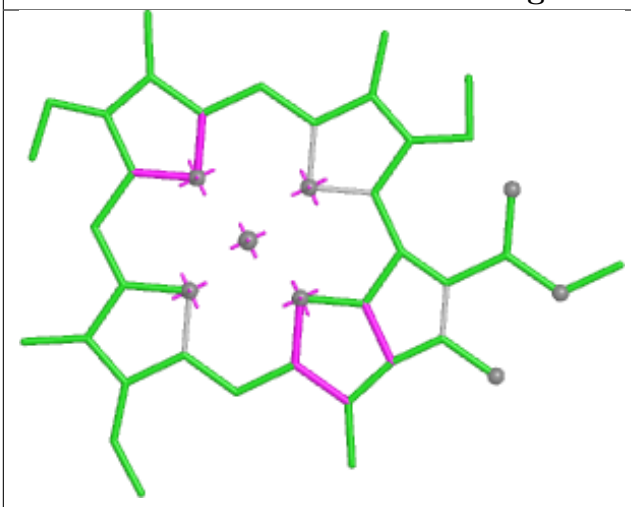


Rings

Ligand CLA p 308



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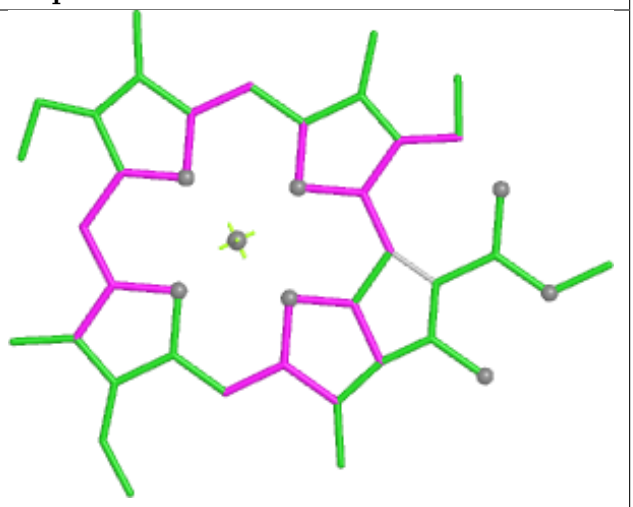
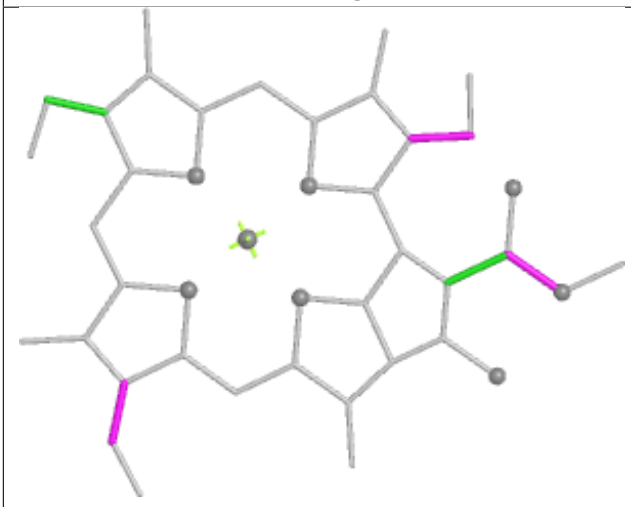


Bond angles



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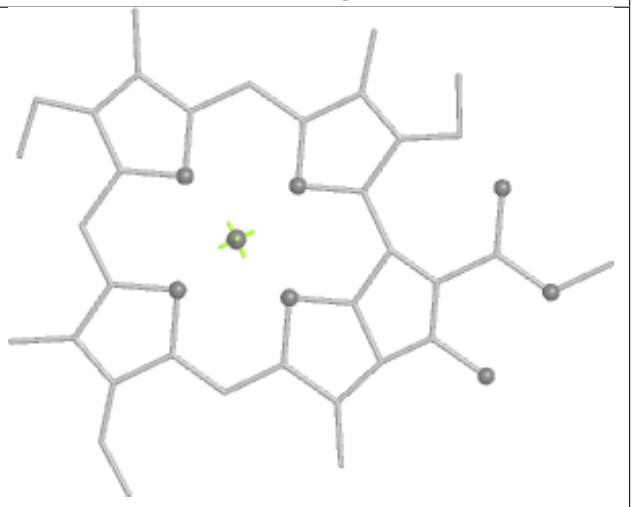
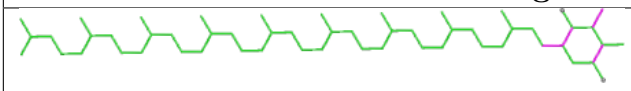
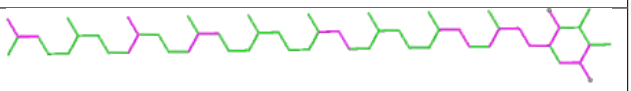
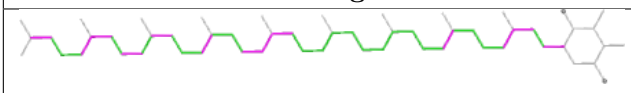
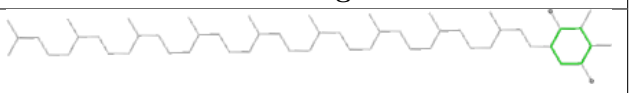
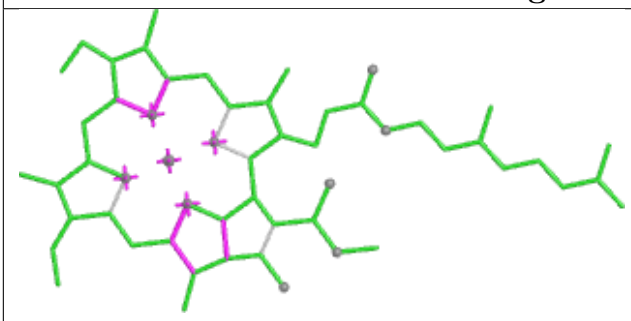
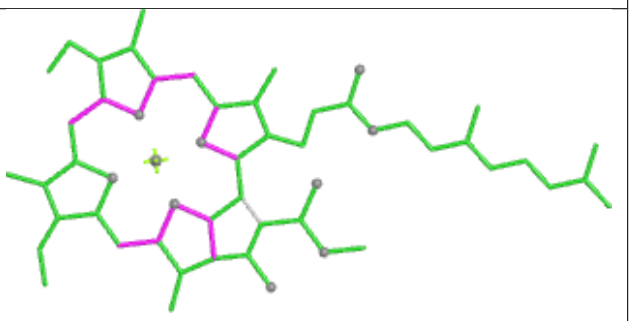
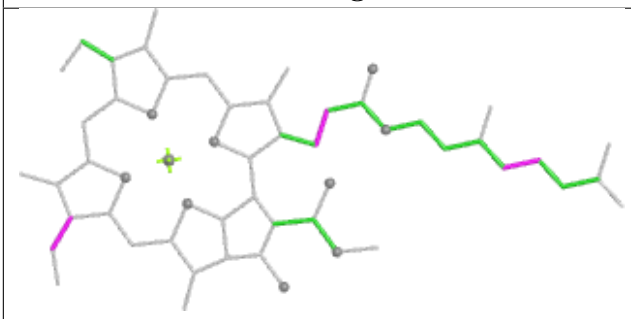
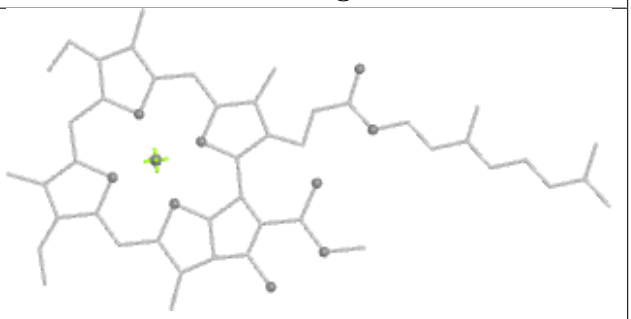
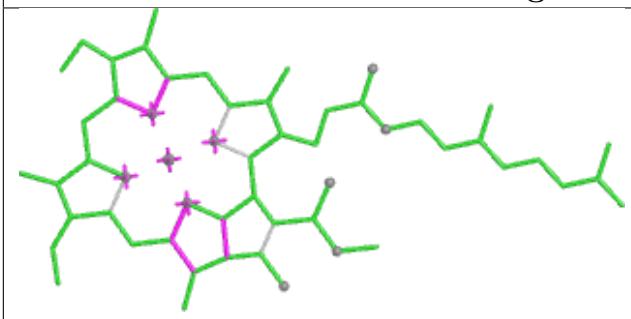


Rings

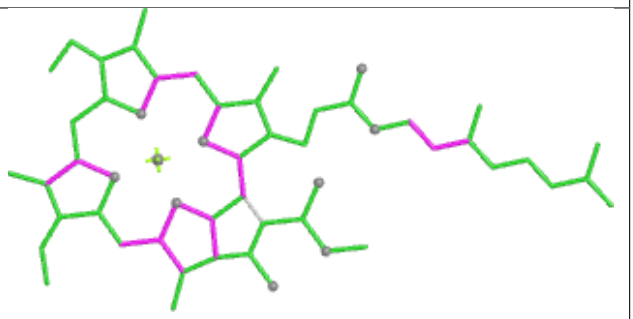
Ligand PL9 d 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

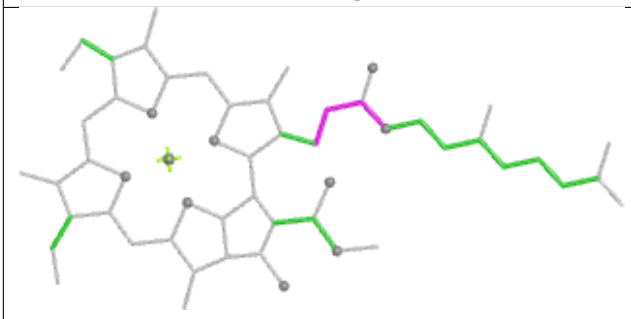
Ligand CLA n 304



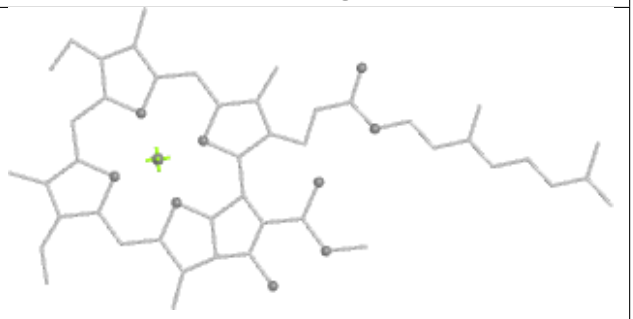
Bond lengths



Bond angles

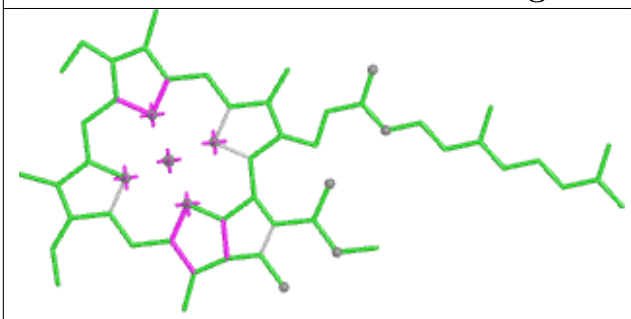


Torsions



Rings

Ligand CLA 9 309



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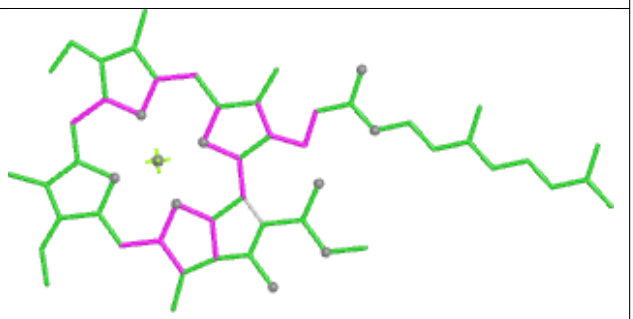
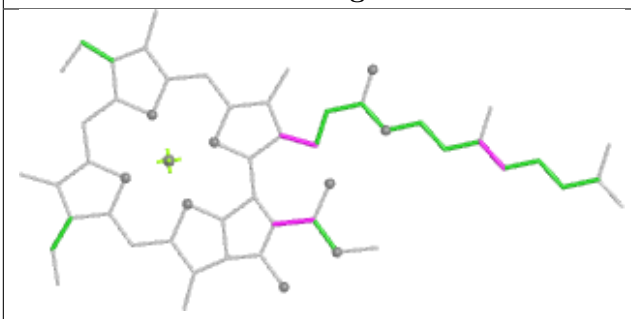
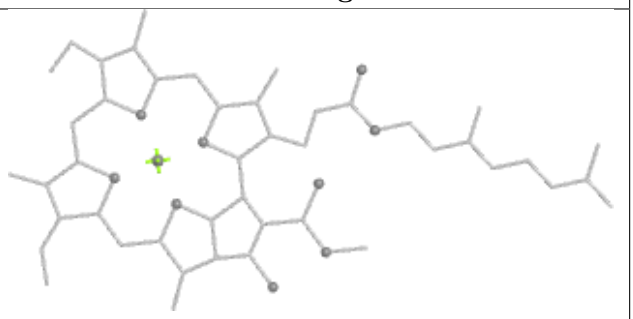


Bond angles

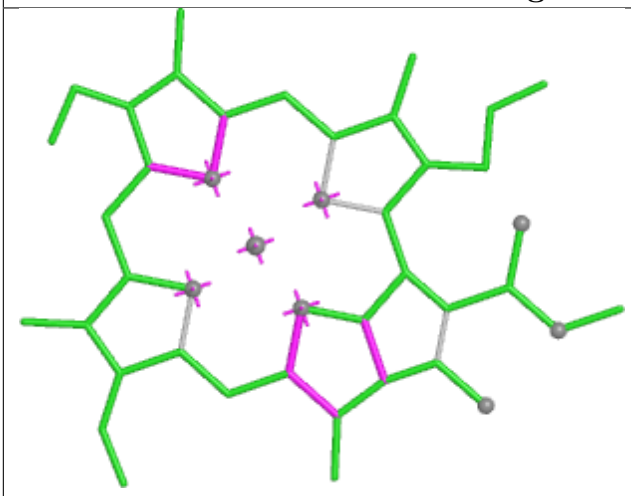


Torsions

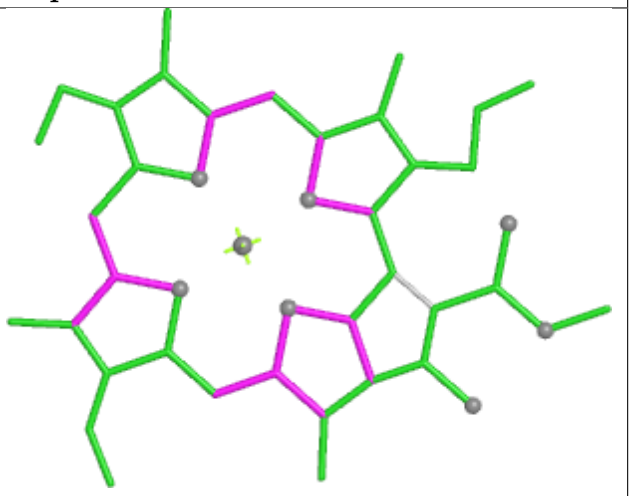


Rings

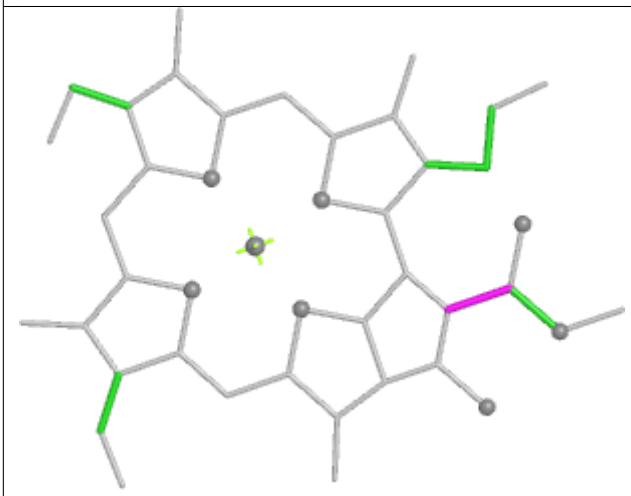
Ligand CLA p 307



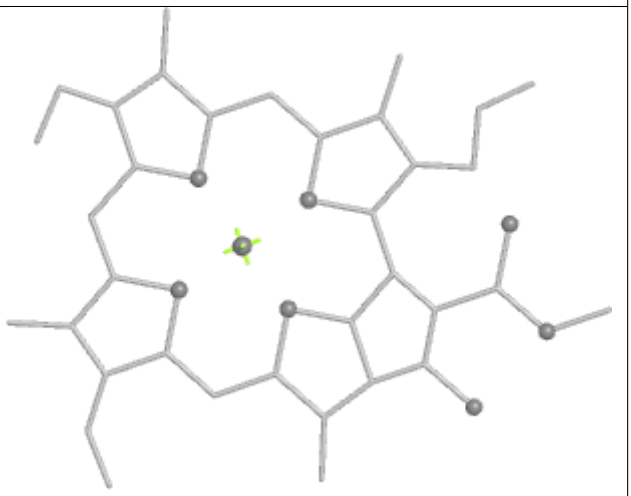
Bond lengths



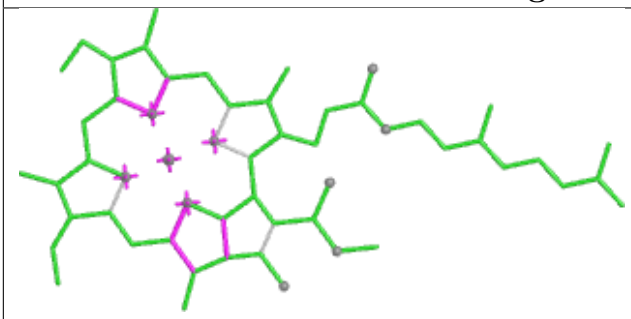
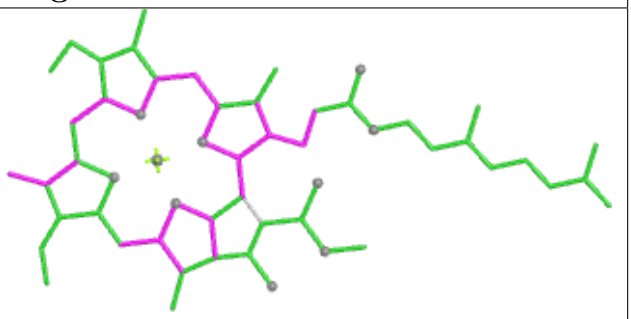
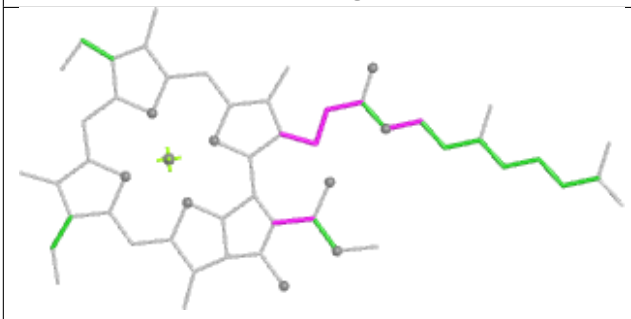
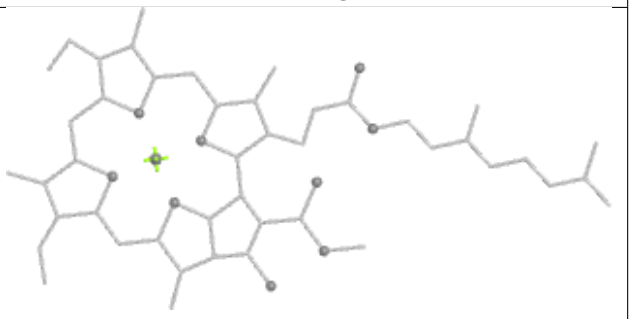
Bond angles

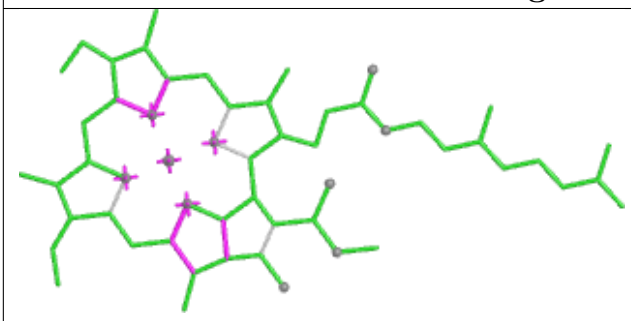
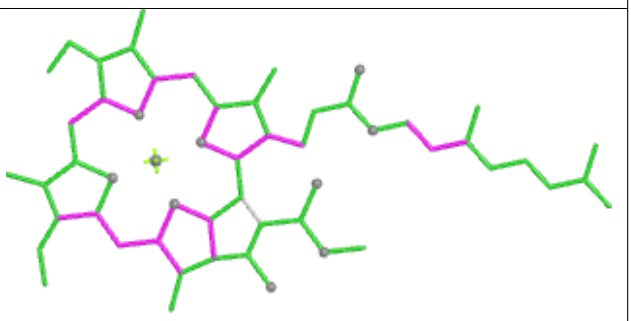
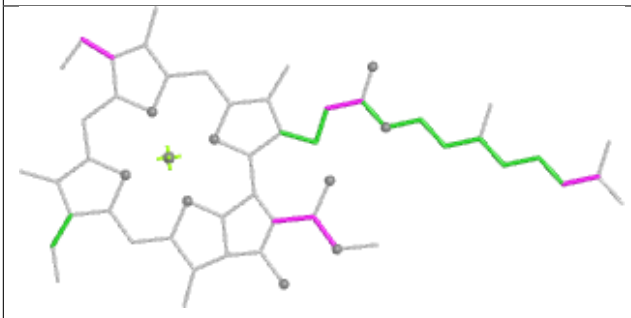
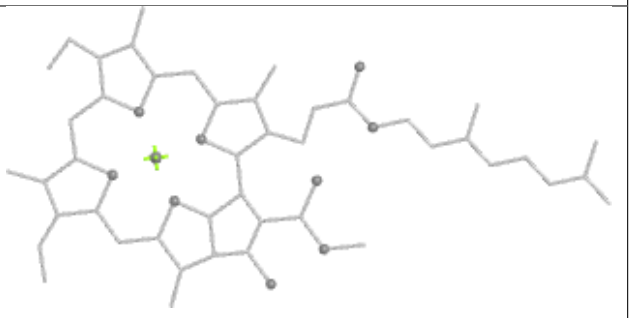


Torsions

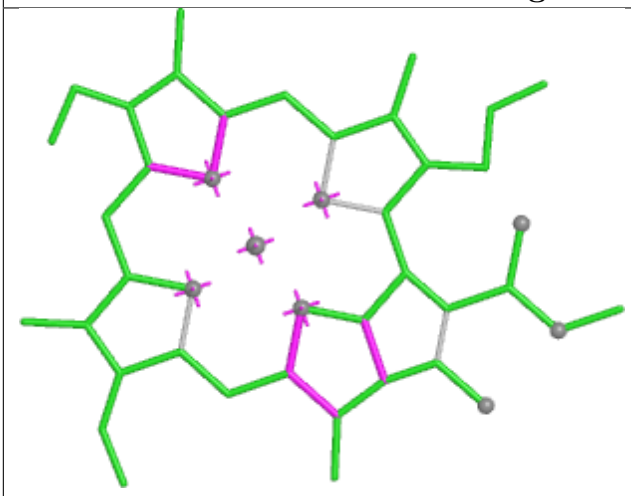


Rings

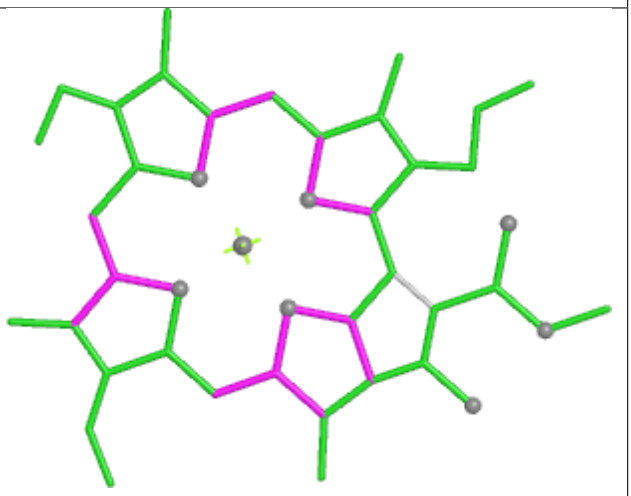
Ligand CLA g 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

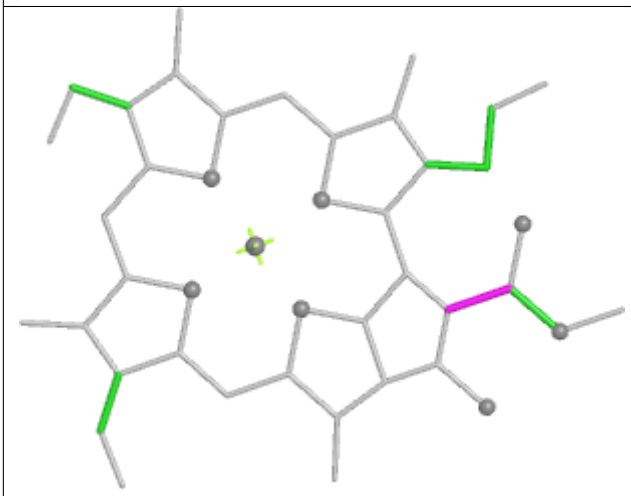
Ligand CLA 6 307



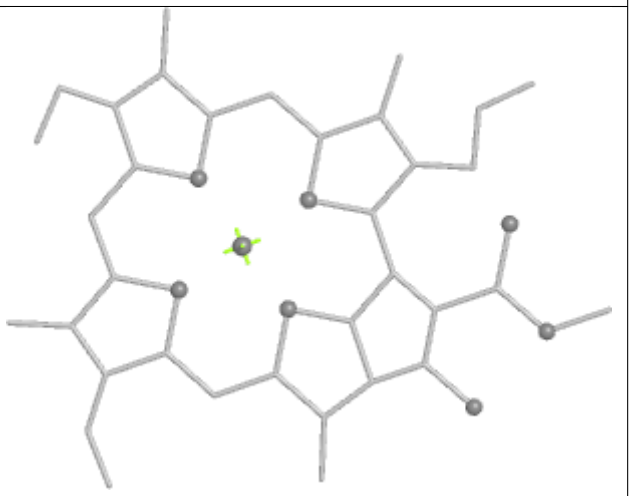
Bond lengths



Bond angles

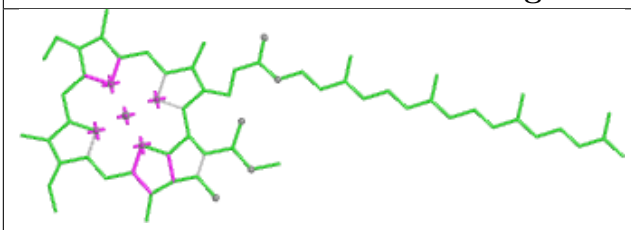


Torsions



Rings

Ligand CLA C 512



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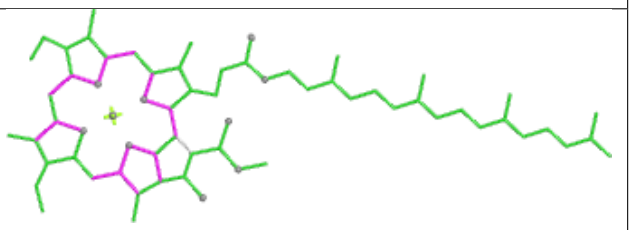
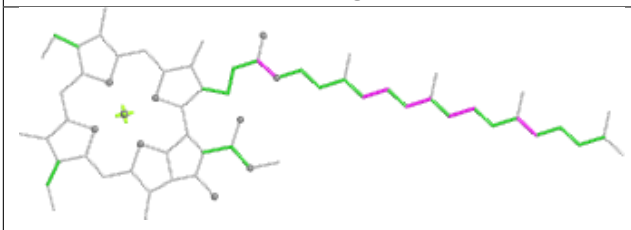


Bond angles



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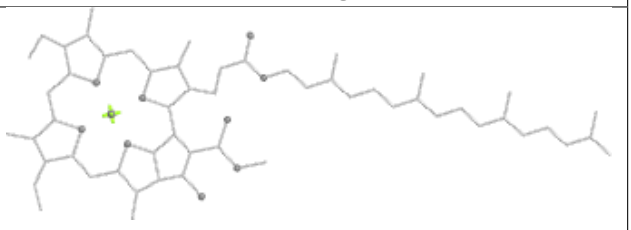
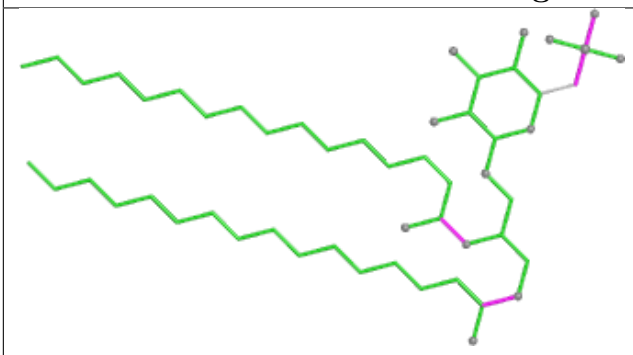


Rings

Ligand SQD l 101



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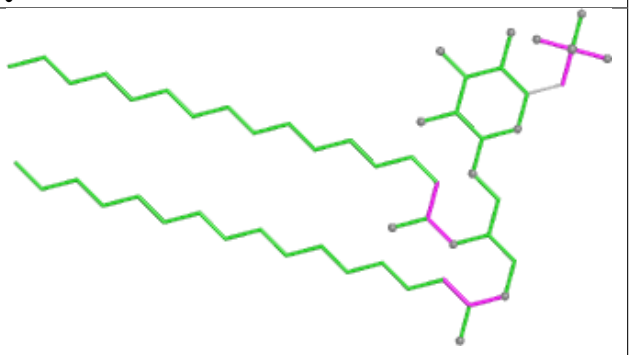
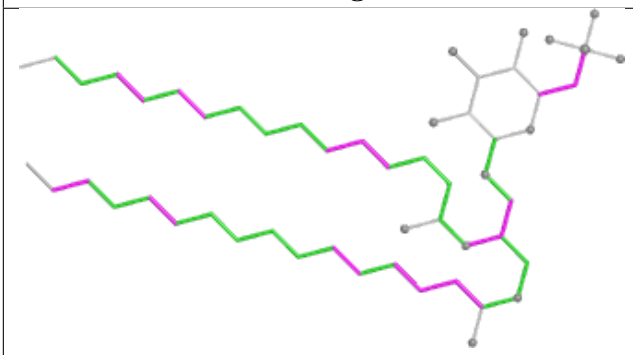


Bond angles



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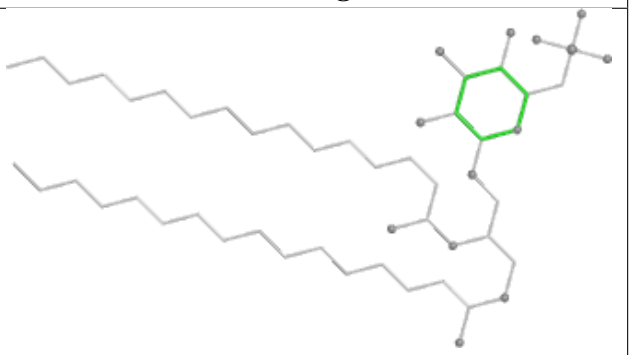
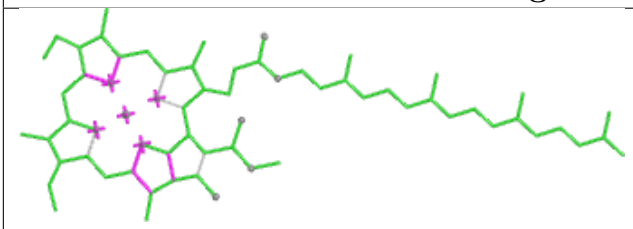


Rings

Ligand CLA c 505



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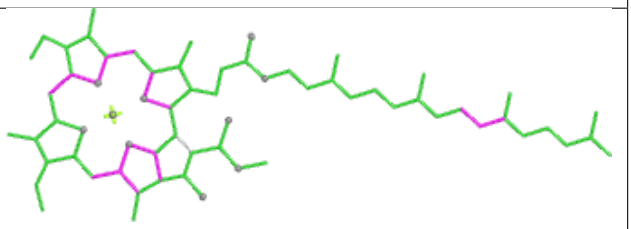
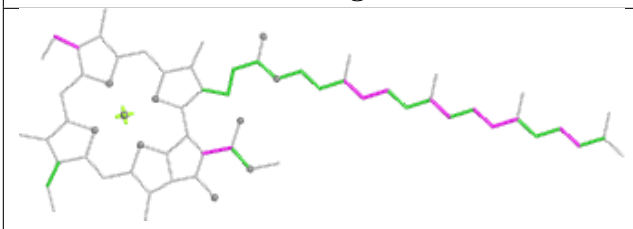


Bond angles



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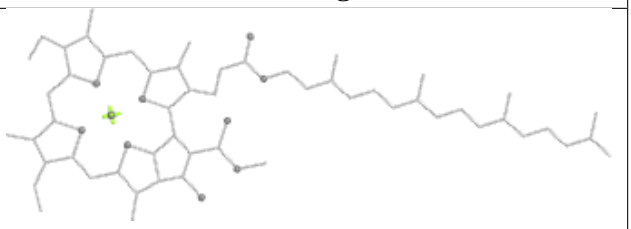
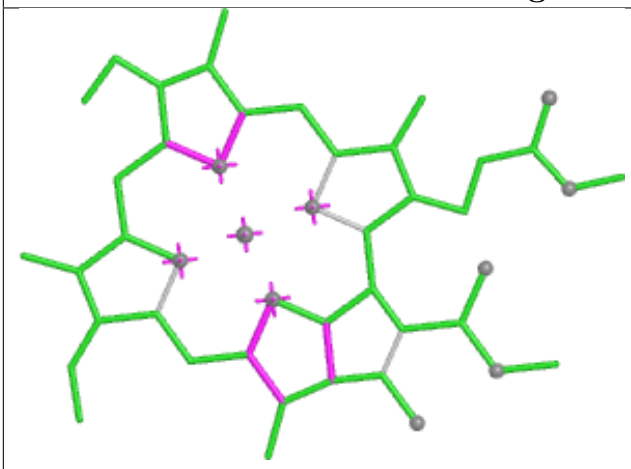


Rings

Ligand CLA 8 310



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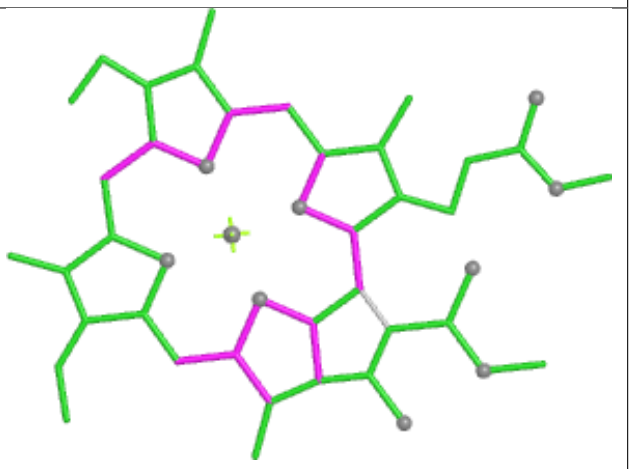

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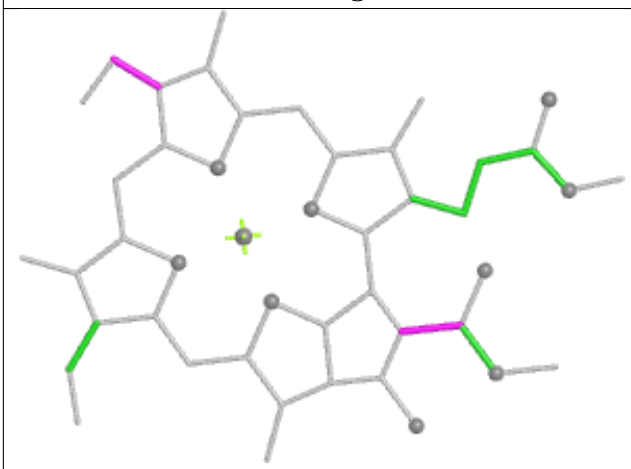

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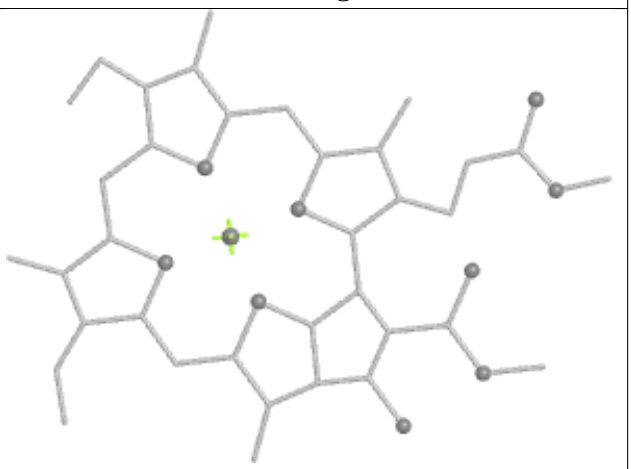
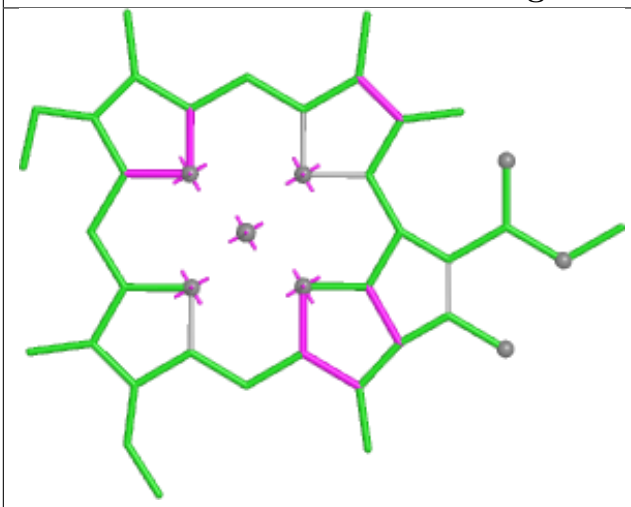


Rings

Ligand CLA p 319



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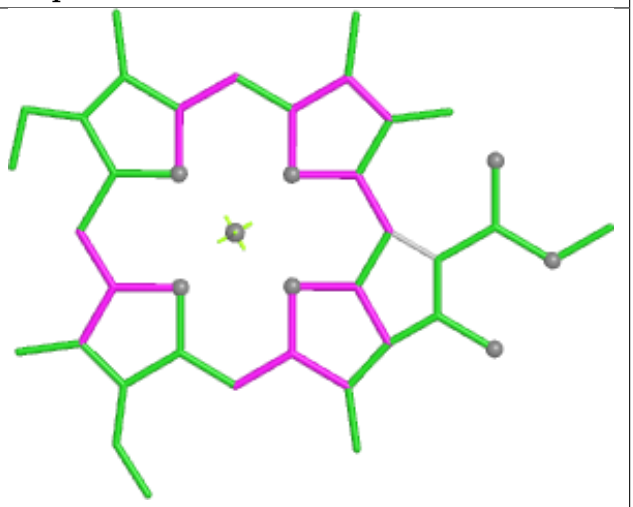

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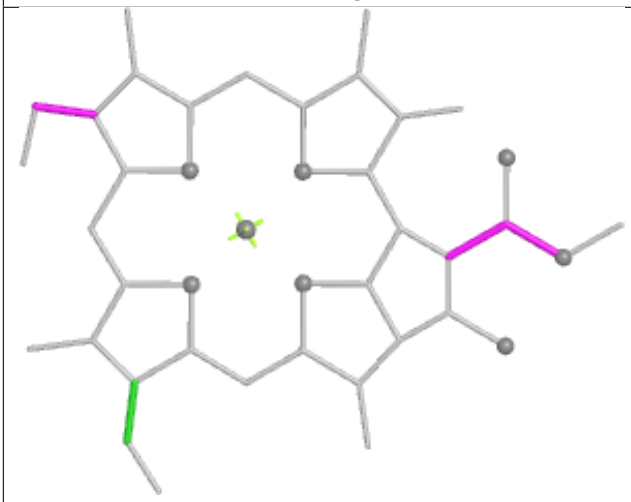

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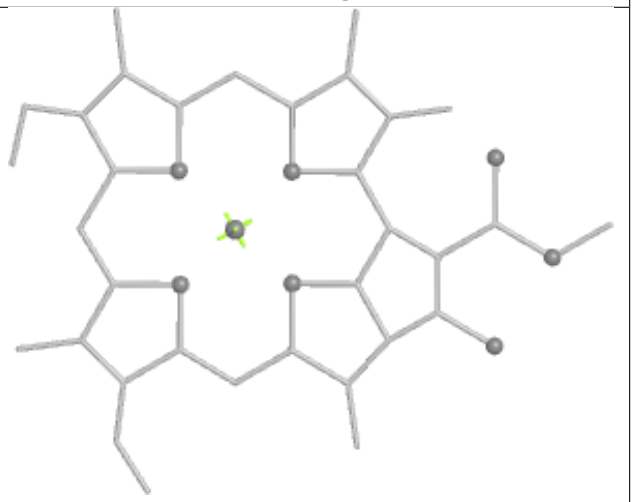
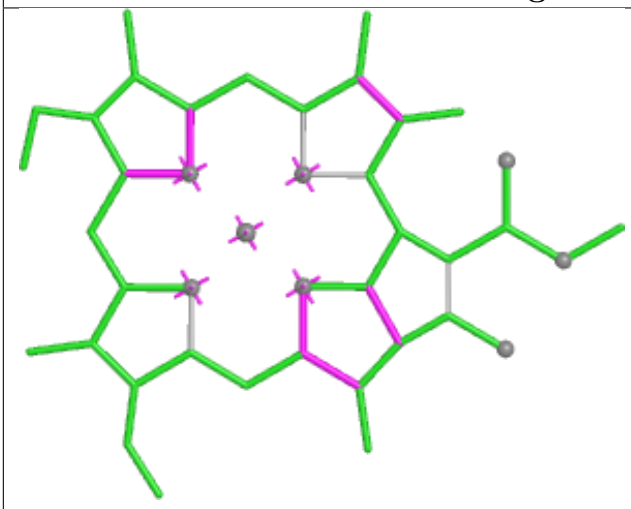


Rings

Ligand CLA 6 310



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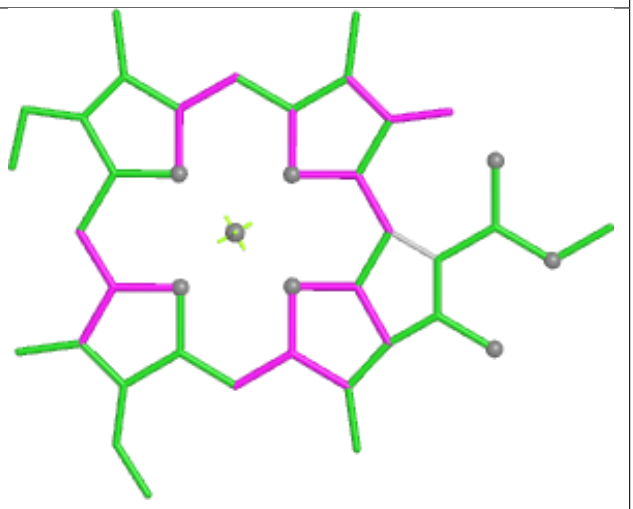

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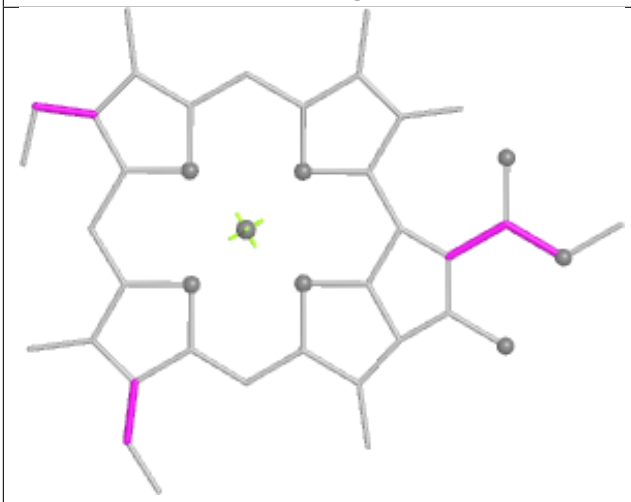

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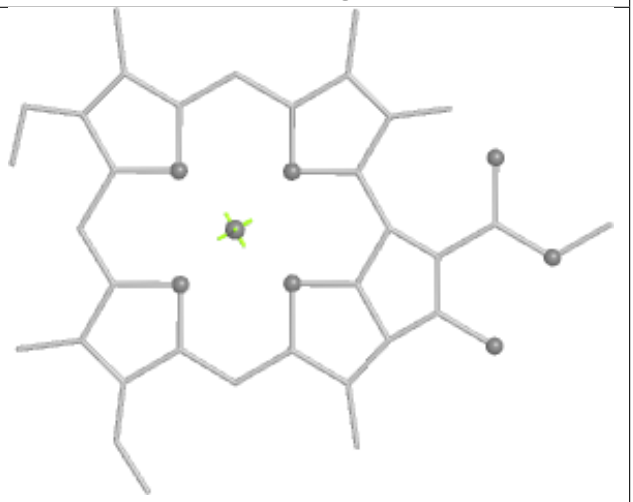
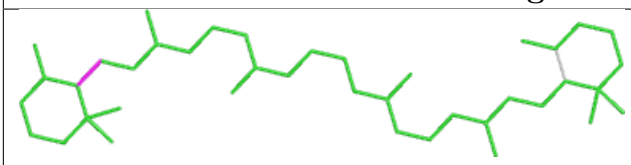


Rings

Ligand 8CT C 515



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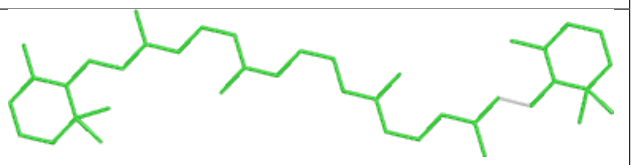
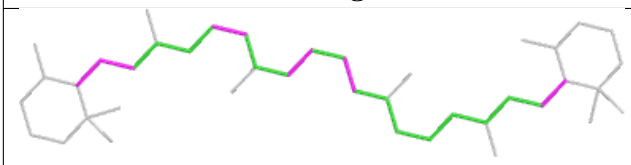


Bond angles



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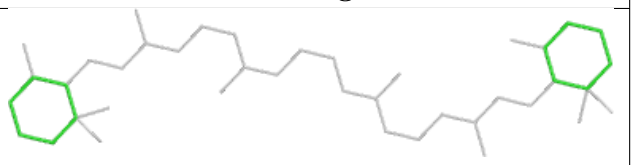
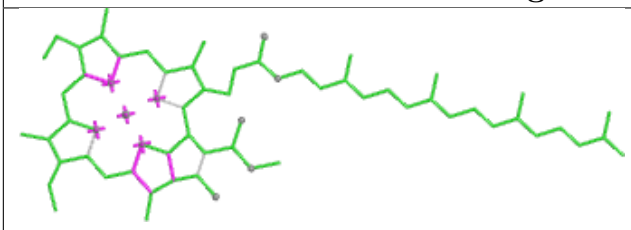


Rings

Ligand CLA b 607



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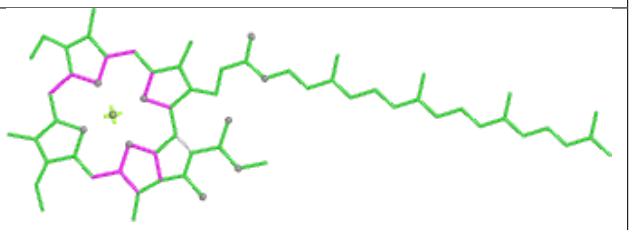
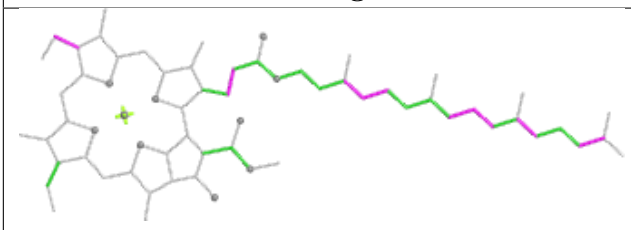
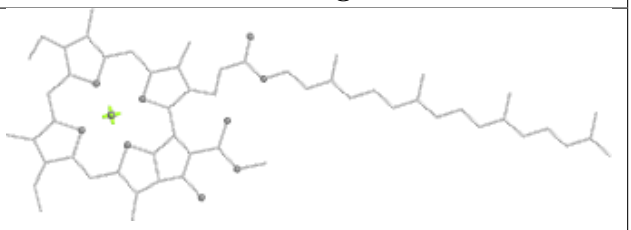


Bond angles



Torsions



Rings

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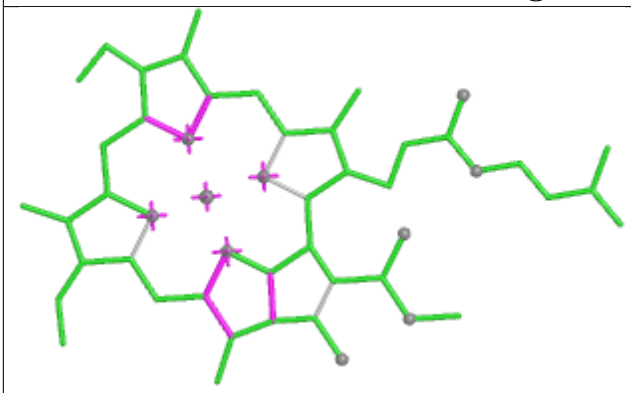

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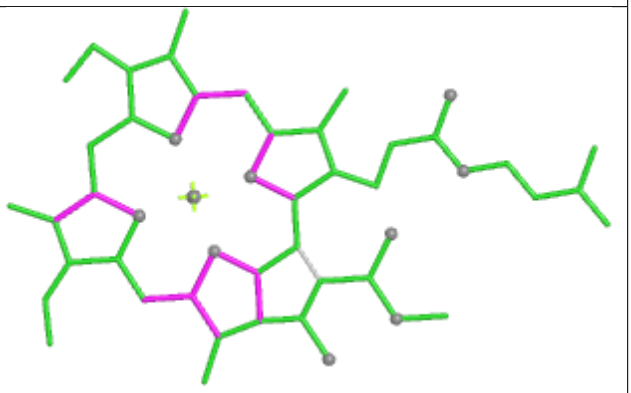
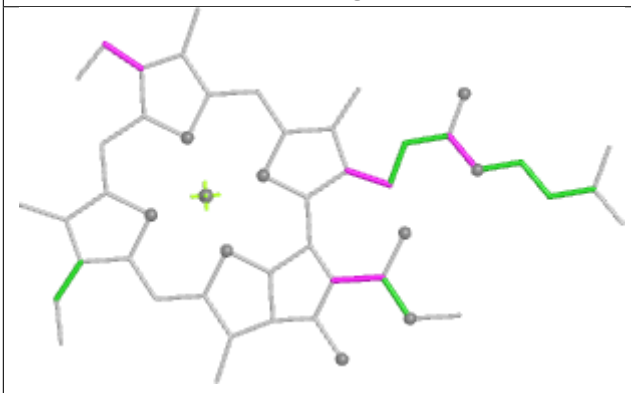


Bond angles



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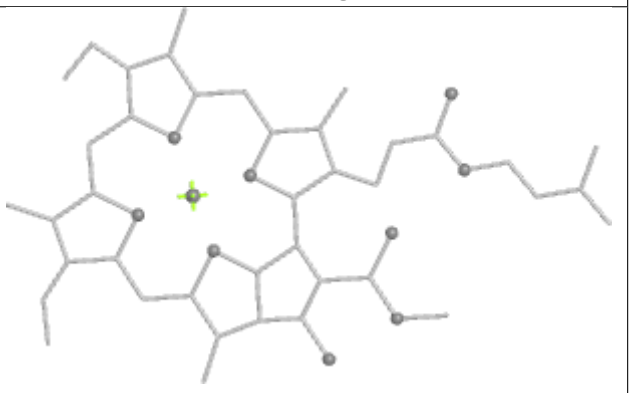
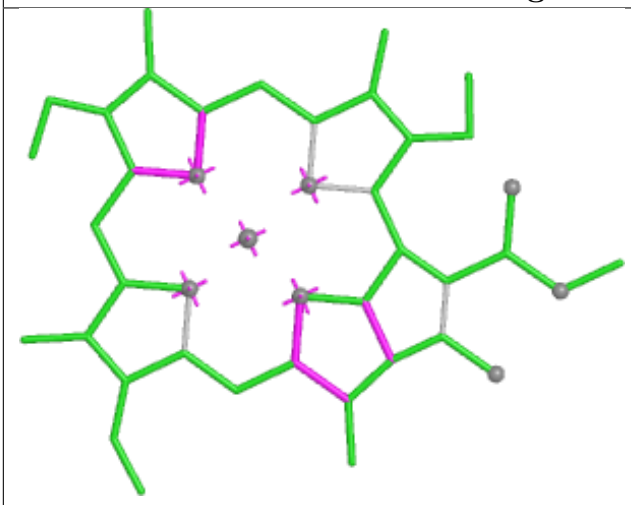


Rings

Ligand CLA p 304



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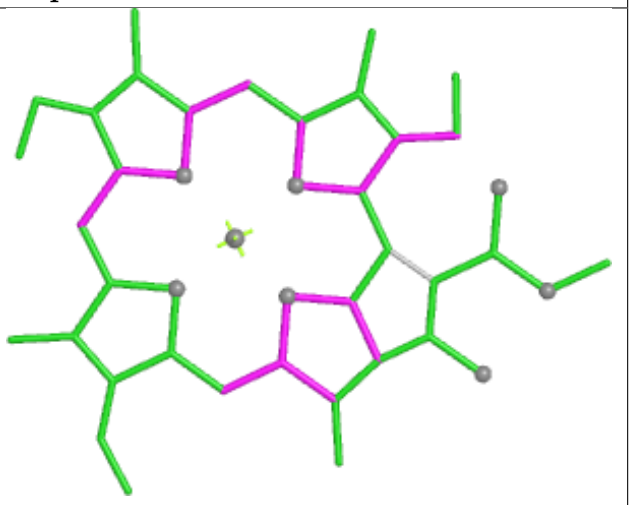
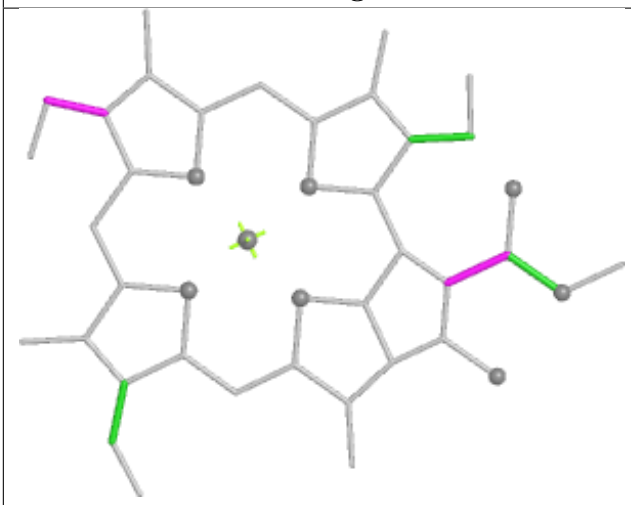
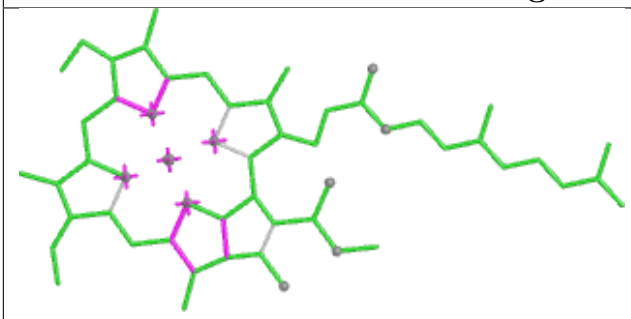
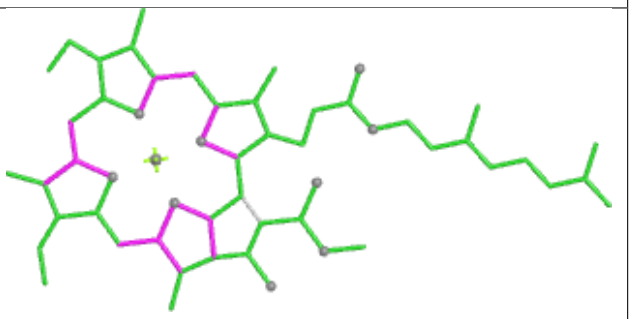
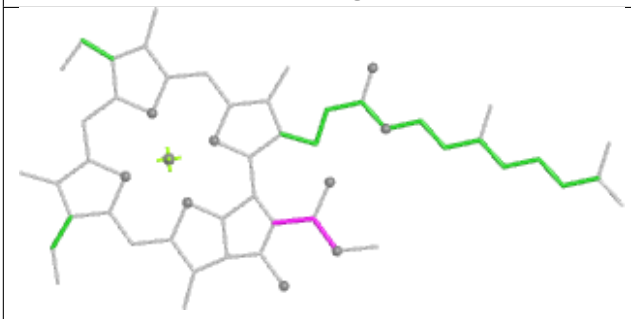
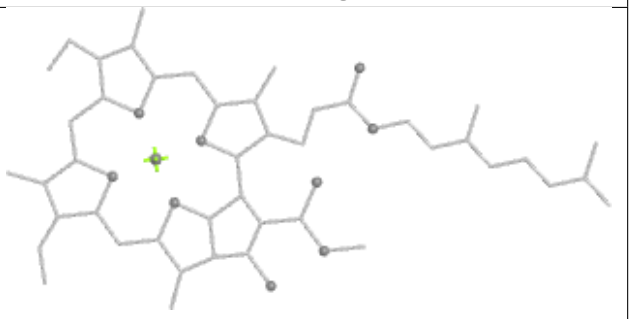


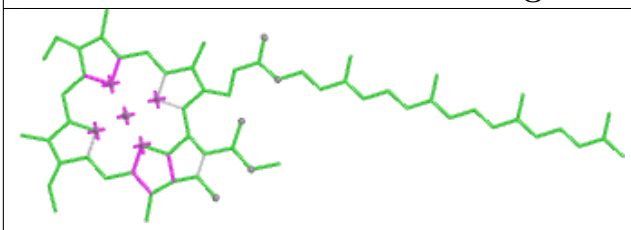
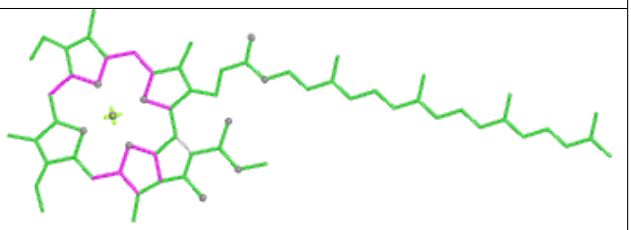
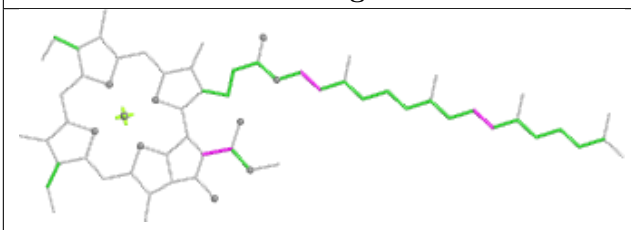
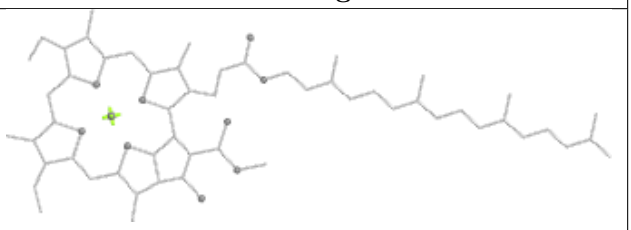
Bond angles



Torsions

Rings

Ligand CLA 6 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

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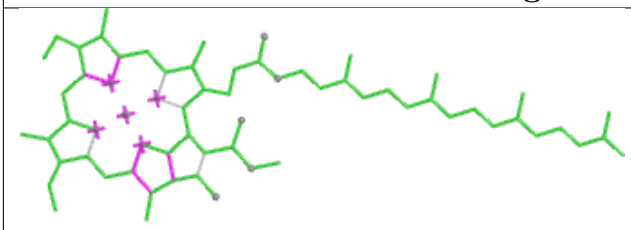
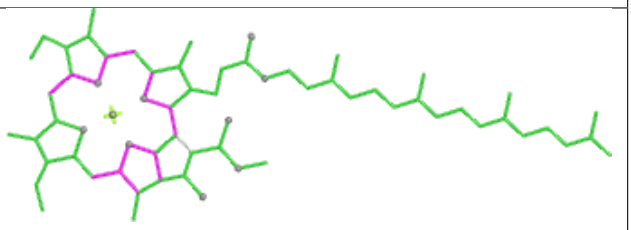
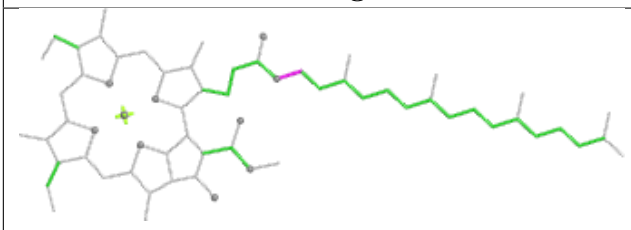
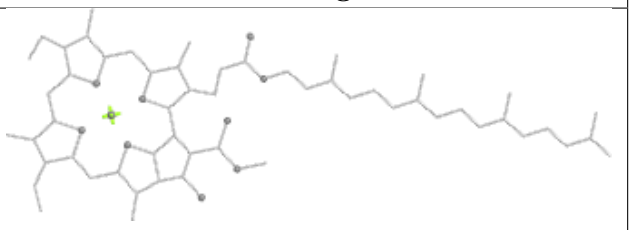
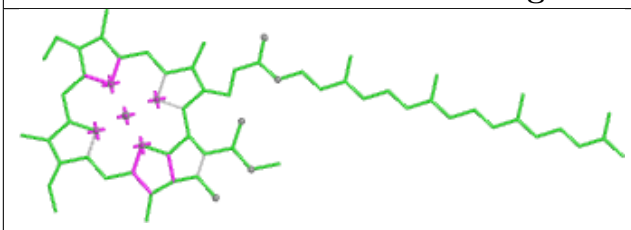
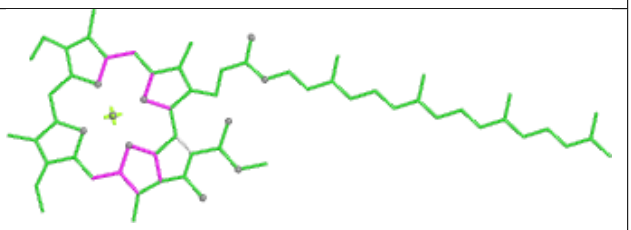
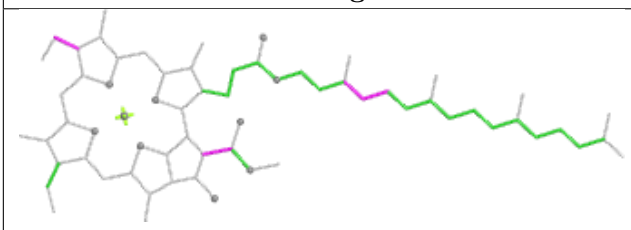
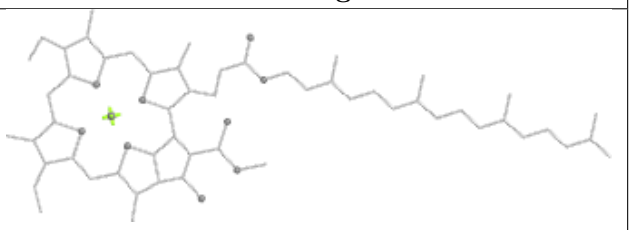
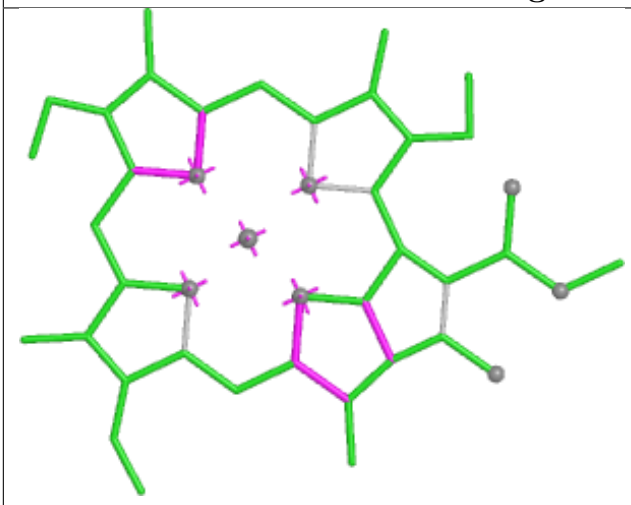
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 6 304



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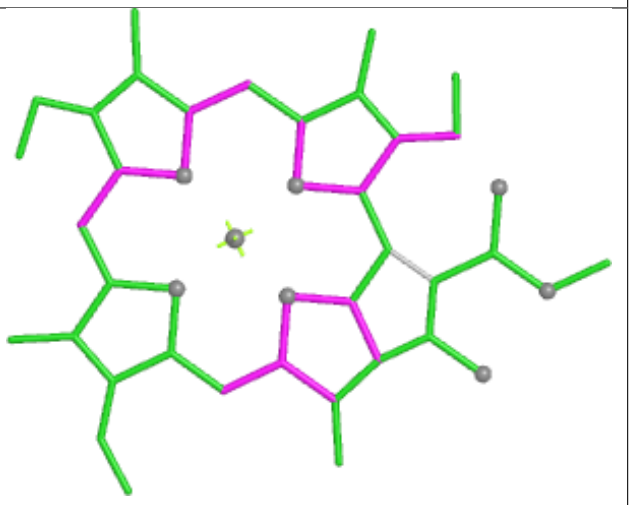

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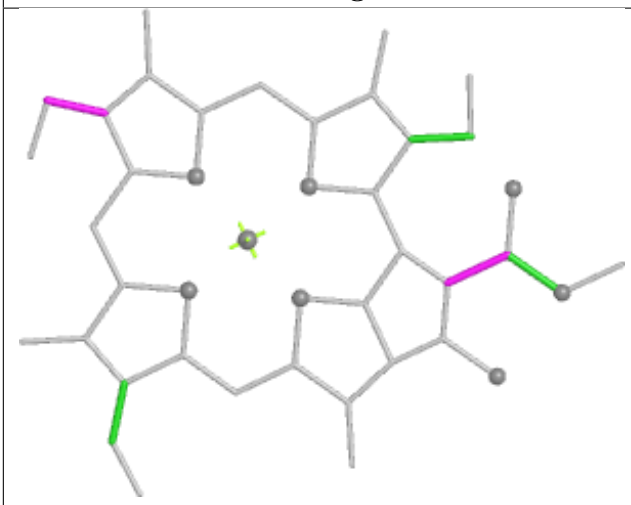
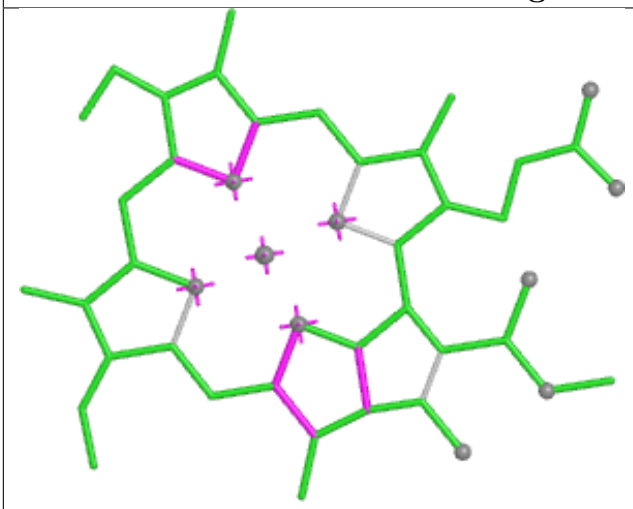


Torsions

Rings

Ligand CLA 9 304



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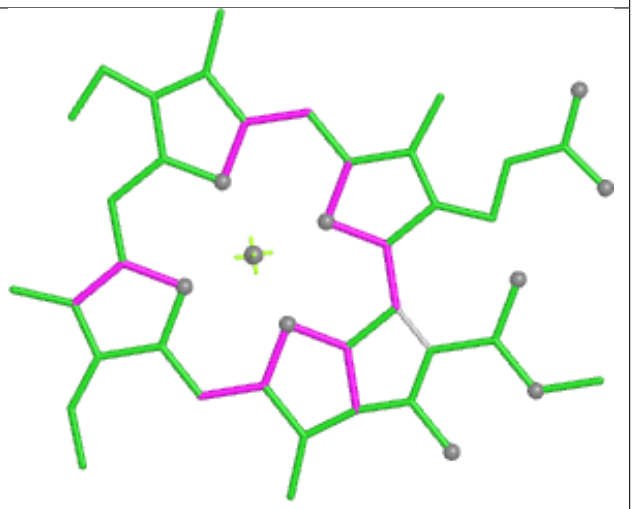

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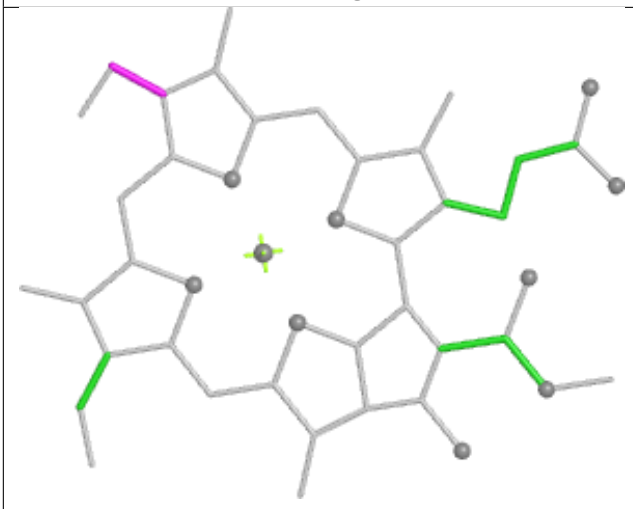
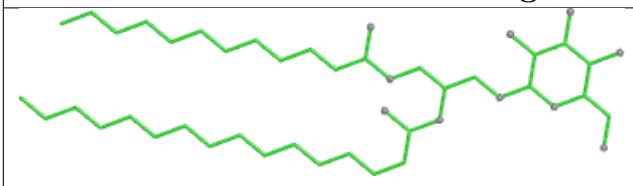


Torsions

Rings

Ligand LMG w 101



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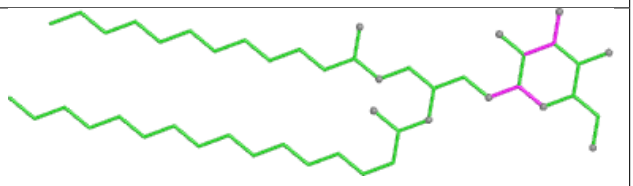

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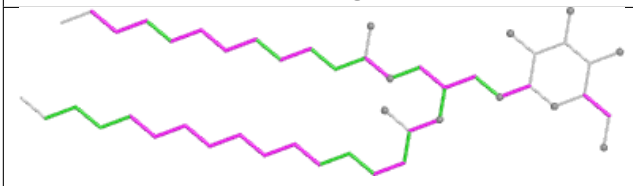

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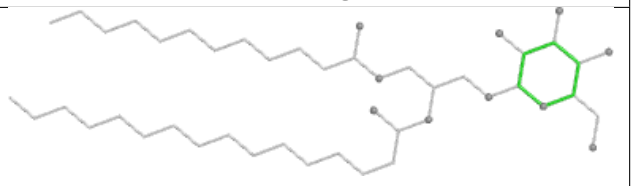
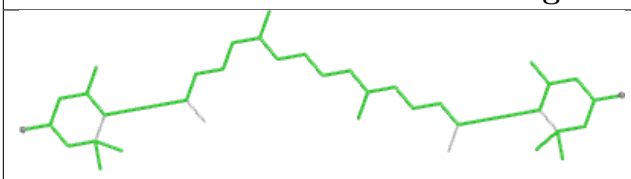


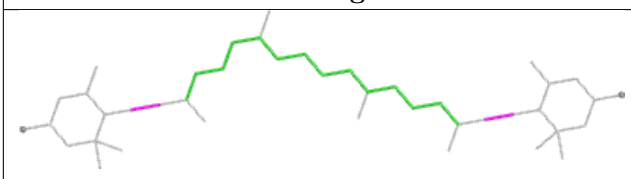
Rings

Ligand II0 0 314



Bond lengths

Bond angles



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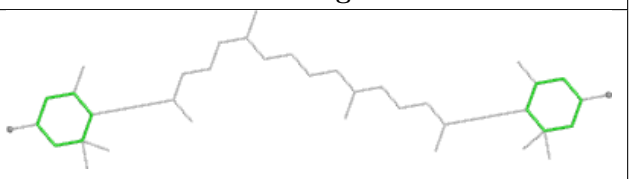
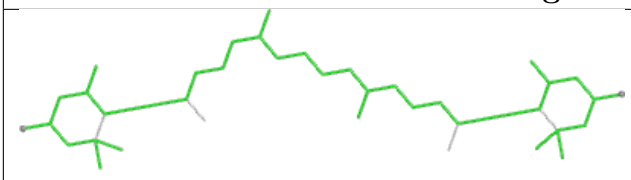


Rings

Ligand II0 9 316



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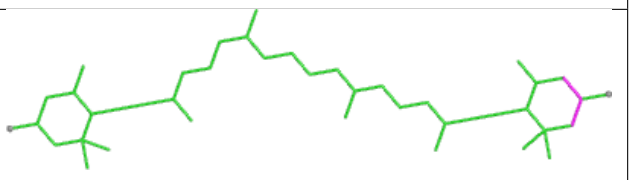

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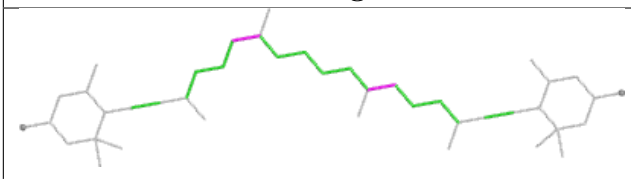

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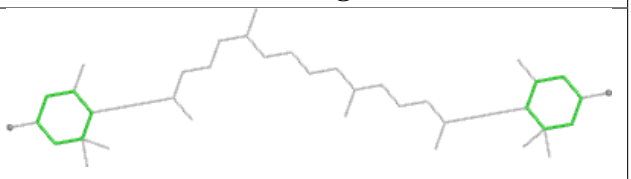
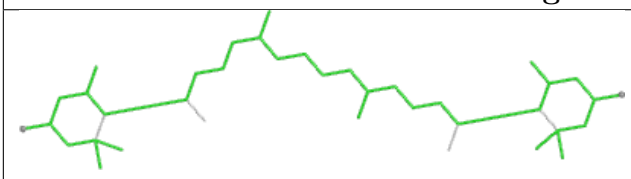


Rings

Ligand II0 5 312



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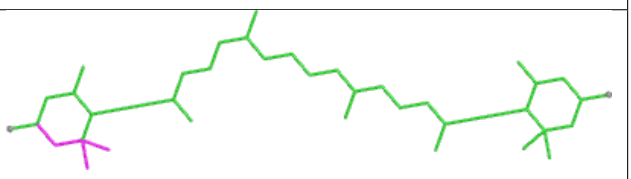

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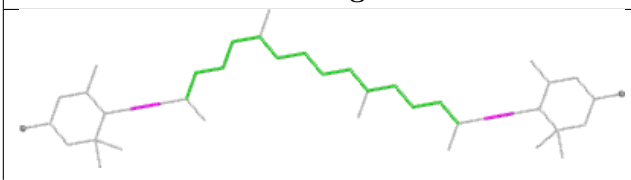

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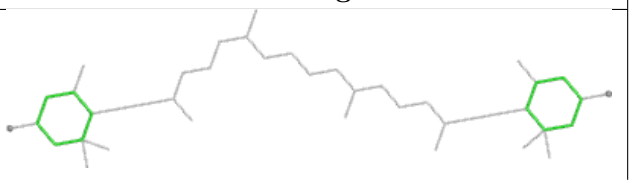
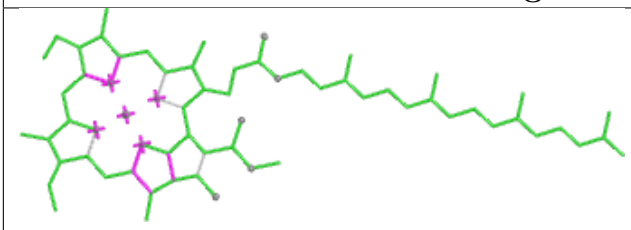


Rings

Ligand CLA B 607



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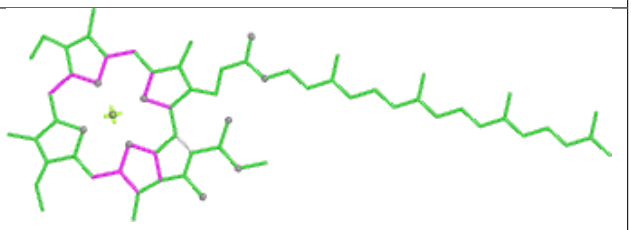
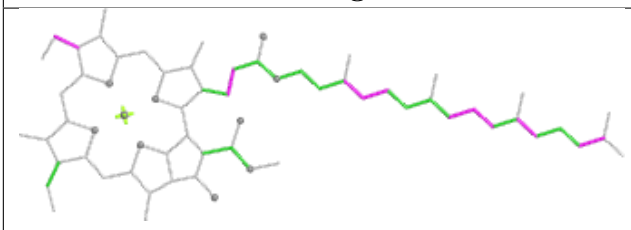


Bond angles



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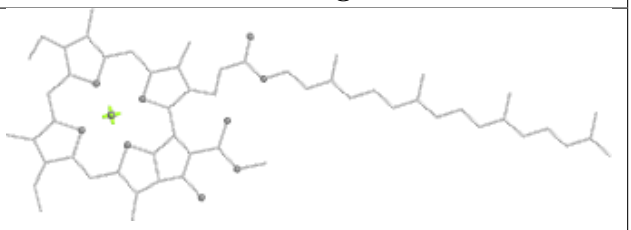
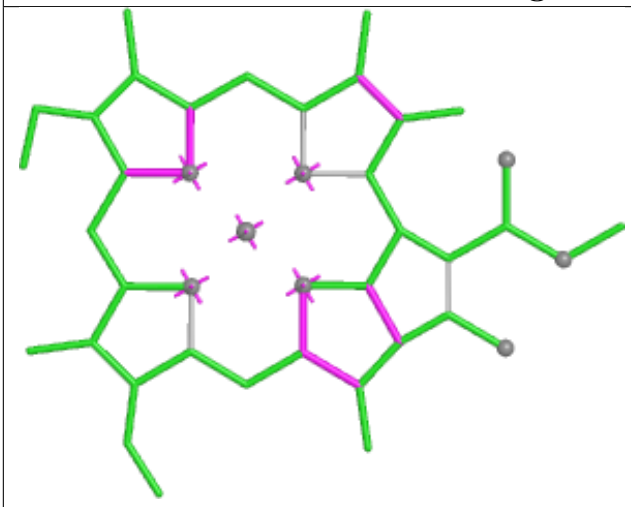


Rings

Ligand CLA 9 306



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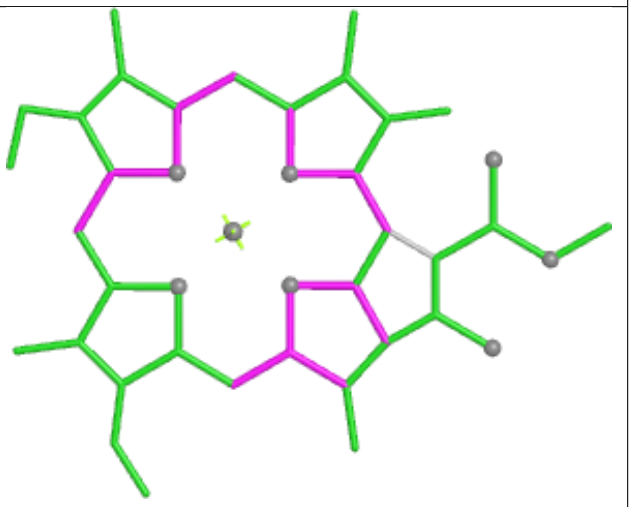
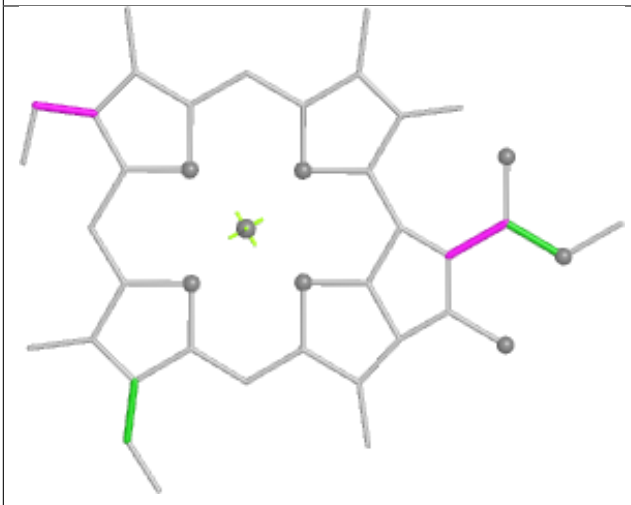


Bond angles



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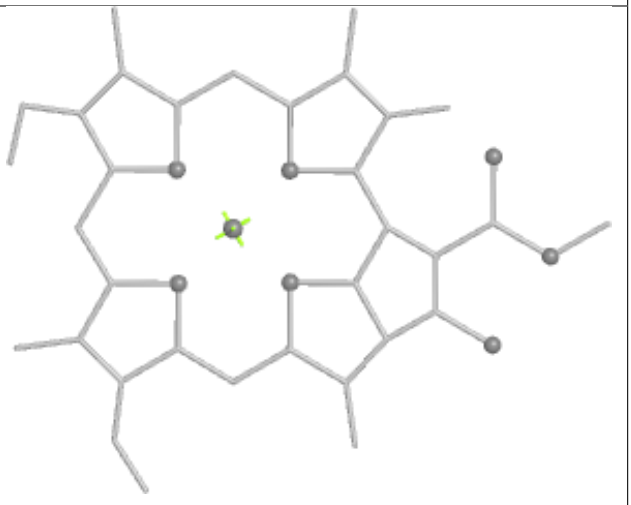
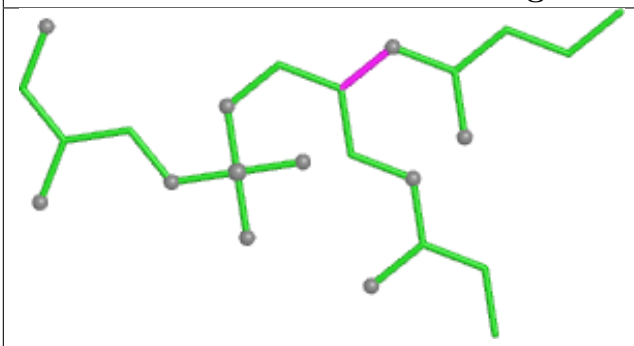


Rings

Ligand LHG a 411



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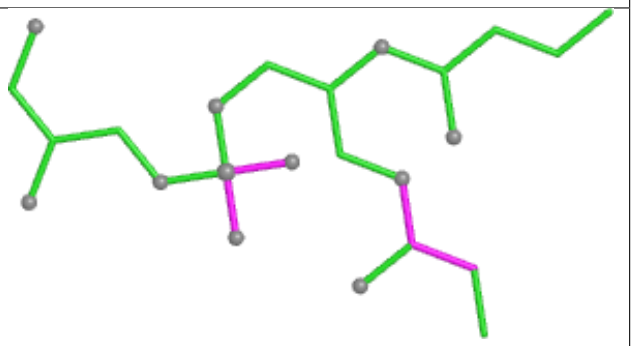
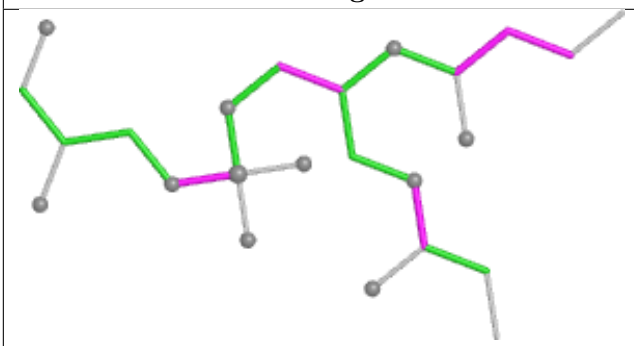


Bond angles



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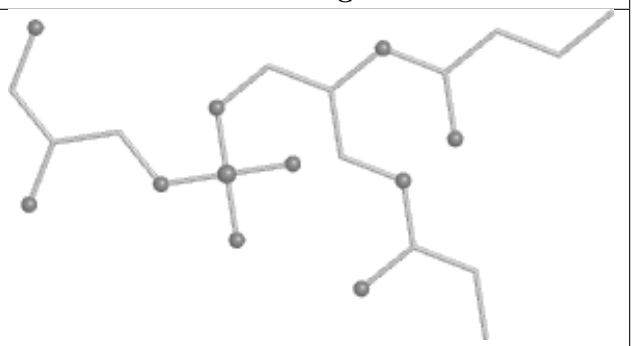
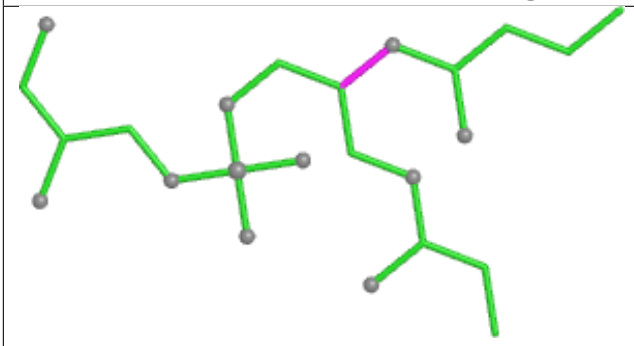


Rings

Ligand LHG A 411



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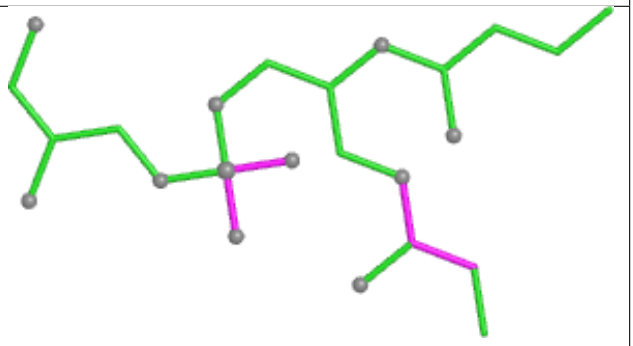
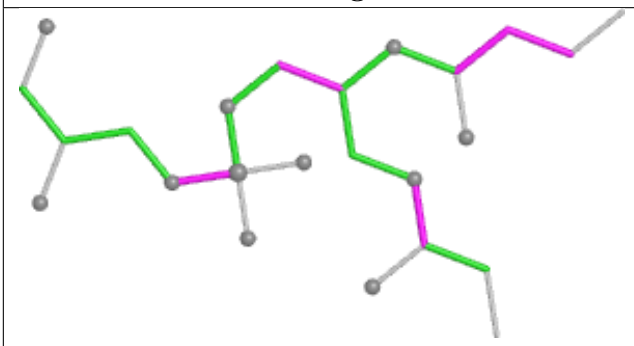


Bond angles



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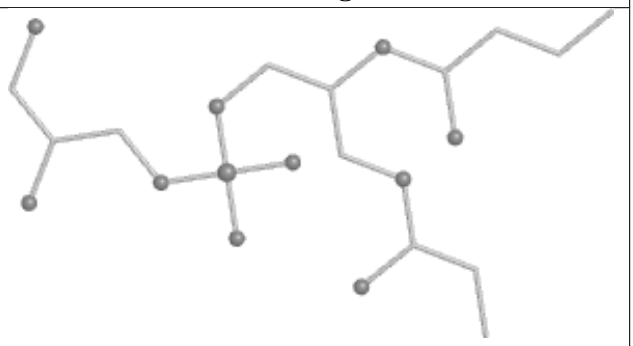
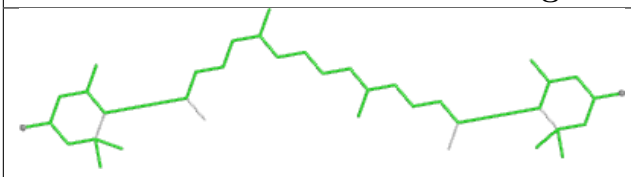
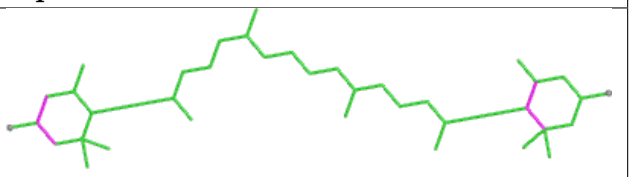
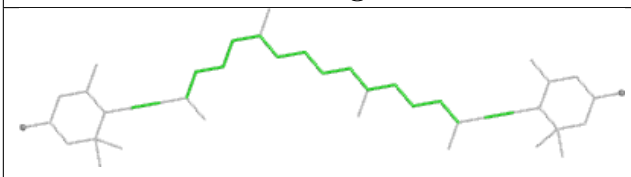
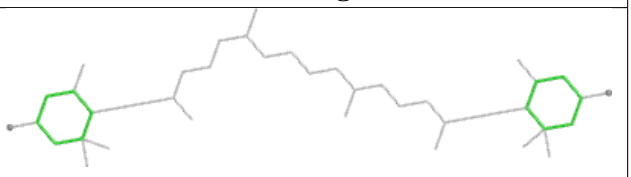
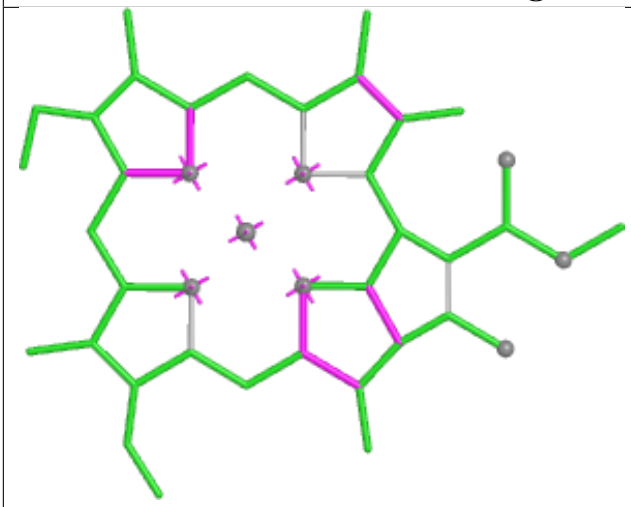
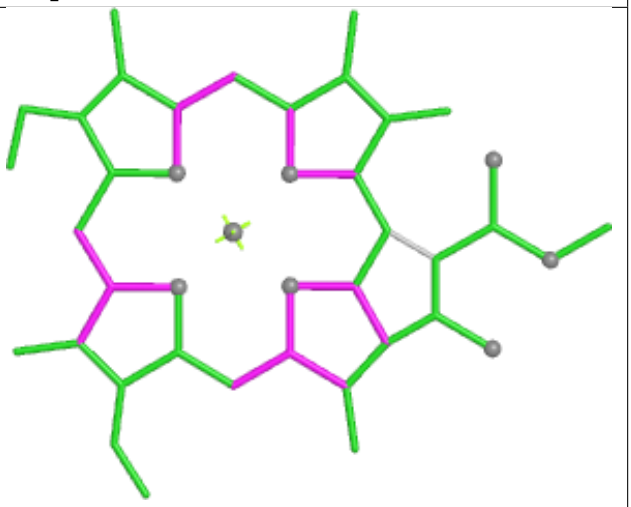
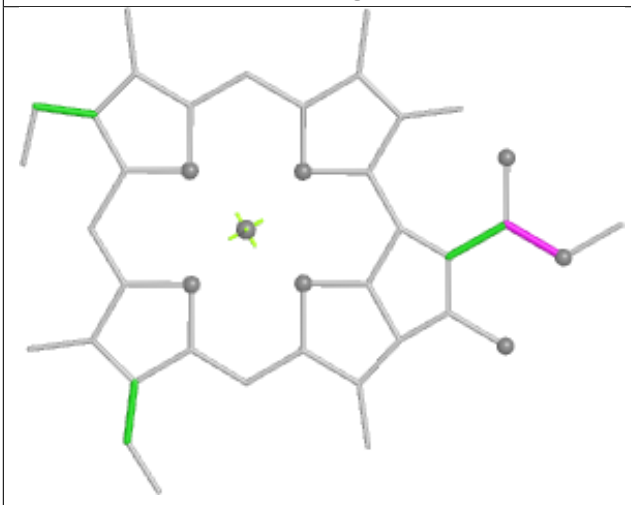
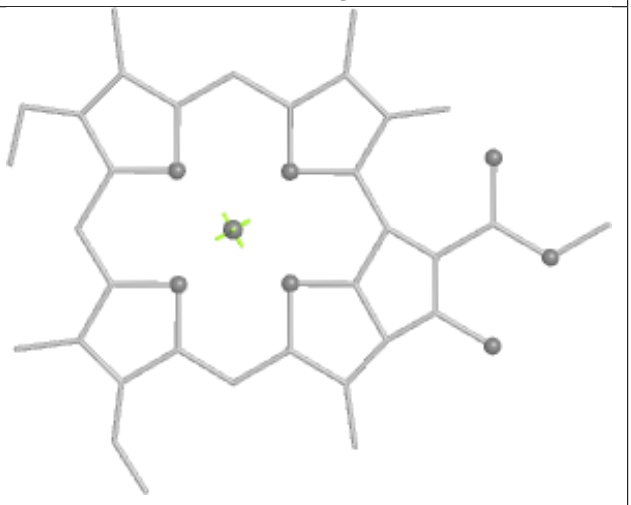
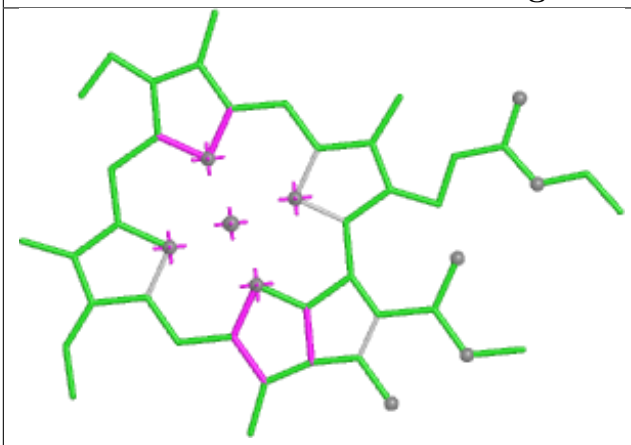


Rings

Ligand II0 p 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 308



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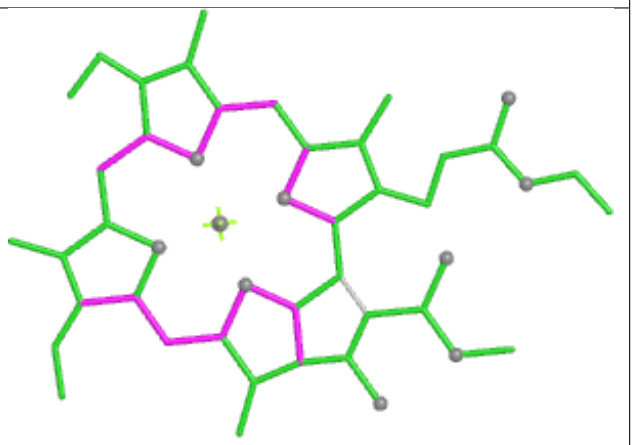

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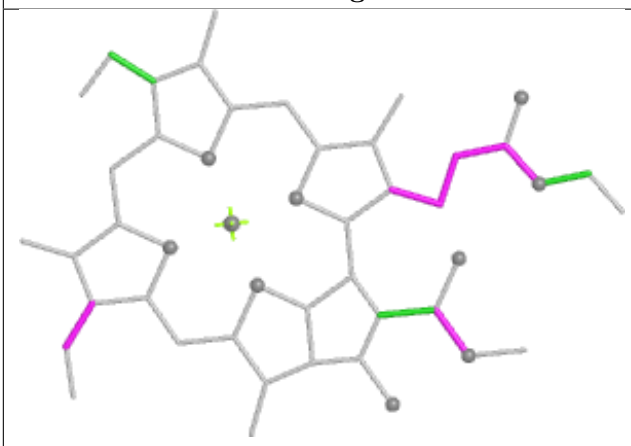

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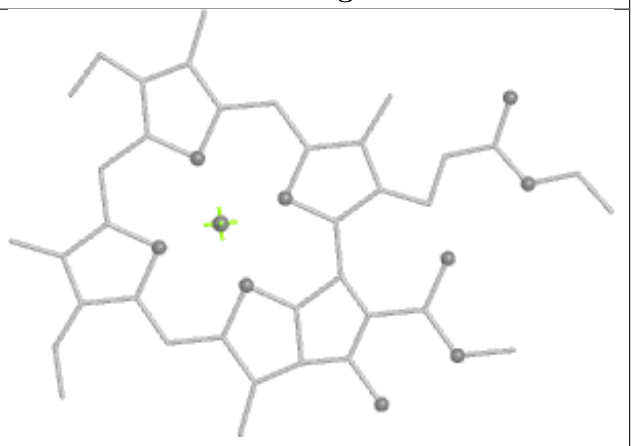
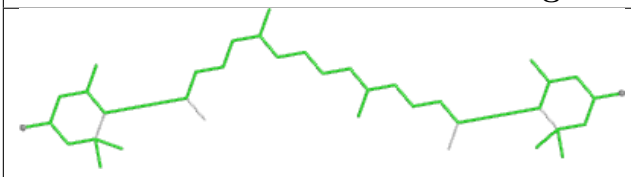


Rings

Ligand II0 6 316



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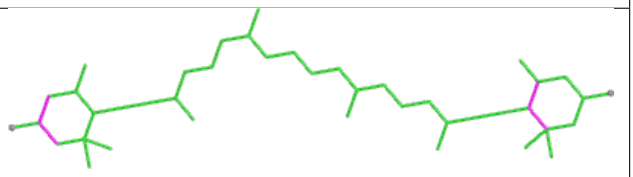

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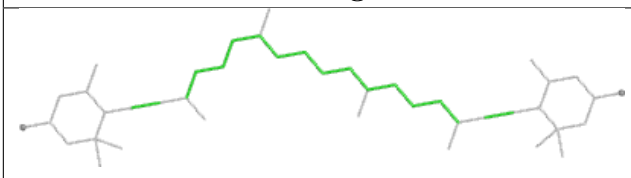

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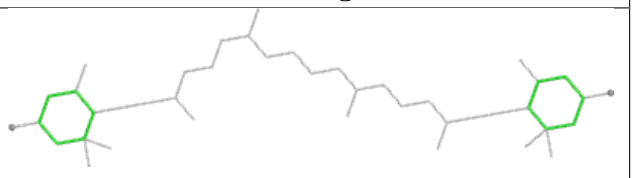
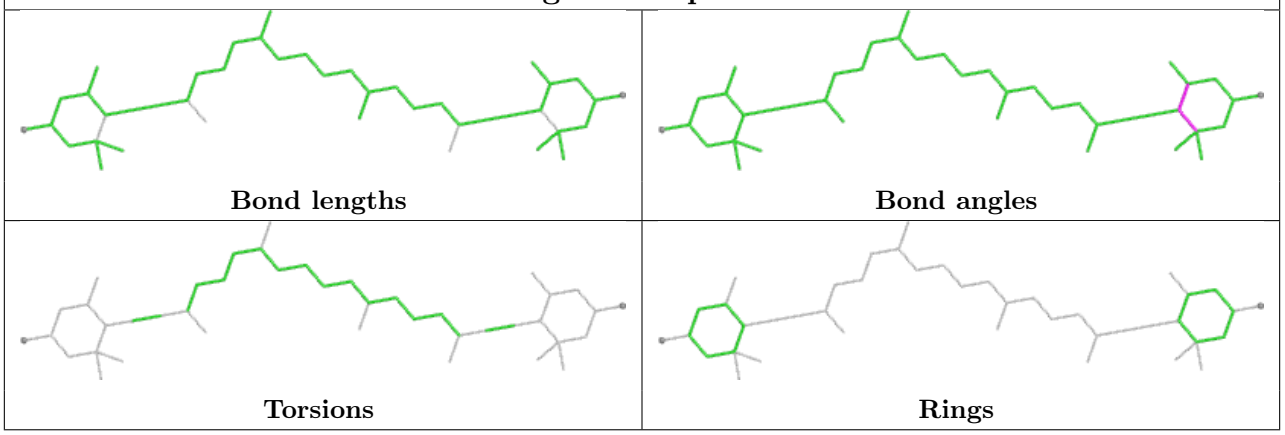
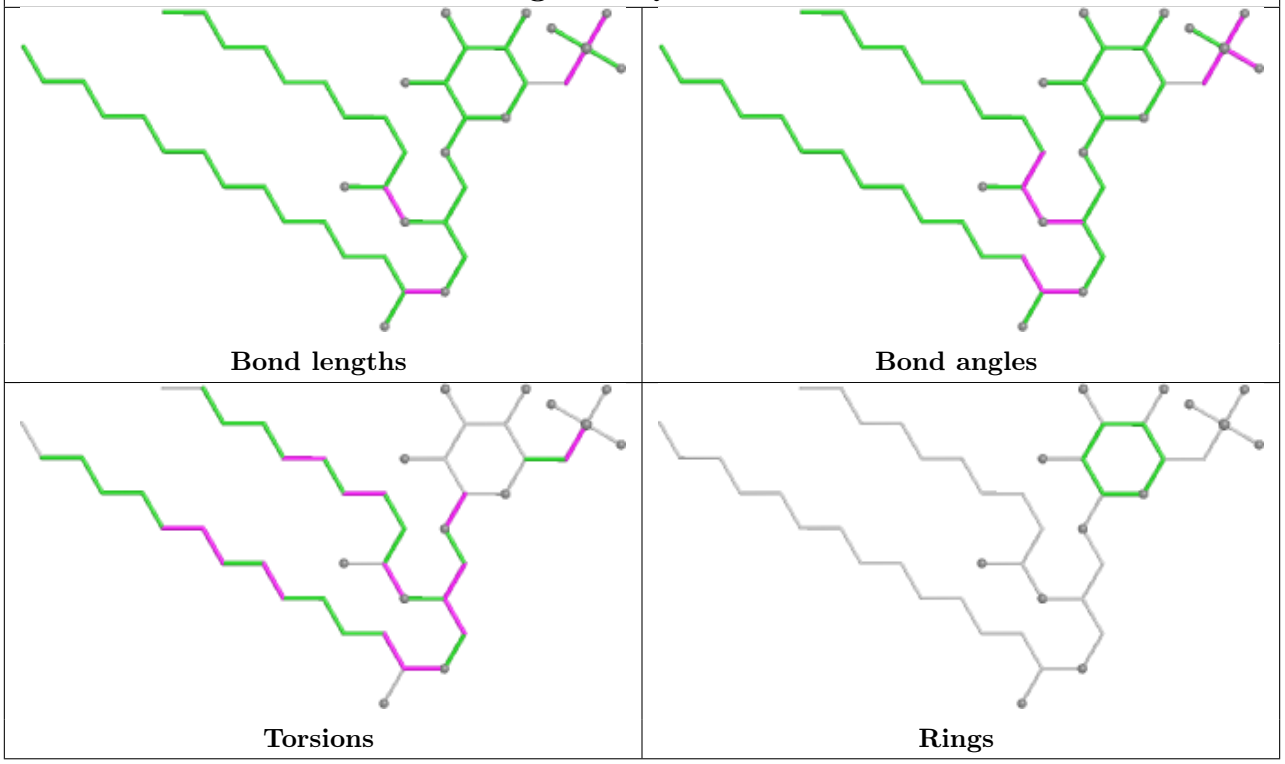


Rings

Ligand II0 p 314



Ligand SQD J 101



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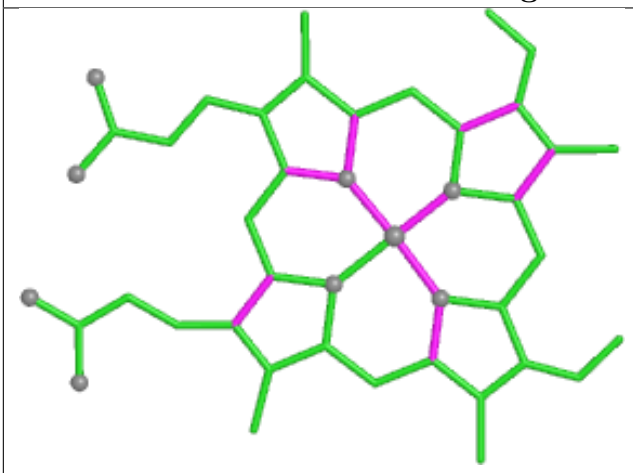

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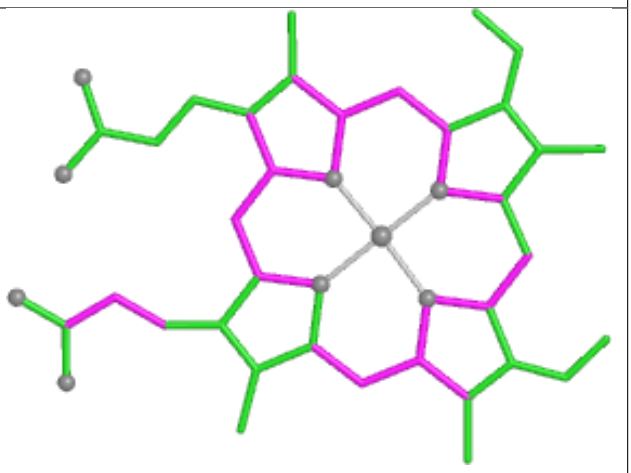

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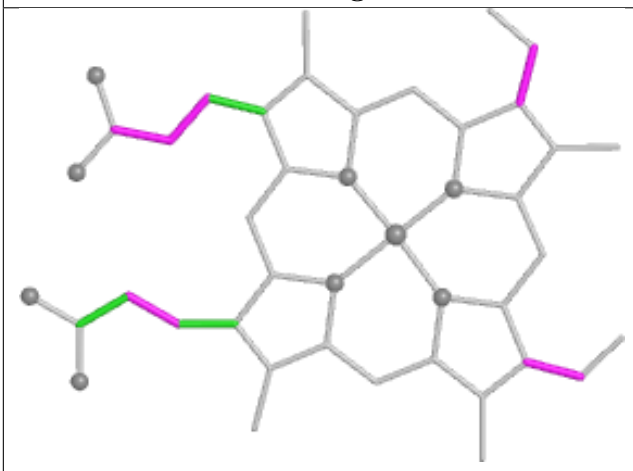

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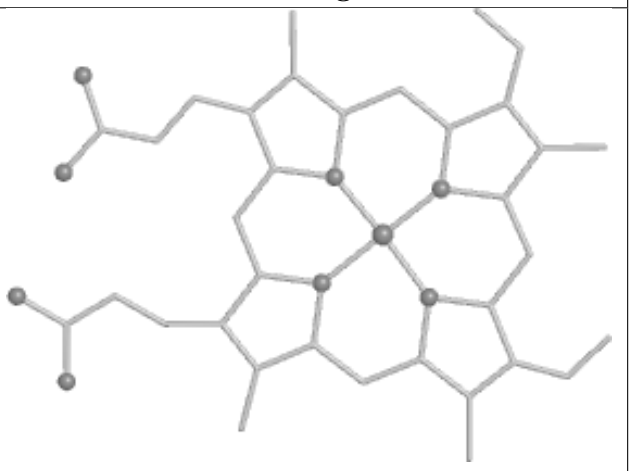
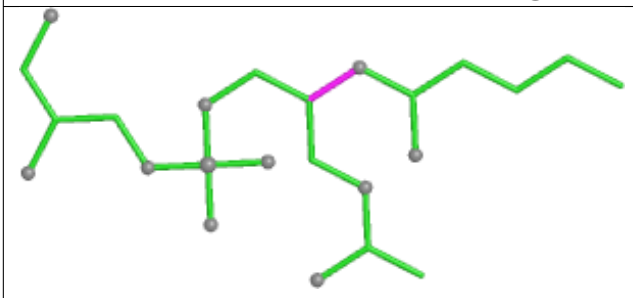


Rings

Ligand LHG 9 321



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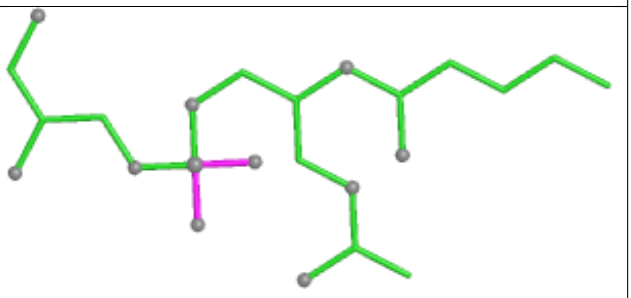

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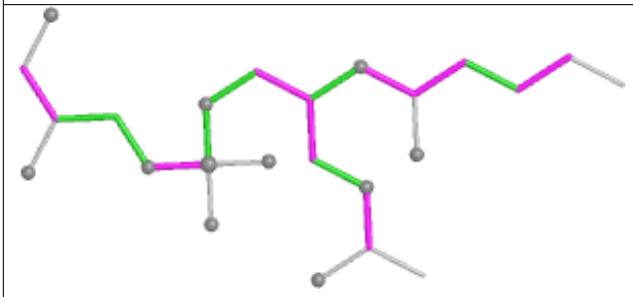

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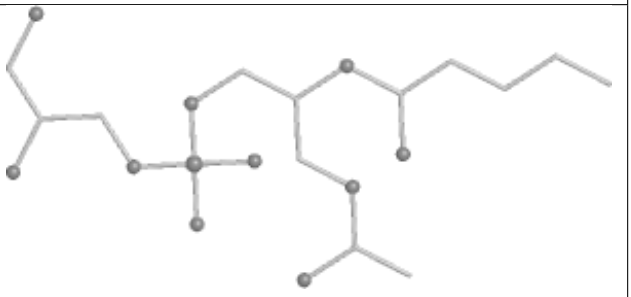
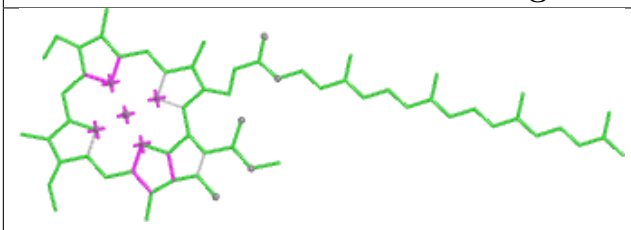


Rings

Ligand CLA c 508



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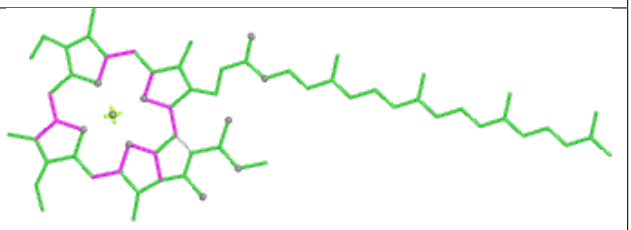

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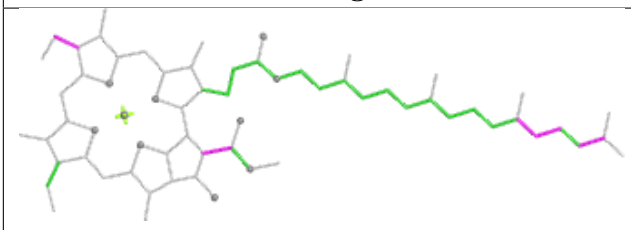

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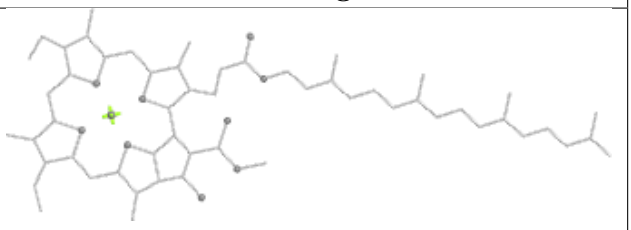
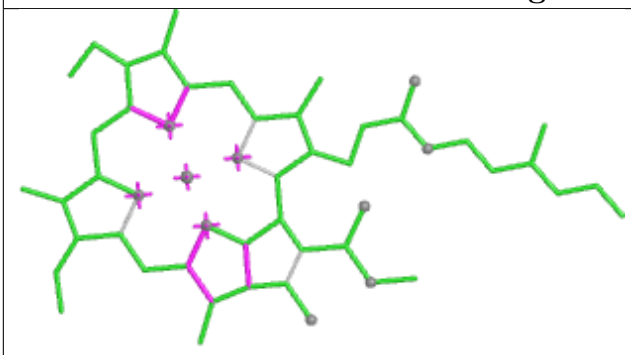


Rings

Ligand CLA 8 303



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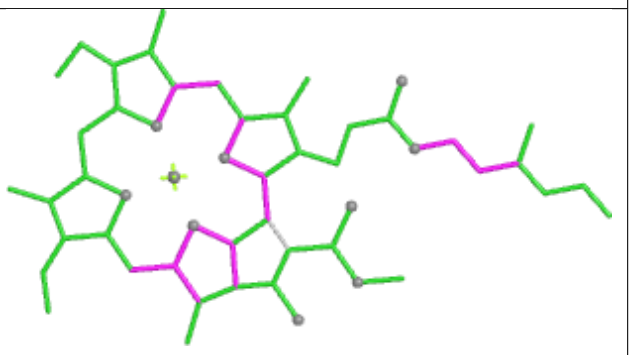

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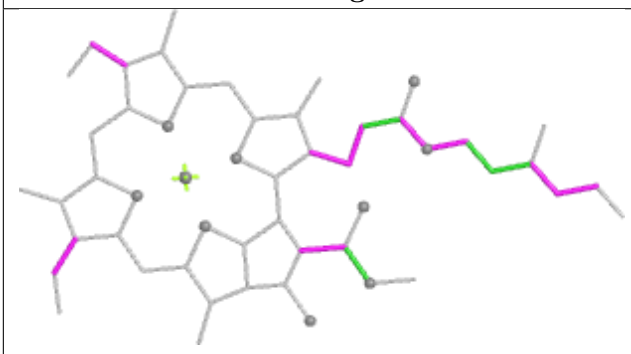

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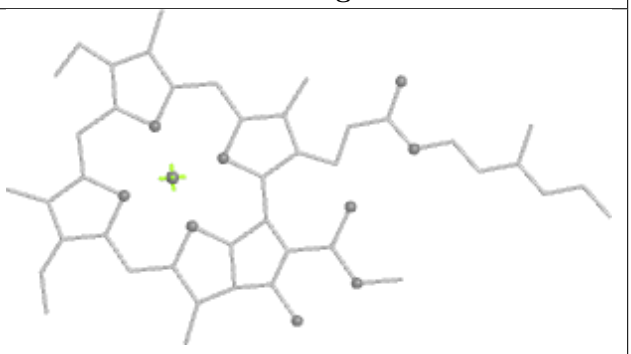
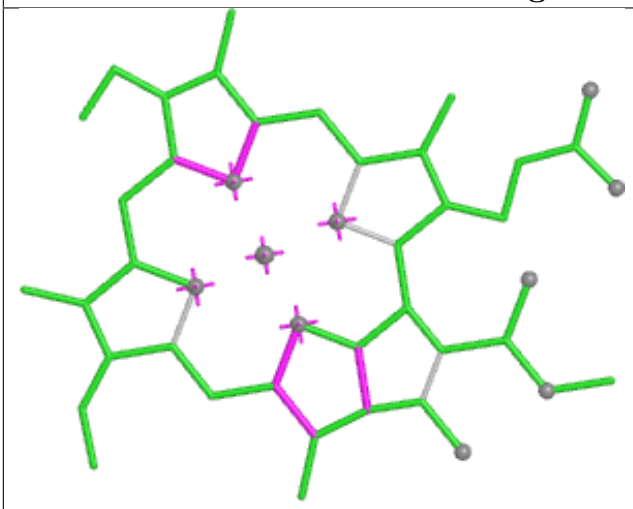


Rings

Ligand CLA g 311



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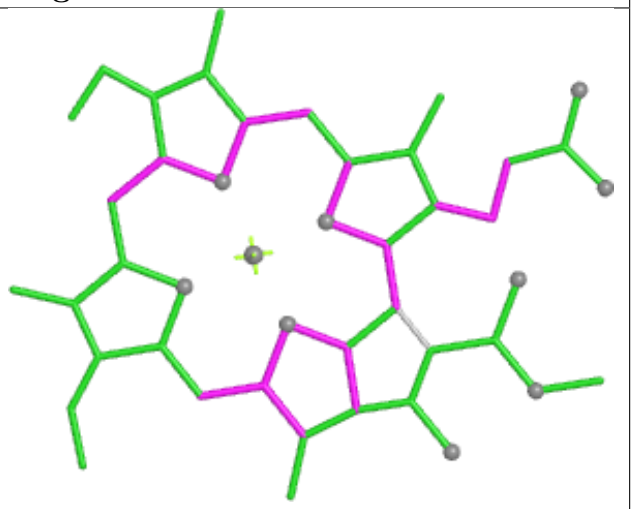

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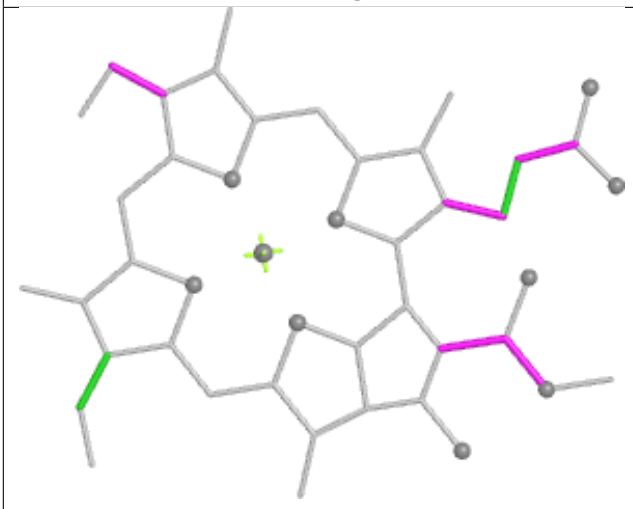
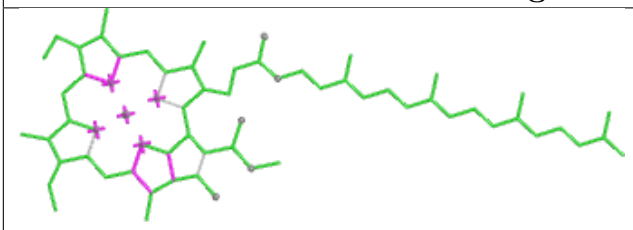


Torsions

Rings

Ligand CLA a 405



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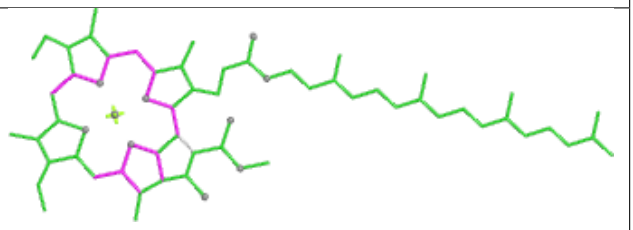

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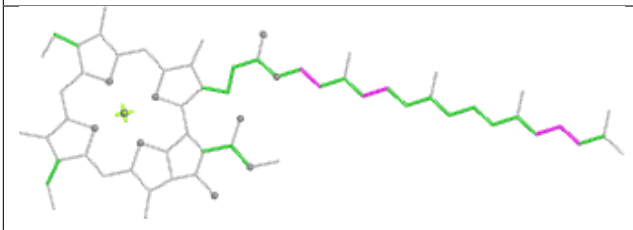

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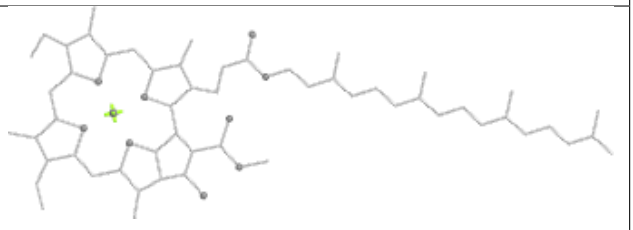
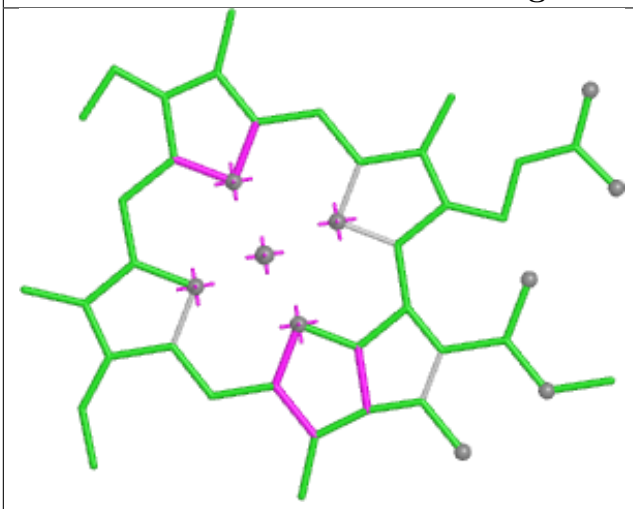


Rings

Ligand CLA 2 301



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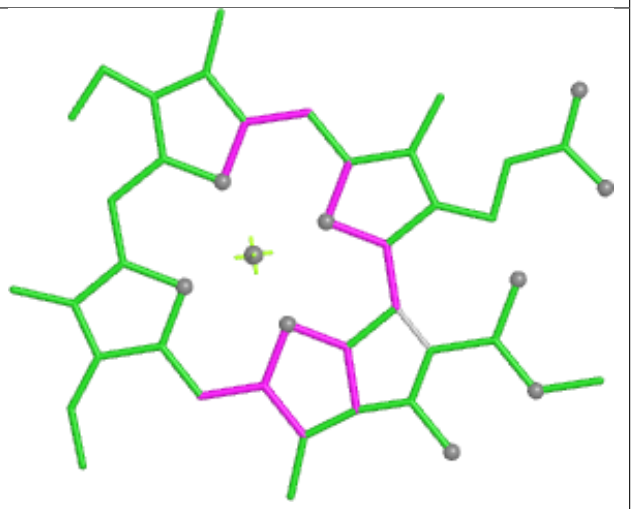

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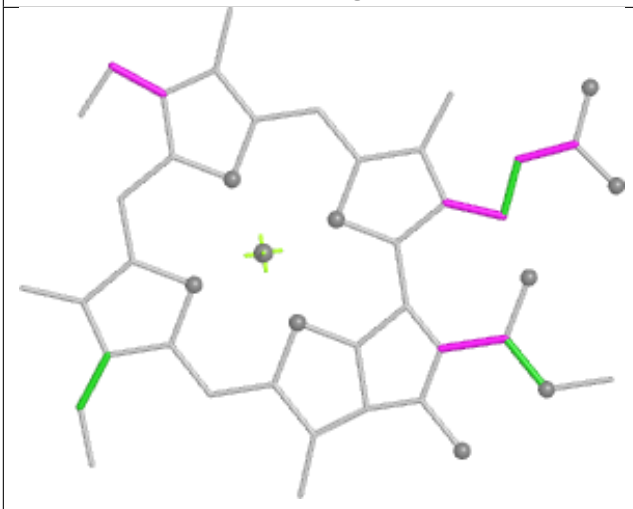
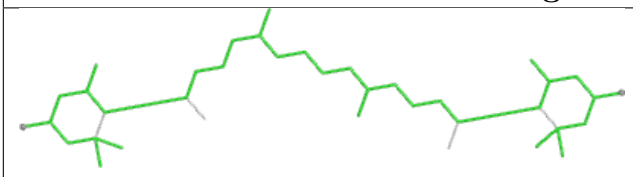


Torsions

Rings

Ligand II0 9 318



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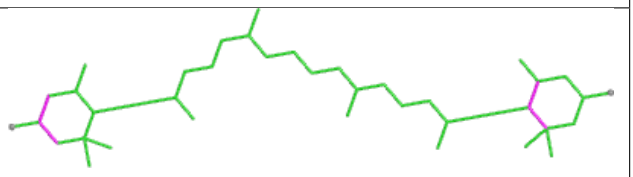

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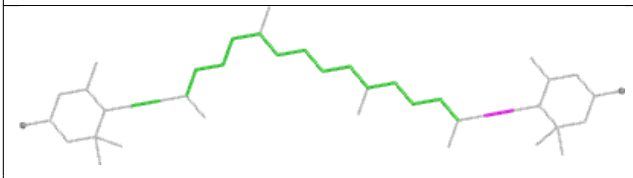

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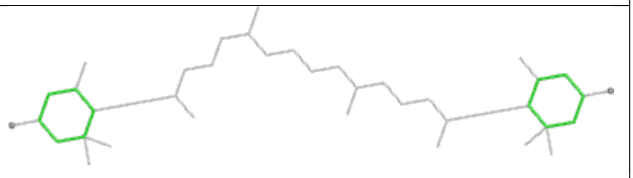
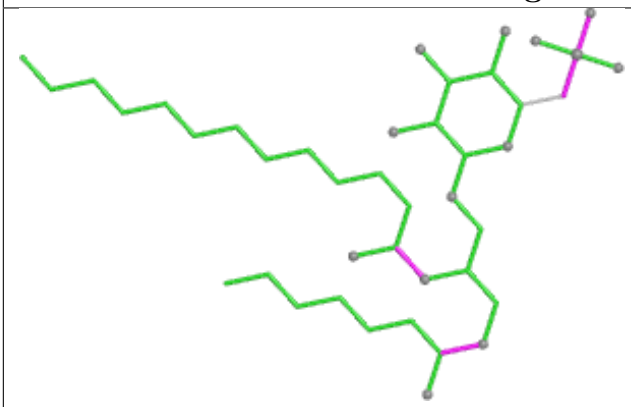


Rings

Ligand SQD C 501



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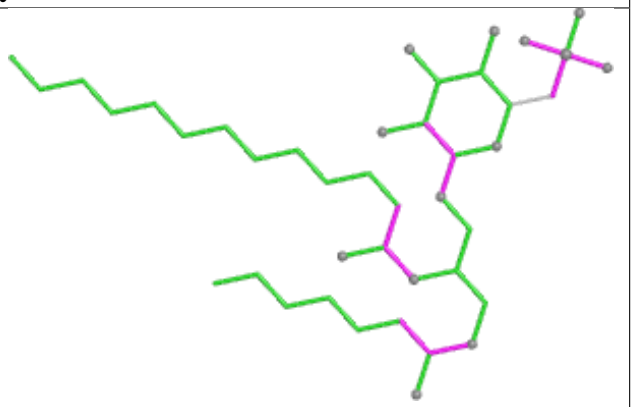

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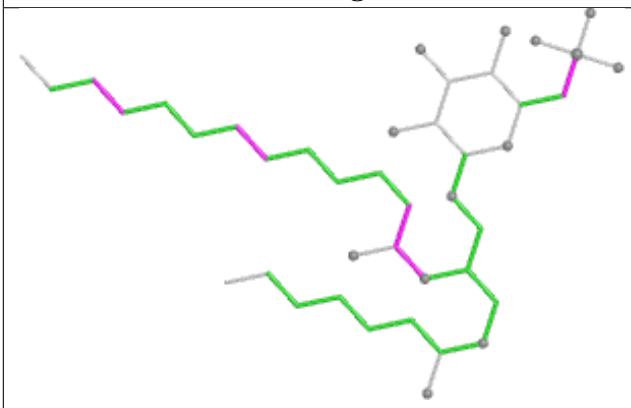

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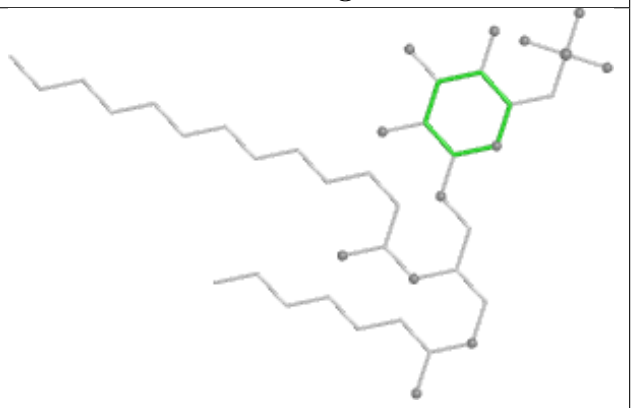
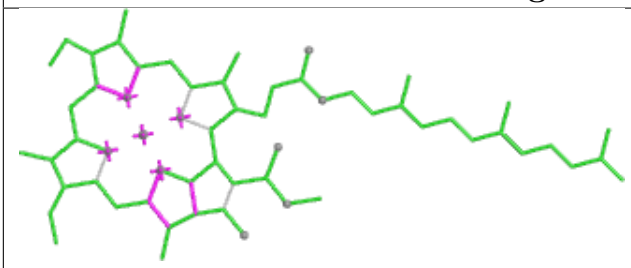


Rings

Ligand CLA 2 307



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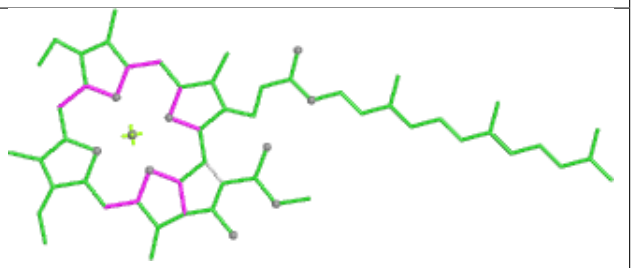
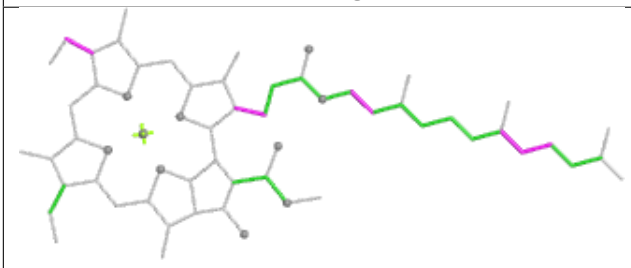


Bond angles



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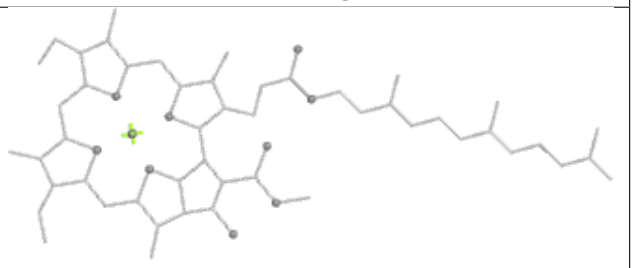
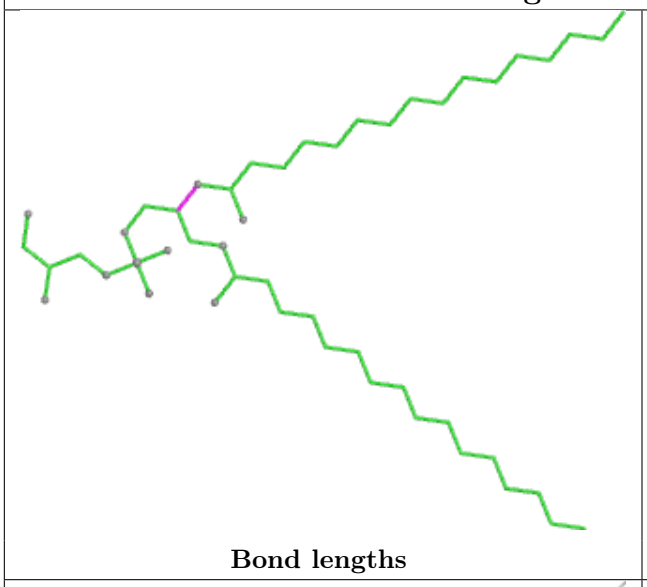


Rings

Ligand LHG B 623



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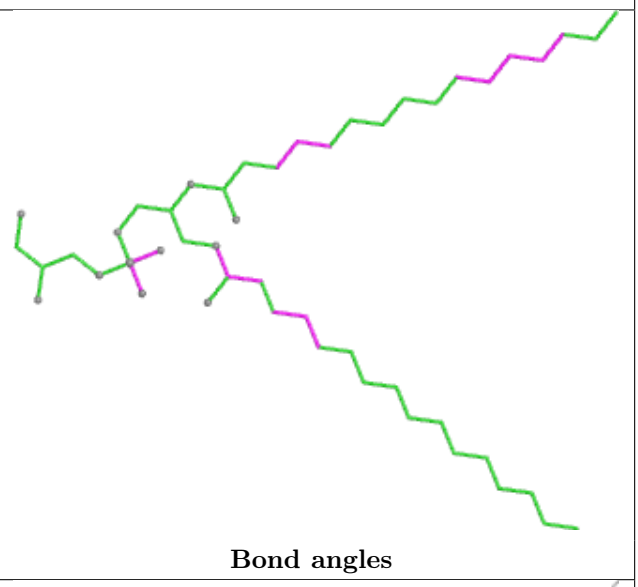
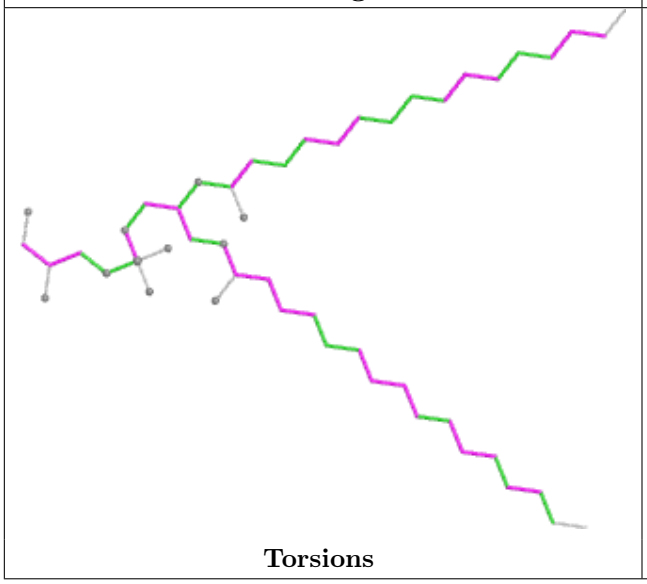
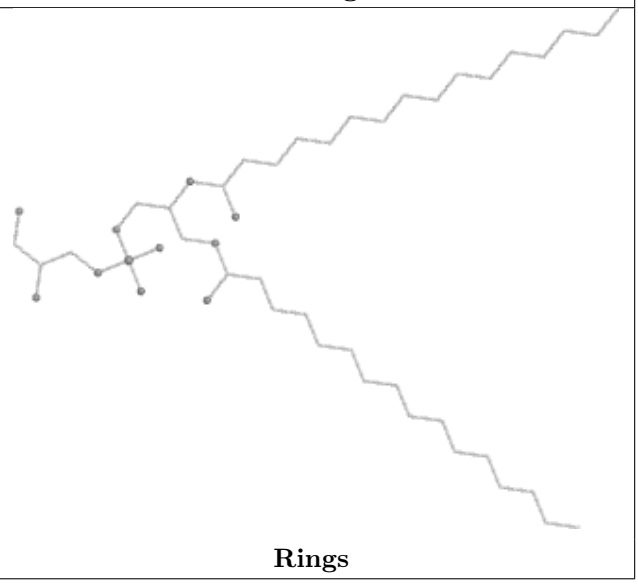


Bond angles

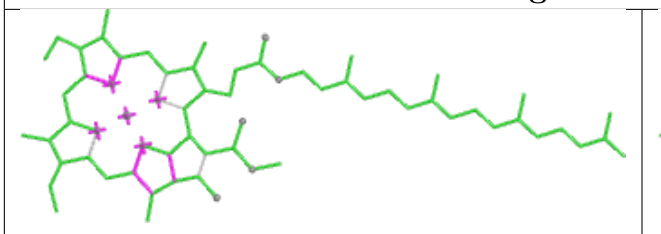


Torsions



Rings

Ligand CLA 7 307



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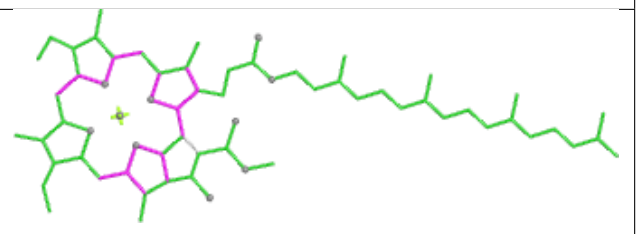

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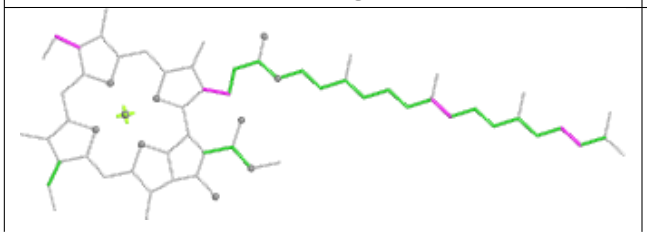

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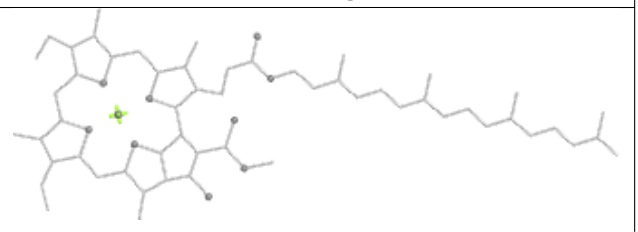
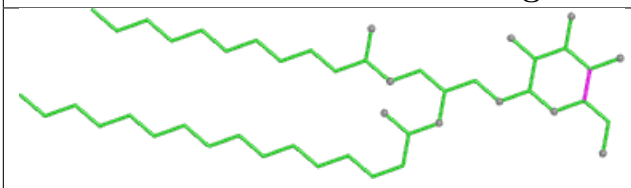


Rings

Ligand LMG d 410



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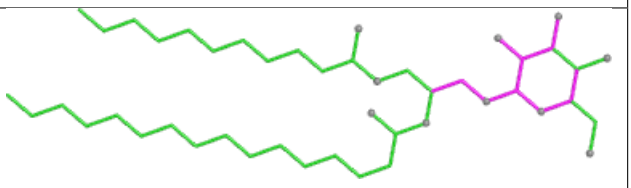

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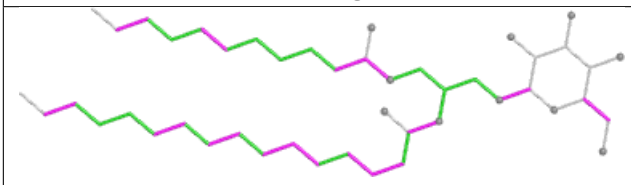

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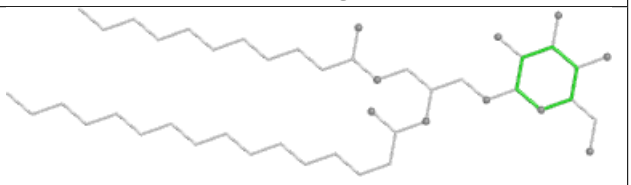
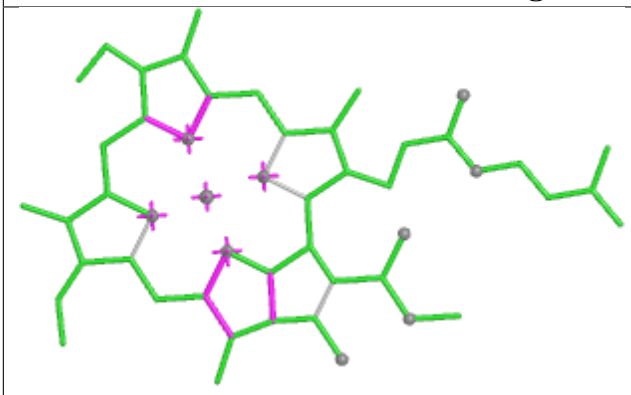


Rings

Ligand CLA n 306



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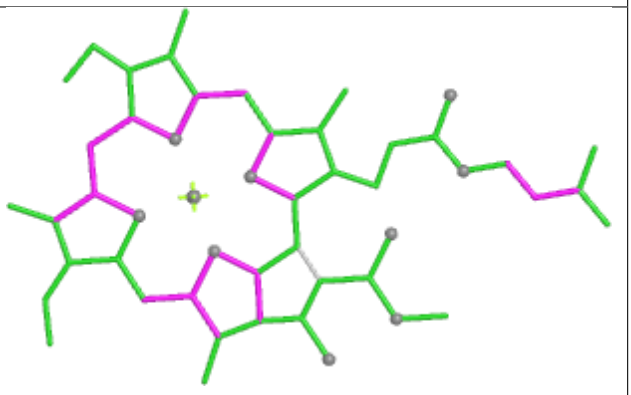

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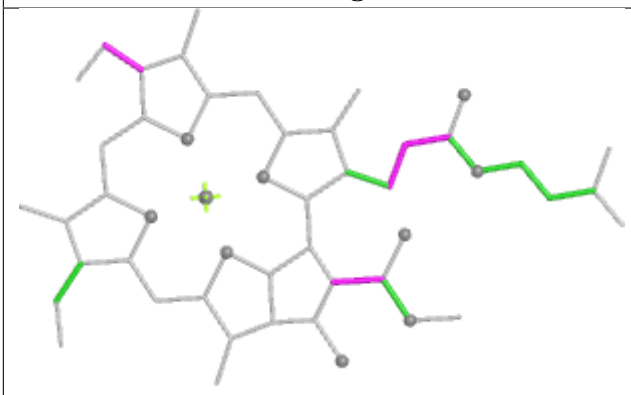

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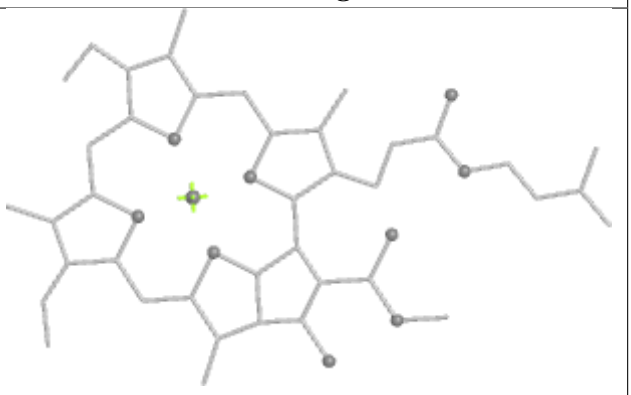
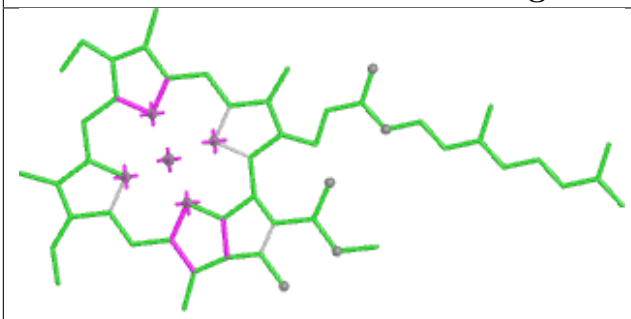


Rings

Ligand CLA 9 312



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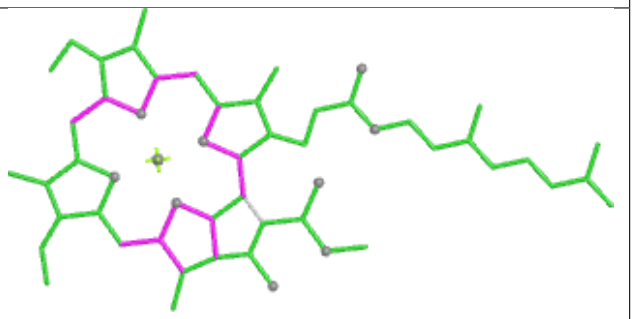

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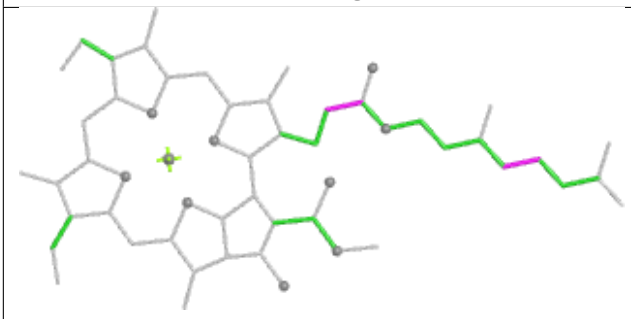

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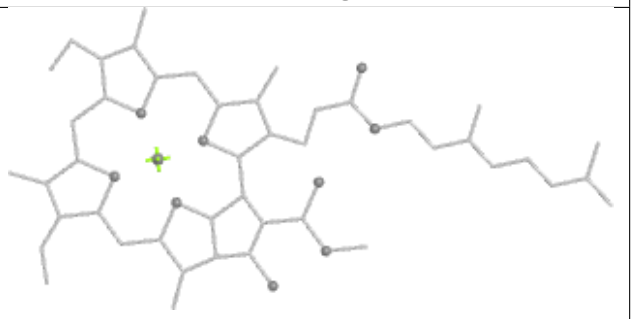
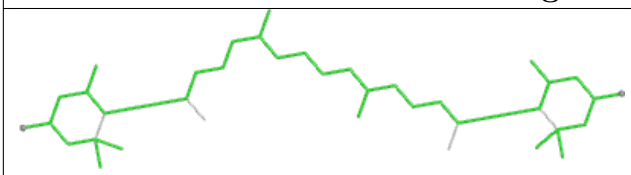


Rings

Ligand II0 p 301



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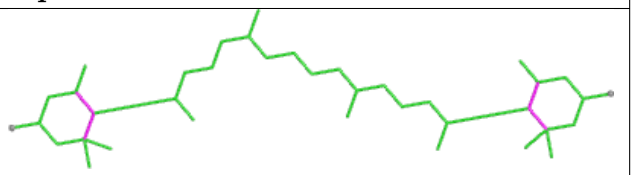

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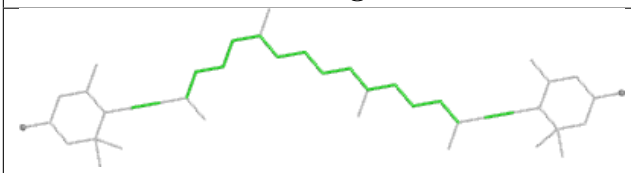

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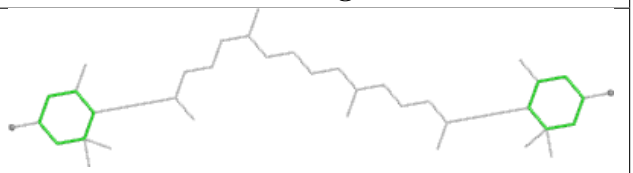

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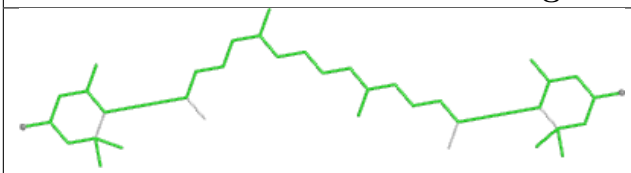

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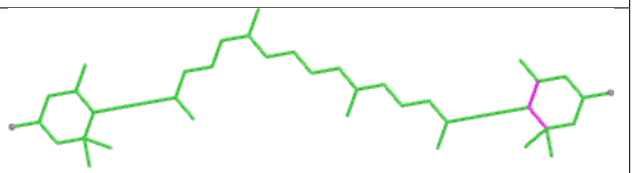

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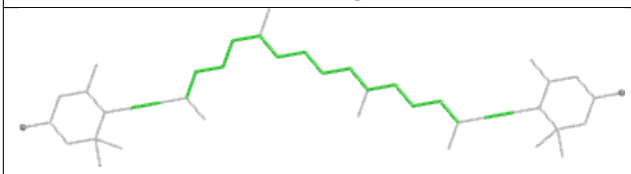

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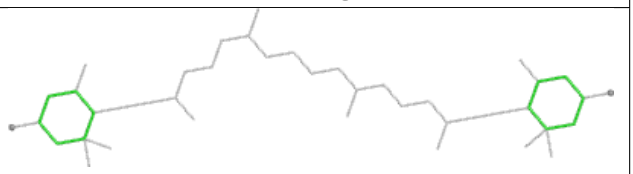
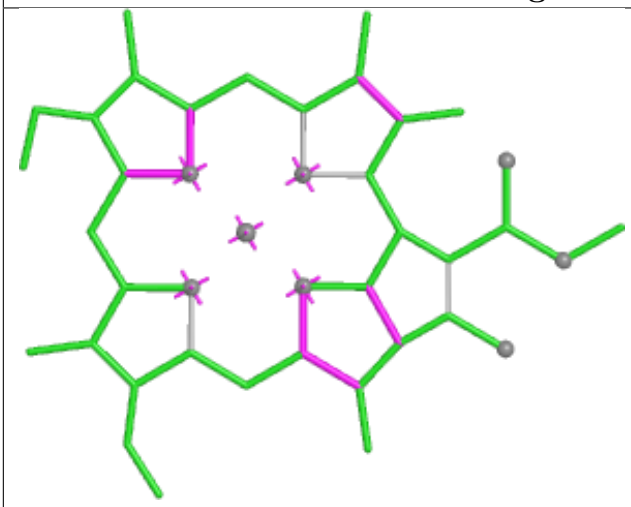


Rings

Ligand CLA 5 308



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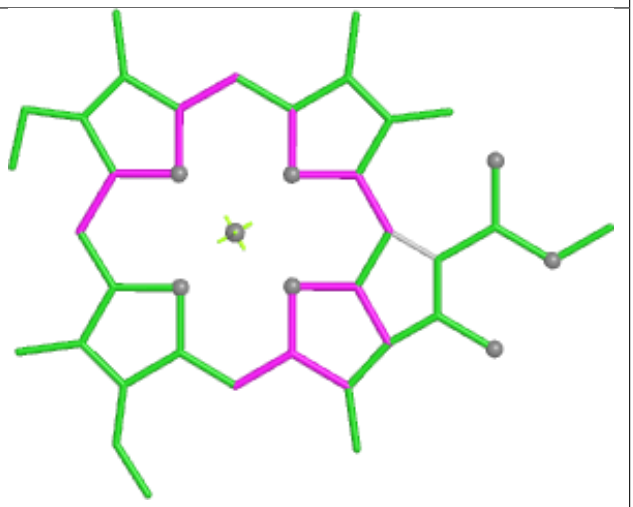

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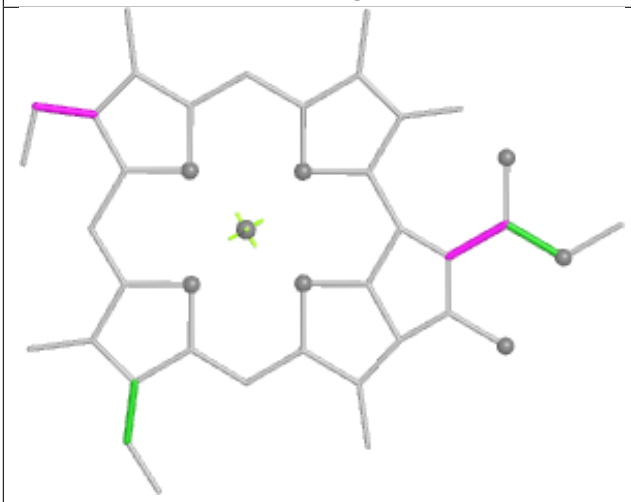

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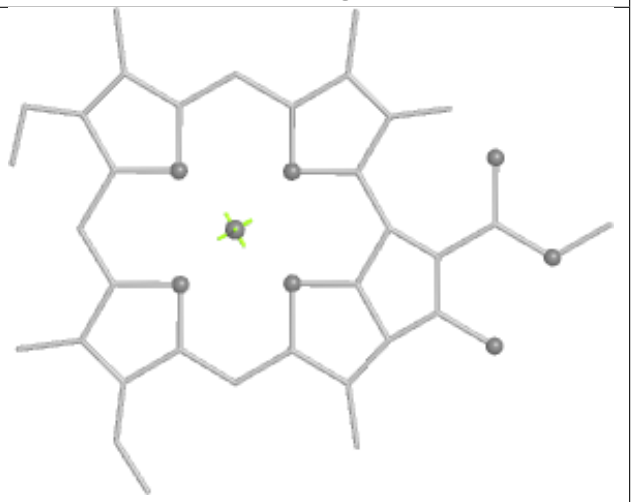

Rings

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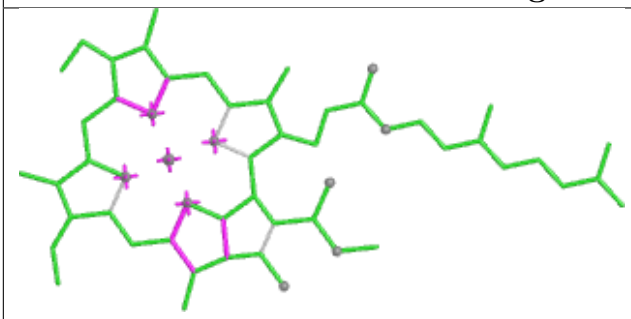

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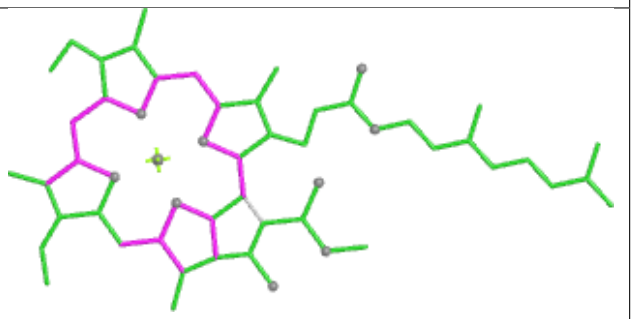

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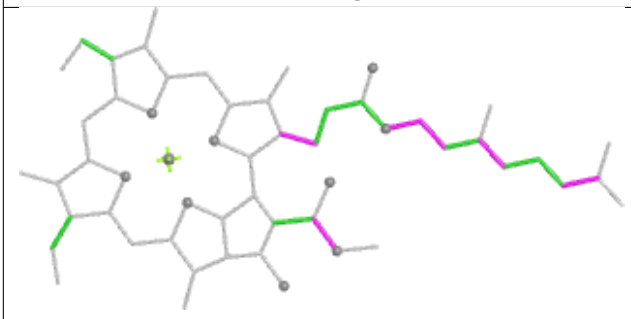

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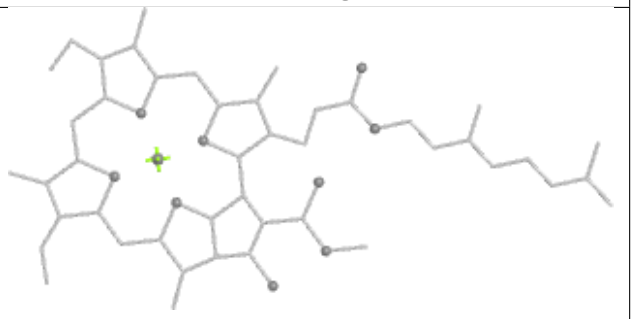
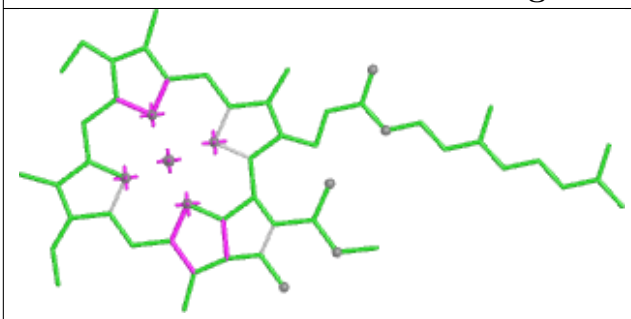


Rings

Ligand CLA 2 305



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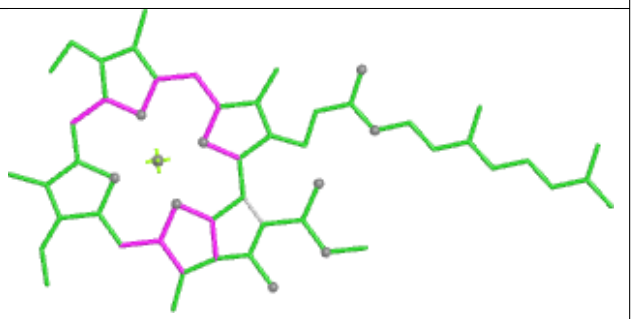

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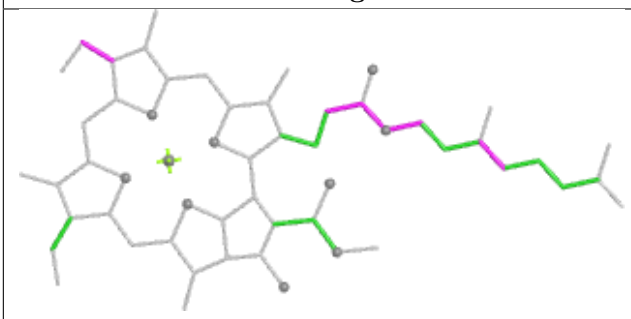

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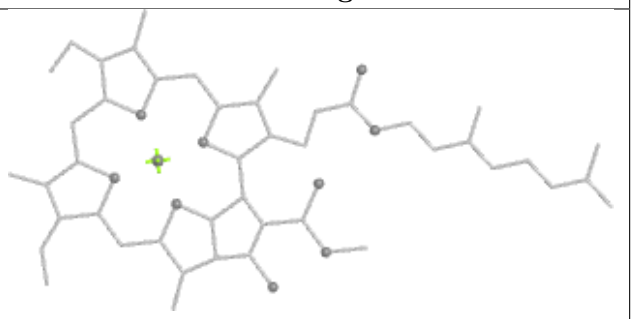
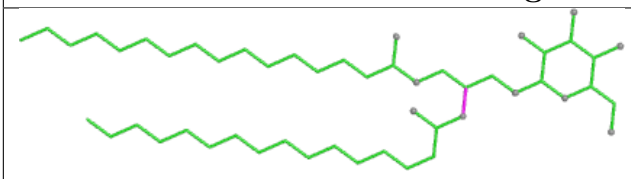


Rings

Ligand LMG c 520



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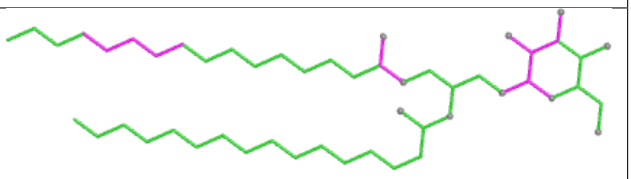
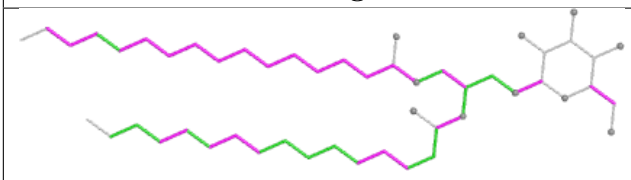


Bond angles



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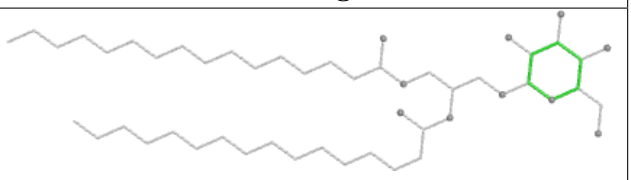
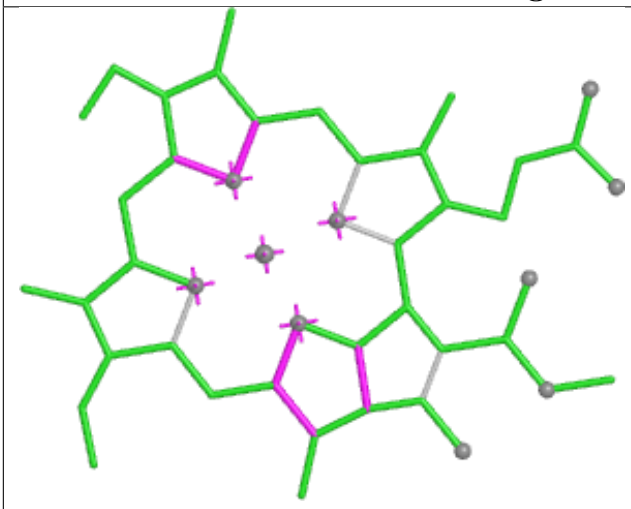


Rings

Ligand CLA b 615



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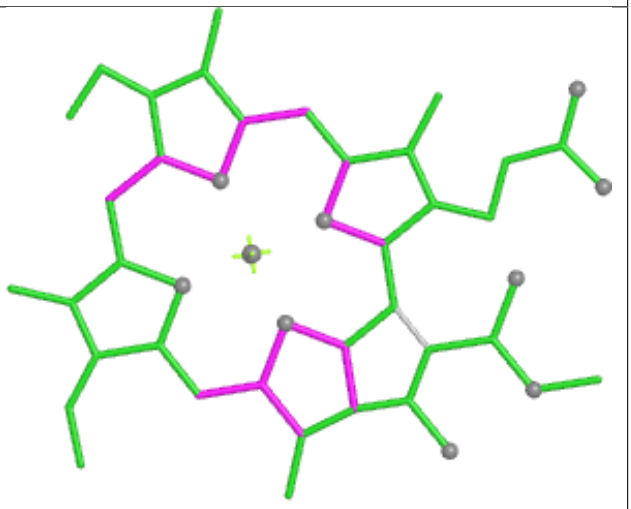

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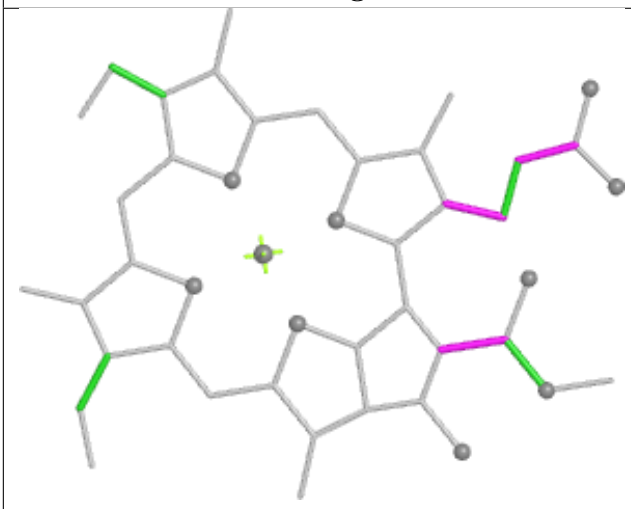
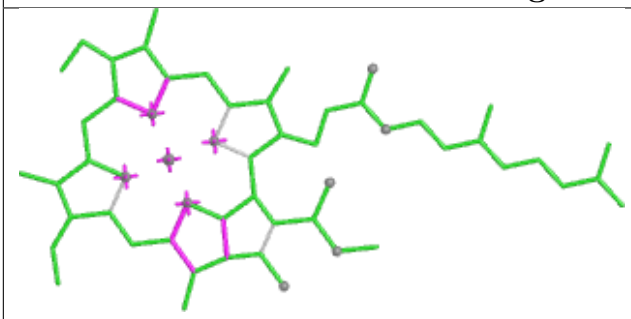


Torsions

Rings

Ligand CLA g 307



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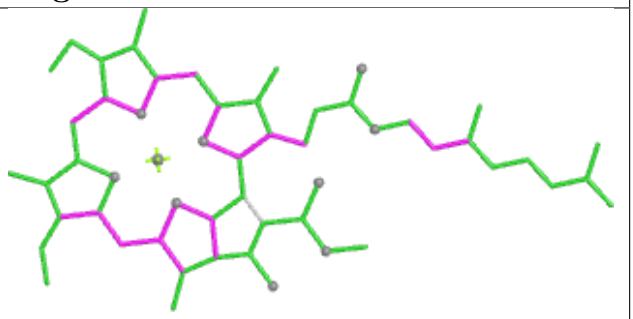

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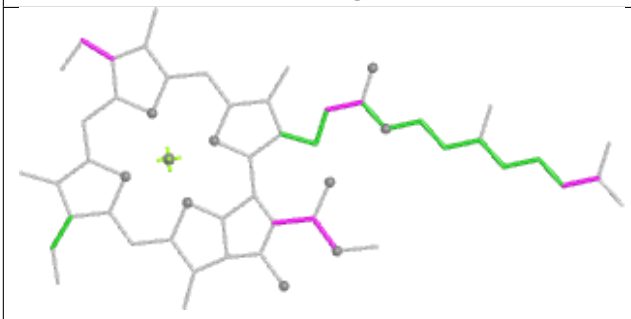

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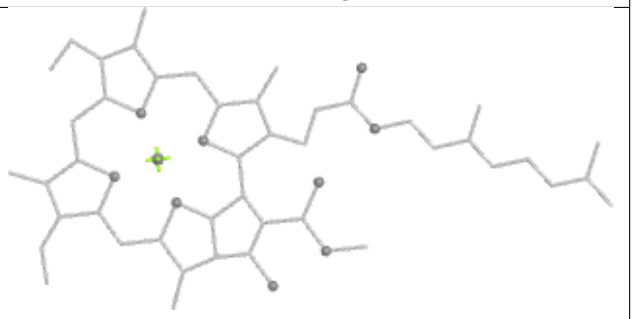
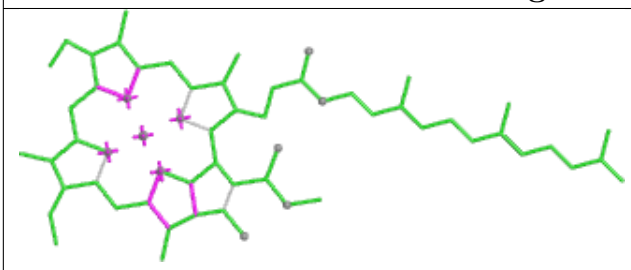


Rings

Ligand CLA 2 304



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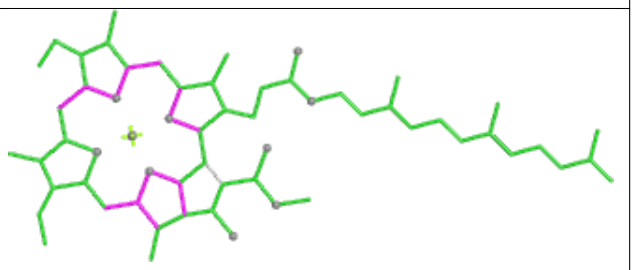
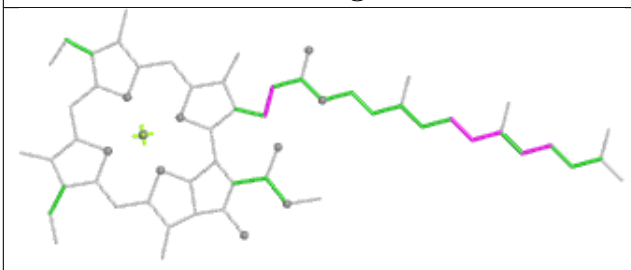


Bond angles



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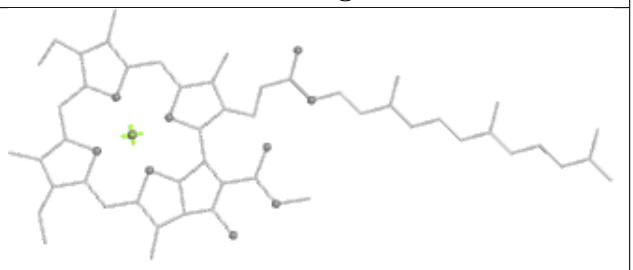
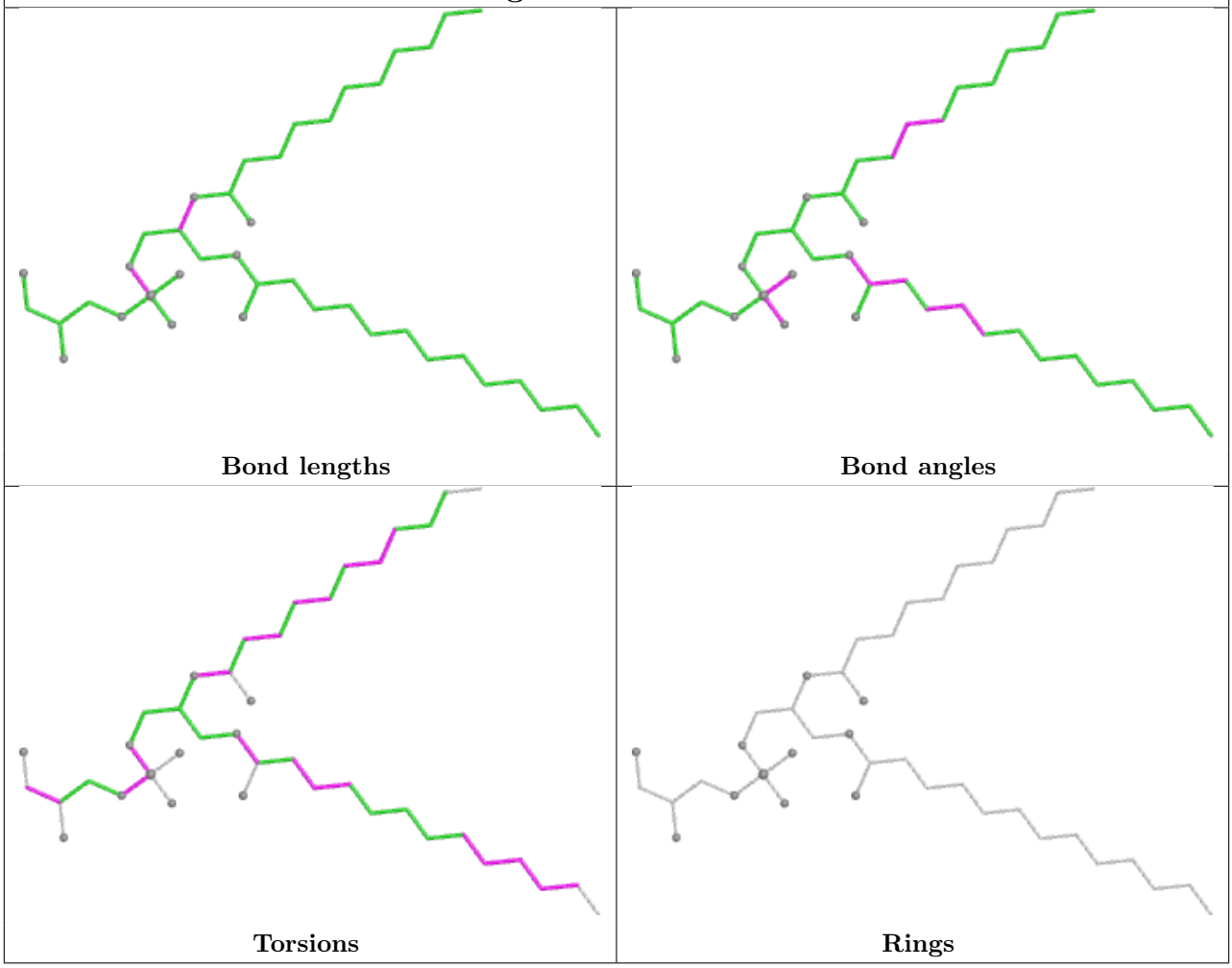
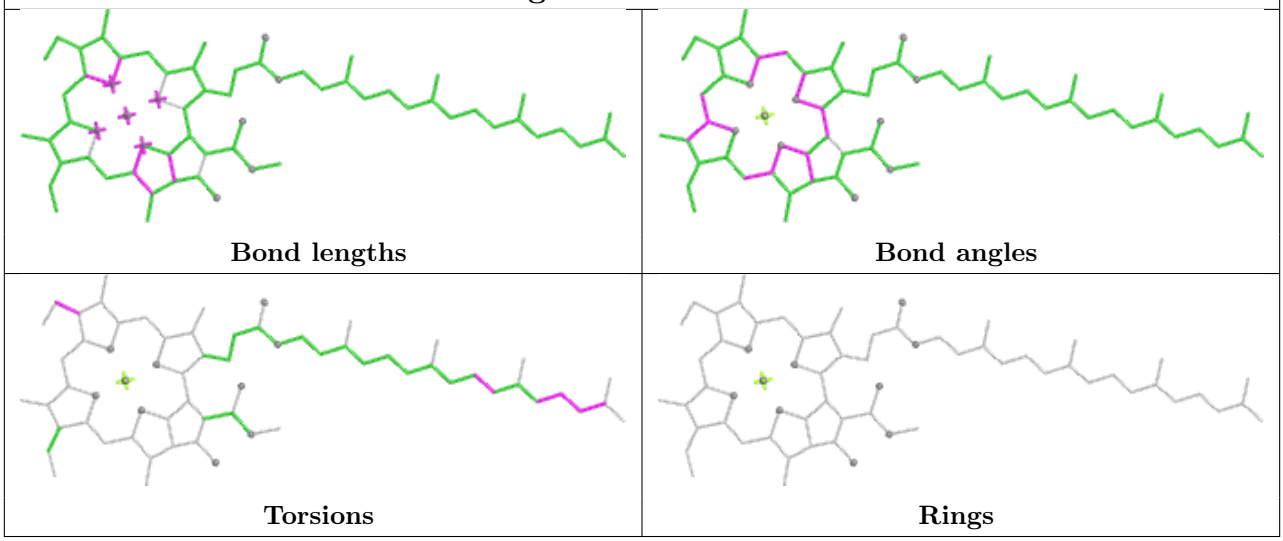


Rings

Ligand LHG 9 322



Ligand CLA b 616



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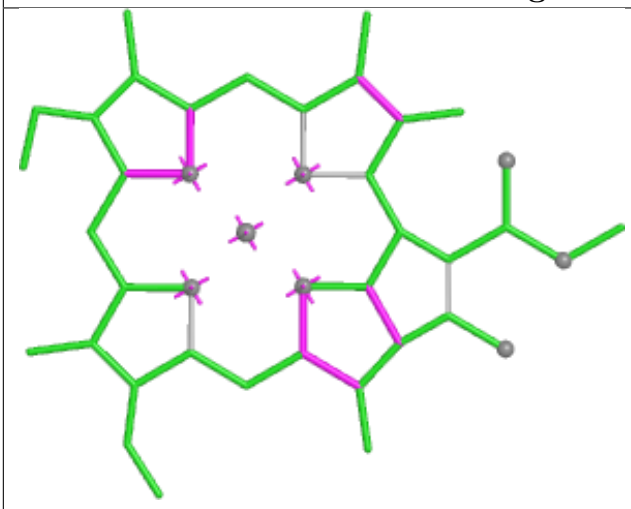

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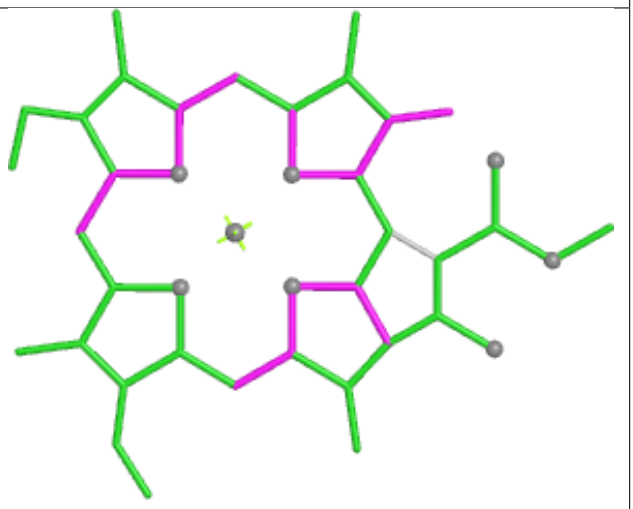
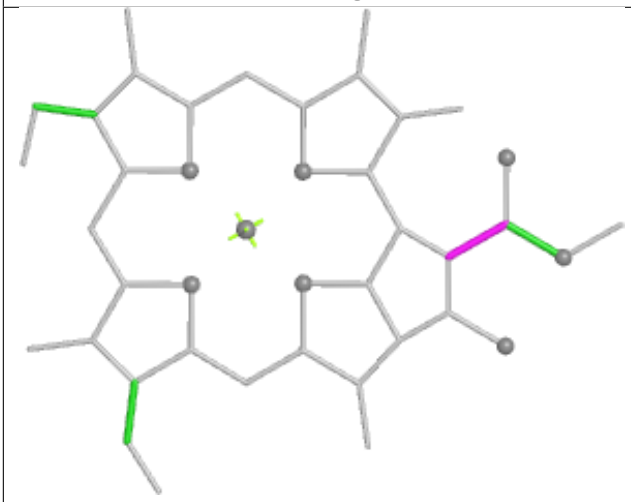
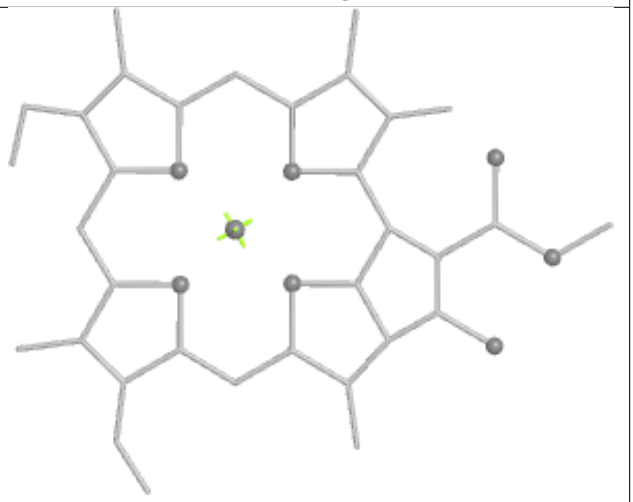


Bond angles

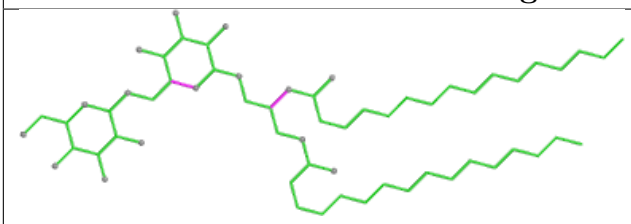


Torsions

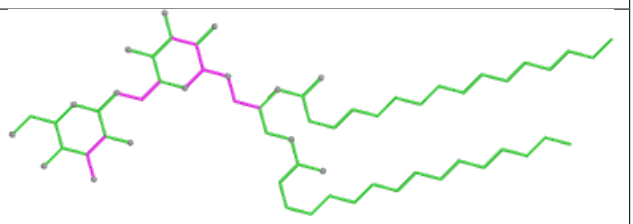


Rings

Ligand DGD C 519



Bond lengths



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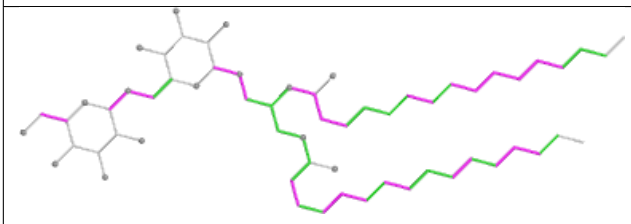

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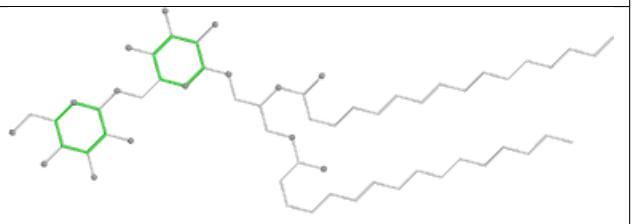
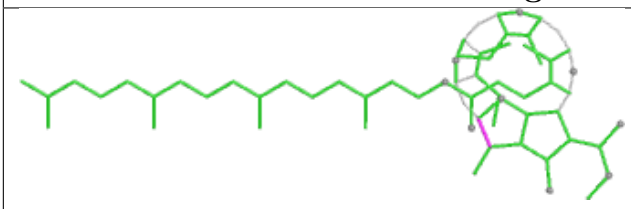


Rings

Ligand PHO d 403



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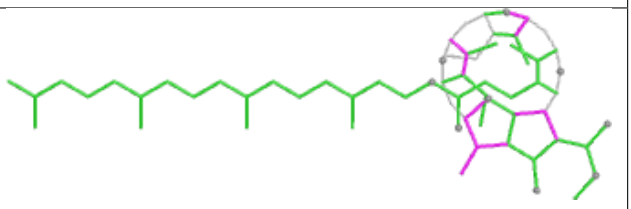

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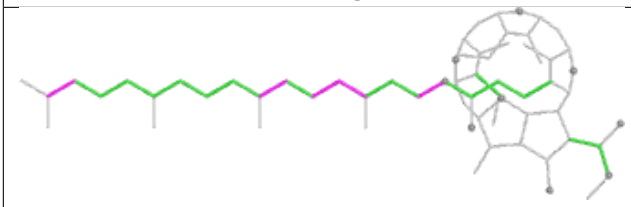

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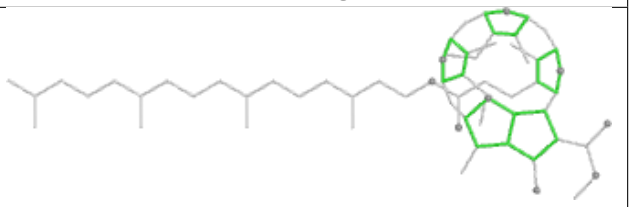
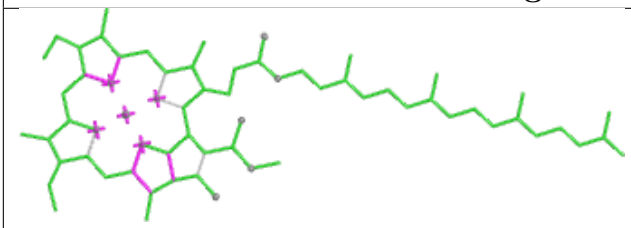


Rings

Ligand CLA C 502



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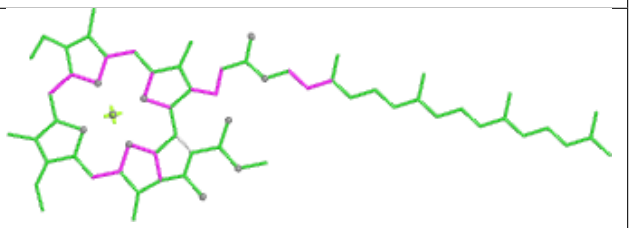
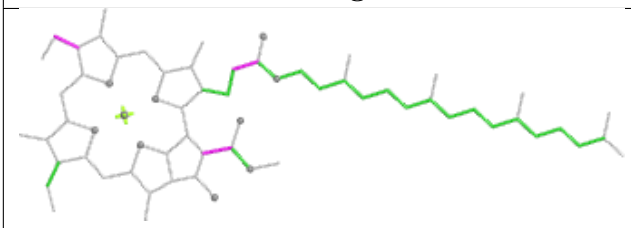


Bond angles



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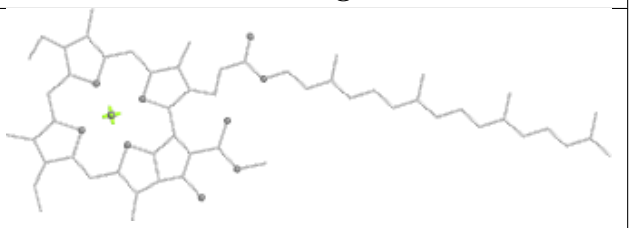
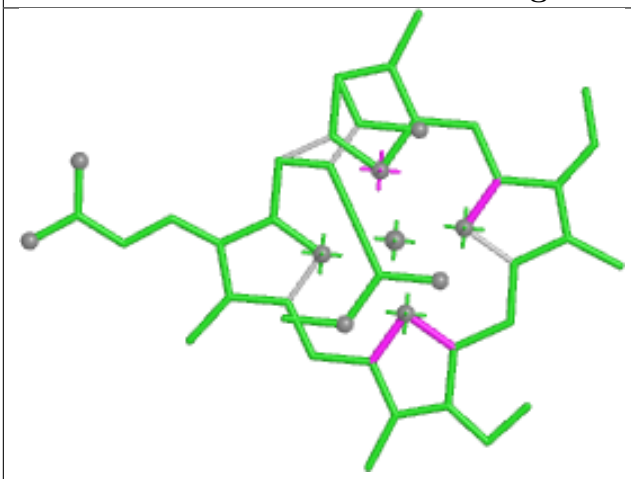


Rings

Ligand KC2 1 311



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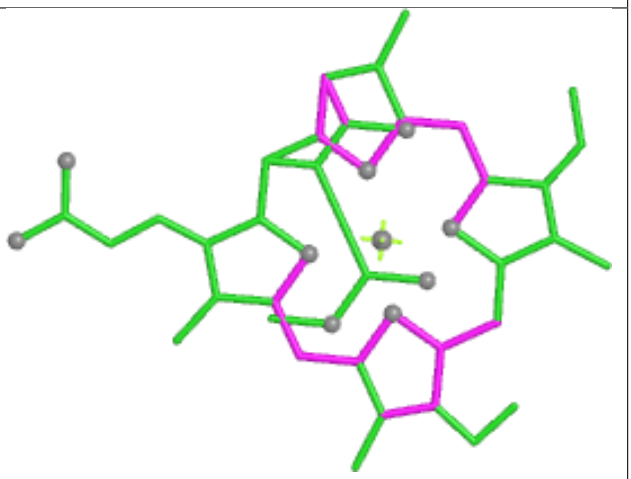

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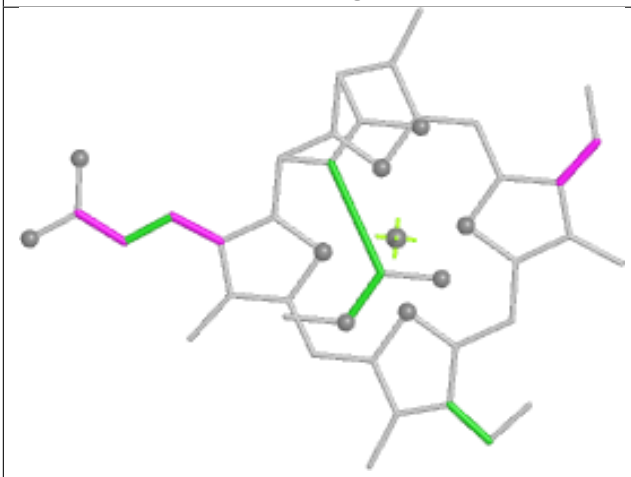

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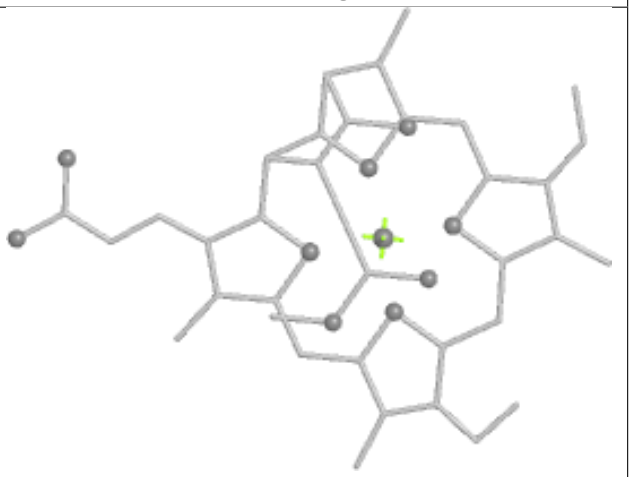
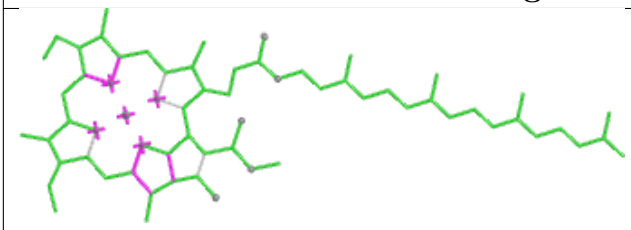


Rings

Ligand CLA A 405



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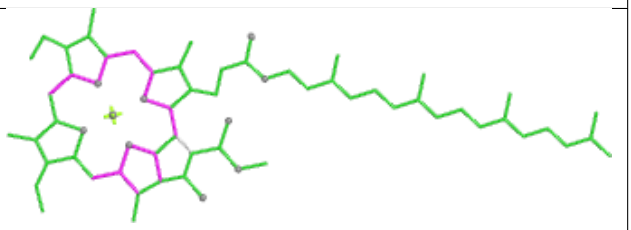

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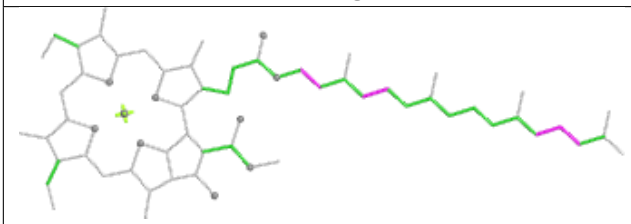

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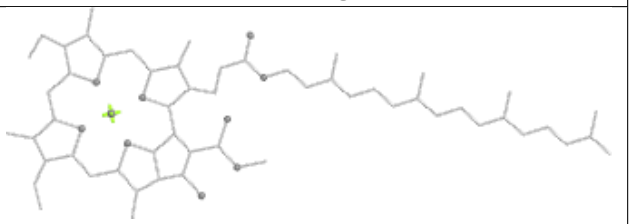
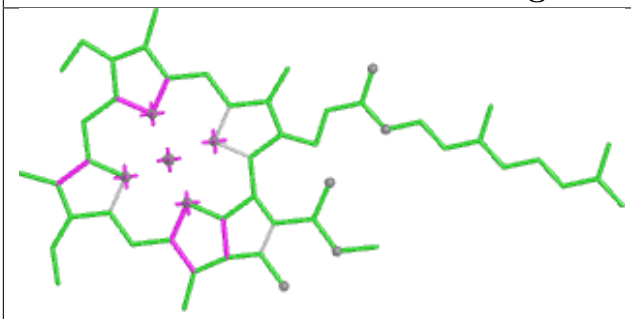


Rings

Ligand CLA 5 303



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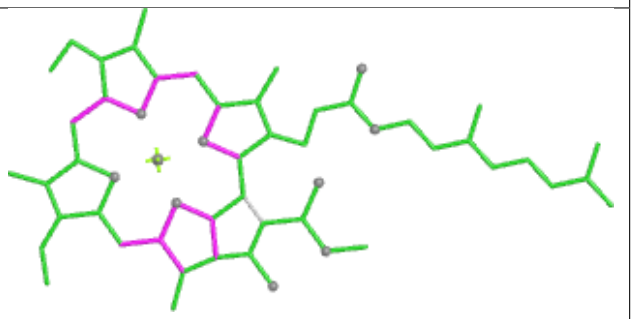

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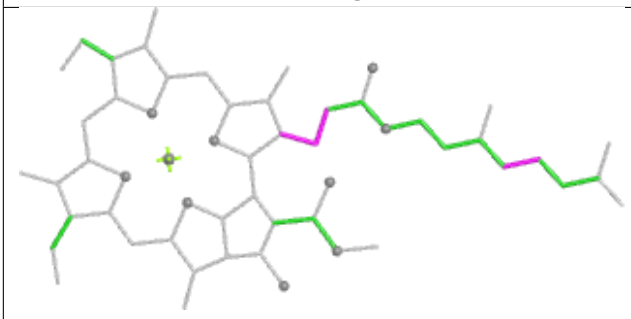

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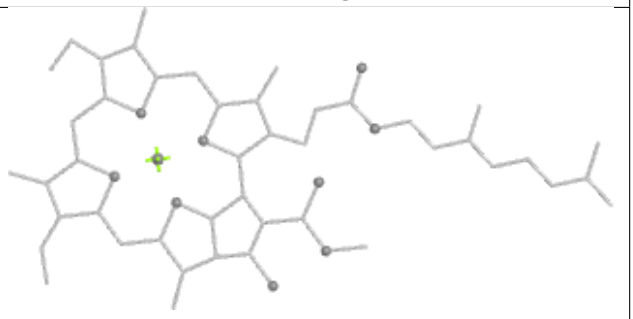
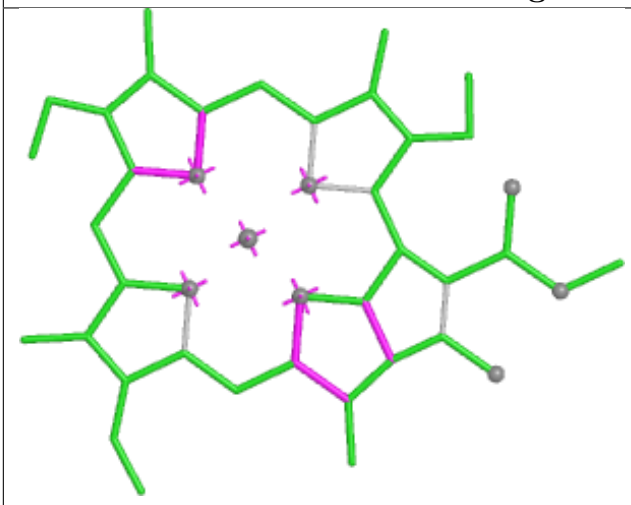


Rings

Ligand CLA 6 309



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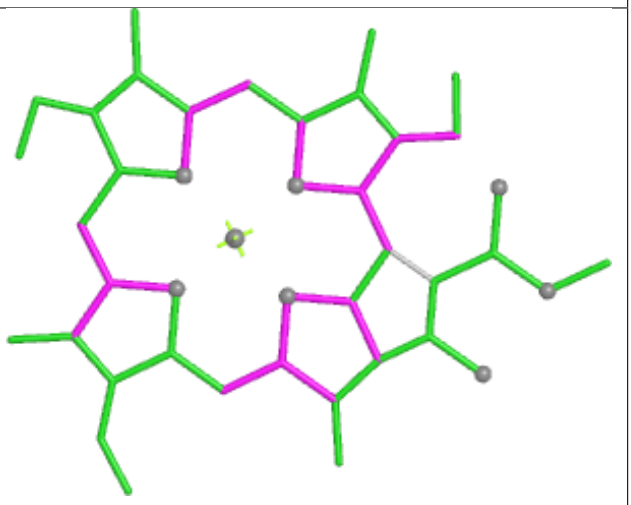

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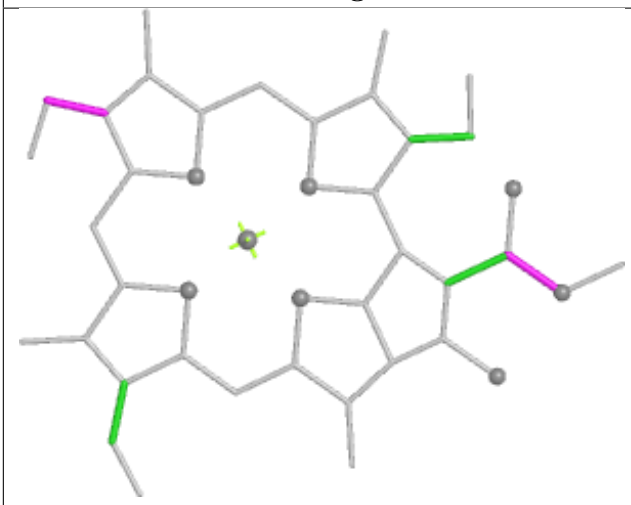

Torsions

Rings

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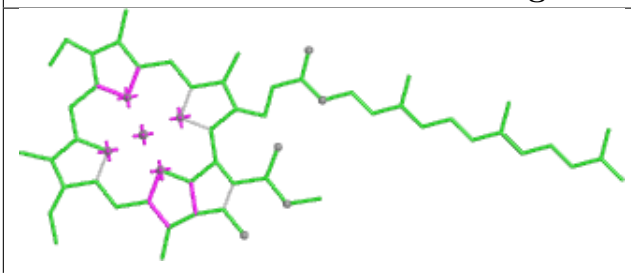

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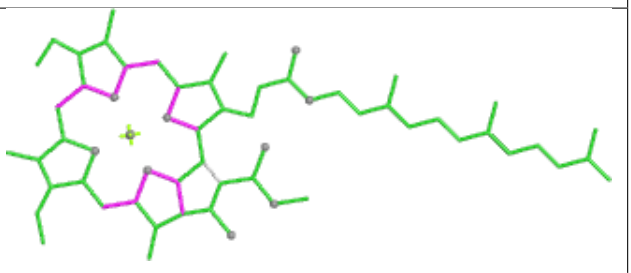

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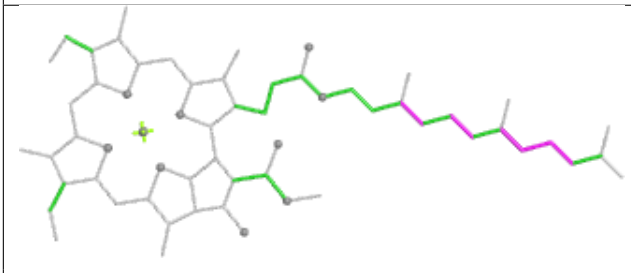

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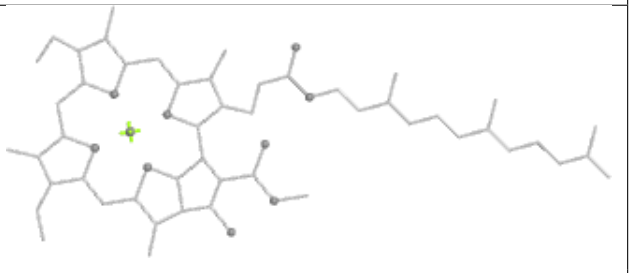
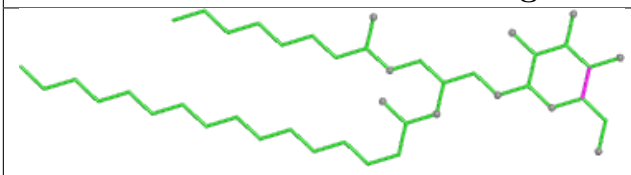
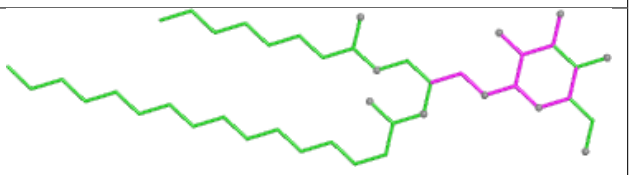
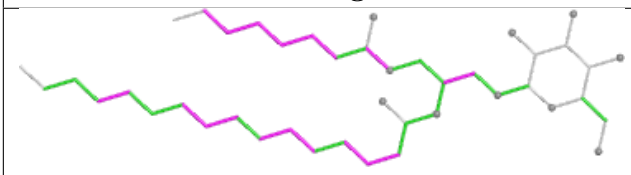
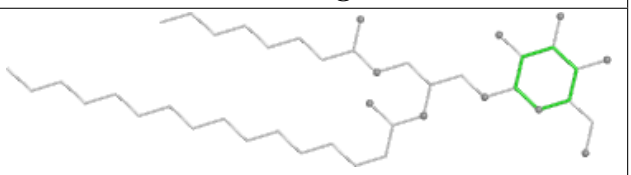
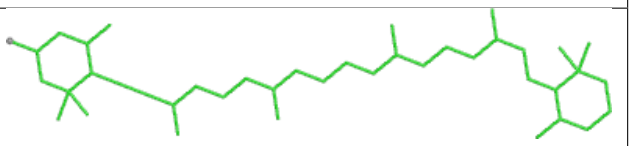


Rings

Ligand LMG B 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand IHT 3 320	
	
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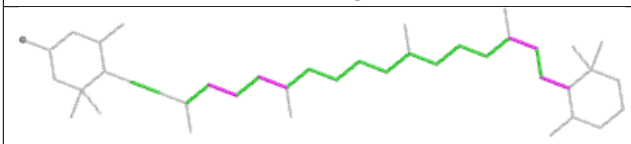
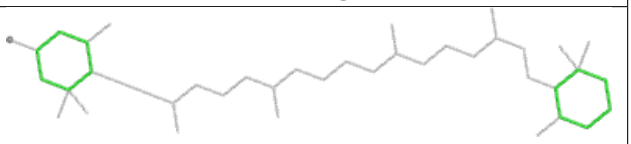
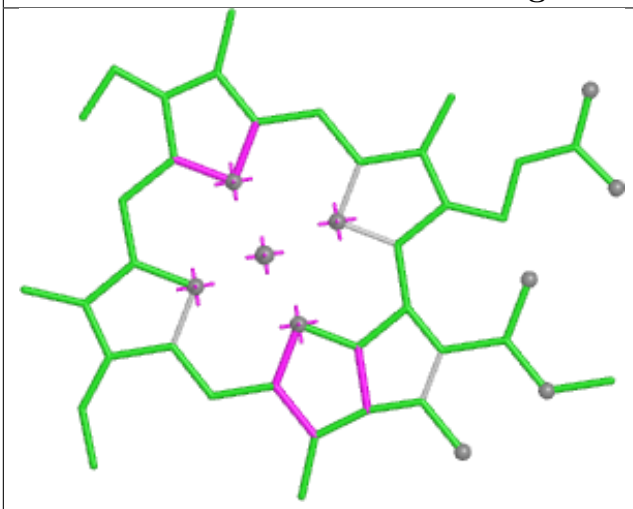
	
Torsions	Rings

Ligand CLA 3 304



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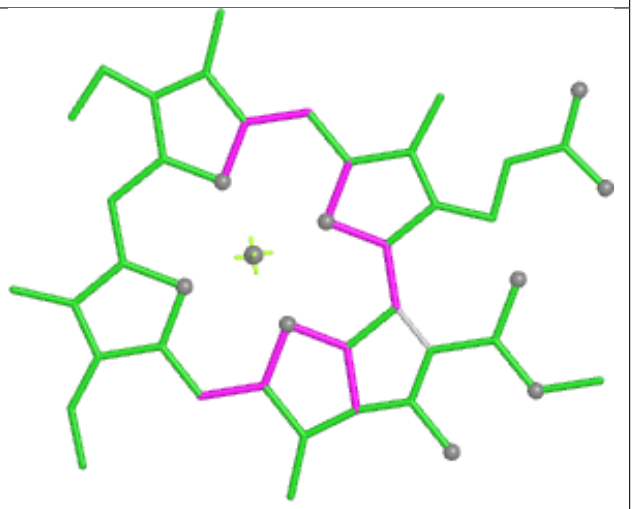

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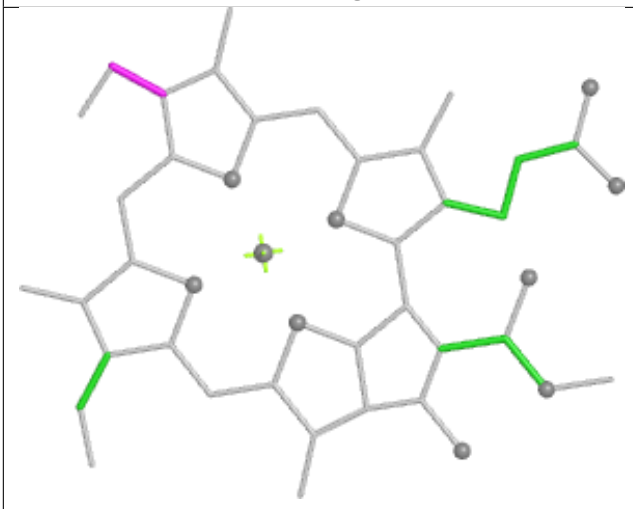

Torsions

Rings

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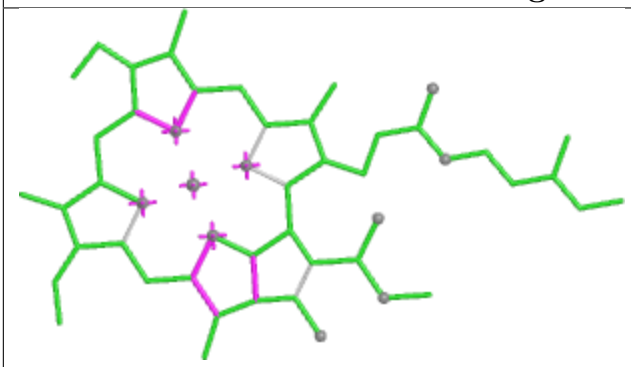

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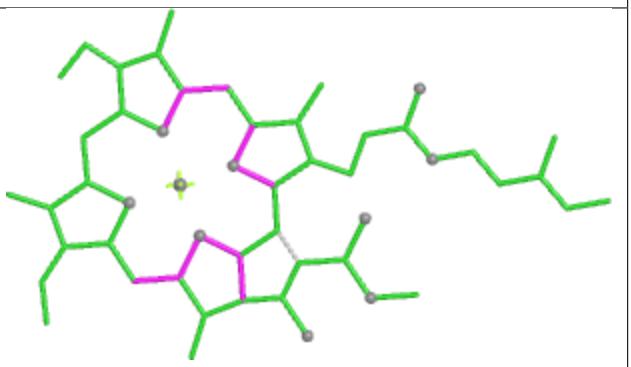

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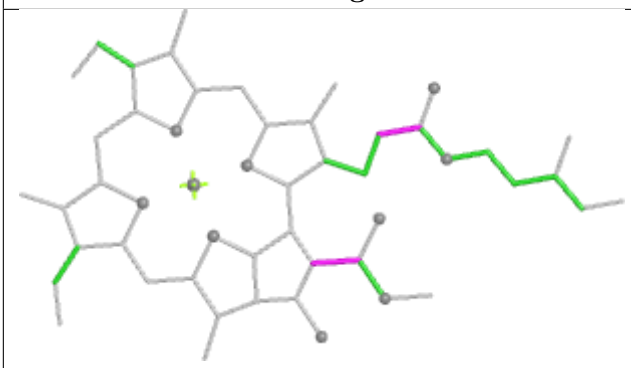

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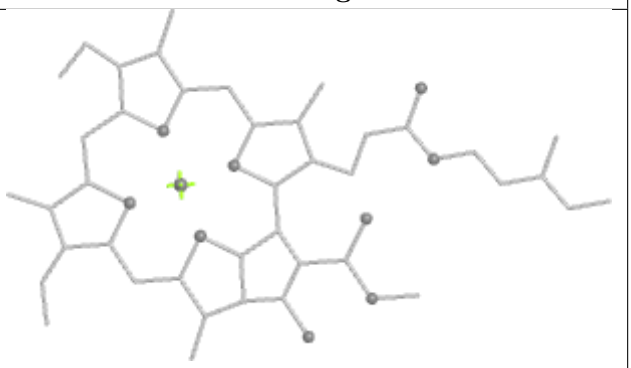
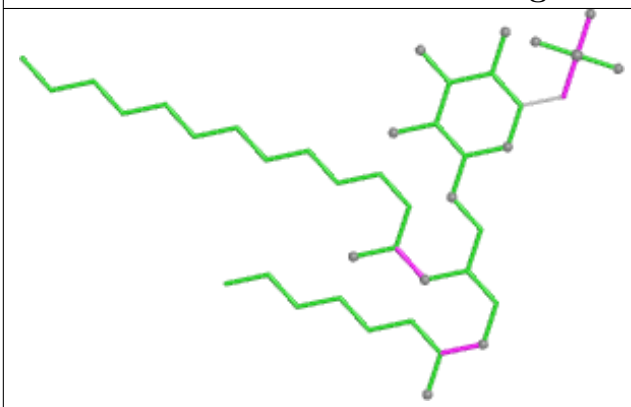


Rings

Ligand SQD c 501



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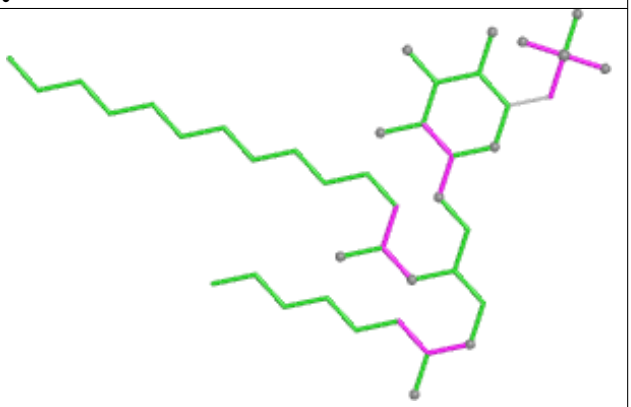
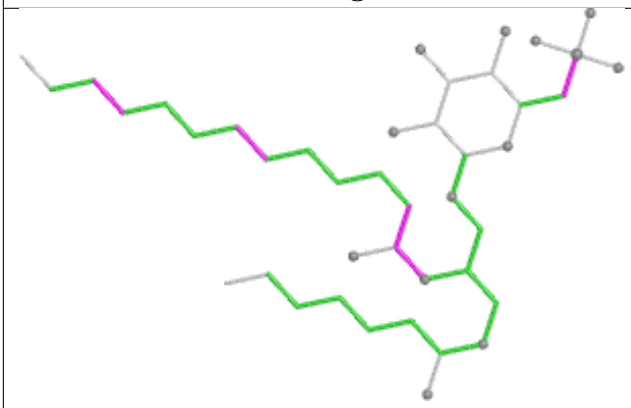


Bond angles



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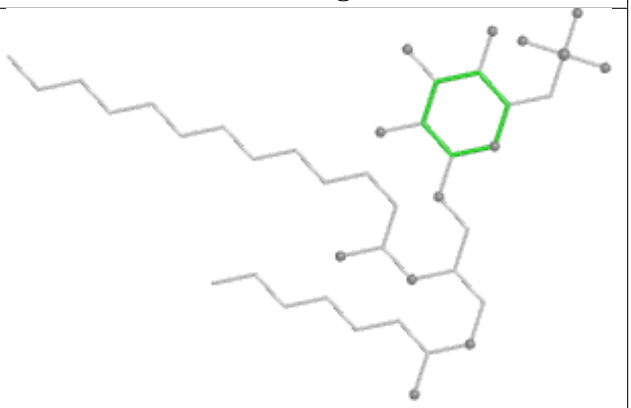
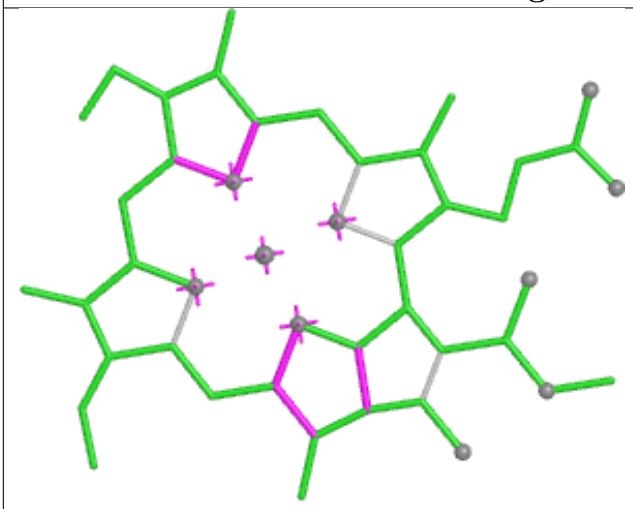


Rings

Ligand CLA 5 304



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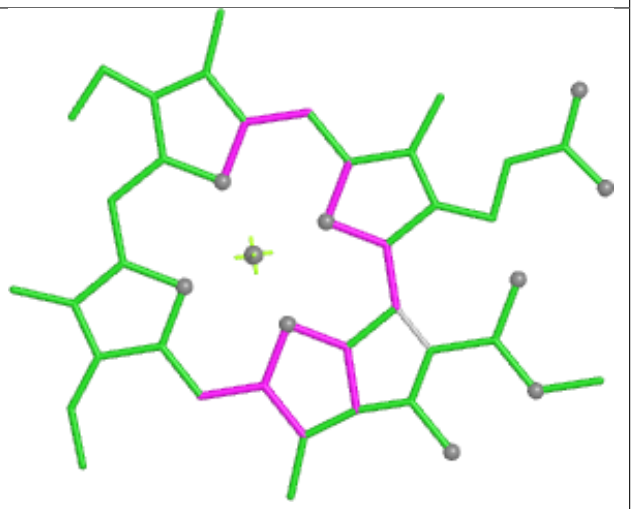
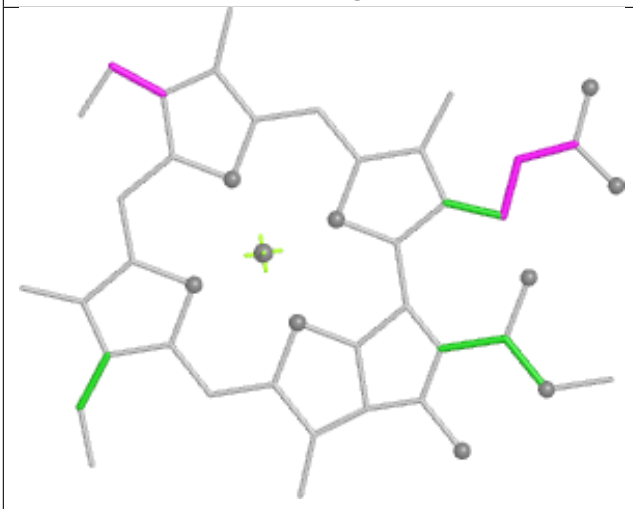


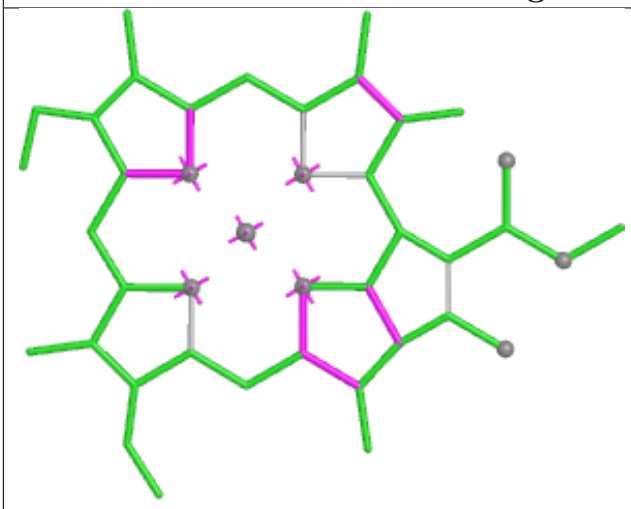
Bond angles



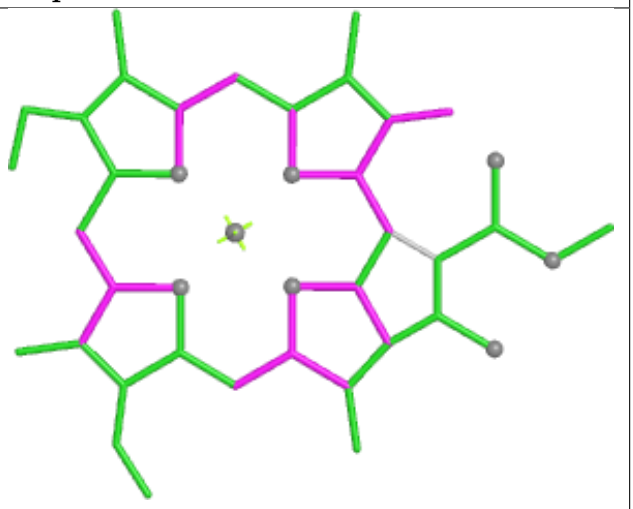
Torsions

Rings

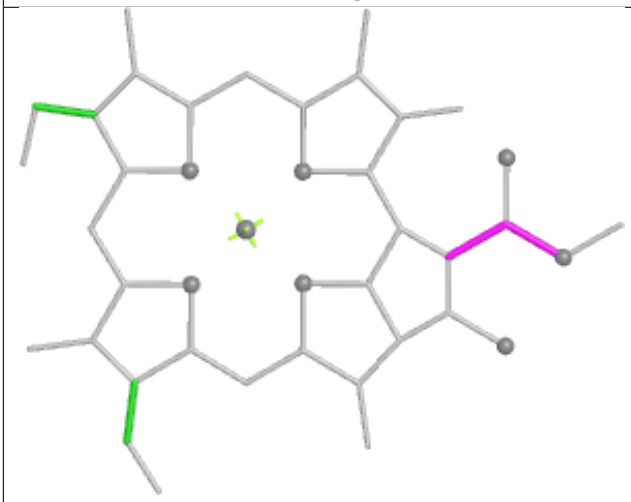
Ligand CLA p 313



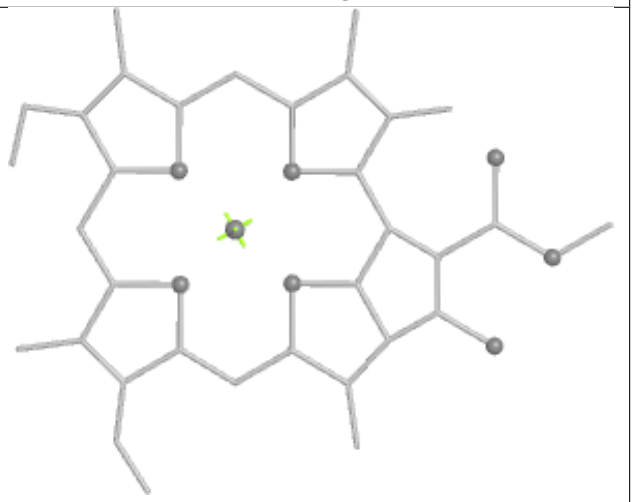
Bond lengths



Bond angles

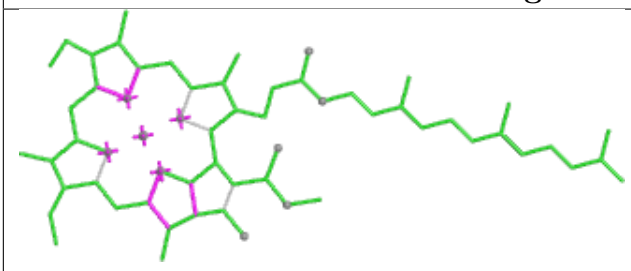


Torsions



Rings

Ligand CLA B 617



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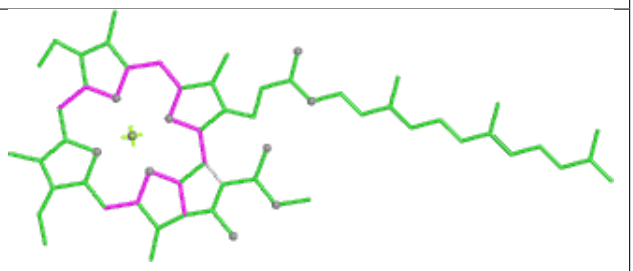
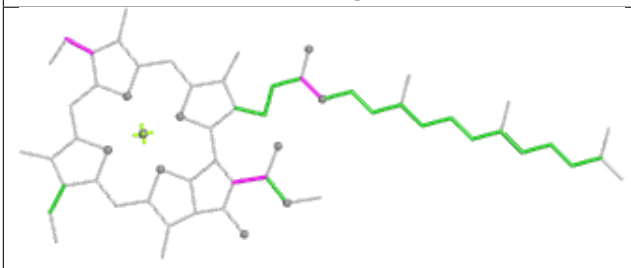
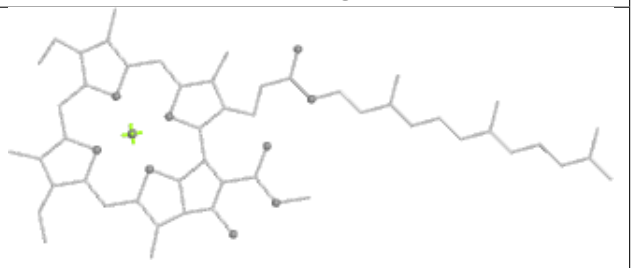


Bond angles

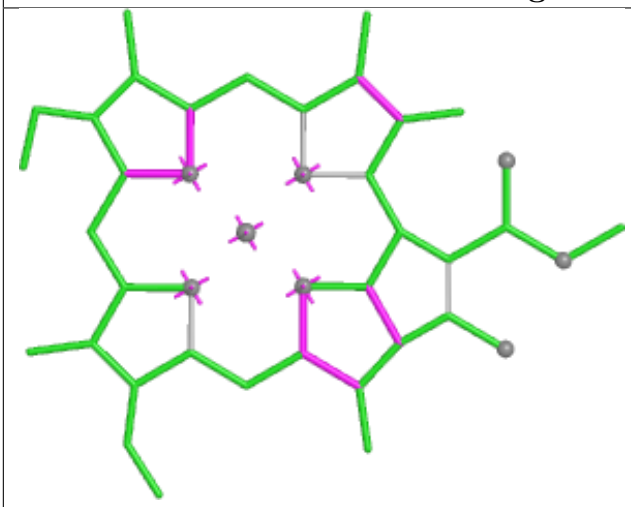


Torsions



Rings

Ligand CLA 6 313



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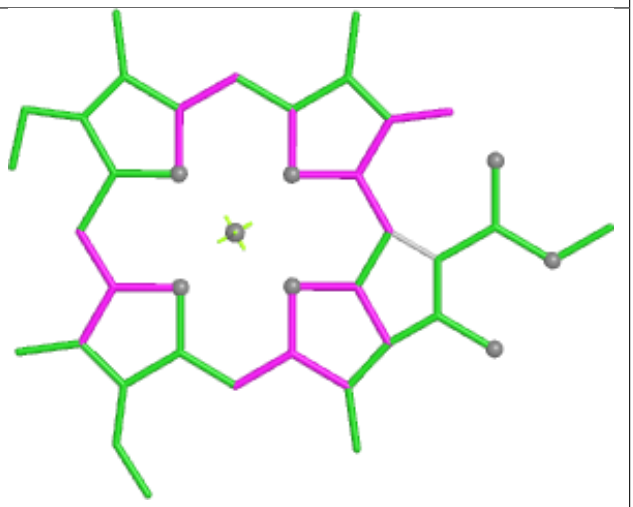
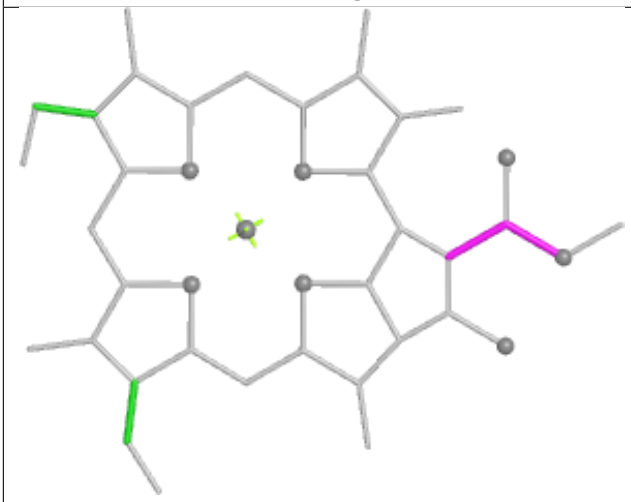


Bond angles



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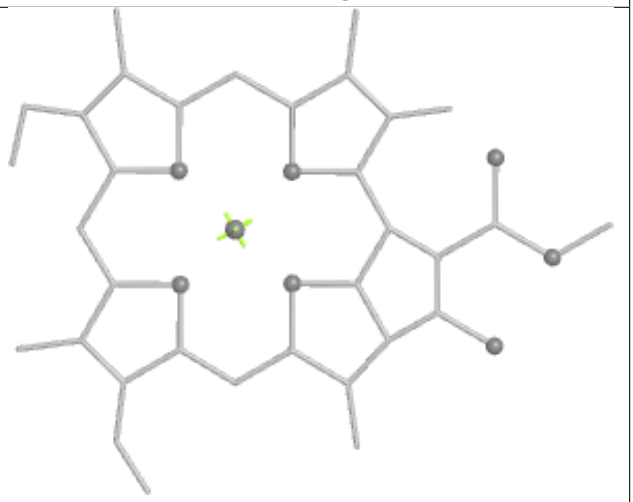
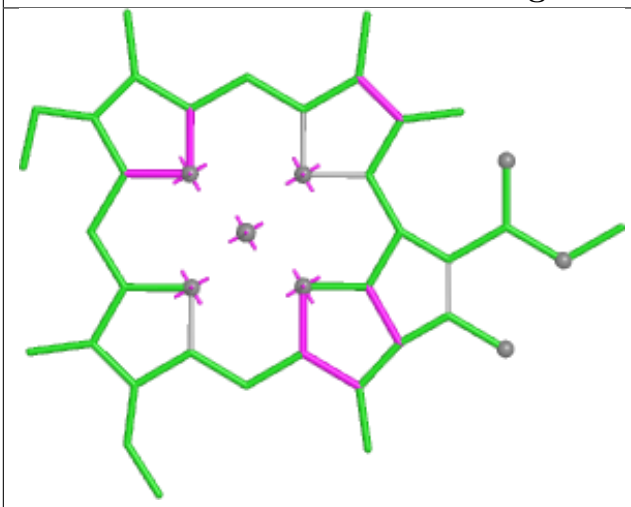


Rings

Ligand CLA 6 319



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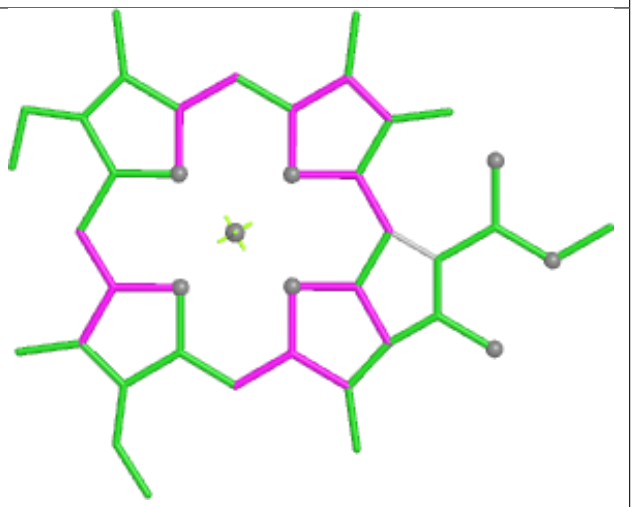
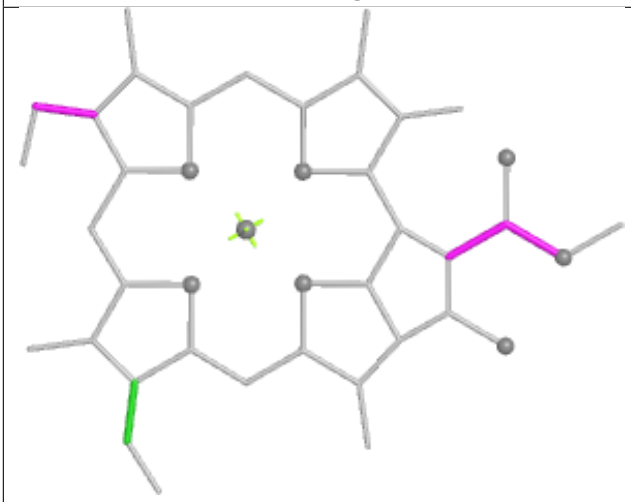


Bond angles



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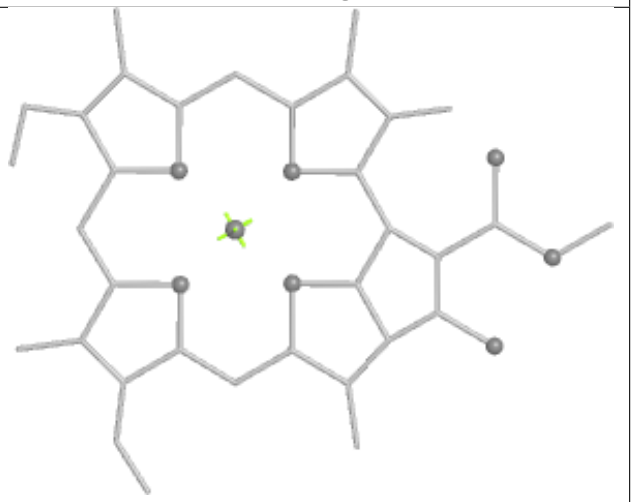
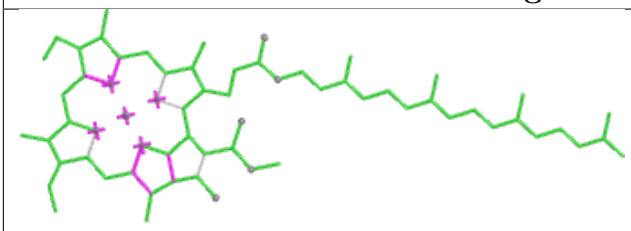
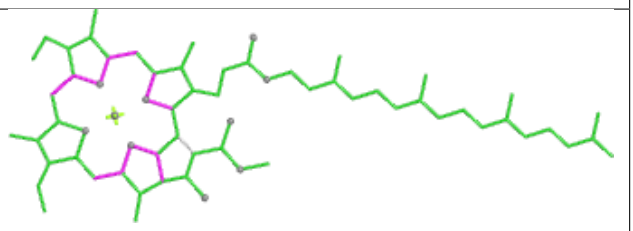


Rings

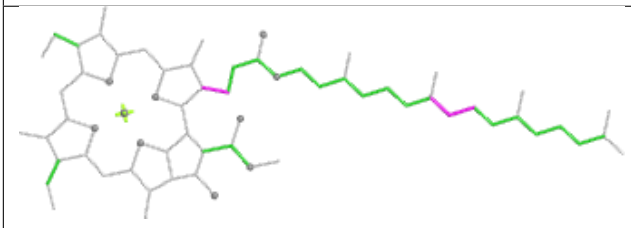
Ligand CLA C 509



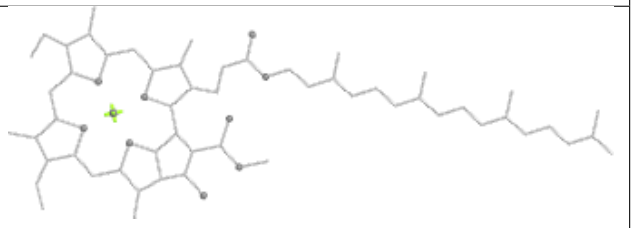
Bond lengths



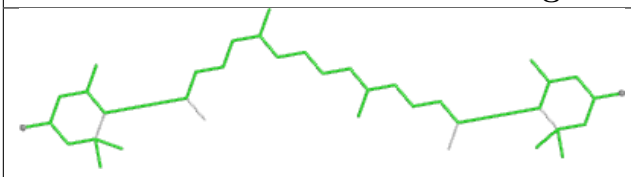
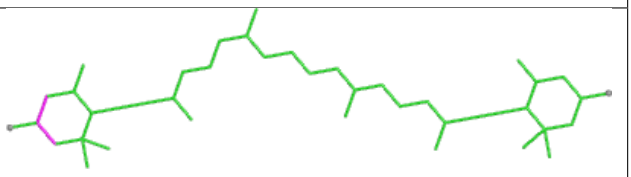
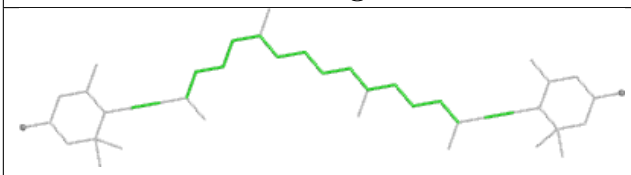
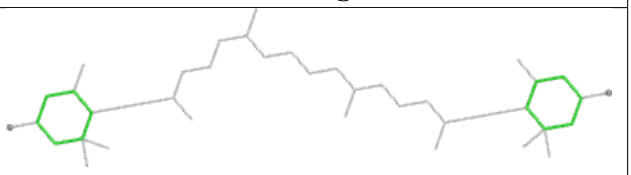
Bond angles

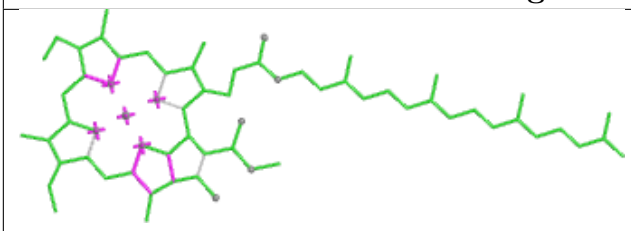
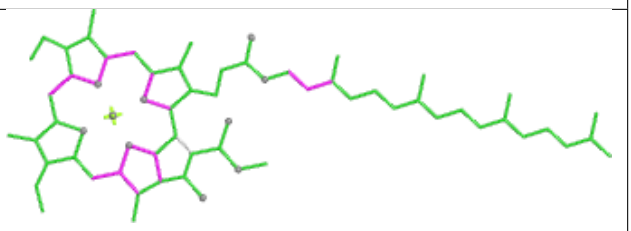
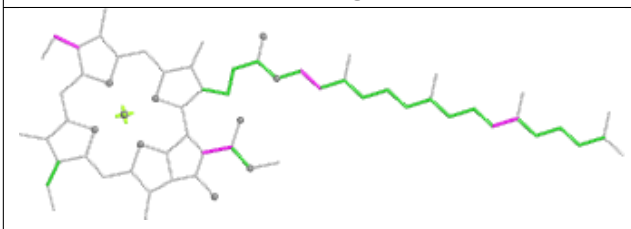
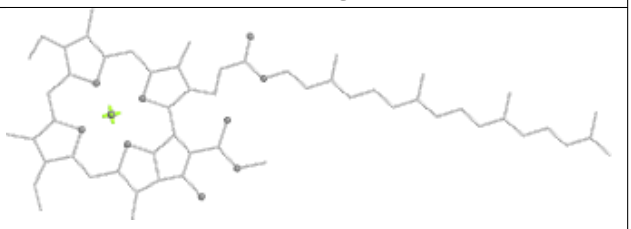


Torsions

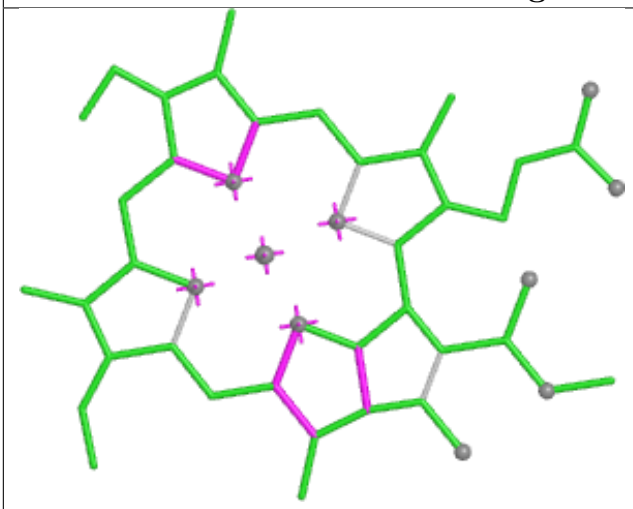


Rings

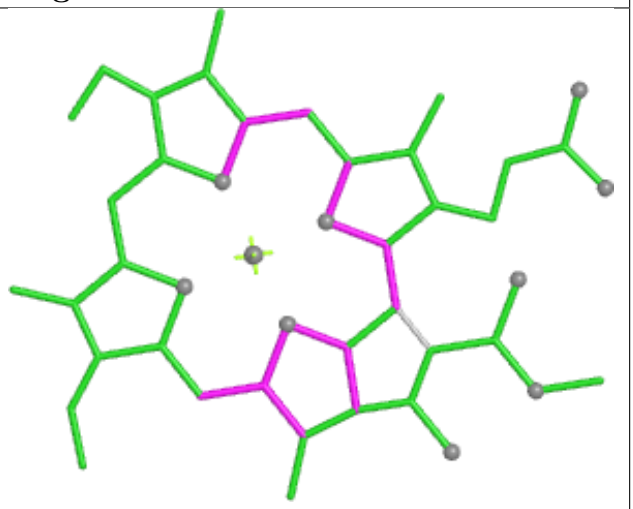
Ligand II0 2 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

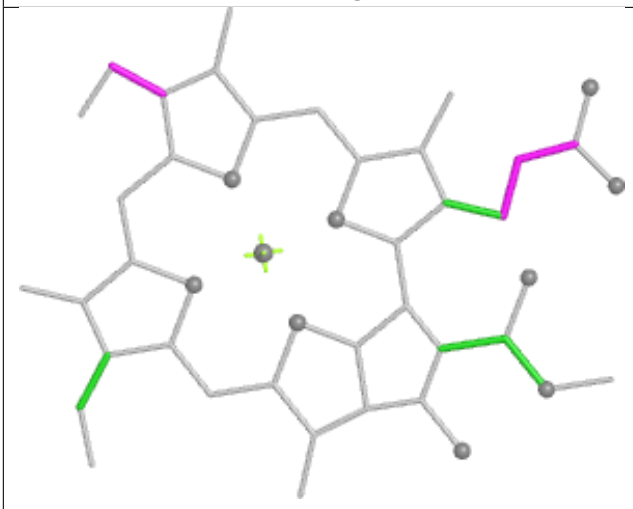
Ligand CLA g 304



Bond lengths



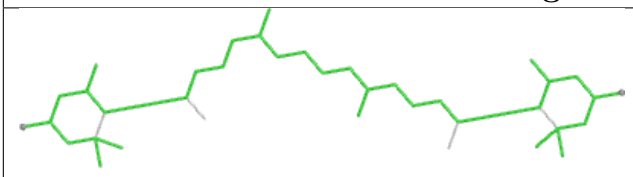
Bond angles



Torsions

Rings

Ligand II0 1 313



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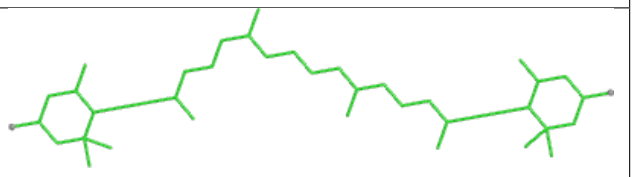
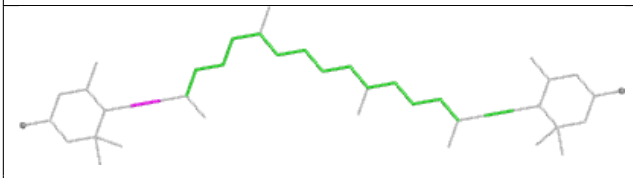
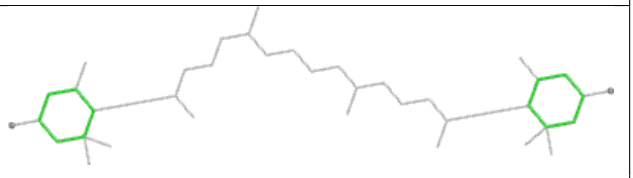


Bond angles

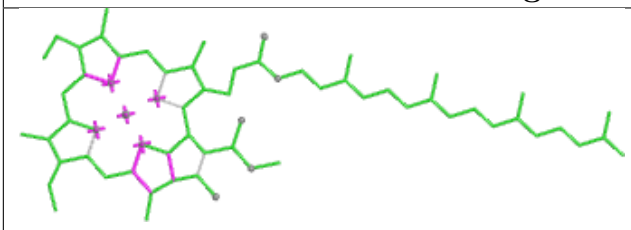


Torsions



Rings

Ligand CLA N 301



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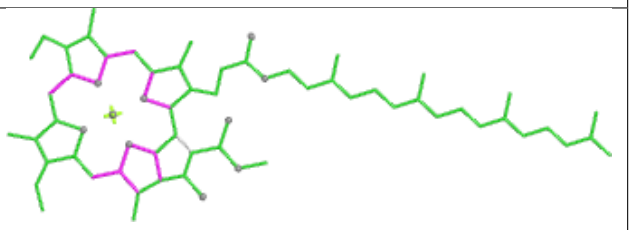
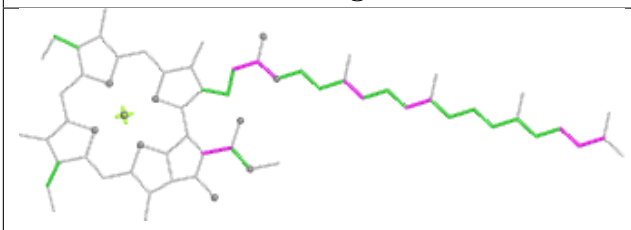


Bond angles



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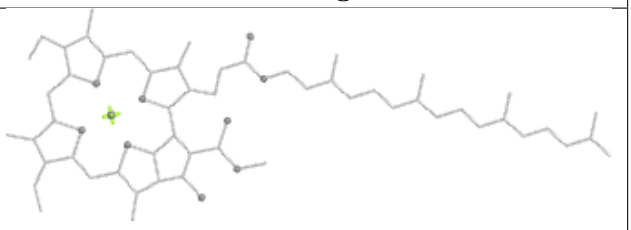
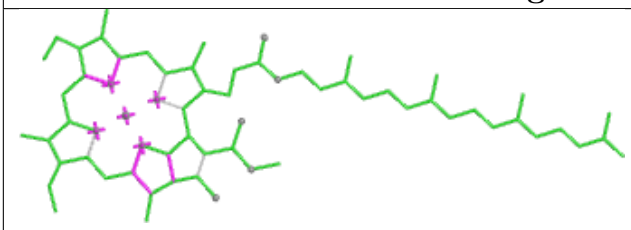


Rings

Ligand CLA b 613



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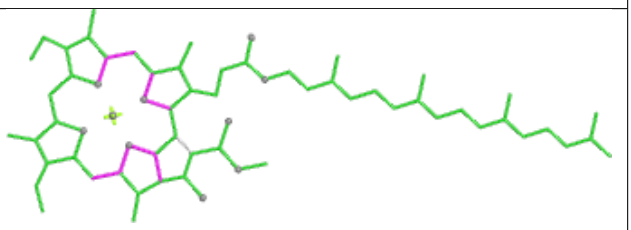
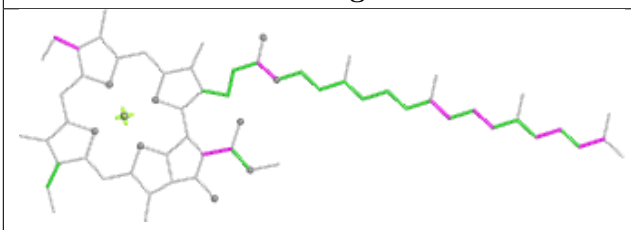
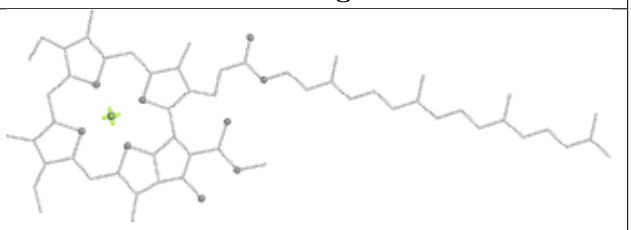


Bond angles

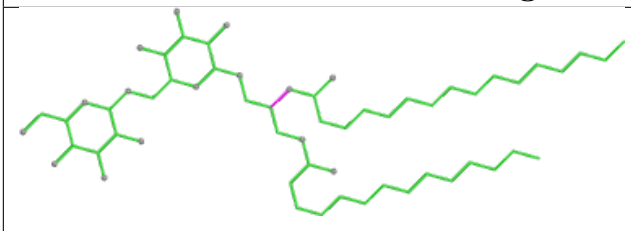


Torsions



Rings

Ligand DGD H 101



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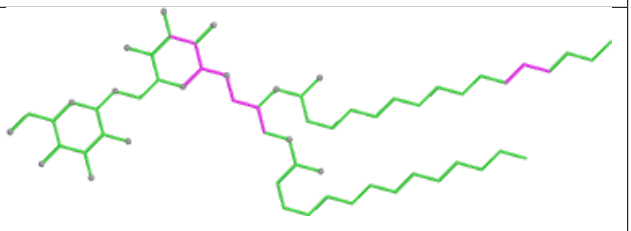
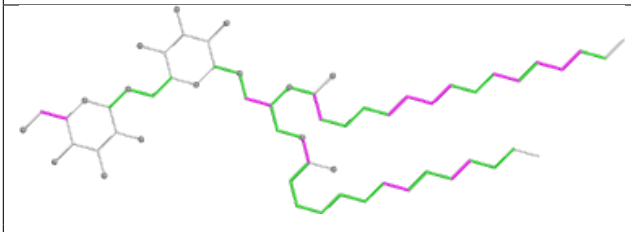


Bond angles



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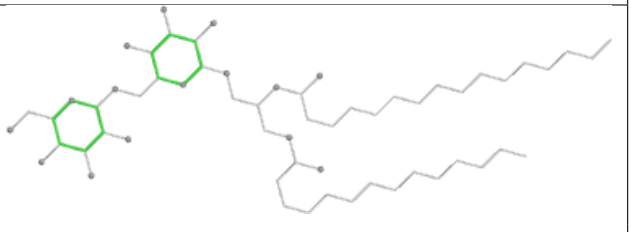
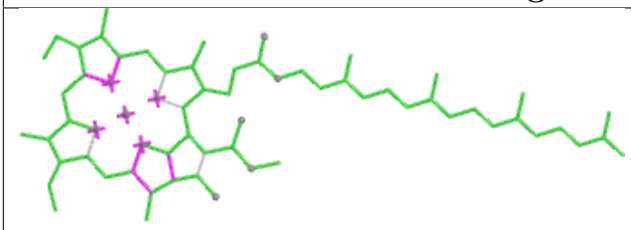


Rings

Ligand CLA n 301



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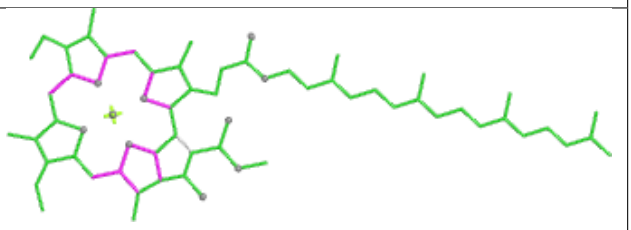
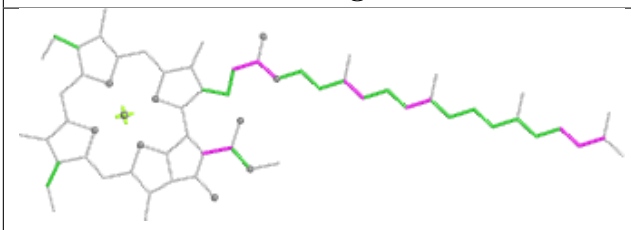
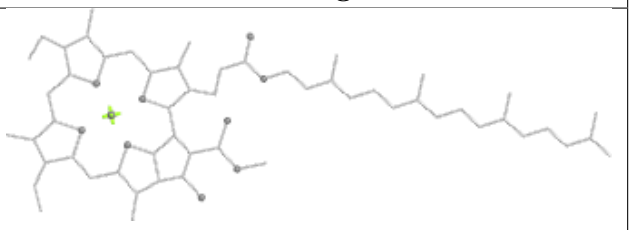


Bond angles

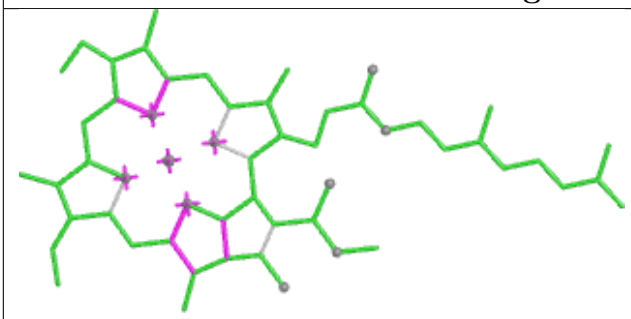


Torsions



Rings

Ligand CLA N 306



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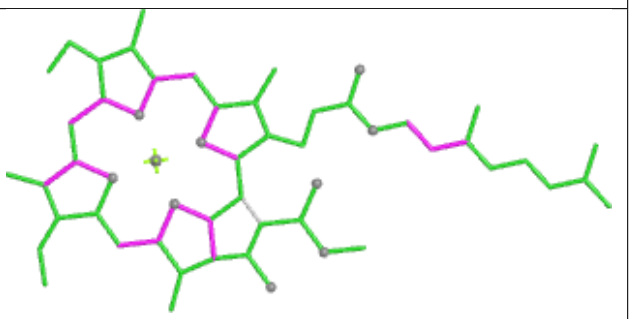
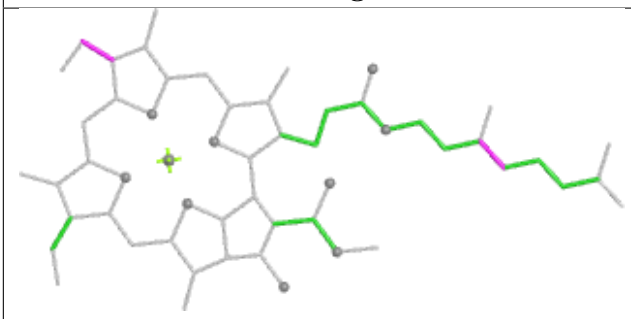
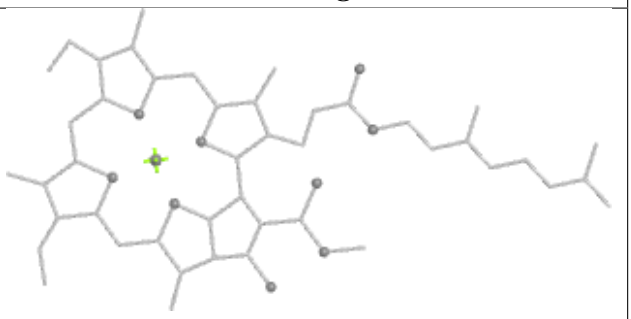


Bond angles

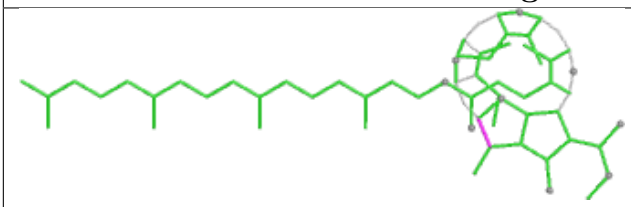


Torsions

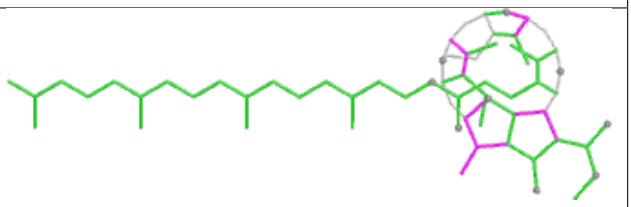


Rings

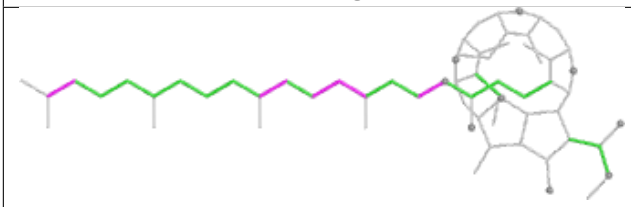
Ligand PHO D 403



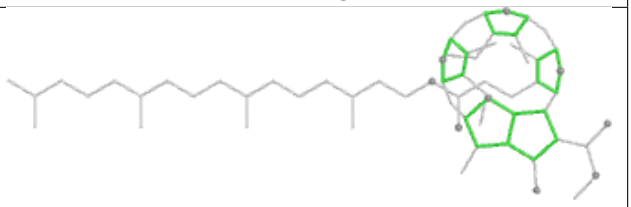
Bond lengths



Bond angles

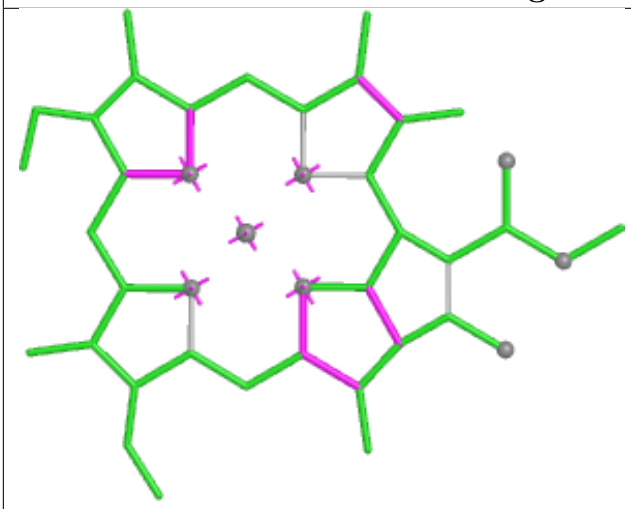


Torsions

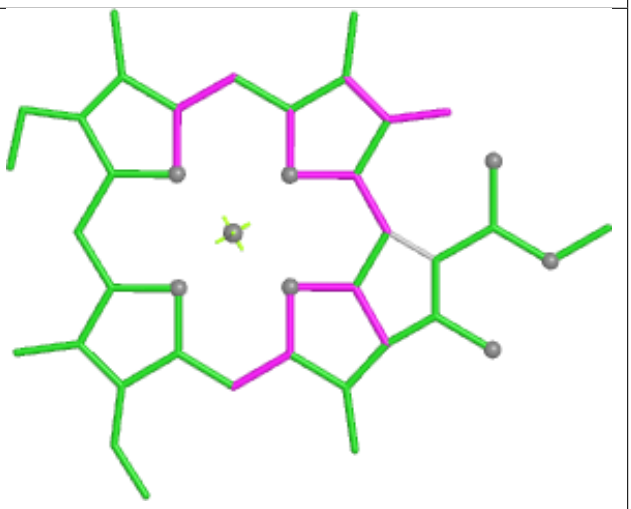


Rings

Ligand CLA 9 315



Bond lengths



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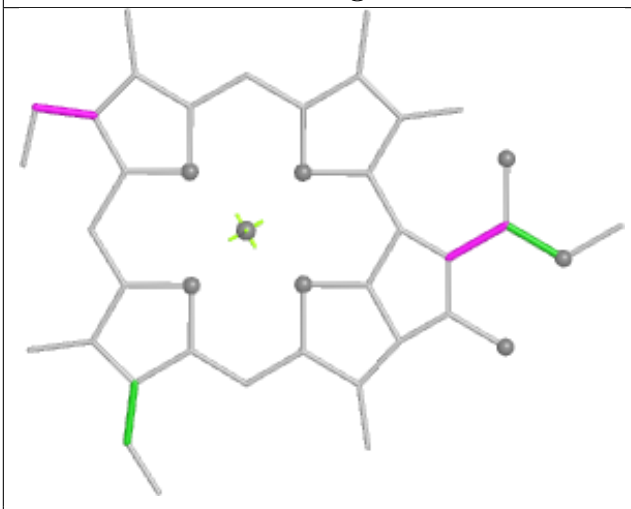

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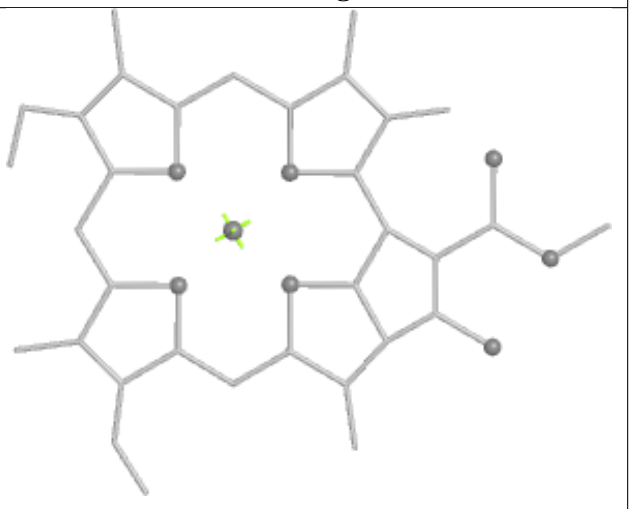
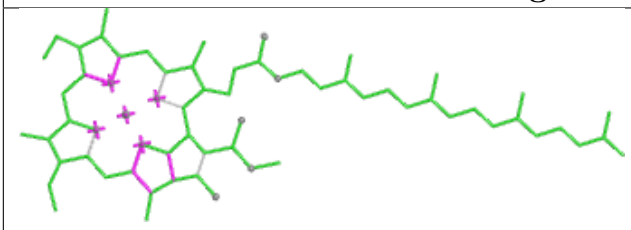


Rings

Ligand CLA c 509



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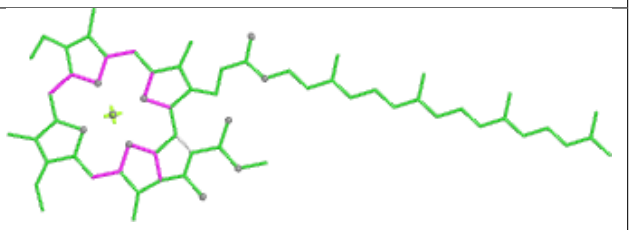
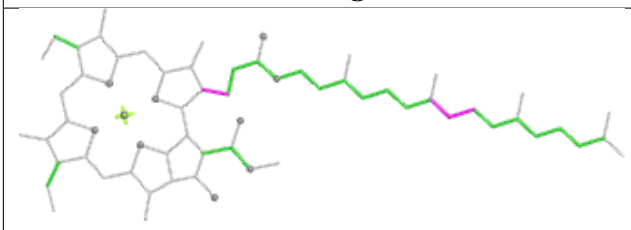


Bond angles



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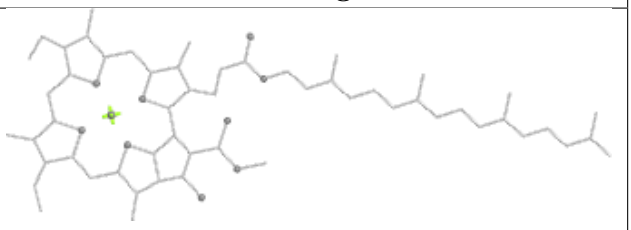
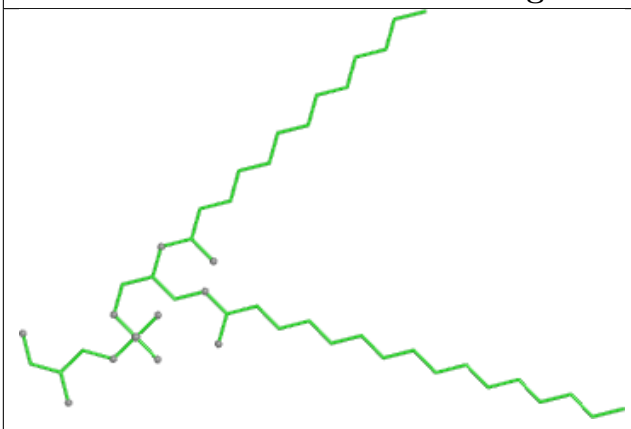


Rings

Ligand LHG 8 315



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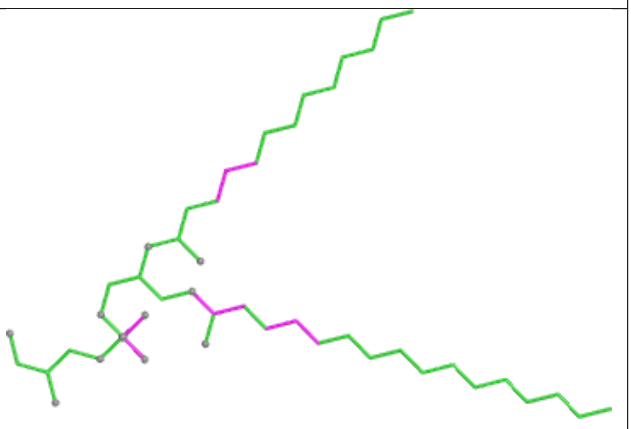

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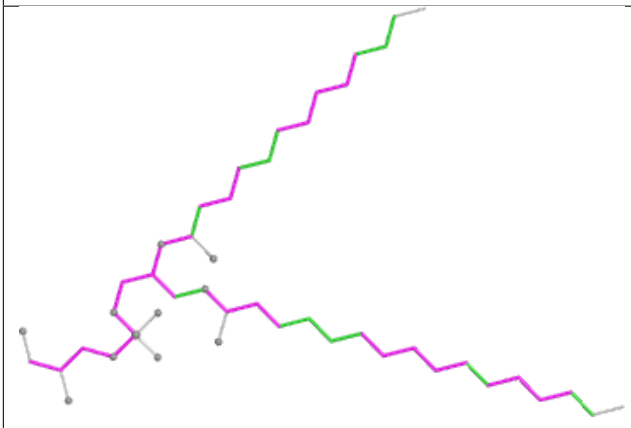

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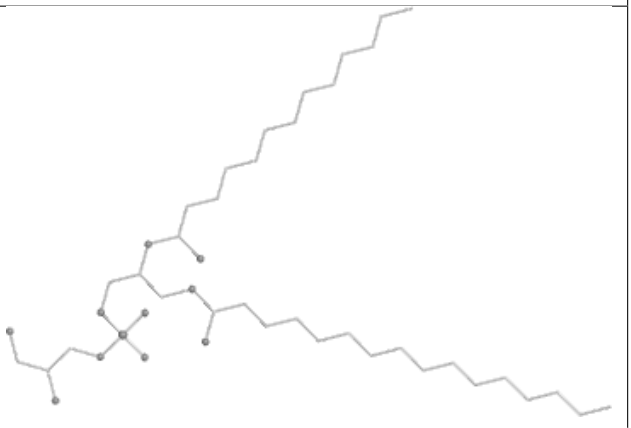
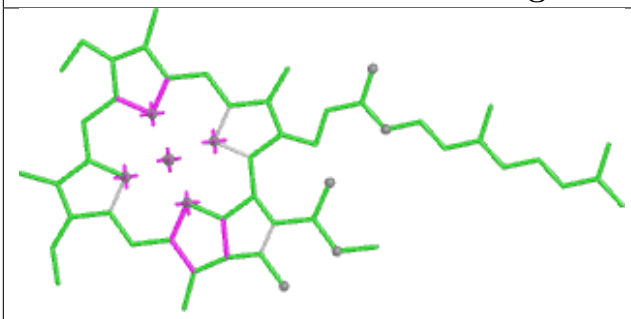


Rings

Ligand CLA 8 305



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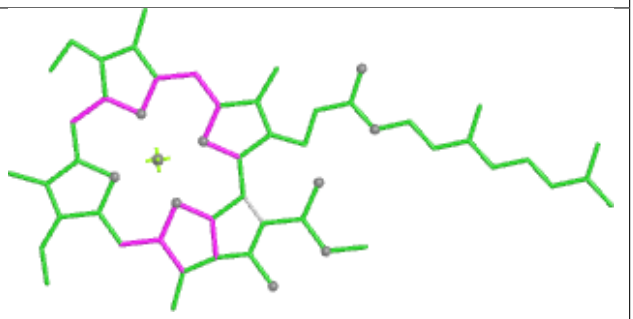

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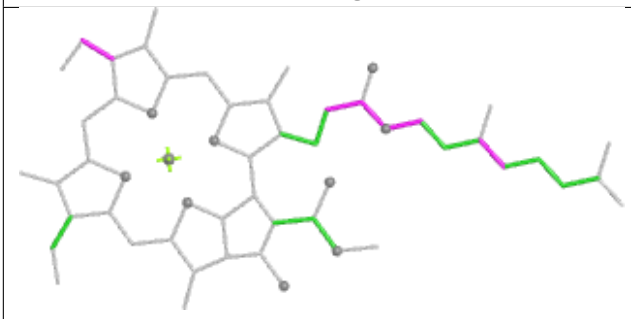

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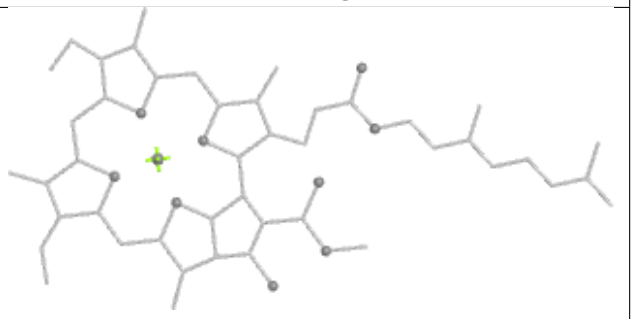
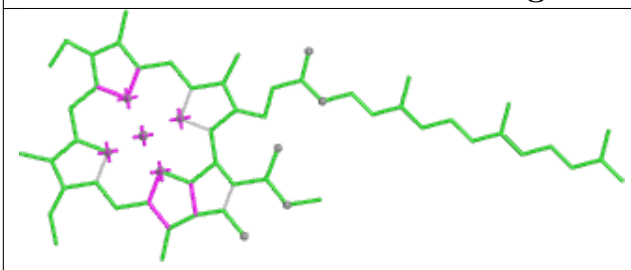


Rings

Ligand CLA b 617



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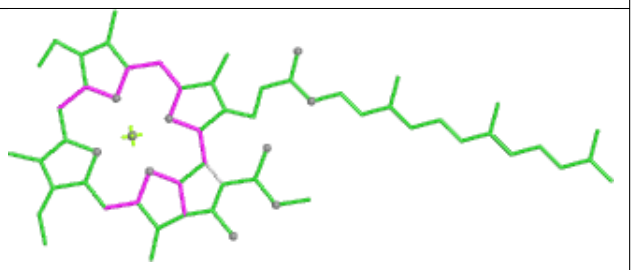
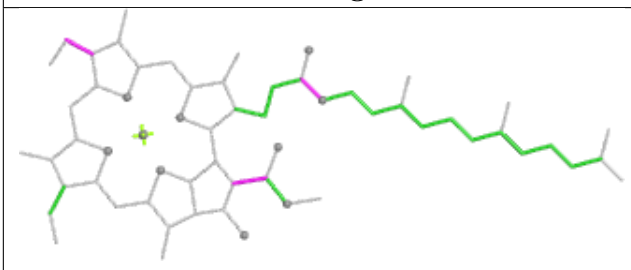


Bond angles



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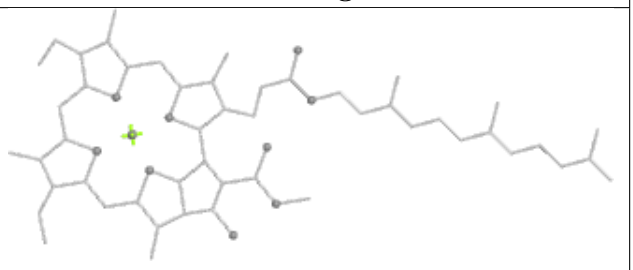
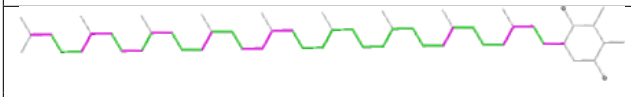


Rings

Ligand PL9 D 407

Bond lengths

Bond angles



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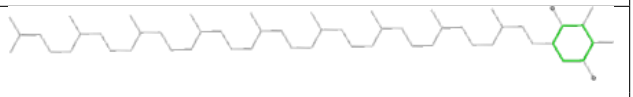
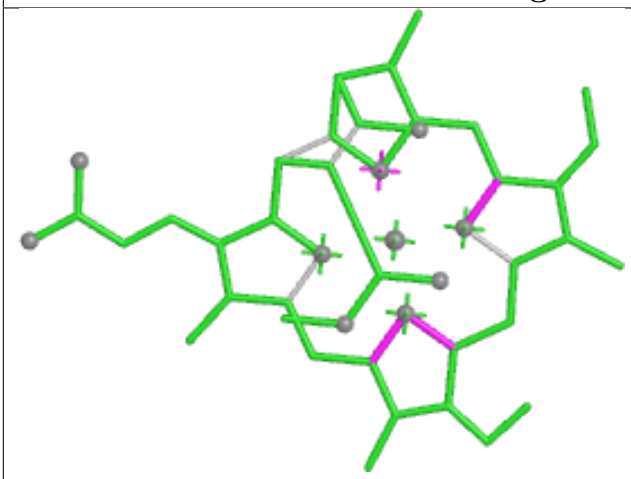


Rings

Ligand KC2 2 309



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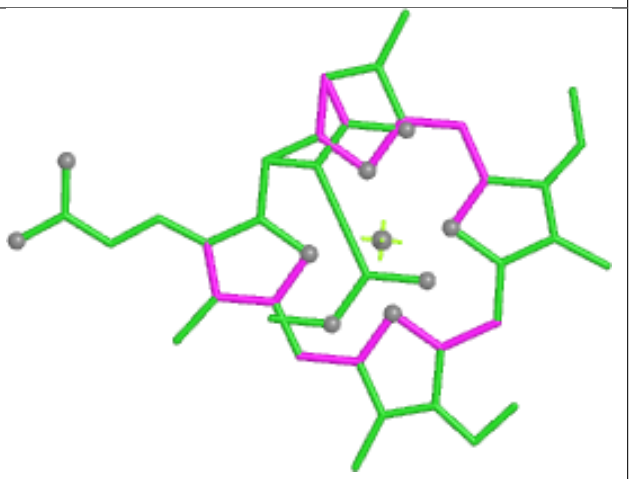

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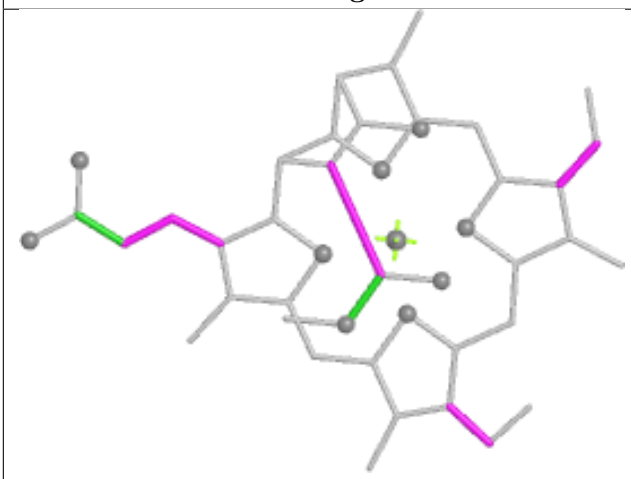

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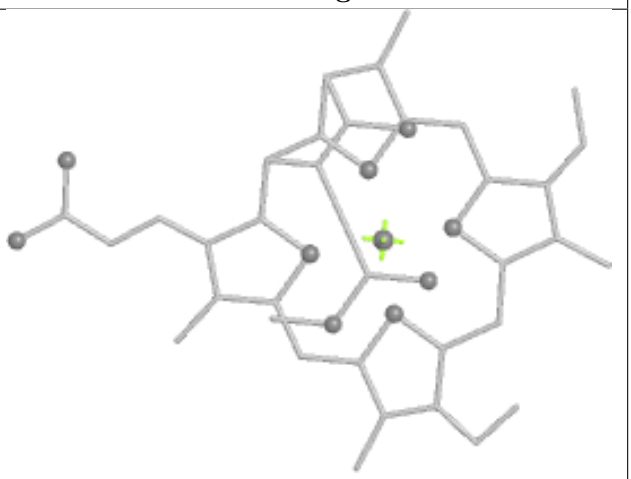
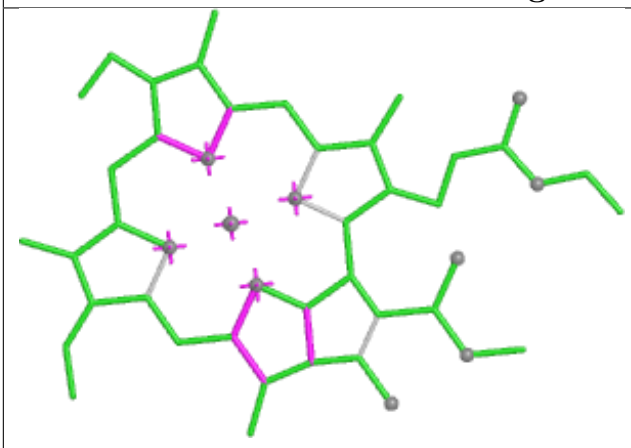


Rings

Ligand CLA 0 309



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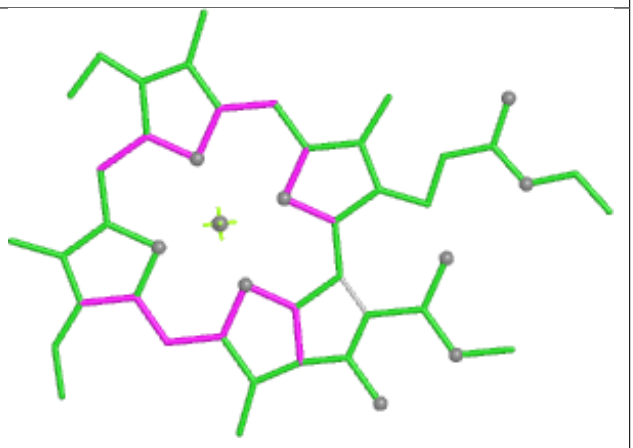

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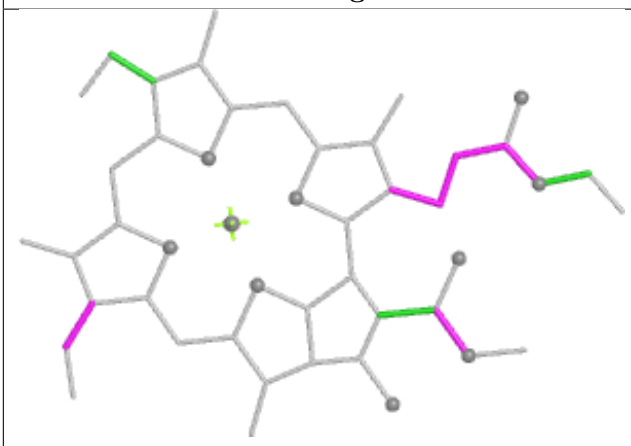

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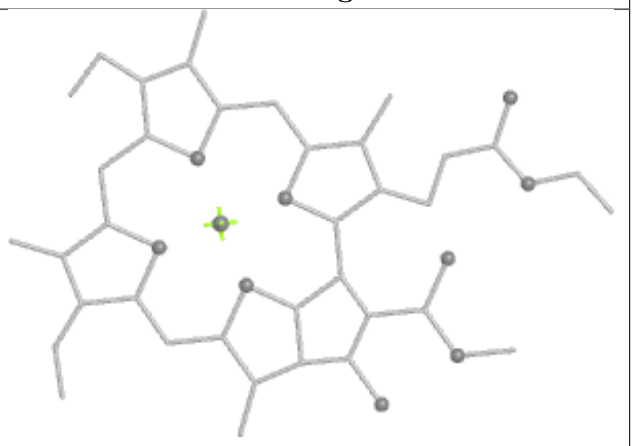
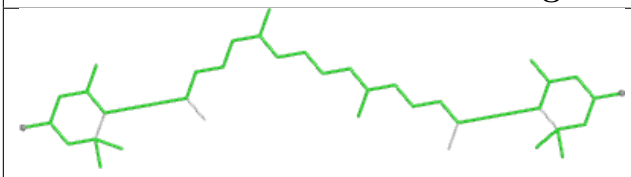


Rings

Ligand II0 4 313



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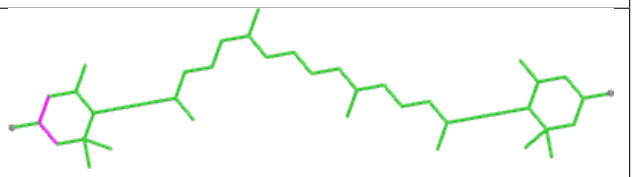

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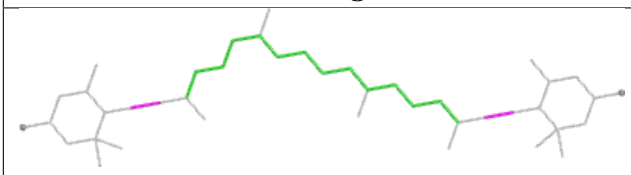

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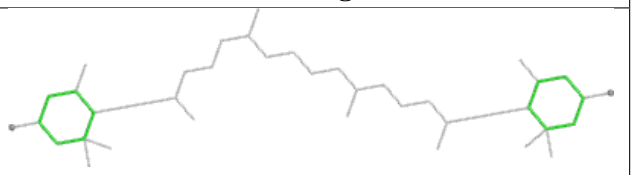
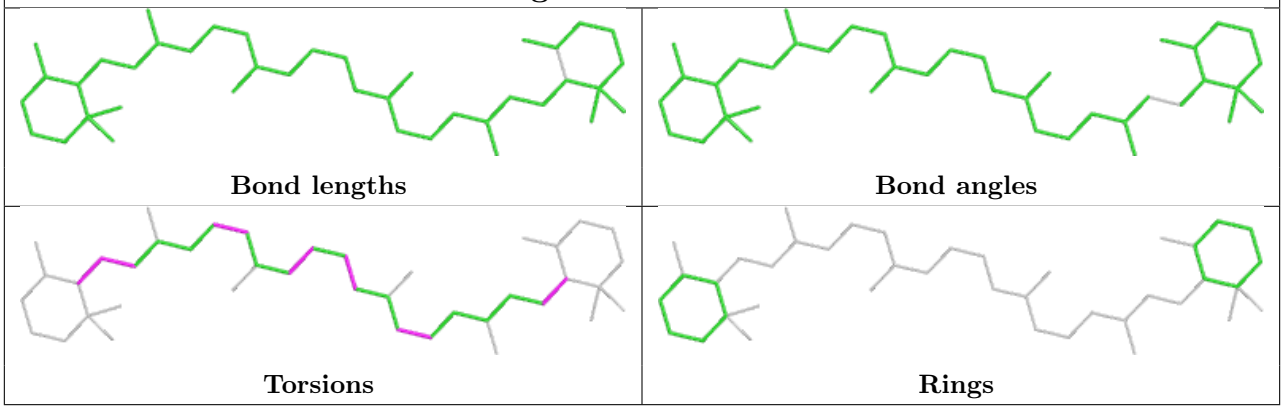
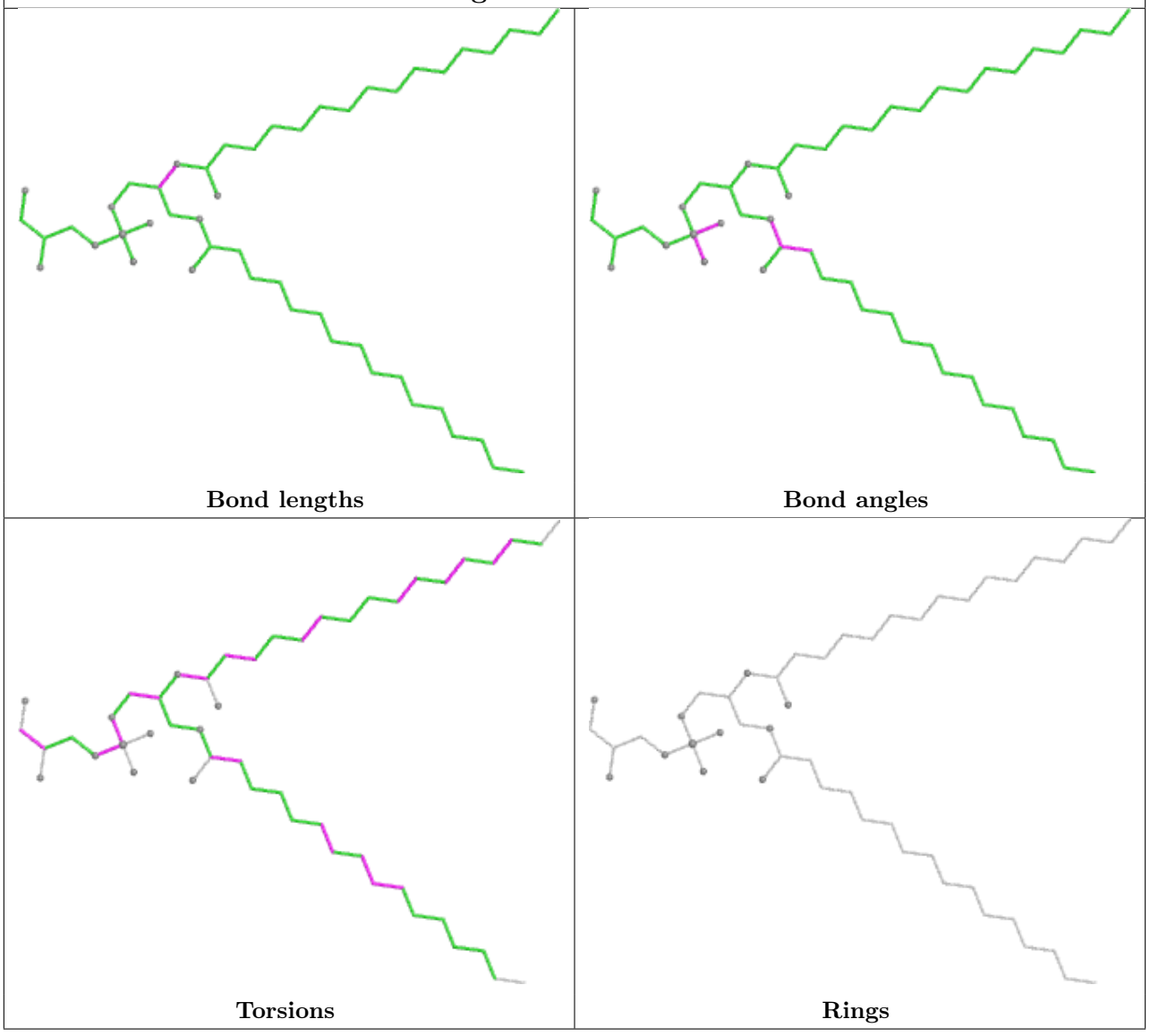


Rings

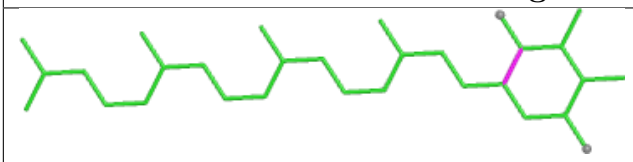
Ligand 8CT b 621



Ligand LHG d 408



Ligand PL9 A 410



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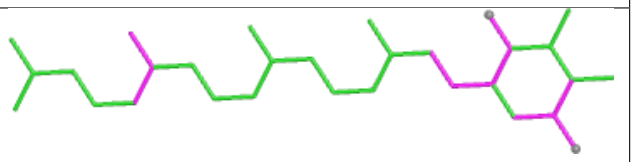
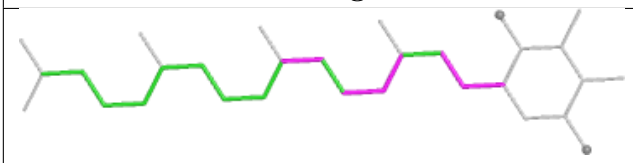


Bond angles



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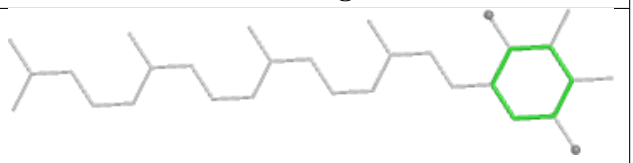
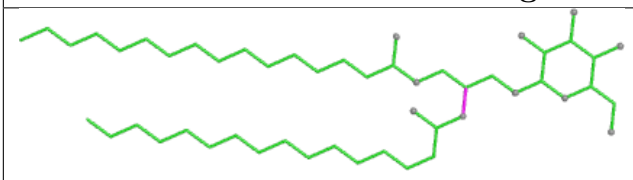


Rings

Ligand LMG C 520



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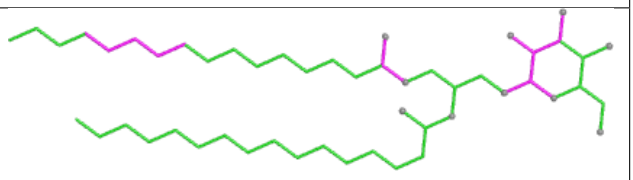
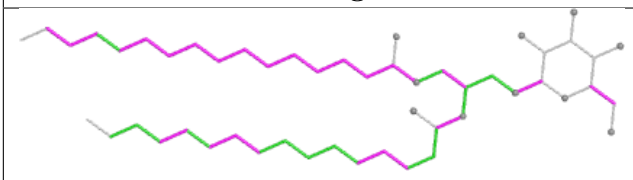


Bond angles



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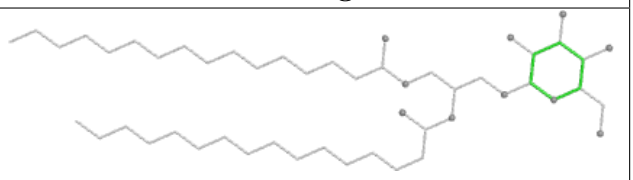
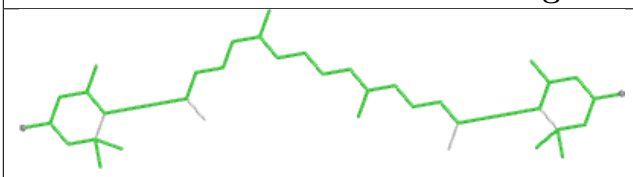


Rings

Ligand II0 8 313



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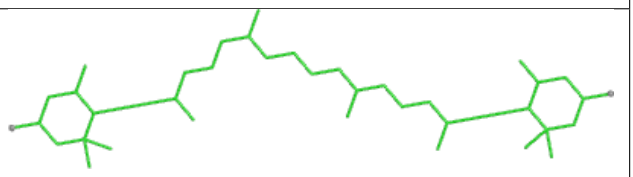
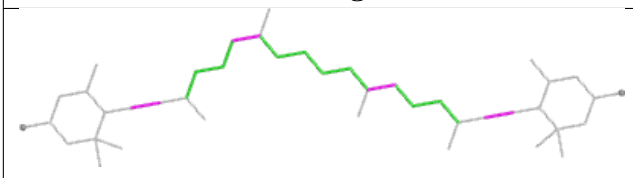


Bond angles



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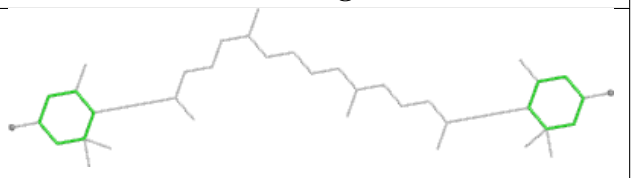
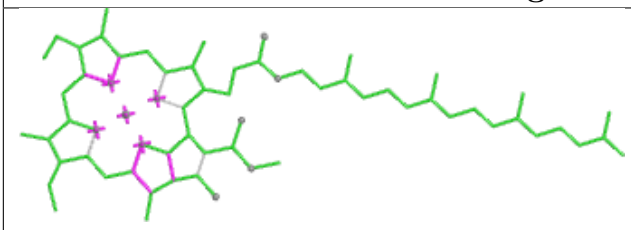


Rings

Ligand CLA b 604



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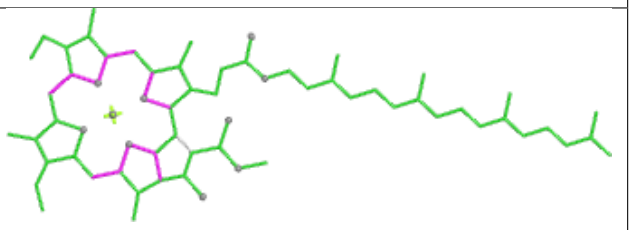
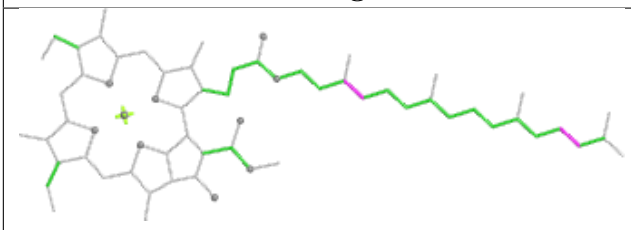
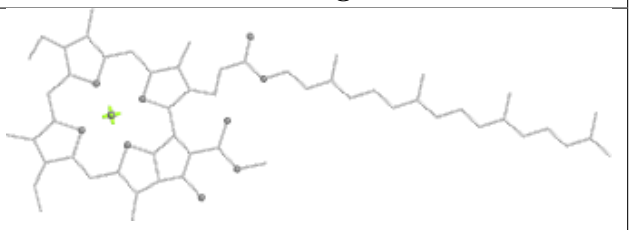


Bond angles

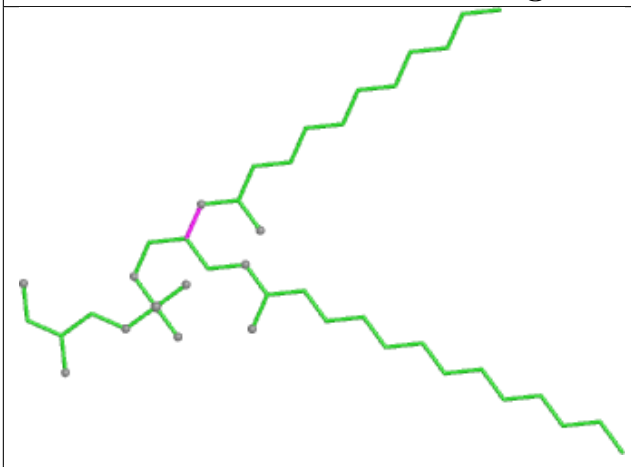


Torsions

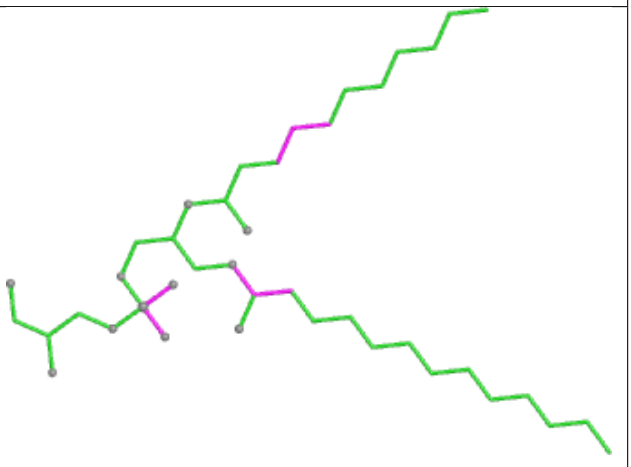


Rings

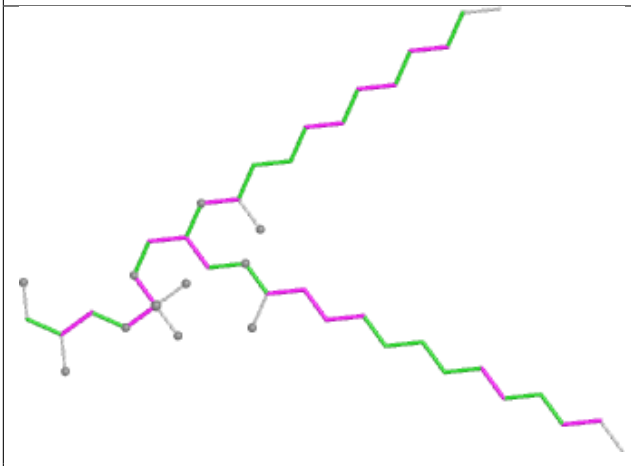
Ligand LHG 3 302



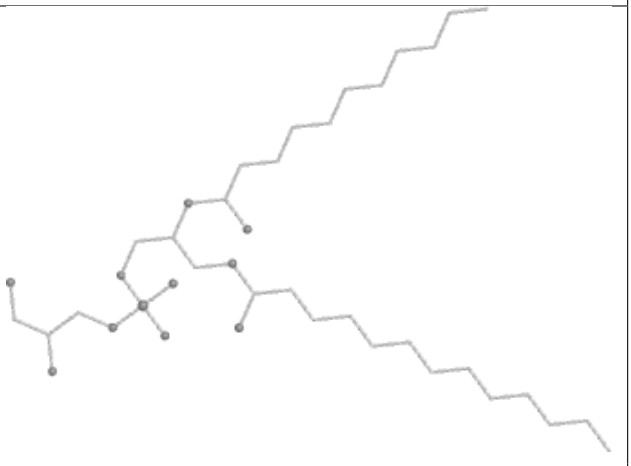
Bond lengths



Bond angles

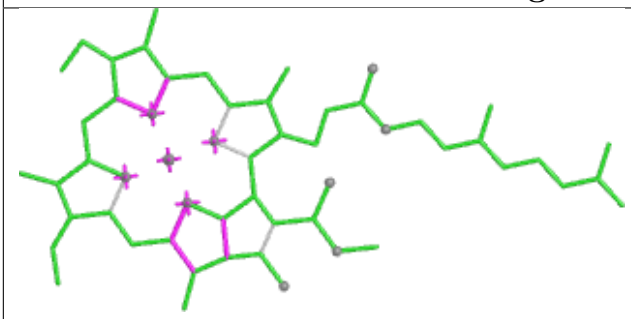


Torsions



Rings

Ligand CLA 2 308



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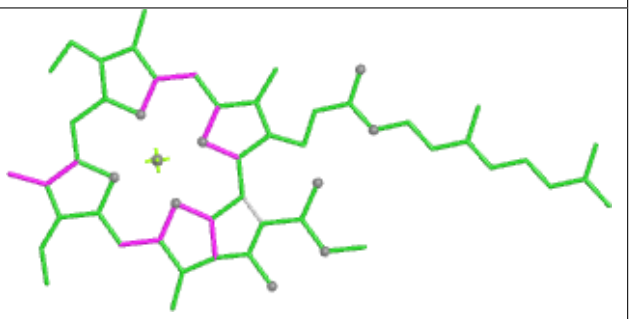

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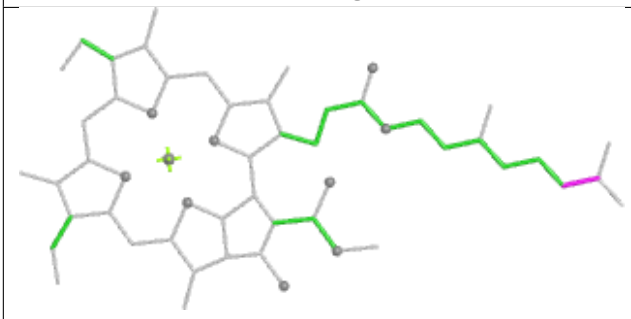

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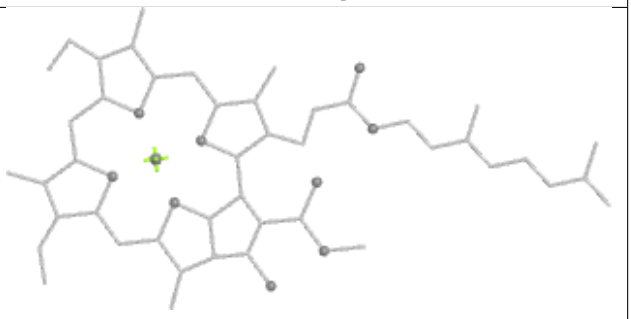
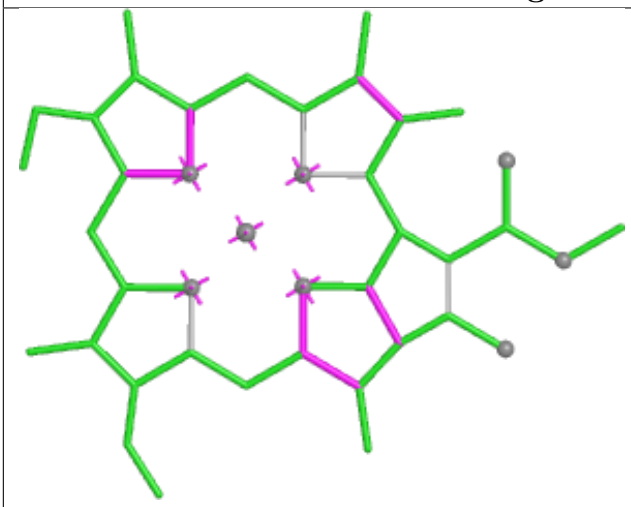


Rings

Ligand CLA p 312



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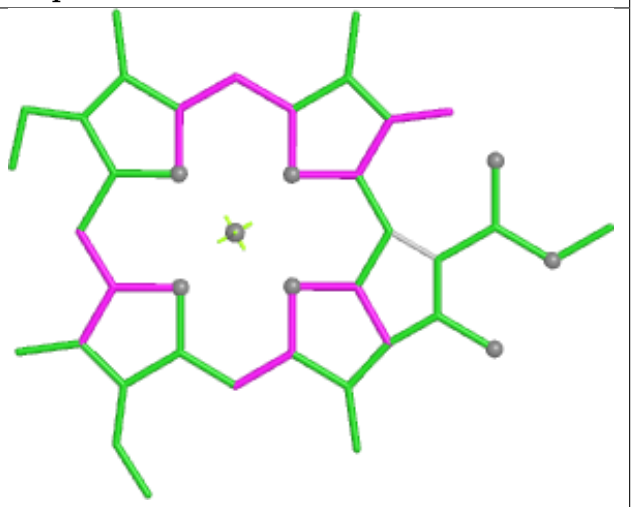
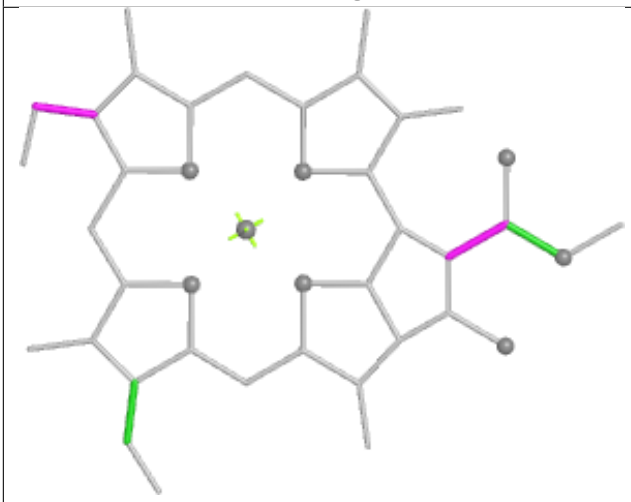


Bond angles



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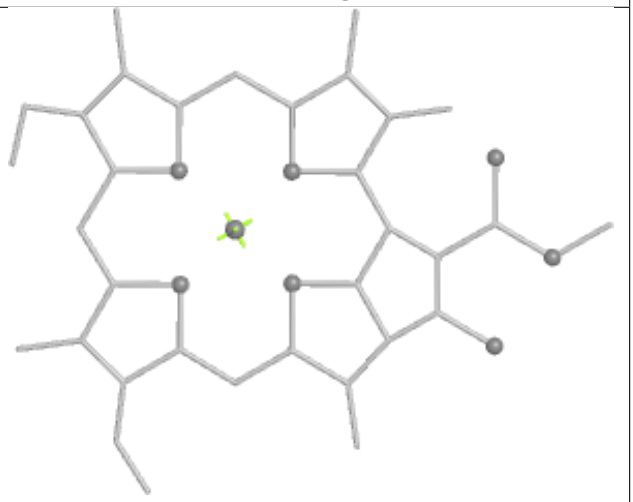
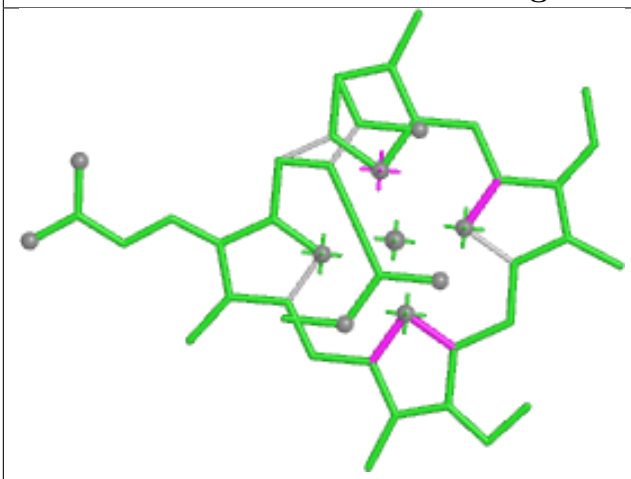


Rings

Ligand KC2 g 309



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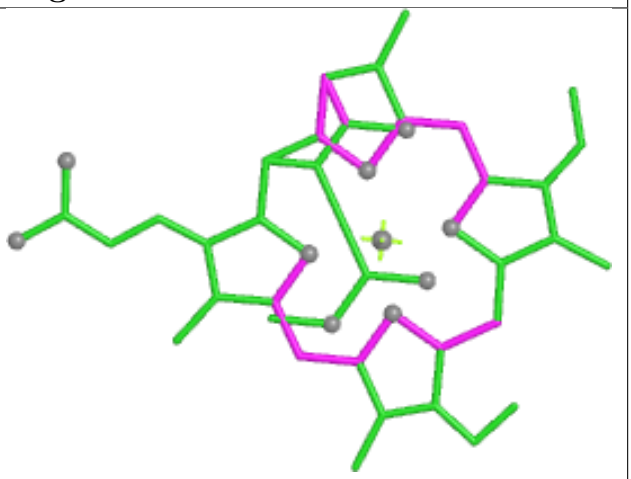
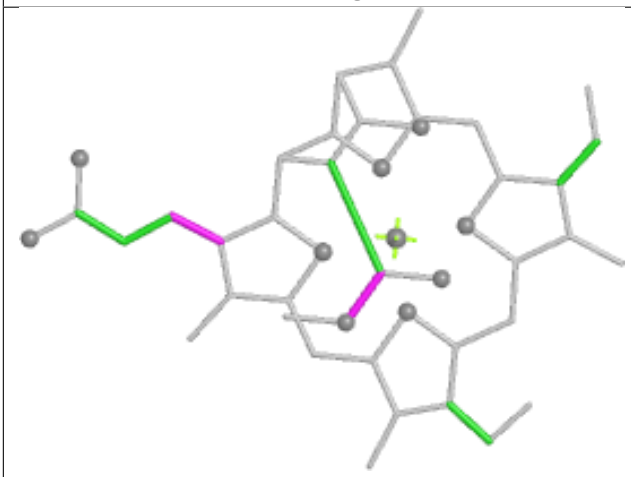


Bond angles



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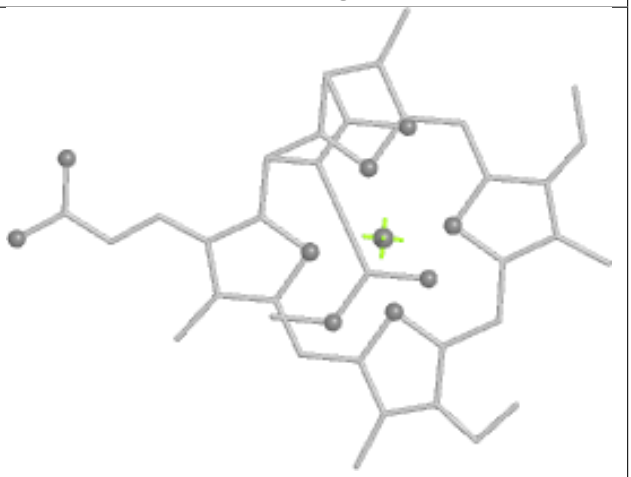
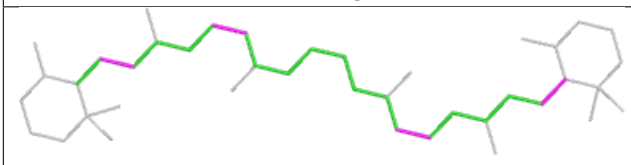


Rings

Ligand 8CT 1 312

Bond lengths

Bond angles



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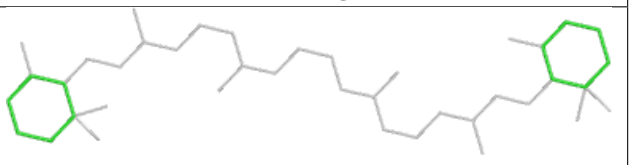
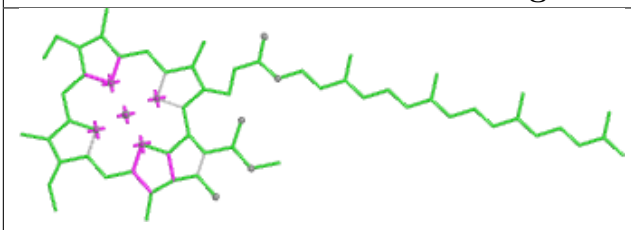
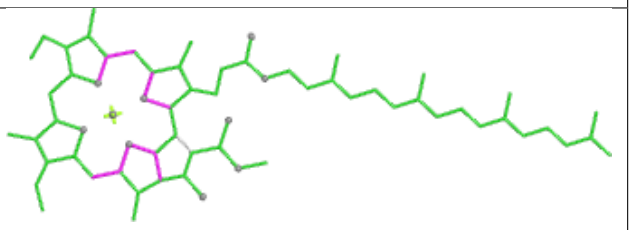


Rings

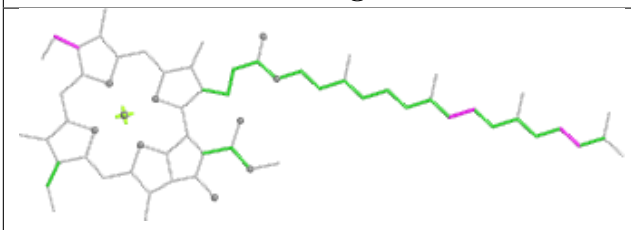
Ligand CLA c 504



Bond lengths



Bond angles



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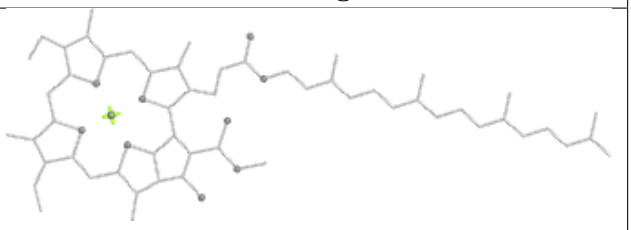
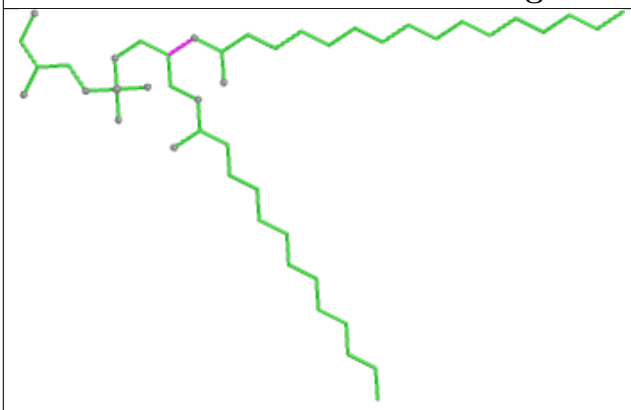


Rings

Ligand LHG d 401



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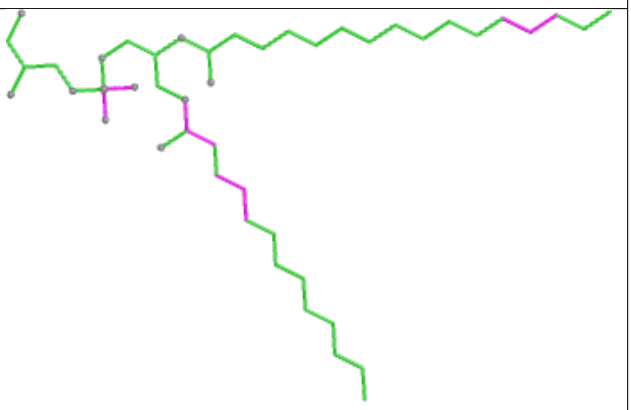
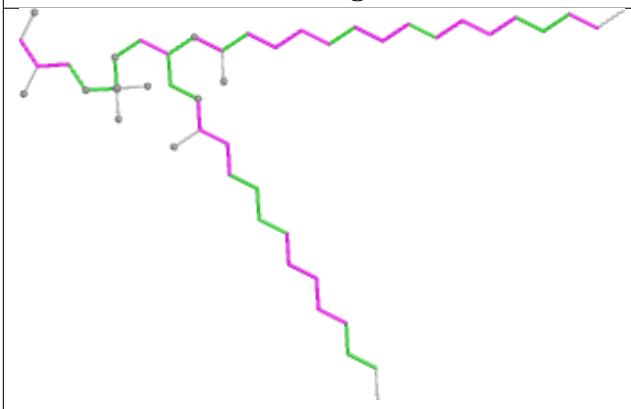


Bond angles



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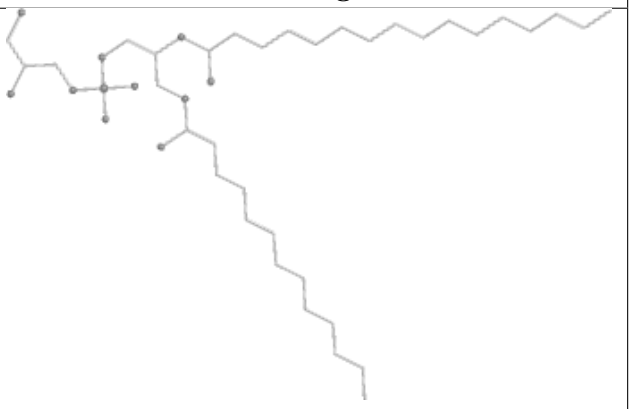
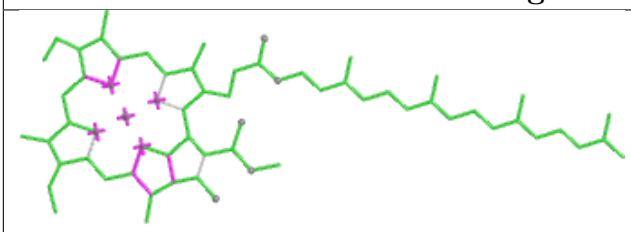
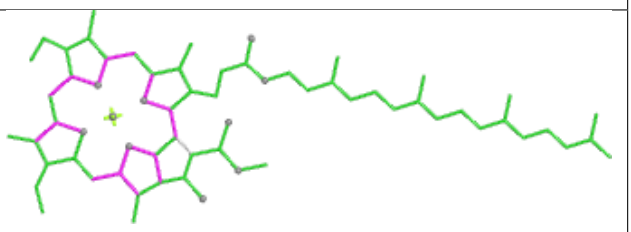


Rings

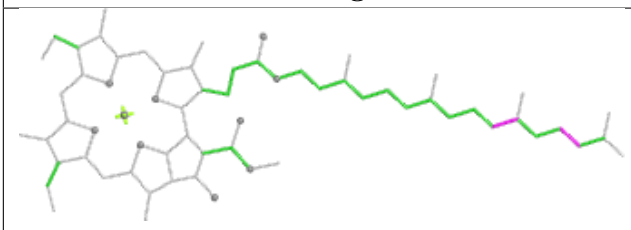
Ligand CLA b 609



Bond lengths



Bond angles



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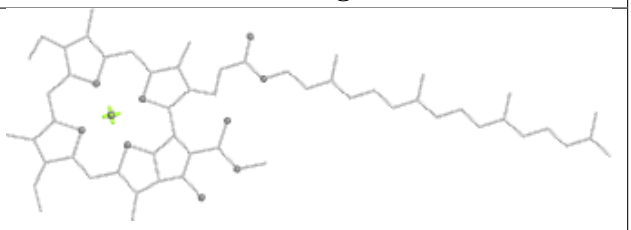
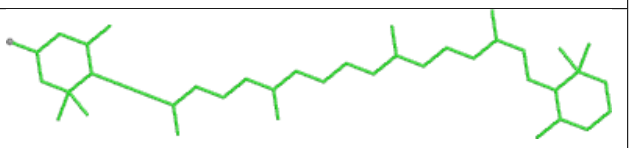


Rings

Ligand IHT 9 320

Bond lengths



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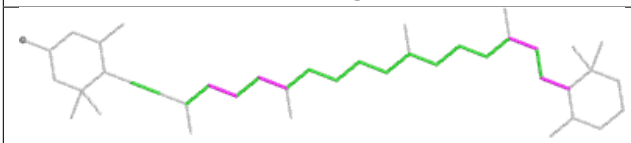

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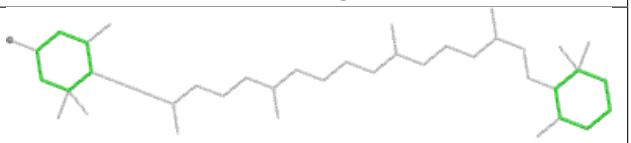
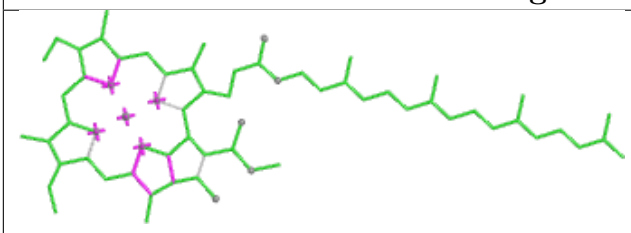


Rings

Ligand CLA c 503



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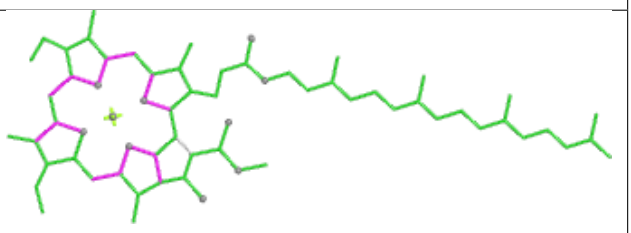
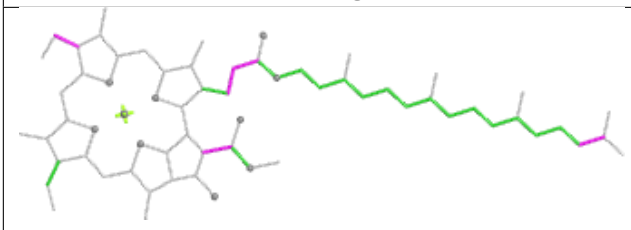


Bond angles



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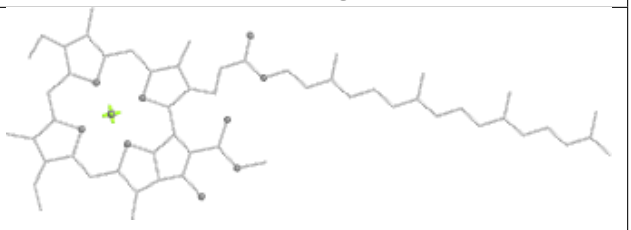
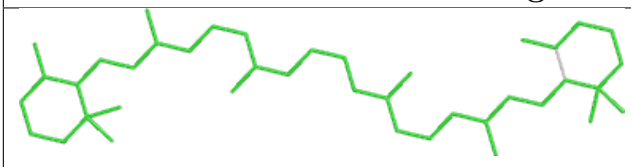


Rings

Ligand 8CT B 619



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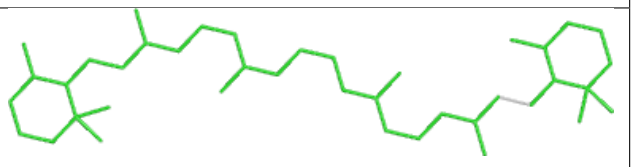

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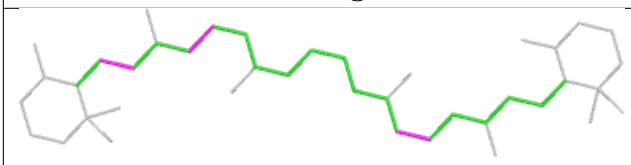

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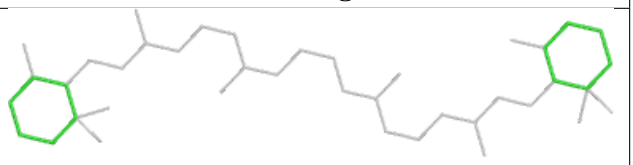
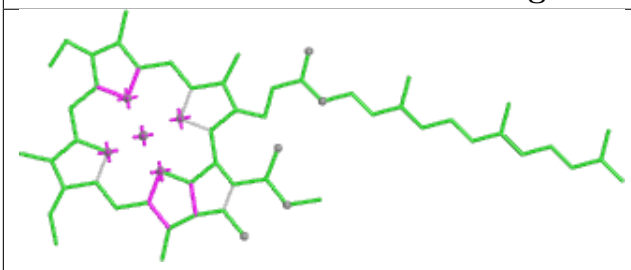


Rings

Ligand CLA 2 306



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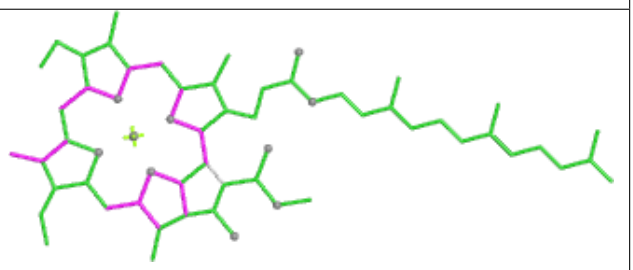
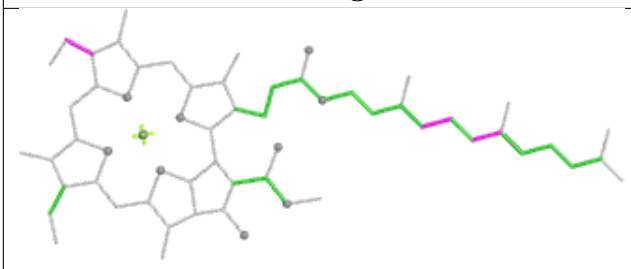
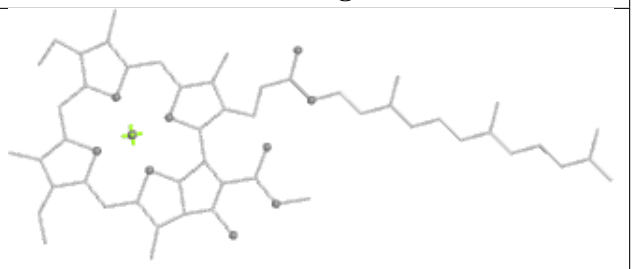


Bond angles

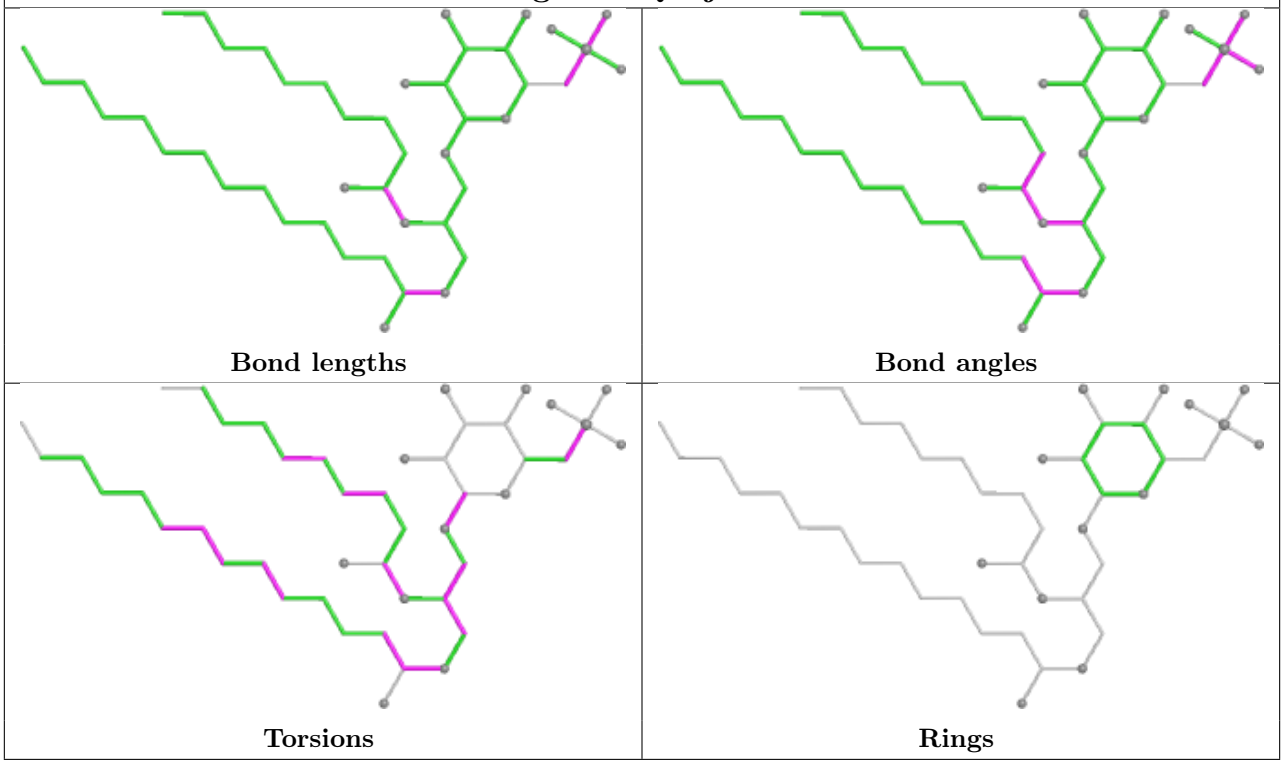


Torsions

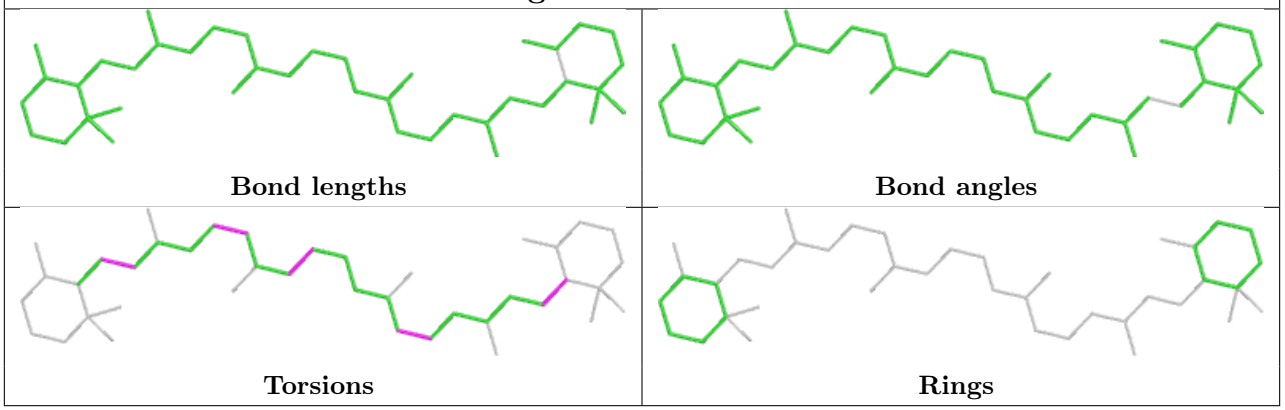


Rings

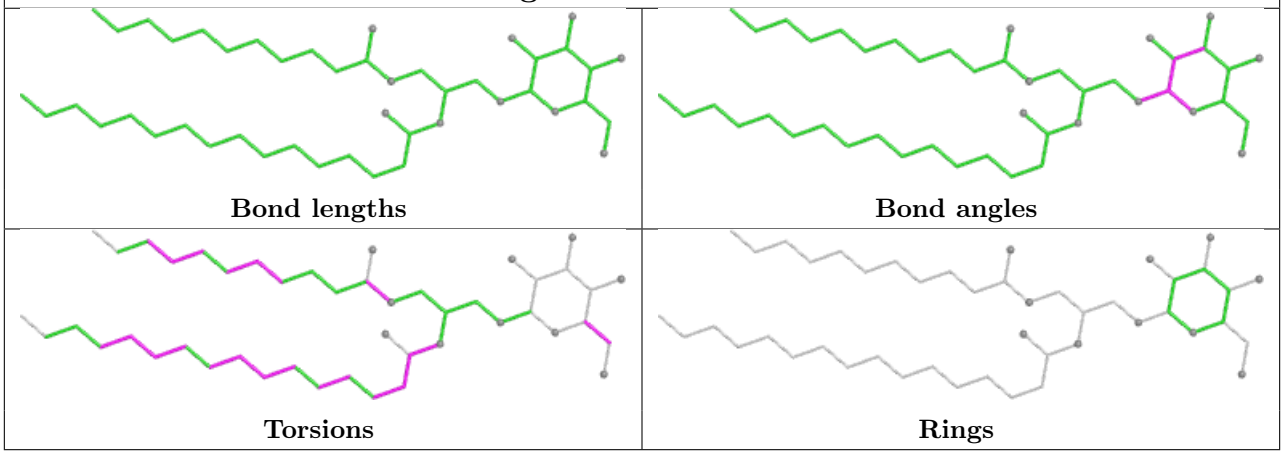
Ligand SQD j 101



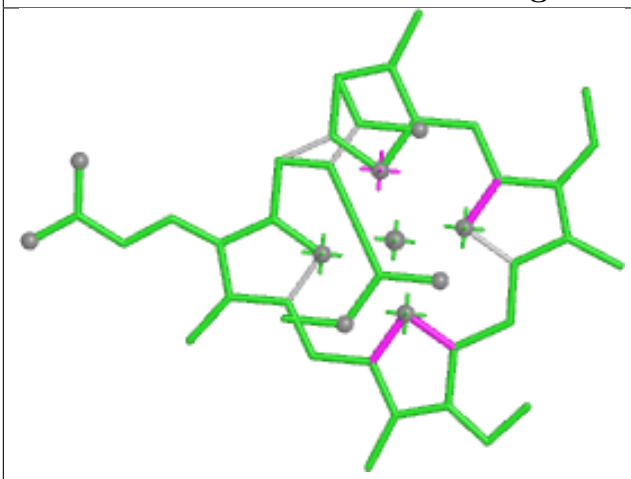
Ligand 8CT C 517



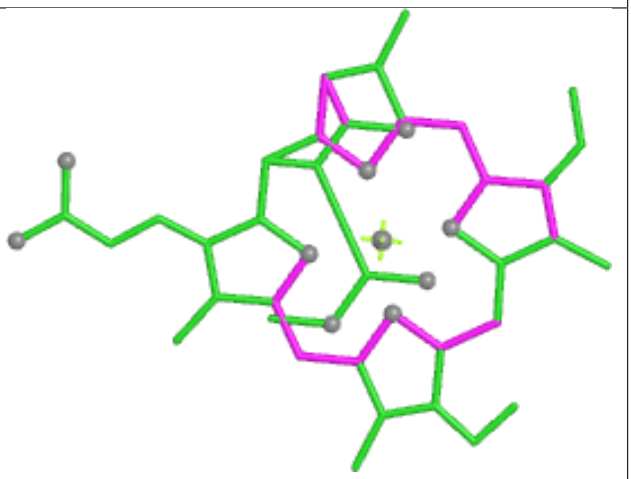
Ligand LMG D 409



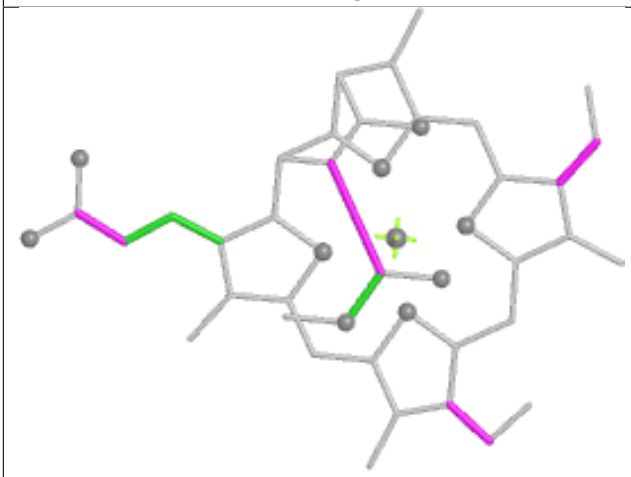
Ligand KC2 7 310



Bond lengths



Bond angles



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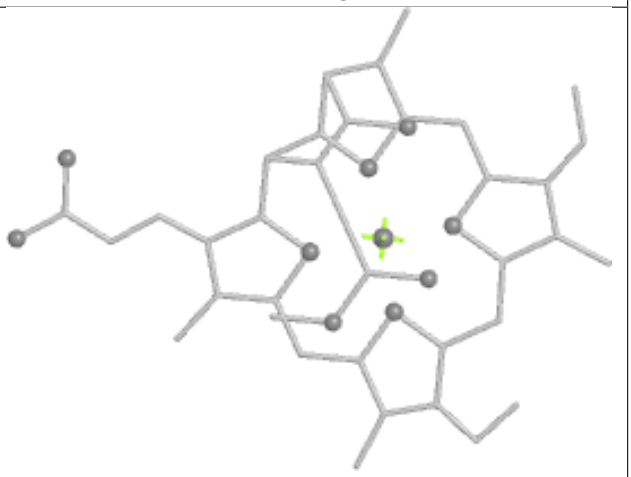
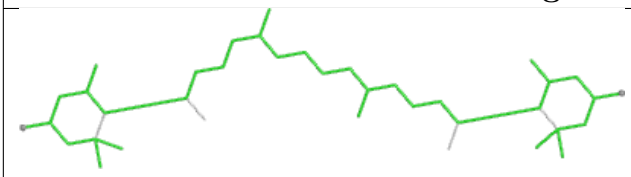


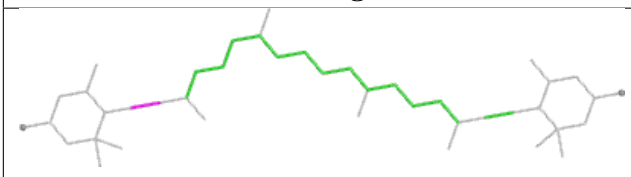
Rings

Ligand II0 g 313



Bond lengths

Bond angles



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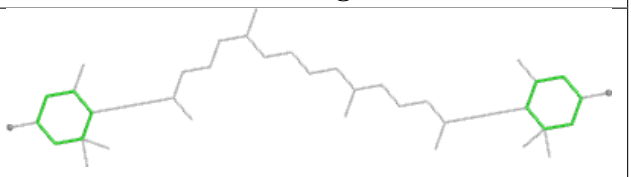
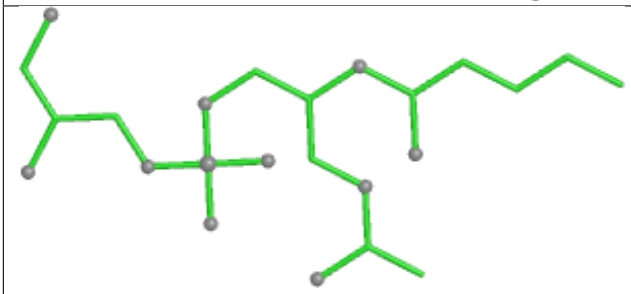
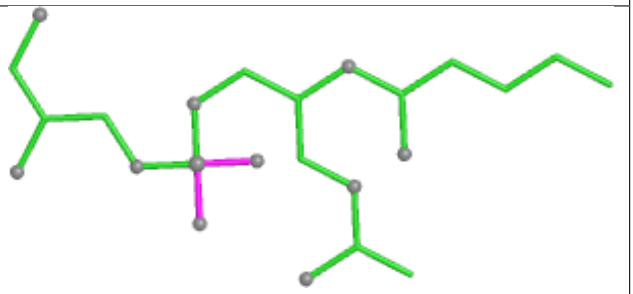


Rings

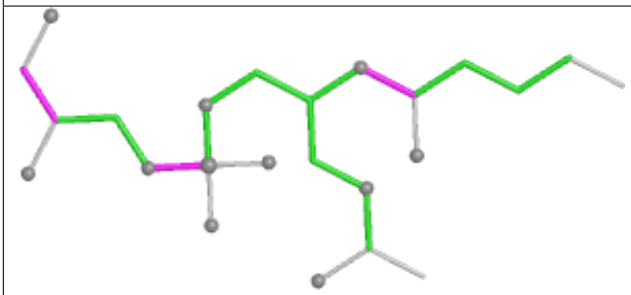
Ligand LHG 4 316



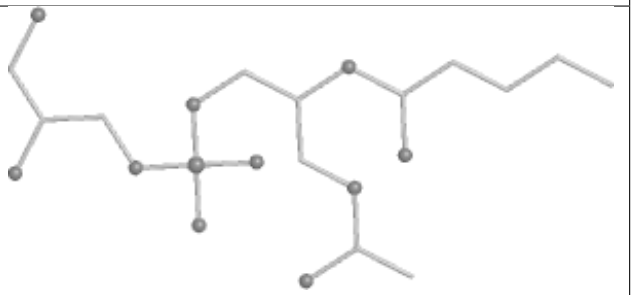
Bond lengths



Bond angles

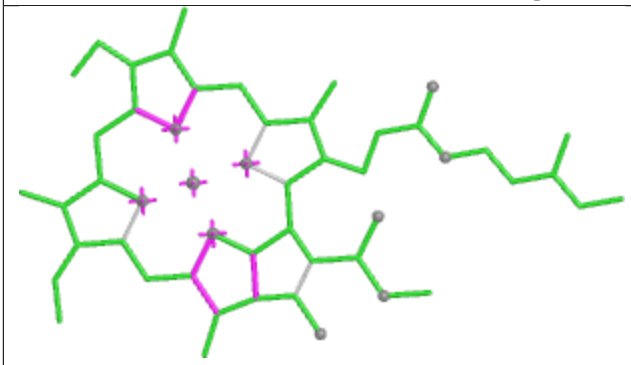


Torsions



Rings

Ligand CLA 1 308



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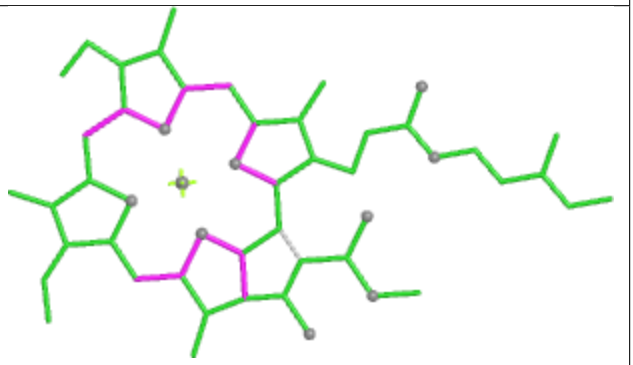

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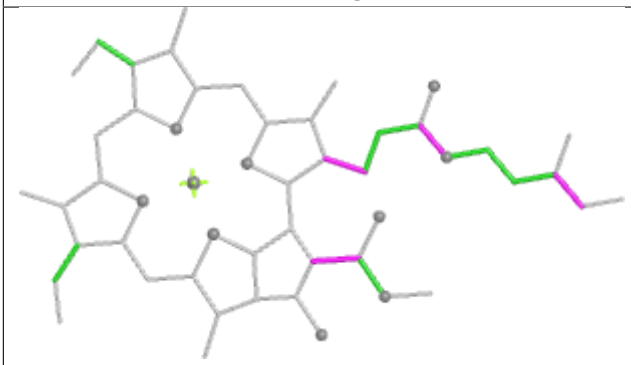

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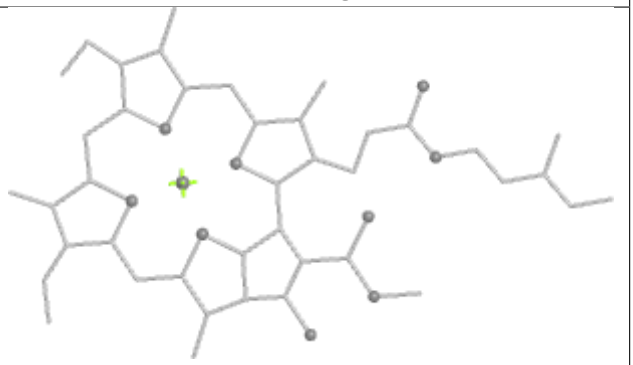
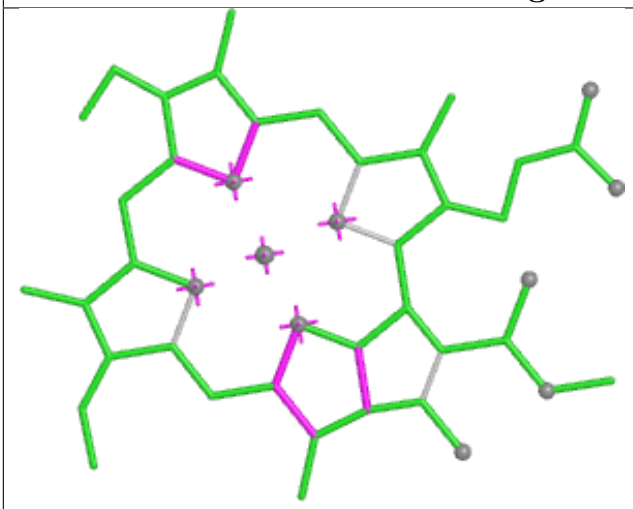


Rings

Ligand CLA 5 311



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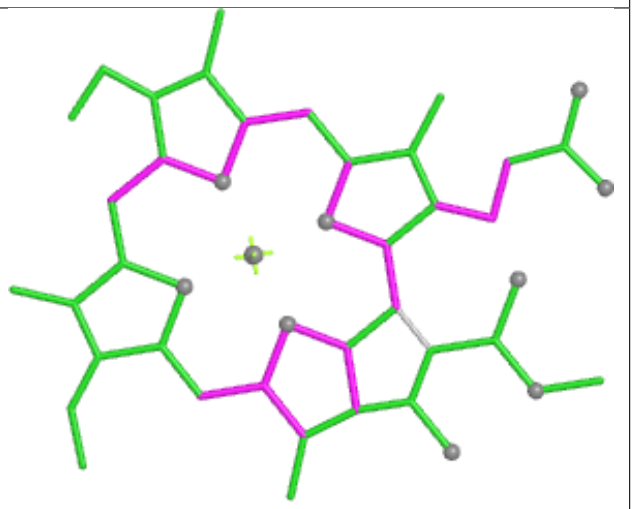

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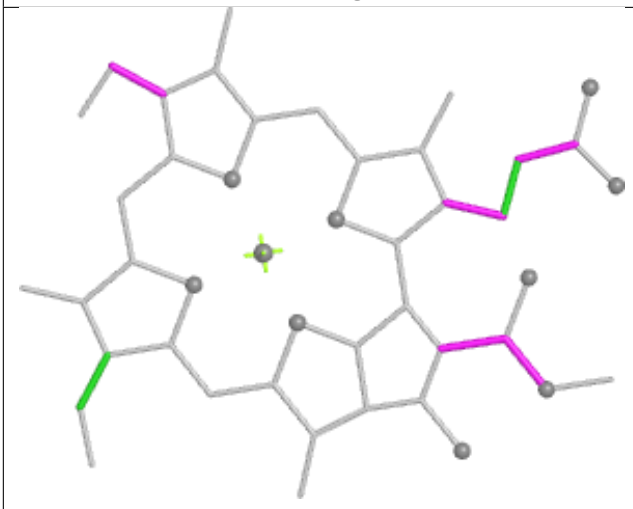
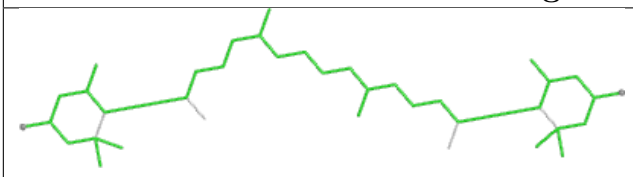


Torsions

Rings

Ligand II0 4 315



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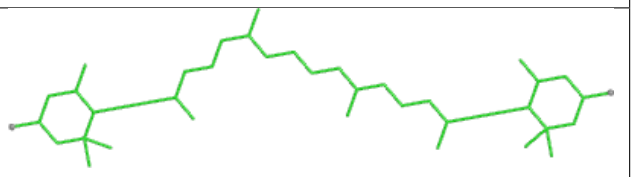

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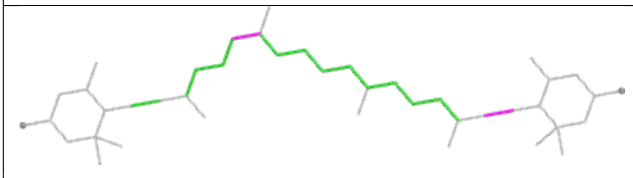

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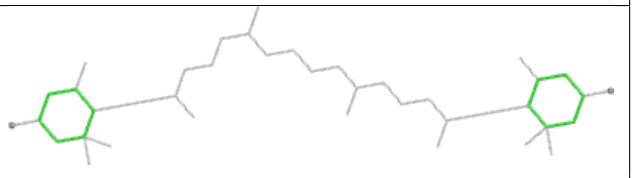
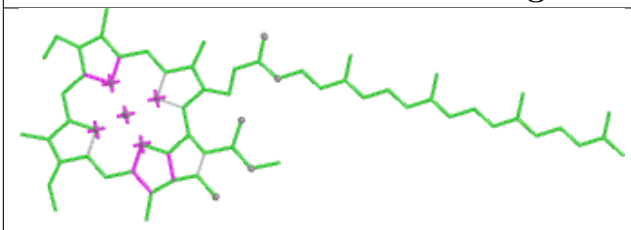


Rings

Ligand CLA d 405



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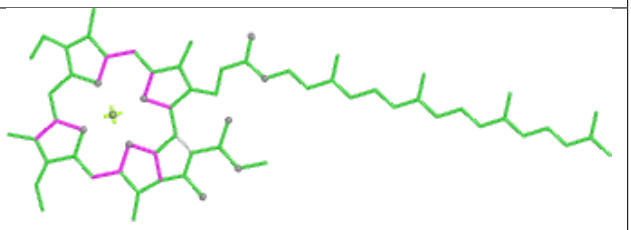

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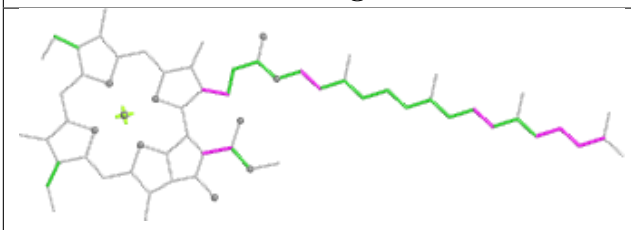

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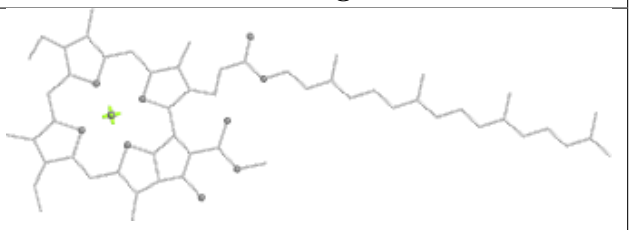
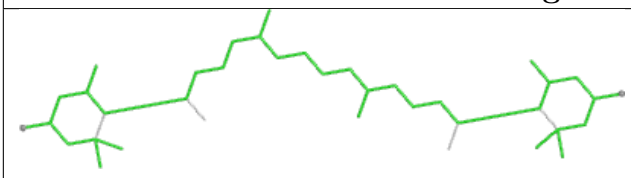


Rings

Ligand II0 6 301



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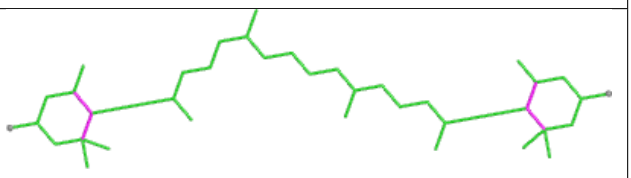

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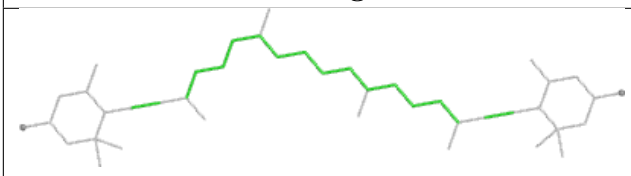

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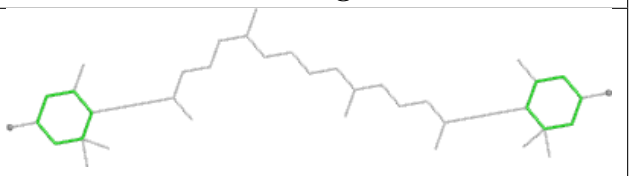
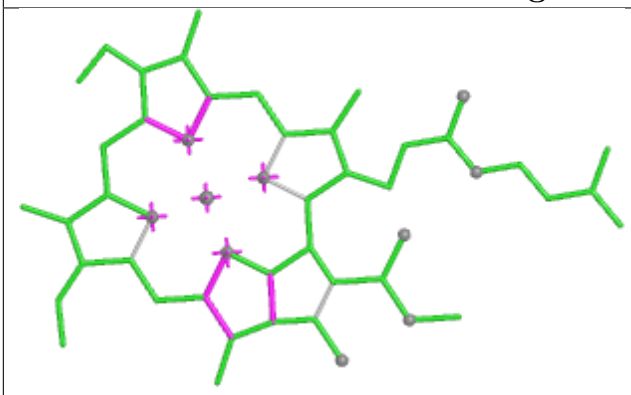


Rings

Ligand CLA 0 303



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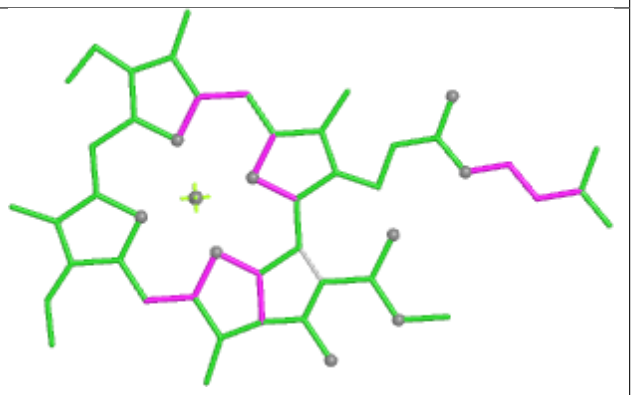
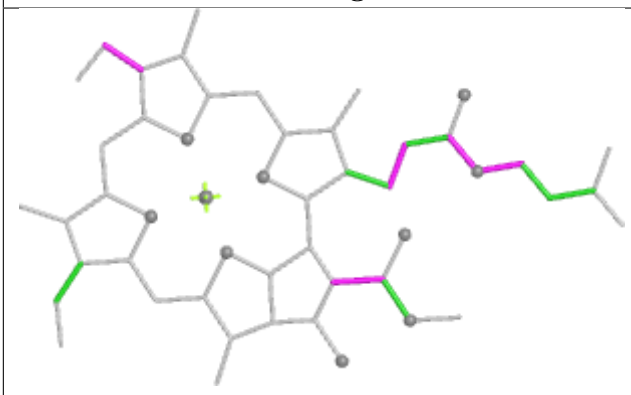


Bond angles



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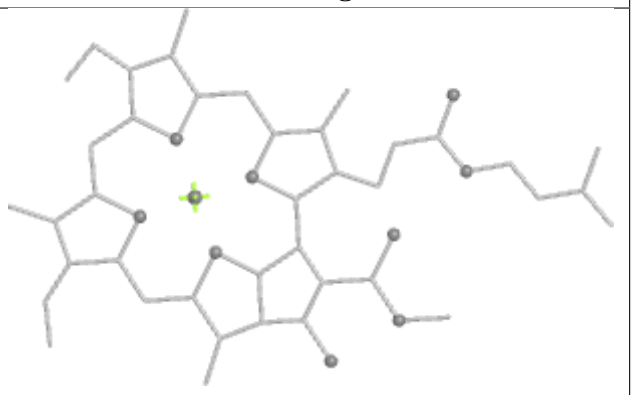
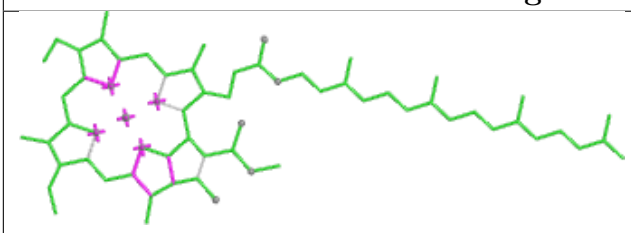


Rings

Ligand CLA C 511



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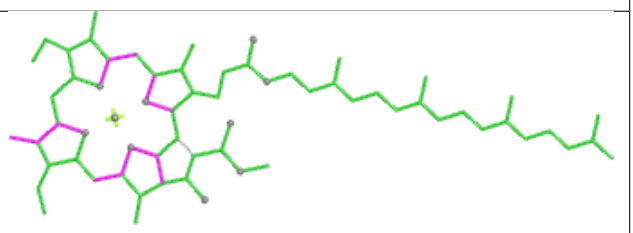

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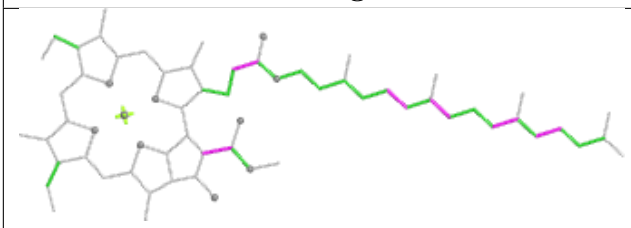

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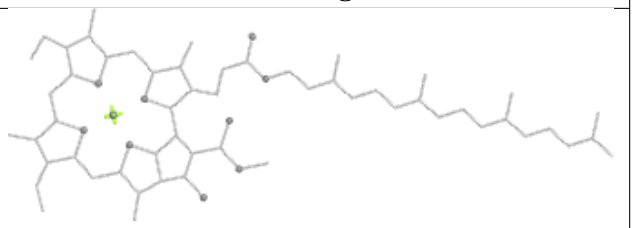
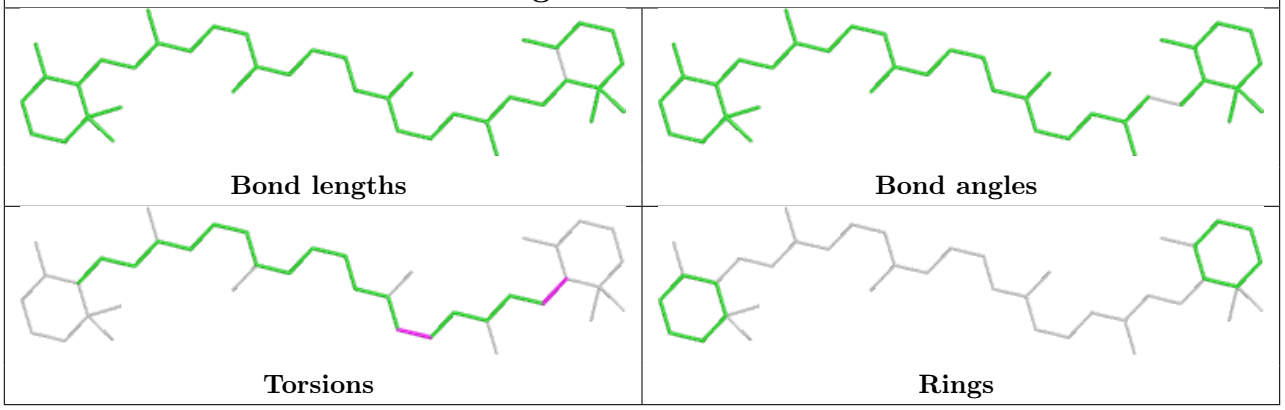


Rings

Ligand 8CT a 409



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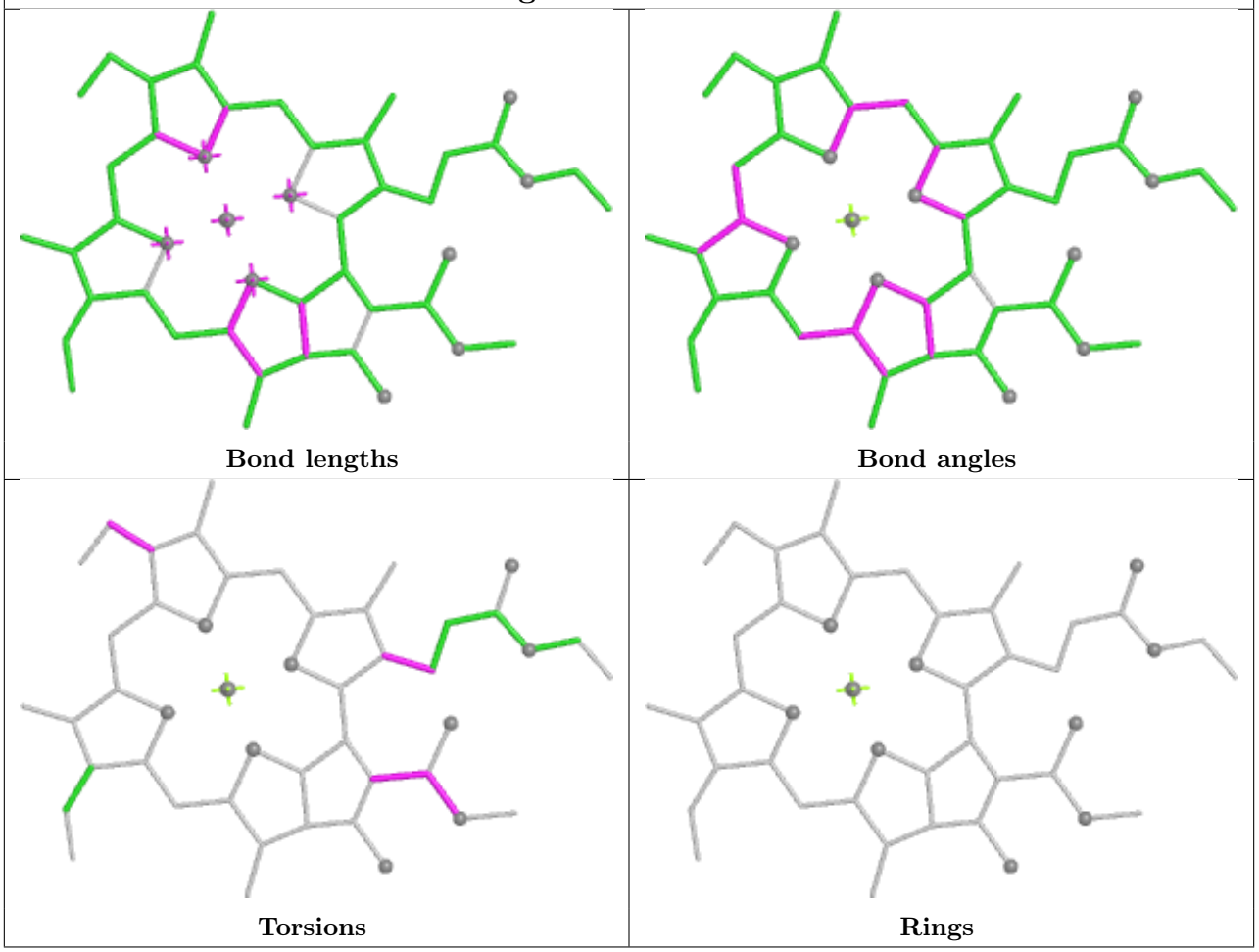
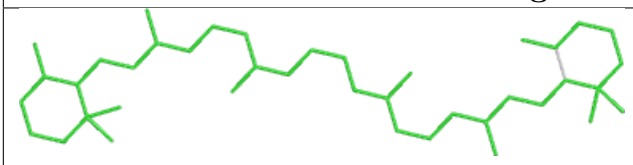


Ligand 8CT d 406



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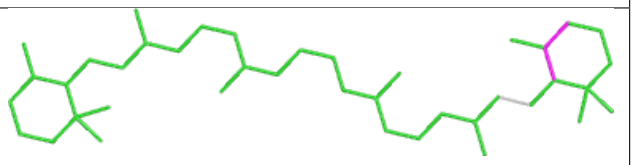
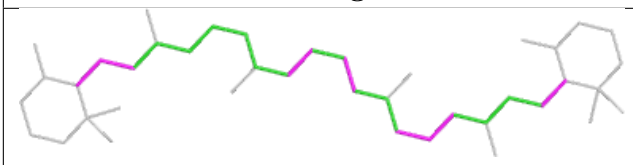


Bond angles



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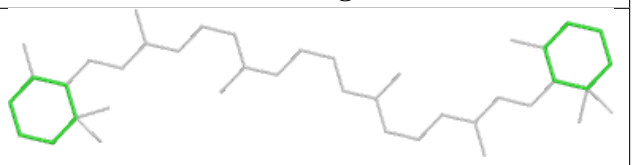
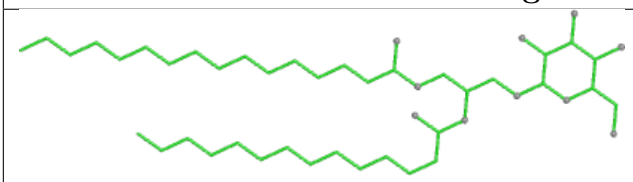


Rings

Ligand LMG b 622



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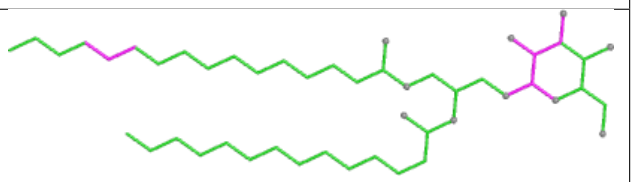
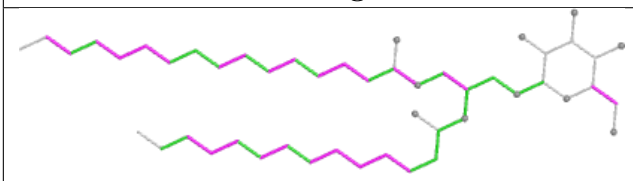


Bond angles



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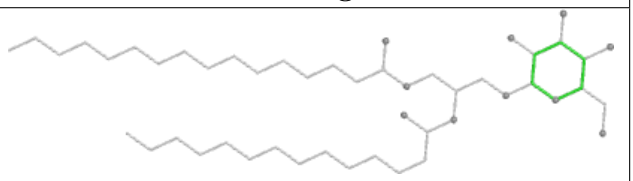
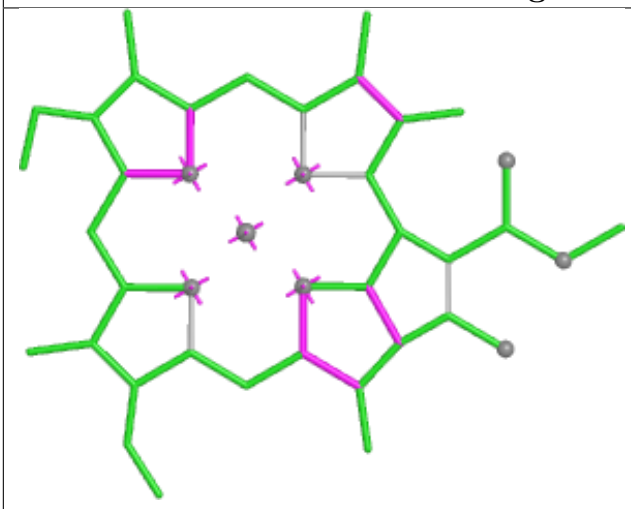


Rings

Ligand CLA 6 312



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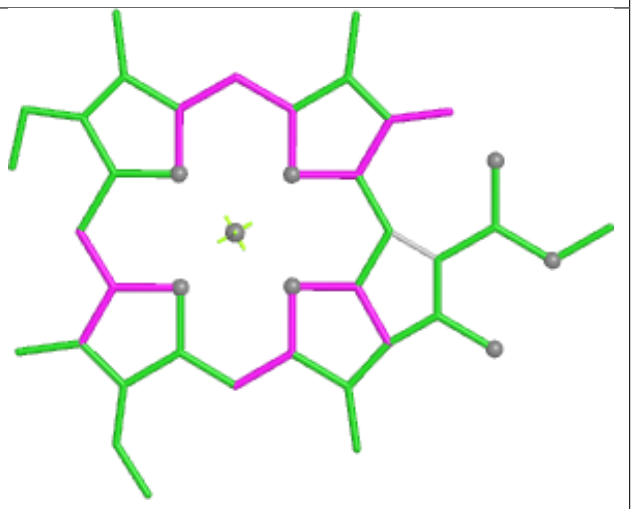
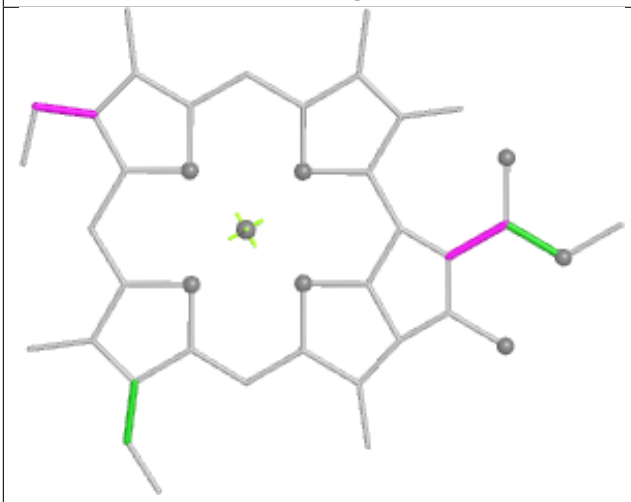


Bond angles



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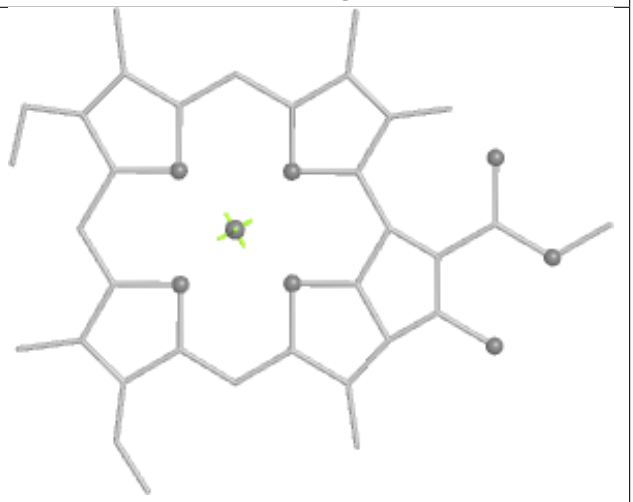
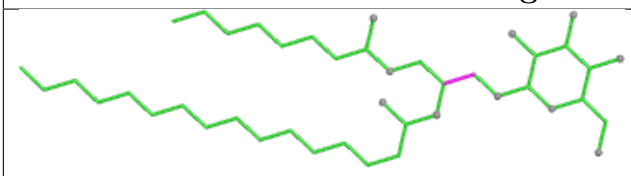


Rings

Ligand LMG T 101



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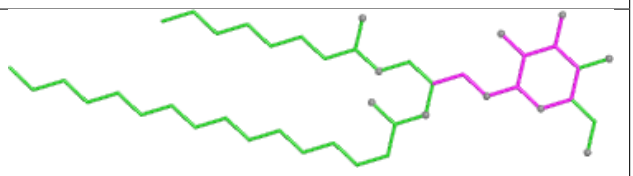
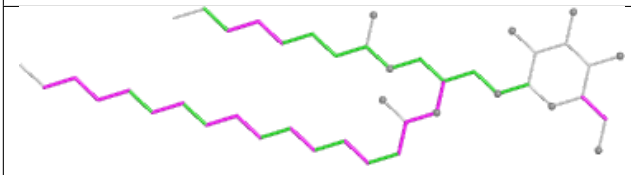


Bond angles



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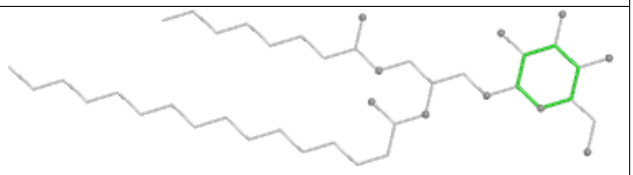
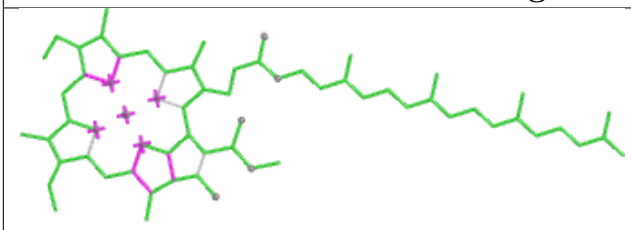


Rings

Ligand CLA a 412



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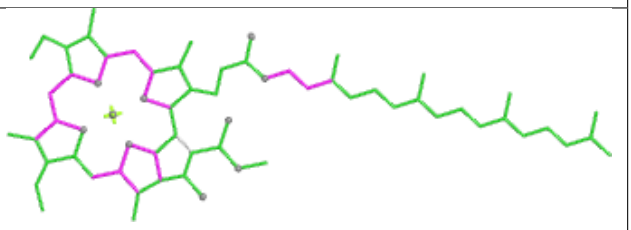
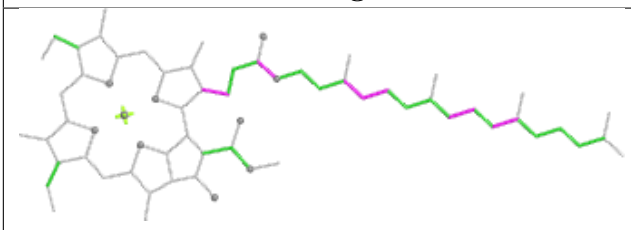


Bond angles



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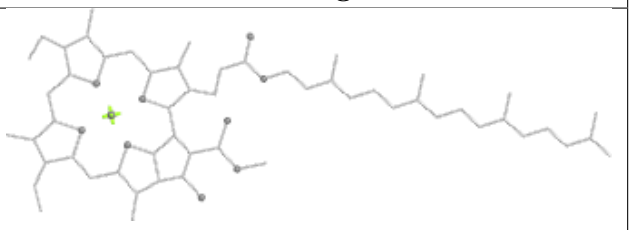
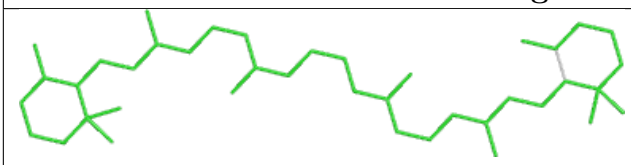


Rings

Ligand 8CT 7 312



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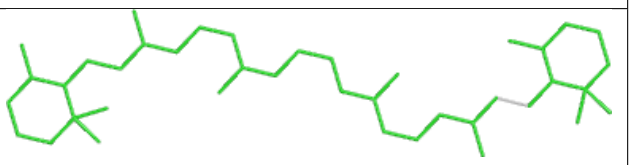
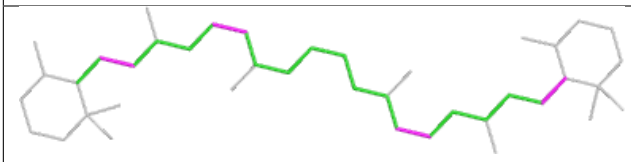


Bond angles



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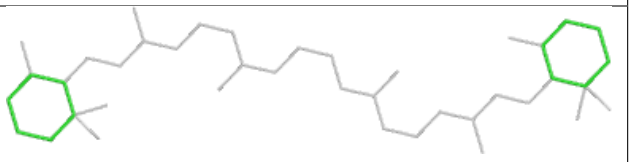
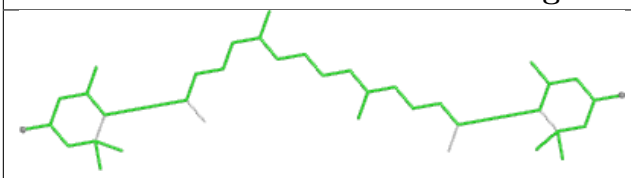


Rings

Ligand II0 1 315



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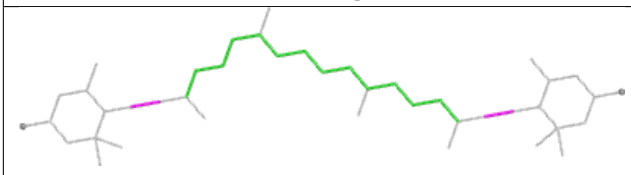

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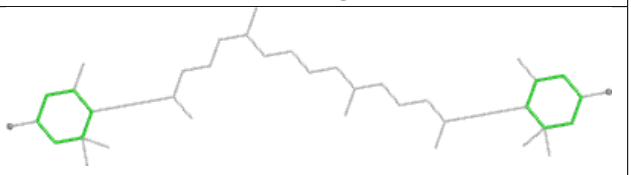
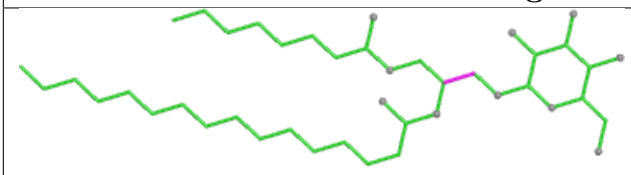


Rings

Ligand LMG t 101



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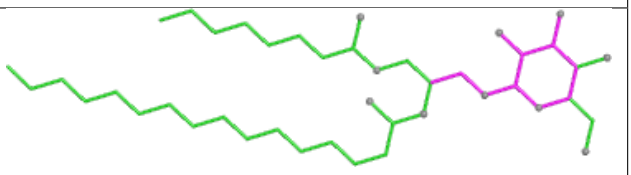

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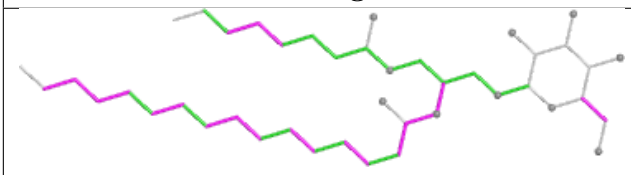

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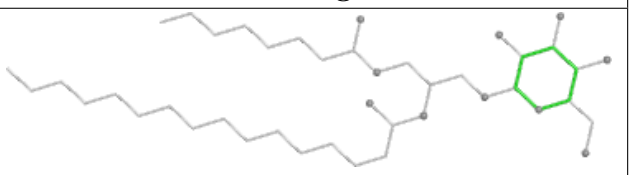
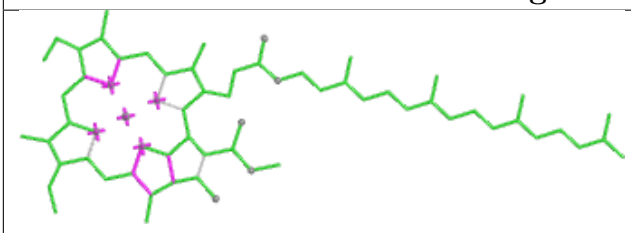


Rings

Ligand CLA c 514



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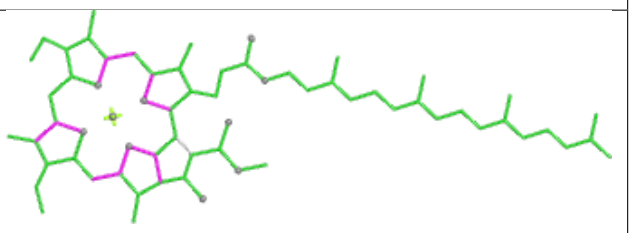

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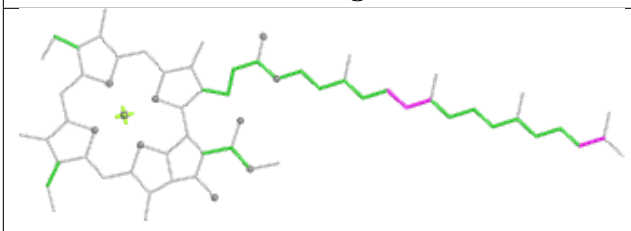

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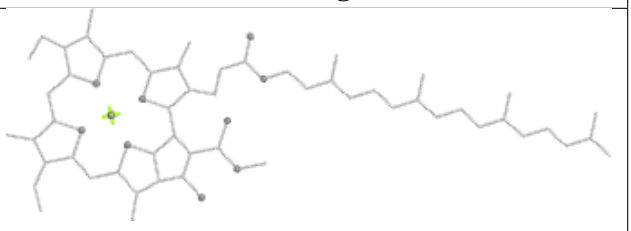

Rings

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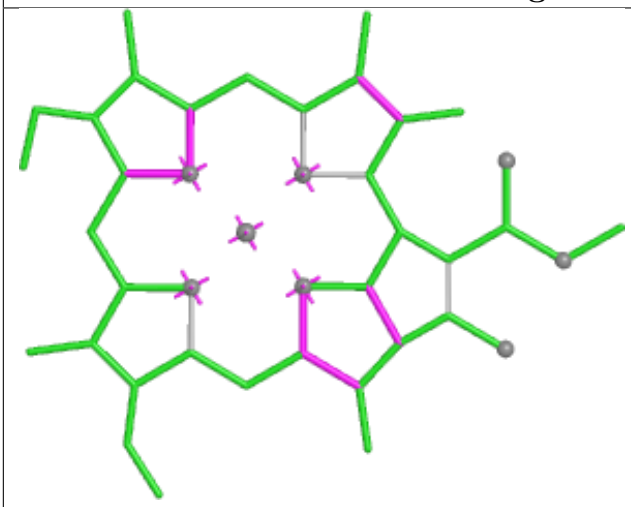

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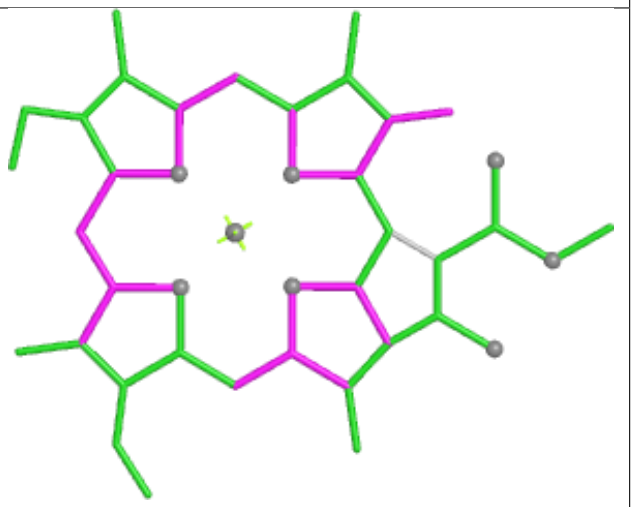

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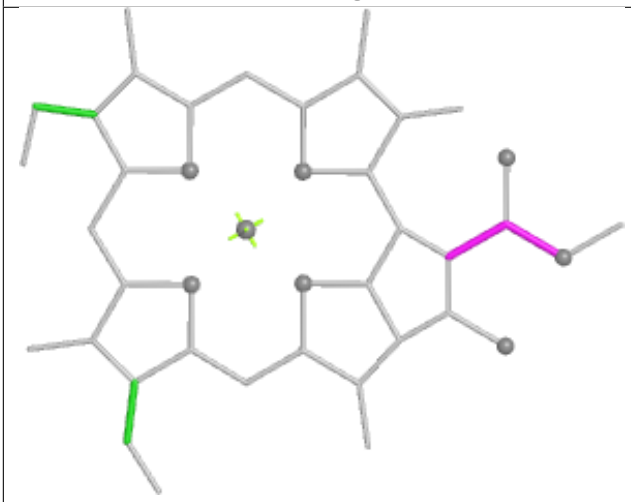

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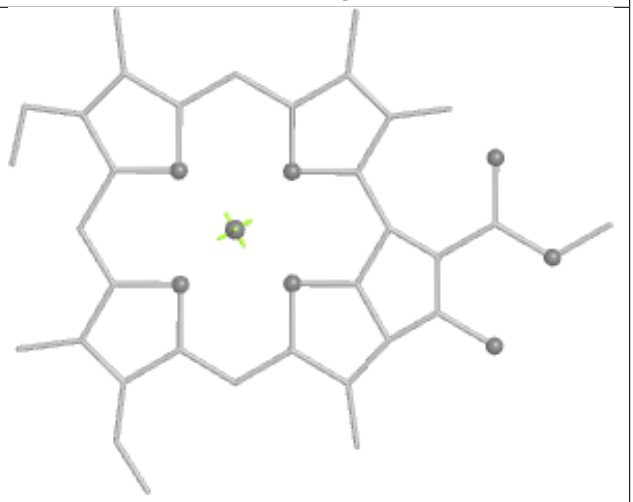

Rings

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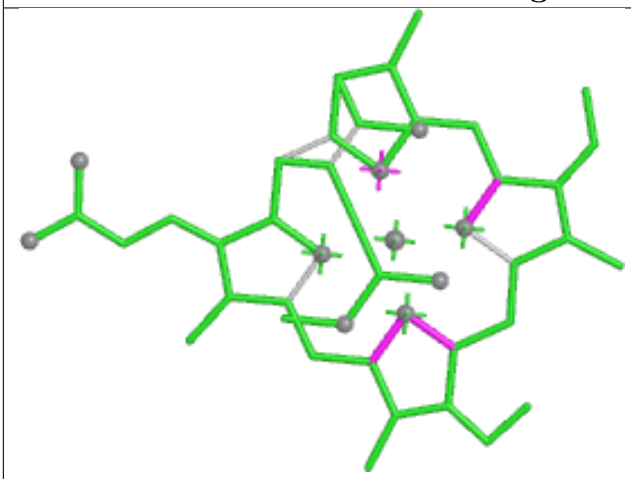

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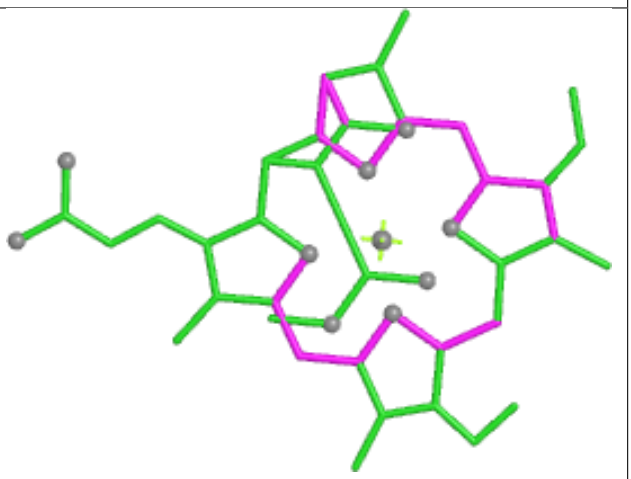

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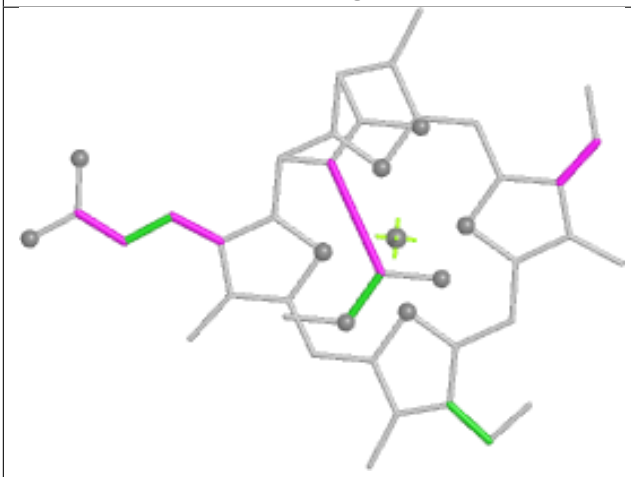

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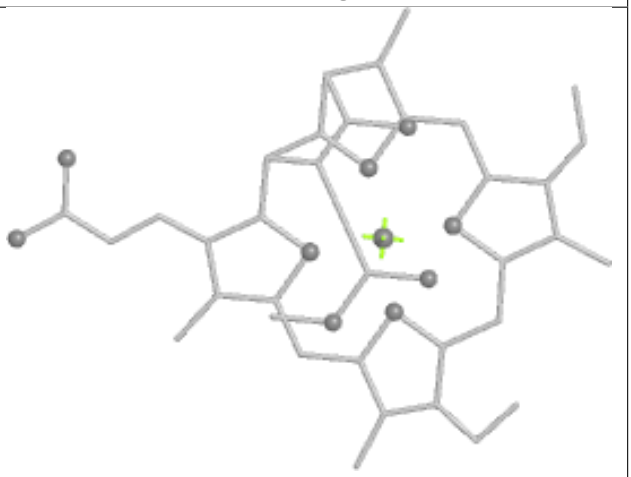
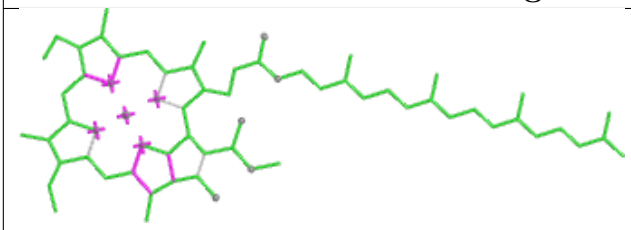


Rings

Ligand CLA B 605



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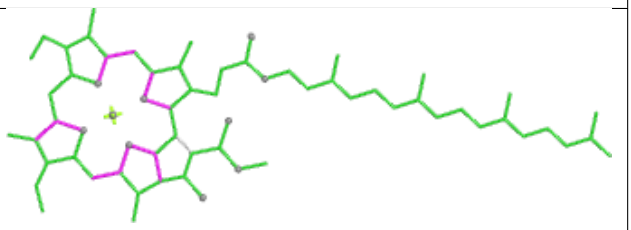

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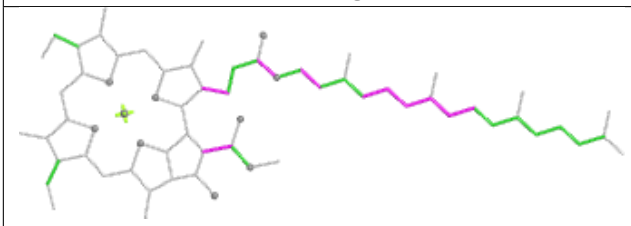

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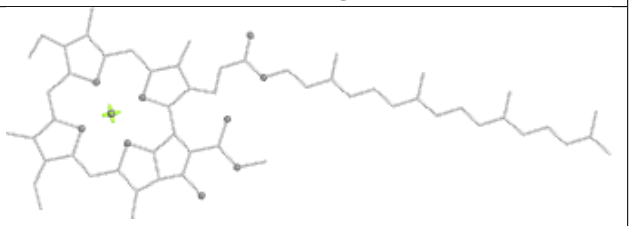
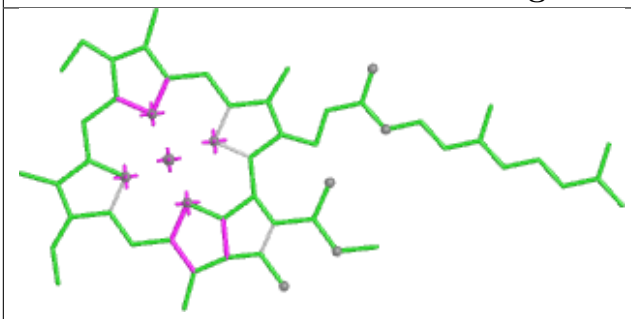


Rings

Ligand CLA g 303



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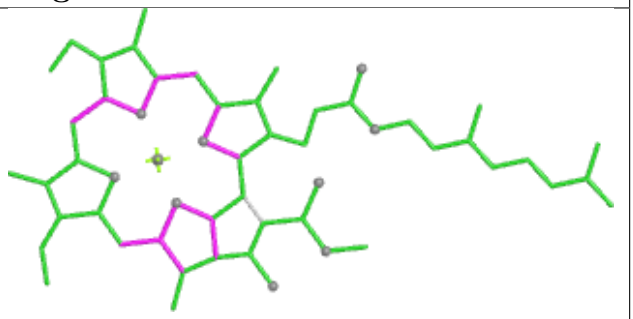

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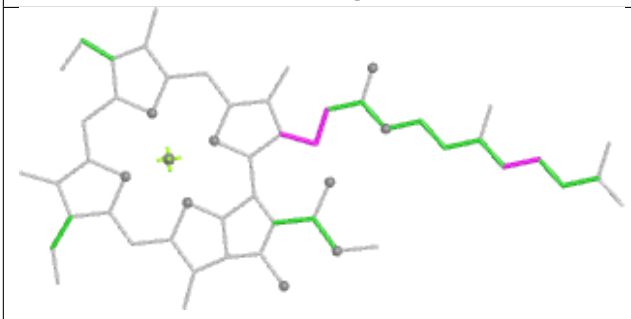

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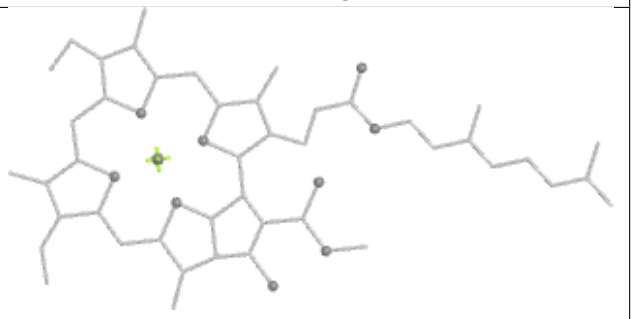
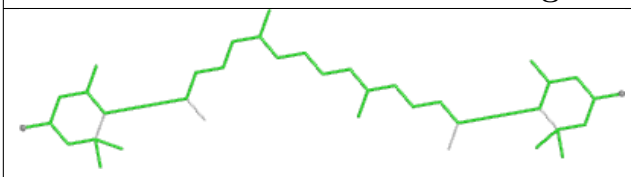


Rings

Ligand II0 p 317



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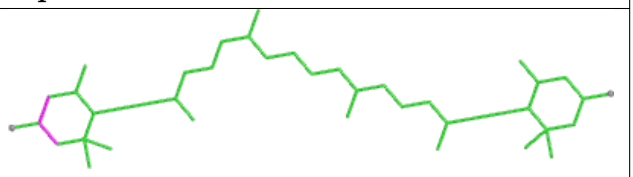

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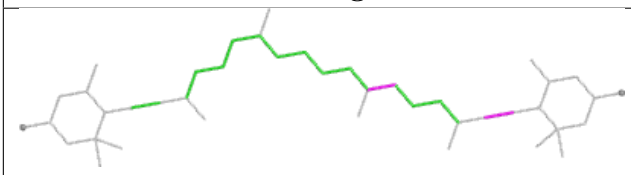

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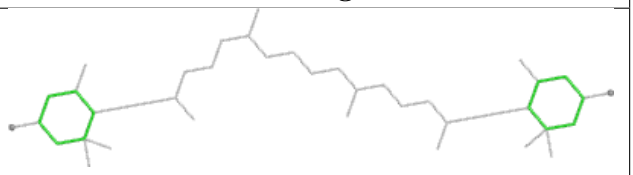

Rings

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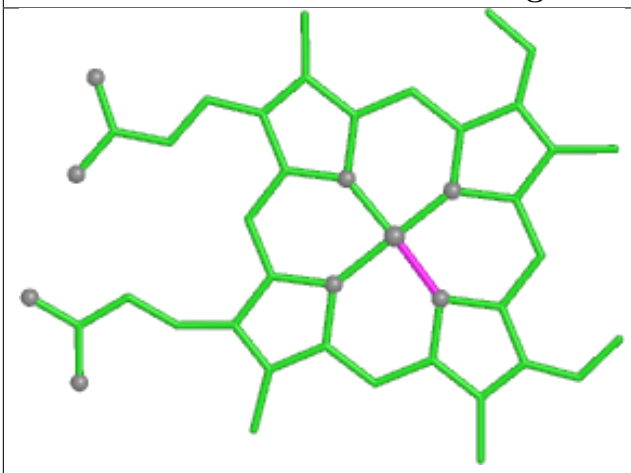

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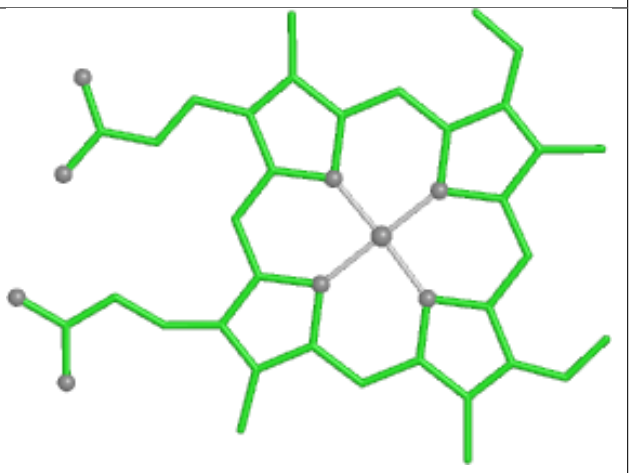

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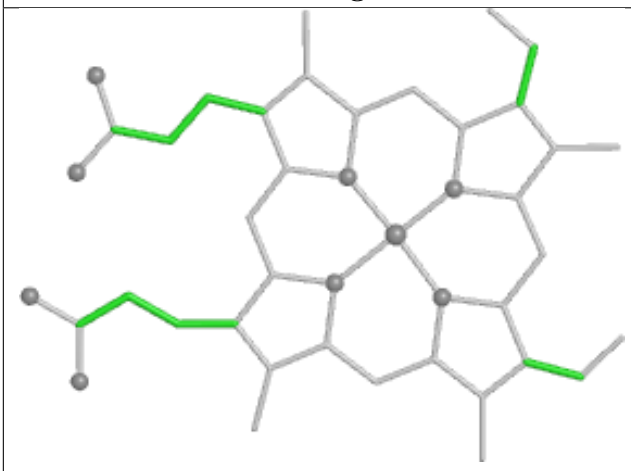

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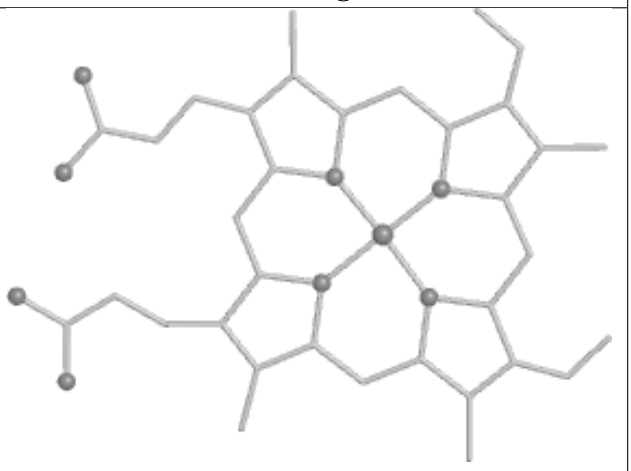
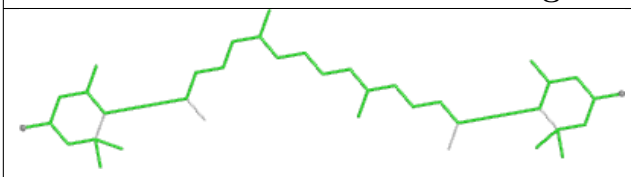


Rings

Ligand II0 9 317



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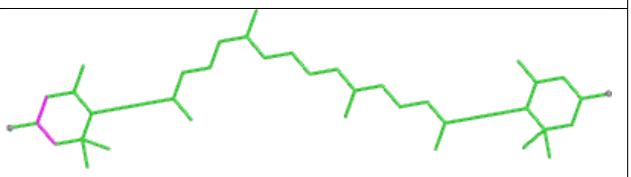

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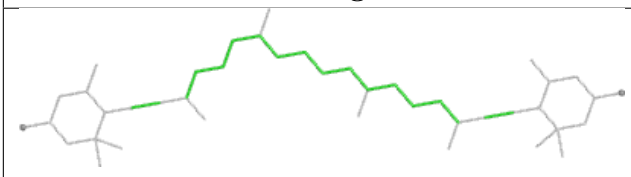

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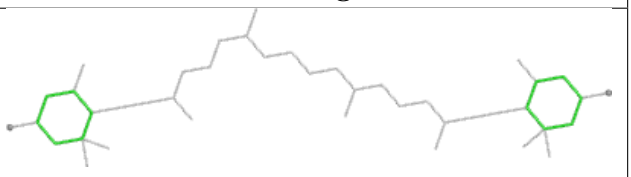
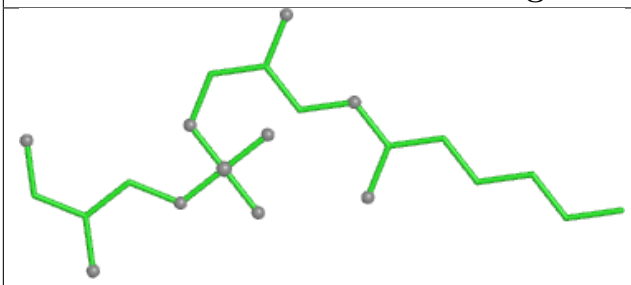


Rings

Ligand LHG g 316



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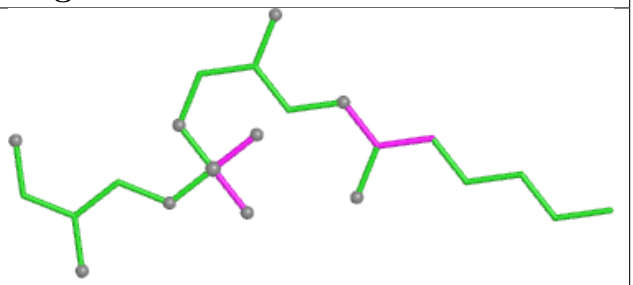

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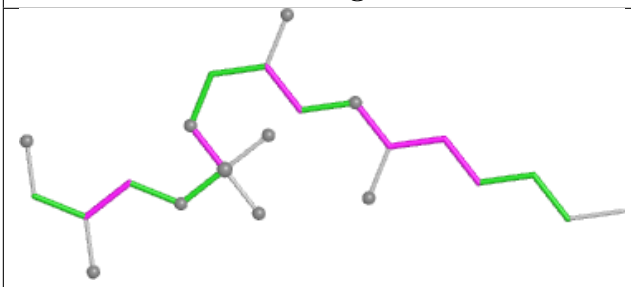

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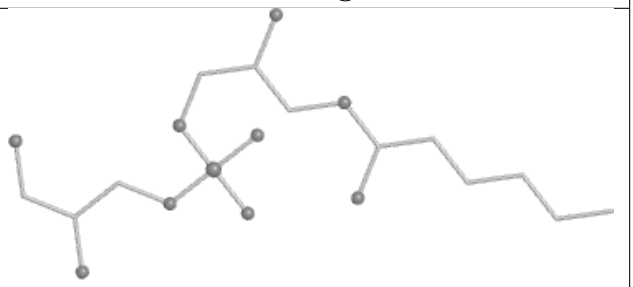
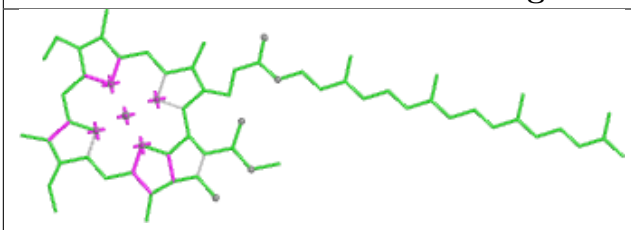


Rings

Ligand CLA b 606



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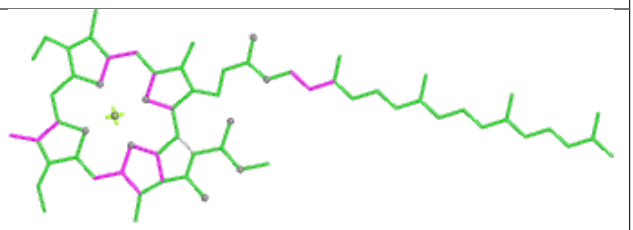

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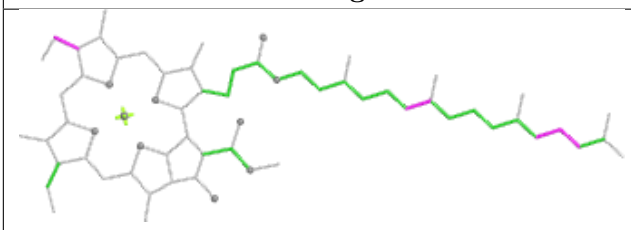

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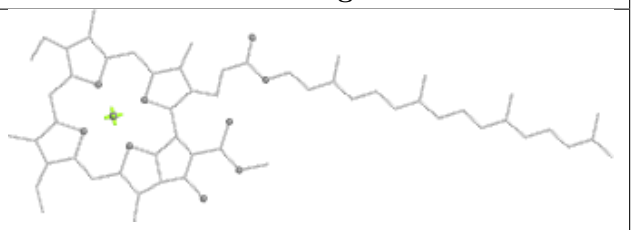
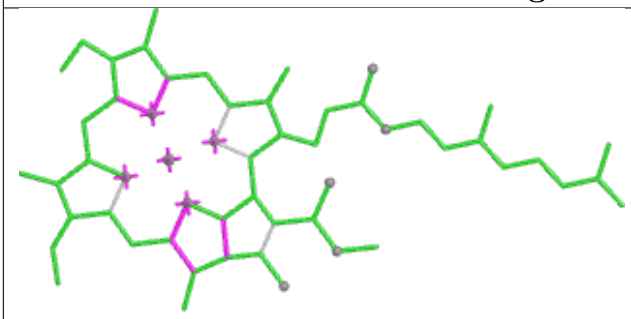


Rings

Ligand CLA 7 309



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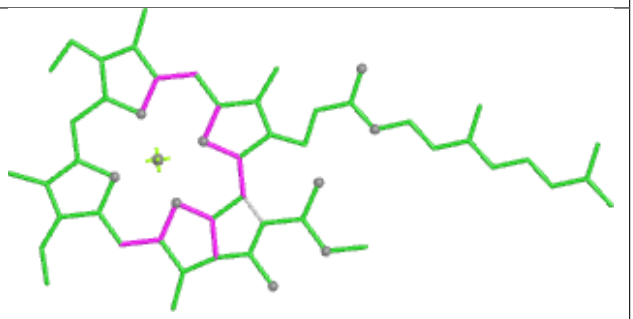
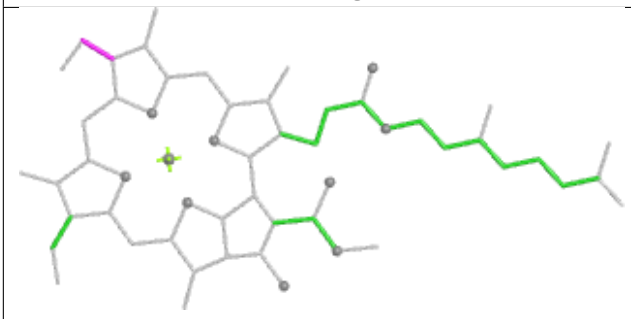


Bond angles



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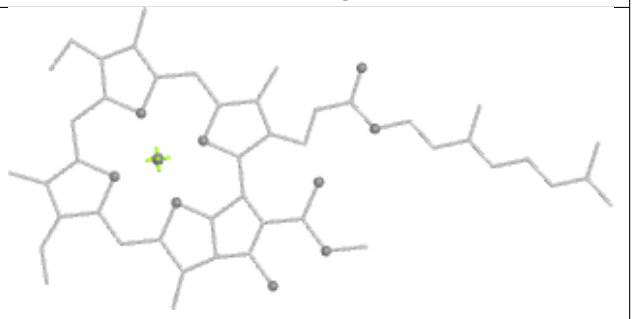
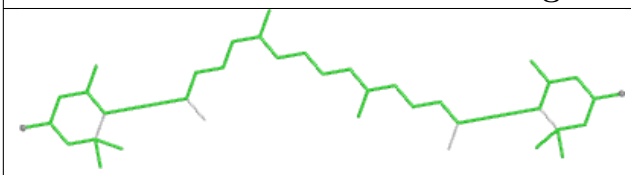


Rings

Ligand II0 3 318



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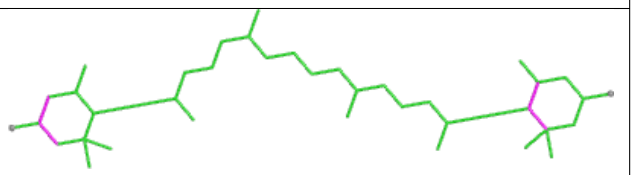

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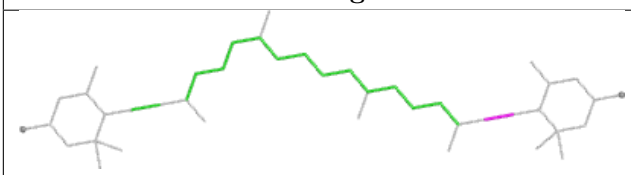

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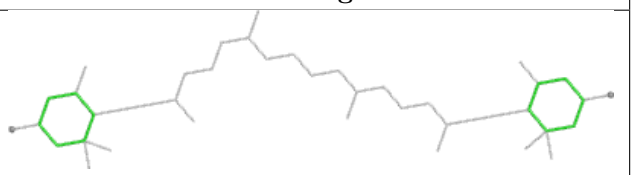
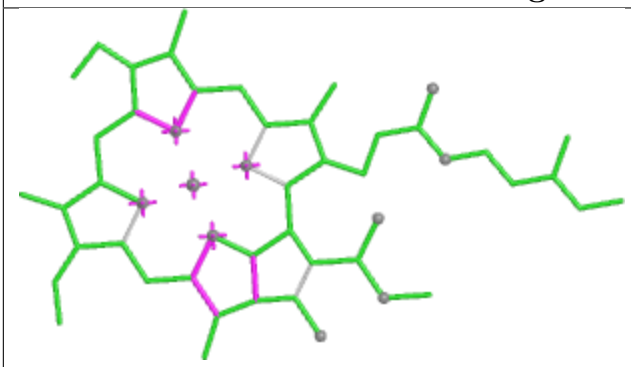
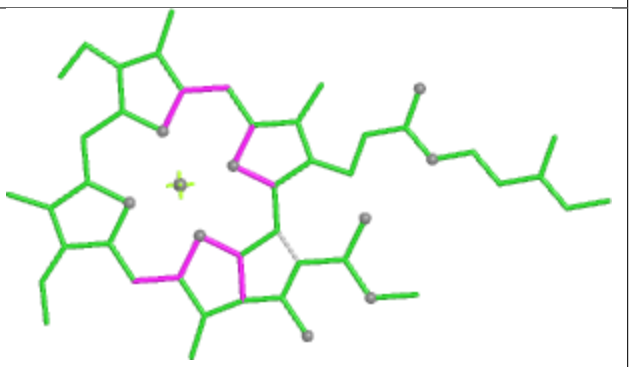
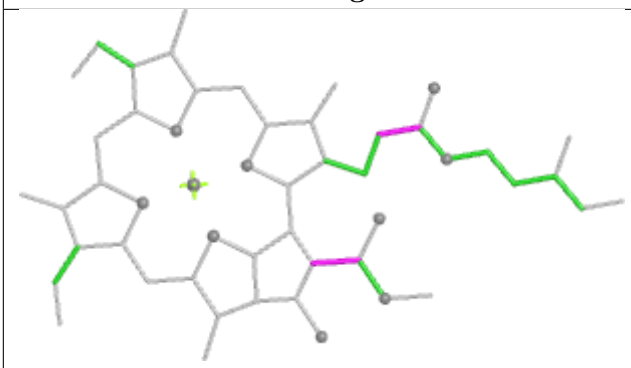
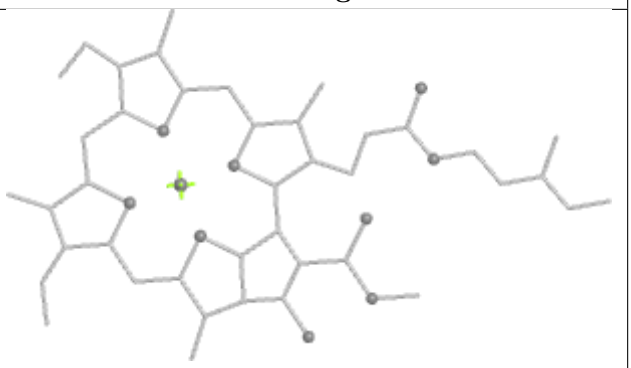


Rings

Ligand CLA 7 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

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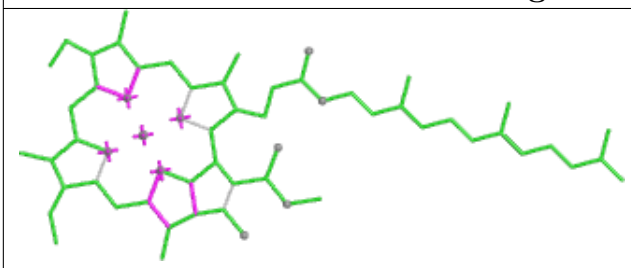
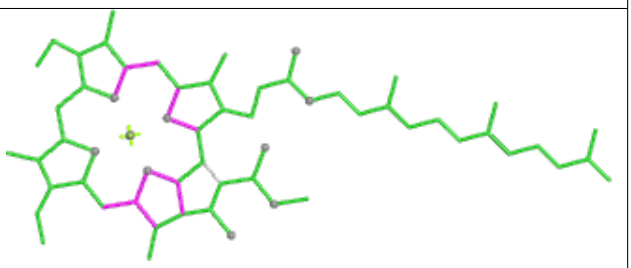
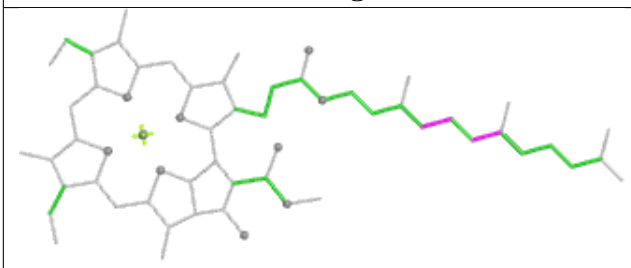
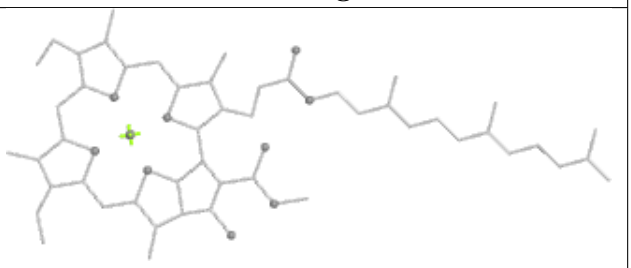
 Bond lengths	 Bond angles
 Torsions	 Rings

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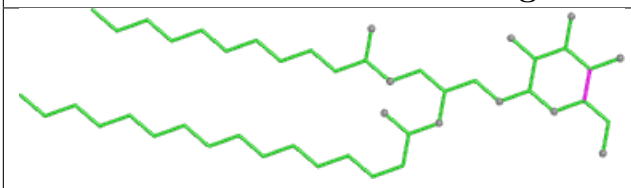
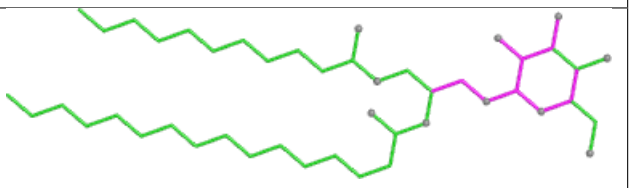
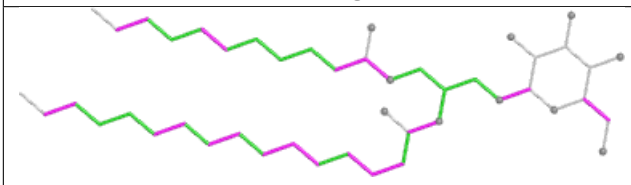
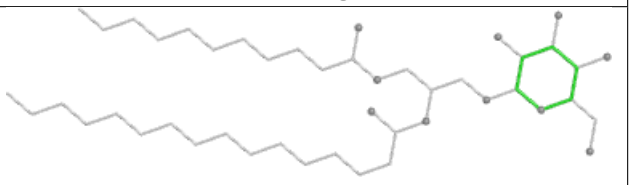
 Bond lengths	 Bond angles
 Torsions	 Rings

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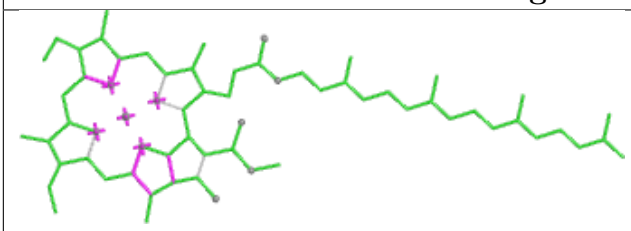
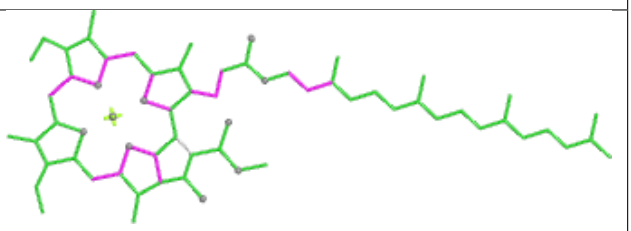
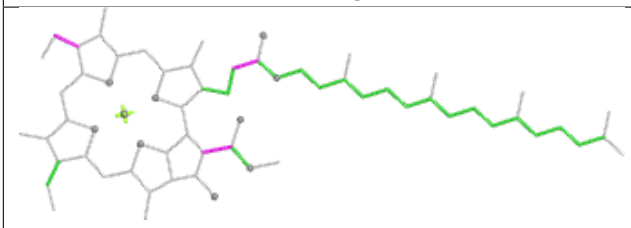
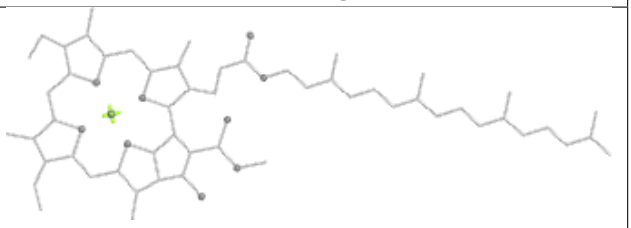
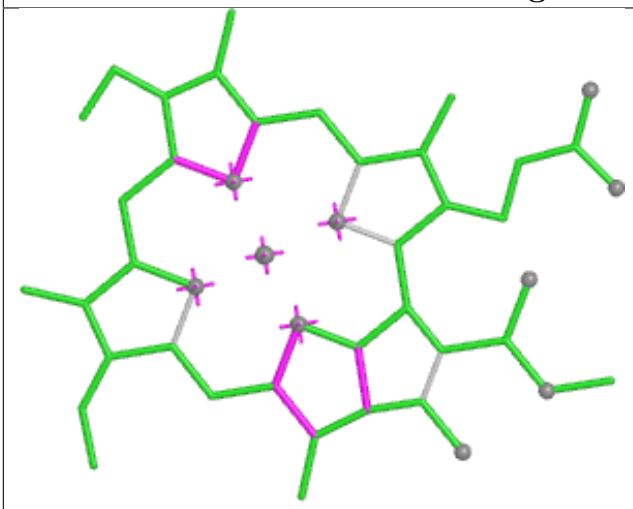
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 301



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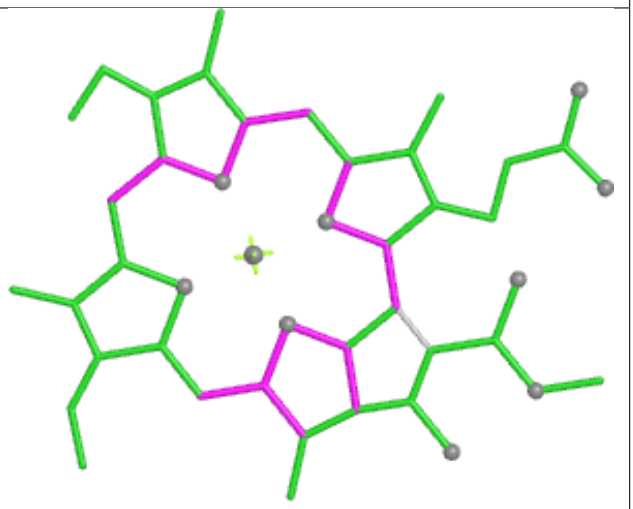
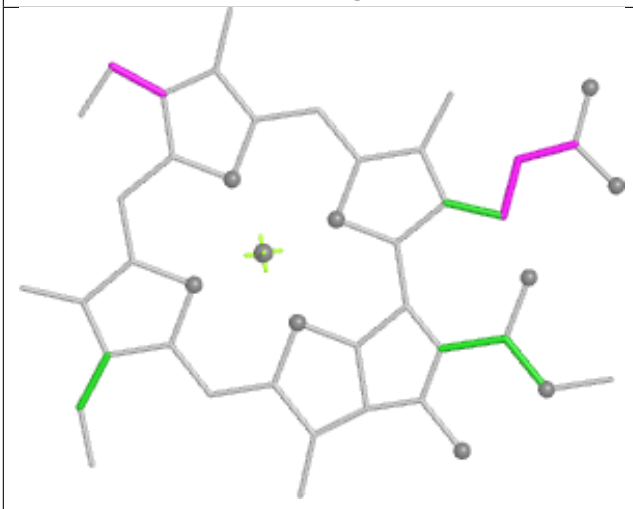


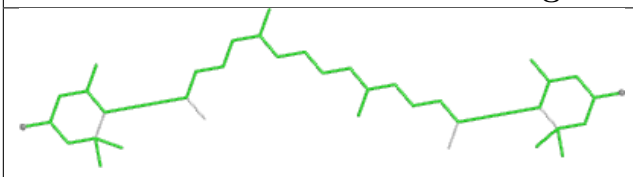
Bond angles



Torsions

Rings

Ligand II0 2 312



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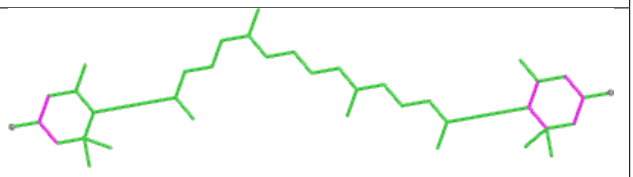

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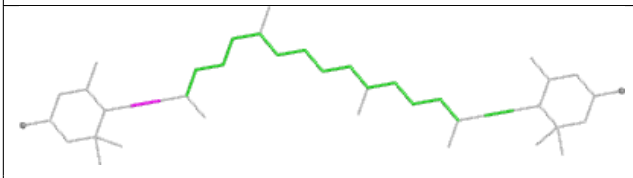

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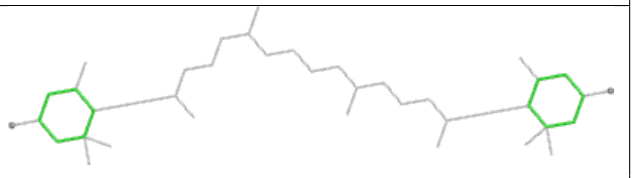
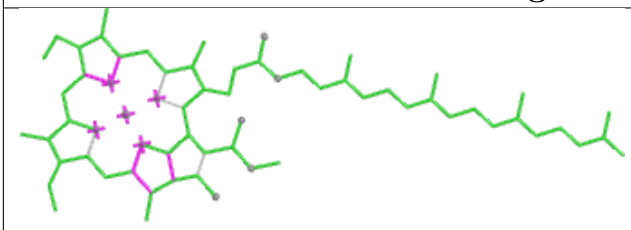
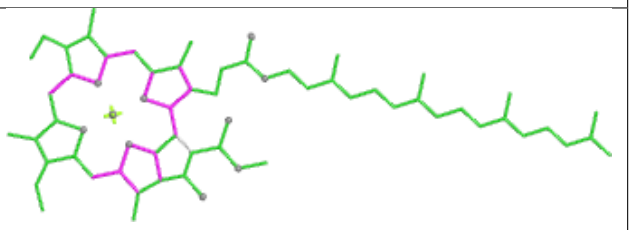


Rings

Ligand CLA 1 307	
	
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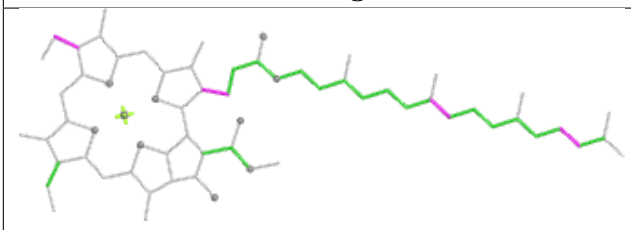	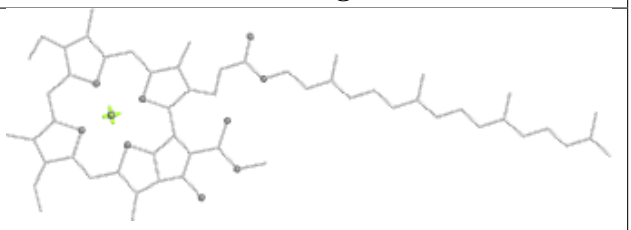
Torsions	Rings

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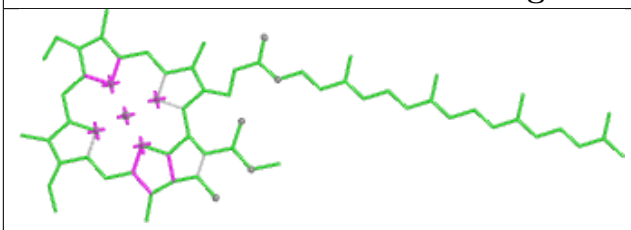
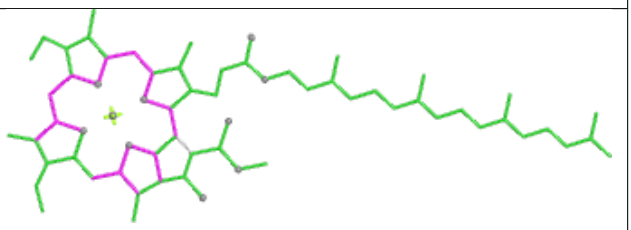
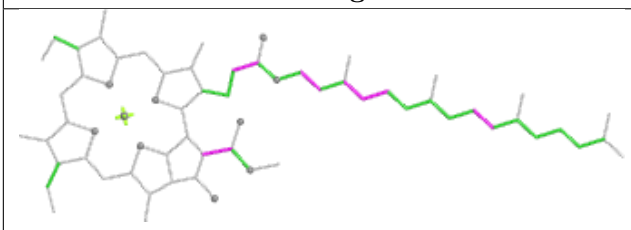
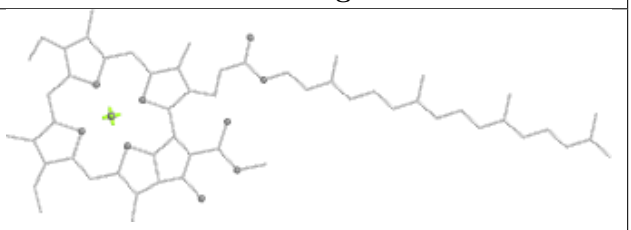
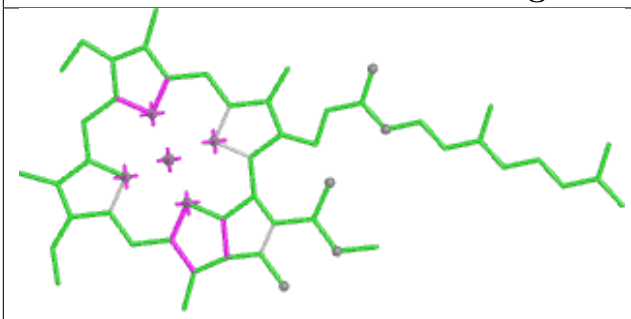
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 302



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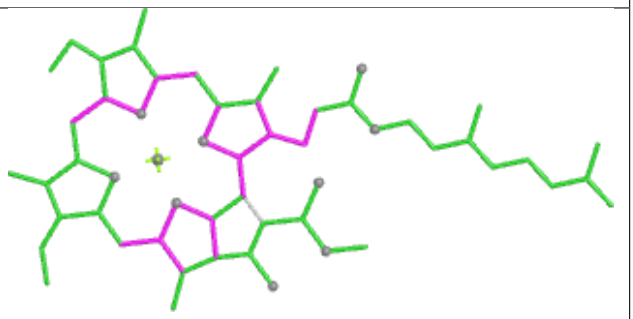
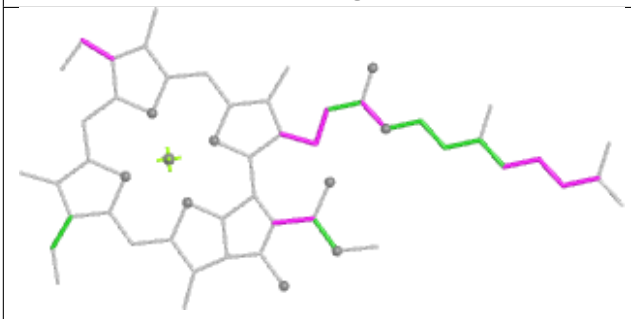
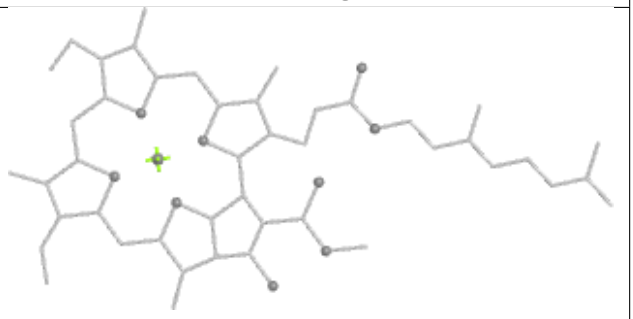


Bond angles

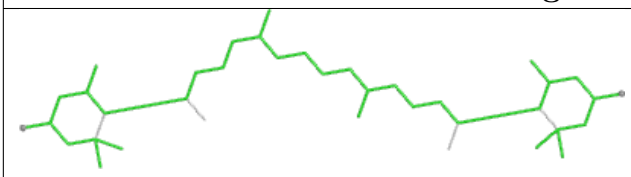


Torsions



Rings

Ligand II0 6 317



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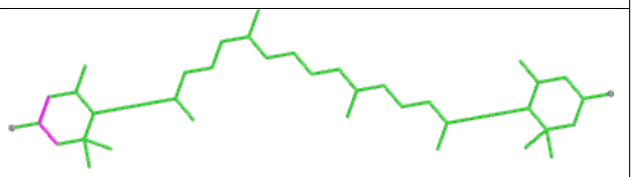

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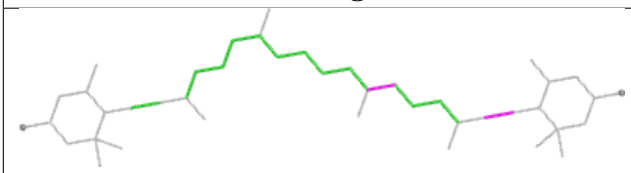

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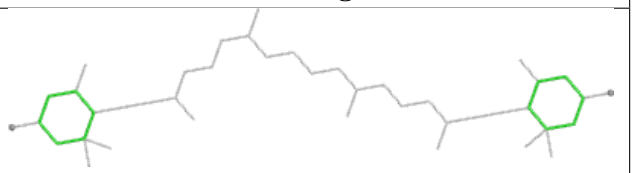
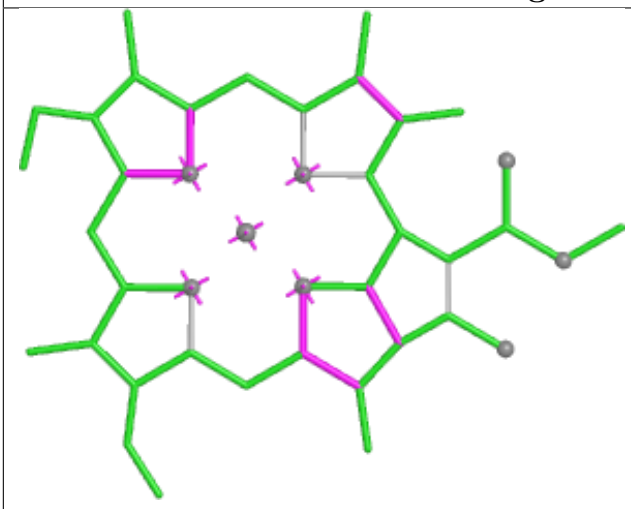


Rings

Ligand CLA 3 313



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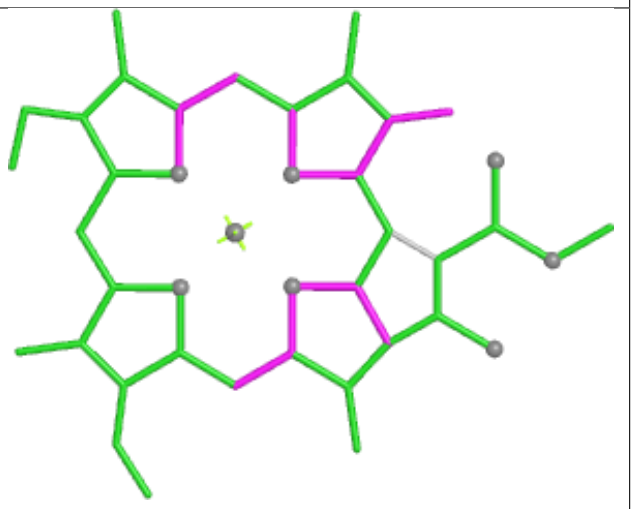

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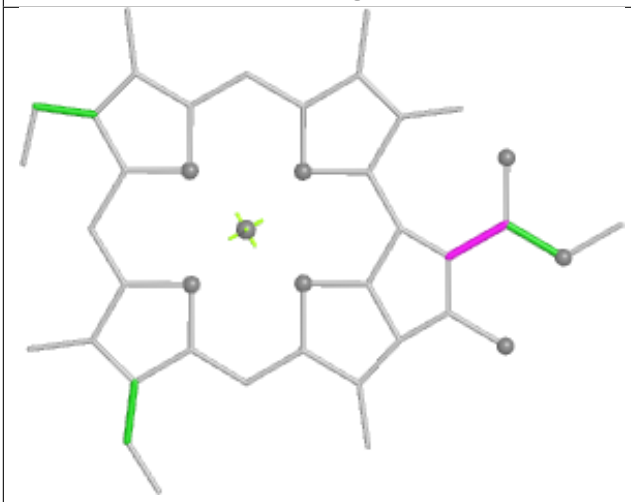

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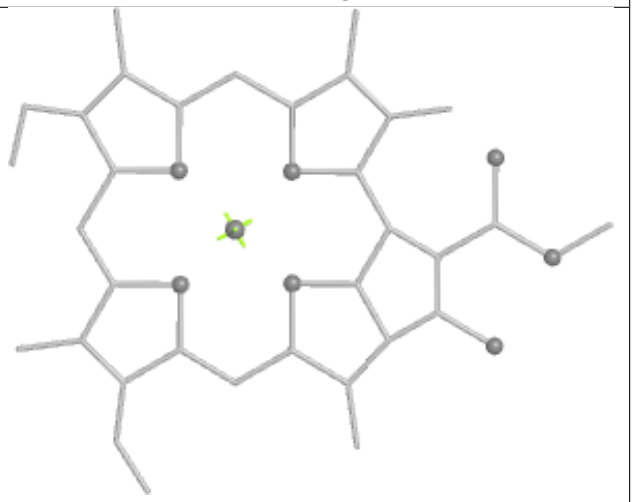
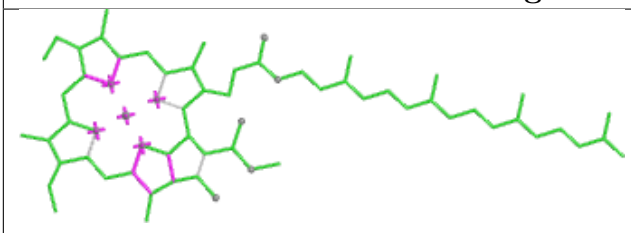


Rings

Ligand CLA B 616



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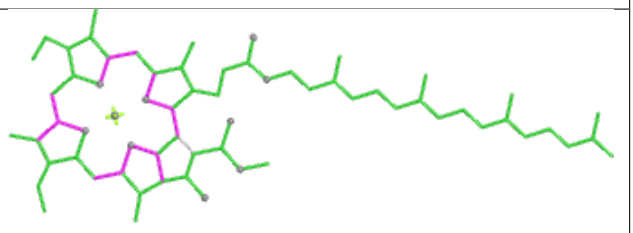

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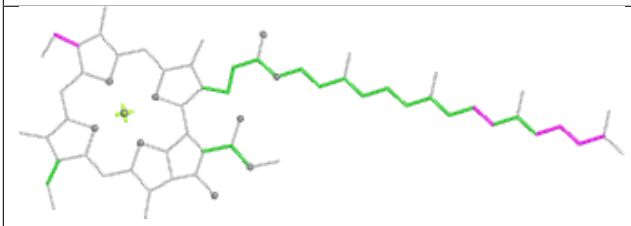

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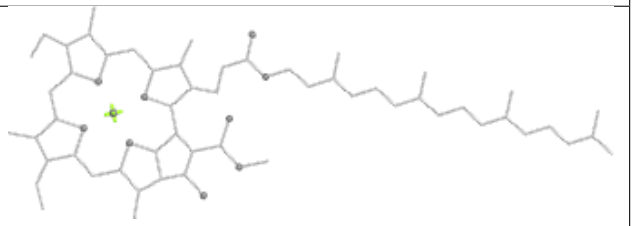
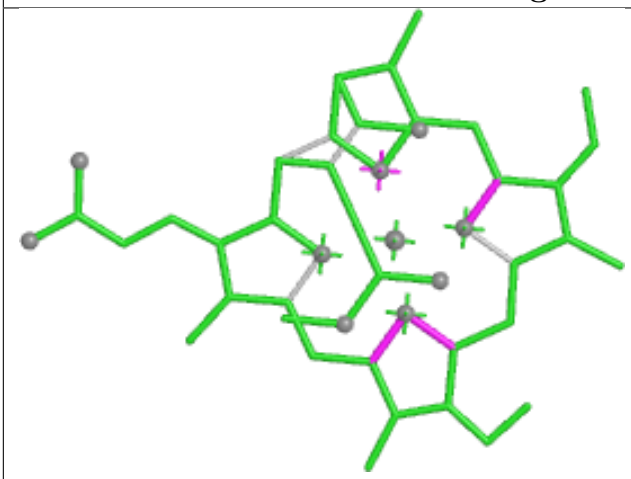


Rings

Ligand KC2 6 311



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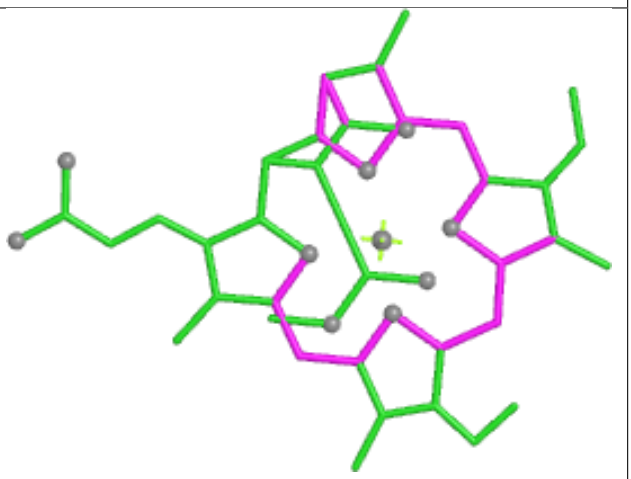

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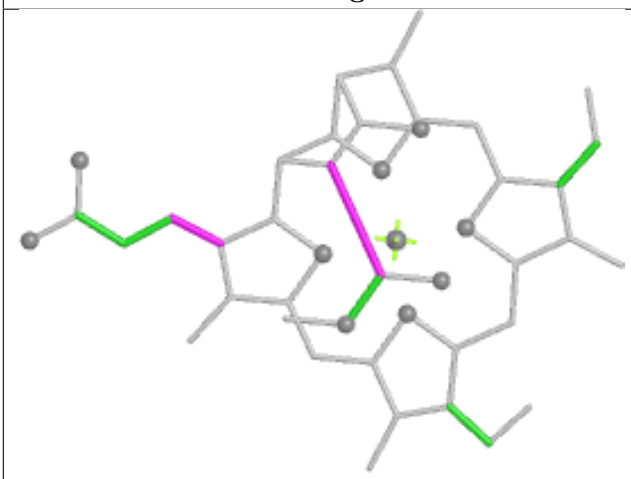

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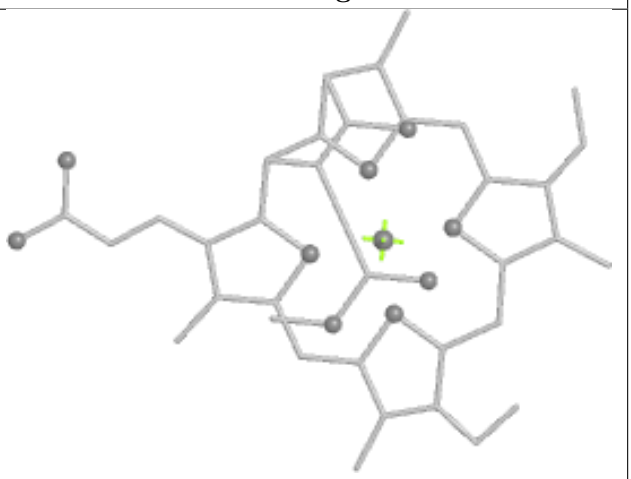
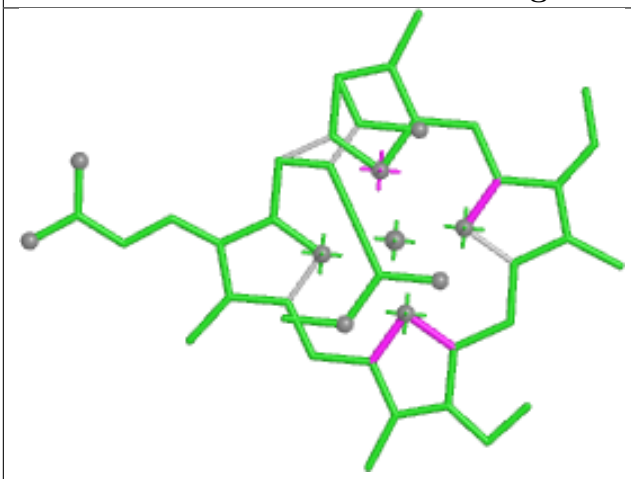


Rings

Ligand KC2 1 310



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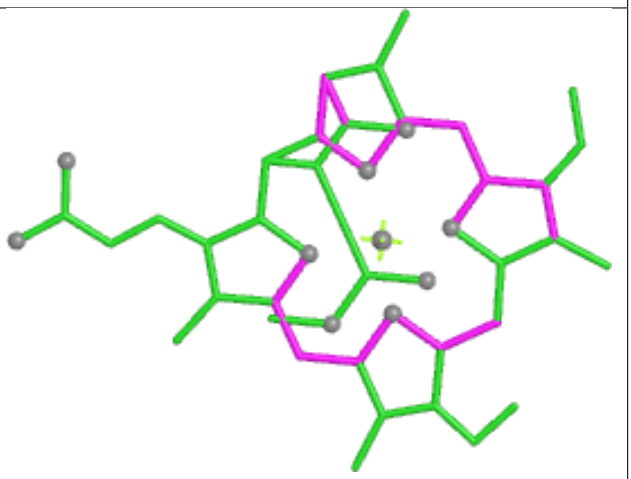
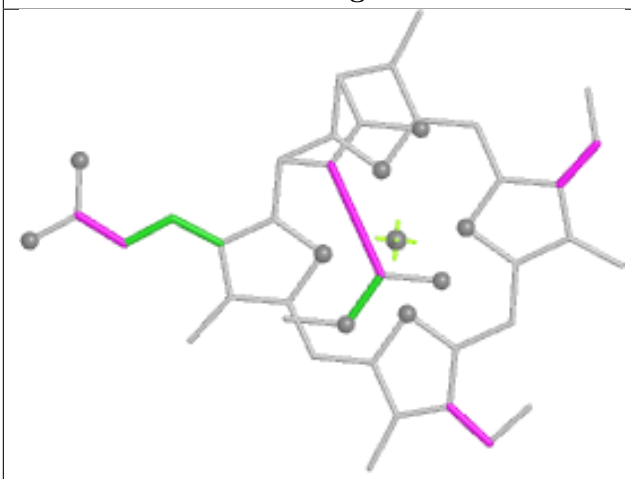


Bond angles



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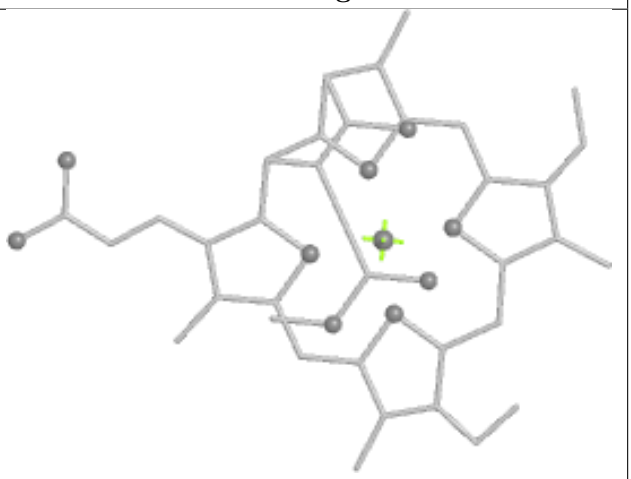
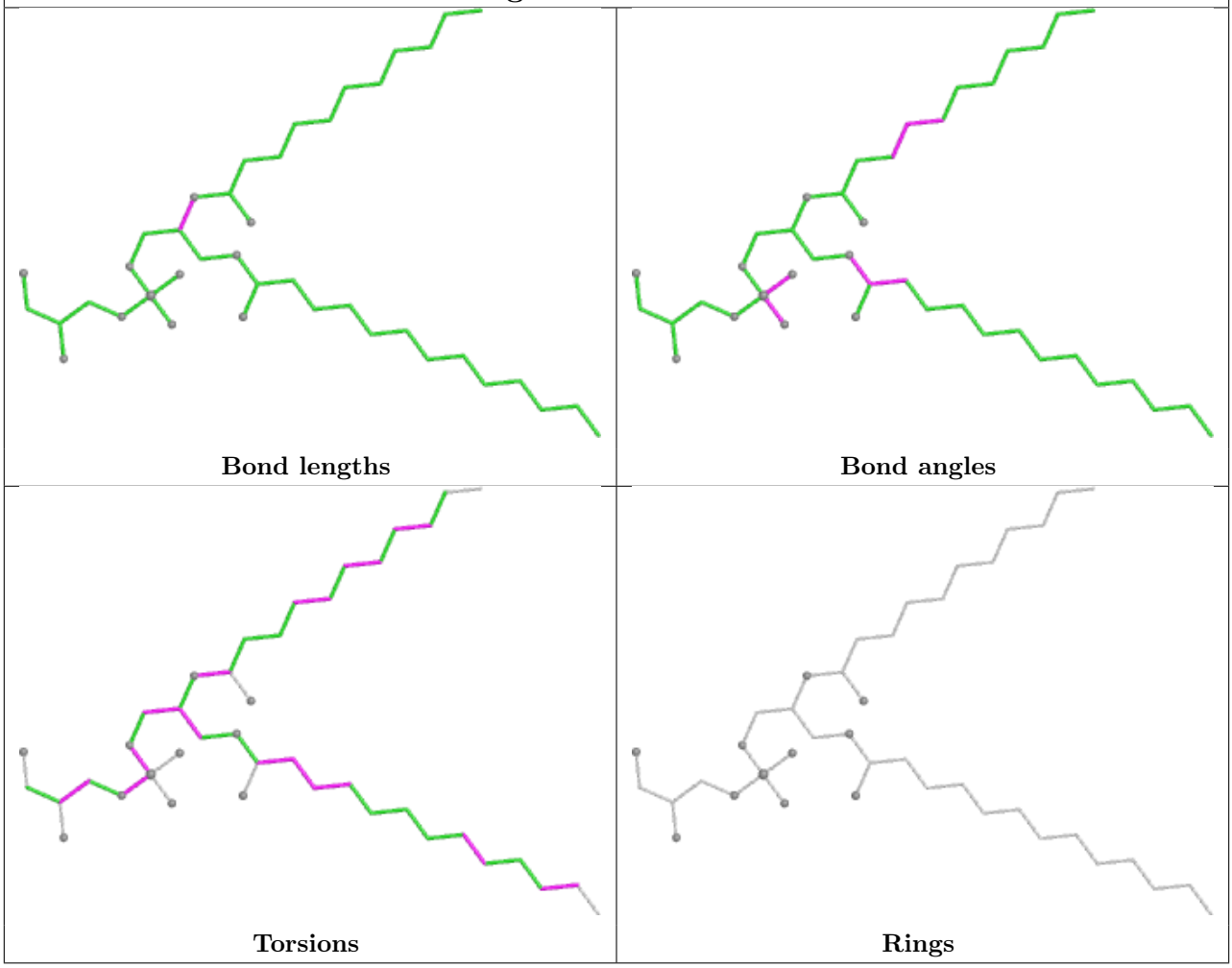
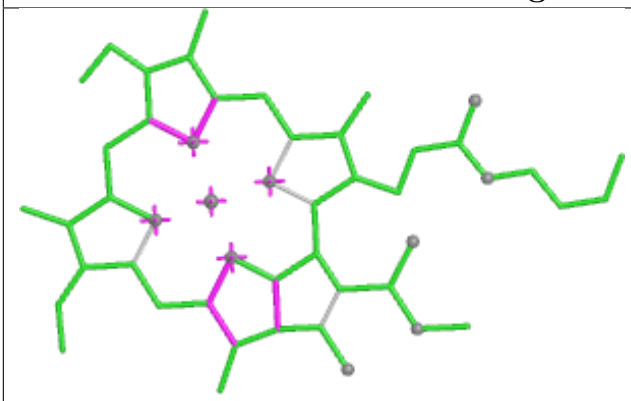


Rings

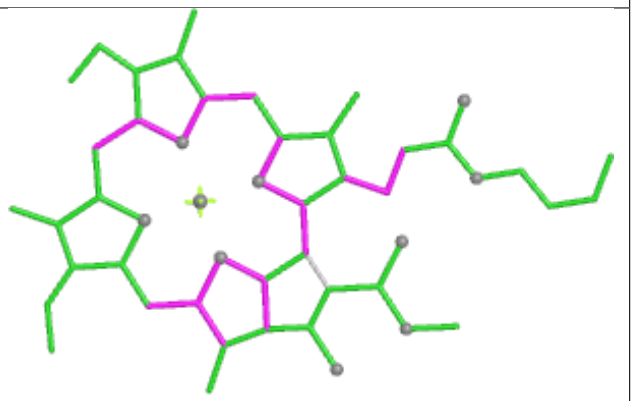
Ligand LHG 9 302



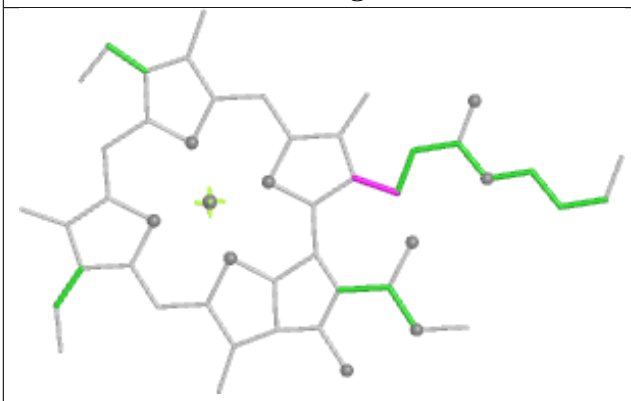
Ligand CLA 9 308



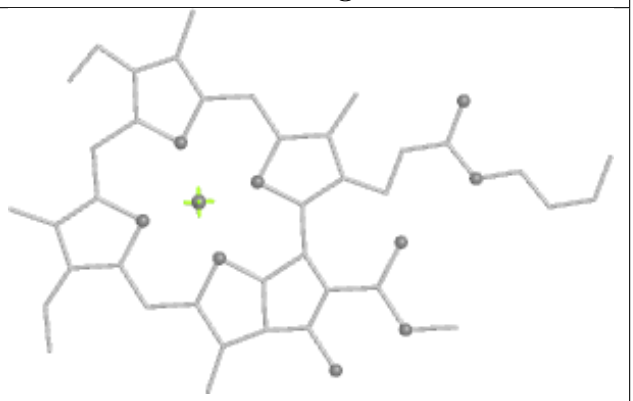
Bond lengths



Bond angles

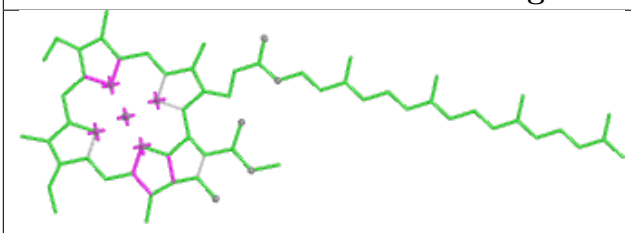


Torsions

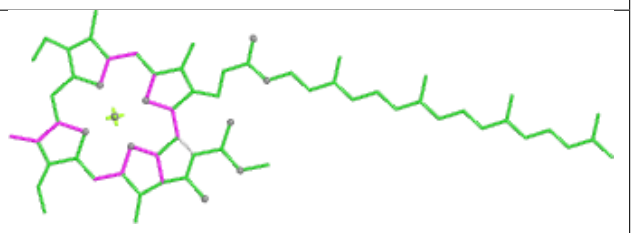


Rings

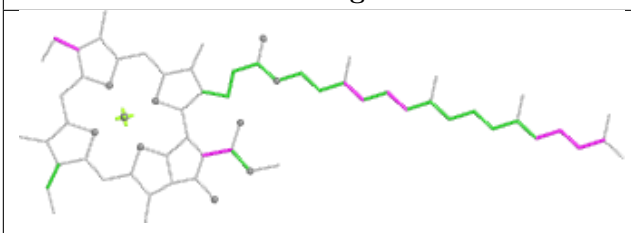
Ligand CLA b 610



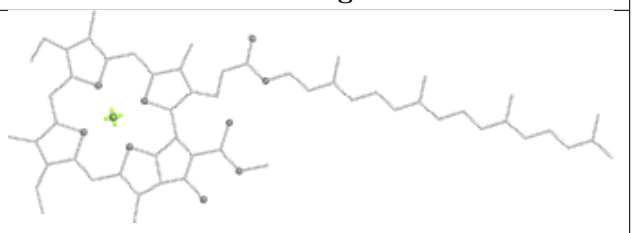
Bond lengths



Bond angles

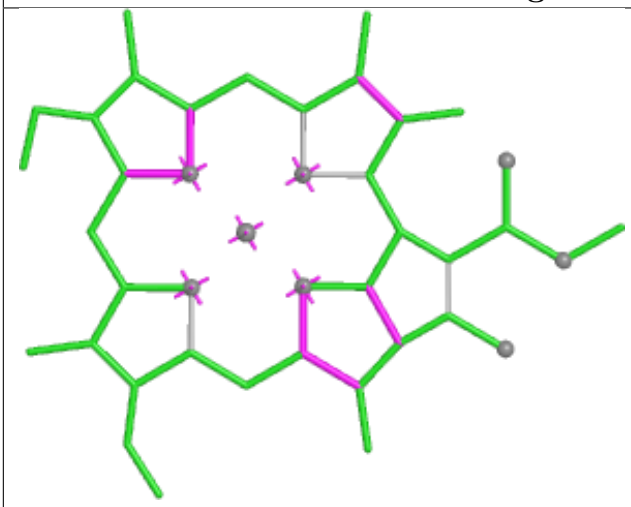


Torsions

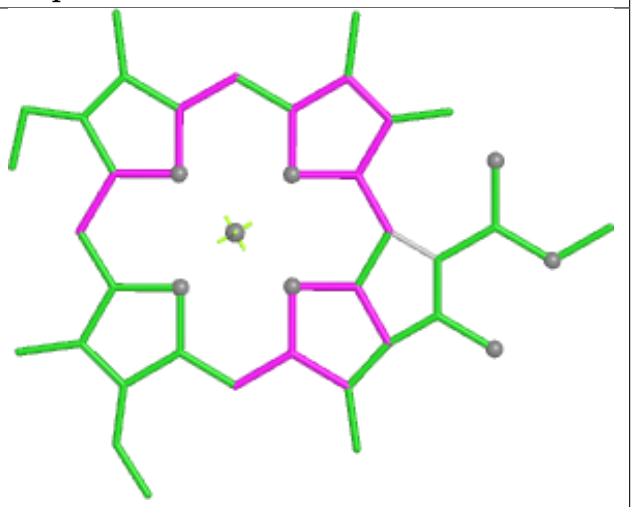


Rings

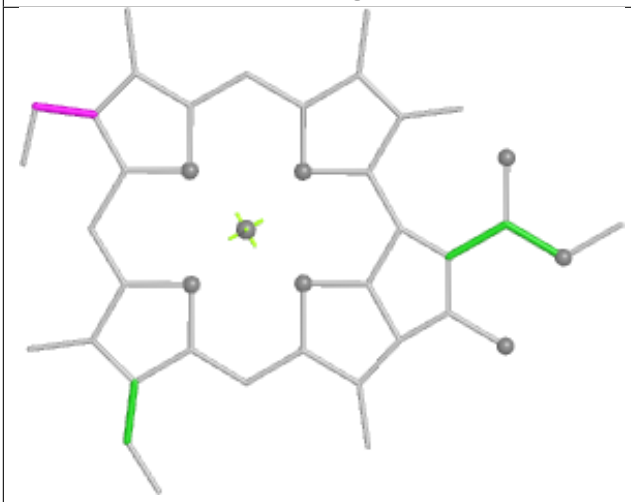
Ligand CLA p 302



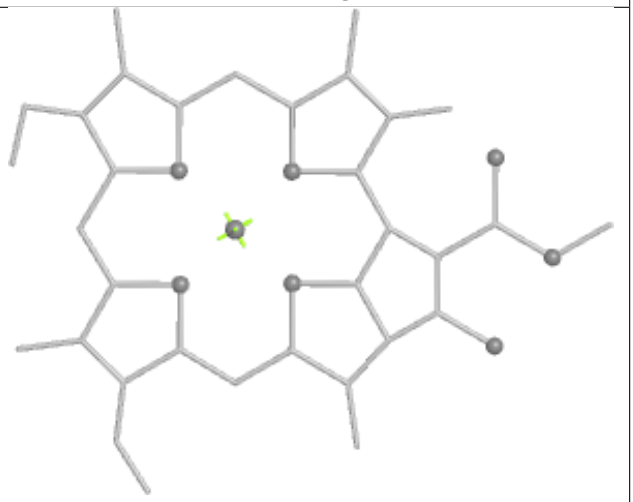
Bond lengths



Bond angles

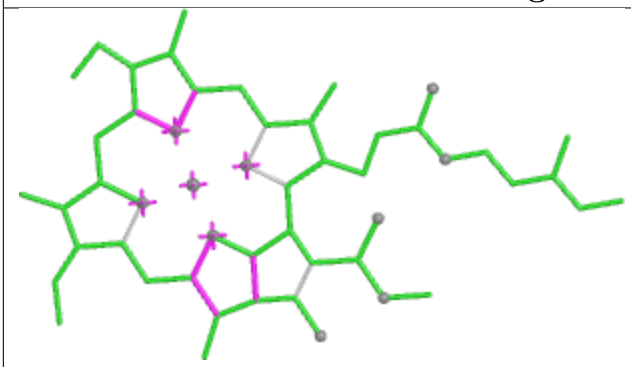


Torsions

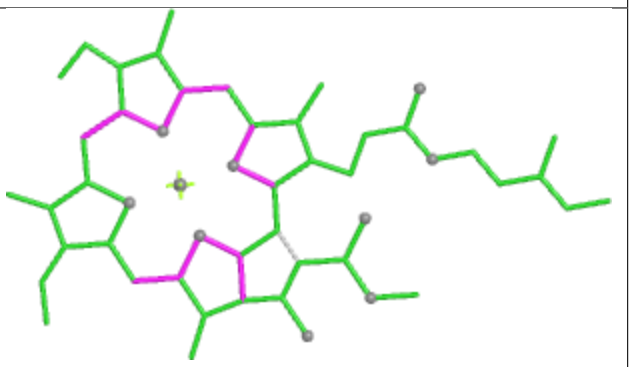


Rings

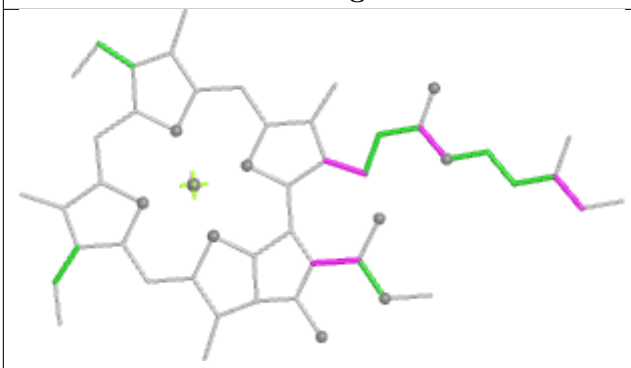
Ligand CLA 7 308



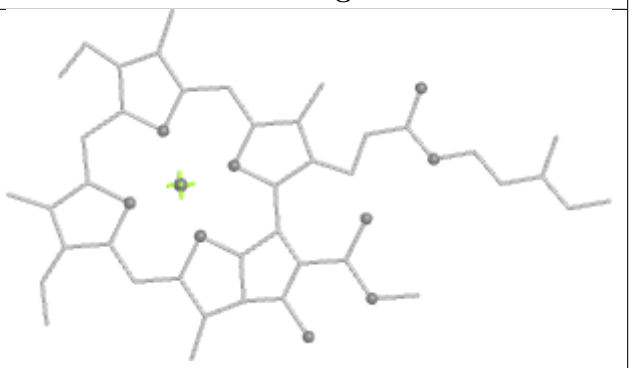
Bond lengths



Bond angles

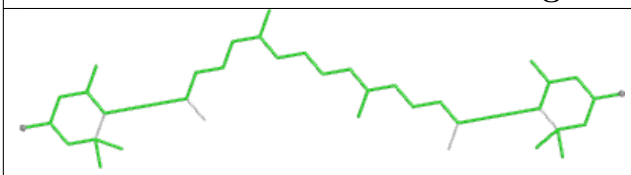


Torsions

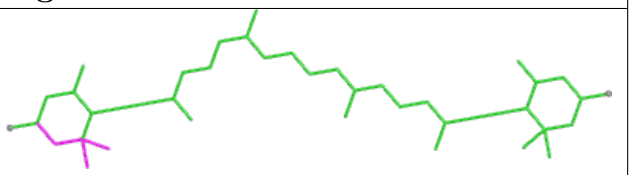


Rings

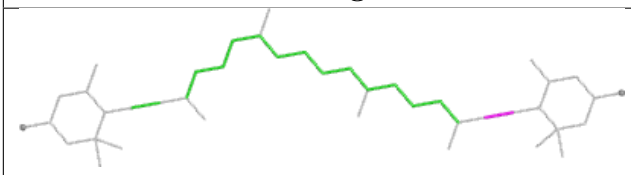
Ligand II0 g 312



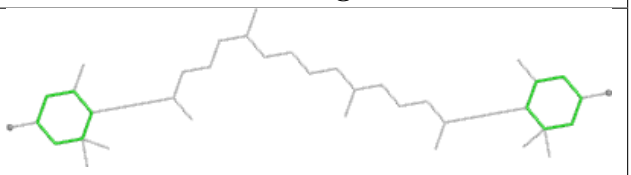
Bond lengths



Bond angles

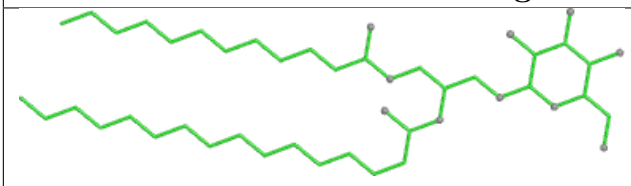


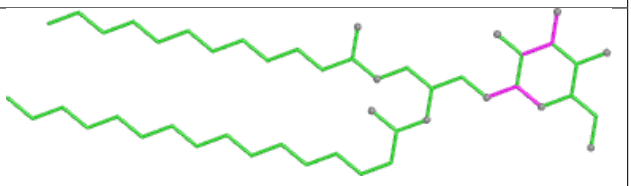
Torsions

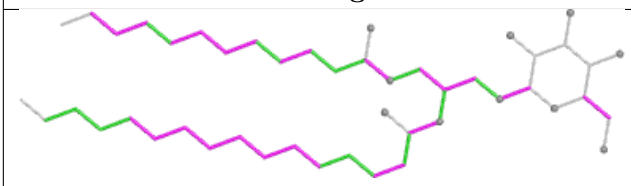


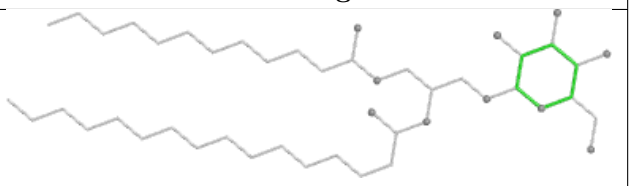
Rings

Ligand LMG W 101

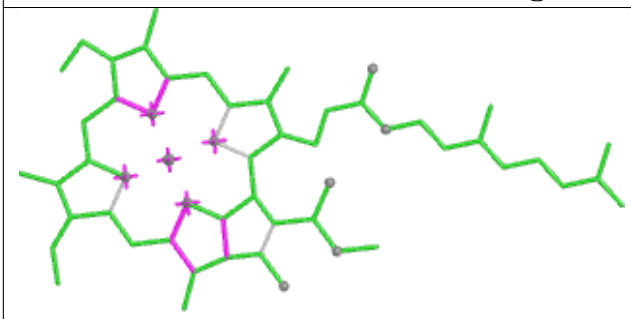

Bond lengths

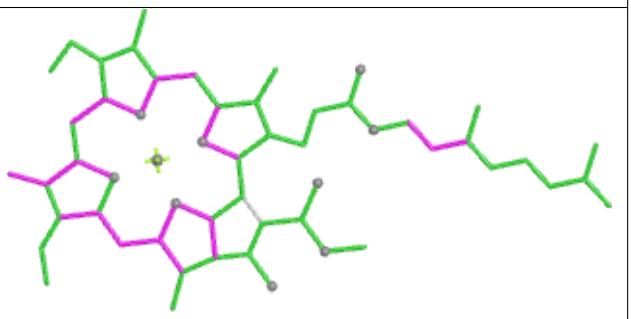

Bond angles

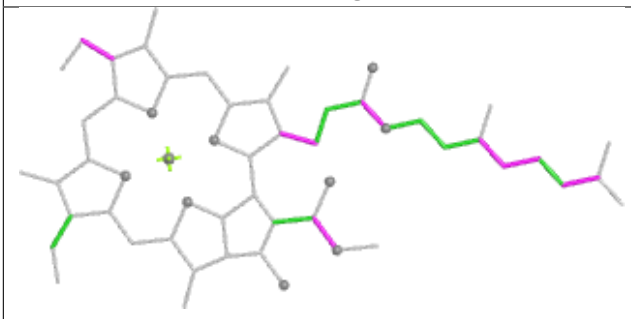

Torsions

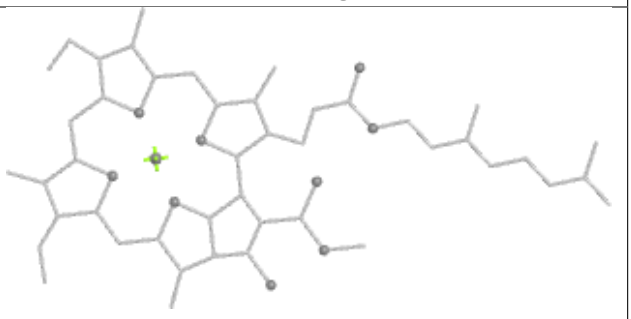

Rings

Ligand CLA 4 307

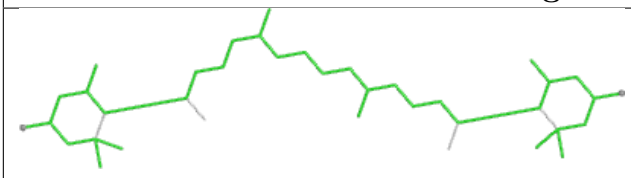

Bond lengths

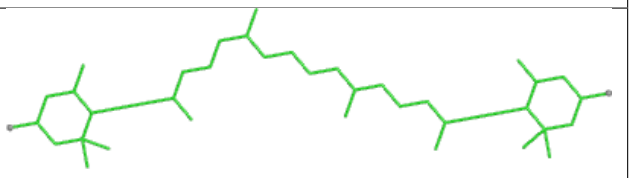

Bond angles

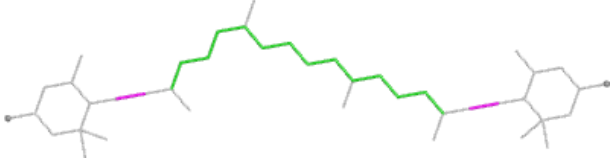

Torsions

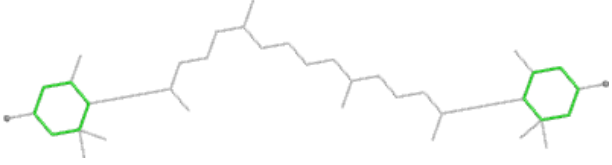

Rings

Ligand II0 7 316


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.

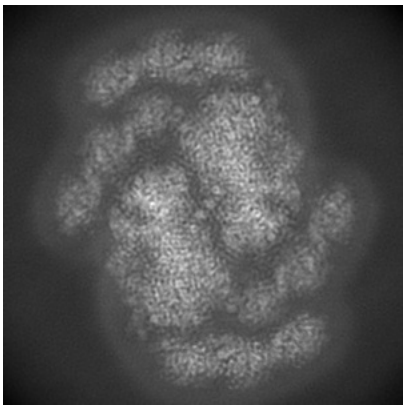
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38596. These allow visual inspection of the internal detail of the map and identification of artifacts.

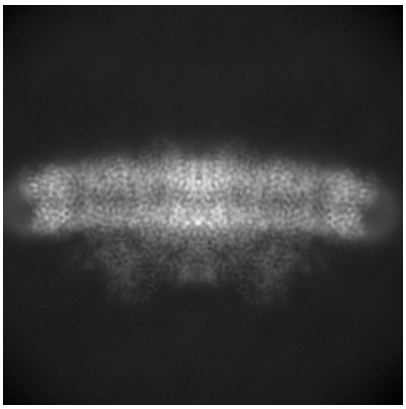
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

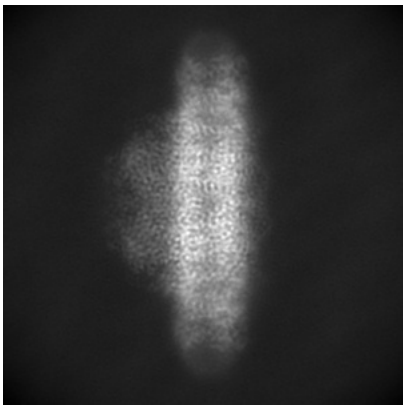
6.1.1 Primary map



X

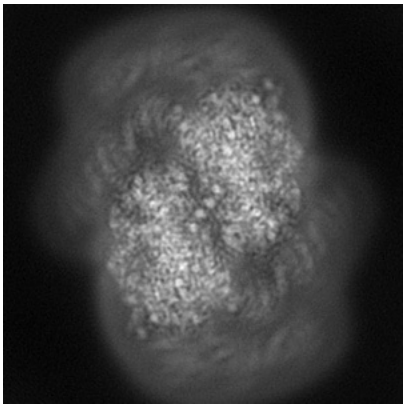


Y

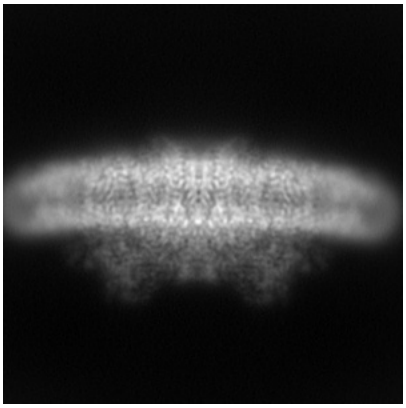


Z

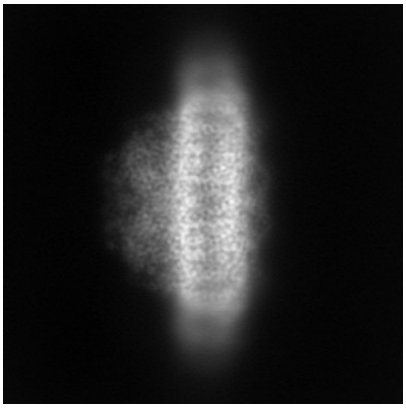
6.1.2 Raw map



X



Y

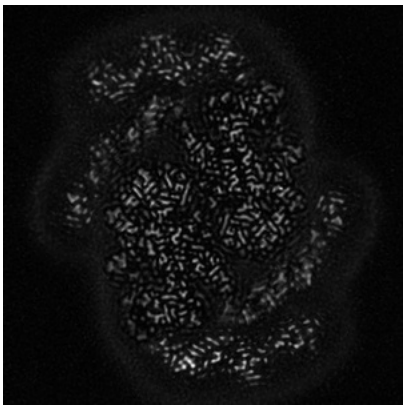


Z

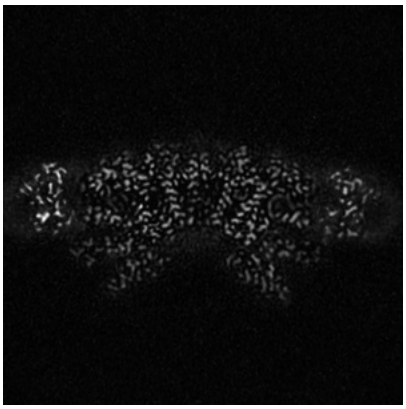
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

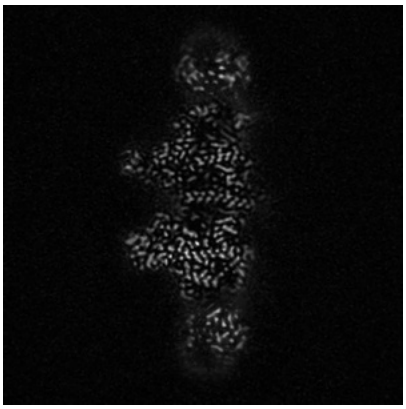
6.2.1 Primary map



X Index: 128

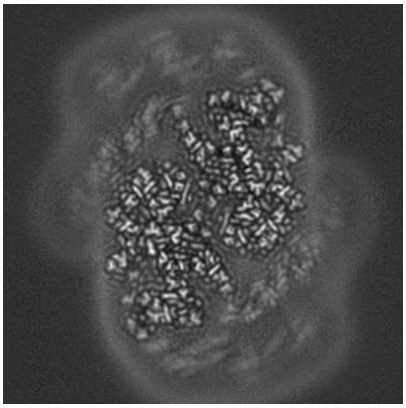


Y Index: 128

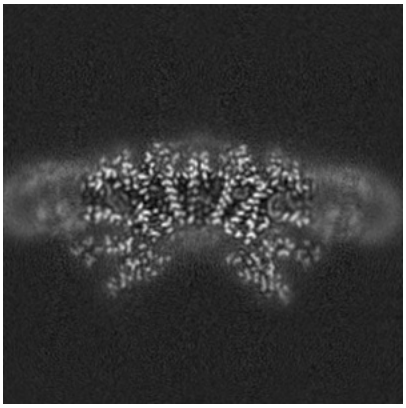


Z Index: 128

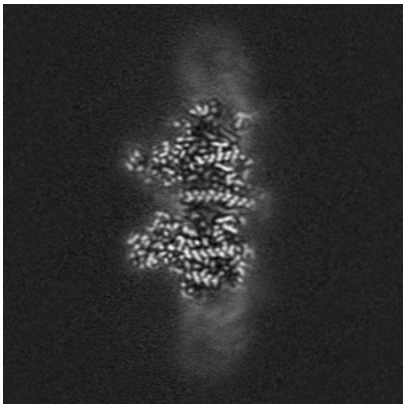
6.2.2 Raw map



X Index: 128



Y Index: 128

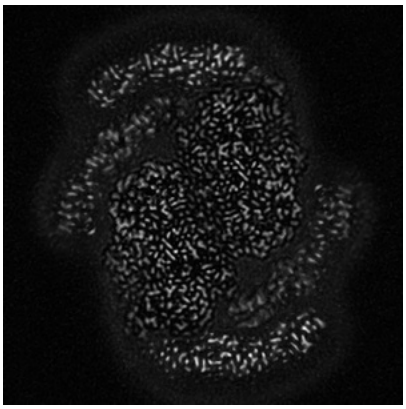


Z Index: 128

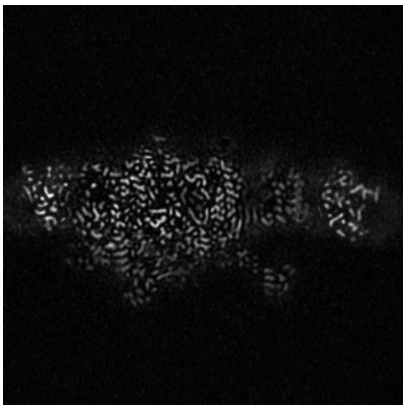
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

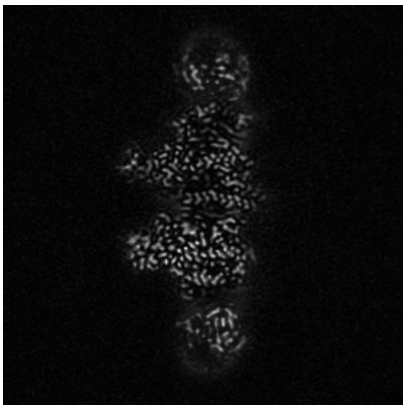
6.3.1 Primary map



X Index: 120

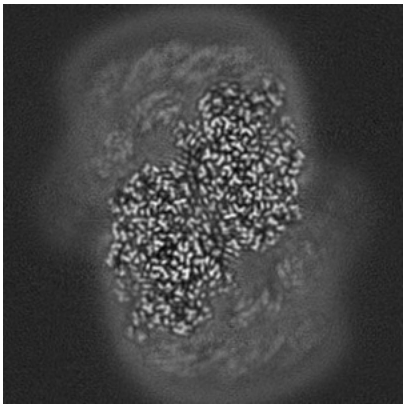


Y Index: 113

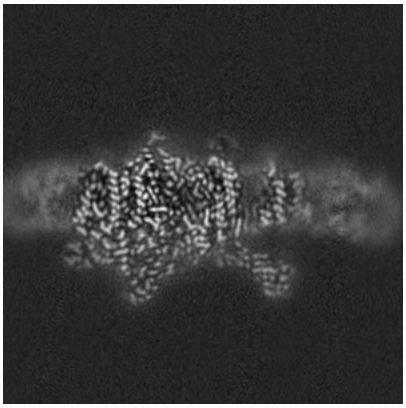


Z Index: 129

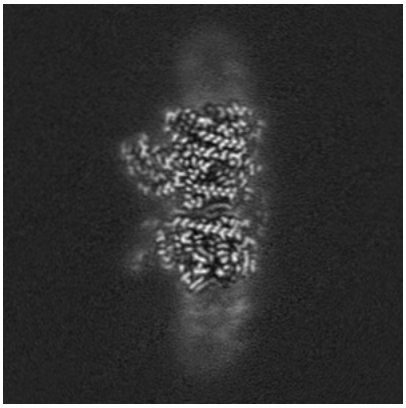
6.3.2 Raw map



X Index: 117



Y Index: 114

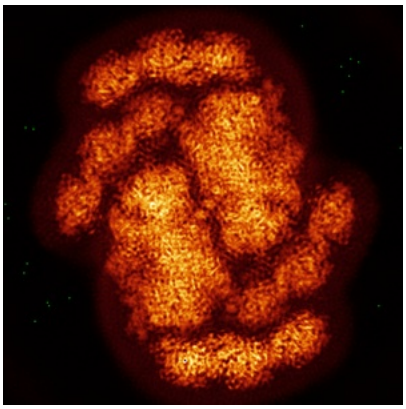


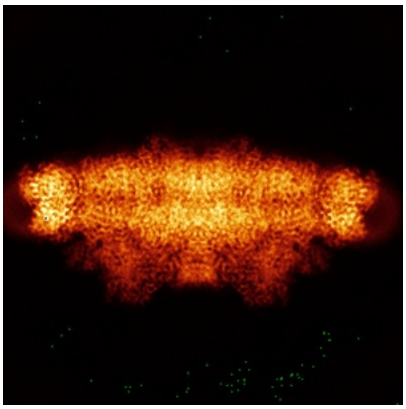
Z Index: 137

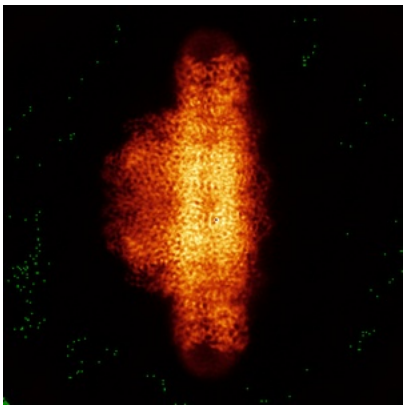
The images above show the largest variance slices of the map in three orthogonal directions.

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

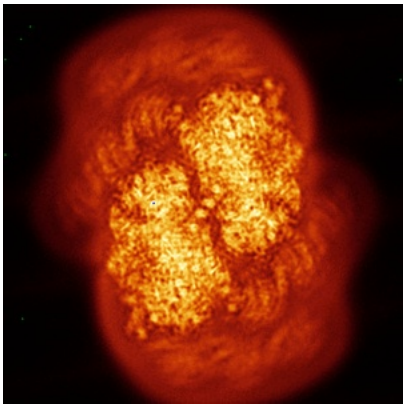
6.4.1 Primary map

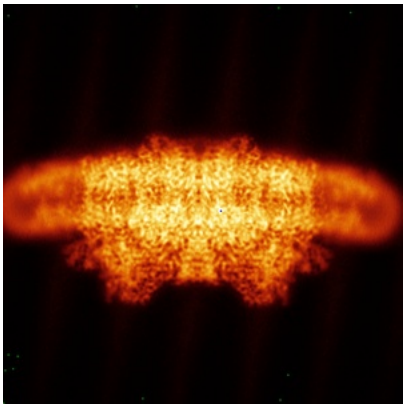

X

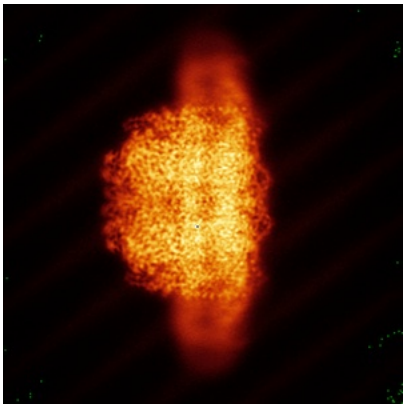

Y


Z

6.4.2 Raw map


X

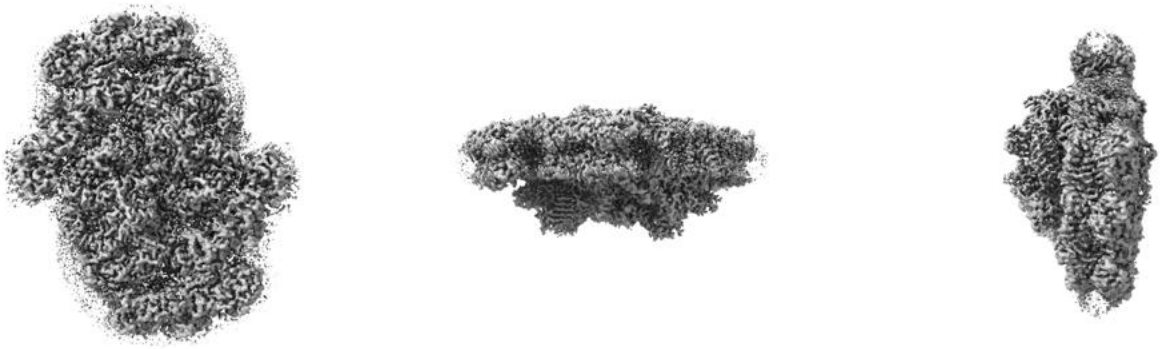

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

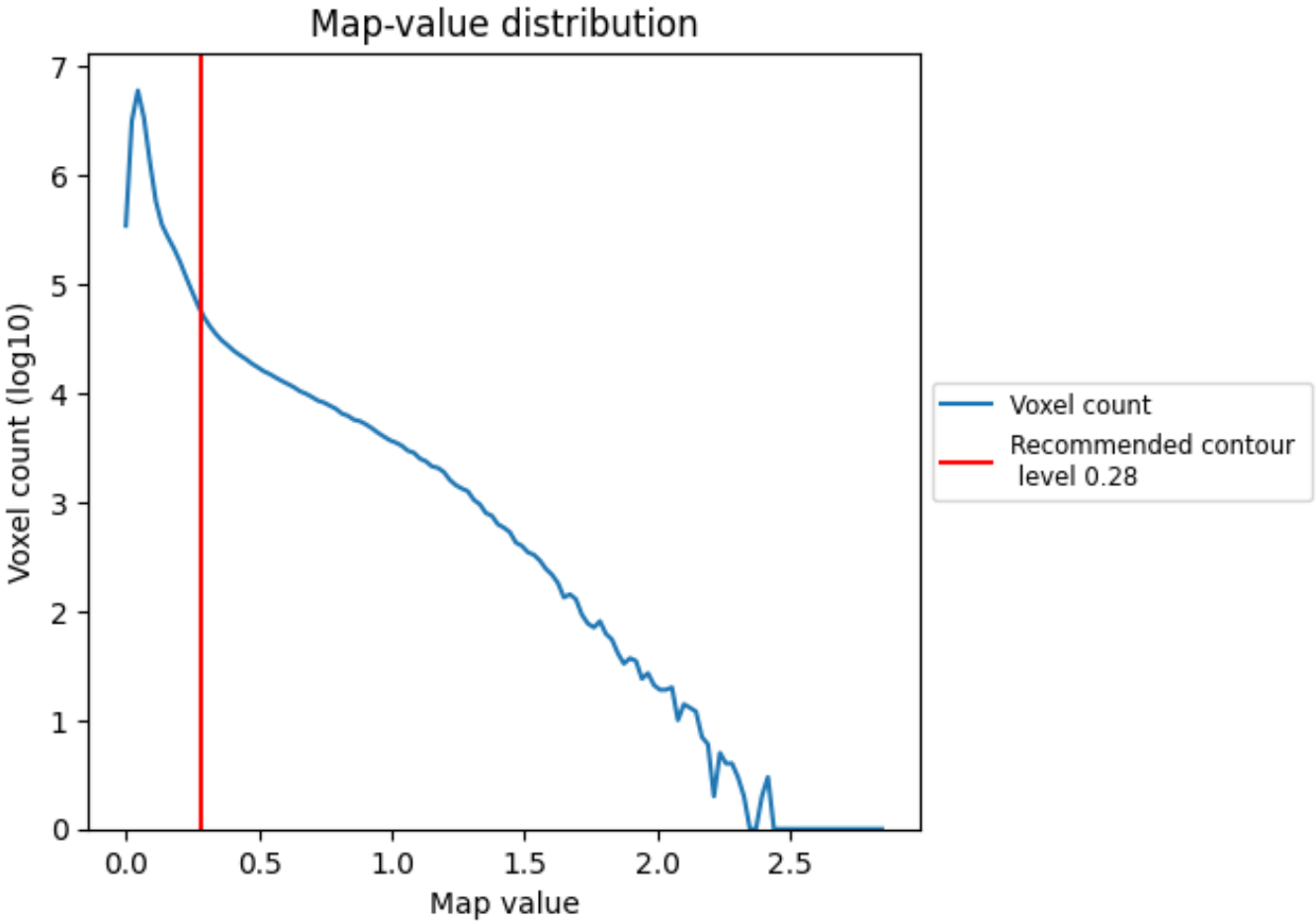
6.6 Mask visualisation (i)

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

7 Map analysis

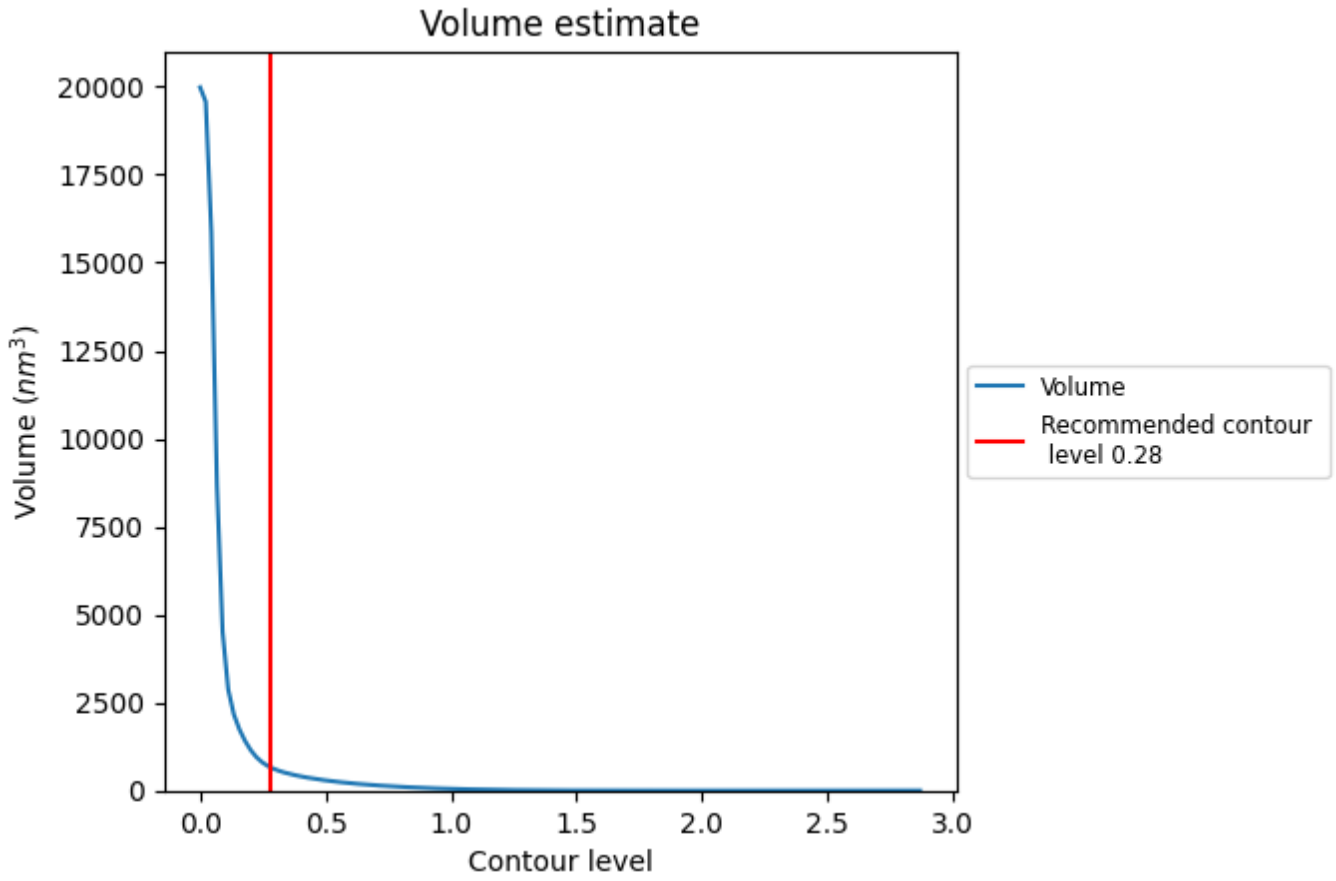
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

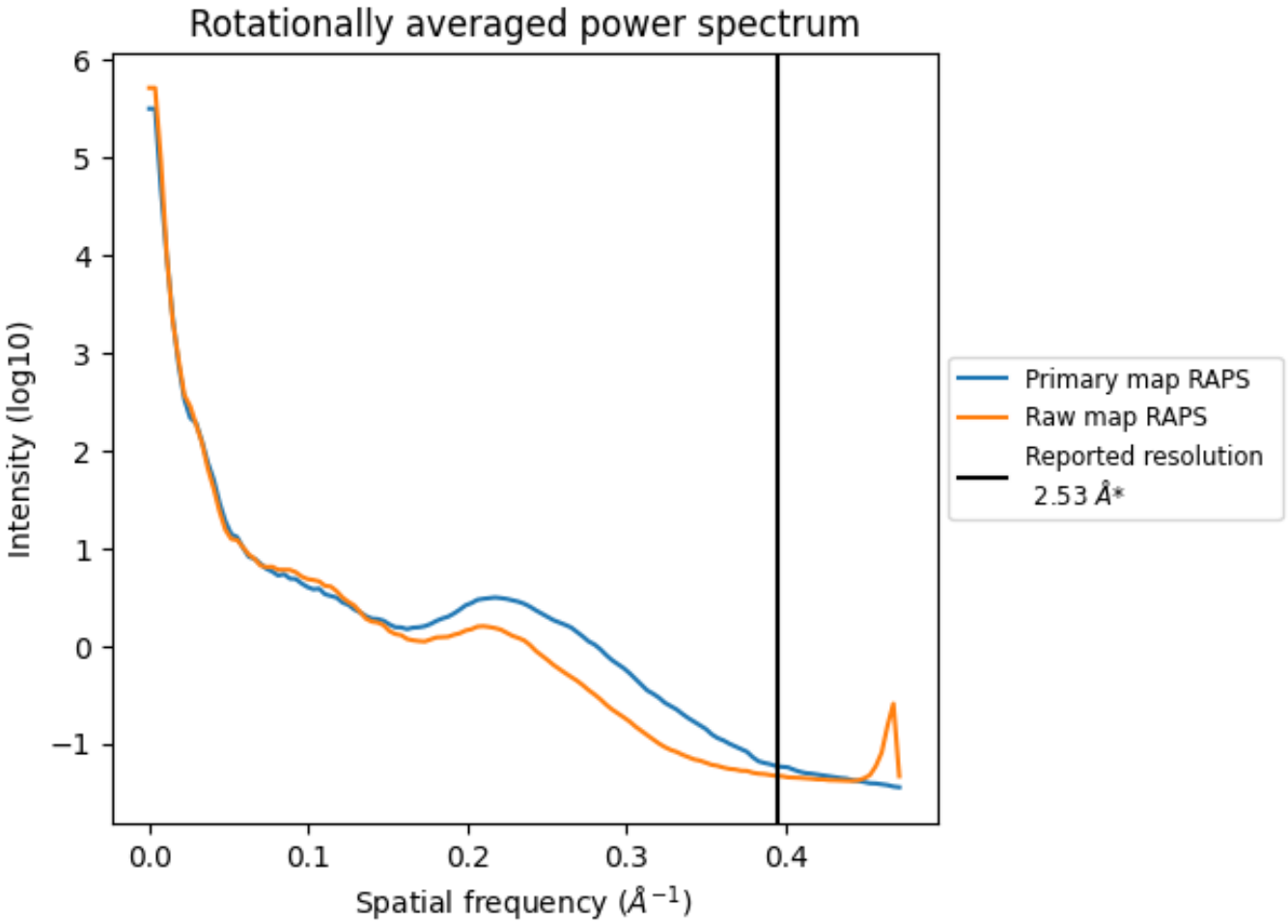
7.2 Volume estimate



The volume at the recommended contour level is 663 nm^3; this corresponds to an approximate mass of 599 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)

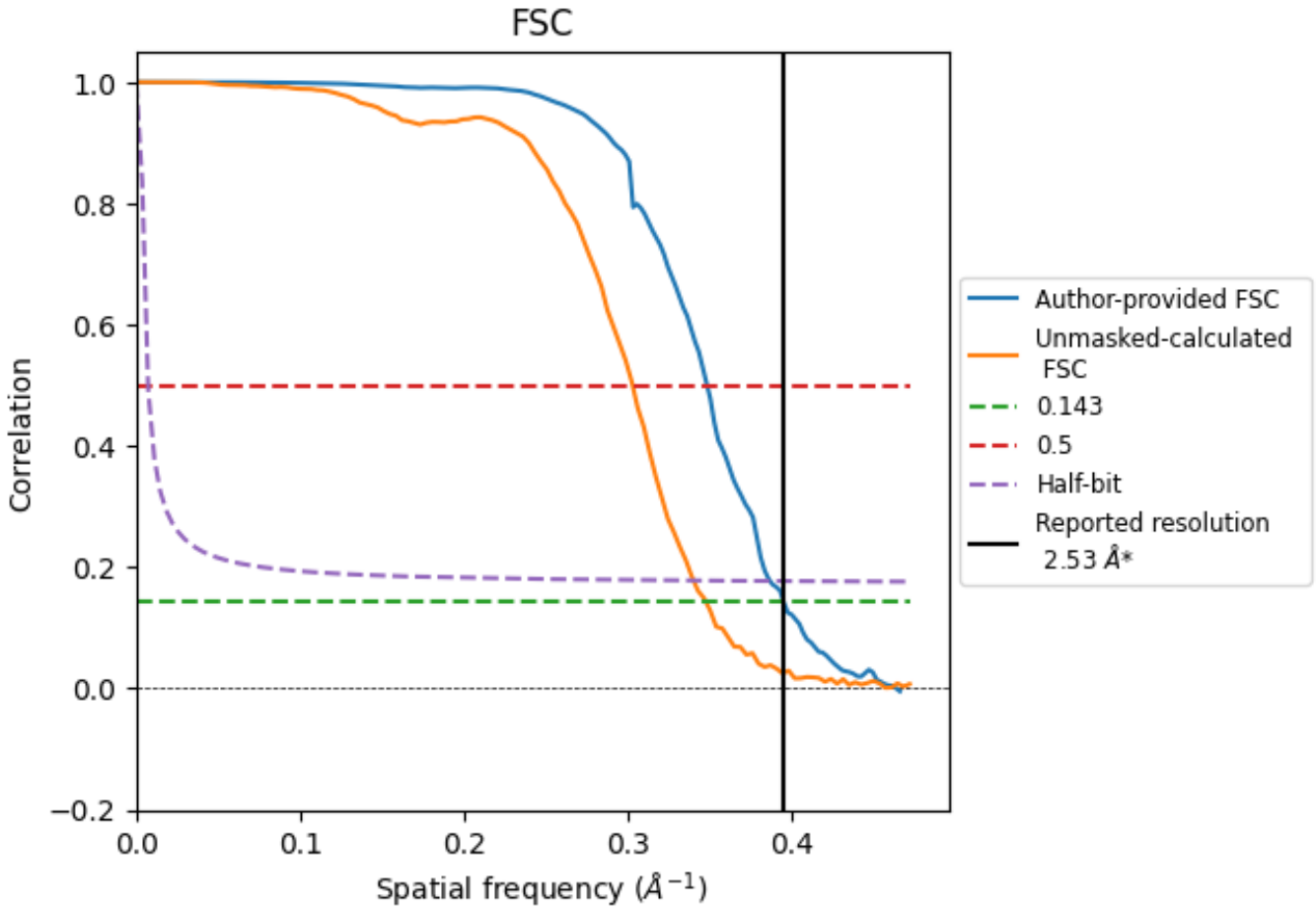


*Reported resolution corresponds to spatial frequency of 0.395 $Å^{-1}$

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 0.395 Å^{-1}

8.2 Resolution estimates (i)

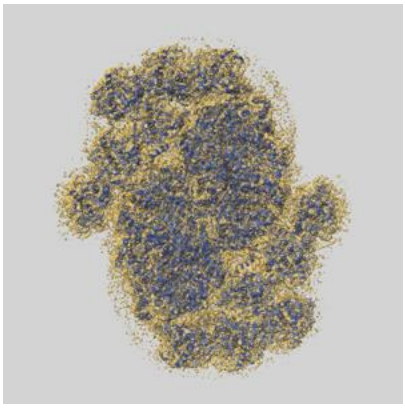
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.53	2.87	2.58
Unmasked-calculated*	2.88	3.30	2.94

*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 2.88 differs from the reported value 2.53 by more than 10 %

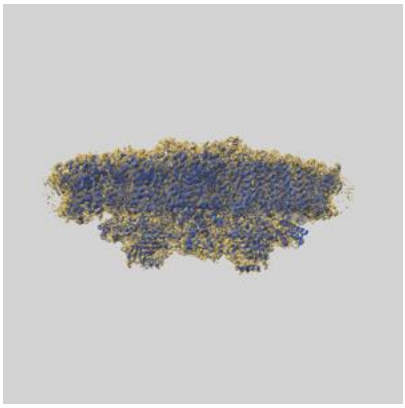
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38596 and PDB model 8XR6. Per-residue inclusion information can be found in section 3 on page 38.

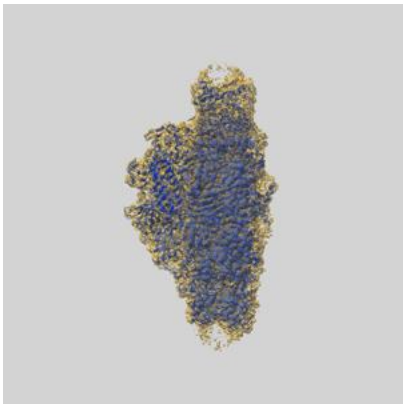
9.1 Map-model overlay



X



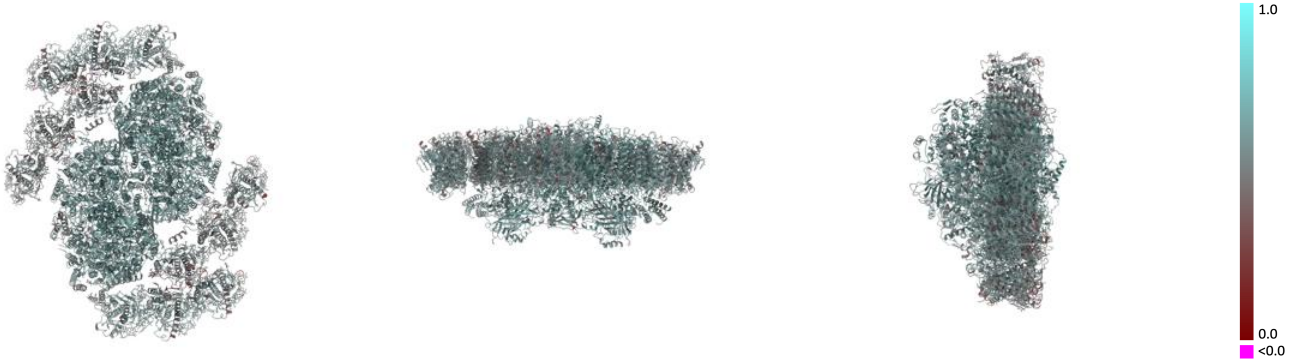
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

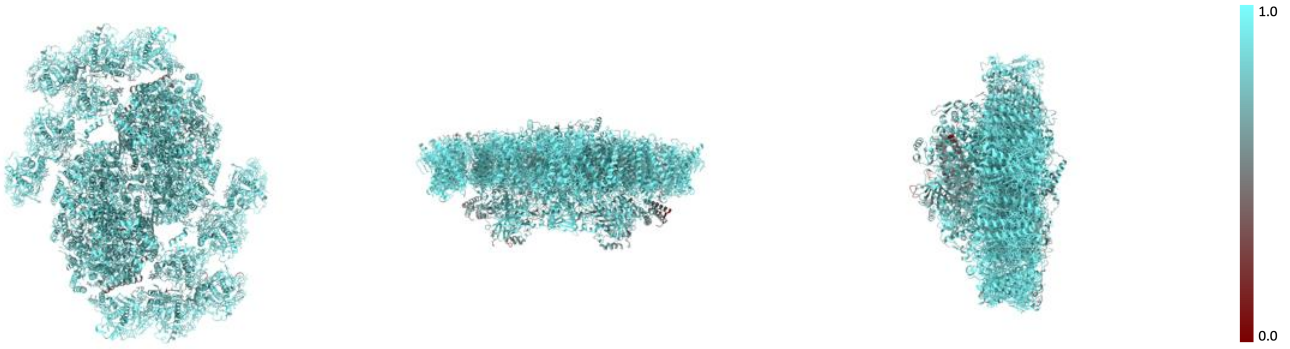
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

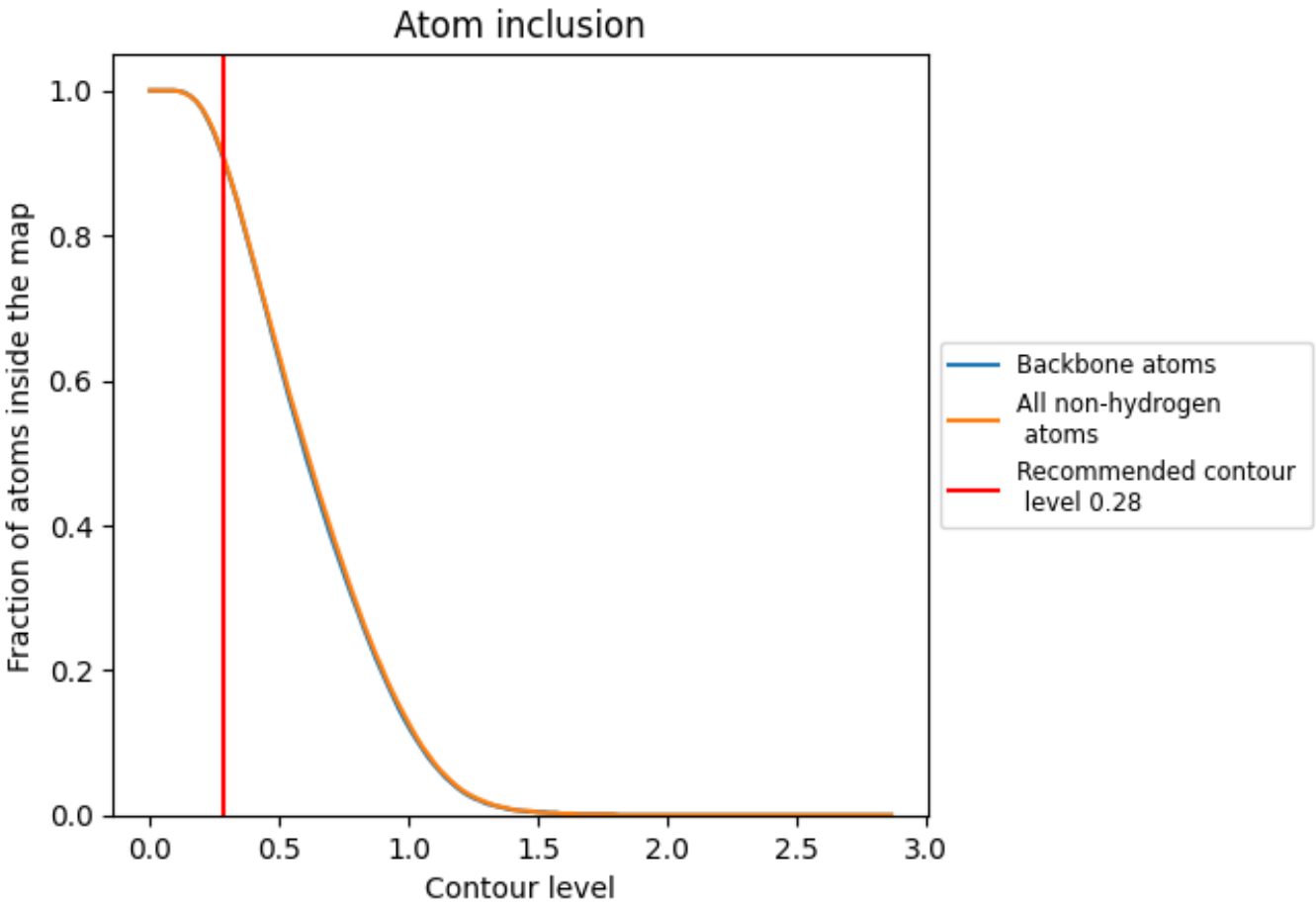
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9130	0.5740
0	0.9020	0.4810
1	0.9410	0.5430
2	0.9370	0.5470
3	0.9060	0.5260
4	0.9110	0.4900
5	0.9330	0.4860
6	0.8940	0.4950
7	0.9330	0.5320
8	0.9330	0.5380
9	0.8910	0.5130
A	0.9770	0.6470
B	0.9650	0.6220
C	0.9710	0.6230
D	0.9780	0.6400
E	0.8900	0.5270
F	0.8810	0.4910
H	0.9720	0.5900
I	0.9930	0.6410
J	0.8830	0.5920
K	0.9660	0.5930
L	0.9490	0.6280
M	0.9410	0.6170
N	0.8100	0.5080
O	0.7700	0.5860
Q	0.6440	0.5550
T	0.9410	0.6320
U	0.8080	0.5790
V	0.8390	0.5930
W	0.8880	0.5950
X	0.9130	0.5520
Y	0.8070	0.5410
Z	0.8440	0.5250
a	0.9790	0.6480
b	0.9610	0.6220

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Chain	Atom inclusion	Q-score
c	0.9660	0.6210
d	0.9780	0.6490
e	0.8830	0.5340
f	0.8920	0.5070
g	0.9380	0.4850
h	0.9670	0.5910
i	0.9930	0.6280
j	0.8860	0.5910
k	0.9660	0.5930
l	0.9540	0.6220
m	0.9290	0.6140
n	0.8110	0.5030
o	0.7570	0.5870
p	0.8960	0.4850
q	0.6280	0.5630
t	0.9440	0.6370
u	0.7990	0.5820
v	0.8430	0.5960
w	0.8980	0.6000
x	0.9230	0.5670
y	0.8240	0.5470
z	0.8440	0.5290