Full wwPDB EM Validation Report ⓘ

Jul 9, 2026 – 11:38 AM JST

PDB ID	:	9JJ8 / pdb_00009jj8
EMDB ID	:	EMD-61519
Title	:	Structural insights into the PSI-FCPI supercomplex from the coccolithophore Emiliania huxleyi
Authors	:	Shen, L.L.; Li, Z.H.; Wang, W.D.
Deposited on	:	2024-09-13
Resolution	:	2.79 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:

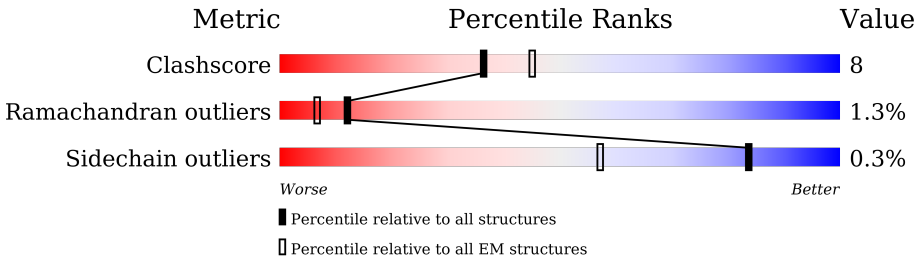
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

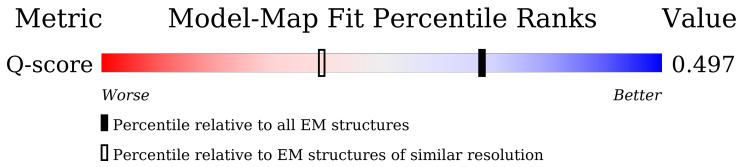
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.79 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	10811 (2.29 - 3.29)

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	752	84% 15%
2	b	734	88% 12%
3	c	81	85% 12%
4	d	142	87% 10%

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Mol	Chain	Length	Quality of chain
5	e	131	46% 52%
6	f	184	79% 8% 12%
7	i	36	78% 14% 8%
8	j	40	78% 22%
9	l	145	86% 13%
10	m	30	80% 20%
11	k	145	40% 10% 50%
12	o	123	7% 32% 7% 61%
13	A	201	77% 14% 9%
14	B	177	24% 78% 19%
15	C	233	6% 65% 10% 24%
16	D	231	71% 11% 18%
17	E	217	73% 13% 14%
18	F	239	59% 18% 21%
19	G	204	68% 16% 16%
20	H	210	5% 66% 14% 20%
21	J	251	13% 53% 15% 32%
22	K	198	75% 7% 15%
23	L	244	6% 76% 9% 14%
24	M	224	71% 15% 14%
24	P	224	71% 15% 14%
24	W	224	72% 12% 14%
25	O	219	6% 57% 12% 29%
26	Q	257	63% 18% 16%
27	5	219	67% 14% 19%

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Mol	Chain	Length	Quality of chain
27	R	219	69% 11% 19%
27	V	219	69% 16% 14%
27	X	219	67% 14% 19%
28	4	255	76% 13% 11%
28	7	255	16% 80% 10% 11%
28	S	255	74% 14% 11%
28	x	255	60% 87% 11%
28	y	255	47% 87% 11%
28	z	255	56% 86% 11%
29	T	211	78% 15% 7%
30	U	198	63% 16% 20%
31	0	254	70% 15% 14%
32	1	253	27% 67% 12% 21%
33	3	268	18% 74% 14% 12%
34	6	250	53% 84% 6% 10%
34	8	250	22% 82% 7% 10%
35	9	245	14% 76% 9% 15%
36	I	209	65% 10% 25%
37	h	133	64% 35%
38	2	260	53% 75% 12% 14%
38	Y	260	85% 82% 5% 13%
38	Z	260	82% 83% 13%

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
46	LMG	4	326	-	-	X	-
48	A86	Q	304	-	-	X	-
49	KC2	5	313	-	-	X	-
51	A1ECV	0	321	X	-	-	-
51	A1ECV	1	318	X	-	-	-
51	A1ECV	2	311	X	-	-	-
51	A1ECV	4	315	X	-	-	-
51	A1ECV	4	321	X	-	-	-
51	A1ECV	5	309	X	-	-	-
51	A1ECV	5	312	X	-	-	-
51	A1ECV	6	320	X	-	-	-
51	A1ECV	7	317	X	-	-	-
51	A1ECV	7	323	X	-	-	-
51	A1ECV	9	314	X	-	-	-
51	A1ECV	9	317	X	-	-	-
51	A1ECV	E	311	X	-	-	-
51	A1ECV	G	316	X	-	-	-
51	A1ECV	L	318	X	-	-	-
51	A1ECV	M	316	X	-	-	-
51	A1ECV	O	315	X	-	-	-
51	A1ECV	P	315	X	-	-	-
51	A1ECV	Q	316	X	-	-	-
51	A1ECV	Q	319	X	-	-	-
51	A1ECV	R	310	X	-	-	-
51	A1ECV	R	313	X	-	-	-
51	A1ECV	S	312	X	-	-	-
51	A1ECV	S	318	X	-	-	-
51	A1ECV	T	317	X	-	-	-
51	A1ECV	V	317	X	-	-	-
51	A1ECV	W	317	X	-	-	-
51	A1ECV	X	310	X	-	-	-
51	A1ECV	X	313	X	-	-	-
51	A1ECV	Y	306	X	-	-	-
51	A1ECV	Y	312	X	-	-	-
51	A1ECV	Z	308	X	-	-	-
51	A1ECV	Z	314	X	-	-	-
51	A1ECV	x	310	X	-	-	-
51	A1ECV	x	316	X	-	-	-
51	A1ECV	y	311	X	-	-	-
51	A1ECV	y	317	X	-	-	-
51	A1ECV	z	310	X	-	-	-
51	A1ECV	z	316	X	-	-	-

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 114135 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	741	5835	3817	993	995	30	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	733	5818	3828	982	987	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	80	598	365	105	117	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	140	1103	710	184	206	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	63	491	314	86	90	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	161	1232	797	207	224	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	33	Total	C	N	O	S	0	0
			254	176	34	43	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	40	Total	C	N	O	S	0	0
			318	211	47	57	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	143	Total	C	N	O	S	0	0
			1084	716	172	195	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	30	Total	C	N	O	S	0	0
			224	149	35	38	2		

- Molecule 11 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	73	Total	C	N	O	S	0	0
			533	347	87	93	6		

- Molecule 12 is a protein called Linker-protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	o	48	Total	C	N	O	S	0	0
			360	231	61	66	2		

- Molecule 13 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	183	Total	C	N	O	S	0	0
			1419	916	229	264	10		

- Molecule 14 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	172	Total	C	N	O	S	0	0
			1255	805	212	231	7		

- Molecule 15 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	176	Total	C	N	O	S	0	0
			1329	857	221	242	9		

- Molecule 16 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	189	Total	C	N	O	S	0	0
			1424	921	226	271	6		

- Molecule 17 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	187	Total	C	N	O	S	0	0
			1384	896	222	258	8		

- Molecule 18 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	188	Total	C	N	O	S	0	0
			1411	907	244	251	9		

- Molecule 19 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	171	Total	C	N	O	S	0	0
			1340	875	226	232	7		

- Molecule 20 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	168	Total	C	N	O	S	0	0
			1263	810	206	235	12		

- Molecule 21 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	171	Total	C	N	O	S	0	0
			1270	810	223	230	7		

- Molecule 22 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	168	Total	C	N	O	S	0	0
			1251	806	206	231	8		

- Molecule 23 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	210	Total	C	N	O	S	0	0
			1626	1064	273	281	8		

- Molecule 24 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
24	P	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
24	W	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		

- Molecule 25 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	155	Total	C	N	O	S	0	0
			1133	717	200	209	7		

- Molecule 26 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	215	Total	C	N	O	S	0	0
			1666	1094	273	294	5		

- Molecule 27 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	188	Total	C	N	O	S	0	0
			1353	872	227	248	6		
27	X	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		
27	5	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		

- Molecule 28 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	4	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	7	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	x	228	Total	C	N	O		0	0
			1113	657	228	228			
28	y	228	Total	C	N	O		0	0
			1113	657	228	228			
28	z	228	Total	C	N	O		0	0
			1113	657	228	228			

- Molecule 29 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	197	Total	C	N	O	S	0	0
			1482	973	246	257	6		

- Molecule 30 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	158	Total	C	N	O	S	0	0
			1240	801	207	226	6		

- Molecule 31 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	0	218	Total	C	N	O	S	0	0
			1706	1114	278	309	5		

- Molecule 32 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1	201	Total	C	N	O	S	0	0
			1255	794	223	237	1		

- Molecule 33 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	3	236	Total	C	N	O	S	0	0
			1775	1155	294	318	8		

- Molecule 34 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	224	Total	C	N	O	S	0	0
			1415	892	255	261	7		
34	6	224	Total	C	N	O	S	0	0
			1326	825	249	250	2		

- Molecule 35 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	209	Total	C	N	O	S	0	0
			1490	970	246	267	7		

- Molecule 36 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	I	156	Total	C	N	O	S	0	0
			1203	780	201	213	9		

- Molecule 37 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	87	Total	C	N	O	S	0	0
			650	425	104	120	1		

- Molecule 38 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	Y	225	Total	C	N	O	0	0
			1099	649	225	225		
38	Z	225	Total	C	N	O	0	0
			1099	649	225	225		

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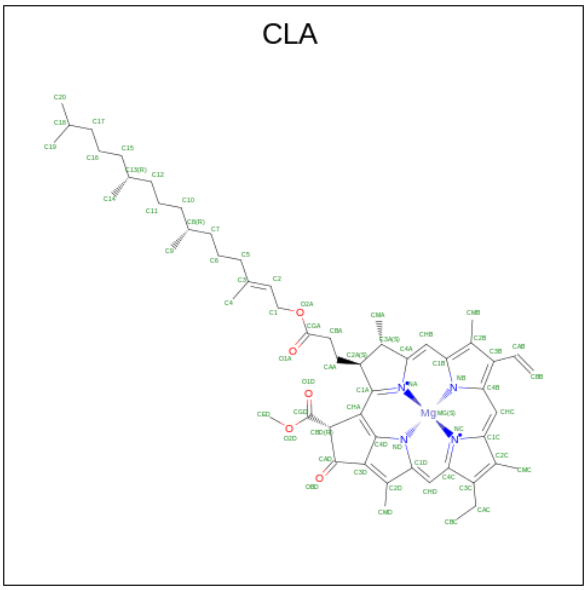
Mol	Chain	Residues	Atoms					AltConf	Trace
38	2	224	Total	C	N	O	S	0	0
			1383	858	256	263	6		

- Molecule 39 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
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	l	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	k	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	o	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	o	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	o	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	o	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	o	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
39	C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	F	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	L	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	L	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	M	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	M	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
39	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	O	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	O	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	P	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	S	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	T	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	W	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
39	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
39	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	x	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	x	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	x	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	x	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	x	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	x	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	y	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	y	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
39	y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			52	44	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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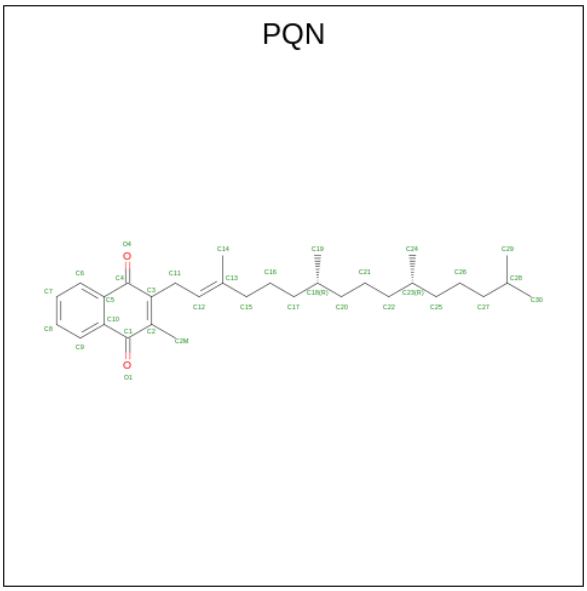
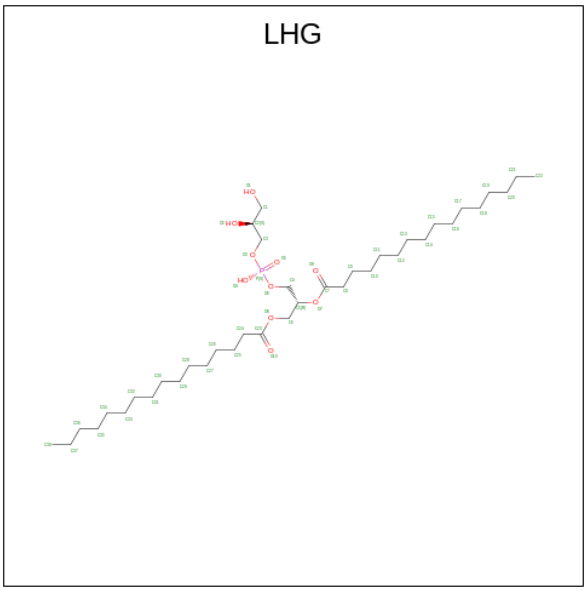
Mol	Chain	Residues	Atoms					AltConf
39	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 40 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



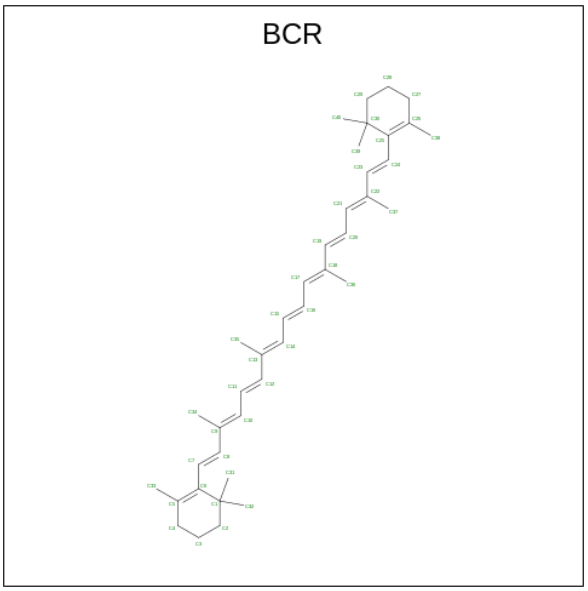
Mol	Chain	Residues	Atoms			AltConf
40	a	1	Total	C	O	0
			33	31	2	
40	b	1	Total	C	O	0
			33	31	2	

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
41	a	1	Total	C	O	P	0
			49	38	10	1	
41	a	1	Total	C	O	P	0
			27	16	10	1	
41	j	1	Total	C	O	P	0
			30	19	10	1	
41	D	1	Total	C	O	P	0
			35	24	10	1	
41	D	1	Total	C	O	P	0
			35	24	10	1	
41	H	1	Total	C	O	P	0
			35	24	10	1	
41	X	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 42 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
42	a	1	Total C 40 40	0
42	a	1	Total C 40 40	0
42	a	1	Total C 40 40	0
42	a	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	f	1	Total C 40 40	0
42	f	1	Total C 40 40	0
42	i	1	Total C 40 40	0
42	j	1	Total C 40 40	0

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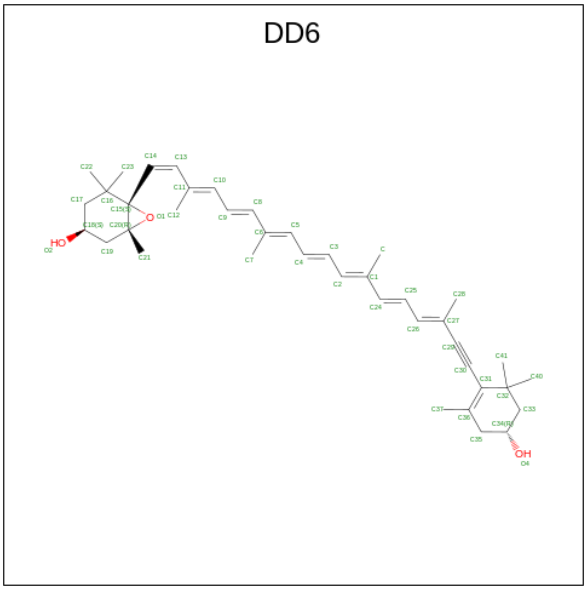
Mol	Chain	Residues	Atoms	AltConf
42	l	1	Total C 40 40	0
42	l	1	Total C 40 40	0
42	l	1	Total C 40 40	0
42	m	1	Total C 40 40	0
42	k	1	Total C 40 40	0
42	h	1	Total C 40 40	0

- Molecule 43 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
43	a	1	Total C O 43 40 3	0
43	j	1	Total C O 43 40 3	0
43	o	1	Total C O 43 40 3	0
43	A	1	Total C O 43 40 3	0

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Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	C	O	0
			43	40	3	
43	A	1	Total	C	O	0
			43	40	3	
43	A	1	Total	C	O	0
			43	40	3	
43	B	1	Total	C	O	0
			43	40	3	
43	C	1	Total	C	O	0
			43	40	3	
43	D	1	Total	C	O	0
			43	40	3	
43	D	1	Total	C	O	0
			43	40	3	
43	D	1	Total	C	O	0
			43	40	3	
43	E	1	Total	C	O	0
			43	40	3	
43	E	1	Total	C	O	0
			43	40	3	
43	E	1	Total	C	O	0
			43	40	3	
43	F	1	Total	C	O	0
			43	40	3	
43	F	1	Total	C	O	0
			43	40	3	
43	G	1	Total	C	O	0
			43	40	3	
43	G	1	Total	C	O	0
			43	40	3	
43	H	1	Total	C	O	0
			43	40	3	
43	H	1	Total	C	O	0
			43	40	3	
43	J	1	Total	C	O	0
			43	40	3	
43	J	1	Total	C	O	0
			43	40	3	
43	J	1	Total	C	O	0
			43	40	3	
43	K	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
43	M	1	Total	C	O	0
			43	40	3	
43	O	1	Total	C	O	0
			43	40	3	
43	O	1	Total	C	O	0
			43	40	3	
43	O	1	Total	C	O	0
			43	40	3	
43	P	1	Total	C	O	0
			43	40	3	
43	Q	1	Total	C	O	0
			43	40	3	
43	Q	1	Total	C	O	0
			43	40	3	
43	R	1	Total	C	O	0
			43	40	3	
43	S	1	Total	C	O	0
			43	40	3	
43	T	1	Total	C	O	0
			43	40	3	
43	U	1	Total	C	O	0
			43	40	3	
43	V	1	Total	C	O	0
			43	40	3	
43	W	1	Total	C	O	0
			43	40	3	
43	X	1	Total	C	O	0
			43	40	3	
43	1	1	Total	C	O	0
			43	40	3	
43	3	1	Total	C	O	0
			43	40	3	
43	3	1	Total	C	O	0
			43	40	3	
43	4	1	Total	C	O	0
			43	40	3	
43	4	1	Total	C	O	0
			43	40	3	
43	5	1	Total	C	O	0
			43	40	3	
43	7	1	Total	C	O	0
			43	40	3	

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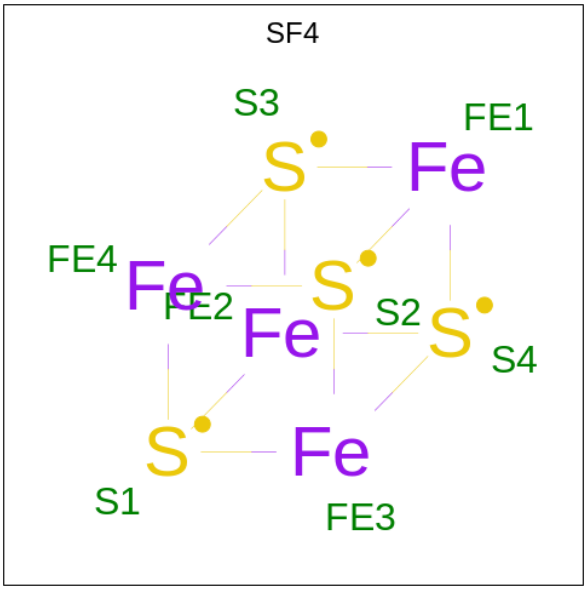
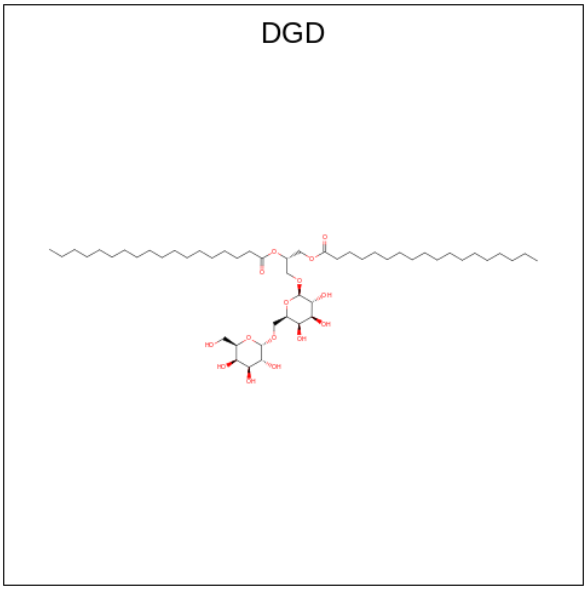
Mol	Chain	Residues	Atoms	AltConf
43	7	1	Total C O 43 40 3	0
43	I	1	Total C O 43 40 3	0
43	I	1	Total C O 43 40 3	0
43	I	1	Total C O 43 40 3	0
43	x	1	Total C O 43 40 3	0
43	x	1	Total C O 43 40 3	0
43	y	1	Total C O 43 40 3	0
43	y	1	Total C O 43 40 3	0
43	z	1	Total C O 43 40 3	0
43	z	1	Total C O 43 40 3	0
43	Z	1	Total C O 43 40 3	0
43	2	1	Total C O 43 40 3	0

- Molecule 44 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



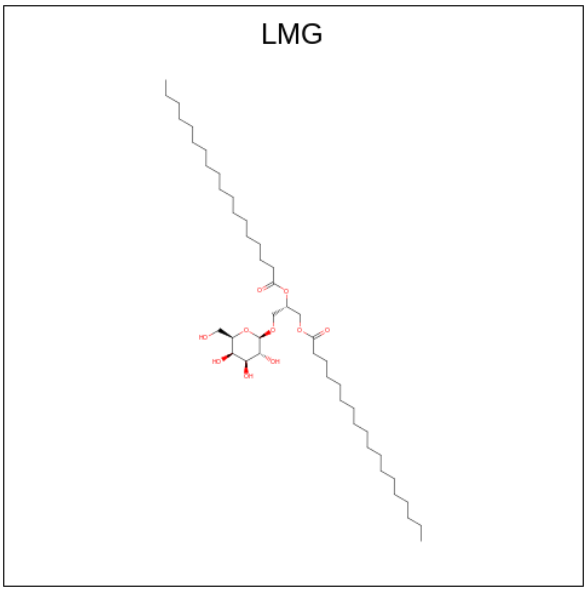
Mol	Chain	Residues	Atoms	AltConf
44	b	1	Total Fe S 8 4 4	0
44	c	1	Total Fe S 8 4 4	0
44	c	1	Total Fe S 8 4 4	0

- Molecule 45 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
45	b	1	Total C O 60 45 15	0
45	C	1	Total C O 40 25 15	0

- Molecule 46 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
46	l	1	Total	C	O	0
			39	29	10	
46	A	1	Total	C	O	0
			29	19	10	
46	D	1	Total	C	O	0
			37	27	10	
46	F	1	Total	C	O	0
			39	29	10	
46	F	1	Total	C	O	0
			34	24	10	
46	M	1	Total	C	O	0
			39	29	10	
46	M	1	Total	C	O	0
			33	23	10	
46	P	1	Total	C	O	0
			39	29	10	
46	Q	1	Total	C	O	0
			28	18	10	
46	S	1	Total	C	O	0
			32	22	10	
46	S	1	Total	C	O	0
			46	36	10	
46	W	1	Total	C	O	0
			39	29	10	
46	W	1	Total	C	O	0
			33	23	10	
46	0	1	Total	C	O	0
			27	17	10	

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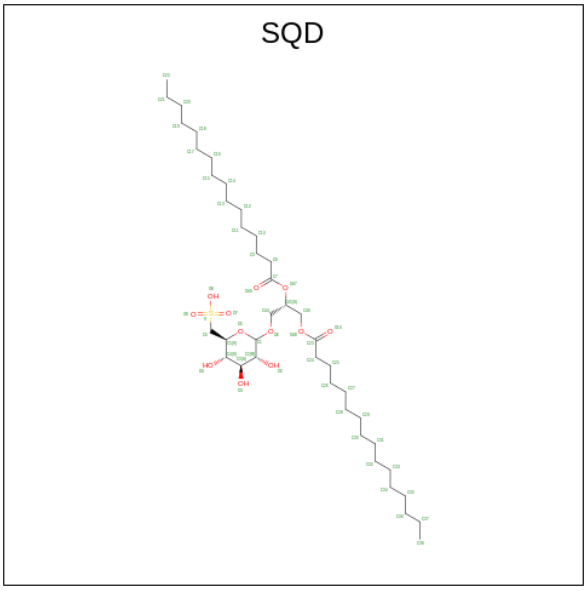
Mol	Chain	Residues	Atoms	AltConf
46	4	1	Total C O 32 22 10	0
46	4	1	Total C O 46 36 10	0
46	7	1	Total C O 46 36 10	0
46	7	1	Total C O 32 22 10	0
46	9	1	Total C O 36 26 10	0
46	I	1	Total C O 42 32 10	0

- Molecule 47 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
47	k	1	Total C O S 38 25 12 1	0
47	D	1	Total C O S 38 25 12 1	0
47	D	1	Total C O S 37 24 12 1	0
47	D	1	Total C O S 39 26 12 1	0

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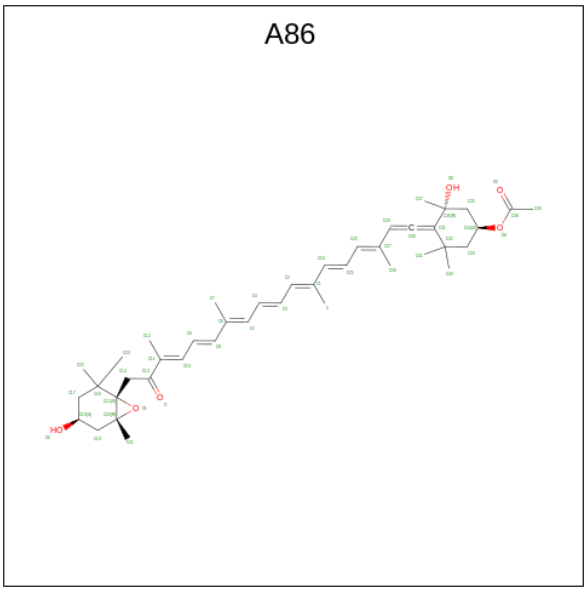
Mol	Chain	Residues	Atoms				AltConf
47	E	1	Total 35	C 22	O 12	S 1	0
47	F	1	Total 42	C 29	O 12	S 1	0
47	F	1	Total 37	C 24	O 12	S 1	0
47	H	1	Total 38	C 25	O 12	S 1	0
47	M	1	Total 39	C 26	O 12	S 1	0
47	P	1	Total 38	C 25	O 12	S 1	0
47	S	1	Total 39	C 26	O 12	S 1	0
47	T	1	Total 36	C 23	O 12	S 1	0
47	W	1	Total 28	C 15	O 12	S 1	0
47	4	1	Total 39	C 26	O 12	S 1	0
47	7	1	Total 39	C 26	O 12	S 1	0
47	9	1	Total 36	C 23	O 12	S 1	0

- Molecule 48 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
48	k	1	Total C O 48 42 6	0
48	B	1	Total C O 48 42 6	0
48	C	1	Total C O 48 42 6	0
48	D	1	Total C O 48 42 6	0
48	E	1	Total C O 48 42 6	0
48	F	1	Total C O 48 42 6	0
48	F	1	Total C O 48 42 6	0
48	G	1	Total C O 48 42 6	0
48	G	1	Total C O 48 42 6	0
48	H	1	Total C O 48 42 6	0
48	J	1	Total C O 48 42 6	0
48	J	1	Total C O 48 42 6	0
48	K	1	Total C O 48 42 6	0
48	L	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
48	L	1	Total C O 48 42 6	0
48	L	1	Total C O 48 42 6	0
48	L	1	Total C O 48 42 6	0
48	L	1	Total C O 48 42 6	0
48	L	1	Total C O 48 42 6	0
48	M	1	Total C O 48 42 6	0
48	M	1	Total C O 48 42 6	0
48	M	1	Total C O 48 42 6	0
48	O	1	Total C O 48 42 6	0
48	O	1	Total C O 48 42 6	0
48	O	1	Total C O 48 42 6	0
48	P	1	Total C O 48 42 6	0
48	P	1	Total C O 48 42 6	0
48	Q	1	Total C O 48 42 6	0
48	Q	1	Total C O 48 42 6	0
48	Q	1	Total C O 48 42 6	0
48	Q	1	Total C O 48 42 6	0
48	Q	1	Total C O 48 42 6	0
48	R	1	Total C O 48 42 6	0
48	R	1	Total C O 48 42 6	0
48	R	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
48	S	1	Total C O 48 42 6	0
48	S	1	Total C O 48 42 6	0
48	S	1	Total C O 48 42 6	0
48	T	1	Total C O 48 42 6	0
48	T	1	Total C O 48 42 6	0
48	T	1	Total C O 48 42 6	0
48	U	1	Total C O 48 42 6	0
48	U	1	Total C O 48 42 6	0
48	V	1	Total C O 48 42 6	0
48	V	1	Total C O 48 42 6	0
48	W	1	Total C O 48 42 6	0
48	W	1	Total C O 48 42 6	0
48	W	1	Total C O 48 42 6	0
48	X	1	Total C O 48 42 6	0
48	X	1	Total C O 48 42 6	0
48	0	1	Total C O 48 42 6	0
48	0	1	Total C O 48 42 6	0
48	0	1	Total C O 48 42 6	0
48	0	1	Total C O 48 42 6	0
48	0	1	Total C O 48 42 6	0
48	1	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
48	1	1	Total C O 48 42 6	0
48	1	1	Total C O 48 42 6	0
48	1	1	Total C O 48 42 6	0
48	3	1	Total C O 48 42 6	0
48	3	1	Total C O 48 42 6	0
48	3	1	Total C O 48 42 6	0
48	3	1	Total C O 48 42 6	0
48	4	1	Total C O 48 42 6	0
48	4	1	Total C O 48 42 6	0
48	4	1	Total C O 48 42 6	0
48	4	1	Total C O 48 42 6	0
48	4	1	Total C O 48 42 6	0
48	5	1	Total C O 48 42 6	0
48	7	1	Total C O 48 42 6	0
48	7	1	Total C O 48 42 6	0
48	7	1	Total C O 48 42 6	0
48	7	1	Total C O 48 42 6	0
48	8	1	Total C O 48 42 6	0
48	8	1	Total C O 48 42 6	0
48	8	1	Total C O 48 42 6	0
48	8	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
48	8	1	Total C O 48 42 6	0
48	8	1	Total C O 48 42 6	0
48	9	1	Total C O 48 42 6	0
48	9	1	Total C O 48 42 6	0
48	9	1	Total C O 48 42 6	0
48	9	1	Total C O 48 42 6	0
48	9	1	Total C O 48 42 6	0
48	I	1	Total C O 48 42 6	0
48	x	1	Total C O 48 42 6	0
48	y	1	Total C O 48 42 6	0
48	y	1	Total C O 48 42 6	0
48	z	1	Total C O 48 42 6	0
48	Y	1	Total C O 48 42 6	0
48	Z	1	Total C O 48 42 6	0
48	Z	1	Total C O 48 42 6	0
48	2	1	Total C O 48 42 6	0
48	2	1	Total C O 48 42 6	0
48	2	1	Total C O 48 42 6	0
48	6	1	Total C O 48 42 6	0
48	6	1	Total C O 48 42 6	0
48	6	1	Total C O 48 42 6	0

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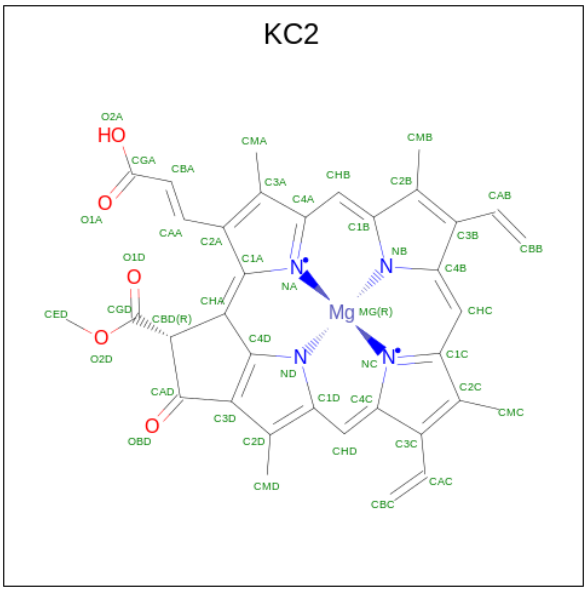
Mol	Chain	Residues	Atoms	AltConf
48	6	1	Total C O 48 42 6	0
48	6	1	Total C O 48 42 6	0

- Molecule 49 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
49	A	1	Total C Mg N O 45 35 1 4 5	0
49	A	1	Total C Mg N O 45 35 1 4 5	0
49	B	1	Total C Mg N O 45 35 1 4 5	0
49	C	1	Total C Mg N O 45 35 1 4 5	0
49	C	1	Total C Mg N O 45 35 1 4 5	0
49	F	1	Total C Mg N O 45 35 1 4 5	0
49	F	1	Total C Mg N O 44 35 1 4 4	0
49	G	1	Total C Mg N O 45 35 1 4 5	0
49	G	1	Total C Mg N O 45 35 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
49	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	M	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	O	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	P	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
49	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Q	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	R	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
49	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	W	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	X	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	0	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
49	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	5	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	I	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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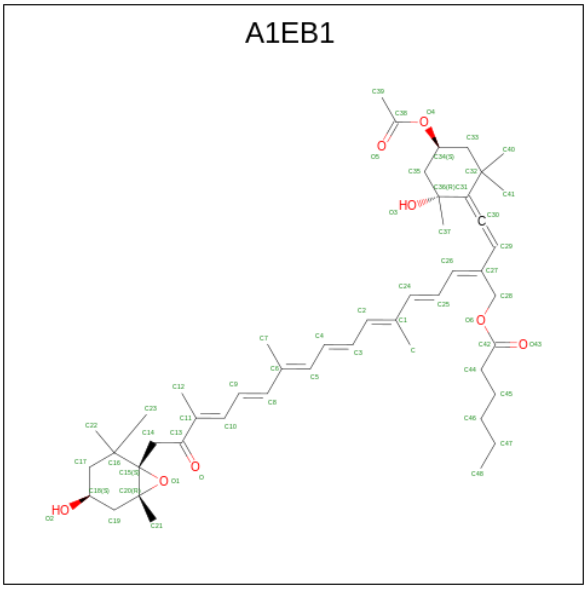
Mol	Chain	Residues	Atoms					AltConf
49	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	z	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
49	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
49	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 50 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-2-[2-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]ethenyl]-6,11,15-trimethyl-16-oxidanylidene-17-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]heptadec

a-2,4,6,8,10,12,14-heptaenyl] hexanoate (CCD ID: A1EB1) (formula: $C_{48}H_{68}O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
50	C	1	Total C O 56 48 8	0
50	D	1	Total C O 56 48 8	0
50	E	1	Total C O 56 48 8	0
50	F	1	Total C O 56 48 8	0
50	G	1	Total C O 56 48 8	0
50	G	1	Total C O 56 48 8	0
50	G	1	Total C O 56 48 8	0
50	G	1	Total C O 56 48 8	0
50	H	1	Total C O 56 48 8	0
50	H	1	Total C O 56 48 8	0
50	J	1	Total C O 56 48 8	0
50	K	1	Total C O 56 48 8	0

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Mol	Chain	Residues	Atoms	AltConf
50	K	1	Total C O 56 48 8	0
50	K	1	Total C O 56 48 8	0
50	L	1	Total C O 56 48 8	0
50	O	1	Total C O 56 48 8	0
50	Q	1	Total C O 56 48 8	0
50	Q	1	Total C O 56 48 8	0
50	R	1	Total C O 56 48 8	0
50	S	1	Total C O 56 48 8	0
50	S	1	Total C O 56 48 8	0
50	T	1	Total C O 56 48 8	0
50	T	1	Total C O 56 48 8	0
50	U	1	Total C O 56 48 8	0
50	U	1	Total C O 56 48 8	0
50	V	1	Total C O 56 48 8	0
50	V	1	Total C O 56 48 8	0
50	V	1	Total C O 56 48 8	0
50	V	1	Total C O 56 48 8	0
50	0	1	Total C O 56 48 8	0
50	0	1	Total C O 56 48 8	0
50	0	1	Total C O 56 48 8	0
50	0	1	Total C O 56 48 8	0

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Mol	Chain	Residues	Atoms	AltConf
50	1	1	Total C O 56 48 8	0
50	1	1	Total C O 56 48 8	0
50	3	1	Total C O 56 48 8	0
50	3	1	Total C O 56 48 8	0
50	3	1	Total C O 56 48 8	0
50	3	1	Total C O 56 48 8	0
50	3	1	Total C O 56 48 8	0
50	4	1	Total C O 56 48 8	0
50	4	1	Total C O 56 48 8	0
50	4	1	Total C O 56 48 8	0
50	4	1	Total C O 56 48 8	0
50	5	1	Total C O 56 48 8	0
50	7	1	Total C O 56 48 8	0
50	7	1	Total C O 56 48 8	0
50	7	1	Total C O 56 48 8	0
50	7	1	Total C O 56 48 8	0
50	8	1	Total C O 56 48 8	0
50	8	1	Total C O 56 48 8	0
50	8	1	Total C O 56 48 8	0
50	8	1	Total C O 56 48 8	0
50	9	1	Total C O 56 48 8	0

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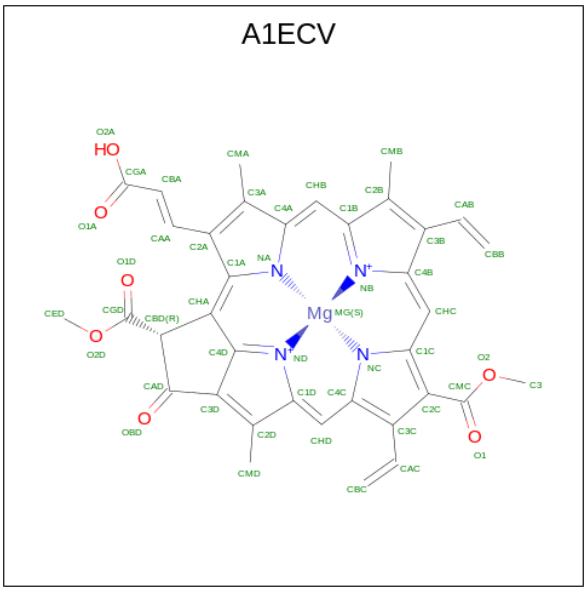
Mol	Chain	Residues	Atoms	AltConf
50	h	1	Total C O 56 48 8	0
50	x	1	Total C O 56 48 8	0
50	x	1	Total C O 56 48 8	0
50	y	1	Total C O 56 48 8	0
50	y	1	Total C O 56 48 8	0
50	z	1	Total C O 48 42 6	0
50	z	1	Total C O 56 48 8	0
50	2	1	Total C O 56 48 8	0
50	2	1	Total C O 56 48 8	0
50	6	1	Total C O 56 48 8	0
50	6	1	Total C O 53 45 8	0
50	6	1	Total C O 48 42 6	0
50	6	1	Total C O 56 48 8	0

- Molecule 51 is Chlorophyll C3 (CCD ID: A1ECV) (formula: $C_{36}H_{28}MgN_4O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
51	E	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	G	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	L	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	M	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	O	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	P	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Q	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Q	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	R	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	R	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	S	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	S	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	T	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	V	1	Total	C	Mg	N	O	0
			48	36	1	4	7	

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Mol	Chain	Residues	Atoms					AltConf
51	W	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	X	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	X	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	0	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	1	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	4	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	4	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	5	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	5	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	7	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	7	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	9	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	9	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	x	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	x	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	y	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	y	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Y	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Y	1	Total	C	Mg	N	O	0
			48	36	1	4	7	

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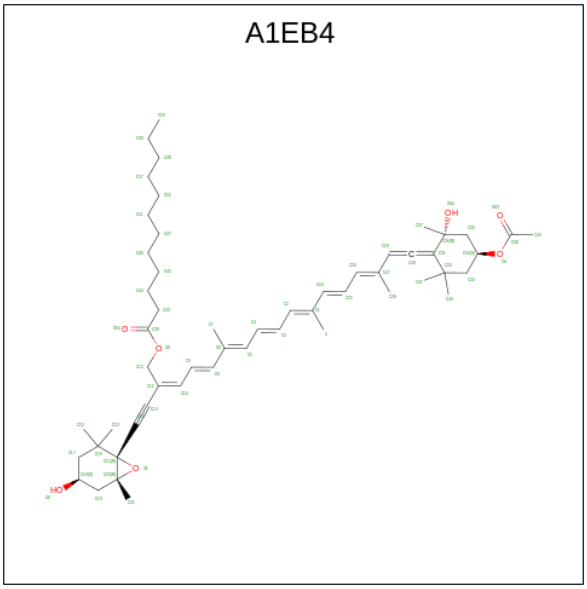
Mol	Chain	Residues	Atoms					AltConf
51	Z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	2	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	6	1	Total	C	Mg	N	O	0
			48	36	1	4	7	

- Molecule 52 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[2-[(1 {R},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethynyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] dodecanoate (CCD ID: A1EB4) (formula: $C_{54}H_{78}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	C	O	0
			58	51	7	
52	M	1	Total	C	O	0
			57	50	7	
52	P	1	Total	C	O	0
			56	49	7	
52	P	1	Total	C	O	0
			54	47	7	
52	P	1	Total	C	O	0
			57	50	7	

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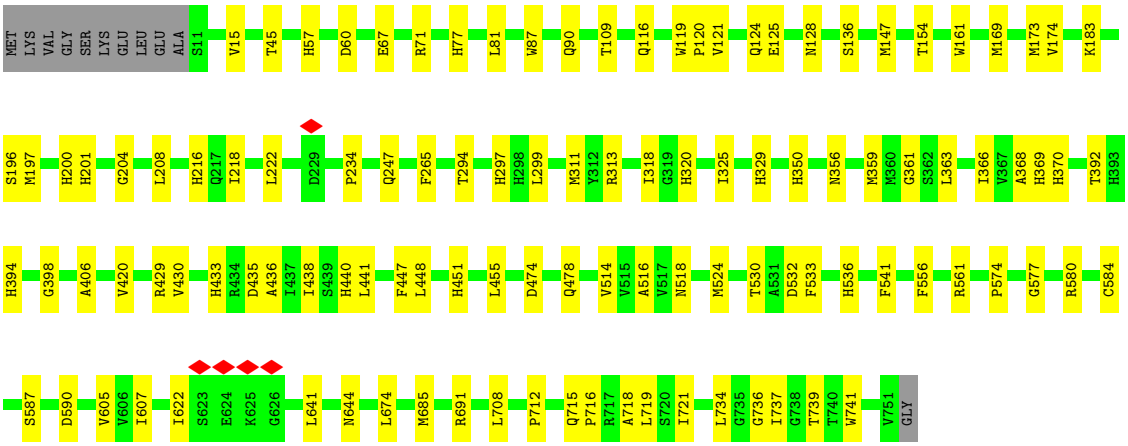
Mol	Chain	Residues	Atoms			AltConf
52	R	1	Total	C	O	0
			57	50	7	
52	T	1	Total	C	O	0
			55	48	7	
52	W	1	Total	C	O	0
			56	49	7	
52	W	1	Total	C	O	0
			57	50	7	
52	X	1	Total	C	O	0
			57	50	7	
52	5	1	Total	C	O	0
			57	50	7	

3 Residue-property plots (i)

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

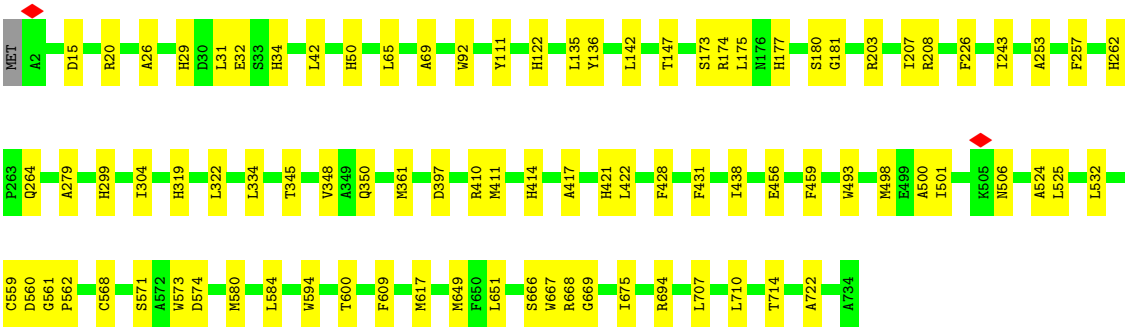
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:



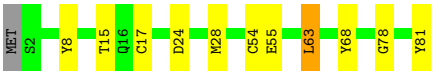
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



• Molecule 3: Photosystem I iron-sulfur center

Chain c:



• Molecule 4: Photosystem I reaction center subunit II

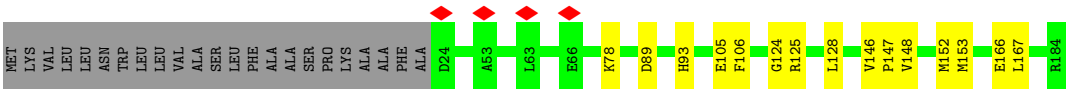
Chain d:

• Molecule 5: Photosystem I reaction center subunit IV

Chain e:

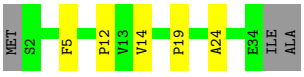
• Molecule 6: Photosystem I reaction center subunit III

Chain f:



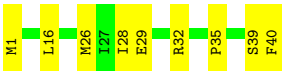
• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:



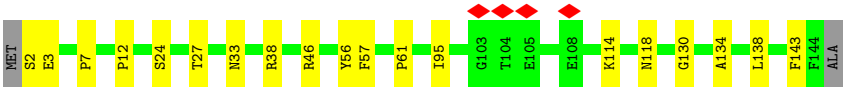
• Molecule 8: Photosystem I reaction center subunit IX

Chain j:



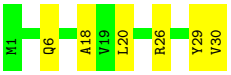
• Molecule 9: Photosystem I reaction center subunit XI

Chain l:



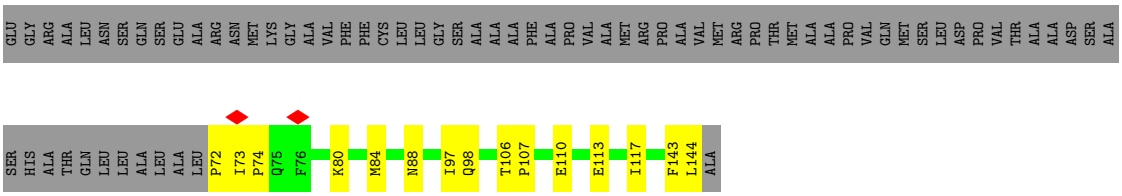
• Molecule 10: Photosystem I reaction center subunit XII

Chain m:



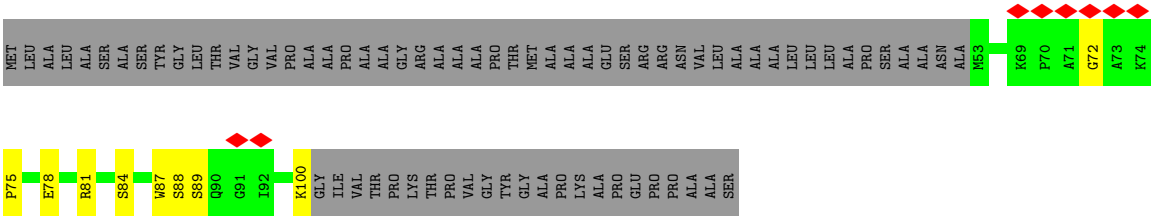
• Molecule 11: PSI-K

Chain k:



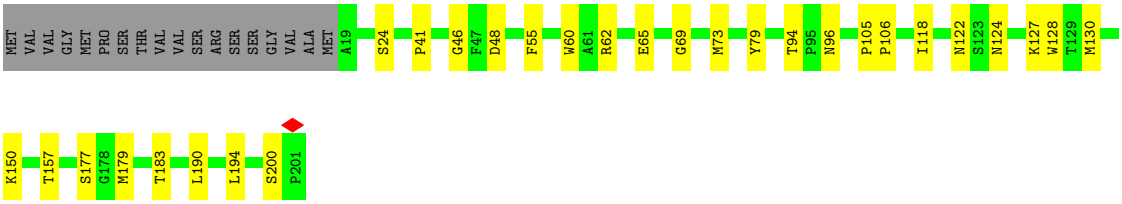
• Molecule 12: Linker-protein

Chain o:



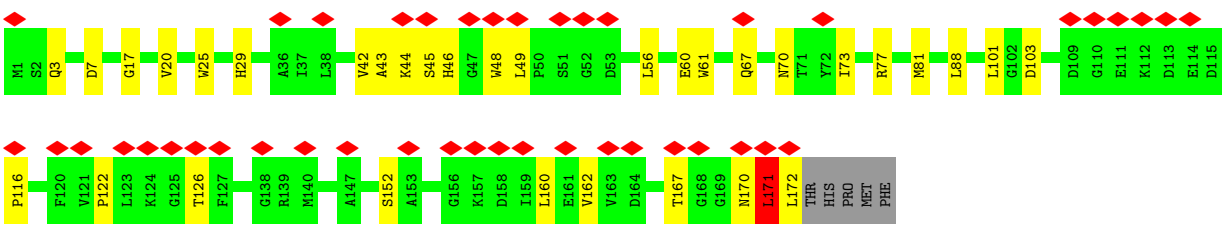
• Molecule 13: Light harvesting protein

Chain A:



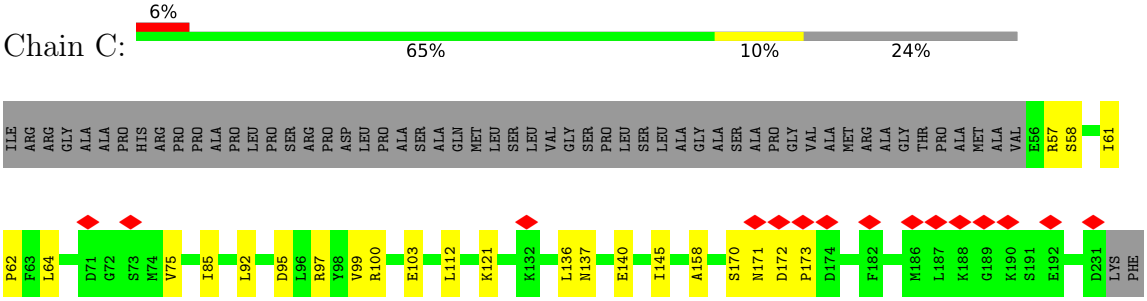
• Molecule 14: Light harvesting protein

Chain B:



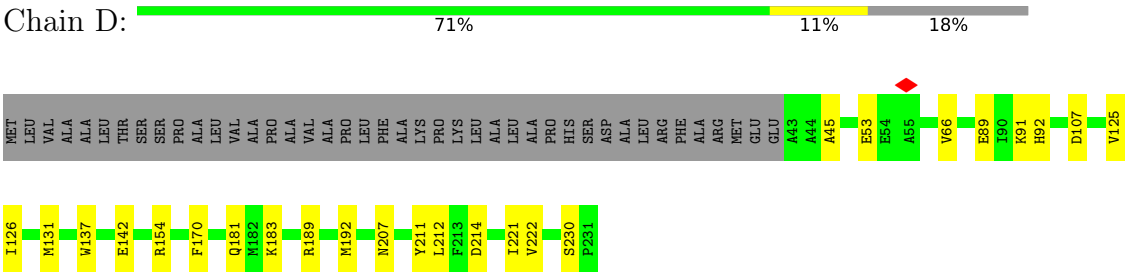
• Molecule 15: Light harvesting protein

Chain C:



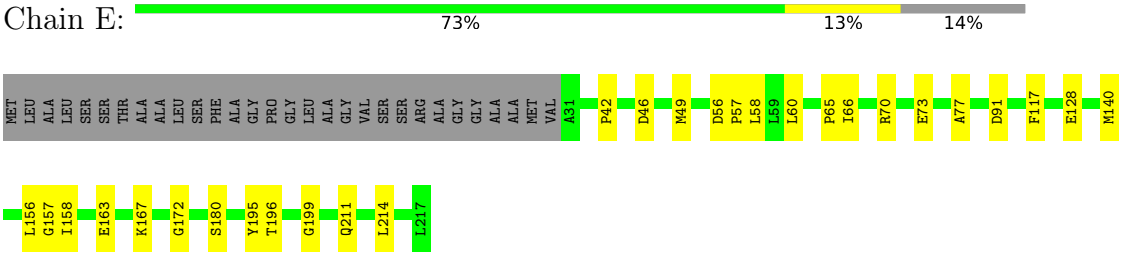
• Molecule 16: Light harvesting protein

Chain D:



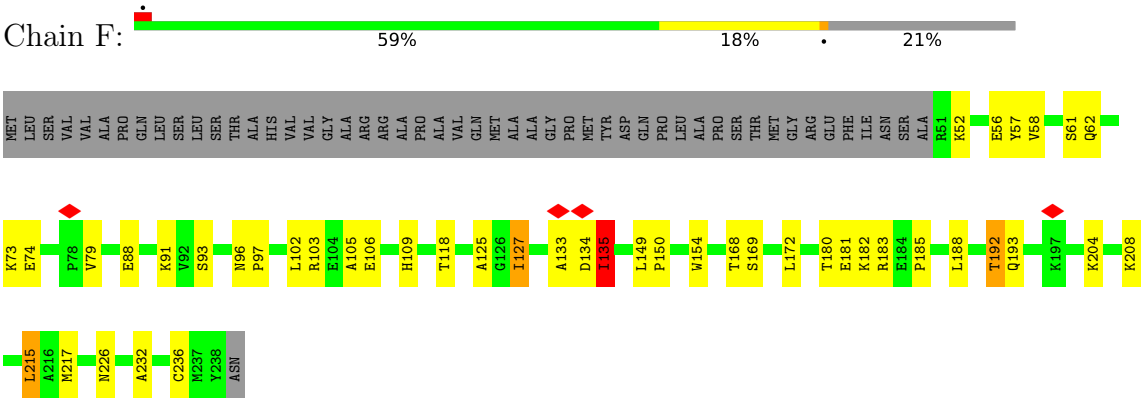
• Molecule 17: Light harvesting protein

Chain E:



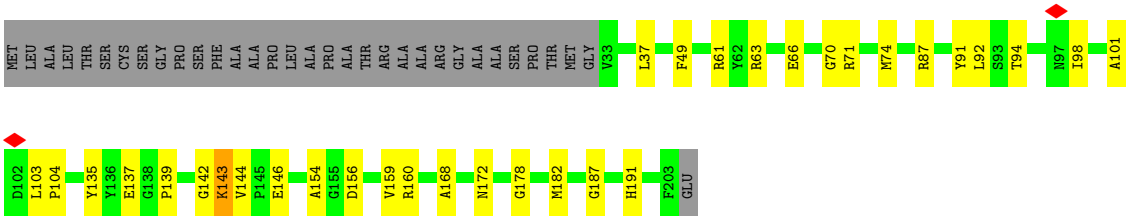
• Molecule 18: Light harvesting protein

Chain F:



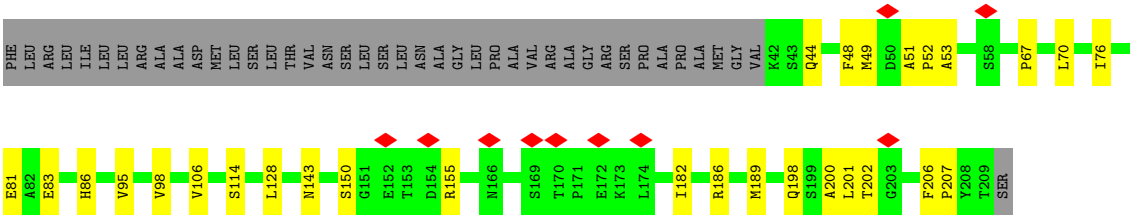
• Molecule 19: Light harvesting protein

Chain G:



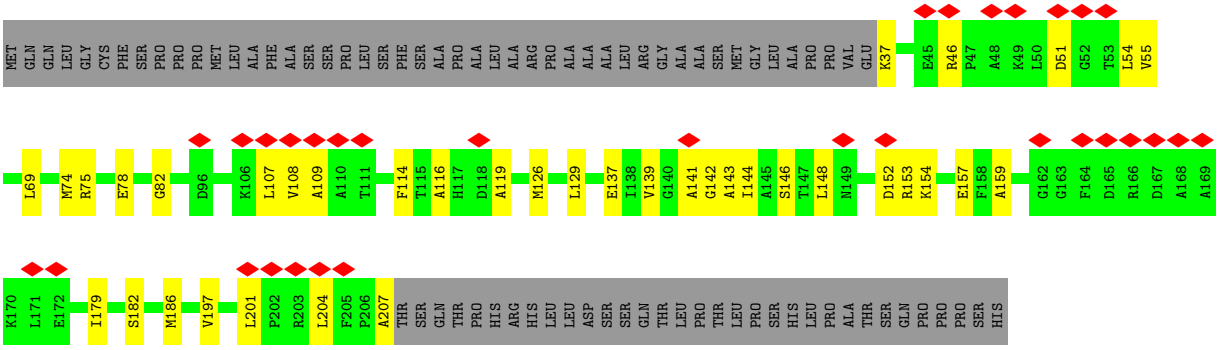
• Molecule 20: Light harvesting protein

Chain H:



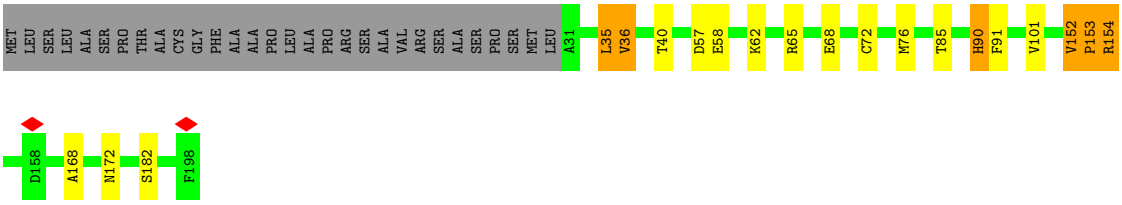
• Molecule 21: Light harvesting protein

Chain J:



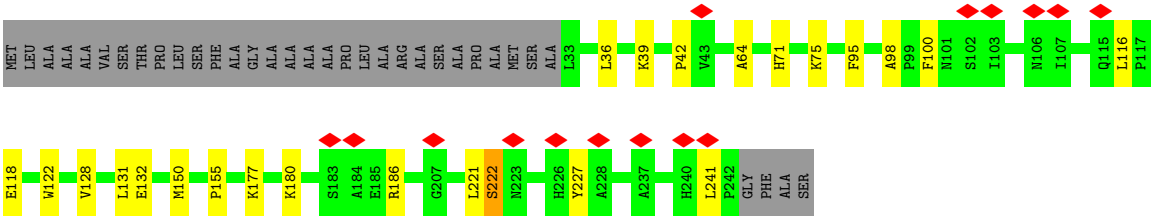
• Molecule 22: Light harvesting protein

Chain K:



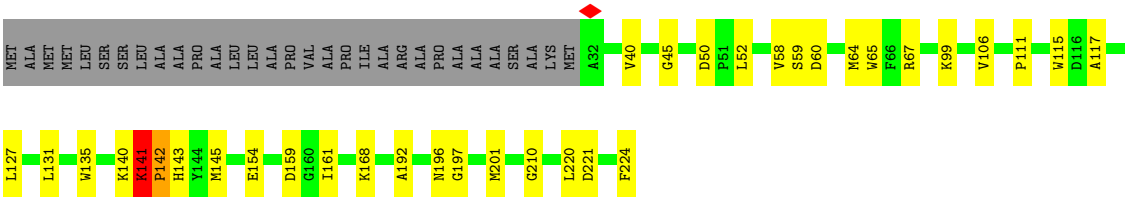
• Molecule 23: Light harvesting protein

Chain L:



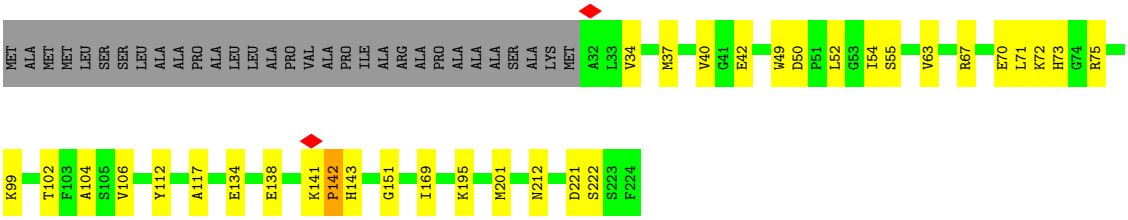
• Molecule 24: Light harvesting protein

Chain M:



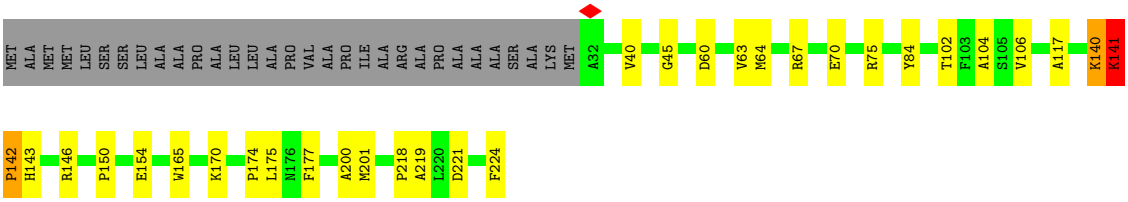
• Molecule 24: Light harvesting protein

Chain P:



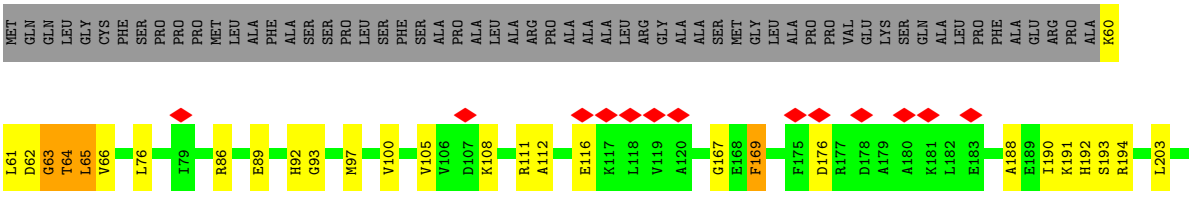
• Molecule 24: Light harvesting protein

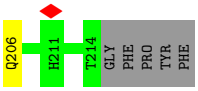
Chain W:



• Molecule 25: Light harvesting protein

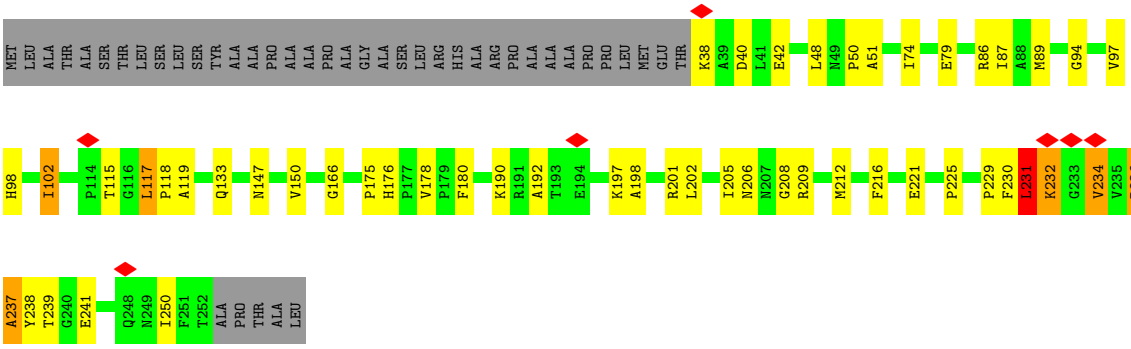
Chain O:





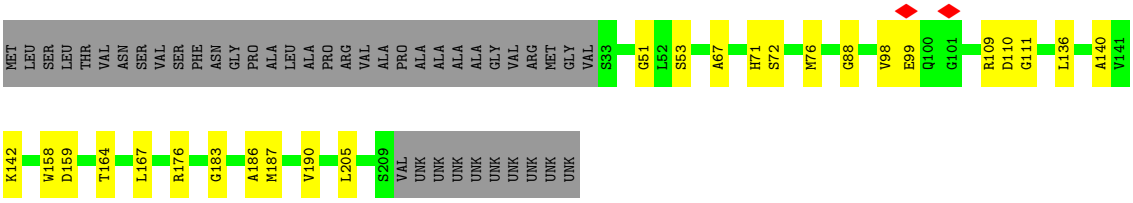
• Molecule 26: Light harvesting protein

Chain Q:



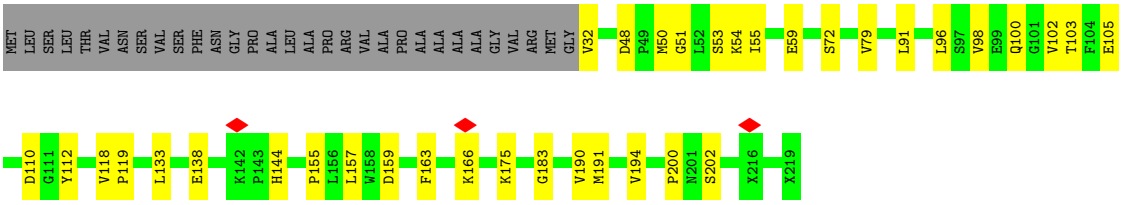
• Molecule 27: Light harvesting protein

Chain R:



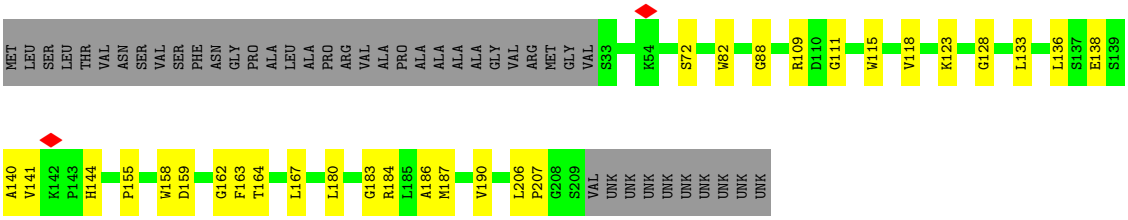
• Molecule 27: Light harvesting protein

Chain V:



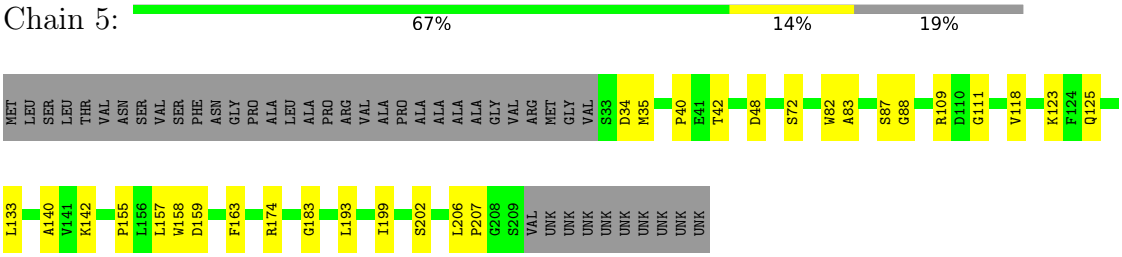
• Molecule 27: Light harvesting protein

Chain X:



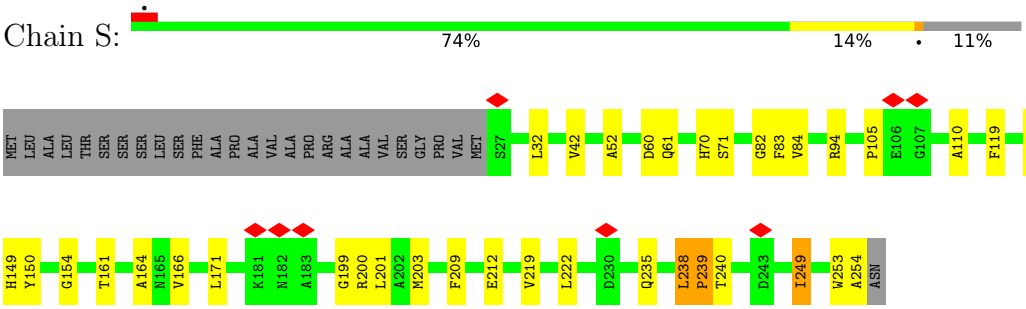
• Molecule 27: Light harvesting protein

Chain 5:



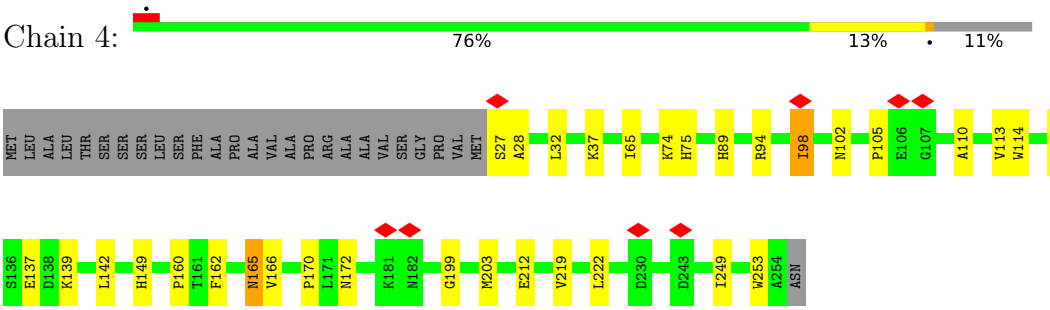
• Molecule 28: Light harvesting protein

Chain S:



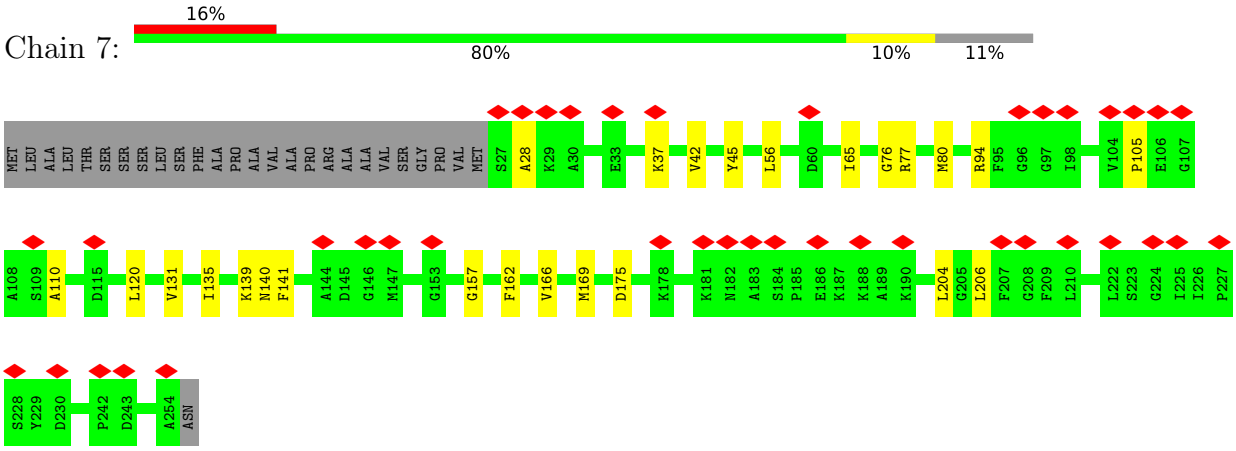
• Molecule 28: Light harvesting protein

Chain 4:



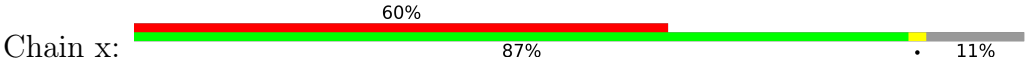
• Molecule 28: Light harvesting protein

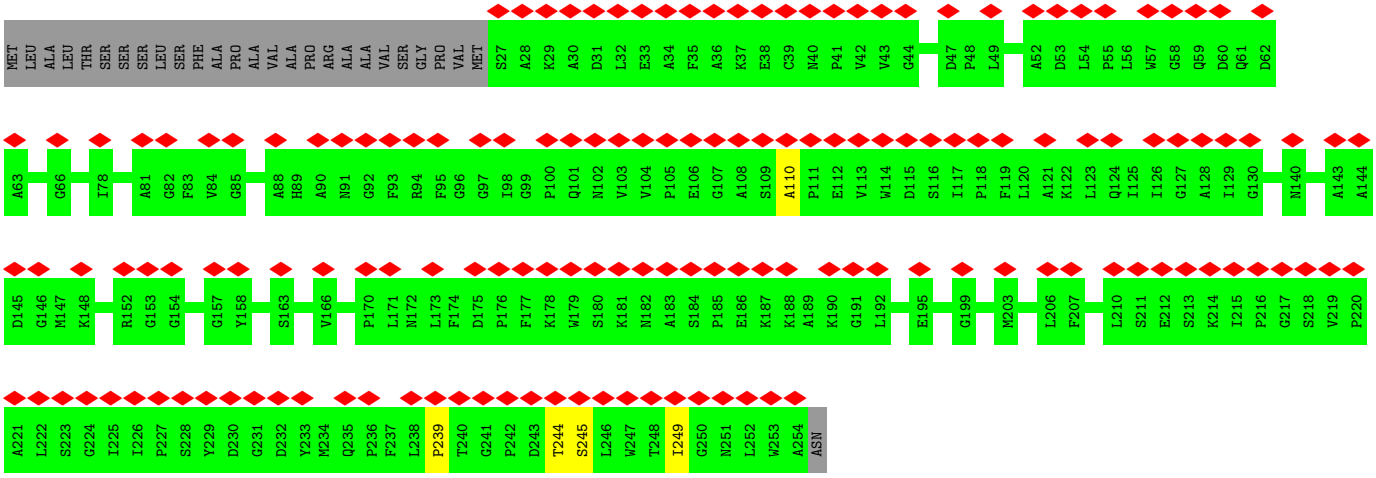
Chain 7:



• Molecule 28: Light harvesting protein

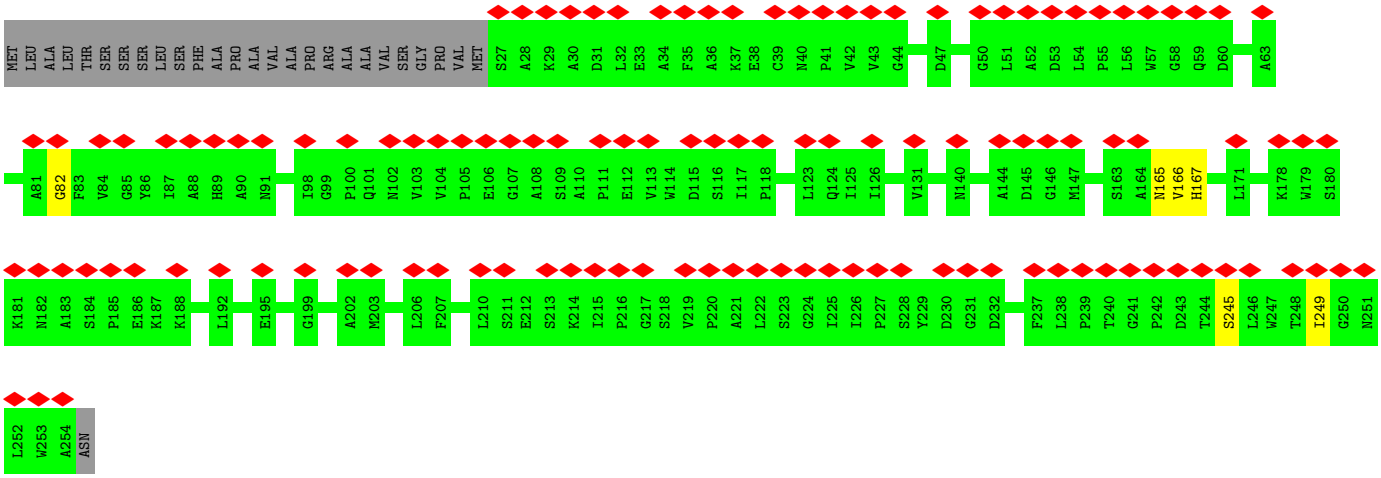
Chain x:





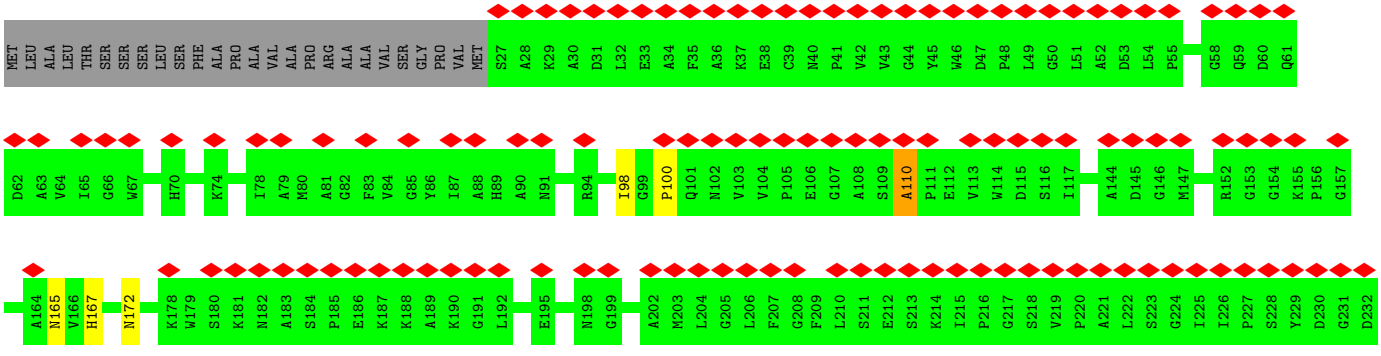
• Molecule 28: Light harvesting protein

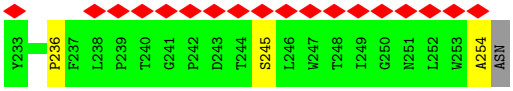
Chain y:



• Molecule 28: Light harvesting protein

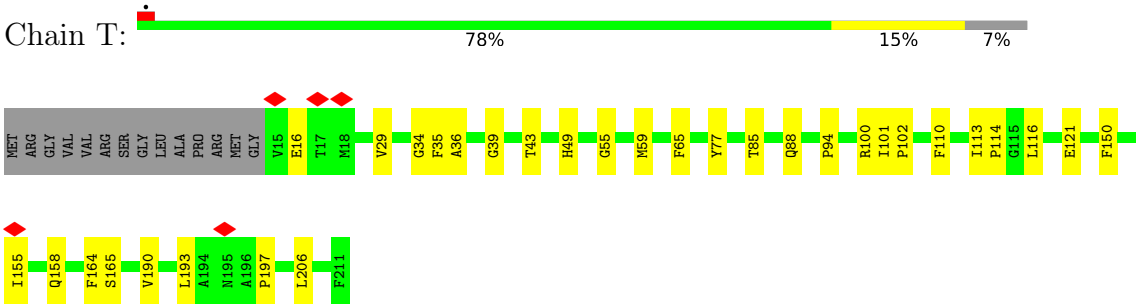
Chain z:





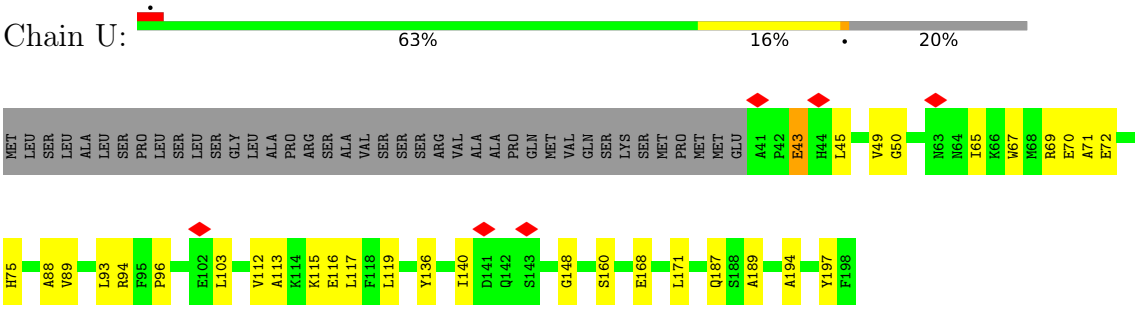
• Molecule 29: Light harvesting protein

Chain T:



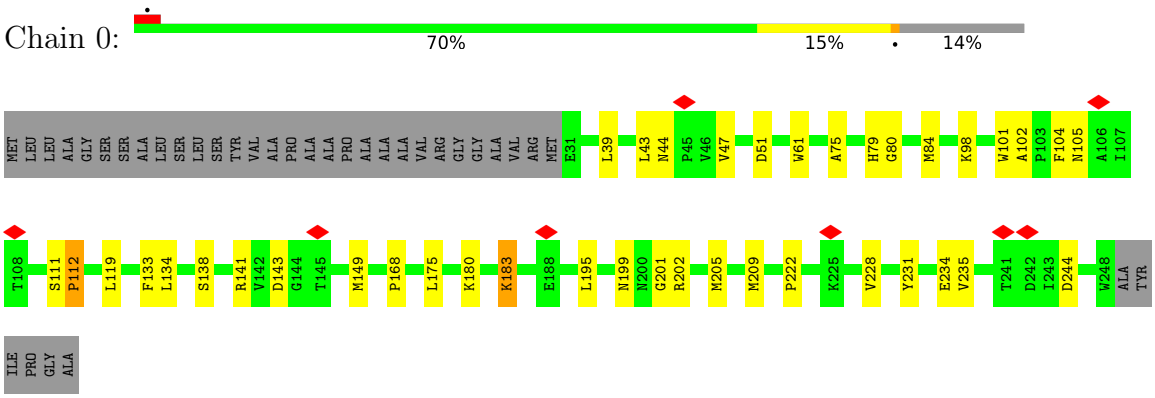
• Molecule 30: Light harvesting protein

Chain U:



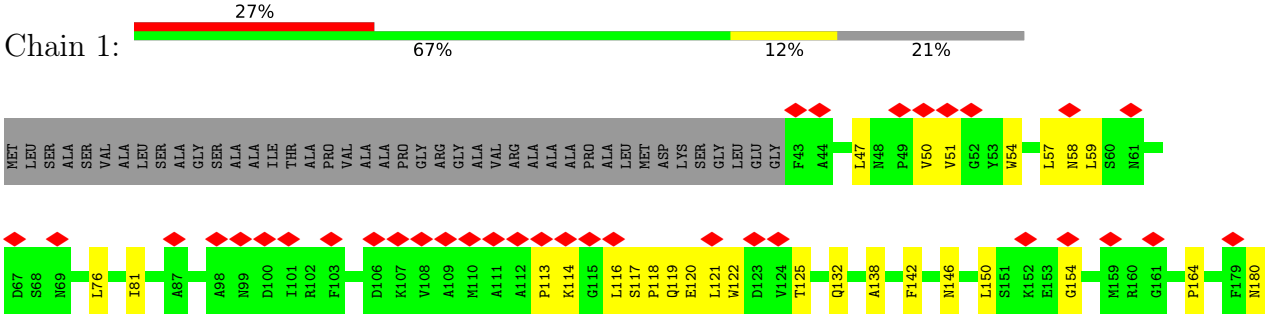
• Molecule 31: Light harvesting protein

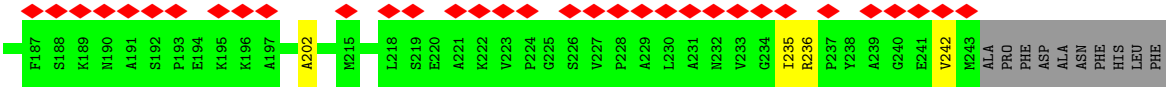
Chain 0:



• Molecule 32: Light harvesting protein

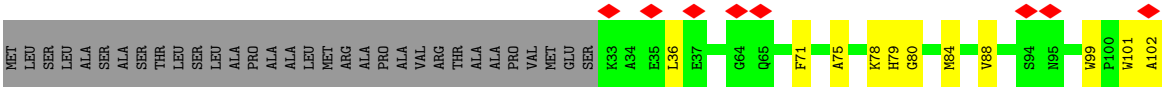
Chain 1:

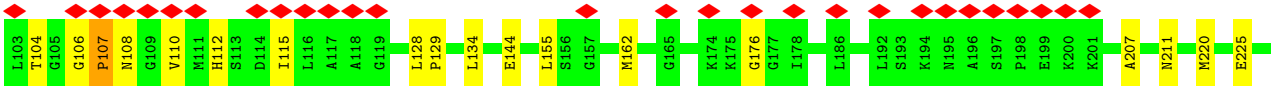


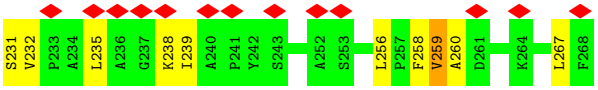


• Molecule 33: Light harvesting protein

Chain 3:

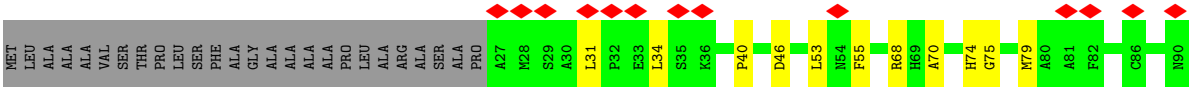


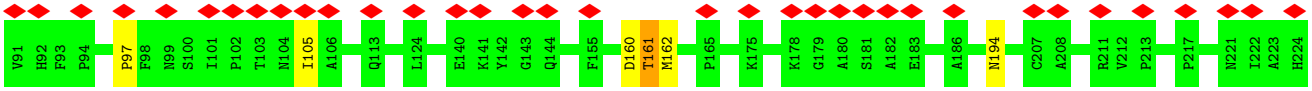


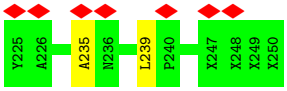


• Molecule 34: Light harvesting protein

Chain 8:

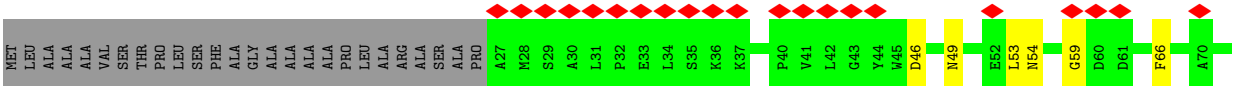


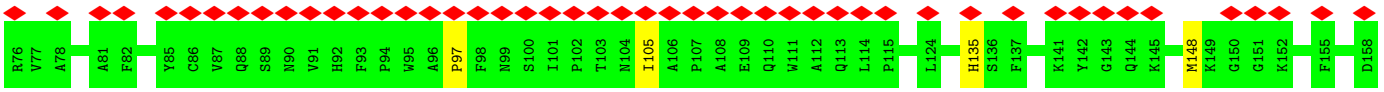


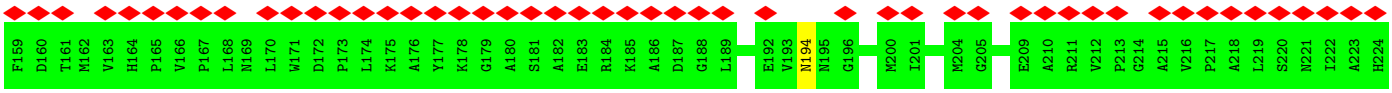


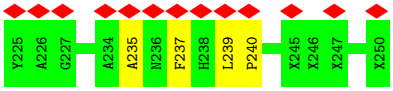
• Molecule 34: Light harvesting protein

Chain 6:



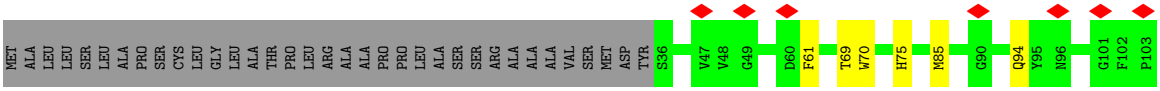


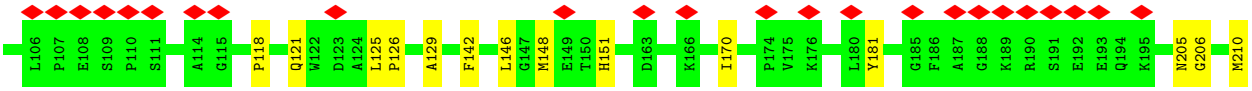


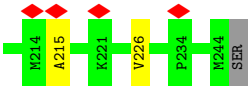


• Molecule 35: Light harvesting protein

Chain 9:

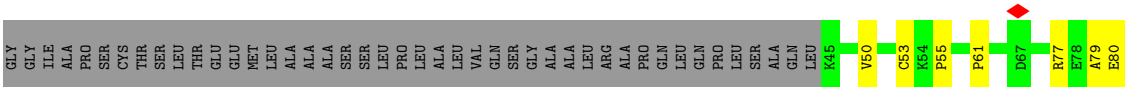


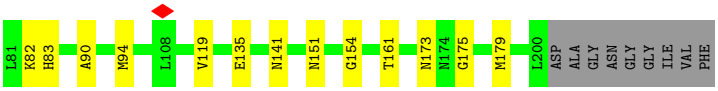




• Molecule 36: Light harvesting protein

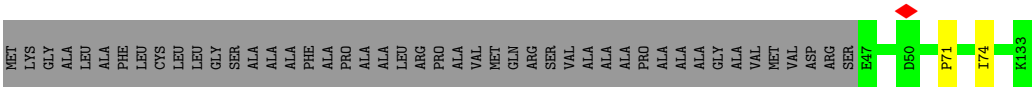
Chain I:





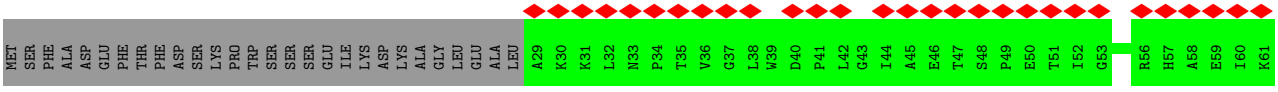
• Molecule 37: PsaR

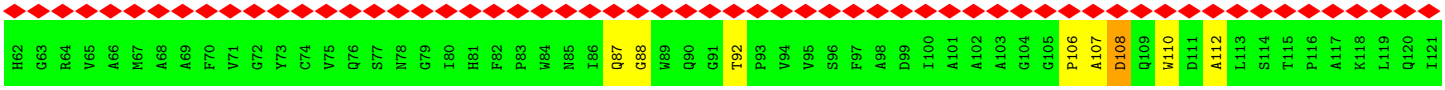
Chain h:

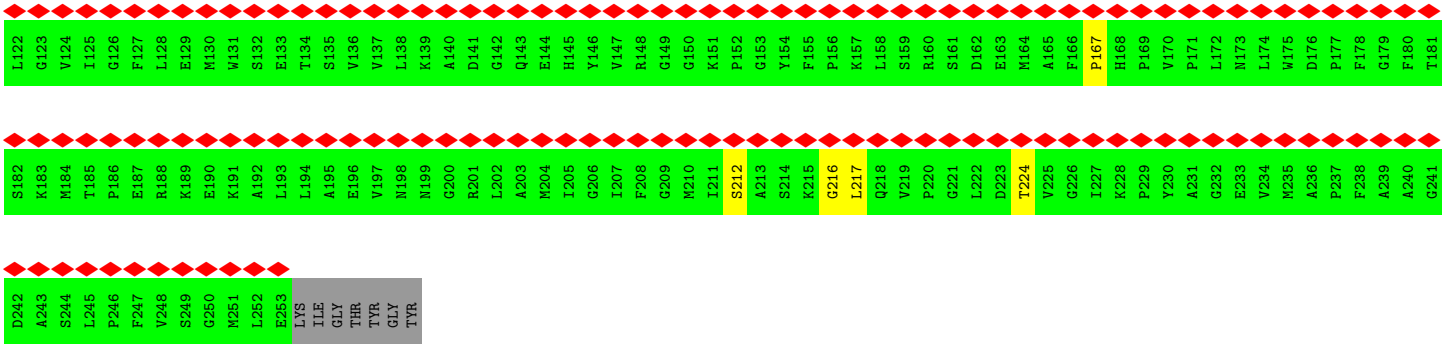


• Molecule 38: Light harvesting protein

Chain Y:

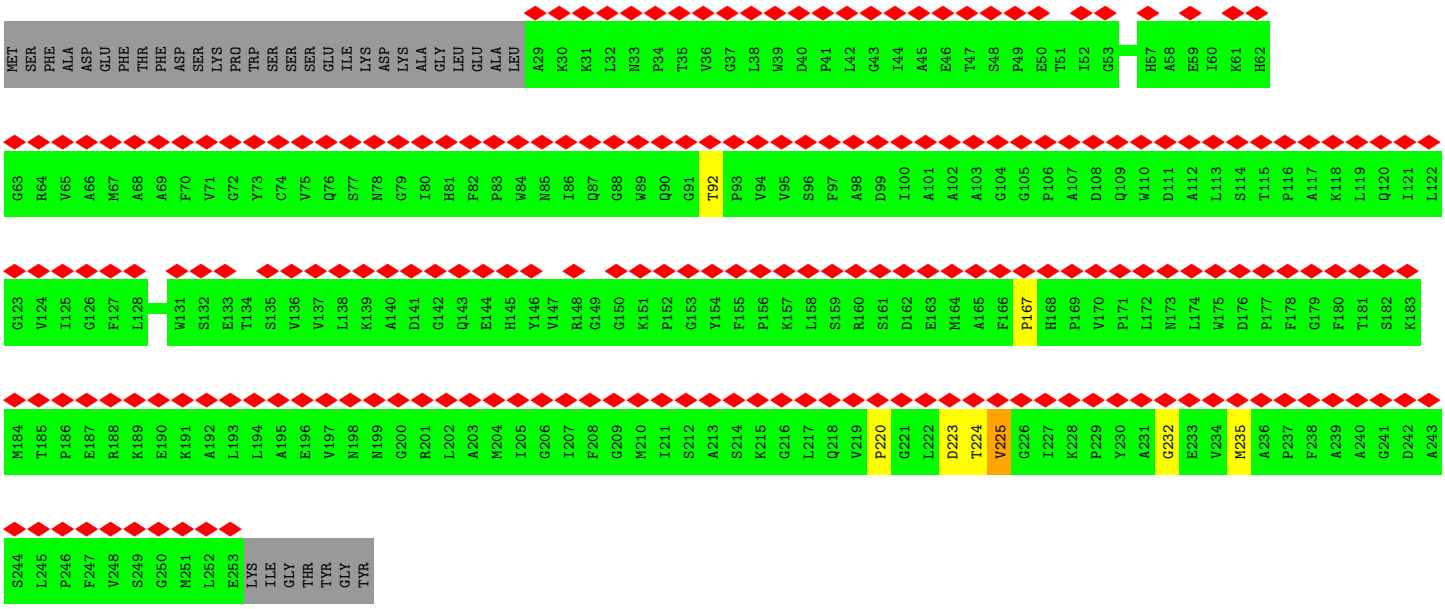






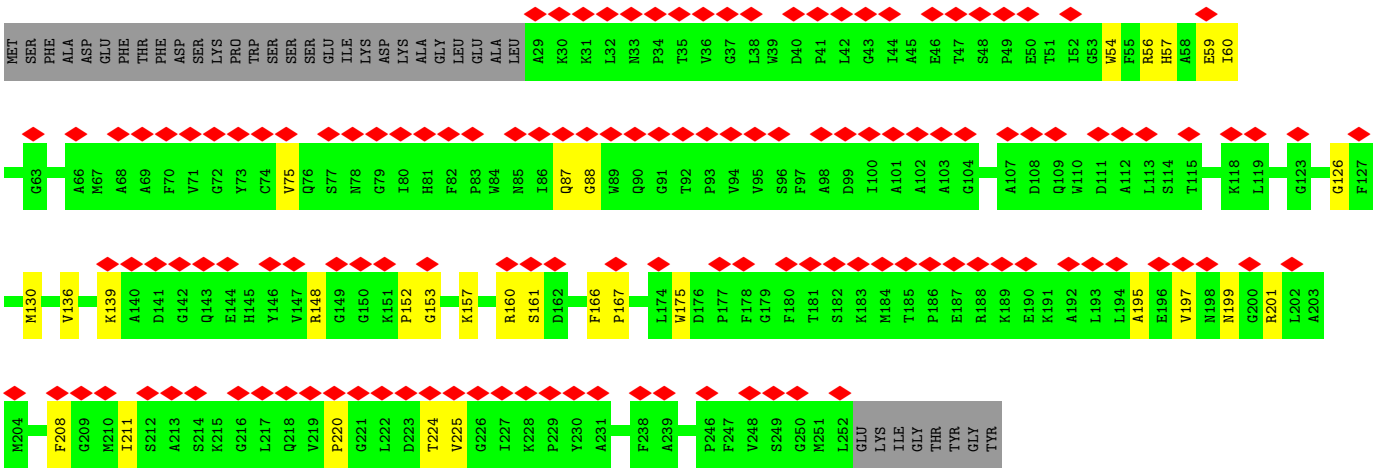
• Molecule 38: Light harvesting protein

Chain Z:



• Molecule 38: Light harvesting protein

Chain 2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70606	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.066	Depositor
Map size (Å)	533.28, 533.28, 533.28	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.808, 0.808, 0.808	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, DD6, BCR, CLA, A1EB4, A86, LHG, PQN, A1EB1, A1ECV, SQD, SF4, KC2, DGD

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	0.18	0/6028	0.40	0/8207
2	b	0.22	0/6028	0.46	1/8222 (0.0%)
3	c	0.16	0/608	0.54	0/824
4	d	0.18	0/1128	0.47	0/1525
5	e	0.24	0/503	0.45	0/683
6	f	0.18	0/1263	0.45	0/1714
7	i	0.30	0/261	0.56	0/357
8	j	0.14	0/325	0.33	0/438
9	l	0.19	0/1113	0.41	0/1513
10	m	0.21	0/226	0.62	0/306
11	k	0.19	0/545	0.43	0/737
12	o	0.21	0/371	0.59	0/503
13	A	0.18	0/1458	0.43	0/1979
14	B	0.20	0/1285	0.49	0/1750
15	C	0.21	0/1357	0.48	0/1836
16	D	0.19	0/1462	0.47	0/1988
17	E	0.22	0/1417	0.51	0/1933
18	F	0.28	0/1449	0.64	3/1967 (0.2%)
19	G	0.22	0/1386	0.55	2/1885 (0.1%)
20	H	0.25	0/1296	0.54	0/1757
21	J	0.23	0/1294	0.54	0/1749
22	K	0.24	0/1281	0.56	1/1744 (0.1%)
23	L	0.20	0/1684	0.49	0/2298
24	M	0.21	0/1491	0.42	0/2020
24	P	0.18	0/1491	0.42	0/2020
24	W	0.21	0/1491	0.45	0/2020
25	O	0.25	0/1152	0.60	0/1555
26	Q	0.26	0/1719	0.60	0/2340
27	5	0.24	0/1346	0.60	0/1830
27	R	0.22	0/1346	0.57	0/1830
27	V	0.23	0/1339	0.57	0/1820
27	X	0.23	0/1346	0.54	0/1830

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
28	4	0.21	0/1801	0.51	2/2451 (0.1%)
28	7	0.20	0/1801	0.48	0/2451
28	S	0.21	0/1801	0.49	0/2451
28	x	0.17	0/1112	0.43	0/1539
28	y	0.16	0/1112	0.38	0/1539
28	z	0.15	0/1112	0.41	0/1539
29	T	0.24	0/1534	0.55	1/2091 (0.0%)
30	U	0.21	0/1274	0.48	0/1726
31	0	0.24	0/1764	0.59	2/2410 (0.1%)
32	1	0.26	0/1284	0.56	0/1770
33	3	0.21	0/1828	0.54	3/2483 (0.1%)
34	6	0.16	0/1317	0.42	0/1813
34	8	0.20	0/1413	0.48	0/1941
35	9	0.25	0/1537	0.57	0/2106
36	I	0.23	0/1233	0.50	0/1666
37	h	0.17	0/669	0.37	0/915
38	2	0.23	0/1401	0.64	0/1911
38	Y	0.19	0/1098	0.59	1/1520 (0.1%)
38	Z	0.18	0/1098	0.58	0/1520
All	All	0.21	0/72678	0.50	16/99022 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	668	ARG	N-CA-C	10.45	123.65	111.11
22	K	36	VAL	N-CA-C	-6.07	107.94	113.71
28	4	165	ASN	CA-C-N	5.99	132.74	121.97
28	4	165	ASN	C-N-CA	5.99	132.74	121.97
33	3	231	SER	CA-C-N	5.66	132.60	122.13
33	3	231	SER	C-N-CA	5.66	132.60	122.13
31	0	112	PRO	CA-C-N	-5.59	112.85	119.05
31	0	112	PRO	C-N-CA	-5.59	112.85	119.05
33	3	107	PRO	N-CA-C	5.59	123.98	112.47
38	Y	217	LEU	CB-CA-C	-5.43	109.33	115.79
18	F	192	THR	CA-C-N	5.25	131.56	121.54
18	F	192	THR	C-N-CA	5.25	131.56	121.54
19	G	143	LYS	CA-C-N	5.21	131.77	122.13
19	G	143	LYS	C-N-CA	5.21	131.77	122.13
18	F	232	ALA	N-CA-C	-5.17	106.78	114.64
29	T	114	PRO	CA-N-CD	-5.11	104.84	112.00

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	5835	0	5733	90	0
2	b	5818	0	5640	71	0
3	c	598	0	581	7	0
4	d	1103	0	1113	20	0
5	e	491	0	480	1	0
6	f	1232	0	1231	13	0
7	i	254	0	262	5	0
8	j	318	0	333	7	0
9	l	1084	0	1090	15	0
10	m	224	0	243	7	0
11	k	533	0	547	11	0
12	o	360	0	363	6	0
13	A	1419	0	1408	20	0
14	B	1255	0	1223	28	0
15	C	1329	0	1352	16	0
16	D	1424	0	1361	20	0
17	E	1384	0	1399	22	0
18	F	1411	0	1407	41	0
19	G	1340	0	1303	17	0
20	H	1263	0	1232	23	0
21	J	1270	0	1295	33	0
22	K	1251	0	1249	16	0
23	L	1626	0	1560	19	0
24	M	1455	0	1468	40	0
24	P	1455	0	1468	26	0
24	W	1455	0	1468	29	0
25	O	1133	0	1141	28	0
26	Q	1666	0	1649	69	0
27	5	1311	0	1326	19	0
27	R	1311	0	1326	18	0
27	V	1353	0	1332	22	0
27	X	1311	0	1326	20	0
28	4	1744	0	1703	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	7	1744	0	1703	19	0
28	S	1744	0	1703	34	0
28	x	1113	0	529	2	0
28	y	1113	0	529	3	0
28	z	1113	0	529	4	0
29	T	1482	0	1457	22	0
30	U	1240	0	1212	22	0
31	0	1706	0	1662	24	0
32	1	1255	0	932	19	0
33	3	1775	0	1765	22	0
34	6	1326	0	910	8	0
34	8	1415	0	1126	9	0
35	9	1490	0	1326	17	0
36	I	1203	0	1215	15	0
37	h	650	0	636	1	0
38	2	1383	0	1078	18	0
38	Y	1099	0	529	4	0
38	Z	1099	0	529	2	0
39	0	457	0	379	18	0
39	1	384	0	279	6	0
39	2	385	0	275	5	0
39	3	477	0	425	12	0
39	4	460	0	454	14	0
39	5	339	0	320	7	0
39	6	345	0	258	3	0
39	7	410	0	353	19	0
39	8	353	0	266	7	0
39	9	347	0	258	10	0
39	A	531	0	527	12	0
39	B	287	0	228	7	0
39	C	470	0	474	13	0
39	D	685	0	725	25	0
39	E	728	0	683	20	0
39	F	551	0	512	13	0
39	G	280	0	257	3	0
39	H	479	0	430	13	0
39	I	520	0	512	12	0
39	J	576	0	506	15	0
39	K	418	0	427	13	0
39	L	420	0	364	7	0
39	M	444	0	424	11	0
39	O	423	0	332	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	P	352	0	358	8	0
39	Q	437	0	399	13	0
39	R	339	0	320	7	0
39	S	456	0	452	18	0
39	T	406	0	330	15	0
39	U	498	0	410	8	0
39	V	357	0	357	22	0
39	W	398	0	391	13	0
39	X	339	0	320	11	0
39	Y	374	0	265	2	0
39	Z	374	0	265	3	0
39	a	2327	0	2356	90	0
39	b	2553	0	2635	106	0
39	f	120	0	121	2	0
39	h	55	0	49	0	0
39	i	130	0	144	10	0
39	j	65	0	72	5	0
39	k	162	0	141	3	0
39	l	229	0	222	13	0
39	o	258	0	219	6	0
39	x	337	0	240	5	0
39	y	339	0	244	2	0
39	z	335	0	240	2	0
40	a	33	0	46	4	0
40	b	33	0	46	3	0
41	D	70	0	80	3	0
41	H	35	0	40	3	0
41	X	41	0	55	2	0
41	a	76	0	98	3	0
41	j	30	0	30	1	0
42	a	160	0	224	16	0
42	b	240	0	336	23	0
42	f	80	0	112	6	0
42	h	40	0	56	4	0
42	i	40	0	56	6	0
42	j	40	0	56	1	0
42	k	40	0	56	2	0
42	l	120	0	168	10	0
42	m	40	0	56	5	0
43	1	43	0	0	2	0
43	2	43	0	0	1	0
43	3	86	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	4	86	0	0	1	0
43	5	43	0	0	1	0
43	7	86	0	0	5	0
43	A	172	0	0	1	0
43	B	43	0	0	0	0
43	C	43	0	0	0	0
43	D	129	0	0	1	0
43	E	129	0	0	1	0
43	F	86	0	0	7	0
43	G	86	0	0	0	0
43	H	86	0	0	1	0
43	I	129	0	0	1	0
43	J	129	0	0	1	0
43	K	43	0	0	0	0
43	M	43	0	0	2	0
43	O	129	0	0	2	0
43	P	43	0	0	2	0
43	Q	86	0	0	5	0
43	R	43	0	0	0	0
43	S	43	0	0	1	0
43	T	43	0	0	0	0
43	U	43	0	0	1	0
43	V	43	0	0	0	0
43	W	43	0	0	0	0
43	X	43	0	0	0	0
43	Z	43	0	0	0	0
43	a	43	0	0	0	0
43	j	43	0	0	0	0
43	o	43	0	0	0	0
43	x	86	0	0	0	0
43	y	86	0	0	0	0
43	z	86	0	0	1	0
44	b	8	0	0	0	0
44	c	16	0	0	0	0
45	C	40	0	38	0	0
45	b	60	0	81	3	0
46	0	27	0	23	4	0
46	4	78	0	93	35	0
46	7	78	0	93	22	0
46	9	36	0	42	0	0
46	A	29	0	28	1	0
46	D	37	0	44	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	F	73	0	84	21	0
46	I	42	0	54	1	0
46	M	72	0	82	10	0
46	P	39	0	46	5	0
46	Q	28	0	25	2	0
46	S	78	0	93	23	0
46	W	72	0	82	14	0
46	l	39	0	47	4	0
47	4	39	0	42	1	0
47	7	39	0	42	1	0
47	9	36	0	36	1	0
47	D	114	0	119	6	0
47	E	35	0	34	0	0
47	F	79	0	86	1	0
47	H	38	0	40	3	0
47	M	39	0	42	3	0
47	P	38	0	40	1	0
47	S	39	0	42	4	0
47	T	36	0	35	1	0
47	W	28	0	20	1	0
47	k	38	0	40	2	0
48	0	240	0	0	1	0
48	1	192	0	0	1	0
48	2	144	0	0	1	0
48	3	192	0	0	0	0
48	4	240	0	0	0	0
48	5	48	0	0	2	0
48	6	240	0	0	0	0
48	7	192	0	0	1	0
48	8	288	0	0	0	0
48	9	240	0	0	1	0
48	B	48	0	0	0	0
48	C	48	0	0	0	0
48	D	48	0	0	1	0
48	E	48	0	0	1	0
48	F	96	0	0	9	0
48	G	96	0	0	0	0
48	H	48	0	0	0	0
48	I	48	0	0	1	0
48	J	96	0	0	0	0
48	K	48	0	0	0	0
48	L	288	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	M	144	0	0	0	0
48	O	144	0	0	0	0
48	P	96	0	0	0	0
48	Q	240	0	0	31	0
48	R	144	0	0	2	0
48	S	144	0	0	0	0
48	T	144	0	0	0	0
48	U	96	0	0	1	0
48	V	96	0	0	0	0
48	W	144	0	0	6	0
48	X	96	0	0	0	0
48	Y	48	0	0	0	0
48	Z	96	0	0	1	0
48	k	48	0	0	0	0
48	x	48	0	0	0	0
48	y	96	0	0	0	0
48	z	48	0	0	0	0
49	0	179	0	0	2	0
49	1	135	0	0	0	0
49	2	134	0	0	1	0
49	3	180	0	0	1	0
49	4	180	0	0	1	0
49	5	179	0	0	27	0
49	6	180	0	0	1	0
49	7	135	0	0	1	0
49	8	225	0	0	1	0
49	9	180	0	0	0	0
49	A	90	0	0	0	0
49	B	45	0	0	0	0
49	C	90	0	0	0	0
49	F	89	0	0	8	0
49	G	180	0	0	0	0
49	H	90	0	0	0	0
49	I	89	0	0	0	0
49	J	45	0	0	0	0
49	K	90	0	0	0	0
49	L	225	0	0	1	0
49	M	179	0	0	1	0
49	O	44	0	0	1	0
49	P	224	0	0	3	0
49	Q	134	0	0	1	0
49	R	179	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	S	135	0	0	0	0
49	T	180	0	0	2	0
49	V	270	0	0	1	0
49	W	179	0	0	3	0
49	X	224	0	0	20	0
49	Y	90	0	0	1	0
49	Z	90	0	0	0	0
49	x	135	0	0	1	0
49	y	135	0	0	0	0
49	z	134	0	0	0	0
50	0	224	0	0	4	0
50	1	112	0	0	0	0
50	2	112	0	0	1	0
50	3	280	0	0	0	0
50	4	224	0	0	1	0
50	5	56	0	0	0	0
50	6	213	0	0	0	0
50	7	224	0	0	1	0
50	8	224	0	0	0	0
50	9	56	0	0	1	0
50	C	56	0	0	0	0
50	D	56	0	0	0	0
50	E	56	0	0	0	0
50	F	56	0	0	4	0
50	G	224	0	0	0	0
50	H	112	0	0	1	0
50	J	56	0	0	0	0
50	K	168	0	0	0	0
50	L	56	0	0	0	0
50	O	56	0	0	0	0
50	Q	112	0	0	0	0
50	R	56	0	0	0	0
50	S	112	0	0	1	0
50	T	112	0	0	0	0
50	U	112	0	0	0	0
50	V	224	0	0	0	0
50	h	56	0	0	0	0
50	x	112	0	0	2	0
50	y	112	0	0	0	0
50	z	104	0	0	1	0
51	0	48	0	0	2	0
51	1	48	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	2	48	0	0	1	0
51	4	96	0	0	0	0
51	5	96	0	0	0	0
51	6	48	0	0	0	0
51	7	96	0	0	6	0
51	9	96	0	0	2	0
51	E	48	0	0	0	0
51	G	48	0	0	0	0
51	L	48	0	0	0	0
51	M	48	0	0	0	0
51	O	48	0	0	0	0
51	P	48	0	0	0	0
51	Q	96	0	0	0	0
51	R	96	0	0	0	0
51	S	96	0	0	0	0
51	T	48	0	0	1	0
51	V	48	0	0	0	0
51	W	48	0	0	0	0
51	X	96	0	0	0	0
51	Y	96	0	0	1	0
51	Z	96	0	0	0	0
51	x	96	0	0	1	0
51	y	96	0	0	1	0
51	z	96	0	0	1	0
52	5	57	0	0	1	0
52	M	115	0	0	0	0
52	P	167	0	0	5	0
52	R	57	0	0	1	0
52	T	55	0	0	0	0
52	W	113	0	0	5	0
52	X	57	0	0	0	0
All	All	114135	0	89288	1556	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 8.

All (1556) 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)
46:4:326:LMG:H311	49:5:313:KC2:C3A	1.15	1.56
49:X:314:KC2:C3A	46:7:301:LMG:H311	1.26	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:4:326:LMG:C31	49:5:313:KC2:C3A	2.03	1.35
46:4:326:LMG:C32	49:5:313:KC2:C4A	2.09	1.30
46:4:326:LMG:C31	49:5:313:KC2:C4A	2.12	1.27
49:X:314:KC2:C2A	46:7:301:LMG:H311	1.65	1.25
49:F:311:KC2:O1A	46:F:317:LMG:C6	1.86	1.24
49:X:314:KC2:C3A	46:7:301:LMG:C31	2.18	1.22
46:4:326:LMG:H321	49:5:313:KC2:CHB	1.71	1.20
46:4:326:LMG:H311	49:5:313:KC2:C2A	1.70	1.19
49:R:314:KC2:C2A	46:S:322:LMG:H311	1.73	1.19
46:4:326:LMG:H312	49:5:313:KC2:C1A	1.72	1.17
49:X:314:KC2:CAA	46:7:301:LMG:O10	1.92	1.16
46:4:326:LMG:C31	49:5:313:KC2:C2A	2.22	1.16
46:4:326:LMG:H311	49:5:313:KC2:C4A	1.75	1.16
46:4:326:LMG:O10	49:5:313:KC2:CAA	1.93	1.15
24:M:99:LYS:NZ	46:M:319:LMG:HC91	1.62	1.15
24:M:141:LYS:HB3	24:M:142:PRO:HD2	1.19	1.14
49:X:314:KC2:C2A	46:7:301:LMG:C31	2.24	1.13
49:X:314:KC2:C4A	46:7:301:LMG:C32	2.28	1.12
50:0:307:A1EB1:O43	46:0:324:LMG:H312	1.49	1.11
26:Q:232:LYS:HE2	48:Q:304:A86:C33	1.80	1.11
39:a:801:CLA:H2A	39:a:801:CLA:HED2	1.10	1.10
49:X:314:KC2:C1A	46:7:301:LMG:H312	1.81	1.09
49:X:314:KC2:C4A	46:7:301:LMG:C31	2.30	1.09
49:X:314:KC2:C4A	46:7:301:LMG:H311	1.82	1.08
49:F:311:KC2:O1A	46:F:317:LMG:HC62	1.50	1.06
39:V:316:CLA:HBA2	46:W:302:LMG:H161	1.38	1.03
46:4:326:LMG:C32	49:5:313:KC2:CHB	2.33	1.03
24:W:141:LYS:HB3	24:W:142:PRO:HD3	1.38	1.03
24:M:99:LYS:CE	46:M:319:LMG:HC91	1.88	1.02
39:V:316:CLA:HBA2	46:W:302:LMG:H181	1.39	1.02
49:X:314:KC2:CHB	46:7:301:LMG:H321	1.92	1.00
24:M:99:LYS:HD2	46:M:319:LMG:HC71	1.44	1.00
49:0:314:KC2:O1A	46:0:324:LMG:O6	1.80	0.98
24:M:141:LYS:HB3	24:M:142:PRO:CD	1.95	0.97
49:X:314:KC2:C1A	46:7:301:LMG:C31	2.41	0.97
4:d:100:HIS:CG	4:d:101:PRO:HD2	2.00	0.96
24:M:99:LYS:HZ3	46:M:319:LMG:HC91	1.28	0.95
49:R:314:KC2:C3A	46:S:322:LMG:H311	1.96	0.95
46:4:326:LMG:H322	49:5:313:KC2:C4A	1.96	0.94
46:4:326:LMG:C31	49:5:313:KC2:C1A	2.42	0.94
26:Q:230:PHE:CE2	48:Q:304:A86:C39	2.51	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:l:205:CLA:O1A	46:l:208:LMG:HC61	1.68	0.93
49:F:311:KC2:CGA	46:F:317:LMG:C6	2.46	0.93
46:4:326:LMG:H312	49:5:313:KC2:C2A	1.94	0.93
39:V:316:CLA:CBA	46:W:302:LMG:H161	1.99	0.93
48:R:302:A86:C7	46:S:322:LMG:C25	2.47	0.92
46:4:326:LMG:H322	49:5:313:KC2:NA	1.83	0.92
49:R:314:KC2:C2A	46:S:322:LMG:C31	2.49	0.90
26:Q:232:LYS:HE2	48:Q:304:A86:C31	2.01	0.90
48:F:302:A86:C41	46:F:317:LMG:H111	2.02	0.90
26:Q:232:LYS:HE2	48:Q:304:A86:C32	2.02	0.89
24:M:99:LYS:NZ	46:M:319:LMG:C9	2.36	0.88
46:4:326:LMG:H311	49:5:313:KC2:CMA	2.02	0.88
49:0:314:KC2:O1A	46:0:324:LMG:C5	1.98	0.88
26:Q:216:PHE:HE2	43:Q:303:DD6:C5	1.87	0.88
39:a:801:CLA:H2A	39:a:801:CLA:CED	2.03	0.87
33:3:220:MET:HE2	43:3:304:DD6:C2	2.02	0.87
27:V:194:VAL:HG11	39:V:313:CLA:H201	1.56	0.86
39:a:830:CLA:HBB1	39:a:831:CLA:H2	1.59	0.85
46:4:326:LMG:C31	49:5:313:KC2:NA	2.40	0.84
49:X:314:KC2:NA	46:7:301:LMG:H322	1.92	0.84
46:4:326:LMG:C32	49:5:313:KC2:NA	2.41	0.82
49:R:314:KC2:C4A	46:S:322:LMG:H322	2.10	0.82
24:P:99:LYS:HE2	46:P:317:LMG:HC72	1.59	0.81
18:F:127:ILE:CD1	46:F:320:LMG:O9	2.28	0.81
26:Q:230:PHE:CE2	48:Q:304:A86:C38	2.63	0.80
25:O:76:LEU:HD11	39:O:310:CLA:H2	1.62	0.80
18:F:125:ALA:HB3	46:F:320:LMG:HC3	1.64	0.80
24:W:141:LYS:HB3	24:W:142:PRO:CD	2.10	0.79
46:W:302:LMG:C32	48:W:304:A86:C41	2.59	0.79
35:9:210:MET:HE1	39:9:308:CLA:HAB	1.65	0.79
24:M:141:LYS:O	24:M:142:PRO:C	2.26	0.79
49:X:314:KC2:C4A	46:7:301:LMG:H321	2.05	0.78
49:X:314:KC2:NA	46:7:301:LMG:C32	2.45	0.78
39:0:312:CLA:H43	39:0:312:CLA:HMA3	1.64	0.78
1:a:739:THR:HB	39:a:801:CLA:HED1	1.63	0.78
24:M:99:LYS:HZ3	46:M:319:LMG:C9	1.95	0.78
43:F:305:DD6:C21	39:F:316:CLA:HBB1	2.14	0.78
46:W:302:LMG:H322	48:W:304:A86:C41	2.15	0.77
39:V:316:CLA:CBA	46:W:302:LMG:H181	2.14	0.76
49:X:314:KC2:NA	46:7:301:LMG:C31	2.47	0.76
21:J:186:MET:HE1	39:J:309:CLA:HAB	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:217:MET:HE2	43:F:303:DD6:C6	2.16	0.76
52:5:304:A1EB4:C42	49:5:313:KC2:CBB	2.65	0.75
24:P:99:LYS:HE2	46:P:317:LMG:C7	2.17	0.75
26:Q:230:PHE:CD2	48:Q:304:A86:C39	2.70	0.75
24:M:99:LYS:HE2	46:M:319:LMG:HC91	1.69	0.75
39:b:840:CLA:H152	42:l:202:BCR:H17C	1.70	0.74
39:4:323:CLA:H121	46:4:326:LMG:H171	1.69	0.74
46:W:302:LMG:H321	48:W:304:A86:C41	2.18	0.73
27:5:72:SER:HB2	27:5:183:GLY:HA3	1.69	0.73
12:o:72:GLY:HA2	16:D:214:ASP:HB3	1.69	0.73
26:Q:230:PHE:CD2	48:Q:304:A86:O4	2.41	0.73
43:2:303:DD6:C12	39:2:308:CLA:HMC2	2.18	0.73
49:X:314:KC2:C2A	46:7:301:LMG:H312	2.04	0.73
39:l:205:CLA:HMC2	46:l:208:LMG:H352	1.71	0.72
39:b:826:CLA:HMA1	42:b:847:BCR:H14C	1.72	0.72
26:Q:232:LYS:CE	48:Q:304:A86:C33	2.66	0.72
18:F:127:ILE:HD13	46:F:320:LMG:O9	1.89	0.72
25:O:93:GLY:HA3	25:O:193:SER:HB2	1.71	0.72
49:X:314:KC2:CHB	46:7:301:LMG:C32	2.62	0.71
26:Q:230:PHE:HD2	48:Q:304:A86:C34	2.02	0.71
4:d:100:HIS:CB	4:d:101:PRO:HD2	2.20	0.71
28:S:238:LEU:HB3	28:S:239:PRO:HD2	1.73	0.71
52:R:305:A1EB4:C42	49:R:314:KC2:CBB	2.69	0.71
39:V:316:CLA:CGA	46:W:302:LMG:H161	2.20	0.70
46:W:302:LMG:H362	48:W:304:A86:C28	2.21	0.70
48:F:302:A86:C33	46:F:317:LMG:C11	2.70	0.70
43:J:305:DD6:C24	39:J:314:CLA:HAB	2.22	0.70
4:d:100:HIS:O	4:d:101:PRO:C	2.35	0.70
18:F:215:LEU:HD11	50:F:304:A1EB1:C12	2.22	0.70
48:F:302:A86:C33	46:F:317:LMG:H111	2.21	0.69
49:R:314:KC2:CAA	46:S:322:LMG:H311	2.21	0.69
24:W:219:ALA:HB2	52:W:306:A1EB4:C42	2.23	0.69
18:F:217:MET:HE3	43:F:303:DD6:C5	2.22	0.69
22:K:153:PRO:O	22:K:154:ARG:HB2	1.92	0.69
11:k:74:PRO:HB3	11:k:80:LYS:HD2	1.75	0.69
48:F:302:A86:C5	49:F:311:KC2:CBC	2.70	0.69
28:S:238:LEU:O	28:S:239:PRO:C	2.36	0.69
30:U:43:GLU:HG3	30:U:45:LEU:H	1.58	0.68
25:O:188:ALA:O	25:O:192:HIS:ND1	2.25	0.68
21:J:153:ARG:HG2	21:J:154:LYS:N	2.07	0.68
27:V:72:SER:HB2	27:V:183:GLY:HA3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:436:ALA:O	1:a:440:HIS:ND1	2.25	0.67
27:R:72:SER:HB2	27:R:183:GLY:HA3	1.76	0.67
49:F:311:KC2:O1A	46:F:317:LMG:O5	2.08	0.67
26:Q:230:PHE:HD2	48:Q:304:A86:O4	1.76	0.67
21:J:114:PHE:HB2	21:J:201:LEU:HD13	1.76	0.67
21:J:157:GLU:HG2	21:J:159:ALA:H	1.59	0.67
48:R:302:A86:C12	46:S:322:LMG:H212	2.25	0.67
30:U:49:VAL:HG13	30:U:168:GLU:HG3	1.77	0.67
2:b:417:ALA:O	2:b:421:HIS:ND1	2.26	0.66
39:j:101:CLA:H101	39:j:101:CLA:H193	1.77	0.66
30:U:112:VAL:HB	30:U:116:GLU:HB2	1.77	0.66
4:d:100:HIS:CG	4:d:101:PRO:CD	2.78	0.66
18:F:103:ARG:NH1	18:F:106:GLU:OE2	2.28	0.66
49:F:311:KC2:CGA	46:F:317:LMG:HC61	2.24	0.66
42:b:850:BCR:HC7	39:b:851:CLA:H151	1.78	0.66
28:S:238:LEU:CB	28:S:239:PRO:HD2	2.25	0.66
26:Q:232:LYS:CE	48:Q:304:A86:C31	2.73	0.66
49:R:314:KC2:C3A	46:S:322:LMG:C31	2.73	0.66
27:X:133:LEU:HD21	41:X:301:LHG:H281	1.77	0.66
36:I:179:MET:HE1	39:I:309:CLA:HAB	1.78	0.66
10:m:18:ALA:HB2	42:m:101:BCR:C14	2.26	0.66
26:Q:216:PHE:CE2	43:Q:303:DD6:C5	2.75	0.66
24:W:140:LYS:HG3	24:W:154:GLU:HB2	1.78	0.66
49:X:314:KC2:CMA	46:7:301:LMG:H311	2.20	0.65
9:l:33:ASN:HB3	39:l:203:CLA:HAC1	1.78	0.65
27:X:72:SER:HB2	27:X:183:GLY:HA3	1.78	0.65
32:1:116:LEU:O	32:1:117:SER:C	2.39	0.65
39:4:323:CLA:H121	46:4:326:LMG:C17	2.26	0.65
24:P:49:TRP:CD1	52:P:318:A1EB4:C17	2.80	0.65
1:a:605:VAL:HG21	39:a:801:CLA:H202	1.79	0.65
47:D:304:SQD:H2	24:W:146:ARG:HH21	1.61	0.65
33:3:134:LEU:HD11	33:3:256:LEU:HD11	1.77	0.65
29:T:116:LEU:HD11	39:T:320:CLA:HBB1	1.79	0.65
24:P:49:TRP:HD1	52:P:318:A1EB4:C17	2.10	0.65
39:9:312:CLA:H3A	51:9:317:A1ECV:O1	1.97	0.65
14:B:44:LYS:HB3	14:B:172:LEU:HD22	1.79	0.64
1:a:116:GLN:NE2	39:a:807:CLA:OBD	2.29	0.64
18:F:133:ALA:O	18:F:135:ILE:HG22	1.98	0.64
39:6:313:CLA:HED3	39:6:313:CLA:H2A	1.79	0.64
39:a:804:CLA:H151	39:a:826:CLA:HBB2	1.78	0.64
18:F:217:MET:CE	43:F:303:DD6:C5	2.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5:34:ASP:OD2	27:5:35:MET:N	2.31	0.64
14:B:67:GLN:HE22	14:B:73:ILE:HB	1.63	0.64
39:V:316:CLA:HBA2	46:W:302:LMG:C16	2.23	0.64
39:b:801:CLA:H193	39:j:101:CLA:H142	1.77	0.64
12:o:78:GLU:HG3	12:o:81:ARG:HH21	1.63	0.64
13:A:124:ASN:HB2	13:A:127:LYS:HB2	1.79	0.64
26:Q:232:LYS:HE2	48:Q:304:A86:C35	2.27	0.64
27:X:206:LEU:HD12	27:X:207:PRO:HD2	1.79	0.63
24:W:140:LYS:HD2	24:W:154:GLU:HG2	1.79	0.63
18:F:217:MET:CE	43:F:303:DD6:C6	2.75	0.63
29:T:197:PRO:HD2	39:T:318:CLA:HAC1	1.81	0.63
30:U:112:VAL:HG21	39:U:209:CLA:HAA2	1.79	0.63
24:W:140:LYS:HG3	24:W:154:GLU:CB	2.29	0.63
27:V:194:VAL:CG1	39:V:313:CLA:H201	2.28	0.63
26:Q:230:PHE:C	26:Q:232:LYS:H	2.07	0.63
49:X:314:KC2:C4A	46:7:301:LMG:H322	2.21	0.63
4:d:89:ARG:HB2	4:d:99:LEU:HD11	1.80	0.62
48:F:302:A86:C33	46:F:317:LMG:O9	2.46	0.62
14:B:42:VAL:HG12	14:B:48:TRP:HE1	1.64	0.62
39:a:816:CLA:H92	39:a:826:CLA:H91	1.82	0.62
39:V:316:CLA:HBA2	46:W:302:LMG:C18	2.23	0.62
18:F:58:VAL:O	18:F:103:ARG:NH2	2.33	0.62
24:M:135:TRP:HE1	47:M:301:SQD:H461	1.65	0.62
27:X:187:MET:HE1	39:X:307:CLA:HAB	1.81	0.62
23:L:71:HIS:ND1	23:L:155:PRO:O	2.33	0.62
23:L:221:LEU:HD21	48:L:304:A86:C18	2.30	0.62
33:3:36:LEU:HB2	39:3:312:CLA:HED1	1.82	0.62
39:5:306:CLA:H202	49:5:313:KC2:CBC	2.30	0.62
26:Q:230:PHE:HE2	48:Q:304:A86:C38	2.12	0.62
27:X:88:GLY:O	27:X:109:ARG:NH2	2.33	0.61
28:7:28:ALA:HB1	28:7:65:ILE:HD11	1.82	0.61
34:8:70:ALA:O	34:8:74:HIS:ND1	2.33	0.61
25:O:64:THR:HG23	25:O:65:LEU:HD23	1.82	0.61
31:0:98:LYS:NZ	31:0:105:ASN:OD1	2.34	0.61
32:1:138:ALA:HB2	39:1:313:CLA:HAB	1.80	0.61
19:G:37:LEU:O	19:G:63:ARG:NH2	2.32	0.61
32:1:57:LEU:O	32:1:58:ASN:C	2.43	0.61
22:K:35:LEU:HB3	22:K:65:ARG:HH21	1.66	0.61
39:R:307:CLA:H202	49:R:314:KC2:CBC	2.30	0.61
24:P:99:LYS:CE	46:P:317:LMG:HC72	2.29	0.61
30:U:71:ALA:O	30:U:75:HIS:ND1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1:150:LEU:O	32:1:154:GLY:N	2.31	0.61
39:a:822:CLA:HBA1	39:a:826:CLA:H193	1.83	0.61
48:F:302:A86:C33	46:F:317:LMG:C10	2.79	0.61
25:O:65:LEU:HD21	35:9:146:LEU:HD21	1.81	0.61
49:R:314:KC2:CAA	46:S:322:LMG:O10	2.49	0.60
9:l:2:SER:N	36:I:161:THR:HG1	1.99	0.60
39:a:838:CLA:H161	42:l:206:BCR:H17C	1.82	0.60
28:7:77:ARG:NH1	28:7:157:GLY:O	2.33	0.60
14:B:77:ARG:HH12	39:B:209:CLA:H11	1.67	0.60
33:3:220:MET:CE	43:3:304:DD6:C2	2.77	0.60
31:0:202:ARG:NH2	39:0:311:CLA:O1D	2.34	0.60
32:1:142:PHE:O	32:1:146:ASN:ND2	2.34	0.60
19:G:87:ARG:NH1	19:G:103:LEU:O	2.35	0.60
1:a:685:MET:HE1	39:b:801:CLA:HMA3	1.84	0.60
49:M:313:KC2:CBC	39:M:317:CLA:H3A	2.32	0.60
46:4:326:LMG:H321	49:5:313:KC2:C4A	2.00	0.60
38:Y:106:PRO:O	38:Y:110:TRP:CB	2.50	0.60
39:0:312:CLA:H43	39:0:312:CLA:CMA	2.32	0.59
2:b:431:PHE:CD1	39:b:801:CLA:H12	2.37	0.59
39:D:317:CLA:H72	39:W:310:CLA:H101	1.83	0.59
18:F:125:ALA:CB	46:F:320:LMG:HC3	2.31	0.59
29:T:39:GLY:HA3	29:T:43:THR:HG21	1.82	0.59
39:a:816:CLA:HAB	39:a:816:CLA:H8	1.82	0.59
39:a:838:CLA:H93	39:a:838:CLA:HBB1	1.84	0.59
2:b:29:HIS:ND1	39:b:810:CLA:O1A	2.35	0.59
25:O:63:GLY:O	25:O:64:THR:HB	2.02	0.59
39:b:819:CLA:HBA2	39:b:827:CLA:HBB2	1.83	0.59
39:O:309:CLA:HAB	35:9:142:PHE:HE2	1.68	0.59
29:T:110:PHE:O	29:T:113:ILE:N	2.34	0.59
1:a:691:ARG:H	2:b:568:CYS:HB2	1.68	0.58
26:Q:232:LYS:HD2	48:Q:304:A86:C41	2.33	0.58
36:I:50:VAL:O	36:I:77:ARG:NH2	2.36	0.58
1:a:154:THR:HB	1:a:234:PRO:HB3	1.85	0.58
2:b:15:ASP:HB3	2:b:20:ARG:HB2	1.86	0.58
16:D:45:ALA:HA	16:D:53:GLU:HA	1.85	0.58
27:R:164:THR:HA	27:R:167:LEU:HD23	1.84	0.58
39:0:315:CLA:H3A	51:0:321:A1ECV:CMC	2.33	0.58
1:a:420:VAL:HG12	4:d:43:ILE:HB	1.85	0.58
28:S:52:ALA:O	28:S:61:GLN:NE2	2.35	0.58
27:V:103:THR:HG22	27:V:105:GLU:H	1.68	0.58
43:P:304:DD6:C23	39:P:307:CLA:H2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:U:89:VAL:O	30:U:94:ARG:NH1	2.34	0.58
13:A:79:TYR:OH	13:A:183:THR:OG1	2.22	0.58
17:E:57:PRO:O	43:E:303:DD6:O2	2.21	0.58
38:2:157:LYS:NZ	38:2:175:TRP:O	2.37	0.58
38:2:208:PHE:HA	38:2:211:ILE:HG22	1.86	0.58
13:A:41:PRO:O	13:A:62:ARG:NH2	2.37	0.58
21:J:129:LEU:HB2	39:J:311:CLA:H12	1.85	0.58
24:P:67:ARG:NH1	24:P:70:GLU:OE1	2.37	0.58
29:T:34:GLY:O	29:T:36:ALA:N	2.37	0.58
39:T:308:CLA:CED	39:T:308:CLA:H2A	2.33	0.58
39:l:205:CLA:CMC	46:l:208:LMG:H352	2.33	0.58
28:4:94:ARG:NH2	28:4:105:PRO:O	2.37	0.58
20:H:49:MET:HE3	21:J:143:ALA:HB1	1.86	0.58
39:a:824:CLA:H152	39:a:836:CLA:H191	1.85	0.57
26:Q:232:LYS:NZ	48:Q:304:A86:C30	2.67	0.57
27:R:88:GLY:O	27:R:109:ARG:NH2	2.37	0.57
46:4:326:LMG:H322	49:5:313:KC2:CHB	2.27	0.57
39:7:316:CLA:H72	39:7:324:CLA:HBB1	1.85	0.57
22:K:40:THR:HG21	39:K:306:CLA:HMA3	1.86	0.57
23:L:118:GLU:OE2	23:L:122:TRP:NE1	2.37	0.57
38:2:59:GLU:OE2	38:2:201:ARG:NH1	2.36	0.57
20:H:83:GLU:OE2	20:H:186:ARG:NH1	2.37	0.57
24:W:67:ARG:NH1	24:W:70:GLU:OE1	2.37	0.57
39:a:813:CLA:HAA2	39:E:316:CLA:HBA1	1.86	0.57
2:b:31:LEU:HA	2:b:34:HIS:CD2	2.39	0.57
14:B:25:TRP:O	14:B:29:HIS:ND1	2.33	0.57
39:b:801:CLA:C19	39:j:101:CLA:H142	2.34	0.57
21:J:82:GLY:HA3	21:J:182:SER:HB3	1.86	0.57
52:P:319:A1EB4:C24	39:R:311:CLA:HBB1	2.34	0.57
27:X:115:TRP:O	27:X:123:LYS:NZ	2.38	0.57
39:1:313:CLA:H3A	51:1:318:A1ECV:O1	2.03	0.57
28:7:139:LYS:N	51:7:323:A1ECV:OBD	2.37	0.57
39:a:818:CLA:H101	42:a:845:BCR:H10C	1.86	0.57
22:K:65:ARG:NH1	22:K:68:GLU:OE1	2.38	0.57
27:5:88:GLY:O	27:5:109:ARG:NH1	2.38	0.57
1:a:218:ILE:HA	1:a:222:LEU:HD12	1.87	0.57
14:B:43:ALA:HA	14:B:48:TRP:HD1	1.68	0.57
17:E:65:PRO:HG2	17:E:140:MET:HE1	1.85	0.57
25:O:61:LEU:HD22	25:O:194:ARG:HH12	1.70	0.57
43:7:310:DD6:C23	39:7:324:CLA:HAB	2.34	0.57
1:a:359:MET:HG3	39:a:822:CLA:HHB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:b:841:CLA:HHC	39:b:841:CLA:HBB1	1.86	0.57
30:U:115:LYS:NZ	39:U:201:CLA:O1A	2.38	0.57
27:V:48:ASP:HB3	27:V:51:GLY:HA2	1.86	0.57
27:X:164:THR:HA	27:X:167:LEU:HD23	1.85	0.57
27:X:158:TRP:CG	27:X:159:ASP:H	2.23	0.57
27:5:118:VAL:O	27:5:123:LYS:NZ	2.37	0.57
1:a:370:HIS:ND1	39:a:815:CLA:OBD	2.37	0.57
13:A:128:TRP:HD1	39:A:311:CLA:HMA1	1.70	0.57
19:G:63:ARG:NH1	19:G:66:GLU:OE1	2.37	0.57
30:U:88:ALA:HB1	30:U:93:LEU:HD12	1.86	0.57
39:z:306:CLA:H2A	39:z:306:CLA:HED3	1.87	0.57
2:b:580:MET:HG3	2:b:710:LEU:HD21	1.87	0.56
39:P:307:CLA:H92	39:P:308:CLA:H8	1.87	0.56
31:0:75:ALA:O	31:0:79:HIS:ND1	2.31	0.56
2:b:438:ILE:HG22	39:b:834:CLA:HAC1	1.87	0.56
22:K:152:VAL:HG22	39:K:312:CLA:HBD	1.87	0.56
26:Q:230:PHE:CD2	48:Q:304:A86:C38	2.87	0.56
30:U:50:GLY:HA3	30:U:171:LEU:HD23	1.87	0.56
28:S:249:ILE:HD11	33:3:267:LEU:HD22	1.86	0.56
43:1:304:DD6:C7	39:1:310:CLA:HAB	2.35	0.56
33:3:106:GLY:O	33:3:108:ASN:N	2.38	0.56
28:4:74:LYS:NZ	28:4:133:GLU:OE1	2.38	0.56
6:f:125:ARG:NH1	6:f:166:GLU:OE1	2.39	0.56
13:A:79:TYR:HE2	13:A:190:LEU:HB2	1.70	0.56
2:b:122:HIS:HB2	2:b:361:MET:HE3	1.87	0.56
2:b:350:GLN:HG3	39:b:826:CLA:HED1	1.88	0.56
27:X:159:ASP:OD2	27:X:163:PHE:N	2.39	0.56
27:5:206:LEU:HD12	27:5:207:PRO:HD2	1.87	0.56
34:8:40:PRO:HD3	39:8:310:CLA:HMA1	1.87	0.56
2:b:500:ALA:O	2:b:506:ASN:ND2	2.39	0.56
7:i:14:VAL:HG21	39:i:101:CLA:H12	1.88	0.56
29:T:55:GLY:O	29:T:59:MET:HG3	2.06	0.56
27:V:96:LEU:HD21	27:V:118:VAL:HG13	1.88	0.56
1:a:532:ASP:O	1:a:536:HIS:ND1	2.30	0.56
16:D:91:LYS:NZ	48:D:305:A86:O5	2.37	0.56
33:3:155:LEU:HD23	33:3:176:GLY:HA2	1.87	0.56
34:8:31:LEU:HD22	39:8:311:CLA:HED1	1.86	0.56
1:a:448:LEU:HB3	1:a:541:PHE:HB2	1.87	0.56
18:F:149:LEU:HD23	18:F:154:TRP:HB3	1.88	0.56
6:f:78:LYS:NZ	8:j:35:PRO:O	2.38	0.56
17:E:49:MET:HE3	17:E:70:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:137:GLU:O	21:J:141:ALA:HB3	2.06	0.56
23:L:64:ALA:HA	23:L:150:MET:HB2	1.86	0.56
39:Z:306:CLA:HBC1	39:Z:309:CLA:HAC1	1.88	0.56
34:6:66:PHE:HB2	34:6:148:MET:HE3	1.86	0.56
14:B:20:VAL:HG11	14:B:116:PRO:HD2	1.88	0.55
26:Q:216:PHE:CE2	43:Q:303:DD6:C3	2.89	0.55
39:4:323:CLA:C12	46:4:326:LMG:C17	2.84	0.55
1:a:174:VAL:HG12	41:D:302:LHG:H142	1.89	0.55
2:b:666:SER:C	2:b:667:TRP:HD1	2.14	0.55
26:Q:230:PHE:O	26:Q:232:LYS:N	2.38	0.55
27:R:159:ASP:HB3	39:R:316:CLA:HED2	1.89	0.55
9:l:61:PRO:HB3	39:l:205:CLA:HBB1	1.88	0.55
25:O:64:THR:HG22	39:O:308:CLA:CGD	2.36	0.55
35:9:181:TYR:HD1	39:9:319:CLA:HED2	1.71	0.55
36:I:77:ARG:NH1	36:I:80:GLU:OE1	2.39	0.55
46:I:302:LMG:H341	39:I:315:CLA:H42	1.87	0.55
1:a:435:ASP:OD2	1:a:561:ARG:NH1	2.40	0.55
14:B:170:ASN:O	14:B:171:LEU:C	2.49	0.55
39:D:317:CLA:H101	39:W:310:CLA:H121	1.88	0.55
18:F:118:THR:HG22	39:F:310:CLA:HBC2	1.89	0.55
38:2:56:ARG:HD2	38:2:152:PRO:HG2	1.88	0.55
13:A:62:ARG:NH1	13:A:65:GLU:OE1	2.39	0.55
15:C:75:VAL:O	15:C:100:ARG:NH2	2.40	0.55
24:M:141:LYS:CB	24:M:142:PRO:CD	2.80	0.55
27:V:133:LEU:HD22	27:V:157:LEU:HD13	1.89	0.55
46:4:326:LMG:C22	48:5:301:A86:C7	2.85	0.55
49:R:314:KC2:CHB	46:S:322:LMG:H351	2.37	0.55
36:I:119:VAL:HG22	39:I:311:CLA:HAA2	1.89	0.55
1:a:712:PRO:HG2	1:a:716:PRO:HD3	1.88	0.55
15:C:100:ARG:NH1	15:C:103:GLU:OE1	2.40	0.55
31:0:138:SER:O	31:0:141:ARG:NH1	2.39	0.55
24:W:75:ARG:NH2	49:W:314:KC2:O1D	2.40	0.55
33:3:99:TRP:HB3	33:3:101:TRP:HE3	1.71	0.55
35:9:75:HIS:HD2	39:9:312:CLA:HED2	1.72	0.55
18:F:215:LEU:CD1	50:F:304:A1EB1:C12	2.85	0.54
32:1:117:SER:O	32:1:118:PRO:C	2.48	0.54
1:a:120:PRO:HB3	1:a:125:GLU:HB3	1.89	0.54
26:Q:209:ARG:HA	26:Q:212:MET:HE3	1.89	0.54
30:U:187:GLN:NE2	30:U:197:TYR:O	2.39	0.54
39:V:316:CLA:HMB2	27:X:128:GLY:HA3	1.89	0.54
15:C:97:ARG:HH12	15:C:173:PRO:HA	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:K:90:HIS:ND1	22:K:91:PHE:O	2.33	0.54
39:Q:311:CLA:HMD3	39:Q:314:CLA:HBA2	1.89	0.54
28:S:164:ALA:O	46:S:321:LMG:O3	2.25	0.54
36:I:61:PRO:O	43:I:306:DD6:O2	2.26	0.54
39:Q:321:CLA:HHC	39:Q:321:CLA:HBB1	1.90	0.54
29:T:121:GLU:HG2	51:T:317:A1ECV:ND	2.23	0.54
39:z:311:CLA:H3A	51:z:316:A1ECV:O1	2.07	0.54
17:E:49:MET:HE1	17:E:66:ILE:HG13	1.89	0.54
38:2:57:HIS:CD2	38:2:153:GLY:H	2.25	0.54
20:H:207:PRO:O	50:H:304:A1EB1:O2	2.25	0.54
25:O:111:ARG:NH1	25:O:112:ALA:O	2.40	0.54
27:R:176:ARG:NH1	49:R:312:KC2:O2A	2.41	0.54
16:D:207:ASN:ND2	16:D:212:LEU:O	2.40	0.54
24:M:65:TRP:HB2	24:M:145:MET:HE2	1.90	0.54
26:Q:94:GLY:O	26:Q:98:HIS:ND1	2.41	0.54
24:W:141:LYS:O	24:W:143:HIS:N	2.40	0.54
28:4:131:VAL:HG22	46:4:325:LMG:H111	1.89	0.54
39:x:306:CLA:H2A	39:x:306:CLA:HED3	1.90	0.54
31:0:61:TRP:HE1	31:0:149:MET:HE1	1.73	0.54
39:a:827:CLA:H42	41:a:840:LHG:H252	1.90	0.54
3:c:24:ASP:OD2	4:d:100:HIS:HD2	1.91	0.54
4:d:100:HIS:ND1	4:d:101:PRO:HD2	2.23	0.54
28:4:139:LYS:NZ	49:4:324:KC2:O1D	2.41	0.54
16:D:221:ILE:HG13	16:D:222:VAL:HG23	1.91	0.53
22:K:57:ASP:OD1	22:K:58:GLU:N	2.41	0.53
25:O:64:THR:CG2	25:O:65:LEU:HD23	2.38	0.53
26:Q:232:LYS:HZ1	48:Q:304:A86:C30	2.21	0.53
1:a:196:SER:O	1:a:200:HIS:ND1	2.34	0.53
32:1:202:ALA:HB2	39:1:308:CLA:HED3	1.89	0.53
28:7:135:ILE:HG21	28:7:162:PHE:HE1	1.72	0.53
49:F:311:KC2:O1A	46:F:317:LMG:HC61	1.95	0.53
25:O:191:LYS:HA	25:O:194:ARG:HH21	1.74	0.53
39:9:319:CLA:HED3	39:9:319:CLA:H2A	1.89	0.53
49:6:316:KC2:CBC	39:6:321:CLA:H3A	2.39	0.53
39:b:827:CLA:H13	42:b:847:BCR:H15C	1.90	0.53
39:o:205:CLA:HAB	39:D:312:CLA:HAC1	1.90	0.53
28:S:137:GLU:OE1	28:S:149:HIS:NE2	2.33	0.53
39:0:315:CLA:H3A	51:0:321:A1ECV:O1	2.08	0.53
28:z:172:ASN:O	43:z:305:DD6:O2	2.27	0.53
39:b:840:CLA:HAB	40:b:843:PQN:H151	1.91	0.53
8:j:29:GLU:OE1	8:j:32:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B:206:CLA:HBB2	39:B:209:CLA:HBC2	1.90	0.53
39:M:310:CLA:H202	39:M:317:CLA:HAC1	1.91	0.53
27:5:158:TRP:CG	27:5:159:ASP:H	2.27	0.53
3:c:55:GLU:HB3	3:c:63:LEU:HD22	1.91	0.53
24:P:42:GLU:OE1	24:P:195:LYS:NZ	2.41	0.53
28:4:212:GLU:HG3	28:4:222:LEU:HB2	1.90	0.53
46:4:326:LMG:H312	49:5:313:KC2:NA	2.06	0.53
39:b:832:CLA:HAB	39:b:833:CLA:H203	1.90	0.53
39:S:320:CLA:H202	46:S:322:LMG:H151	1.91	0.53
49:8:316:KC2:CBC	39:8:321:CLA:H3A	2.39	0.53
39:a:820:CLA:HAB	39:I:301:CLA:HBB1	1.90	0.53
39:E:314:CLA:H42	39:M:309:CLA:H71	1.89	0.53
18:F:217:MET:CE	43:F:303:DD6:C8	2.87	0.53
47:H:318:SQD:H282	21:J:146:SER:HA	1.91	0.53
39:b:810:CLA:H151	39:b:829:CLA:HBB2	1.91	0.53
17:E:180:SER:HB3	39:E:315:CLA:HBC2	1.91	0.53
20:H:76:ILE:HD11	39:H:308:CLA:HAA2	1.90	0.53
21:J:153:ARG:HD2	21:J:157:GLU:HB3	1.90	0.53
23:L:221:LEU:HD23	48:L:304:A86:O2	2.09	0.53
28:S:212:GLU:HG3	28:S:222:LEU:HB2	1.90	0.53
29:T:39:GLY:HA2	30:U:160:SER:HB3	1.90	0.53
39:x:307:CLA:H2A	39:x:307:CLA:HED3	1.90	0.53
39:7:318:CLA:H3A	51:7:323:A1ECV:O2	2.09	0.53
39:A:306:CLA:HBA1	47:W:301:SQD:H1	1.91	0.52
22:K:152:VAL:O	22:K:153:PRO:C	2.51	0.52
49:R:314:KC2:C1A	46:S:322:LMG:C31	2.87	0.52
1:a:533:PHE:HA	39:a:835:CLA:HED1	1.90	0.52
1:a:580:ARG:NH1	4:d:67:GLU:OE1	2.41	0.52
39:b:807:CLA:H152	42:b:848:BCR:H362	1.90	0.52
26:Q:206:ASN:ND2	39:Q:309:CLA:O1D	2.38	0.52
33:3:110:VAL:HG12	33:3:112:HIS:H	1.73	0.52
28:S:131:VAL:HG11	39:S:320:CLA:HBA1	1.91	0.52
28:S:171:LEU:O	43:S:306:DD6:O2	2.28	0.52
39:S:308:CLA:H11	38:2:166:PHE:HA	1.91	0.52
27:X:118:VAL:O	27:X:123:LYS:NZ	2.42	0.52
39:a:818:CLA:H202	42:a:844:BCR:H272	1.91	0.52
24:W:45:GLY:HA3	27:5:142:LYS:HE3	1.91	0.52
2:b:111:TYR:HA	14:B:70:ASN:HB2	1.91	0.52
41:H:317:LHG:H152	41:H:317:LHG:H251	1.91	0.52
28:S:238:LEU:HD13	28:S:239:PRO:HD2	1.91	0.52
46:4:326:LMG:C32	49:5:313:KC2:C1B	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:7:310:DD6:C13	43:7:310:DD6:C21	2.87	0.52
39:9:312:CLA:H3A	51:9:317:A1ECV:CMC	2.39	0.52
1:a:584:CYS:O	2:b:669:GLY:N	2.42	0.52
1:a:741:TRP:NE1	39:a:825:CLA:O1A	2.40	0.52
14:B:3:GLN:NE2	14:B:7:ASP:OD2	2.42	0.52
48:F:302:A86:C41	46:F:317:LMG:H132	2.40	0.52
26:Q:206:ASN:OD1	48:Q:301:A86:O2	2.28	0.52
32:1:117:SER:O	32:1:120:GLU:N	2.42	0.52
28:4:75:HIS:HB3	28:4:203:MET:HE2	1.92	0.52
36:I:79:ALA:O	36:I:83:HIS:ND1	2.30	0.52
42:b:850:BCR:H323	39:b:851:CLA:H202	1.92	0.52
39:A:305:CLA:H3A	47:D:304:SQD:H442	1.92	0.52
26:Q:216:PHE:HE2	43:Q:303:DD6:C3	2.22	0.52
26:Q:221:GLU:HA	26:Q:225:PRO:HA	1.91	0.52
28:S:42:VAL:HA	38:2:136:VAL:HG21	1.91	0.52
49:2:313:KC2:CBC	39:2:318:CLA:H3A	2.39	0.52
39:a:802:CLA:HAB	39:a:809:CLA:H142	1.92	0.52
13:A:94:THR:O	13:A:96:ASN:N	2.39	0.52
22:K:58:GLU:OE1	22:K:62:LYS:NZ	2.39	0.52
25:O:86:ARG:NH1	25:O:89:GLU:OE1	2.40	0.52
30:U:45:LEU:HD12	30:U:65:ILE:HG21	1.91	0.52
30:U:69:ARG:NH1	30:U:72:GLU:OE1	2.43	0.52
4:d:100:HIS:HB3	4:d:101:PRO:HD2	1.90	0.52
14:B:45:SER:OG	14:B:46:HIS:N	2.41	0.52
18:F:88:GLU:OE1	18:F:91:LYS:NZ	2.43	0.52
47:F:319:SQD:H241	47:F:319:SQD:H81	1.91	0.52
22:K:85:THR:HG23	39:K:309:CLA:HED1	1.91	0.52
50:0:303:A1EB1:C3	39:0:312:CLA:HAB	2.40	0.52
39:a:831:CLA:H61	42:l:202:BCR:H363	1.90	0.51
39:i:103:CLA:OBD	14:B:77:ARG:NH2	2.43	0.51
10:m:26:ARG:HH12	14:B:7:ASP:HB3	1.74	0.51
18:F:134:ASP:OD2	46:F:317:LMG:HC4	2.10	0.51
39:K:308:CLA:H102	39:I:309:CLA:H143	1.90	0.51
24:M:192:ALA:O	24:M:196:ASN:ND2	2.35	0.51
26:Q:40:ASP:OD2	26:Q:40:ASP:N	2.43	0.51
28:S:94:ARG:NH2	28:S:105:PRO:O	2.40	0.51
24:W:219:ALA:HB2	52:W:306:A1EB4:C38	2.40	0.51
27:X:183:GLY:O	27:X:187:MET:HG3	2.10	0.51
27:5:159:ASP:OD2	27:5:163:PHE:N	2.43	0.51
2:b:410:ARG:O	2:b:414:HIS:ND1	2.41	0.51
11:k:97:ILE:HG22	11:k:98:GLN:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:103:ASP:HB2	39:B:207:CLA:HED2	1.92	0.51
18:F:61:SER:OG	48:F:301:A86:O2	2.26	0.51
18:F:204:LYS:NZ	49:F:307:KC2:O1A	2.41	0.51
26:Q:230:PHE:CD2	48:Q:304:A86:C34	2.88	0.51
33:3:220:MET:HE3	39:3:313:CLA:HAB	1.92	0.51
1:a:719:LEU:HD21	40:a:839:PQN:H151	1.91	0.51
39:b:807:CLA:H13	42:i:102:BCR:H271	1.92	0.51
21:J:142:GLY:O	21:J:146:SER:HB3	2.10	0.51
28:4:110:ALA:O	50:4:304:A1EB1:O2	2.29	0.51
38:2:57:HIS:CD2	38:2:148:ARG:HB3	2.45	0.51
25:O:194:ARG:HD2	39:O:310:CLA:C4C	2.41	0.51
43:O:304:DD6:C12	39:O:310:CLA:H143	2.40	0.51
46:7:326:LMG:O5	46:7:326:LMG:O4	2.26	0.51
34:8:46:ASP:OD1	34:8:46:ASP:N	2.43	0.51
39:b:838:CLA:H161	42:f:804:BCR:H23C	1.93	0.51
12:o:100:LYS:HB2	46:D:322:LMG:HC5	1.93	0.51
15:C:137:ASN:HB3	15:C:140:GLU:HB2	1.91	0.51
17:E:49:MET:HG2	17:E:70:ARG:HH21	1.74	0.51
29:T:165:SER:HB3	39:T:308:CLA:O1D	2.10	0.51
28:7:76:GLY:O	28:7:80:MET:HG3	2.10	0.51
2:b:694:ARG:HG2	39:b:840:CLA:HED2	1.92	0.51
25:O:62:ASP:O	25:O:63:GLY:C	2.52	0.51
39:0:312:CLA:H42	39:0:312:CLA:O1D	2.11	0.51
33:3:258:PHE:O	33:3:260:ALA:N	2.43	0.51
34:6:237:PHE:HB3	34:6:239:LEU:HD23	1.92	0.51
1:a:516:ALA:HB2	1:a:622:ILE:HD12	1.92	0.51
26:Q:232:LYS:NZ	48:Q:304:A86:C31	2.74	0.51
31:0:134:LEU:HD22	31:0:175:LEU:HD22	1.92	0.51
33:3:225:GLU:HB3	33:3:239:ILE:HG13	1.93	0.51
43:3:304:DD6:C22	39:3:312:CLA:H52	2.41	0.51
39:b:824:CLA:HBA1	42:h:202:BCR:H16C	1.92	0.51
17:E:158:ILE:HG23	24:M:58:VAL:HG12	1.93	0.51
23:L:42:PRO:HD3	39:L:308:CLA:HMA1	1.93	0.51
29:T:164:PHE:HD2	39:T:308:CLA:CED	2.24	0.51
46:4:326:LMG:H222	48:5:301:A86:C7	2.41	0.51
1:a:366:ILE:HG21	39:a:816:CLA:H191	1.93	0.51
39:b:824:CLA:HAB	39:b:831:CLA:HMD2	1.93	0.51
3:c:8:TYR:HH	3:c:68:TYR:HH	1.57	0.51
19:G:168:ALA:O	19:G:172:ASN:ND2	2.44	0.51
48:Q:302:A86:O5	46:Q:322:LMG:C9	2.58	0.51
25:O:100:VAL:HG23	25:O:203:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:V:309:CLA:HMB3	39:V:310:CLA:HBA2	1.92	0.51
50:0:303:A1EB1:C2	39:0:312:CLA:C3B	2.88	0.51
39:a:816:CLA:H203	39:a:824:CLA:H3A	1.93	0.50
9:l:114:LYS:O	9:l:118:ASN:ND2	2.45	0.50
17:E:214:LEU:O	24:P:212:ASN:ND2	2.40	0.50
31:0:133:PHE:CE2	39:0:323:CLA:H3A	2.46	0.50
36:I:173:ASN:ND2	39:I:308:CLA:O1D	2.44	0.50
28:4:27:SER:OG	28:4:28:ALA:N	2.44	0.50
39:8:313:CLA:H2A	39:8:313:CLA:HED2	1.93	0.50
38:2:160:ARG:HG2	38:2:161:SER:H	1.77	0.50
1:a:369:HIS:NE2	39:a:823:CLA:OBD	2.44	0.50
39:0:311:CLA:HMB1	39:0:312:CLA:HAA1	1.93	0.50
38:2:195:ALA:O	38:2:199:ASN:ND2	2.42	0.50
39:b:821:CLA:H71	39:b:827:CLA:H11	1.93	0.50
14:B:167:THR:HB	14:B:170:ASN:CG	2.37	0.50
39:4:314:CLA:H52	39:4:314:CLA:H142	1.93	0.50
34:8:194:ASN:ND2	39:8:310:CLA:O1D	2.41	0.50
29:T:101:ILE:HD11	39:T:311:CLA:H3A	1.92	0.50
39:l:203:CLA:HBA2	42:l:207:BCR:H352	1.94	0.50
39:k:201:CLA:HAB	47:k:205:SQD:H241	1.92	0.50
15:C:99:VAL:HG22	39:C:306:CLA:HHB	1.93	0.50
20:H:198:GLN:O	20:H:202:THR:OG1	2.27	0.50
24:P:50:ASP:OD1	43:P:304:DD6:O2	2.29	0.50
1:a:169:MET:HG3	42:a:842:BCR:H322	1.94	0.50
39:i:101:CLA:H71	42:i:102:BCR:HC32	1.94	0.50
39:C:305:CLA:H91	39:C:305:CLA:H152	1.93	0.50
52:P:318:A1EB4:C28	39:Q:311:CLA:HBC1	2.42	0.50
26:Q:231:LEU:HD23	26:Q:234:VAL:H	1.76	0.50
28:S:124:GLN:NE2	47:S:301:SQD:O10	2.37	0.50
39:U:207:CLA:HED3	39:U:207:CLA:H2A	1.93	0.50
33:3:75:ALA:O	33:3:79:HIS:ND1	2.40	0.50
39:7:314:CLA:HAA1	39:7:314:CLA:HED2	1.94	0.50
34:6:194:ASN:ND2	39:6:310:CLA:O1D	2.43	0.50
1:a:363:LEU:HD21	39:a:816:CLA:H93	1.93	0.50
24:W:102:THR:HG22	24:W:104:ALA:H	1.76	0.50
38:2:88:GLY:O	51:2:311:A1ECV:O2A	2.30	0.50
2:b:174:ARG:HB2	39:b:815:CLA:HBC2	1.93	0.50
4:d:43:ILE:HG12	4:d:53:ILE:HG13	1.93	0.50
10:m:18:ALA:HB2	42:m:101:BCR:C15	2.42	0.50
39:D:310:CLA:H43	47:M:301:SQD:H92	1.93	0.50
24:M:161:ILE:HD13	47:M:301:SQD:H82	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Q:176:HIS:HB3	26:Q:178:VAL:HG23	1.93	0.50
33:3:207:ALA:O	33:3:211:ASN:ND2	2.39	0.50
27:5:140:ALA:HB3	27:5:155:PRO:HG3	1.94	0.50
35:9:125:LEU:HB3	35:9:129:ALA:HB3	1.94	0.50
21:J:197:VAL:HG11	39:J:318:CLA:H2A	1.92	0.49
24:M:99:LYS:HE2	46:M:319:LMG:C9	2.41	0.49
33:3:71:PHE:HB2	33:3:162:MET:SD	2.52	0.49
39:L:308:CLA:H2A	39:L:308:CLA:HED3	1.93	0.49
24:P:75:ARG:NH2	49:P:312:KC2:O1D	2.45	0.49
39:a:831:CLA:H51	9:l:61:PRO:HG2	1.93	0.49
49:P:312:KC2:CBC	39:P:316:CLA:H3A	2.43	0.49
28:4:172:ASN:O	43:4:308:DD6:O2	2.29	0.49
39:b:830:CLA:H42	45:b:849:DGD:HB42	1.94	0.49
18:F:169:SER:HA	18:F:172:LEU:HD13	1.93	0.49
20:H:95:VAL:HG12	39:H:310:CLA:HBC2	1.93	0.49
26:Q:230:PHE:CE2	48:Q:304:A86:O4	2.65	0.49
27:V:175:LYS:NZ	49:V:315:KC2:O1A	2.45	0.49
33:3:102:ALA:HB1	33:3:104:THR:HG23	1.93	0.49
1:a:204:GLY:HA3	39:a:811:CLA:HBB1	1.93	0.49
1:a:441:LEU:HD22	39:a:836:CLA:HBB1	1.95	0.49
2:b:92:TRP:HE1	14:B:67:GLN:HB2	1.77	0.49
39:A:311:CLA:H202	39:A:315:CLA:HBB1	1.95	0.49
15:C:170:SER:OG	15:C:172:ASP:OD1	2.30	0.49
24:M:106:VAL:HG13	24:M:117:ALA:HB3	1.95	0.49
26:Q:230:PHE:HD2	48:Q:304:A86:C33	2.25	0.49
26:Q:236:PRO:O	26:Q:237:ALA:HB2	2.10	0.49
29:T:88:GLN:O	29:T:100:ARG:NH1	2.46	0.49
33:3:88:VAL:HG12	39:3:314:CLA:HBC2	1.93	0.49
39:5:308:CLA:HBC3	39:5:316:CLA:H51	1.94	0.49
50:2:304:A1EB1:O43	50:2:304:A1EB1:O3	2.30	0.49
1:a:644:ASN:HB2	2:b:651:LEU:HD11	1.94	0.49
18:F:127:ILE:HD11	46:F:320:LMG:O9	2.12	0.49
24:P:138:GLU:OE1	24:P:143:HIS:NE2	2.34	0.49
39:Q:320:CLA:H2A	39:Q:320:CLA:HED3	1.94	0.49
24:W:141:LYS:O	24:W:142:PRO:C	2.55	0.49
3:c:81:TYR:HB3	4:d:23:LEU:HD12	1.94	0.49
18:F:217:MET:HE2	43:F:303:DD6:C8	2.41	0.49
24:W:219:ALA:CB	52:W:306:A1EB4:C42	2.90	0.49
1:a:119:TRP:O	1:a:124:GLN:NE2	2.36	0.49
1:a:447:PHE:HE2	39:a:835:CLA:HAB	1.77	0.49
2:b:50:HIS:ND1	39:b:815:CLA:OBD	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:l:24:SER:HB2	9:l:27:THR:HG23	1.94	0.49
46:A:316:LMG:H291	46:A:316:LMG:H122	1.94	0.49
16:D:183:LYS:HD3	39:D:317:CLA:HBD	1.93	0.49
39:7:318:CLA:H3A	51:7:323:A1ECV:CMC	2.42	0.49
28:x:110:ALA:O	50:x:302:A1EB1:O2	2.30	0.49
1:a:674:LEU:HD11	2:b:617:MET:HB2	1.95	0.49
13:A:79:TYR:CE2	13:A:190:LEU:HB2	2.48	0.49
21:J:107:LEU:HG	21:J:109:ALA:H	1.78	0.49
28:4:253:TRP:O	47:4:327:SQD:O3	2.27	0.49
1:a:580:ARG:HG2	3:c:78:GLY:HA3	1.95	0.49
39:b:841:CLA:H203	39:l:201:CLA:H192	1.95	0.49
16:D:183:LYS:HD2	39:D:317:CLA:HBA2	1.94	0.49
20:H:150:SER:OG	41:H:317:LHG:O4	2.29	0.49
26:Q:79:GLU:OE1	26:Q:166:GLY:N	2.42	0.49
26:Q:230:PHE:C	26:Q:232:LYS:N	2.67	0.49
39:S:311:CLA:H52	39:S:311:CLA:H142	1.94	0.49
28:4:98:ILE:H	28:4:102:ASN:HD21	1.61	0.49
1:a:15:VAL:HG11	39:a:808:CLA:HAA2	1.95	0.48
1:a:57:HIS:ND1	39:a:803:CLA:HBB2	2.28	0.48
39:b:801:CLA:H162	39:b:801:CLA:H141	1.67	0.48
13:A:69:GLY:O	13:A:73:MET:HG3	2.13	0.48
18:F:215:LEU:HG	50:F:304:A1EB1:C12	2.43	0.48
39:b:833:CLA:HBB2	42:f:801:BCR:HC41	1.94	0.48
2:b:319:HIS:HB3	2:b:322:LEU:HD12	1.95	0.48
20:H:201:LEU:HD12	20:H:202:THR:HG23	1.94	0.48
28:S:199:GLY:O	28:S:203:MET:HG3	2.13	0.48
1:a:128:ASN:HB3	1:a:136:SER:HB3	1.95	0.48
2:b:573:TRP:HZ2	2:b:707:LEU:HD12	1.78	0.48
2:b:707:LEU:HD11	45:b:849:DGD:HB41	1.95	0.48
20:H:98:VAL:HG13	20:H:206:PHE:HE1	1.77	0.48
24:M:99:LYS:HZ1	46:M:319:LMG:C9	2.26	0.48
32:1:59:LEU:HB3	32:1:76:LEU:HD21	1.95	0.48
39:A:315:CLA:HBA1	39:A:315:CLA:H3A	1.47	0.48
16:D:107:ASP:OD2	16:D:211:TYR:OH	2.27	0.48
48:F:302:A86:C41	46:F:317:LMG:C11	2.85	0.48
43:7:310:DD6:C8	51:7:317:A1ECV:O1	2.62	0.48
39:b:801:CLA:CGA	39:b:801:CLA:H3A	2.44	0.48
17:E:46:ASP:OD1	17:E:46:ASP:N	2.43	0.48
19:G:70:GLY:O	19:G:74:MET:HG3	2.13	0.48
19:G:143:LYS:HG3	19:G:144:VAL:H	1.79	0.48
20:H:51:ALA:O	20:H:53:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:102:THR:HG22	24:P:104:ALA:H	1.78	0.48
27:R:98:VAL:HG23	27:R:99:GLU:HG3	1.96	0.48
49:R:314:KC2:C1A	46:S:322:LMG:H312	2.43	0.48
28:S:110:ALA:O	50:S:303:A1EB1:O2	2.31	0.48
29:T:206:LEU:HD11	30:U:96:PRO:HG2	1.95	0.48
38:Y:88:GLY:O	51:Y:306:A1ECV:O2A	2.31	0.48
1:a:60:ASP:OD2	1:a:350:HIS:NE2	2.47	0.48
39:H:310:CLA:H101	39:H:310:CLA:H61	1.70	0.48
24:P:73:HIS:HB3	24:P:201:MET:SD	2.54	0.48
29:T:65:PHE:HE1	29:T:94:PRO:HG3	1.79	0.48
39:T:313:CLA:HHC	39:T:313:CLA:HBB1	1.96	0.48
1:a:121:VAL:HG21	8:j:28:ILE:HG23	1.94	0.48
15:C:58:SER:OG	15:C:61:ILE:O	2.32	0.48
17:E:157:GLY:O	24:M:59:SER:OG	2.30	0.48
39:H:310:CLA:HMC3	39:H:313:CLA:H171	1.94	0.48
24:P:34:VAL:HG11	24:P:55:SER:HB2	1.95	0.48
26:Q:232:LYS:CE	48:Q:304:A86:C41	2.92	0.48
31:0:104:PHE:HB3	39:0:313:CLA:HED3	1.94	0.48
36:I:175:GLY:O	36:I:179:MET:HG3	2.14	0.48
1:a:313:ARG:NH2	11:k:98:GLN:OE1	2.46	0.48
39:b:831:CLA:HAB	39:b:839:CLA:HBB2	1.95	0.48
8:j:1:MET:O	16:D:154:ARG:NH1	2.46	0.48
39:F:313:CLA:H3A	39:F:313:CLA:HBA2	1.54	0.48
21:J:108:VAL:HG23	21:J:119:ALA:HB2	1.94	0.48
26:Q:133:GLN:HG2	39:Q:321:CLA:H41	1.96	0.48
26:Q:232:LYS:CE	48:Q:304:A86:C35	2.92	0.48
39:F:313:CLA:H93	39:F:313:CLA:H61	1.78	0.47
26:Q:42:GLU:HB3	39:Q:310:CLA:HED1	1.95	0.47
26:Q:201:ARG:NH1	49:Q:315:KC2:O1A	2.47	0.47
26:Q:232:LYS:HE2	48:Q:304:A86:C36	2.42	0.47
48:W:307:A86:O3	49:W:315:KC2:O1A	2.32	0.47
31:0:111:SER:O	31:0:112:PRO:C	2.55	0.47
46:4:326:LMG:H132	46:4:326:LMG:HC91	1.96	0.47
16:D:92:HIS:HB3	16:D:192:MET:HE2	1.96	0.47
39:D:316:CLA:H93	39:W:310:CLA:H43	1.96	0.47
18:F:105:ALA:O	18:F:109:HIS:ND1	2.35	0.47
39:V:313:CLA:H141	39:V:313:CLA:H161	1.69	0.47
24:W:221:ASP:OD1	24:W:221:ASP:N	2.47	0.47
39:b:823:CLA:HBA1	39:b:823:CLA:H3A	1.52	0.47
12:o:84:SER:O	12:o:89:SER:OG	2.24	0.47
23:L:36:LEU:HD12	23:L:39:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:W:314:KC2:CBC	39:W:318:CLA:H3A	2.44	0.47
35:9:85:MET:HG2	48:9:303:A86:C3	2.43	0.47
39:a:815:CLA:H3A	39:a:815:CLA:HBA2	1.51	0.47
39:b:832:CLA:HBC2	39:b:839:CLA:HMC2	1.95	0.47
39:b:842:CLA:H161	39:b:842:CLA:H141	1.71	0.47
13:A:157:THR:HG21	27:V:55:ILE:HA	1.96	0.47
39:L:310:CLA:HBC1	39:L:313:CLA:HAC1	1.95	0.47
26:Q:192:ALA:HB3	26:Q:197:LYS:HE3	1.95	0.47
46:S:322:LMG:H172	46:S:322:LMG:H301	1.97	0.47
24:W:175:LEU:O	24:W:177:PHE:N	2.48	0.47
33:3:235:LEU:HA	33:3:238:LYS:HE3	1.96	0.47
28:7:56:LEU:O	48:7:312:A86:O2	2.31	0.47
2:b:26:ALA:HA	39:b:830:CLA:H43	1.95	0.47
39:b:820:CLA:H3A	39:b:820:CLA:HBA2	1.44	0.47
39:b:827:CLA:H141	39:b:827:CLA:H161	1.72	0.47
39:D:319:CLA:H143	39:D:319:CLA:H111	1.78	0.47
47:D:321:SQD:H262	47:D:321:SQD:H101	1.96	0.47
24:P:106:VAL:HG13	24:P:117:ALA:HB3	1.96	0.47
24:W:140:LYS:HA	24:W:140:LYS:HD3	1.55	0.47
14:B:43:ALA:HA	14:B:48:TRP:CD1	2.49	0.47
26:Q:232:LYS:CD	48:Q:304:A86:C41	2.92	0.47
27:R:136:LEU:O	27:R:140:ALA:CB	2.63	0.47
27:V:91:LEU:HD22	27:V:105:GLU:HA	1.97	0.47
27:V:191:MET:SD	39:V:310:CLA:HBB2	2.54	0.47
39:X:317:CLA:H62	39:X:317:CLA:H41	1.73	0.47
32:1:180:ASN:O	48:1:307:A86:O2	2.33	0.47
27:5:174:ARG:NH1	49:5:305:KC2:O1A	2.47	0.47
2:b:65:LEU:HD11	42:b:846:BCR:H271	1.96	0.47
39:b:829:CLA:H3A	39:b:829:CLA:HBA2	1.63	0.47
39:D:318:CLA:H3A	39:D:318:CLA:HBA2	1.53	0.47
39:E:314:CLA:H41	39:E:314:CLA:H61	1.55	0.47
39:F:313:CLA:H72	39:F:314:CLA:H42	1.96	0.47
22:K:153:PRO:O	22:K:154:ARG:CB	2.63	0.47
24:W:218:PRO:HB2	27:5:125:GLN:HG3	1.96	0.47
1:a:530:THR:HG23	1:a:641:LEU:HD21	1.97	0.47
39:a:804:CLA:H2	39:a:804:CLA:HED2	1.97	0.47
9:l:130:GLY:HA2	42:l:207:BCR:H10C	1.97	0.47
43:Q:303:DD6:C24	39:Q:310:CLA:HAB	2.45	0.47
28:S:235:GLN:OE1	28:S:238:LEU:HG	2.14	0.47
33:3:80:GLY:O	33:3:84:MET:HG3	2.15	0.47
28:y:245:SER:O	51:y:311:A1ECV:O2A	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:a:802:CLA:H12	39:a:809:CLA:H92	1.97	0.47
39:b:814:CLA:H3A	39:b:814:CLA:HBA2	1.75	0.47
39:b:817:CLA:H52	20:H:128:LEU:HD21	1.97	0.47
39:b:827:CLA:H152	42:b:847:BCR:H17C	1.96	0.47
39:A:312:CLA:HBA2	39:A:312:CLA:H3A	1.51	0.47
17:E:196:THR:OG1	17:E:199:GLY:O	2.33	0.47
28:x:245:SER:O	51:x:310:A1ECV:O2A	2.33	0.47
1:a:438:ILE:HG13	1:a:556:PHE:HE2	1.80	0.47
14:B:44:LYS:HD3	14:B:160:LEU:HD23	1.96	0.47
17:E:77:ALA:HB1	17:E:172:GLY:HA3	1.96	0.47
39:J:309:CLA:H152	39:J:309:CLA:H111	1.72	0.47
39:L:308:CLA:HBD	39:L:308:CLA:HBA1	1.96	0.47
49:R:314:KC2:C4A	46:S:322:LMG:C32	2.89	0.47
28:S:249:ILE:HD13	39:3:320:CLA:H3A	1.95	0.47
29:T:85:THR:OG1	29:T:88:GLN:OE1	2.26	0.47
39:8:311:CLA:H61	39:8:311:CLA:H41	1.58	0.47
35:9:94:GLN:NE2	50:9:302:A1EB1:O2	2.43	0.47
14:B:56:LEU:HB2	14:B:73:ILE:HG23	1.96	0.46
18:F:57:TYR:HB3	18:F:103:ARG:HH21	1.80	0.46
18:F:182:LYS:HG2	18:F:183:ARG:H	1.79	0.46
18:F:226:ASN:ND2	18:F:236:CYS:SG	2.88	0.46
19:G:49:PHE:HE2	39:P:308:CLA:H42	1.80	0.46
39:S:319:CLA:O2D	39:S:319:CLA:H2A	2.15	0.46
52:W:321:A1EB4:C24	39:X:311:CLA:HBB1	2.45	0.46
11:k:80:LYS:HE2	11:k:144:LEU:HD23	1.97	0.46
39:E:315:CLA:HAA2	39:E:318:CLA:HED3	1.97	0.46
18:F:73:LYS:HB3	18:F:204:LYS:HZ3	1.80	0.46
24:M:141:LYS:O	24:M:143:HIS:N	2.48	0.46
25:O:105:VAL:HA	25:O:108:LYS:HD2	1.97	0.46
39:V:311:CLA:H142	39:V:319:CLA:HBA2	1.98	0.46
24:W:170:LYS:HB2	24:W:174:PRO:HA	1.96	0.46
46:7:301:LMG:H132	46:7:301:LMG:HC91	1.96	0.46
39:b:813:CLA:HMA2	15:C:92:LEU:HD21	1.97	0.46
39:b:821:CLA:H203	39:b:821:CLA:HBC3	1.96	0.46
7:i:14:VAL:O	7:i:19:PRO:HD3	2.15	0.46
10:m:26:ARG:HH22	14:B:7:ASP:HA	1.79	0.46
16:D:137:TRP:CZ2	39:D:314:CLA:HBB1	2.51	0.46
19:G:61:ARG:NH1	19:G:142:GLY:O	2.48	0.46
39:K:306:CLA:HBA1	31:0:168:PRO:HA	1.98	0.46
24:M:99:LYS:CE	46:M:319:LMG:C9	2.79	0.46
39:5:306:CLA:H41	39:5:306:CLA:H62	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:a:821:CLA:H2	39:a:836:CLA:H121	1.97	0.46
39:a:847:CLA:H61	6:f:153:MET:HE1	1.98	0.46
15:C:85:ILE:HG21	39:C:306:CLA:H11	1.97	0.46
15:C:112:LEU:HD13	39:C:308:CLA:H91	1.98	0.46
17:E:163:GLU:OE1	17:E:167:LYS:NZ	2.43	0.46
39:E:312:CLA:H41	39:E:312:CLA:H61	1.57	0.46
21:J:51:ASP:OD1	21:J:51:ASP:N	2.44	0.46
39:J:309:CLA:H62	39:J:309:CLA:H41	1.60	0.46
24:P:72:LYS:NZ	24:P:134:GLU:OE1	2.47	0.46
26:Q:232:LYS:HE2	48:Q:304:A86:C34	2.42	0.46
29:T:16:GLU:HB3	29:T:29:VAL:HG11	1.97	0.46
48:U:206:A86:C4	39:U:208:CLA:HBB2	2.45	0.46
27:V:138:GLU:OE1	27:V:144:HIS:NE2	2.41	0.46
39:a:824:CLA:HED1	39:a:832:CLA:HAB	1.98	0.46
42:b:848:BCR:H15C	42:b:848:BCR:H351	1.83	0.46
13:A:48:ASP:OD1	43:A:302:DD6:O2	2.34	0.46
16:D:89:GLU:OE2	16:D:189:ARG:NH2	2.37	0.46
18:F:208:LYS:HB3	39:F:314:CLA:HBA1	1.97	0.46
28:S:84:VAL:HG11	39:S:319:CLA:H52	1.98	0.46
39:U:207:CLA:H2A	39:U:207:CLA:CED	2.46	0.46
39:V:316:CLA:O1A	46:W:302:LMG:H142	2.16	0.46
31:0:51:ASP:OD1	31:0:51:ASP:N	2.47	0.46
39:0:310:CLA:H93	39:0:310:CLA:H61	1.81	0.46
39:7:318:CLA:HHB	51:7:323:A1ECV:O1	2.16	0.46
12:o:88:SER:OG	12:o:89:SER:N	2.46	0.46
39:o:205:CLA:HED2	16:D:126:ILE:HG21	1.96	0.46
47:D:321:SQD:H131	47:D:321:SQD:H281	1.96	0.46
20:H:48:PHE:HD2	20:H:49:MET:HE2	1.81	0.46
24:M:197:GLY:O	24:M:201:MET:HG3	2.15	0.46
24:P:221:ASP:OD2	24:P:222:SER:N	2.48	0.46
39:T:319:CLA:HBB2	39:T:320:CLA:C4C	2.46	0.46
39:5:316:CLA:H62	39:5:316:CLA:H41	1.71	0.46
36:I:141:ASN:ND2	36:I:151:ASN:O	2.45	0.46
4:d:85:TYR:HE1	4:d:100:HIS:ND1	2.13	0.46
39:k:201:CLA:HBB2	47:k:205:SQD:H271	1.97	0.46
39:C:311:CLA:H92	39:C:311:CLA:H61	1.73	0.46
47:H:318:SQD:H251	21:J:146:SER:HA	1.98	0.46
25:O:65:LEU:HD11	35:9:146:LEU:HD11	1.97	0.46
27:V:32:VAL:N	27:V:54:LYS:HD3	2.31	0.46
39:X:308:CLA:H41	39:X:308:CLA:H62	1.58	0.46
31:0:143:ASP:OD1	31:0:143:ASP:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Y:212:SER:O	38:Y:216:GLY:N	2.49	0.46
1:a:577:GLY:HA2	2:b:562:PRO:HD3	1.97	0.46
8:j:26:MET:HE2	8:j:26:MET:HB3	1.86	0.46
16:D:66:VAL:HG21	16:D:181:GLN:HB3	1.97	0.46
39:M:310:CLA:H152	39:M:310:CLA:H111	1.59	0.46
39:X:309:CLA:HBC3	39:X:317:CLA:H51	1.98	0.46
36:I:151:ASN:OD1	36:I:154:GLY:N	2.47	0.46
39:b:803:CLA:HBB2	6:f:124:GLY:HA3	1.96	0.46
9:l:38:ARG:O	9:l:46:ARG:NH2	2.49	0.46
14:B:152:SER:HB2	14:B:162:VAL:HG11	1.96	0.46
39:D:310:CLA:HAB	47:D:320:SQD:H441	1.98	0.46
17:E:156:LEU:N	48:E:304:A86:O5	2.49	0.46
24:M:111:PRO:O	43:M:304:DD6:O4	2.34	0.46
25:O:167:GLY:O	25:O:169:PHE:N	2.46	0.46
27:R:67:ALA:O	27:R:71:HIS:ND1	2.43	0.46
29:T:155:ILE:HG13	29:T:158:GLN:H	1.81	0.46
47:T:321:SQD:H2	39:I:313:CLA:HAA2	1.98	0.46
31:0:119:LEU:HD11	39:0:313:CLA:HAA2	1.96	0.46
32:1:57:LEU:CB	32:1:59:LEU:CD1	2.94	0.46
27:5:82:TRP:CZ3	27:5:111:GLY:HA3	2.51	0.46
28:7:45:TYR:CE1	39:7:314:CLA:HED1	2.51	0.46
28:7:131:VAL:HG11	39:7:325:CLA:HBA1	1.98	0.46
39:x:308:CLA:HMD3	39:x:311:CLA:HBA2	1.98	0.46
39:a:807:CLA:H161	39:a:807:CLA:H193	1.82	0.46
2:b:397:ASP:OD1	4:d:134:LYS:NZ	2.38	0.46
12:o:84:SER:OG	12:o:87:TRP:O	2.34	0.46
23:L:221:LEU:CD2	48:L:304:A86:O2	2.64	0.46
24:P:37:MET:HG2	24:P:67:ARG:HH21	1.81	0.46
27:R:205:LEU:HD11	47:S:301:SQD:H92	1.97	0.46
39:R:307:CLA:H62	39:R:307:CLA:H41	1.62	0.46
39:T:308:CLA:HBD	49:T:315:KC2:OBD	2.16	0.46
2:b:428:PHE:CE2	39:b:838:CLA:HAB	2.51	0.45
39:b:840:CLA:H72	39:b:841:CLA:H121	1.98	0.45
13:A:105:PRO:HA	13:A:106:PRO:HD3	1.88	0.45
21:J:141:ALA:HA	21:J:144:ILE:HG22	1.98	0.45
24:M:221:ASP:OD1	24:M:221:ASP:N	2.49	0.45
39:M:312:CLA:H91	39:M:312:CLA:H112	1.73	0.45
27:V:112:TYR:HE2	27:V:194:VAL:HG22	1.81	0.45
39:I:308:CLA:H41	39:I:308:CLA:H61	1.77	0.45
28:z:110:ALA:O	50:z:302:A1EB1:O2	2.34	0.45
39:a:817:CLA:HBA1	39:a:817:CLA:H3A	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:b:833:CLA:H62	39:b:833:CLA:H2	1.73	0.45
39:f:802:CLA:H72	39:f:802:CLA:H112	1.59	0.45
39:D:318:CLA:H143	39:D:318:CLA:H162	1.88	0.45
39:E:313:CLA:H61	39:E:313:CLA:H41	1.54	0.45
39:J:311:CLA:H13	39:J:311:CLA:H102	1.69	0.45
39:K:306:CLA:H92	39:K:306:CLA:H41	1.99	0.45
28:S:200:ARG:HA	28:S:203:MET:HE3	1.97	0.45
30:U:94:ARG:NH2	30:U:103:LEU:O	2.49	0.45
39:4:323:CLA:H152	46:4:326:LMG:H161	1.97	0.45
39:7:314:CLA:H41	39:7:314:CLA:H62	1.58	0.45
38:2:136:VAL:HG12	38:2:139:LYS:HE2	1.97	0.45
1:a:183:LYS:HD3	41:D:302:LHG:HC32	1.98	0.45
1:a:429:ARG:O	1:a:433:HIS:ND1	2.42	0.45
9:l:138:LEU:HG	39:l:205:CLA:HED3	1.99	0.45
39:J:307:CLA:H3A	39:J:307:CLA:HBA2	1.72	0.45
24:P:169:ILE:HD12	52:P:319:A1EB4:C21	2.47	0.45
28:S:137:GLU:OE2	28:S:150:TYR:OH	2.28	0.45
39:U:207:CLA:H41	39:U:207:CLA:H62	1.56	0.45
39:8:310:CLA:HBD	39:8:310:CLA:HBA1	1.98	0.45
28:z:245:SER:HA	28:z:254:ALA:HB2	1.98	0.45
2:b:181:GLY:HA3	39:b:815:CLA:HBB1	1.97	0.45
39:b:806:CLA:H72	39:b:806:CLA:H112	1.63	0.45
6:f:146:VAL:HB	41:j:104:LHG:HC61	1.98	0.45
18:F:192:THR:O	18:F:193:GLN:HG3	2.16	0.45
20:H:200:ALA:HB2	39:H:316:CLA:HED3	1.98	0.45
23:L:177:LYS:HA	23:L:180:LYS:HZ3	1.80	0.45
39:P:308:CLA:H202	39:P:308:CLA:H141	1.98	0.45
29:T:190:VAL:HB	29:T:193:LEU:HB2	1.98	0.45
46:W:302:LMG:H341	48:W:304:A86:C28	2.47	0.45
39:X:308:CLA:H3A	39:X:308:CLA:HBA1	1.63	0.45
39:0:323:CLA:H2A	39:0:323:CLA:CED	2.46	0.45
28:4:32:LEU:HD22	39:4:312:CLA:HED1	1.97	0.45
39:a:830:CLA:CAD	42:l:202:BCR:H10C	2.46	0.45
39:b:832:CLA:H52	39:b:832:CLA:H8	1.69	0.45
16:D:142:GLU:HG2	39:D:315:CLA:NB	2.31	0.45
39:E:310:CLA:H112	39:E:310:CLA:H71	1.73	0.45
19:G:87:ARG:HG2	19:G:101:ALA:HA	1.98	0.45
39:H:306:CLA:HBC2	21:J:139:VAL:HG11	1.97	0.45
24:P:71:LEU:HD13	24:P:151:GLY:HA3	1.99	0.45
30:U:113:ALA:HA	30:U:117:LEU:HB2	1.99	0.45
49:Y:308:KC2:CBC	39:Y:313:CLA:H3A	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:737:ILE:HG23	39:a:825:CLA:HAB	1.98	0.45
39:a:827:CLA:H41	41:a:840:LHG:H121	1.98	0.45
2:b:262:HIS:HD1	2:b:264:GLN:H	1.63	0.45
4:d:103:ASP:OD1	4:d:103:ASP:N	2.45	0.45
21:J:69:LEU:HB2	21:J:74:MET:HE2	1.98	0.45
39:M:309:CLA:H143	39:M:309:CLA:H111	1.84	0.45
39:X:309:CLA:H143	39:X:309:CLA:H161	1.87	0.45
49:x:312:KC2:CBC	39:x:317:CLA:H3A	2.47	0.45
39:a:816:CLA:HAB	39:a:816:CLA:H111	1.98	0.45
2:b:32:GLU:HG2	2:b:42:LEU:HD11	1.98	0.45
39:b:826:CLA:H172	39:b:832:CLA:HBC1	1.97	0.45
16:D:170:PHE:CZ	39:W:310:CLA:H42	2.51	0.45
39:E:314:CLA:H93	24:M:52:LEU:HD13	1.98	0.45
21:J:55:VAL:HG23	21:J:179:ILE:HD13	1.99	0.45
26:Q:38:LYS:HB3	26:Q:74:ILE:HD11	1.98	0.45
26:Q:238:TYR:HE2	26:Q:241:GLU:C	2.25	0.45
28:S:131:VAL:HG22	46:S:321:LMG:H112	1.99	0.45
28:S:212:GLU:OE2	28:S:219:VAL:N	2.48	0.45
29:T:164:PHE:CD2	39:T:308:CLA:CED	2.99	0.45
27:X:136:LEU:O	27:X:140:ALA:CB	2.65	0.45
39:X:308:CLA:H92	39:X:308:CLA:H61	1.85	0.45
46:4:326:LMG:H322	49:5:313:KC2:C1B	2.46	0.45
1:a:356:ASN:ND2	39:a:803:CLA:OBD	2.36	0.45
39:a:829:CLA:HBC2	39:a:836:CLA:HMC2	1.99	0.45
39:i:103:CLA:H91	39:i:103:CLA:H111	1.80	0.45
39:l:205:CLA:C2C	46:l:208:LMG:H352	2.47	0.45
24:M:140:LYS:HD3	24:M:140:LYS:HA	1.70	0.45
24:W:106:VAL:HG13	24:W:117:ALA:HB3	1.97	0.45
39:W:311:CLA:HED2	39:W:311:CLA:HBD	1.87	0.45
1:a:247:GLN:HG3	39:a:813:CLA:HED2	1.98	0.45
41:a:840:LHG:H281	41:a:840:LHG:H312	1.83	0.45
39:b:851:CLA:HBA2	39:b:851:CLA:H3A	1.74	0.45
11:k:117:ILE:HD13	17:E:58:LEU:HB3	1.99	0.45
14:B:122:PRO:O	14:B:126:THR:OG1	2.30	0.45
39:D:309:CLA:O1A	47:D:320:SQD:O2	2.35	0.45
39:E:314:CLA:H41	39:E:314:CLA:H92	1.99	0.45
18:F:102:LEU:HD22	39:F:308:CLA:H43	1.98	0.45
21:J:204:LEU:HD23	21:J:207:ALA:HB2	1.99	0.45
27:V:51:GLY:C	27:V:53:SER:H	2.25	0.45
43:7:310:DD6:C3	51:7:317:A1ECV:C3B	2.95	0.45
2:b:345:THR:HA	2:b:348:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:b:844:BCR:H371	42:b:844:BCR:H24C	1.76	0.45
5:e:42:LYS:HB3	5:e:97:GLU:HB3	1.98	0.45
23:L:221:LEU:CD2	48:L:304:A86:C18	2.94	0.45
39:O:310:CLA:H41	39:O:310:CLA:H62	1.68	0.45
26:Q:238:TYR:HE2	26:Q:241:GLU:O	1.99	0.45
39:3:311:CLA:H112	39:Z:316:CLA:HBB2	1.98	0.45
39:y:307:CLA:H2A	39:y:307:CLA:HED3	1.99	0.45
1:a:77:HIS:ND1	39:a:811:CLA:OBD	2.35	0.44
1:a:691:ARG:NH1	1:a:718:ALA:O	2.51	0.44
2:b:26:ALA:HB2	45:b:849:DGD:HA32	1.99	0.44
2:b:348:VAL:HG12	39:b:820:CLA:H2	1.99	0.44
39:b:827:CLA:H111	42:h:202:BCR:H373	1.99	0.44
42:b:845:BCR:H16C	39:C:307:CLA:H172	1.98	0.44
39:3:314:CLA:H112	39:3:314:CLA:H52	1.99	0.44
28:4:37:LYS:HA	28:4:37:LYS:HD3	1.78	0.44
28:7:120:LEU:HD22	47:7:302:SQD:H441	2.00	0.44
42:a:842:BCR:H362	42:a:843:BCR:H21C	1.98	0.44
39:b:830:CLA:H141	39:b:830:CLA:H162	1.79	0.44
19:G:92:LEU:HB3	19:G:98:ILE:HG23	1.99	0.44
39:G:309:CLA:H61	39:G:309:CLA:H41	1.80	0.44
21:J:137:GLU:HG2	39:J:313:CLA:C1B	2.47	0.44
26:Q:117:LEU:HD12	26:Q:117:LEU:HA	1.76	0.44
39:S:311:CLA:H161	39:S:311:CLA:H202	1.79	0.44
39:W:310:CLA:H51	39:W:310:CLA:H8	1.72	0.44
50:0:307:A1EB1:O3	50:0:307:A1EB1:O6	2.35	0.44
46:4:326:LMG:H321	49:5:313:KC2:C1B	2.38	0.44
2:b:226:PHE:HE1	42:b:850:BCR:H313	1.81	0.44
2:b:559:CYS:SG	2:b:560:ASP:N	2.90	0.44
2:b:594:TRP:HB2	39:b:837:CLA:HMC1	1.98	0.44
39:b:801:CLA:H151	39:b:801:CLA:H111	1.56	0.44
18:F:215:LEU:CG	50:F:304:A1EB1:C12	2.95	0.44
24:M:210:GLY:HA3	24:M:220:LEU:HD12	2.00	0.44
28:4:89:HIS:CG	28:4:113:VAL:HG21	2.52	0.44
28:7:94:ARG:NH2	28:7:105:PRO:O	2.33	0.44
35:9:61:PHE:CD2	35:9:69:THR:HG23	2.52	0.44
1:a:87:TRP:O	1:a:90:GLN:HG3	2.18	0.44
9:l:56:TYR:CD1	9:l:134:ALA:HB2	2.52	0.44
16:D:222:VAL:HG12	24:M:115:TRP:HE1	1.82	0.44
39:D:316:CLA:H193	39:D:316:CLA:H162	1.83	0.44
39:E:310:CLA:H92	39:E:310:CLA:H61	1.83	0.44
21:J:126:MET:HE1	39:J:311:CLA:H3A	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:K:168:ALA:O	22:K:172:ASN:ND2	2.35	0.44
25:O:176:ASP:OD1	43:O:305:DD6:O4	2.36	0.44
39:V:309:CLA:H62	39:V:309:CLA:H41	1.61	0.44
24:W:175:LEU:HD11	39:X:308:CLA:HED1	1.99	0.44
33:3:78:LYS:NZ	33:3:144:GLU:OE1	2.48	0.44
38:2:54:TRP:HZ2	39:2:309:CLA:HED1	1.81	0.44
39:a:829:CLA:H41	39:a:829:CLA:H61	1.56	0.44
2:b:524:ALA:HB2	39:b:838:CLA:HMA1	1.99	0.44
42:b:850:BCR:H20C	42:b:850:BCR:H361	1.85	0.44
7:i:24:ALA:HB1	9:l:95:ILE:HG21	1.99	0.44
42:i:102:BCR:H15C	42:i:102:BCR:H351	1.82	0.44
21:J:54:LEU:HD13	21:J:75:ARG:HE	1.83	0.44
23:L:186:ARG:NH2	49:L:315:KC2:O2A	2.51	0.44
29:T:49:HIS:HD2	39:T:313:CLA:HED2	1.83	0.44
27:X:136:LEU:O	27:X:140:ALA:HB3	2.18	0.44
1:a:87:TRP:HZ3	42:a:843:BCR:H322	1.82	0.44
1:a:587:SER:OG	1:a:590:ASP:OD2	2.31	0.44
39:a:838:CLA:HBC1	40:b:843:PQN:H193	2.00	0.44
42:a:843:BCR:H11C	42:a:843:BCR:H341	1.83	0.44
2:b:69:ALA:HB2	2:b:135:LEU:HB2	1.98	0.44
39:b:824:CLA:H2A	39:b:824:CLA:HED3	1.99	0.44
39:b:834:CLA:H41	39:b:834:CLA:H61	1.57	0.44
40:b:843:PQN:H171	40:b:843:PQN:H212	1.76	0.44
42:b:845:BCR:H11C	42:b:845:BCR:H341	1.77	0.44
39:i:103:CLA:H102	14:B:81:MET:HE2	2.00	0.44
39:C:310:CLA:H11	39:C:310:CLA:H52	1.78	0.44
21:J:144:ILE:HG13	21:J:153:ARG:CZ	2.48	0.44
26:Q:48:LEU:HD22	26:Q:202:LEU:HD22	1.98	0.44
26:Q:232:LYS:HE2	48:Q:304:A86:C41	2.47	0.44
39:V:310:CLA:H92	39:V:310:CLA:H62	1.84	0.44
31:0:80:GLY:O	31:0:84:MET:HG3	2.18	0.44
28:4:212:GLU:OE2	28:4:219:VAL:N	2.50	0.44
39:I:313:CLA:H112	39:I:313:CLA:H71	1.68	0.44
38:2:75:VAL:HG21	39:2:310:CLA:HBC3	1.99	0.44
39:a:821:CLA:HBA2	39:a:821:CLA:H3A	1.36	0.44
39:i:103:CLA:H143	14:B:88:LEU:HD13	2.00	0.44
11:k:73:ILE:HG12	39:E:317:CLA:H61	1.99	0.44
13:A:79:TYR:CE2	13:A:179:MET:HB3	2.53	0.44
20:H:114:SER:O	43:H:303:DD6:O4	2.36	0.44
22:K:72:CYS:O	22:K:76:MET:HG3	2.18	0.44
39:M:310:CLA:HED2	39:M:310:CLA:HBD	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:S:309:CLA:H62	39:S:309:CLA:H41	1.57	0.44
36:I:90:ALA:O	36:I:94:MET:HG3	2.17	0.44
42:h:202:BCR:H15C	42:h:202:BCR:H351	1.83	0.44
39:a:818:CLA:HBC3	39:a:824:CLA:H171	2.00	0.44
2:b:571:SER:OG	2:b:574:ASP:OD2	2.34	0.44
39:b:812:CLA:H102	39:b:828:CLA:H193	1.98	0.44
39:b:832:CLA:H42	6:f:167:LEU:HD13	2.00	0.44
15:C:145:ILE:HD12	39:C:308:CLA:HAA2	2.00	0.44
46:F:320:LMG:O10	49:O:317:KC2:C3A	2.66	0.44
39:H:309:CLA:HBC1	39:H:312:CLA:H111	1.99	0.44
39:M:312:CLA:H141	39:M:312:CLA:H161	1.75	0.44
26:Q:230:PHE:CD1	26:Q:230:PHE:N	2.84	0.44
41:X:301:LHG:H172	41:X:301:LHG:H262	2.00	0.44
39:7:313:CLA:H62	39:7:313:CLA:H41	1.76	0.44
39:I:301:CLA:HBA2	39:I:301:CLA:H3A	1.78	0.44
37:h:71:PRO:HD2	37:h:74:ILE:HD13	2.00	0.44
1:a:451:HIS:O	1:a:455:LEU:HG	2.18	0.44
39:a:811:CLA:H102	39:a:811:CLA:H61	1.82	0.44
39:a:830:CLA:H141	39:a:830:CLA:H161	1.79	0.44
42:a:842:BCR:H20C	42:a:842:BCR:H361	1.84	0.44
39:b:802:CLA:H151	39:l:201:CLA:HBC3	1.98	0.44
39:b:838:CLA:H102	39:b:838:CLA:H62	1.90	0.44
6:f:128:LEU:HD23	6:f:128:LEU:HA	1.90	0.44
42:i:102:BCR:H392	42:i:102:BCR:H24C	1.81	0.44
18:F:125:ALA:HB3	46:F:320:LMG:C3	2.43	0.44
21:J:37:LYS:HB3	21:J:46:ARG:HB2	2.00	0.44
39:J:311:CLA:H93	39:J:311:CLA:H111	1.86	0.44
24:M:131:LEU:HB2	39:M:312:CLA:HAB	1.99	0.44
26:Q:48:LEU:HD11	26:Q:205:ILE:HB	1.99	0.44
28:S:254:ALA:O	47:S:301:SQD:O3	2.33	0.44
39:S:313:CLA:H18	39:S:313:CLA:H151	1.80	0.44
43:1:304:DD6:C8	39:1:309:CLA:HAB	2.48	0.44
39:7:316:CLA:H142	39:7:316:CLA:H52	1.99	0.44
34:8:53:LEU:HG	34:8:55:PHE:HB3	1.99	0.44
38:Z:232:GLY:O	48:Z:303:A86:O2	2.35	0.44
1:a:514:VAL:HG13	1:a:524:MET:HB3	1.99	0.43
1:a:708:LEU:HD11	42:f:804:BCR:H342	1.99	0.43
39:b:805:CLA:H61	39:b:805:CLA:H41	1.65	0.43
39:C:310:CLA:H92	39:C:310:CLA:H61	1.83	0.43
16:D:214:ASP:OD1	16:D:214:ASP:N	2.51	0.43
18:F:168:THR:HB	18:F:188:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:178:GLY:O	19:G:182:MET:HG3	2.18	0.43
25:O:61:LEU:HD13	25:O:190:ILE:HB	2.00	0.43
27:V:191:MET:SD	39:V:313:CLA:H193	2.58	0.43
24:W:84:TYR:OH	24:W:224:PHE:O	2.33	0.43
39:4:314:CLA:H93	39:4:314:CLA:H62	1.80	0.43
39:4:323:CLA:H111	39:4:323:CLA:H142	1.76	0.43
40:a:839:PQN:H162	39:a:847:CLA:HAB	1.99	0.43
2:b:411:MET:HE2	42:h:202:BCR:H402	2.00	0.43
39:b:817:CLA:HBA2	39:b:817:CLA:H3A	1.61	0.43
39:b:841:CLA:H18	42:i:102:BCR:H362	2.00	0.43
39:b:842:CLA:H141	39:b:842:CLA:H192	1.99	0.43
4:d:86:LYS:HB3	4:d:98:TYR:HE1	1.83	0.43
6:f:147:PRO:HG3	13:A:55:PHE:HB3	2.00	0.43
8:j:39:SER:OG	8:j:40:PHE:N	2.51	0.43
16:D:125:VAL:HG11	39:D:313:CLA:HAA2	1.99	0.43
27:V:79:VAL:HG23	27:V:190:VAL:HG13	2.00	0.43
39:W:313:CLA:H41	39:W:313:CLA:H61	1.54	0.43
39:0:312:CLA:HBA1	39:0:312:CLA:H11	1.43	0.43
32:1:81:ILE:HD12	32:1:164:PRO:HB2	2.00	0.43
39:7:316:CLA:H143	39:7:316:CLA:H111	1.78	0.43
48:2:305:A86:C25	39:2:316:CLA:HBB2	2.48	0.43
1:a:147:MET:HE2	1:a:147:MET:HB3	1.86	0.43
1:a:201:HIS:HB3	39:a:822:CLA:HED3	2.00	0.43
2:b:207:ILE:O	2:b:208:ARG:NH1	2.46	0.43
2:b:422:LEU:HG	39:b:839:CLA:HBB1	1.99	0.43
39:b:828:CLA:H3A	39:b:828:CLA:HBA2	1.50	0.43
15:C:57:ARG:NH1	15:C:62:PRO:O	2.41	0.43
39:C:307:CLA:H91	39:C:307:CLA:H112	1.77	0.43
18:F:149:LEU:HD12	18:F:150:PRO:HD2	1.98	0.43
19:G:159:VAL:HG12	22:K:154:ARG:C	2.43	0.43
20:H:81:GLU:OE1	20:H:155:ARG:NH2	2.51	0.43
20:H:86:HIS:HB3	20:H:189:MET:HE2	1.98	0.43
26:Q:232:LYS:HD2	26:Q:232:LYS:HA	1.85	0.43
1:a:299:LEU:HD23	1:a:299:LEU:HA	1.80	0.43
2:b:600:THR:HG21	2:b:609:PHE:HB2	2.00	0.43
6:f:89:ASP:OD1	6:f:89:ASP:N	2.45	0.43
39:D:312:CLA:H12	39:D:312:CLA:HBA2	1.72	0.43
24:M:141:LYS:CE	24:M:141:LYS:HA	2.40	0.43
27:R:72:SER:O	27:R:76:MET:HG3	2.18	0.43
24:W:201:MET:HE1	39:W:309:CLA:HAB	2.00	0.43
39:X:307:CLA:H62	39:X:307:CLA:H41	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:3:115:ILE:HG21	33:3:128:LEU:HD23	1.99	0.43
27:5:193:LEU:HD23	27:5:206:LEU:HD21	1.99	0.43
35:9:70:TRP:HH2	39:9:308:CLA:HED1	1.84	0.43
1:a:197:MET:HB2	39:a:811:CLA:HBC2	2.01	0.43
1:a:736:GLY:HA2	39:a:801:CLA:CED	2.48	0.43
42:a:842:BCR:H11C	42:a:842:BCR:H341	1.86	0.43
17:E:70:ARG:NH1	17:E:73:GLU:OE1	2.51	0.43
19:G:187:GLY:O	19:G:191:HIS:ND1	2.51	0.43
24:M:50:ASP:OD1	43:M:304:DD6:O2	2.36	0.43
28:S:70:HIS:HD2	39:S:313:CLA:HED2	1.82	0.43
31:0:209:MET:HE2	39:0:312:CLA:HBB2	1.99	0.43
39:3:312:CLA:H142	39:3:312:CLA:H112	1.86	0.43
28:4:137:GLU:HG2	28:4:149:HIS:HE2	1.84	0.43
38:2:126:GLY:O	38:2:130:MET:HG2	2.19	0.43
34:6:46:ASP:OD1	34:6:46:ASP:N	2.51	0.43
1:a:169:MET:O	1:a:173:MET:HG2	2.18	0.43
39:a:814:CLA:H41	39:a:814:CLA:H61	1.73	0.43
39:b:828:CLA:H142	39:b:828:CLA:H112	1.88	0.43
42:b:846:BCR:H24C	42:b:846:BCR:H371	1.70	0.43
3:c:17:CYS:HB2	3:c:54:CYS:HB2	2.01	0.43
39:H:306:CLA:HBA2	39:H:306:CLA:H3A	1.53	0.43
21:J:144:ILE:HG13	21:J:153:ARG:NH2	2.33	0.43
27:R:186:ALA:O	27:R:190:VAL:HG23	2.19	0.43
39:R:316:CLA:H3A	39:R:316:CLA:HBA1	1.76	0.43
30:U:94:ARG:HD3	30:U:94:ARG:HA	1.87	0.43
30:U:189:ALA:HB2	39:U:215:CLA:HED3	2.01	0.43
28:4:114:TRP:HE3	39:4:314:CLA:HMA3	1.82	0.43
36:I:55:PRO:HG3	39:I:308:CLA:C4B	2.48	0.43
2:b:92:TRP:CH2	7:i:12:PRO:HG3	2.53	0.43
42:b:844:BCR:H11C	42:b:844:BCR:H341	1.92	0.43
39:D:317:CLA:H112	39:D:317:CLA:H91	1.77	0.43
18:F:180:THR:O	18:F:182:LYS:N	2.51	0.43
19:G:71:ARG:NH1	19:G:135:TYR:OH	2.45	0.43
20:H:48:PHE:HB3	21:J:159:ALA:HB2	2.00	0.43
41:H:317:LHG:H111	41:H:317:LHG:HC81	1.75	0.43
21:J:75:ARG:NH1	21:J:78:GLU:OE1	2.52	0.43
26:Q:50:PRO:HG2	39:Q:309:CLA:HMB3	2.01	0.43
26:Q:86:ARG:HA	26:Q:89:MET:HE3	2.00	0.43
26:Q:147:ASN:HB3	26:Q:150:VAL:HG22	2.00	0.43
39:V:310:CLA:HBA1	39:V:310:CLA:H3A	1.51	0.43
28:4:199:GLY:O	28:4:203:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:7:321:CLA:H2A	34:6:240:PRO:HG2	2.01	0.43
1:a:318:ILE:HD11	39:a:817:CLA:H2A	2.00	0.43
39:a:820:CLA:CAB	39:I:301:CLA:HBB1	2.48	0.43
39:a:825:CLA:H121	39:a:825:CLA:H161	1.81	0.43
39:b:807:CLA:H121	39:b:807:CLA:H8	1.88	0.43
39:b:809:CLA:HBD	39:b:809:CLA:H122	2.00	0.43
42:b:846:BCR:H341	42:b:846:BCR:H11C	1.76	0.43
3:c:15:THR:HA	3:c:28:MET:HE3	1.99	0.43
42:j:103:BCR:H15C	42:j:103:BCR:H351	1.79	0.43
11:k:72:PRO:HA	39:E:317:CLA:H52	2.01	0.43
15:C:158:ALA:HA	39:C:310:CLA:HAB	2.00	0.43
43:D:306:DD6:O1	39:D:311:CLA:H43	2.19	0.43
26:Q:118:PRO:HD3	26:Q:236:PRO:HD2	2.00	0.43
48:Q:302:A86:C39	46:Q:322:LMG:HC71	2.49	0.43
27:V:50:MET:HE1	24:W:165:TRP:H	1.84	0.43
1:a:361:GLY:HA2	1:a:398:GLY:HA2	2.01	0.43
39:a:809:CLA:HAB	41:D:302:LHG:H122	2.01	0.43
39:a:830:CLA:H51	39:a:830:CLA:H12	1.75	0.43
2:b:459:PHE:CZ	39:f:803:CLA:HBB1	2.54	0.43
42:f:801:BCR:H11C	42:f:801:BCR:H341	1.91	0.43
39:o:201:CLA:HBA2	39:o:201:CLA:H3A	1.65	0.43
17:E:91:ASP:OD2	17:E:195:TYR:OH	2.28	0.43
39:J:314:CLA:H51	39:J:314:CLA:H12	1.77	0.43
39:K:306:CLA:H41	39:K:306:CLA:H61	1.58	0.43
28:S:149:HIS:O	28:S:154:GLY:N	2.48	0.43
27:X:138:GLU:OE1	27:X:144:HIS:NE2	2.41	0.43
34:8:75:GLY:O	34:8:79:MET:HG3	2.19	0.43
1:a:433:HIS:HA	4:d:19:THR:HB	2.00	0.43
40:a:839:PQN:H222	40:a:839:PQN:H18	1.68	0.43
2:b:334:LEU:HD12	39:b:809:CLA:CHD	2.49	0.43
42:b:850:BCR:H11C	42:b:850:BCR:H341	1.83	0.43
42:l:202:BCR:H24C	42:l:202:BCR:H371	1.88	0.43
13:A:150:LYS:HD2	27:V:59:GLU:HG3	2.01	0.43
39:K:306:CLA:HBB1	31:0:133:PHE:CE1	2.54	0.43
23:L:221:LEU:HB2	23:L:222:SER:H	1.70	0.43
39:P:307:CLA:H91	39:P:308:CLA:H143	2.01	0.43
39:W:310:CLA:HMA2	39:W:310:CLA:H12	2.01	0.43
32:1:118:PRO:O	32:1:121:LEU:HB2	2.19	0.43
32:1:120:GLU:O	32:1:121:LEU:C	2.60	0.43
27:5:40:PRO:C	27:5:42:THR:H	2.27	0.43
27:5:48:ASP:OD1	43:5:303:DD6:O2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:7:313:CLA:H93	39:7:313:CLA:H61	1.86	0.43
39:7:316:CLA:H18	39:7:316:CLA:H152	1.85	0.43
1:a:474:ASP:HA	1:a:478:GLN:HG2	2.01	0.42
2:b:180:SER:HB2	39:b:822:CLA:HAC2	2.01	0.42
2:b:493:TRP:HE1	39:b:835:CLA:HED1	1.84	0.42
19:G:137:GLU:O	19:G:142:GLY:HA2	2.19	0.42
26:Q:97:VAL:HG13	26:Q:102:ILE:HB	2.01	0.42
26:Q:190:LYS:HD3	26:Q:190:LYS:HA	1.93	0.42
39:R:308:CLA:H62	39:R:308:CLA:H41	1.60	0.42
39:W:309:CLA:HMB3	39:W:310:CLA:HBA2	2.01	0.42
35:9:205:ASN:ND2	39:9:307:CLA:OBD	2.52	0.42
2:b:559:CYS:SG	2:b:561:GLY:N	2.75	0.42
2:b:722:ALA:HB2	39:b:828:CLA:HBB1	2.00	0.42
39:b:809:CLA:HBA1	39:b:809:CLA:H3A	1.53	0.42
39:b:826:CLA:HED2	39:b:827:CLA:CAD	2.49	0.42
42:b:845:BCR:H15C	42:b:845:BCR:H351	1.72	0.42
39:o:206:CLA:H41	39:o:206:CLA:H62	1.65	0.42
24:M:45:GLY:HA3	27:R:142:LYS:HE3	1.99	0.42
27:R:51:GLY:C	27:R:53:SER:H	2.27	0.42
39:T:308:CLA:H2A	39:T:308:CLA:O2D	2.18	0.42
43:U:204:DD6:C3	39:U:208:CLA:HBB1	2.48	0.42
39:V:316:CLA:O1A	46:W:302:LMG:C15	2.67	0.42
32:1:50:VAL:HG13	32:1:51:VAL:HG23	2.00	0.42
1:a:294:THR:HG23	39:a:816:CLA:HMA3	2.01	0.42
39:a:814:CLA:H61	39:a:814:CLA:H93	1.82	0.42
39:a:823:CLA:HAB	42:a:845:BCR:H311	2.00	0.42
6:f:148:VAL:O	6:f:152:MET:HG2	2.20	0.42
42:f:804:BCR:H11C	42:f:804:BCR:H341	1.70	0.42
39:D:311:CLA:H111	39:D:311:CLA:H152	1.48	0.42
39:F:321:CLA:H61	39:F:321:CLA:H41	1.69	0.42
39:G:310:CLA:H143	39:G:310:CLA:H161	1.89	0.42
24:P:141:LYS:HB3	24:P:142:PRO:HD2	2.01	0.42
27:R:110:ASP:OD1	27:R:111:GLY:N	2.52	0.42
46:S:322:LMG:H322	46:S:322:LMG:H351	1.45	0.42
46:S:322:LMG:H172	46:S:322:LMG:H202	1.78	0.42
33:3:256:LEU:HB2	33:3:259:VAL:HG21	2.00	0.42
39:3:312:CLA:H8	39:3:312:CLA:H121	1.74	0.42
28:z:165:ASN:O	28:z:167:HIS:N	2.51	0.42
38:Y:108:ASP:O	38:Y:112:ALA:HB2	2.19	0.42
39:a:831:CLA:H141	39:a:831:CLA:H161	1.83	0.42
2:b:279:ALA:HA	39:b:818:CLA:HMC2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:422:LEU:HD13	2:b:532:LEU:HA	2.00	0.42
39:b:818:CLA:H61	39:b:818:CLA:H41	1.63	0.42
4:d:100:HIS:CB	4:d:101:PRO:CD	2.95	0.42
13:A:177:SER:HB3	39:A:314:CLA:HBC2	2.00	0.42
39:D:318:CLA:H18	39:D:318:CLA:H122	2.01	0.42
28:S:253:TRP:HB2	47:S:301:SQD:H2	2.01	0.42
27:V:112:TYR:CE2	27:V:194:VAL:HG22	2.54	0.42
1:a:574:PRO:HB3	1:a:721:ILE:HB	2.01	0.42
39:a:822:CLA:H121	39:a:822:CLA:H8	1.97	0.42
42:a:844:BCR:H11C	42:a:844:BCR:H341	1.85	0.42
2:b:498:MET:HA	2:b:501:ILE:HG22	2.00	0.42
2:b:666:SER:C	2:b:667:TRP:CD1	2.95	0.42
42:b:847:BCR:H15C	42:b:847:BCR:H351	1.72	0.42
39:F:308:CLA:H93	39:F:308:CLA:H61	1.86	0.42
39:H:309:CLA:HED3	39:H:309:CLA:H12	2.02	0.42
49:P:310:KC2:C4B	46:P:317:LMG:H361	2.50	0.42
46:S:321:LMG:O5	46:S:321:LMG:O4	2.32	0.42
27:X:180:LEU:HD22	27:X:184:ARG:HH21	1.84	0.42
39:5:315:CLA:HBA1	39:5:315:CLA:H3A	1.85	0.42
28:7:175:ASP:OD1	28:7:175:ASP:N	2.47	0.42
49:7:319:KC2:CBC	39:7:324:CLA:H3A	2.50	0.42
42:a:843:BCR:H15C	42:a:843:BCR:H351	1.83	0.42
39:b:812:CLA:HED1	39:i:101:CLA:HAA2	2.01	0.42
39:b:822:CLA:H12	20:H:143:ASN:HD21	1.85	0.42
39:b:825:CLA:H141	39:b:825:CLA:H161	1.78	0.42
39:b:826:CLA:H3A	39:b:826:CLA:HBA2	1.77	0.42
42:m:101:BCR:H15C	42:m:101:BCR:H351	1.81	0.42
39:C:308:CLA:H93	39:C:308:CLA:H111	1.87	0.42
19:G:91:TYR:HD2	19:G:94:THR:HG22	1.85	0.42
23:L:128:VAL:HA	23:L:131:LEU:HD12	2.02	0.42
24:W:60:ASP:HA	24:W:63:VAL:HG22	2.01	0.42
24:W:60:ASP:O	24:W:64:MET:HG3	2.19	0.42
32:1:116:LEU:H	32:1:121:LEU:HD21	1.84	0.42
49:3:317:KC2:CBC	39:3:322:CLA:H3A	2.50	0.42
28:4:135:ILE:HD13	28:4:162:PHE:HE1	1.84	0.42
39:5:308:CLA:H143	39:5:308:CLA:H161	1.87	0.42
39:a:815:CLA:H91	39:a:815:CLA:H111	1.83	0.42
9:l:7:PRO:HB3	9:l:12:PRO:HA	2.01	0.42
39:B:207:CLA:HBB1	39:B:207:CLA:H92	2.01	0.42
15:C:64:LEU:HD23	15:C:64:LEU:HA	1.92	0.42
39:C:304:CLA:H3A	39:C:304:CLA:HBA2	1.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:F:316:CLA:H3A	39:F:316:CLA:HBA2	1.75	0.42
20:H:67:PRO:HG3	21:J:139:VAL:HG23	2.01	0.42
39:L:311:CLA:H2A	39:L:311:CLA:HED3	2.00	0.42
24:M:67:ARG:NH2	39:M:308:CLA:O1D	2.53	0.42
27:R:158:TRP:CG	27:R:159:ASP:H	2.38	0.42
28:S:71:SER:OG	39:S:313:CLA:OBD	2.26	0.42
28:7:204:LEU:HD11	39:7:314:CLA:HAC1	2.01	0.42
39:7:314:CLA:HED3	39:7:314:CLA:HBD	1.80	0.42
1:a:368:ALA:HB2	1:a:394:HIS:HB2	2.02	0.42
2:b:257:PHE:HB3	39:b:818:CLA:HED1	2.01	0.42
14:B:60:GLU:HG3	14:B:61:TRP:CD1	2.54	0.42
14:B:101:LEU:HD11	30:U:67:TRP:CD2	2.54	0.42
24:M:140:LYS:HD2	24:M:154:GLU:OE2	2.20	0.42
39:Q:312:CLA:H62	39:Q:312:CLA:H93	1.83	0.42
28:S:119:PHE:CZ	46:S:322:LMG:HC91	2.55	0.42
39:V:310:CLA:H61	39:V:310:CLA:H2	1.67	0.42
31:0:201:GLY:O	31:0:205:MET:HG3	2.18	0.42
31:0:231:TYR:HE2	31:0:235:VAL:HG22	1.85	0.42
39:9:308:CLA:H2	39:9:308:CLA:H61	1.88	0.42
1:a:297:HIS:HB2	39:a:815:CLA:C1B	2.49	0.42
1:a:299:LEU:HD21	39:a:813:CLA:HMC3	2.01	0.42
39:a:801:CLA:H102	39:a:801:CLA:H62	1.75	0.42
42:a:842:BCR:H15C	42:a:842:BCR:H351	1.82	0.42
2:b:175:LEU:HD12	2:b:175:LEU:HA	1.87	0.42
2:b:584:LEU:HD21	2:b:714:THR:HG23	2.02	0.42
39:A:306:CLA:H92	39:A:306:CLA:H61	1.78	0.42
17:E:117:PHE:CE1	39:E:310:CLA:H3A	2.55	0.42
39:E:314:CLA:H61	39:E:314:CLA:H92	1.83	0.42
20:H:70:LEU:HD12	39:H:308:CLA:H2	2.02	0.42
25:O:176:ASP:OD1	25:O:176:ASP:N	2.47	0.42
24:P:52:LEU:HB3	24:P:54:ILE:HG13	2.01	0.42
26:Q:208:GLY:O	26:Q:212:MET:HG3	2.19	0.42
27:5:82:TRP:HE1	39:5:315:CLA:HMD2	1.85	0.42
27:5:83:ALA:O	27:5:87:SER:HB3	2.20	0.42
1:a:109:THR:HG21	1:a:518:ASN:HD22	1.84	0.42
39:b:803:CLA:H171	6:f:124:GLY:HA2	2.02	0.42
42:i:102:BCR:H11C	42:i:102:BCR:H341	1.87	0.42
42:m:101:BCR:H24C	42:m:101:BCR:H371	1.88	0.42
39:A:306:CLA:H111	39:A:306:CLA:H71	1.73	0.42
39:K:307:CLA:H61	39:K:307:CLA:H41	1.71	0.42
23:L:186:ARG:HD2	23:L:186:ARG:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:99:LYS:HE2	46:P:317:LMG:HC71	1.97	0.42
27:R:159:ASP:OD2	27:R:159:ASP:N	2.51	0.42
39:R:309:CLA:H143	39:R:309:CLA:H161	1.87	0.42
49:R:314:KC2:C3A	46:S:322:LMG:C32	2.97	0.42
28:S:60:ASP:HB3	28:S:61:GLN:H	1.75	0.42
39:T:308:CLA:OBD	49:T:315:KC2:CAD	2.67	0.42
39:0:310:CLA:H61	39:0:310:CLA:H41	1.71	0.42
35:9:75:HIS:CD2	39:9:312:CLA:HED2	2.54	0.42
1:a:216:HIS:HB2	39:a:812:CLA:C1C	2.49	0.41
1:a:430:VAL:HA	1:a:433:HIS:CE1	2.55	0.41
42:a:844:BCR:H15C	42:a:844:BCR:H351	1.80	0.41
7:i:5:PHE:HB3	39:i:103:CLA:HED1	2.02	0.41
39:P:308:CLA:H61	39:P:308:CLA:H92	1.80	0.41
26:Q:229:PRO:O	26:Q:230:PHE:HB2	2.20	0.41
28:S:201:LEU:HD12	39:S:308:CLA:HAC2	2.02	0.41
39:S:311:CLA:H143	39:S:311:CLA:H111	1.90	0.41
39:S:313:CLA:H112	39:S:313:CLA:H152	1.87	0.41
24:W:64:MET:HB3	24:W:150:PRO:HG3	2.02	0.41
24:W:200:ALA:HB2	52:W:306:A1EB4:C1	2.50	0.41
39:3:311:CLA:H62	39:3:311:CLA:H41	1.82	0.41
28:4:32:LEU:HD11	28:4:65:ILE:HD12	2.00	0.41
46:4:326:LMG:H301	46:4:326:LMG:H332	1.29	0.41
27:5:133:LEU:HD13	27:5:157:LEU:HD11	2.02	0.41
38:2:197:VAL:O	38:2:201:ARG:HG3	2.20	0.41
1:a:119:TRP:CD2	39:a:807:CLA:HED3	2.56	0.41
1:a:265:PHE:HB3	11:k:72:PRO:HB3	2.02	0.41
39:a:825:CLA:H151	39:b:805:CLA:H202	2.02	0.41
39:j:101:CLA:H112	39:j:101:CLA:H91	1.81	0.41
14:B:170:ASN:H	14:B:170:ASN:HD22	1.67	0.41
39:E:310:CLA:HBC3	39:E:313:CLA:H171	2.03	0.41
39:H:312:CLA:H3A	39:H:312:CLA:HBA2	1.47	0.41
22:K:35:LEU:HB3	22:K:36:VAL:H	1.64	0.41
47:P:301:SQD:H81	47:P:301:SQD:H112	1.83	0.41
39:S:311:CLA:H62	39:S:311:CLA:H93	1.80	0.41
27:V:100:GLN:HB2	27:V:102:VAL:HG23	2.02	0.41
27:X:82:TRP:HZ3	27:X:111:GLY:HA3	1.85	0.41
28:7:162:PHE:HB3	28:7:169:MET:HG3	2.02	0.41
35:9:118:PRO:HA	35:9:121:GLN:HB2	2.02	0.41
2:b:50:HIS:HE1	39:b:809:CLA:H171	1.85	0.41
39:b:828:CLA:H93	39:b:828:CLA:H111	1.89	0.41
42:f:801:BCR:H361	42:f:801:BCR:H20C	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:k:204:BCR:H341	42:k:204:BCR:H11C	1.71	0.41
13:A:118:ILE:O	13:A:122:ASN:ND2	2.46	0.41
15:C:95:ASP:OD1	15:C:95:ASP:N	2.54	0.41
19:G:160:ARG:HA	19:G:160:ARG:HD3	1.90	0.41
23:L:95:PHE:HB2	23:L:100:PHE:HE2	1.85	0.41
27:R:183:GLY:O	27:R:187:MET:HG3	2.21	0.41
39:W:311:CLA:H152	39:W:311:CLA:H111	1.79	0.41
31:0:180:LYS:HB3	31:0:183:LYS:HD3	2.01	0.41
39:4:314:CLA:H111	39:4:314:CLA:H71	1.90	0.41
27:5:199:ILE:O	27:5:202:SER:OG	2.37	0.41
1:a:204:GLY:O	1:a:208:LEU:HB2	2.20	0.41
1:a:406:ALA:HB2	42:a:845:BCR:H323	2.02	0.41
39:a:836:CLA:H72	42:a:845:BCR:H373	2.02	0.41
42:a:845:BCR:H15C	42:a:845:BCR:H351	1.82	0.41
42:l:202:BCR:C11	39:l:204:CLA:HAB	2.51	0.41
42:m:101:BCR:H11C	42:m:101:BCR:H341	1.91	0.41
13:A:194:LEU:HD23	13:A:194:LEU:HA	1.95	0.41
39:A:309:CLA:H92	39:A:309:CLA:H61	1.90	0.41
18:F:62:GLN:N	18:F:74:GLU:O	2.53	0.41
39:K:306:CLA:H112	39:K:306:CLA:H71	1.76	0.41
24:M:60:ASP:O	24:M:64:MET:HG3	2.20	0.41
27:R:136:LEU:O	27:R:140:ALA:HB2	2.20	0.41
39:S:320:CLA:H142	39:S:320:CLA:H111	1.78	0.41
29:T:77:TYR:O	29:T:85:THR:HA	2.19	0.41
39:1:308:CLA:HED2	39:1:308:CLA:HBD	1.95	0.41
28:7:42:VAL:HG13	34:6:135:HIS:CD2	2.55	0.41
36:I:53:CYS:SG	48:I:304:A86:O2	2.60	0.41
38:2:157:LYS:HB2	38:2:160:ARG:NH1	2.36	0.41
1:a:325:ILE:O	1:a:329:HIS:ND1	2.42	0.41
2:b:136:TYR:CZ	10:m:6:GLN:HB3	2.56	0.41
2:b:173:SER:O	2:b:177:HIS:ND1	2.31	0.41
39:b:809:CLA:H61	39:b:815:CLA:H61	2.03	0.41
42:b:848:BCR:H371	42:b:848:BCR:H24C	1.89	0.41
39:i:103:CLA:HBC1	39:B:209:CLA:H93	2.02	0.41
42:k:204:BCR:H15C	42:k:204:BCR:H351	1.86	0.41
39:A:314:CLA:H71	39:D:314:CLA:H142	2.03	0.41
39:B:209:CLA:H2A	39:B:209:CLA:HED2	2.03	0.41
39:D:318:CLA:H172	39:M:312:CLA:H102	2.02	0.41
17:E:42:PRO:HG2	17:E:56:ASP:HB3	2.01	0.41
39:F:308:CLA:H152	39:F:308:CLA:H18	1.69	0.41
21:J:148:LEU:CD2	21:J:153:ARG:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:141:LYS:HA	24:M:141:LYS:HD3	1.60	0.41
24:M:220:LEU:HB3	24:M:224:PHE:HB2	2.02	0.41
28:S:83:PHE:HE1	28:S:209:PHE:HE2	1.68	0.41
39:4:316:CLA:H152	39:4:316:CLA:H112	1.82	0.41
1:a:67:GLU:OE2	1:a:71:ARG:NH2	2.54	0.41
2:b:299:HIS:HB3	2:b:304:ILE:HD11	2.02	0.41
39:b:851:CLA:H93	39:b:851:CLA:H62	1.79	0.41
42:l:207:BCR:H11C	42:l:207:BCR:H341	1.88	0.41
14:B:17:GLY:N	39:B:204:CLA:OBD	2.44	0.41
39:F:309:CLA:HBC1	39:F:312:CLA:HAC1	2.02	0.41
22:K:182:SER:HB2	39:K:314:CLA:HMC1	2.03	0.41
39:K:311:CLA:H142	39:K:311:CLA:H111	1.83	0.41
23:L:75:LYS:NZ	23:L:132:GLU:OE1	2.50	0.41
25:O:64:THR:HG23	25:O:65:LEU:N	2.35	0.41
25:O:203:LEU:HD23	25:O:203:LEU:HA	1.82	0.41
24:P:37:MET:HE1	24:P:63:VAL:HG12	2.01	0.41
31:0:195:LEU:O	31:0:199:ASN:ND2	2.41	0.41
31:0:234:GLU:HB3	31:0:244:ASP:HA	2.03	0.41
28:7:206:LEU:HD23	28:7:206:LEU:HA	1.88	0.41
39:b:825:CLA:H52	39:b:825:CLA:H12	1.82	0.41
9:l:57:PHE:O	9:l:61:PRO:HD3	2.21	0.41
13:A:24:SER:OG	13:A:46:GLY:O	2.37	0.41
24:M:159:ASP:OD1	24:M:168:LYS:NZ	2.53	0.41
49:X:312:KC2:CBC	39:X:317:CLA:H3A	2.51	0.41
46:0:324:LMG:O1	46:0:324:LMG:HC61	2.21	0.41
32:1:119:GLN:O	32:1:122:TRP:N	2.53	0.41
32:1:122:TRP:O	32:1:125:THR:OG1	2.39	0.41
35:9:215:ALA:HB1	35:9:226:VAL:HG11	2.02	0.41
50:x:302:A1EB1:C24	39:x:307:CLA:HAB	2.50	0.41
28:y:165:ASN:O	28:y:167:HIS:N	2.53	0.41
1:a:81:LEU:HD22	39:a:803:CLA:H92	2.03	0.41
2:b:649:MET:HE2	42:b:848:BCR:H333	2.01	0.41
2:b:675:ILE:HD11	42:b:848:BCR:H282	2.02	0.41
39:b:826:CLA:H141	39:b:826:CLA:H162	1.79	0.41
4:d:102:LYS:C	4:d:104:GLY:H	2.29	0.41
39:i:101:CLA:H93	39:i:101:CLA:H61	1.81	0.41
39:F:314:CLA:H61	39:F:314:CLA:H41	1.87	0.41
20:H:182:ILE:O	20:H:186:ARG:HG3	2.21	0.41
21:J:109:ALA:HA	21:J:116:ALA:HA	2.02	0.41
21:J:197:VAL:CG1	39:J:318:CLA:H2A	2.51	0.41
24:P:50:ASP:OD2	24:P:54:ILE:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S:82:GLY:HA2	39:S:311:CLA:HBB1	2.03	0.41
29:T:164:PHE:HD2	39:T:308:CLA:HED3	1.85	0.41
31:0:222:PRO:O	48:0:304:A86:O2	2.38	0.41
28:4:165:ASN:O	46:4:325:LMG:O3	2.36	0.41
1:a:87:TRP:NE1	39:a:825:CLA:OBD	2.53	0.41
39:a:825:CLA:H142	39:a:825:CLA:H111	1.88	0.41
2:b:142:LEU:HG	42:b:846:BCR:H382	2.02	0.41
2:b:203:ARG:NH2	2:b:253:ALA:O	2.43	0.41
2:b:456:GLU:OE1	6:f:93:HIS:ND1	2.54	0.41
39:b:810:CLA:H112	39:b:810:CLA:H71	1.90	0.41
39:b:811:CLA:HAB	39:b:812:CLA:HAA2	2.03	0.41
39:b:826:CLA:H112	39:b:826:CLA:H142	1.81	0.41
8:j:16:LEU:HD11	39:j:101:CLA:H93	2.03	0.41
39:l:205:CLA:HBC1	42:l:207:BCR:H372	2.03	0.41
11:k:84:MET:O	11:k:88:ASN:ND2	2.41	0.41
39:k:203:CLA:H11	39:k:203:CLA:H52	1.78	0.41
39:o:206:CLA:H93	39:o:206:CLA:H61	1.79	0.41
17:E:60:LEU:HD13	39:E:308:CLA:H42	2.02	0.41
17:E:128:GLU:HG2	39:E:312:CLA:NB	2.36	0.41
39:E:317:CLA:H3A	39:E:317:CLA:HBA2	1.81	0.41
20:H:44:GLN:HG2	39:H:306:CLA:HED2	2.01	0.41
39:K:312:CLA:H142	39:K:312:CLA:H111	1.90	0.41
23:L:116:LEU:HD11	39:L:311:CLA:HAA2	2.02	0.41
23:L:241:LEU:HD23	23:L:241:LEU:HA	1.94	0.41
25:O:60:LYS:HB3	25:O:61:LEU:H	1.63	0.41
26:Q:87:ILE:HD12	39:Q:314:CLA:HMD3	2.03	0.41
39:T:308:CLA:H3A	39:T:308:CLA:HBA2	1.87	0.41
39:W:313:CLA:H112	39:W:313:CLA:H142	1.84	0.41
27:X:141:VAL:HG22	27:X:155:PRO:HD2	2.03	0.41
36:I:82:LYS:NZ	36:I:135:GLU:OE1	2.51	0.41
39:Y:305:CLA:H2A	39:Y:305:CLA:HED2	2.02	0.41
2:b:147:THR:HG23	10:m:20:LEU:HD12	2.03	0.41
6:f:105:GLU:HB3	6:f:106:PHE:H	1.71	0.41
15:C:121:LYS:HD2	15:C:136:LEU:HB2	2.02	0.41
39:E:312:CLA:H143	39:E:312:CLA:H111	1.86	0.41
39:J:310:CLA:H61	39:J:310:CLA:H92	1.89	0.41
39:Q:321:CLA:H3A	39:Q:321:CLA:HBA2	1.74	0.41
39:4:323:CLA:C12	46:4:326:LMG:H172	2.51	0.41
28:7:110:ALA:O	50:7:306:A1EB1:O2	2.39	0.41
28:y:82:GLY:HA2	39:y:310:CLA:HBB1	2.01	0.41
1:a:311:MET:O	1:a:320:HIS:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:a:823:CLA:H93	39:a:836:CLA:H52	2.03	0.40
39:a:824:CLA:H61	39:a:824:CLA:H2	1.69	0.40
39:b:811:CLA:O1A	39:b:828:CLA:HBD	2.21	0.40
39:l:201:CLA:H93	39:l:201:CLA:H61	1.82	0.40
39:G:318:CLA:H11	39:G:318:CLA:HBA2	1.84	0.40
23:L:71:HIS:CD2	23:L:75:LYS:HD2	2.55	0.40
28:S:32:LEU:HD12	39:S:309:CLA:HED1	2.03	0.40
30:U:70:GLU:OE1	30:U:148:GLY:N	2.48	0.40
39:V:313:CLA:H142	39:V:313:CLA:H112	1.96	0.40
27:X:186:ALA:O	27:X:190:VAL:HG23	2.22	0.40
28:4:142:LEU:HD13	28:4:160:PRO:HG3	2.03	0.40
39:4:312:CLA:H141	39:4:312:CLA:H162	1.92	0.40
39:4:323:CLA:H61	39:4:323:CLA:H41	1.89	0.40
28:7:37:LYS:HA	28:7:37:LYS:HD3	1.88	0.40
47:9:322:SQD:H241	47:9:322:SQD:H272	1.87	0.40
1:a:161:TRP:CG	39:o:201:CLA:HBA1	2.56	0.40
1:a:392:THR:HG22	1:a:607:ILE:HB	2.03	0.40
39:b:808:CLA:HBD	10:m:30:VAL:HG22	2.03	0.40
4:d:87:ILE:HB	4:d:100:HIS:HB2	2.03	0.40
11:k:110:GLU:HA	11:k:113:GLU:HB3	2.02	0.40
39:A:314:CLA:H93	39:A:314:CLA:H112	1.91	0.40
39:D:318:CLA:H143	39:D:319:CLA:H203	2.02	0.40
25:O:93:GLY:O	25:O:97:MET:HG3	2.21	0.40
25:O:188:ALA:HB1	25:O:192:HIS:HE1	1.85	0.40
26:Q:198:ALA:O	26:Q:202:LEU:HG	2.21	0.40
49:R:314:KC2:CHB	46:S:322:LMG:H322	2.51	0.40
31:0:43:LEU:HD12	31:0:47:VAL:HG22	2.04	0.40
28:7:140:ASN:HD22	46:7:326:LMG:HC61	1.87	0.40
34:6:54:ASN:HD21	34:6:59:GLY:H	1.70	0.40
1:a:45:THR:HG22	1:a:715:GLN:HB2	2.03	0.40
1:a:734:LEU:HD22	39:a:837:CLA:HMA1	2.03	0.40
39:a:806:CLA:HBA2	39:a:806:CLA:H3A	1.43	0.40
39:a:822:CLA:H162	39:a:822:CLA:H202	1.83	0.40
39:a:825:CLA:H3A	39:a:825:CLA:HBA2	1.86	0.40
39:a:835:CLA:H51	39:a:835:CLA:H11	1.88	0.40
2:b:348:VAL:HG12	39:b:820:CLA:C2	2.51	0.40
39:b:814:CLA:HBB1	39:b:814:CLA:H72	2.03	0.40
39:b:824:CLA:H62	39:b:824:CLA:H41	1.85	0.40
9:l:143:PHE:HZ	30:U:119:LEU:HG	1.87	0.40
39:D:319:CLA:HMC3	24:M:127:LEU:HD13	2.03	0.40
17:E:211:GLN:NE2	24:P:112:TYR:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:52:PRO:HB3	47:H:318:SQD:H3	2.03	0.40
25:O:92:HIS:HA	39:O:313:CLA:HMD1	2.04	0.40
39:P:309:CLA:H111	39:P:309:CLA:H152	1.67	0.40
30:U:136:TYR:O	30:U:140:ILE:HG12	2.21	0.40
27:V:159:ASP:OD1	27:V:163:PHE:N	2.46	0.40
39:3:314:CLA:H151	39:3:322:CLA:C1C	2.51	0.40
34:8:34:LEU:HD22	34:8:68:ARG:HH12	1.85	0.40
35:9:206:GLY:O	35:9:210:MET:HG3	2.21	0.40
39:a:811:CLA:H61	39:a:811:CLA:H41	1.87	0.40
39:b:813:CLA:H62	39:b:813:CLA:H41	1.89	0.40
39:J:314:CLA:H143	39:J:314:CLA:H111	1.89	0.40
39:L:310:CLA:H3A	39:L:310:CLA:HBA1	1.87	0.40
39:Q:310:CLA:H71	39:Q:311:CLA:HMA3	2.03	0.40
27:X:162:GLY:O	34:8:53:LEU:HD13	2.21	0.40
28:7:135:ILE:HG12	28:7:141:PHE:CE2	2.57	0.40
38:Z:223:ASP:O	38:Z:225:VAL:N	2.54	0.40
39:Z:313:CLA:OBD	39:Z:313:CLA:HED3	2.21	0.40
1:a:429:ARG:NH2	9:l:3:GLU:OE1	2.53	0.40
1:a:719:LEU:N	40:a:839:PQN:O4	2.49	0.40
2:b:525:LEU:HD21	39:b:805:CLA:HBB1	2.02	0.40
39:b:817:CLA:H91	39:b:817:CLA:H112	1.85	0.40
11:k:106:THR:HA	11:k:107:PRO:HD3	1.90	0.40
13:A:60:TRP:CD2	13:A:130:MET:HG2	2.56	0.40
16:D:126:ILE:HG13	16:D:131:MET:HG3	2.04	0.40
18:F:52:LYS:HE2	18:F:56:GLU:HB2	2.02	0.40
18:F:57:TYR:HB3	18:F:103:ARG:NH2	2.37	0.40
18:F:96:ASN:HA	18:F:97:PRO:HD3	1.95	0.40
39:H:313:CLA:H193	39:H:313:CLA:H161	1.86	0.40
25:O:206:GLN:HG2	39:O:316:CLA:C4D	2.51	0.40
26:Q:117:LEU:CG	26:Q:118:PRO:HD2	2.52	0.40
26:Q:230:PHE:HE1	32:1:132:GLN:CG	2.34	0.40
26:Q:232:LYS:CE	48:Q:304:A86:C32	2.87	0.40
31:0:39:LEU:HD21	39:0:311:CLA:CGD	2.51	0.40
28:4:170:PRO:HA	34:6:53:LEU:HD13	2.04	0.40
43:7:310:DD6:C21	39:7:324:CLA:HMC3	2.52	0.40
35:9:148:MET:SD	35:9:151:HIS:HA	2.62	0.40
38:2:60:ILE:HD12	38:2:152:PRO:HB2	2.04	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	739/752 (98%)	706 (96%)	33 (4%)	0	100	100
2	b	731/734 (100%)	698 (96%)	32 (4%)	1 (0%)	48	77
3	c	78/81 (96%)	74 (95%)	3 (4%)	1 (1%)	9	31
4	d	138/142 (97%)	125 (91%)	12 (9%)	1 (1%)	18	47
5	e	61/131 (47%)	58 (95%)	2 (3%)	1 (2%)	7	27
6	f	159/184 (86%)	154 (97%)	5 (3%)	0	100	100
7	i	31/36 (86%)	29 (94%)	2 (6%)	0	100	100
8	j	38/40 (95%)	38 (100%)	0	0	100	100
9	l	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
10	m	28/30 (93%)	27 (96%)	0	1 (4%)	2	10
11	k	71/145 (49%)	69 (97%)	1 (1%)	1 (1%)	9	30
12	o	46/123 (37%)	36 (78%)	9 (20%)	1 (2%)	5	19
13	A	181/201 (90%)	167 (92%)	13 (7%)	1 (1%)	21	51
14	B	170/177 (96%)	153 (90%)	15 (9%)	2 (1%)	10	34
15	C	174/233 (75%)	164 (94%)	9 (5%)	1 (1%)	21	51
16	D	187/231 (81%)	172 (92%)	14 (8%)	1 (0%)	24	55
17	E	185/217 (85%)	169 (91%)	16 (9%)	0	100	100
18	F	186/239 (78%)	157 (84%)	23 (12%)	6 (3%)	3	11
19	G	169/204 (83%)	148 (88%)	16 (10%)	5 (3%)	3	12
20	H	166/210 (79%)	147 (89%)	18 (11%)	1 (1%)	21	51
21	J	169/251 (67%)	150 (89%)	18 (11%)	1 (1%)	21	51
22	K	166/198 (84%)	149 (90%)	12 (7%)	5 (3%)	3	12
23	L	208/244 (85%)	182 (88%)	24 (12%)	2 (1%)	12	38
24	M	191/224 (85%)	170 (89%)	18 (9%)	3 (2%)	7	27
24	P	191/224 (85%)	175 (92%)	14 (7%)	2 (1%)	12	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
24	W	191/224 (85%)	176 (92%)	12 (6%)	3 (2%)	7 27
25	O	153/219 (70%)	135 (88%)	13 (8%)	5 (3%)	3 11
26	Q	213/257 (83%)	178 (84%)	24 (11%)	11 (5%)	1 5
27	5	175/219 (80%)	153 (87%)	22 (13%)	0	100 100
27	R	175/219 (80%)	151 (86%)	24 (14%)	0	100 100
27	V	178/219 (81%)	147 (83%)	24 (14%)	7 (4%)	2 8
27	X	175/219 (80%)	157 (90%)	18 (10%)	0	100 100
28	4	226/255 (89%)	202 (89%)	21 (9%)	3 (1%)	9 31
28	7	226/255 (89%)	201 (89%)	24 (11%)	1 (0%)	30 60
28	S	226/255 (89%)	204 (90%)	18 (8%)	4 (2%)	6 23
28	x	226/255 (89%)	203 (90%)	20 (9%)	3 (1%)	9 31
28	y	226/255 (89%)	211 (93%)	13 (6%)	2 (1%)	14 41
28	z	226/255 (89%)	203 (90%)	19 (8%)	4 (2%)	6 23
29	T	195/211 (92%)	169 (87%)	23 (12%)	3 (2%)	8 28
30	U	156/198 (79%)	138 (88%)	16 (10%)	2 (1%)	9 31
31	0	216/254 (85%)	186 (86%)	25 (12%)	5 (2%)	5 18
32	1	199/253 (79%)	163 (82%)	29 (15%)	7 (4%)	3 10
33	3	234/268 (87%)	204 (87%)	26 (11%)	4 (2%)	7 25
34	6	217/250 (87%)	182 (84%)	31 (14%)	4 (2%)	6 23
34	8	217/250 (87%)	186 (86%)	25 (12%)	6 (3%)	4 14
35	9	207/245 (84%)	173 (84%)	32 (16%)	2 (1%)	12 38
36	I	154/209 (74%)	142 (92%)	12 (8%)	0	100 100
37	h	85/133 (64%)	83 (98%)	2 (2%)	0	100 100
38	2	222/260 (85%)	186 (84%)	31 (14%)	5 (2%)	5 18
38	Y	223/260 (86%)	186 (83%)	31 (14%)	6 (3%)	4 15
38	Z	223/260 (86%)	191 (86%)	26 (12%)	6 (3%)	4 15
All	All	9768/11553 (84%)	8765 (90%)	873 (9%)	130 (1%)	12 31

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	101	PRO
13	A	200	SER

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Mol	Chain	Res	Type
15	C	171	ASN
18	F	135	ILE
18	F	181	GLU
18	F	185	PRO
22	K	35	LEU
22	K	153	PRO
22	K	154	ARG
23	L	98	ALA
24	M	40	VAL
24	M	141	LYS
24	M	142	PRO
25	O	64	THR
25	O	116	GLU
24	P	40	VAL
24	P	142	PRO
26	Q	119	ALA
26	Q	236	PRO
28	S	239	PRO
29	T	102	PRO
29	T	150	PHE
27	V	119	PRO
27	V	200	PRO
24	W	141	LYS
31	0	101	TRP
31	0	228	VAL
32	1	114	LYS
33	3	107	PRO
33	3	129	PRO
28	4	166	VAL
28	7	166	VAL
34	8	97	PRO
34	8	162	MET
28	x	239	PRO
28	z	100	PRO
28	z	110	ALA
28	z	236	PRO
38	Y	92	THR
38	Y	167	PRO
38	Z	92	THR
38	Z	167	PRO
38	Z	220	PRO
38	2	167	PRO

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Mol	Chain	Res	Type
38	2	220	PRO
34	6	97	PRO
11	k	143	PHE
14	B	49	LEU
14	B	171	LEU
25	O	63	GLY
25	O	169	PHE
26	Q	231	LEU
26	Q	237	ALA
28	S	166	VAL
29	T	35	PHE
27	V	98	VAL
27	V	202	SER
24	W	40	VAL
31	0	44	ASN
32	1	47	LEU
32	1	236	ARG
32	1	242	VAL
34	8	105	ILE
35	9	170	ILE
38	Y	107	ALA
38	Y	224	THR
38	Z	224	THR
38	2	224	THR
34	6	235	ALA
3	c	63	LEU
16	D	230	SER
19	G	104	PRO
19	G	139	PRO
19	G	156	ASP
21	J	152	ASP
27	V	166	LYS
31	0	102	ALA
31	0	183	LYS
32	1	54	TRP
32	1	235	ILE
28	x	244	THR
28	z	98	ILE
38	Z	235	MET
34	6	49	ASN
5	e	95	GLU
22	K	90	HIS

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Mol	Chain	Res	Type
28	S	161	THR
34	8	161	THR
34	8	235	ALA
38	Y	87	GLN
38	2	87	GLN
34	6	105	ILE
2	b	243	ILE
10	m	29	TYR
18	F	93	SER
19	G	154	ALA
20	H	106	VAL
22	K	101	VAL
23	L	227	TYR
26	Q	115	THR
26	Q	175	PRO
28	S	249	ILE
30	U	43	GLU
30	U	194	ALA
24	W	142	PRO
33	3	259	VAL
28	4	249	ILE
35	9	126	PRO
28	x	249	ILE
38	Y	108	ASP
19	G	146	GLU
25	O	66	VAL
26	Q	51	ALA
26	Q	234	VAL
27	V	110	ASP
26	Q	250	ILE
27	V	155	PRO
28	y	249	ILE
18	F	79	VAL
12	o	75	PRO
26	Q	102	ILE
26	Q	180	PHE
33	3	232	VAL
28	4	98	ILE
34	8	239	LEU
28	y	166	VAL
38	Z	225	VAL
38	2	225	VAL

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Mol	Chain	Res	Type
18	F	127	ILE
32	1	113	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	608/616 (99%)	608 (100%)	0	100 100
2	b	591/592 (100%)	591 (100%)	0	100 100
3	c	68/69 (99%)	68 (100%)	0	100 100
4	d	120/122 (98%)	118 (98%)	2 (2%)	53 83
5	e	51/91 (56%)	51 (100%)	0	100 100
6	f	126/144 (88%)	126 (100%)	0	100 100
7	i	29/32 (91%)	29 (100%)	0	100 100
8	j	36/36 (100%)	36 (100%)	0	100 100
9	l	114/115 (99%)	114 (100%)	0	100 100
10	m	23/23 (100%)	23 (100%)	0	100 100
11	k	56/107 (52%)	56 (100%)	0	100 100
12	o	40/85 (47%)	40 (100%)	0	100 100
13	A	155/170 (91%)	155 (100%)	0	100 100
14	B	120/131 (92%)	119 (99%)	1 (1%)	73 90
15	C	140/181 (77%)	140 (100%)	0	100 100
16	D	140/171 (82%)	140 (100%)	0	100 100
17	E	146/163 (90%)	146 (100%)	0	100 100
18	F	140/180 (78%)	138 (99%)	2 (1%)	59 85
19	G	132/153 (86%)	132 (100%)	0	100 100
20	H	131/163 (80%)	131 (100%)	0	100 100
21	J	128/194 (66%)	128 (100%)	0	100 100
22	K	127/149 (85%)	126 (99%)	1 (1%)	73 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	L	161/183 (88%)	160 (99%)	1 (1%)	78 92
24	M	146/165 (88%)	145 (99%)	1 (1%)	76 91
24	P	146/165 (88%)	146 (100%)	0	100 100
24	W	146/165 (88%)	144 (99%)	2 (1%)	59 85
25	O	112/160 (70%)	111 (99%)	1 (1%)	70 89
26	Q	171/199 (86%)	167 (98%)	4 (2%)	44 78
27	5	134/157 (85%)	134 (100%)	0	100 100
27	R	134/157 (85%)	134 (100%)	0	100 100
27	V	132/157 (84%)	132 (100%)	0	100 100
27	X	134/157 (85%)	134 (100%)	0	100 100
28	4	179/199 (90%)	179 (100%)	0	100 100
28	7	179/199 (90%)	179 (100%)	0	100 100
28	S	179/199 (90%)	177 (99%)	2 (1%)	65 87
29	T	150/161 (93%)	150 (100%)	0	100 100
30	U	128/162 (79%)	128 (100%)	0	100 100
31	0	177/198 (89%)	177 (100%)	0	100 100
32	1	74/194 (38%)	74 (100%)	0	100 100
33	3	181/204 (89%)	181 (100%)	0	100 100
34	6	58/183 (32%)	58 (100%)	0	100 100
34	8	91/183 (50%)	89 (98%)	2 (2%)	45 78
35	9	126/188 (67%)	126 (100%)	0	100 100
36	I	126/163 (77%)	126 (100%)	0	100 100
37	h	67/94 (71%)	67 (100%)	0	100 100
38	2	82/204 (40%)	82 (100%)	0	100 100
All	All	6434/7883 (82%)	6415 (100%)	19 (0%)	84 95

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	100	HIS
4	d	102	LYS
14	B	171	LEU
18	F	135	ILE
18	F	215	LEU

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Mol	Chain	Res	Type
22	K	152	VAL
23	L	222	SER
24	M	141	LYS
25	O	65	LEU
26	Q	117	LEU
26	Q	231	LEU
26	Q	232	LYS
26	Q	239	THR
28	S	238	LEU
28	S	240	THR
24	W	140	LYS
24	W	141	LYS
34	8	160	ASP
34	8	161	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	80	GLN
1	a	193	ASN
1	a	320	HIS
1	a	393	HIS
1	a	442	ASN
1	a	451	HIS
1	a	723	GLN
2	b	10	GLN
2	b	41	ASN
2	b	114	ASN
2	b	158	GLN
2	b	266	GLN
2	b	299	HIS
2	b	627	ASN
4	d	9	GLN
4	d	93	ASN
4	d	100	HIS
6	f	67	GLN
6	f	68	GLN
6	f	129	GLN
9	l	73	ASN
9	l	102	GLN
9	l	118	ASN
11	k	75	GLN

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Mol	Chain	Res	Type
13	A	82	GLN
14	B	67	GLN
14	B	170	ASN
15	C	194	GLN
17	E	67	GLN
17	E	208	GLN
18	F	132	ASN
18	F	212	ASN
18	F	226	ASN
19	G	55	ASN
20	H	198	GLN
21	J	67	ASN
22	K	44	ASN
22	K	139	ASN
22	K	157	GLN
22	K	166	GLN
23	L	92	ASN
24	M	73	HIS
24	M	155	GLN
24	M	212	ASN
25	O	136	HIS
24	P	155	GLN
26	Q	207	ASN
26	Q	249	ASN
28	S	140	ASN
28	S	251	ASN
29	T	70	ASN
24	W	185	GLN
24	W	212	ASN
27	X	125	GLN
31	0	65	ASN
31	0	118	GLN
32	1	58	ASN
33	3	54	ASN
33	3	135	GLN
33	3	210	ASN
28	4	61	GLN
27	5	125	GLN
27	5	182	ASN
27	5	197	HIS
28	7	61	GLN
28	7	140	ASN

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Mol	Chain	Res	Type
34	8	164	HIS
35	9	132	GLN
35	9	220	GLN
38	2	57	HIS
38	2	198	ASN
34	6	195	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

869 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	A86	S	307	-	44,50,50	1.19	2 (4%)	51,76,76	2.32	18 (35%)
39	CLA	G	314	19	62,66,73	1.31	7 (11%)	74,104,113	1.45	6 (8%)
43	DD6	E	302	-	39,45,45	1.98	3 (7%)	52,67,67	1.77	8 (15%)
46	LMG	M	320	-	33,33,55	0.94	0	41,41,63	1.19	4 (9%)
39	CLA	I	308	-	65,69,73	1.27	7 (10%)	78,108,113	1.29	7 (8%)
49	KC2	A	310	13	49,53,53	1.81	9 (18%)	62,89,89	2.04	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	1	316	-	45,49,73	1.53	6 (13%)	54,84,113	1.54	5 (9%)
50	A1EB1	E	301	-	51,58,58	1.31	4 (7%)	60,85,85	1.91	19 (31%)
39	CLA	R	309	-	69,73,73	1.25	6 (8%)	83,113,113	1.32	7 (8%)
49	KC2	V	312	-	49,53,53	1.77	10 (20%)	62,89,89	2.18	18 (29%)
39	CLA	a	837	-	69,73,73	1.27	7 (10%)	83,113,113	1.26	5 (6%)
39	CLA	G	312	-	56,60,73	1.39	6 (10%)	67,97,113	1.47	6 (8%)
39	CLA	I	309	-	69,73,73	1.27	7 (10%)	83,113,113	1.29	4 (4%)
39	CLA	6	313	-	46,50,73	1.50	6 (13%)	55,85,113	1.48	4 (7%)
46	LMG	Q	322	49	28,28,55	1.26	2 (7%)	36,36,63	1.44	6 (16%)
39	CLA	b	827	-	69,73,73	1.26	7 (10%)	83,113,113	1.31	4 (4%)
48	A86	P	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.25	18 (35%)
39	CLA	D	309	16	53,57,73	1.43	8 (15%)	62,93,113	1.53	7 (11%)
48	A86	7	307	-	44,50,50	1.24	3 (6%)	51,76,76	2.22	17 (33%)
49	KC2	z	312	-	49,53,53	1.78	10 (20%)	62,89,89	2.04	15 (24%)
39	CLA	X	307	-	69,73,73	1.26	6 (8%)	83,113,113	1.27	6 (7%)
39	CLA	b	803	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
39	CLA	4	319	-	45,49,73	1.53	7 (15%)	54,84,113	1.56	5 (9%)
43	DD6	Q	303	-	39,45,45	2.12	3 (7%)	52,67,67	2.59	17 (32%)
39	CLA	f	802	-	69,73,73	1.27	7 (10%)	83,113,113	1.26	7 (8%)
43	DD6	y	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.84	14 (26%)
50	A1EB1	S	302	-	51,58,58	1.30	3 (5%)	60,85,85	1.97	17 (28%)
39	CLA	6	310	-	46,50,73	1.53	7 (15%)	55,85,113	1.44	5 (9%)
39	CLA	F	313	-	61,65,73	1.34	9 (14%)	73,103,113	1.35	6 (8%)
39	CLA	a	818	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	6 (7%)
48	A86	9	305	-	44,50,50	1.19	3 (6%)	51,76,76	1.91	17 (33%)
50	A1EB1	J	302	-	51,58,58	1.26	4 (7%)	60,85,85	2.25	23 (38%)
41	LHG	H	317	-	34,34,48	0.71	0	37,40,54	1.19	3 (8%)
39	CLA	O	312	-	50,54,73	1.47	8 (16%)	60,90,113	1.45	4 (6%)
43	DD6	Q	306	-	39,45,45	2.01	3 (7%)	52,67,67	1.83	14 (26%)
46	LMG	M	319	49	39,39,55	1.08	2 (5%)	47,47,63	1.56	8 (17%)
39	CLA	Y	307	-	45,49,73	1.53	7 (15%)	54,84,113	1.40	5 (9%)
48	A86	R	301	-	44,50,50	1.22	3 (6%)	51,76,76	2.06	16 (31%)
48	A86	y	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.00	16 (31%)
39	CLA	T	309	-	60,64,73	1.37	7 (11%)	72,102,113	1.34	9 (12%)
50	A1EB1	4	301	-	51,58,58	1.25	3 (5%)	60,85,85	1.93	18 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	X	317	-	56,60,73	1.40	9 (16%)	67,97,113	1.45	6 (8%)
39	CLA	5	307	-	64,68,73	1.32	7 (10%)	77,107,113	1.30	6 (7%)
39	CLA	y	309	-	50,54,73	1.47	7 (14%)	60,90,113	1.43	5 (8%)
49	KC2	y	316	-	49,53,53	1.75	10 (20%)	62,89,89	2.15	18 (29%)
39	CLA	9	319	-	49,53,73	1.50	6 (12%)	59,89,113	1.47	5 (8%)
51	A1ECV	W	317	-	47,56,56	3.34	19 (40%)	32,93,93	3.00	10 (31%)
39	CLA	a	835	-	69,73,73	1.26	8 (11%)	83,113,113	1.32	8 (9%)
39	CLA	H	309	20	56,60,73	1.40	8 (14%)	67,97,113	1.40	6 (8%)
39	CLA	J	316	-	50,54,73	1.46	7 (14%)	60,90,113	1.49	4 (6%)
39	CLA	3	320	-	49,53,73	1.49	6 (12%)	59,89,113	1.53	6 (10%)
49	KC2	y	314	-	49,53,53	1.81	9 (18%)	62,89,89	2.05	14 (22%)
39	CLA	E	312	-	69,73,73	1.27	9 (13%)	83,113,113	1.27	6 (7%)
39	CLA	h	201	-	59,63,73	1.35	8 (13%)	71,101,113	1.35	6 (8%)
39	CLA	i	101	-	69,73,73	1.25	7 (10%)	83,113,113	1.25	5 (6%)
39	CLA	Q	310	-	69,73,73	1.27	8 (11%)	83,113,113	1.27	10 (12%)
48	A86	9	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.01	14 (27%)
39	CLA	y	310	-	45,49,73	1.52	7 (15%)	54,84,113	1.50	5 (9%)
39	CLA	A	312	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	7 (8%)
51	A1ECV	1	318	-	47,56,56	3.33	20 (42%)	32,93,93	3.34	11 (34%)
39	CLA	W	319	-	50,54,73	1.47	6 (12%)	60,90,113	1.44	4 (6%)
50	A1EB1	H	301	-	51,58,58	1.27	3 (5%)	60,85,85	2.10	17 (28%)
39	CLA	1	308	-	45,49,73	1.54	7 (15%)	54,84,113	1.57	5 (9%)
39	CLA	I	310	-	58,62,73	1.36	8 (13%)	69,99,113	1.39	5 (7%)
48	A86	F	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.12	15 (29%)
39	CLA	K	308	22	63,67,73	1.32	8 (12%)	75,105,113	1.30	5 (6%)
49	KC2	R	306	-	49,53,53	1.81	10 (20%)	62,89,89	2.08	14 (22%)
49	KC2	2	317	-	49,53,53	1.78	11 (22%)	62,89,89	2.24	19 (30%)
50	A1EB1	R	303	-	51,58,58	1.31	5 (9%)	60,85,85	2.18	19 (31%)
39	CLA	P	308	24	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
39	CLA	l	203	-	53,57,73	1.44	8 (15%)	62,93,113	1.45	7 (11%)
39	CLA	T	310	29	56,60,73	1.39	9 (16%)	67,97,113	1.39	5 (7%)
39	CLA	H	315	-	45,49,73	1.51	8 (17%)	54,84,113	1.50	6 (11%)
39	CLA	b	828	-	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
39	CLA	F	321	-	69,73,73	1.26	7 (10%)	83,113,113	1.33	8 (9%)
39	CLA	J	308	-	54,58,73	1.42	6 (11%)	65,95,113	1.41	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	y	318	-	46,50,73	1.51	6 (13%)	55,85,113	1.48	4 (7%)
49	KC2	Z	310	-	49,53,53	1.76	10 (20%)	62,89,89	2.15	18 (29%)
48	A86	8	309	-	44,50,50	1.17	3 (6%)	51,76,76	2.32	19 (37%)
50	A1EB1	F	304	-	51,58,58	1.30	4 (7%)	60,85,85	2.12	18 (30%)
39	CLA	O	313	-	54,58,73	1.40	8 (14%)	65,95,113	1.45	5 (7%)
39	CLA	a	808	-	60,64,73	1.34	8 (13%)	72,102,113	1.39	4 (5%)
39	CLA	X	311	27	54,58,73	1.41	6 (11%)	65,95,113	1.42	7 (10%)
39	CLA	0	315	31	54,58,73	1.39	7 (12%)	65,95,113	1.42	9 (13%)
39	CLA	b	851	-	69,73,73	1.27	8 (11%)	83,113,113	1.26	5 (6%)
48	A86	U	206	-	44,50,50	1.20	3 (6%)	51,76,76	2.39	19 (37%)
49	KC2	R	318	-	49,53,53	1.78	10 (20%)	62,89,89	2.13	17 (27%)
49	KC2	L	312	-	49,53,53	1.81	10 (20%)	62,89,89	1.99	14 (22%)
47	SQD	4	327	-	38,39,54	1.14	5 (13%)	47,50,65	1.69	11 (23%)
49	KC2	1	312	-	49,53,53	1.83	11 (22%)	62,89,89	2.02	15 (24%)
39	CLA	8	312	-	49,53,73	1.49	7 (14%)	59,89,113	1.49	4 (6%)
47	SQD	T	321	-	35,36,54	1.15	5 (14%)	44,47,65	1.80	10 (22%)
39	CLA	k	203	-	59,63,73	1.36	7 (11%)	71,101,113	1.37	5 (7%)
48	A86	3	308	-	44,50,50	1.25	3 (6%)	51,76,76	2.33	18 (35%)
50	A1EB1	0	302	-	51,58,58	1.22	3 (5%)	60,85,85	2.11	19 (31%)
49	KC2	Q	315	-	49,53,53	1.75	10 (20%)	62,89,89	2.13	18 (29%)
43	DD6	z	305	-	39,45,45	2.02	2 (5%)	52,67,67	1.89	16 (30%)
48	A86	I	304	-	44,50,50	1.13	3 (6%)	51,76,76	2.14	14 (27%)
39	CLA	b	841	2	69,73,73	1.28	6 (8%)	83,113,113	1.29	6 (7%)
50	A1EB1	x	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.07	19 (31%)
39	CLA	z	308	-	50,54,73	1.46	7 (14%)	60,90,113	1.42	4 (6%)
46	LMG	9	321	-	36,36,55	0.91	0	44,44,63	1.20	3 (6%)
48	A86	Z	301	-	44,50,50	1.17	3 (6%)	51,76,76	2.18	19 (37%)
49	KC2	5	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.16	18 (29%)
39	CLA	L	316	-	45,49,73	1.51	7 (15%)	54,84,113	1.60	6 (11%)
39	CLA	o	201	-	55,59,73	1.40	8 (14%)	66,96,113	1.40	5 (7%)
39	CLA	b	838	-	69,73,73	1.25	6 (8%)	83,113,113	1.33	8 (9%)
39	CLA	8	321	-	46,50,73	1.51	7 (15%)	55,85,113	1.46	4 (7%)
43	DD6	y	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.93	15 (28%)
48	A86	O	306	-	44,50,50	1.18	3 (6%)	51,76,76	2.57	20 (39%)
39	CLA	L	313	-	54,58,73	1.40	8 (14%)	65,95,113	1.40	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	0	322	-	55,59,73	1.42	10 (18%)	66,96,113	1.44	5 (7%)
39	CLA	a	825	-	66,70,73	1.27	7 (10%)	79,109,113	1.34	8 (10%)
39	CLA	b	842	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	5 (6%)
48	A86	J	301	-	44,50,50	1.17	3 (6%)	51,76,76	2.13	18 (35%)
39	CLA	a	831	-	69,73,73	1.25	7 (10%)	83,113,113	1.32	5 (6%)
41	LHG	D	301	-	34,34,48	0.72	0	37,40,54	1.25	3 (8%)
39	CLA	H	307	-	49,53,73	1.50	6 (12%)	59,89,113	1.48	4 (6%)
43	DD6	O	305	-	39,45,45	1.99	2 (5%)	52,67,67	1.62	12 (23%)
49	KC2	L	321	-	49,53,53	1.80	11 (22%)	62,89,89	2.06	15 (24%)
50	A1EB1	8	308	-	51,58,58	1.26	4 (7%)	60,85,85	1.97	18 (30%)
52	A1EB4	P	319	-	52,59,63	2.81	6 (11%)	61,85,89	2.79	21 (34%)
39	CLA	b	801	-	69,73,73	1.23	10 (14%)	83,113,113	1.33	8 (9%)
39	CLA	A	315	-	54,58,73	1.41	6 (11%)	65,95,113	1.42	6 (9%)
49	KC2	M	314	-	49,53,53	1.78	9 (18%)	62,89,89	2.11	19 (30%)
49	KC2	9	313	-	49,53,53	1.78	12 (24%)	62,89,89	2.11	15 (24%)
39	CLA	C	305	-	65,69,73	1.30	6 (9%)	78,108,113	1.29	5 (6%)
39	CLA	W	316	24	45,49,73	1.51	8 (17%)	54,84,113	1.57	9 (16%)
39	CLA	a	804	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
48	A86	B	201	-	44,50,50	1.19	3 (6%)	51,76,76	2.49	19 (37%)
49	KC2	7	320	-	49,53,53	1.79	9 (18%)	62,89,89	2.06	15 (24%)
43	DD6	K	303	-	39,45,45	1.95	3 (7%)	52,67,67	1.73	11 (21%)
39	CLA	H	306	-	52,56,73	1.44	8 (15%)	62,92,113	1.44	5 (8%)
47	SQD	P	301	-	37,38,54	1.11	5 (13%)	46,49,65	1.73	12 (26%)
50	A1EB1	V	306	-	51,58,58	1.25	3 (5%)	60,85,85	1.97	19 (31%)
39	CLA	l	201	-	69,73,73	1.26	8 (11%)	83,113,113	1.23	6 (7%)
39	CLA	S	310	-	46,50,73	1.51	7 (15%)	55,85,113	1.59	6 (10%)
49	KC2	P	306	24	49,53,53	1.82	12 (24%)	62,89,89	2.19	17 (27%)
51	A1ECV	P	315	-	47,56,56	3.34	19 (40%)	32,93,93	3.12	12 (37%)
39	CLA	a	824	-	69,73,73	1.27	10 (14%)	83,113,113	1.31	7 (8%)
39	CLA	R	316	-	56,60,73	1.41	9 (16%)	67,97,113	1.45	5 (7%)
39	CLA	B	204	-	50,54,73	1.47	8 (16%)	60,90,113	1.45	6 (10%)
48	A86	6	303	-	44,50,50	1.15	3 (6%)	51,76,76	2.21	15 (29%)
49	KC2	P	312	-	49,53,53	1.79	10 (20%)	62,89,89	2.17	16 (25%)
39	CLA	a	834	-	55,59,73	1.40	8 (14%)	66,96,113	1.45	8 (12%)
39	CLA	Z	315	-	45,49,73	1.53	7 (15%)	54,84,113	1.53	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	1	309	-	46,50,73	1.52	9 (19%)	55,85,113	1.46	5 (9%)
39	CLA	y	319	-	45,49,73	1.54	8 (17%)	54,84,113	1.59	8 (14%)
43	DD6	A	303	-	39,45,45	2.03	3 (7%)	52,67,67	2.88	20 (38%)
48	A86	1	306	-	44,50,50	1.18	2 (4%)	51,76,76	2.05	13 (25%)
39	CLA	0	318	-	45,49,73	1.54	6 (13%)	54,84,113	1.50	5 (9%)
39	CLA	a	803	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	6 (7%)
39	CLA	T	311	-	60,64,73	1.35	7 (11%)	72,102,113	1.35	5 (6%)
39	CLA	J	311	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	6 (7%)
49	KC2	X	314	46	48,52,53	1.75	9 (18%)	59,87,89	2.20	17 (28%)
49	KC2	1	314	-	49,53,53	1.78	10 (20%)	62,89,89	2.09	16 (25%)
43	DD6	V	303	-	39,45,45	1.97	3 (7%)	52,67,67	1.75	10 (19%)
39	CLA	a	847	-	69,73,73	1.27	9 (13%)	83,113,113	1.27	5 (6%)
39	CLA	3	314	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
39	CLA	4	316	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	5 (6%)
39	CLA	X	316	-	51,55,73	1.45	8 (15%)	61,91,113	1.48	6 (9%)
48	A86	8	305	-	44,50,50	1.20	3 (6%)	51,76,76	2.63	22 (43%)
39	CLA	E	314	-	60,64,73	1.35	9 (15%)	72,102,113	1.36	4 (5%)
39	CLA	T	319	29	50,54,73	1.47	7 (14%)	60,90,113	1.48	5 (8%)
39	CLA	Z	316	-	45,49,73	1.52	6 (13%)	54,84,113	1.61	6 (11%)
42	BCR	l	206	-	41,41,41	0.69	0	56,56,56	1.76	13 (23%)
39	CLA	x	307	-	45,49,73	1.53	7 (15%)	54,84,113	1.48	8 (14%)
50	A1EB1	V	302	-	51,58,58	1.27	4 (7%)	60,85,85	2.00	20 (33%)
49	KC2	L	315	-	49,53,53	1.78	10 (20%)	62,89,89	2.18	15 (24%)
39	CLA	5	308	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
48	A86	S	304	-	44,50,50	1.13	2 (4%)	51,76,76	1.98	11 (21%)
49	KC2	L	314	-	49,53,53	1.75	9 (18%)	62,89,89	2.17	19 (30%)
48	A86	G	301	-	44,50,50	1.18	2 (4%)	51,76,76	2.46	19 (37%)
49	KC2	P	320	-	49,53,53	1.76	10 (20%)	62,89,89	2.17	19 (30%)
42	BCR	m	101	-	41,41,41	1.16	4 (9%)	56,56,56	1.34	7 (12%)
47	SQD	E	320	-	34,35,54	1.17	5 (14%)	43,46,65	1.98	11 (25%)
39	CLA	Z	305	-	45,49,73	1.54	7 (15%)	54,84,113	1.53	6 (11%)
39	CLA	J	313	-	50,54,73	1.47	7 (14%)	60,90,113	1.44	4 (6%)
39	CLA	F	315	18	45,49,73	1.52	6 (13%)	54,84,113	1.66	6 (11%)
39	CLA	9	315	-	45,49,73	1.53	8 (17%)	54,84,113	1.53	5 (9%)
48	A86	Q	304	-	44,50,50	1.19	3 (6%)	51,76,76	2.14	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	Z	306	-	50,54,73	1.46	7 (14%)	60,90,113	1.46	5 (8%)
50	A1EB1	3	324	-	51,58,58	1.29	3 (5%)	60,85,85	2.03	18 (30%)
49	KC2	z	313	-	46,50,53	1.98	11 (23%)	49,80,89	2.25	12 (24%)
49	KC2	P	313	24	49,53,53	1.82	11 (22%)	62,89,89	2.21	19 (30%)
49	KC2	9	316	35	49,53,53	1.79	10 (20%)	62,89,89	2.11	16 (25%)
39	CLA	D	310	47	65,69,73	1.31	8 (12%)	78,108,113	1.33	7 (8%)
50	A1EB1	C	302	-	51,58,58	1.24	3 (5%)	60,85,85	1.81	16 (26%)
50	A1EB1	5	302	-	51,58,58	1.26	3 (5%)	60,85,85	2.12	16 (26%)
46	LMG	4	325	-	32,32,55	0.90	0	40,40,63	1.25	4 (10%)
39	CLA	L	310	23	69,73,73	1.26	7 (10%)	83,113,113	1.29	5 (6%)
39	CLA	D	312	16	59,63,73	1.35	8 (13%)	71,101,113	1.39	8 (11%)
50	A1EB1	Q	307	-	51,58,58	1.31	5 (9%)	60,85,85	2.01	15 (25%)
39	CLA	1	310	-	49,53,73	1.50	7 (14%)	59,89,113	1.48	4 (6%)
39	CLA	Z	309	-	45,49,73	1.53	6 (13%)	54,84,113	1.46	4 (7%)
46	LMG	l	208	49	39,39,55	1.06	2 (5%)	47,47,63	1.23	5 (10%)
50	A1EB1	h	203	-	51,58,58	1.27	4 (7%)	60,85,85	2.00	19 (31%)
51	A1ECV	y	317	-	47,56,56	3.38	20 (42%)	32,93,93	3.14	13 (40%)
48	A86	L	301	-	44,50,50	1.16	3 (6%)	51,76,76	2.05	14 (27%)
39	CLA	0	310	-	65,69,73	1.32	8 (12%)	78,108,113	1.33	7 (8%)
39	CLA	a	836	-	69,73,73	1.24	7 (10%)	83,113,113	1.32	4 (4%)
48	A86	W	303	-	44,50,50	1.19	2 (4%)	51,76,76	2.16	19 (37%)
51	A1ECV	z	310	-	47,56,56	3.33	20 (42%)	32,93,93	3.43	11 (34%)
39	CLA	4	311	-	65,69,73	1.32	9 (13%)	78,108,113	1.37	8 (10%)
39	CLA	3	323	-	50,54,73	1.46	8 (16%)	60,90,113	1.50	4 (6%)
49	KC2	6	319	-	49,53,53	1.82	11 (22%)	62,89,89	2.05	13 (20%)
49	KC2	P	310	46	48,52,53	1.72	9 (18%)	59,87,89	2.21	18 (30%)
39	CLA	1	311	-	45,49,73	1.53	7 (15%)	54,84,113	1.47	5 (9%)
39	CLA	j	101	-	69,73,73	1.24	7 (10%)	83,113,113	1.33	8 (9%)
47	SQD	D	321	-	38,39,54	1.10	5 (13%)	47,50,65	1.70	11 (23%)
39	CLA	X	308	-	64,68,73	1.31	8 (12%)	77,107,113	1.36	8 (10%)
48	A86	W	304	-	44,50,50	1.21	3 (6%)	51,76,76	2.29	18 (35%)
39	CLA	U	207	-	64,68,73	1.30	8 (12%)	77,107,113	1.33	5 (6%)
39	CLA	x	311	-	49,53,73	1.49	6 (12%)	59,89,113	1.46	4 (6%)
49	KC2	0	314	46,31	48,52,53	1.72	9 (18%)	59,87,89	2.23	17 (28%)
49	KC2	V	315	-	49,53,53	1.79	11 (22%)	62,89,89	2.14	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	2	307	-	45,49,73	1.53	7 (15%)	54,84,113	1.58	5 (9%)
39	CLA	S	319	-	56,60,73	1.39	9 (16%)	67,97,113	1.53	9 (13%)
48	A86	X	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.10	18 (35%)
43	DD6	3	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.91	13 (25%)
51	A1ECV	7	317	-	47,56,56	3.42	20 (42%)	32,93,93	3.31	13 (40%)
48	A86	6	307	-	44,50,50	1.15	3 (6%)	51,76,76	2.11	17 (33%)
43	DD6	4	308	-	39,45,45	2.06	3 (7%)	52,67,67	2.04	14 (26%)
39	CLA	F	310	-	58,62,73	1.37	6 (10%)	69,99,113	1.39	6 (8%)
48	A86	1	307	-	44,50,50	1.24	3 (6%)	51,76,76	2.20	18 (35%)
39	CLA	4	313	-	50,54,73	1.45	7 (14%)	60,90,113	1.41	4 (6%)
39	CLA	z	309	-	45,49,73	1.52	7 (15%)	54,84,113	1.54	6 (11%)
49	KC2	A	313	-	49,53,53	1.79	10 (20%)	62,89,89	2.14	19 (30%)
39	CLA	4	323	-	69,73,73	1.29	9 (13%)	83,113,113	1.27	4 (4%)
39	CLA	C	308	-	64,68,73	1.30	8 (12%)	77,107,113	1.35	6 (7%)
44	SF4	b	804	-	0,12,12	-	-	-		
49	KC2	6	317	-	49,53,53	1.76	9 (18%)	62,89,89	2.13	18 (29%)
39	CLA	b	813	-	58,62,73	1.41	10 (17%)	73,100,113	1.42	6 (8%)
44	SF4	c	101	-	0,12,12	-	-	-		
43	DD6	H	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.76	10 (19%)
46	LMG	W	302	49	39,39,55	1.08	2 (5%)	47,47,63	1.23	4 (8%)
48	A86	3	306	-	44,50,50	1.14	3 (6%)	51,76,76	2.24	13 (25%)
51	A1ECV	7	323	-	47,56,56	3.34	20 (42%)	32,93,93	3.48	12 (37%)
48	A86	T	301	-	44,50,50	1.29	3 (6%)	51,76,76	2.33	17 (33%)
43	DD6	5	303	-	39,45,45	1.90	3 (7%)	52,67,67	1.73	12 (23%)
49	KC2	G	313	-	49,53,53	1.79	10 (20%)	62,89,89	2.23	20 (32%)
49	KC2	B	208	-	49,53,53	1.77	10 (20%)	62,89,89	2.24	19 (30%)
39	CLA	V	310	-	64,68,73	1.31	8 (12%)	77,107,113	1.43	12 (15%)
39	CLA	6	322	-	50,54,73	1.47	6 (12%)	60,90,113	1.46	4 (6%)
50	A1EB1	3	303	-	51,58,58	1.28	4 (7%)	60,85,85	2.05	18 (30%)
50	A1EB1	8	301	-	51,58,58	1.26	4 (7%)	60,85,85	1.95	16 (26%)
49	KC2	W	312	24,46	48,52,53	1.72	9 (18%)	59,87,89	2.21	18 (30%)
51	A1ECV	X	310	-	47,56,56	3.32	19 (40%)	32,93,93	3.28	11 (34%)
48	A86	Y	301	-	44,50,50	1.16	3 (6%)	51,76,76	2.05	15 (29%)
50	A1EB1	1	305	-	51,58,58	1.25	4 (7%)	60,85,85	2.08	16 (26%)
39	CLA	b	814	-	59,63,73	1.36	8 (13%)	71,101,113	1.36	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	A1ECV	x	310	-	47,56,56	3.35	21 (44%)	32,93,93	3.30	11 (34%)
50	A1EB1	K	305	-	51,58,58	1.25	3 (5%)	60,85,85	2.22	18 (30%)
39	CLA	J	312	-	50,54,73	1.48	8 (16%)	60,90,113	1.47	4 (6%)
39	CLA	W	309	-	69,73,73	1.26	9 (13%)	83,113,113	1.27	5 (6%)
39	CLA	D	311	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
49	KC2	W	308	-	49,53,53	1.77	10 (20%)	62,89,89	2.21	17 (27%)
39	CLA	y	312	-	46,50,73	1.52	7 (15%)	55,85,113	1.46	4 (7%)
39	CLA	z	311	-	45,49,73	1.53	7 (15%)	54,84,113	1.49	5 (9%)
39	CLA	D	319	16	69,73,73	1.26	6 (8%)	83,113,113	1.31	7 (8%)
39	CLA	T	308	-	50,54,73	1.45	9 (18%)	60,90,113	1.45	6 (10%)
49	KC2	2	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.16	18 (29%)
39	CLA	L	319	-	55,59,73	1.41	6 (10%)	66,96,113	1.40	4 (6%)
50	A1EB1	3	309	-	51,58,58	1.28	4 (7%)	60,85,85	1.97	15 (25%)
43	DD6	R	304	-	39,45,45	1.95	4 (10%)	52,67,67	1.84	15 (28%)
50	A1EB1	G	304	-	51,58,58	1.31	4 (7%)	60,85,85	2.04	20 (33%)
39	CLA	1	319	-	55,59,73	1.41	9 (16%)	66,96,113	1.43	5 (7%)
39	CLA	7	313	-	65,69,73	1.31	8 (12%)	78,108,113	1.33	7 (8%)
49	KC2	X	312	-	49,53,53	1.76	9 (18%)	62,89,89	2.20	19 (30%)
50	A1EB1	0	305	-	51,58,58	1.27	3 (5%)	60,85,85	2.03	17 (28%)
39	CLA	2	316	-	45,49,73	1.52	7 (15%)	54,84,113	1.58	5 (9%)
39	CLA	M	310	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)
43	DD6	J	305	-	39,45,45	2.05	3 (7%)	52,67,67	2.29	17 (32%)
39	CLA	b	816	-	64,68,73	1.31	8 (12%)	77,107,113	1.31	6 (7%)
49	KC2	V	318	-	49,53,53	1.78	9 (18%)	62,89,89	2.15	17 (27%)
39	CLA	a	832	-	54,58,73	1.42	7 (12%)	65,95,113	1.45	6 (9%)
43	DD6	A	301	-	39,45,45	1.98	3 (7%)	52,67,67	1.88	12 (23%)
39	CLA	B	203	-	50,54,73	1.45	7 (14%)	60,90,113	1.44	5 (8%)
39	CLA	D	313	-	69,73,73	1.24	7 (10%)	83,113,113	1.29	8 (9%)
39	CLA	M	317	-	55,59,73	1.40	9 (16%)	66,96,113	1.41	4 (6%)
43	DD6	U	204	-	39,45,45	2.04	4 (10%)	52,67,67	1.72	12 (23%)
43	DD6	7	309	-	39,45,45	1.99	3 (7%)	52,67,67	1.87	15 (28%)
48	A86	T	306	-	44,50,50	1.19	2 (4%)	51,76,76	2.35	15 (29%)
49	KC2	5	305	27	49,53,53	1.73	9 (18%)	62,89,89	2.17	16 (25%)
39	CLA	T	320	-	56,60,73	1.39	8 (14%)	67,97,113	1.36	5 (7%)
43	DD6	1	304	-	39,45,45	2.22	3 (7%)	52,67,67	3.19	18 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	C	304	-	47,51,73	1.50	8 (17%)	56,86,113	1.44	5 (8%)
39	CLA	3	316	-	54,58,73	1.42	8 (14%)	65,95,113	1.42	6 (9%)
39	CLA	A	306	-	65,69,73	1.30	9 (13%)	78,108,113	1.35	6 (7%)
51	A1ECV	L	318	-	47,56,56	3.35	20 (42%)	32,93,93	3.16	12 (37%)
48	A86	5	301	-	44,50,50	1.21	2 (4%)	51,76,76	2.19	16 (31%)
50	A1EB1	D	308	-	51,58,58	1.28	3 (5%)	60,85,85	2.34	20 (33%)
39	CLA	U	209	-	56,60,73	1.39	8 (14%)	67,97,113	1.43	7 (10%)
39	CLA	M	318	24	50,54,73	1.47	7 (14%)	60,90,113	1.50	4 (6%)
39	CLA	Z	312	-	45,49,73	1.52	6 (13%)	54,84,113	1.51	5 (9%)
46	LMG	7	301	49	46,46,55	0.95	2 (4%)	54,54,63	1.28	6 (11%)
51	A1ECV	4	321	-	47,56,56	3.37	20 (42%)	32,93,93	3.09	13 (40%)
39	CLA	D	317	-	69,73,73	1.25	8 (11%)	83,113,113	1.34	8 (9%)
48	A86	6	305	-	44,50,50	1.17	2 (4%)	51,76,76	2.19	16 (31%)
39	CLA	9	307	-	45,49,73	1.54	8 (17%)	54,84,113	1.51	6 (11%)
48	A86	Q	301	-	44,50,50	1.22	3 (6%)	51,76,76	2.35	19 (37%)
39	CLA	T	313	-	55,59,73	1.44	7 (12%)	66,96,113	1.27	7 (10%)
48	A86	8	307	-	44,50,50	1.23	3 (6%)	51,76,76	2.45	23 (45%)
39	CLA	1	317	-	45,49,73	1.53	6 (13%)	54,84,113	1.53	5 (9%)
39	CLA	a	826	-	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
39	CLA	9	308	-	59,63,73	1.34	8 (13%)	71,101,113	1.51	11 (15%)
39	CLA	I	301	41	56,60,73	1.40	7 (12%)	67,97,113	1.38	7 (10%)
39	CLA	I	315	-	56,60,73	1.39	6 (10%)	67,97,113	1.45	8 (11%)
47	SQD	k	205	-	37,38,54	1.13	5 (13%)	46,49,65	1.66	9 (19%)
51	A1ECV	Z	314	-	47,56,56	3.36	20 (42%)	32,93,93	3.28	11 (34%)
39	CLA	K	314	-	45,49,73	1.52	7 (15%)	54,84,113	1.52	7 (12%)
39	CLA	H	313	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	6 (7%)
39	CLA	M	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.35	6 (7%)
49	KC2	6	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.18	19 (30%)
51	A1ECV	O	315	-	47,56,56	3.34	20 (42%)	32,93,93	3.23	11 (34%)
39	CLA	b	836	-	49,53,73	1.50	8 (16%)	59,89,113	1.51	8 (13%)
39	CLA	J	318	-	50,54,73	1.45	8 (16%)	60,90,113	1.48	7 (11%)
51	A1ECV	4	315	-	47,56,56	3.42	20 (42%)	32,93,93	3.40	11 (34%)
50	A1EB1	7	304	-	51,58,58	1.23	4 (7%)	60,85,85	2.03	19 (31%)
39	CLA	J	314	-	69,73,73	1.27	7 (10%)	83,113,113	1.22	6 (7%)
43	DD6	I	305	-	39,45,45	1.98	3 (7%)	52,67,67	1.86	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	KC2	W	315	-	49,53,53	1.81	9 (18%)	62,89,89	2.05	14 (22%)
52	A1EB4	W	321	-	52,59,63	2.65	5 (9%)	61,85,89	2.25	20 (32%)
39	CLA	V	319	-	56,60,73	1.40	8 (14%)	67,97,113	1.36	5 (7%)
50	A1EB1	8	306	-	51,58,58	1.28	3 (5%)	60,85,85	2.08	19 (31%)
39	CLA	I	313	-	69,73,73	1.26	7 (10%)	83,113,113	1.26	6 (7%)
39	CLA	2	312	-	45,49,73	1.51	9 (20%)	54,84,113	1.56	6 (11%)
50	A1EB1	O	301	-	51,58,58	1.24	4 (7%)	60,85,85	1.95	18 (30%)
39	CLA	8	311	-	59,63,73	1.35	7 (11%)	71,101,113	1.40	6 (8%)
39	CLA	X	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
46	LMG	S	322	49	46,46,55	0.95	2 (4%)	54,54,63	1.32	5 (9%)
49	KC2	G	317	-	49,53,53	1.77	10 (20%)	62,89,89	2.25	19 (30%)
39	CLA	S	308	-	65,69,73	1.30	7 (10%)	78,108,113	1.32	6 (7%)
43	DD6	x	303	-	39,45,45	2.06	3 (7%)	52,67,67	1.96	16 (30%)
39	CLA	b	832	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	5 (6%)
51	A1ECV	Y	312	-	47,56,56	3.33	19 (40%)	32,93,93	3.26	11 (34%)
39	CLA	3	322	-	55,59,73	1.40	8 (14%)	66,96,113	1.45	6 (9%)
48	A86	W	307	-	44,50,50	1.23	4 (9%)	51,76,76	1.94	13 (25%)
50	A1EB1	1	301	-	51,58,58	1.22	3 (5%)	60,85,85	1.92	17 (28%)
43	DD6	P	304	-	39,45,45	2.10	3 (7%)	52,67,67	2.77	14 (26%)
49	KC2	0	319	-	49,53,53	1.91	11 (22%)	62,89,89	2.01	15 (24%)
39	CLA	E	308	-	69,73,73	1.24	7 (10%)	83,113,113	1.28	8 (9%)
48	A86	8	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.04	15 (29%)
48	A86	H	302	-	44,50,50	1.15	3 (6%)	51,76,76	2.29	17 (33%)
49	KC2	Y	308	-	49,53,53	1.83	9 (18%)	62,89,89	2.02	14 (22%)
39	CLA	U	210	-	64,68,73	1.32	9 (14%)	77,107,113	1.31	7 (9%)
49	KC2	O	317	46	48,52,53	1.80	10 (20%)	59,87,89	2.06	13 (22%)
39	CLA	o	202	-	46,50,73	1.51	7 (15%)	55,85,113	1.52	6 (10%)
49	KC2	S	315	28	49,53,53	1.81	10 (20%)	62,89,89	2.15	18 (29%)
39	CLA	L	320	-	50,54,73	1.47	6 (12%)	60,90,113	1.56	7 (11%)
39	CLA	a	807	1	69,73,73	1.27	9 (13%)	83,113,113	1.29	5 (6%)
39	CLA	L	308	-	65,69,73	1.31	7 (10%)	78,108,113	1.37	6 (7%)
50	A1EB1	H	304	-	51,58,58	1.22	3 (5%)	60,85,85	1.63	11 (18%)
39	CLA	o	203	12	59,63,73	1.35	7 (11%)	71,101,113	1.38	5 (7%)
48	A86	3	305	-	44,50,50	1.19	2 (4%)	51,76,76	1.79	10 (19%)
48	A86	Q	308	-	44,50,50	1.15	2 (4%)	51,76,76	2.25	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	K	312	-	69,73,73	1.24	8 (11%)	83,113,113	1.34	6 (7%)
51	A1ECV	T	317	-	47,56,56	3.32	20 (42%)	32,93,93	3.13	11 (34%)
39	CLA	J	310	-	59,63,73	1.37	8 (13%)	71,101,113	1.36	7 (9%)
39	CLA	U	208	-	50,54,73	1.47	9 (18%)	60,90,113	1.39	5 (8%)
43	DD6	O	304	-	39,45,45	2.10	4 (10%)	52,67,67	1.91	15 (28%)
39	CLA	9	309	-	45,49,73	1.51	8 (17%)	54,84,113	1.58	5 (9%)
39	CLA	G	318	-	53,57,73	1.43	8 (15%)	62,93,113	1.36	5 (8%)
46	LMG	0	324	49	27,27,55	1.31	2 (7%)	35,35,63	1.47	4 (11%)
49	KC2	0	317	31	49,53,53	1.79	10 (20%)	62,89,89	2.15	18 (29%)
49	KC2	y	313	-	49,53,53	1.76	10 (20%)	62,89,89	2.13	17 (27%)
50	A1EB1	7	306	-	51,58,58	1.26	3 (5%)	60,85,85	2.11	22 (36%)
39	CLA	R	315	-	51,55,73	1.45	8 (15%)	61,91,113	1.49	8 (13%)
48	A86	L	307	-	44,50,50	1.18	3 (6%)	51,76,76	2.52	20 (39%)
48	A86	M	302	-	44,50,50	1.18	2 (4%)	51,76,76	2.19	17 (33%)
39	CLA	Q	312	-	69,73,73	1.26	7 (10%)	83,113,113	1.27	4 (4%)
50	A1EB1	G	302	-	51,58,58	1.30	4 (7%)	60,85,85	2.07	19 (31%)
50	A1EB1	V	305	-	51,58,58	1.29	4 (7%)	60,85,85	2.09	17 (28%)
39	CLA	b	822	2	54,58,73	1.42	8 (14%)	65,95,113	1.42	5 (7%)
49	KC2	3	321	-	49,53,53	1.74	9 (18%)	62,89,89	2.12	18 (29%)
49	KC2	L	317	-	49,53,53	1.77	10 (20%)	62,89,89	2.18	18 (29%)
49	KC2	G	315	-	49,53,53	1.81	10 (20%)	62,89,89	2.19	19 (30%)
39	CLA	a	809	-	66,70,73	1.27	7 (10%)	79,109,113	1.32	5 (6%)
39	CLA	3	313	-	57,61,73	1.40	8 (14%)	68,98,113	1.35	5 (7%)
49	KC2	X	306	27	49,53,53	1.85	10 (20%)	62,89,89	2.05	15 (24%)
39	CLA	M	321	24	50,54,73	1.46	7 (14%)	60,90,113	1.47	5 (8%)
51	A1ECV	5	312	27	47,56,56	3.35	19 (40%)	32,93,93	3.13	12 (37%)
52	A1EB4	R	305	-	52,59,63	2.56	4 (7%)	61,85,89	1.92	21 (34%)
48	A86	4	305	-	44,50,50	1.16	2 (4%)	51,76,76	1.94	11 (21%)
43	DD6	D	307	-	39,45,45	1.97	3 (7%)	52,67,67	1.79	10 (19%)
47	SQD	H	318	-	37,38,54	1.13	5 (13%)	46,49,65	1.64	8 (17%)
39	CLA	b	839	-	51,55,73	1.45	8 (15%)	61,91,113	1.37	6 (9%)
42	BCR	l	202	-	41,41,41	0.76	0	56,56,56	1.93	13 (23%)
47	SQD	7	302	-	38,39,54	1.13	5 (13%)	47,50,65	1.69	11 (23%)
46	LMG	F	317	49	39,39,55	1.05	2 (5%)	47,47,63	1.23	6 (12%)
48	A86	K	301	-	44,50,50	1.23	3 (6%)	51,76,76	2.15	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	l	204	-	69,73,73	1.24	8 (11%)	83,113,113	1.31	8 (9%)
52	A1EB4	W	306	-	51,58,63	2.60	4 (7%)	60,84,89	2.09	19 (31%)
48	A86	z	303	-	44,50,50	1.14	2 (4%)	51,76,76	1.90	11 (21%)
39	CLA	O	318	-	50,54,73	1.47	7 (14%)	60,90,113	1.50	7 (11%)
47	SQD	9	322	-	35,36,54	1.16	5 (14%)	44,47,65	1.65	9 (20%)
48	A86	S	305	-	44,50,50	1.17	2 (4%)	51,76,76	2.02	14 (27%)
49	KC2	V	320	-	49,53,53	1.76	10 (20%)	62,89,89	2.25	18 (29%)
39	CLA	1	313	32	45,49,73	1.51	8 (17%)	54,84,113	1.51	5 (9%)
43	DD6	O	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	13 (25%)
52	A1EB4	5	304	-	52,59,63	2.56	4 (7%)	61,85,89	1.93	19 (31%)
48	A86	J	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.28	18 (35%)
39	CLA	b	840	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	6 (7%)
39	CLA	S	320	-	69,73,73	1.28	9 (13%)	83,113,113	1.29	6 (7%)
49	KC2	8	314	-	49,53,53	1.79	10 (20%)	62,89,89	2.07	15 (24%)
52	A1EB4	X	305	-	52,59,63	2.59	4 (7%)	61,85,89	1.90	19 (31%)
39	CLA	7	318	28	50,54,73	1.44	8 (16%)	60,90,113	1.38	4 (6%)
39	CLA	G	310	-	69,73,73	1.27	10 (14%)	83,113,113	1.31	6 (7%)
42	BCR	l	207	-	41,41,41	0.69	0	56,56,56	1.81	11 (19%)
39	CLA	E	318	17	50,54,73	1.46	8 (16%)	60,90,113	1.42	5 (8%)
39	CLA	E	309	-	57,61,73	1.38	8 (14%)	68,98,113	1.37	6 (8%)
47	SQD	F	319	-	36,37,54	1.14	5 (13%)	45,48,65	1.72	10 (22%)
47	SQD	W	301	-	27,28,54	1.22	4 (14%)	36,39,65	1.79	9 (25%)
43	DD6	E	303	-	39,45,45	1.93	3 (7%)	52,67,67	1.84	11 (21%)
39	CLA	F	314	18	59,63,73	1.36	6 (10%)	71,101,113	1.48	10 (14%)
49	KC2	Y	309	-	49,53,53	1.77	9 (18%)	62,89,89	2.11	17 (27%)
39	CLA	6	311	-	43,48,73	1.56	7 (16%)	51,83,113	1.53	7 (13%)
48	A86	7	312	-	44,50,50	1.21	2 (4%)	51,76,76	2.29	18 (35%)
39	CLA	U	211	-	64,68,73	1.31	7 (10%)	77,107,113	1.36	8 (10%)
48	A86	E	304	-	44,50,50	1.26	3 (6%)	51,76,76	2.41	19 (37%)
48	A86	R	317	-	44,50,50	1.17	2 (4%)	51,76,76	2.06	12 (23%)
48	A86	9	301	-	44,50,50	1.20	3 (6%)	51,76,76	2.14	15 (29%)
49	KC2	3	315	-	49,53,53	1.81	10 (20%)	62,89,89	2.14	15 (24%)
39	CLA	U	213	-	45,49,73	1.52	7 (15%)	54,84,113	1.56	5 (9%)
52	A1EB4	T	304	-	50,57,63	2.65	5 (10%)	59,83,89	2.20	19 (32%)
40	PQN	a	839	-	34,34,34	1.60	2 (5%)	42,45,45	1.10	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	z	306	-	45,49,73	1.54	7 (15%)	54,84,113	1.52	5 (9%)
43	DD6	B	202	-	39,45,45	2.03	3 (7%)	52,67,67	1.99	12 (23%)
43	DD6	3	304	-	39,45,45	2.05	3 (7%)	52,67,67	3.25	19 (36%)
39	CLA	D	318	-	69,73,73	1.26	6 (8%)	83,113,113	1.31	5 (6%)
39	CLA	a	805	-	69,73,73	1.24	8 (11%)	83,113,113	1.34	9 (10%)
48	A86	R	302	-	44,50,50	1.15	2 (4%)	51,76,76	2.19	13 (25%)
43	DD6	G	306	-	39,45,45	2.02	3 (7%)	52,67,67	2.07	12 (23%)
49	KC2	8	317	-	49,53,53	1.78	9 (18%)	62,89,89	2.12	17 (27%)
39	CLA	z	318	-	45,49,73	1.52	7 (15%)	54,84,113	1.58	7 (12%)
39	CLA	Z	313	-	45,49,73	1.55	8 (17%)	54,84,113	1.89	10 (18%)
50	A1EB1	T	302	-	51,58,58	1.27	3 (5%)	60,85,85	2.04	12 (20%)
43	DD6	A	302	-	39,45,45	1.97	3 (7%)	52,67,67	1.84	11 (21%)
43	DD6	S	306	-	39,45,45	2.01	2 (5%)	52,67,67	1.92	16 (30%)
52	A1EB4	M	305	-	53,60,63	2.51	4 (7%)	62,86,89	2.08	16 (25%)
39	CLA	U	214	-	50,54,73	1.47	7 (14%)	60,90,113	1.42	4 (6%)
50	A1EB1	z	302	-	51,58,58	1.28	3 (5%)	60,85,85	2.12	20 (33%)
39	CLA	a	813	1	54,58,73	1.42	7 (12%)	65,95,113	1.50	6 (9%)
39	CLA	b	830	-	69,73,73	1.27	8 (11%)	83,113,113	1.40	7 (8%)
39	CLA	5	315	-	51,55,73	1.44	8 (15%)	61,91,113	1.44	6 (9%)
43	DD6	A	304	-	39,45,45	2.00	2 (5%)	52,67,67	1.75	13 (25%)
39	CLA	Q	321	-	57,61,73	1.42	7 (12%)	68,98,113	1.33	8 (11%)
39	CLA	8	313	-	45,49,73	1.51	7 (15%)	54,84,113	1.51	6 (11%)
39	CLA	a	814	-	65,69,73	1.28	8 (12%)	78,108,113	1.35	6 (7%)
49	KC2	K	313	22	49,53,53	1.79	10 (20%)	62,89,89	2.19	18 (29%)
49	KC2	C	312	-	49,53,53	1.76	10 (20%)	62,89,89	2.14	17 (27%)
48	A86	9	306	-	44,50,50	1.18	2 (4%)	51,76,76	2.38	15 (29%)
48	A86	6	309	-	44,50,50	1.18	2 (4%)	51,76,76	2.22	17 (33%)
39	CLA	b	818	-	59,63,73	1.35	7 (11%)	71,101,113	1.39	8 (11%)
48	A86	y	306	-	44,50,50	1.16	2 (4%)	51,76,76	2.50	18 (35%)
42	BCR	f	801	-	41,41,41	0.68	0	56,56,56	1.92	14 (25%)
41	LHG	a	840	-	48,48,48	0.62	1 (2%)	51,54,54	1.28	7 (13%)
39	CLA	x	314	-	45,49,73	1.52	7 (15%)	54,84,113	1.56	5 (9%)
39	CLA	M	315	-	45,49,73	1.51	7 (15%)	54,84,113	1.55	9 (16%)
51	A1ECV	E	311	-	47,56,56	3.42	20 (42%)	32,93,93	3.59	12 (37%)
39	CLA	J	317	-	46,50,73	1.53	8 (17%)	55,85,113	1.48	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	LHG	X	301	-	40,40,48	0.67	1 (2%)	43,46,54	1.30	6 (13%)
43	DD6	W	305	-	39,45,45	1.91	3 (7%)	52,67,67	1.78	12 (23%)
43	DD6	j	102	-	39,45,45	1.96	2 (5%)	52,67,67	1.85	12 (23%)
43	DD6	F	305	-	39,45,45	2.14	3 (7%)	52,67,67	2.66	17 (32%)
50	A1EB1	G	307	-	51,58,58	1.29	4 (7%)	60,85,85	1.87	17 (28%)
49	KC2	I	312	46	48,52,53	1.73	9 (18%)	59,87,89	2.31	19 (32%)
47	SQD	D	304	-	37,38,54	1.14	5 (13%)	46,49,65	1.74	10 (21%)
39	CLA	H	310	-	61,65,73	1.32	8 (13%)	73,103,113	1.36	4 (5%)
39	CLA	H	312	20	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
39	CLA	V	316	-	54,58,73	1.42	7 (12%)	65,95,113	1.44	9 (13%)
39	CLA	I	311	-	69,73,73	1.24	7 (10%)	83,113,113	1.35	5 (6%)
46	LMG	A	316	-	29,29,55	1.00	0	37,37,63	1.23	4 (10%)
48	A86	Q	305	-	44,50,50	1.14	3 (6%)	51,76,76	2.03	14 (27%)
39	CLA	C	310	-	69,73,73	1.23	8 (11%)	83,113,113	1.33	5 (6%)
39	CLA	b	817	-	63,67,73	1.31	6 (9%)	75,105,113	1.36	7 (9%)
39	CLA	K	309	-	66,70,73	1.28	6 (9%)	79,109,113	1.30	5 (6%)
39	CLA	x	318	-	45,49,73	1.54	8 (17%)	54,84,113	1.57	8 (14%)
39	CLA	b	820	-	64,68,73	1.31	9 (14%)	77,107,113	1.29	4 (5%)
42	BCR	a	845	-	41,41,41	0.75	0	56,56,56	2.14	15 (26%)
49	KC2	4	318	28	49,53,53	1.79	10 (20%)	62,89,89	2.14	16 (25%)
49	KC2	F	307	-	49,53,53	1.77	10 (20%)	62,89,89	2.19	18 (29%)
49	KC2	x	312	-	49,53,53	1.76	10 (20%)	62,89,89	2.11	17 (27%)
50	A1EB1	L	303	-	51,58,58	1.29	3 (5%)	60,85,85	2.24	19 (31%)
39	CLA	b	809	-	69,73,73	1.24	6 (8%)	83,113,113	1.28	7 (8%)
48	A86	P	302	-	44,50,50	1.23	2 (4%)	51,76,76	2.31	17 (33%)
50	A1EB1	6	308	-	51,58,58	1.29	4 (7%)	60,85,85	2.25	19 (31%)
39	CLA	k	202	-	59,63,73	1.36	9 (15%)	71,101,113	1.35	6 (8%)
39	CLA	J	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
48	A86	L	306	-	44,50,50	1.16	3 (6%)	51,76,76	2.15	15 (29%)
39	CLA	b	810	-	69,73,73	1.26	6 (8%)	83,113,113	1.27	5 (6%)
39	CLA	b	811	-	69,73,73	1.23	10 (14%)	83,113,113	1.40	7 (8%)
39	CLA	2	308	-	50,54,73	1.48	8 (16%)	60,90,113	1.46	6 (10%)
51	A1ECV	9	314	-	47,56,56	3.40	20 (42%)	32,93,93	3.33	12 (37%)
39	CLA	i	103	-	69,73,73	1.27	9 (13%)	83,113,113	1.38	10 (12%)
49	KC2	4	320	-	49,53,53	1.76	10 (20%)	62,89,89	2.17	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	A1ECV	R	313	-	47,56,56	3.40	20 (42%)	32,93,93	3.32	12 (37%)
39	CLA	b	815	-	69,73,73	1.27	8 (11%)	83,113,113	1.28	7 (8%)
39	CLA	W	318	-	55,59,73	1.41	8 (14%)	66,96,113	1.42	4 (6%)
50	A1EB1	2	304	-	51,58,58	1.26	4 (7%)	60,85,85	2.16	20 (33%)
39	CLA	O	314	-	59,63,73	1.37	8 (13%)	71,101,113	1.35	6 (8%)
39	CLA	M	308	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
39	CLA	f	803	-	59,63,73	1.37	7 (11%)	71,101,113	1.33	6 (8%)
52	A1EB4	P	318	-	49,56,63	2.77	5 (10%)	58,82,89	2.27	18 (31%)
50	A1EB1	3	310	-	51,58,58	1.27	4 (7%)	60,85,85	2.05	17 (28%)
49	KC2	9	311	-	49,53,53	1.79	10 (20%)	62,89,89	2.10	15 (24%)
49	KC2	3	318	-	49,53,53	1.80	10 (20%)	62,89,89	2.13	18 (29%)
39	CLA	O	311	-	46,50,73	1.56	7 (15%)	55,85,113	1.48	6 (10%)
42	BCR	a	844	-	41,41,41	0.72	0	56,56,56	1.91	17 (30%)
39	CLA	7	316	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
39	CLA	A	314	-	69,73,73	1.25	6 (8%)	83,113,113	1.35	7 (8%)
39	CLA	K	311	-	69,73,73	1.24	6 (8%)	83,113,113	1.27	5 (6%)
39	CLA	b	807	-	69,73,73	1.24	8 (11%)	83,113,113	1.43	8 (9%)
39	CLA	6	312	-	55,59,73	1.39	8 (14%)	65,95,113	1.39	5 (7%)
48	A86	M	306	-	44,50,50	1.24	3 (6%)	51,76,76	2.08	17 (33%)
49	KC2	8	320	-	49,53,53	1.77	9 (18%)	62,89,89	2.14	16 (25%)
48	A86	0	301	-	44,50,50	1.26	3 (6%)	51,76,76	2.19	19 (37%)
39	CLA	b	825	-	69,73,73	1.27	9 (13%)	83,113,113	1.34	8 (9%)
50	A1EB1	y	301	-	51,58,58	1.23	4 (7%)	60,85,85	2.16	23 (38%)
39	CLA	Y	303	-	45,49,73	1.53	7 (15%)	54,84,113	1.52	6 (11%)
43	DD6	C	301	-	39,45,45	2.32	4 (10%)	52,67,67	2.51	14 (26%)
39	CLA	a	823	-	69,73,73	1.25	8 (11%)	83,113,113	1.32	10 (12%)
39	CLA	F	308	-	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)
48	A86	k	206	-	44,50,50	1.18	3 (6%)	51,76,76	2.00	13 (25%)
39	CLA	A	311	-	69,73,73	1.25	7 (10%)	83,113,113	1.24	6 (7%)
39	CLA	y	315	-	45,49,73	1.52	7 (15%)	54,84,113	1.57	5 (9%)
39	CLA	a	829	-	60,64,73	1.35	6 (10%)	72,102,113	1.39	6 (8%)
49	KC2	V	314	-	49,53,53	1.77	9 (18%)	62,89,89	2.14	19 (30%)
49	KC2	5	313	46	48,52,53	1.74	9 (18%)	59,87,89	2.19	16 (27%)
39	CLA	Q	309	-	65,69,73	1.29	8 (12%)	78,108,113	1.32	4 (5%)
39	CLA	W	313	-	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	a	811	-	69,73,73	1.26	8 (11%)	83,113,113	1.30	5 (6%)
39	CLA	Y	304	-	50,54,73	1.46	6 (12%)	60,90,113	1.47	4 (6%)
39	CLA	o	205	-	56,60,73	1.40	7 (12%)	67,97,113	1.39	5 (7%)
39	CLA	8	315	-	47,51,73	1.49	8 (17%)	56,86,113	1.43	4 (7%)
49	KC2	S	317	-	49,53,53	1.75	10 (20%)	62,89,89	2.17	17 (27%)
49	KC2	X	315	-	49,53,53	1.77	10 (20%)	62,89,89	2.15	17 (27%)
39	CLA	S	311	-	69,73,73	1.26	8 (11%)	83,113,113	1.26	5 (6%)
39	CLA	5	310	27	54,58,73	1.40	6 (11%)	65,95,113	1.46	6 (9%)
43	DD6	T	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.87	13 (25%)
39	CLA	L	311	23	56,60,73	1.39	8 (14%)	67,97,113	1.38	7 (10%)
39	CLA	P	316	-	55,59,73	1.41	8 (14%)	66,96,113	1.43	5 (7%)
39	CLA	a	838	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	5 (6%)
39	CLA	B	209	-	60,64,73	1.36	8 (13%)	72,102,113	1.29	6 (8%)
39	CLA	C	311	-	69,73,73	1.25	6 (8%)	83,113,113	1.29	4 (4%)
49	KC2	0	316	-	49,53,53	1.75	10 (20%)	62,89,89	2.13	19 (30%)
49	KC2	M	313	-	49,53,53	1.79	9 (18%)	62,89,89	2.17	17 (27%)
50	A1EB1	2	306	-	51,58,58	1.24	3 (5%)	60,85,85	2.09	20 (33%)
39	CLA	J	307	21	53,57,73	1.43	7 (13%)	62,93,113	1.45	5 (8%)
39	CLA	H	316	-	50,54,73	1.47	8 (16%)	60,90,113	1.49	4 (6%)
39	CLA	2	309	-	50,54,73	1.47	9 (18%)	60,90,113	1.42	6 (10%)
43	DD6	a	846	-	39,45,45	2.00	3 (7%)	52,67,67	1.84	12 (23%)
51	A1ECV	0	321	48	47,56,56	3.35	19 (40%)	32,93,93	3.32	14 (43%)
51	A1ECV	z	316	-	47,56,56	3.37	20 (42%)	32,93,93	3.37	11 (34%)
39	CLA	a	812	-	49,53,73	1.49	8 (16%)	59,89,113	1.47	8 (13%)
39	CLA	9	320	-	45,49,73	1.53	8 (17%)	54,84,113	1.52	8 (14%)
39	CLA	B	206	-	46,50,73	1.51	8 (17%)	55,85,113	1.47	6 (10%)
49	KC2	3	317	-	49,53,53	1.78	9 (18%)	62,89,89	2.16	19 (30%)
39	CLA	a	816	-	69,73,73	1.27	8 (11%)	83,113,113	1.34	10 (12%)
39	CLA	y	307	-	45,49,73	1.53	8 (17%)	54,84,113	1.54	5 (9%)
48	A86	2	305	-	44,50,50	1.12	2 (4%)	51,76,76	2.43	15 (29%)
52	A1EB4	M	322	-	52,59,63	2.81	6 (11%)	61,85,89	2.80	22 (36%)
39	CLA	a	828	1	54,58,73	1.42	9 (16%)	65,95,113	1.40	5 (7%)
47	SQD	M	301	-	38,39,54	1.11	5 (13%)	47,50,65	1.69	13 (27%)
39	CLA	a	801	-	69,73,73	1.27	9 (13%)	83,113,113	1.35	7 (8%)
49	KC2	Q	313	46	48,52,53	1.81	11 (22%)	59,87,89	2.24	17 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	7	321	-	45,49,73	1.52	7 (15%)	54,84,113	1.59	6 (11%)
39	CLA	a	817	1	49,53,73	1.50	9 (18%)	59,89,113	1.49	4 (6%)
39	CLA	Y	313	-	45,49,73	1.53	8 (17%)	54,84,113	1.54	5 (9%)
49	KC2	7	322	-	49,53,53	1.78	10 (20%)	62,89,89	2.11	17 (27%)
39	CLA	O	316	-	45,49,73	1.53	6 (13%)	54,84,113	1.58	5 (9%)
39	CLA	E	316	-	56,60,73	1.39	9 (16%)	67,97,113	1.43	6 (8%)
45	DGD	b	849	-	61,61,67	0.93	2 (3%)	75,75,81	1.37	8 (10%)
39	CLA	5	306	-	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
49	KC2	7	319	-	49,53,53	1.76	10 (20%)	62,89,89	2.18	17 (27%)
39	CLA	Y	302	-	45,49,73	1.53	7 (15%)	54,84,113	1.56	5 (9%)
39	CLA	b	826	-	69,73,73	1.28	10 (14%)	83,113,113	1.26	7 (8%)
39	CLA	x	306	-	49,53,73	1.50	6 (12%)	59,89,113	1.47	4 (6%)
46	LMG	F	320	49	34,34,55	1.14	2 (5%)	42,42,63	1.20	6 (14%)
39	CLA	K	307	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	4 (4%)
49	KC2	4	324	-	49,53,53	1.78	10 (20%)	62,89,89	2.23	17 (27%)
39	CLA	4	314	-	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
41	LHG	a	841	39	26,26,48	0.85	1 (3%)	29,32,54	1.33	3 (10%)
48	A86	8	323	-	44,50,50	1.19	3 (6%)	51,76,76	2.21	16 (31%)
50	A1EB1	U	203	-	51,58,58	1.25	3 (5%)	60,85,85	2.17	19 (31%)
43	DD6	I	306	-	39,45,45	1.95	3 (7%)	52,67,67	1.76	11 (21%)
43	DD6	D	306	-	39,45,45	2.66	4 (10%)	52,67,67	2.39	12 (23%)
39	CLA	T	318	-	51,55,73	1.44	7 (13%)	61,91,113	1.47	5 (8%)
39	CLA	Q	311	-	50,54,73	1.45	9 (18%)	60,90,113	1.53	6 (10%)
43	DD6	F	303	-	39,45,45	1.93	2 (5%)	52,67,67	1.79	10 (19%)
39	CLA	x	308	-	45,49,73	1.51	7 (15%)	54,84,113	1.61	6 (11%)
49	KC2	4	317	-	49,53,53	1.78	9 (18%)	62,89,89	2.12	17 (27%)
48	A86	O	302	-	44,50,50	1.22	3 (6%)	51,76,76	2.36	20 (39%)
46	LMG	W	320	-	33,33,55	0.94	1 (3%)	41,41,63	1.21	4 (9%)
40	PQN	b	843	-	34,34,34	1.53	2 (5%)	42,45,45	1.26	4 (9%)
48	A86	x	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.26	17 (33%)
39	CLA	b	819	-	63,67,73	1.32	8 (12%)	75,105,113	1.36	5 (6%)
39	CLA	b	833	-	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)
39	CLA	V	311	-	69,73,73	1.25	8 (11%)	83,113,113	1.30	4 (4%)
39	CLA	0	311	-	59,63,73	1.38	9 (15%)	71,101,113	1.39	10 (14%)
39	CLA	8	318	-	45,49,73	1.53	6 (13%)	54,84,113	1.52	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	2	310	-	46,50,73	1.51	7 (15%)	55,85,113	1.53	5 (9%)
39	CLA	U	215	-	45,49,73	1.55	7 (15%)	54,84,113	1.56	6 (11%)
48	A86	9	304	-	44,50,50	1.16	3 (6%)	51,76,76	2.06	16 (31%)
39	CLA	b	829	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
43	DD6	H	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.93	10 (19%)
49	KC2	T	315	29	49,53,53	1.76	10 (20%)	62,89,89	2.10	19 (30%)
49	KC2	S	314	-	49,53,53	1.78	9 (18%)	62,89,89	2.11	17 (27%)
42	BCR	b	846	-	41,41,41	0.74	0	56,56,56	2.13	16 (28%)
39	CLA	Q	314	-	58,62,73	1.36	9 (15%)	69,99,113	1.37	5 (7%)
49	KC2	X	318	-	49,53,53	1.77	9 (18%)	62,89,89	2.15	16 (25%)
51	A1ECV	Q	316	26	47,56,56	3.37	21 (44%)	32,93,93	3.10	11 (34%)
39	CLA	7	325	-	54,58,73	1.43	7 (12%)	65,95,113	1.44	7 (10%)
39	CLA	E	315	-	50,54,73	1.48	8 (16%)	60,90,113	1.45	4 (6%)
42	BCR	b	845	-	41,41,41	0.72	0	56,56,56	1.96	17 (30%)
46	LMG	P	317	49	39,39,55	1.08	2 (5%)	47,47,63	1.23	4 (8%)
39	CLA	b	805	-	69,73,73	1.25	7 (10%)	83,113,113	1.21	6 (7%)
39	CLA	S	316	-	45,49,73	1.53	6 (13%)	54,84,113	1.49	6 (11%)
39	CLA	a	830	-	69,73,73	1.26	7 (10%)	83,113,113	1.27	4 (4%)
50	A1EB1	7	305	-	51,58,58	1.29	4 (7%)	60,85,85	2.22	18 (30%)
50	A1EB1	y	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.21	20 (33%)
39	CLA	2	318	-	45,49,73	1.53	7 (15%)	54,84,113	1.53	5 (9%)
39	CLA	k	201	-	56,60,73	1.37	9 (16%)	67,97,113	1.39	5 (7%)
39	CLA	M	312	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	4 (4%)
48	A86	2	301	-	44,50,50	1.18	3 (6%)	51,76,76	2.31	17 (33%)
43	DD6	E	305	-	39,45,45	1.99	3 (7%)	52,67,67	1.92	14 (26%)
39	CLA	b	802	-	69,73,73	1.26	8 (11%)	83,113,113	1.25	5 (6%)
39	CLA	a	806	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	6 (7%)
42	BCR	a	843	-	41,41,41	0.73	0	56,56,56	1.94	17 (30%)
39	CLA	7	314	-	60,64,73	1.36	7 (11%)	72,102,113	1.47	10 (13%)
50	A1EB1	9	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.05	19 (31%)
42	BCR	j	103	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
43	DD6	x	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.89	16 (30%)
49	KC2	z	315	-	49,53,53	1.76	10 (20%)	62,89,89	2.20	18 (29%)
43	DD6	4	307	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	15 (28%)
39	CLA	C	309	-	50,54,73	1.47	6 (12%)	60,90,113	1.40	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	SQD	D	320	39	36,37,54	1.16	5 (13%)	45,48,65	1.86	10 (22%)
50	A1EB1	7	303	-	51,58,58	1.33	3 (5%)	60,85,85	2.01	20 (33%)
49	KC2	9	318	-	49,53,53	1.82	9 (18%)	62,89,89	2.03	14 (22%)
39	CLA	R	307	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
39	CLA	F	312	-	69,73,73	1.26	7 (10%)	83,113,113	1.29	5 (6%)
39	CLA	a	820	-	55,59,73	1.43	9 (16%)	66,96,113	1.35	5 (7%)
49	KC2	C	313	-	49,53,53	1.75	9 (18%)	62,89,89	2.16	18 (29%)
39	CLA	R	311	27	54,58,73	1.40	8 (14%)	65,95,113	1.41	5 (7%)
39	CLA	W	311	-	69,73,73	1.26	7 (10%)	83,113,113	1.29	7 (8%)
39	CLA	8	310	-	49,53,73	1.51	6 (12%)	59,89,113	1.51	7 (11%)
48	A86	G	305	-	44,50,50	1.19	2 (4%)	51,76,76	2.29	16 (31%)
39	CLA	E	306	17	53,57,73	1.42	8 (15%)	62,93,113	1.43	5 (8%)
39	CLA	Y	314	-	45,49,73	1.53	6 (13%)	54,84,113	1.61	6 (11%)
39	CLA	x	309	-	45,49,73	1.53	8 (17%)	54,84,113	1.55	6 (11%)
39	CLA	F	309	-	56,60,73	1.39	7 (12%)	67,97,113	1.40	4 (5%)
39	CLA	A	308	-	55,59,73	1.42	8 (14%)	66,96,113	1.33	5 (7%)
39	CLA	Z	307	-	45,49,73	1.52	8 (17%)	54,84,113	1.54	6 (11%)
39	CLA	1	320	-	45,49,73	1.53	6 (13%)	54,84,113	1.56	7 (12%)
51	A1ECV	S	318	-	47,56,56	3.38	20 (42%)	32,93,93	3.02	11 (34%)
39	CLA	0	312	31	57,61,73	1.36	9 (15%)	68,98,113	1.41	7 (10%)
39	CLA	0	320	-	49,53,73	1.50	6 (12%)	59,89,113	1.45	5 (8%)
51	A1ECV	y	311	-	47,56,56	3.30	20 (42%)	32,93,93	3.33	12 (37%)
39	CLA	a	821	-	59,63,73	1.35	8 (13%)	71,101,113	1.40	5 (7%)
49	KC2	x	315	-	49,53,53	1.79	9 (18%)	62,89,89	2.05	15 (24%)
39	CLA	7	315	-	54,58,73	1.42	8 (14%)	65,95,113	1.43	7 (10%)
49	KC2	J	315	-	49,53,53	1.79	9 (18%)	62,89,89	2.11	20 (32%)
50	A1EB1	4	303	-	51,58,58	1.27	3 (5%)	60,85,85	1.84	14 (23%)
43	DD6	Z	302	-	39,45,45	2.09	4 (10%)	52,67,67	3.79	20 (38%)
39	CLA	P	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
48	A86	L	305	-	44,50,50	1.22	3 (6%)	51,76,76	2.17	16 (31%)
50	A1EB1	0	307	-	51,58,58	1.25	3 (5%)	60,85,85	2.24	17 (28%)
50	A1EB1	4	302	-	51,58,58	1.24	4 (7%)	60,85,85	2.12	20 (33%)
48	A86	U	202	-	44,50,50	1.17	3 (6%)	51,76,76	2.30	20 (39%)
45	DGD	C	314	-	41,41,67	1.10	2 (4%)	55,55,81	1.38	6 (10%)
51	A1ECV	G	316	-	47,56,56	3.30	19 (40%)	32,93,93	3.24	12 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	b	812	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
50	A1EB1	x	301	-	51,58,58	1.26	4 (7%)	60,85,85	1.97	14 (23%)
39	CLA	2	319	-	50,54,73	1.46	7 (14%)	60,90,113	1.67	9 (15%)
50	A1EB1	4	304	-	51,58,58	1.28	3 (5%)	60,85,85	2.17	21 (35%)
39	CLA	S	313	-	69,73,73	1.25	9 (13%)	83,113,113	1.27	6 (7%)
47	SQD	F	318	-	41,42,54	1.07	5 (12%)	50,53,65	1.70	10 (20%)
39	CLA	O	308	-	41,46,73	1.60	7 (17%)	51,80,113	2.03	11 (21%)
39	CLA	K	306	-	65,69,73	1.31	9 (13%)	78,108,113	1.35	7 (8%)
39	CLA	Y	305	-	45,49,73	1.53	6 (13%)	54,84,113	1.54	5 (9%)
39	CLA	Q	317	-	50,54,73	1.48	7 (14%)	60,90,113	1.40	5 (8%)
39	CLA	U	201	-	50,54,73	1.44	9 (18%)	60,90,113	1.49	7 (11%)
43	DD6	J	304	-	39,45,45	2.23	5 (12%)	52,67,67	2.35	14 (26%)
39	CLA	E	313	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	9 (10%)
49	KC2	I	303	-	49,53,53	1.77	10 (20%)	62,89,89	2.33	21 (33%)
39	CLA	A	305	13	53,57,73	1.44	8 (15%)	62,93,113	1.41	5 (8%)
49	KC2	R	314	46	48,52,53	1.74	9 (18%)	59,87,89	2.20	16 (27%)
50	A1EB1	U	205	-	51,58,58	1.23	4 (7%)	60,85,85	1.99	19 (31%)
39	CLA	I	314	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
50	A1EB1	Q	323	-	51,58,58	1.24	3 (5%)	60,85,85	2.08	15 (25%)
39	CLA	O	309	-	49,53,73	1.48	9 (18%)	59,89,113	1.50	5 (8%)
39	CLA	D	314	-	69,73,73	1.27	8 (11%)	83,113,113	1.23	7 (8%)
39	CLA	D	315	-	69,73,73	1.25	7 (10%)	83,113,113	1.26	5 (6%)
49	KC2	x	313	-	49,53,53	1.77	9 (18%)	62,89,89	2.13	17 (27%)
51	A1ECV	Z	308	-	47,56,56	3.34	20 (42%)	32,93,93	3.27	13 (40%)
44	SF4	c	102	-	0,12,12	-	-	-		
49	KC2	5	311	-	49,53,53	1.78	10 (20%)	62,89,89	2.25	19 (30%)
48	A86	6	302	-	44,50,50	1.16	3 (6%)	51,76,76	2.16	15 (29%)
51	A1ECV	M	316	-	47,56,56	3.32	19 (40%)	32,93,93	3.06	12 (37%)
49	KC2	F	311	46	48,52,53	1.73	9 (18%)	59,87,89	2.31	19 (32%)
50	A1EB1	3	302	-	51,58,58	1.30	4 (7%)	60,85,85	2.09	18 (30%)
51	A1ECV	R	310	-	47,56,56	3.31	19 (40%)	32,93,93	3.55	11 (34%)
39	CLA	B	207	-	59,63,73	1.39	8 (13%)	71,101,113	1.42	7 (9%)
49	KC2	W	314	-	49,53,53	1.76	9 (18%)	62,89,89	2.14	17 (27%)
50	A1EB1	K	302	-	51,58,58	1.29	4 (7%)	60,85,85	2.12	21 (35%)
39	CLA	b	837	-	64,68,73	1.31	9 (14%)	77,107,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	A	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	8 (9%)
39	CLA	E	310	-	69,73,73	1.25	7 (10%)	83,113,113	1.32	7 (8%)
39	CLA	b	823	-	50,54,73	1.46	6 (12%)	60,90,113	1.46	5 (8%)
39	CLA	a	810	-	58,62,73	1.37	8 (13%)	69,99,113	1.37	7 (10%)
49	KC2	T	312	-	49,53,53	1.81	10 (20%)	62,89,89	2.19	17 (27%)
49	KC2	1	315	-	49,53,53	1.80	10 (20%)	62,89,89	2.09	15 (24%)
49	KC2	Z	311	-	49,53,53	1.75	9 (18%)	62,89,89	2.16	17 (27%)
42	BCR	i	102	-	41,41,41	0.72	0	56,56,56	2.26	19 (33%)
43	DD6	2	303	-	39,45,45	2.09	4 (10%)	52,67,67	3.79	20 (38%)
42	BCR	b	844	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
49	KC2	M	311	46	48,52,53	1.72	9 (18%)	59,87,89	2.20	17 (28%)
48	A86	X	302	-	44,50,50	1.17	2 (4%)	51,76,76	2.19	17 (33%)
49	KC2	6	316	-	49,53,53	1.76	9 (18%)	62,89,89	2.14	19 (30%)
39	CLA	L	309	-	57,62,73	1.37	9 (15%)	68,100,113	1.41	7 (10%)
49	KC2	Q	318	26	49,53,53	1.75	10 (20%)	62,89,89	2.19	17 (27%)
48	A86	1	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.18	17 (33%)
39	CLA	7	324	-	45,49,73	1.53	8 (17%)	54,84,113	1.64	8 (14%)
43	DD6	z	304	-	39,45,45	2.05	4 (10%)	52,67,67	1.88	14 (26%)
41	LHG	j	104	-	29,29,48	0.74	1 (3%)	32,35,54	1.23	3 (9%)
48	A86	4	310	-	44,50,50	1.18	2 (4%)	51,76,76	2.34	17 (33%)
39	CLA	S	309	-	69,73,73	1.29	9 (13%)	83,113,113	1.36	10 (12%)
48	A86	4	328	-	44,50,50	1.14	2 (4%)	51,76,76	2.28	15 (29%)
50	A1EB1	V	307	-	51,58,58	1.26	4 (7%)	60,85,85	2.09	21 (35%)
51	A1ECV	Q	319	-	47,56,56	3.32	19 (40%)	32,93,93	3.17	12 (37%)
49	KC2	H	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.13	18 (29%)
49	KC2	H	311	-	49,53,53	1.78	10 (20%)	62,89,89	2.12	15 (24%)
48	A86	0	304	-	44,50,50	1.20	2 (4%)	51,76,76	1.94	15 (29%)
43	DD6	7	310	-	39,45,45	2.06	3 (7%)	52,67,67	2.49	14 (26%)
48	A86	V	304	-	44,50,50	1.18	3 (6%)	51,76,76	2.02	17 (33%)
51	A1ECV	5	309	27	47,56,56	3.32	19 (40%)	32,93,93	3.31	12 (37%)
48	A86	0	308	51	44,50,50	1.27	3 (6%)	51,76,76	2.18	19 (37%)
49	KC2	8	316	-	49,53,53	1.77	10 (20%)	62,89,89	2.20	16 (25%)
39	CLA	a	819	-	53,57,73	1.41	7 (13%)	62,93,113	1.44	7 (11%)
50	A1EB1	z	301	-	44,50,58	1.15	2 (4%)	51,76,85	1.70	12 (23%)
39	CLA	C	307	-	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	BCR	b	848	-	41,41,41	0.75	0	56,56,56	1.78	14 (25%)
39	CLA	b	806	-	69,73,73	1.23	7 (10%)	83,113,113	1.25	7 (8%)
39	CLA	0	313	-	59,63,73	1.36	7 (11%)	71,101,113	1.38	6 (8%)
48	A86	L	304	-	44,50,50	1.21	3 (6%)	51,76,76	2.32	18 (35%)
39	CLA	Y	310	-	45,49,73	1.54	6 (13%)	54,84,113	1.55	5 (9%)
46	LMG	I	302	-	42,42,55	0.89	1 (2%)	50,50,63	1.22	4 (8%)
48	A86	0	309	-	44,50,50	1.20	2 (4%)	51,76,76	2.35	18 (35%)
49	KC2	2	313	-	48,52,53	1.80	10 (20%)	62,88,89	2.19	19 (30%)
47	SQD	S	301	-	38,39,54	1.14	5 (13%)	47,50,65	1.67	10 (21%)
39	CLA	P	314	-	45,49,73	1.53	8 (17%)	54,84,113	1.56	6 (11%)
39	CLA	P	311	-	69,73,73	1.26	6 (8%)	83,113,113	1.28	5 (6%)
39	CLA	4	322	-	56,60,73	1.40	9 (16%)	67,97,113	1.44	7 (10%)
39	CLA	x	317	-	45,49,73	1.53	6 (13%)	54,84,113	1.53	6 (11%)
39	CLA	6	321	-	45,49,73	1.53	8 (17%)	54,84,113	1.52	5 (9%)
39	CLA	a	827	-	69,73,73	1.28	10 (14%)	83,113,113	1.40	8 (9%)
39	CLA	R	308	-	64,68,73	1.30	7 (10%)	77,107,113	1.30	5 (6%)
39	CLA	I	316	36	45,49,73	1.51	6 (13%)	54,84,113	1.50	6 (11%)
51	A1ECV	6	320	-	47,56,56	3.37	20 (42%)	32,93,93	3.14	11 (34%)
39	CLA	D	316	-	69,73,73	1.25	7 (10%)	83,113,113	1.26	5 (6%)
43	DD6	M	304	-	39,45,45	1.92	3 (7%)	52,67,67	1.71	12 (23%)
39	CLA	P	307	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	5 (6%)
51	A1ECV	9	317	-	47,56,56	3.32	20 (42%)	32,93,93	3.25	12 (37%)
46	LMG	7	326	-	32,32,55	0.93	1 (3%)	40,40,63	1.23	3 (7%)
39	CLA	O	310	-	64,68,73	1.32	9 (14%)	77,107,113	1.39	10 (12%)
48	A86	7	311	-	44,50,50	1.19	3 (6%)	51,76,76	2.16	16 (31%)
39	CLA	Z	304	-	45,49,73	1.53	8 (17%)	54,84,113	1.56	5 (9%)
48	A86	Z	303	-	44,50,50	1.16	3 (6%)	51,76,76	2.27	18 (35%)
43	DD6	G	303	-	39,45,45	1.93	3 (7%)	52,67,67	1.82	11 (21%)
51	A1ECV	S	312	-	47,56,56	3.44	20 (42%)	32,93,93	3.45	11 (34%)
39	CLA	a	833	1	49,53,73	1.48	7 (14%)	59,89,113	1.49	5 (8%)
50	A1EB1	K	304	-	51,58,58	1.26	4 (7%)	60,85,85	1.95	18 (30%)
50	A1EB1	6	301	-	51,58,58	1.28	3 (5%)	60,85,85	2.00	16 (26%)
42	BCR	h	202	-	41,41,41	0.74	0	56,56,56	1.87	17 (30%)
39	CLA	b	824	-	64,68,73	1.30	8 (12%)	77,107,113	1.33	4 (5%)
39	CLA	U	212	-	50,54,73	1.48	7 (14%)	60,90,113	1.42	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	A1EB1	0	303	-	51,58,58	1.26	3 (5%)	60,85,85	2.23	17 (28%)
39	CLA	5	316	-	56,60,73	1.41	9 (16%)	67,97,113	1.42	5 (7%)
49	KC2	M	307	-	49,53,53	1.76	10 (20%)	62,89,89	2.21	19 (30%)
43	DD6	X	304	-	39,45,45	1.92	3 (7%)	52,67,67	1.87	16 (30%)
39	CLA	Q	320	-	51,55,73	1.44	7 (13%)	61,91,113	1.41	4 (6%)
51	A1ECV	x	316	-	47,56,56	3.36	19 (40%)	32,93,93	3.12	13 (40%)
48	A86	7	308	-	44,50,50	1.19	2 (4%)	51,76,76	2.06	16 (31%)
39	CLA	2	315	-	45,49,73	1.53	8 (17%)	54,84,113	1.50	5 (9%)
51	A1ECV	2	311	-	47,56,56	3.35	20 (42%)	32,93,93	3.26	12 (37%)
43	DD6	J	306	-	39,45,45	1.99	3 (7%)	52,67,67	2.16	12 (23%)
48	A86	4	306	-	44,50,50	1.18	2 (4%)	51,76,76	1.99	15 (29%)
39	CLA	G	309	-	60,64,73	1.34	9 (15%)	72,102,113	1.40	6 (8%)
50	A1EB1	S	303	-	51,58,58	1.25	3 (5%)	60,85,85	2.14	21 (35%)
39	CLA	V	309	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	8 (9%)
43	DD6	I	307	-	39,45,45	2.01	3 (7%)	52,67,67	1.90	10 (19%)
49	KC2	V	308	27	49,53,53	1.77	10 (20%)	62,89,89	2.20	18 (29%)
39	CLA	a	802	-	59,63,73	1.35	7 (11%)	71,101,113	1.39	8 (11%)
39	CLA	H	308	-	64,68,73	1.30	7 (10%)	77,107,113	1.31	6 (7%)
48	A86	4	309	-	44,50,50	1.21	3 (6%)	51,76,76	2.13	17 (33%)
41	LHG	D	302	-	34,34,48	0.70	0	37,40,54	1.27	3 (8%)
48	A86	8	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.24	19 (37%)
48	A86	Q	302	-	44,50,50	1.21	3 (6%)	51,76,76	2.27	18 (35%)
51	A1ECV	X	313	-	47,56,56	3.38	20 (42%)	32,93,93	3.26	12 (37%)
46	LMG	4	326	49	46,46,55	0.96	2 (4%)	54,54,63	1.28	6 (11%)
50	A1EB1	T	307	-	51,58,58	1.24	4 (7%)	60,85,85	1.95	19 (31%)
39	CLA	b	831	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	8 (12%)
39	CLA	a	815	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	5 (6%)
39	CLA	z	317	-	46,50,73	1.52	6 (13%)	55,85,113	1.48	4 (7%)
39	CLA	6	315	-	45,49,73	1.52	8 (17%)	54,84,113	1.57	7 (12%)
39	CLA	E	307	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	8 (9%)
39	CLA	a	822	-	69,73,73	1.25	7 (10%)	83,113,113	1.34	7 (8%)
48	A86	M	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.16	19 (37%)
39	CLA	3	311	-	65,69,73	1.30	8 (12%)	78,108,113	1.27	5 (6%)
49	KC2	8	319	34	49,53,53	1.79	10 (20%)	62,89,89	2.14	17 (27%)
46	LMG	D	322	-	37,37,55	0.91	0	45,45,63	1.21	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	A1EB4	P	305	-	51,58,63	2.60	4 (7%)	60,84,89	2.09	19 (31%)
50	A1EB1	6	306	-	44,50,58	1.15	2 (4%)	51,76,85	1.86	11 (21%)
42	BCR	b	847	-	41,41,41	0.71	0	56,56,56	2.01	16 (28%)
39	CLA	3	319	-	45,49,73	1.52	6 (13%)	54,84,113	1.57	7 (12%)
42	BCR	k	204	-	41,41,41	0.71	0	56,56,56	1.90	15 (26%)
49	KC2	K	310	-	49,53,53	1.77	10 (20%)	62,89,89	2.19	17 (27%)
39	CLA	Y	311	-	45,49,73	1.52	6 (13%)	54,84,113	1.57	6 (11%)
39	CLA	A	307	-	64,68,73	1.32	8 (12%)	77,107,113	1.30	6 (7%)
46	LMG	S	321	-	32,32,55	0.92	0	40,40,63	1.21	5 (12%)
39	CLA	E	317	-	56,60,73	1.39	6 (10%)	67,97,113	1.43	6 (8%)
50	A1EB1	6	304	-	48,55,58	1.32	3 (6%)	57,82,85	2.32	19 (33%)
42	BCR	b	850	-	41,41,41	0.68	0	56,56,56	1.86	12 (21%)
43	DD6	D	303	-	39,45,45	2.10	2 (5%)	52,67,67	2.77	15 (28%)
49	KC2	R	312	-	49,53,53	1.75	11 (22%)	62,89,89	2.18	19 (30%)
39	CLA	b	834	-	62,66,73	1.33	7 (11%)	74,104,113	1.37	6 (8%)
39	CLA	z	314	-	45,49,73	1.53	7 (15%)	54,84,113	1.52	5 (9%)
42	BCR	f	804	-	41,41,41	0.68	0	56,56,56	1.98	14 (25%)
39	CLA	F	316	-	55,59,73	1.42	8 (14%)	66,96,113	1.40	5 (7%)
48	A86	0	306	-	44,50,50	1.14	3 (6%)	51,76,76	2.25	17 (33%)
39	CLA	B	205	-	46,50,73	1.52	6 (13%)	55,85,113	1.51	6 (10%)
48	A86	3	307	-	44,50,50	1.22	3 (6%)	51,76,76	2.40	20 (39%)
51	A1ECV	Y	306	-	47,56,56	3.33	19 (40%)	32,93,93	3.28	13 (40%)
48	A86	D	305	-	44,50,50	1.21	3 (6%)	51,76,76	2.71	21 (41%)
48	A86	O	307	-	44,50,50	1.17	2 (4%)	51,76,76	2.35	19 (37%)
39	CLA	9	310	-	45,49,73	1.51	8 (17%)	54,84,113	1.57	8 (14%)
39	CLA	C	306	-	69,73,73	1.25	8 (11%)	83,113,113	1.26	5 (6%)
39	CLA	9	312	35	46,50,73	1.49	8 (17%)	55,85,113	1.53	6 (10%)
39	CLA	y	308	-	49,53,73	1.49	8 (16%)	59,89,113	1.51	7 (11%)
39	CLA	z	307	-	46,50,73	1.51	6 (13%)	55,85,113	1.50	6 (10%)
48	A86	1	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.29	18 (35%)
49	KC2	G	311	19	49,53,53	1.78	10 (20%)	62,89,89	2.17	16 (25%)
39	CLA	8	322	-	45,49,73	1.54	7 (15%)	54,84,113	1.63	8 (14%)
49	KC2	T	314	-	49,53,53	1.75	10 (20%)	62,89,89	2.18	18 (29%)
48	A86	F	301	-	44,50,50	1.19	3 (6%)	51,76,76	2.23	15 (29%)
39	CLA	0	323	-	50,54,73	1.43	8 (16%)	60,90,113	1.48	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	DD6	o	204	-	39,45,45	1.99	2 (5%)	52,67,67	1.88	12 (23%)
39	CLA	b	821	-	69,73,73	1.27	8 (11%)	83,113,113	1.31	7 (8%)
39	CLA	V	313	27	69,73,73	1.23	9 (13%)	83,113,113	1.27	4 (4%)
48	A86	C	303	-	44,50,50	1.21	2 (4%)	51,76,76	1.92	14 (27%)
39	CLA	W	310	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
48	A86	L	302	-	44,50,50	1.13	3 (6%)	51,76,76	2.99	22 (43%)
48	A86	T	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.22	19 (37%)
50	A1EB1	G	308	-	51,58,58	1.22	3 (5%)	60,85,85	2.28	16 (26%)
39	CLA	6	318	-	45,49,73	1.52	8 (17%)	54,84,113	1.55	5 (9%)
48	A86	2	302	-	44,50,50	1.17	3 (6%)	51,76,76	2.32	18 (35%)
39	CLA	F	306	-	50,54,73	1.46	7 (14%)	60,90,113	1.43	5 (8%)
39	CLA	b	808	-	49,53,73	1.48	7 (14%)	59,89,113	1.51	6 (10%)
39	CLA	b	835	-	69,73,73	1.26	7 (10%)	83,113,113	1.24	5 (6%)
50	A1EB1	8	304	-	51,58,58	1.25	3 (5%)	60,85,85	2.21	17 (28%)
49	KC2	T	316	-	49,53,53	1.76	9 (18%)	62,89,89	2.13	16 (25%)
39	CLA	l	205	-	54,58,73	1.41	8 (14%)	65,95,113	1.44	8 (12%)
48	A86	V	301	-	44,50,50	1.19	3 (6%)	51,76,76	2.45	17 (33%)
39	CLA	o	206	-	62,66,73	1.32	6 (9%)	74,104,113	1.36	5 (6%)
39	CLA	E	319	17	53,57,73	1.43	7 (13%)	62,93,113	1.40	5 (8%)
39	CLA	4	312	-	69,73,73	1.26	8 (11%)	83,113,113	1.37	10 (12%)
51	A1ECV	V	317	-	47,56,56	3.38	20 (42%)	32,93,93	3.15	11 (34%)
39	CLA	3	312	-	69,73,73	1.27	7 (10%)	83,113,113	1.36	8 (9%)
42	BCR	a	842	-	41,41,41	0.67	0	56,56,56	1.82	14 (25%)

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
48	A86	S	307	-	-	6/34/90/90	0/3/3/3
39	CLA	G	314	19	-	8/31/107/115	-
43	DD6	E	302	-	-	0/26/80/80	0/3/3/3
46	LMG	M	320	-	-	10/28/48/70	0/1/1/1
39	CLA	I	308	-	-	10/35/111/115	-
49	KC2	A	310	13	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	1	316	-	-	5/10/86/115	-
50	A1EB1	E	301	-	-	9/42/100/100	0/3/3/3
39	CLA	R	309	-	-	13/39/115/115	-
49	KC2	V	312	-	-	6/15/71/71	-
39	CLA	a	837	-	-	5/39/115/115	-
39	CLA	G	312	-	-	12/24/100/115	-
39	CLA	I	309	-	-	12/39/115/115	-
39	CLA	6	313	-	-	5/12/88/115	-
46	LMG	Q	322	49	-	13/23/43/70	0/1/1/1
39	CLA	b	827	-	-	10/39/115/115	-
48	A86	P	303	-	-	0/34/90/90	0/3/3/3
39	CLA	D	309	16	-	8/20/96/115	-
48	A86	7	307	-	-	3/34/90/90	0/3/3/3
49	KC2	z	312	-	-	7/15/71/71	-
39	CLA	X	307	-	-	10/39/115/115	-
39	CLA	b	803	-	-	14/39/115/115	-
39	CLA	4	319	-	-	4/10/86/115	-
43	DD6	Q	303	-	-	4/26/80/80	0/3/3/3
39	CLA	f	802	-	-	11/39/115/115	-
43	DD6	y	303	-	-	1/26/80/80	0/3/3/3
50	A1EB1	S	302	-	-	11/42/100/100	0/3/3/3
39	CLA	6	310	-	-	6/12/88/115	-
39	CLA	F	313	-	-	12/30/106/115	-
39	CLA	a	818	-	-	11/39/115/115	-
48	A86	9	305	-	-	6/34/90/90	0/3/3/3
50	A1EB1	J	302	-	-	9/42/100/100	0/3/3/3
41	LHG	H	317	-	-	18/39/39/53	-
39	CLA	O	312	-	-	7/17/93/115	-
43	DD6	Q	306	-	-	1/26/80/80	0/3/3/3
46	LMG	M	319	49	-	13/34/54/70	0/1/1/1
39	CLA	Y	307	-	-	5/10/86/115	-
48	A86	R	301	-	-	2/34/90/90	0/3/3/3
48	A86	y	305	-	-	0/34/90/90	0/3/3/3
39	CLA	T	309	-	-	11/29/105/115	-
50	A1EB1	4	301	-	-	12/42/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	X	317	-	-	10/24/100/115	-
39	CLA	5	307	-	-	5/33/109/115	-
39	CLA	y	309	-	-	6/17/93/115	-
51	A1ECV	W	317	-	3/3/17/24	9/19/117/117	-
39	CLA	9	319	-	-	8/15/91/115	-
49	KC2	y	316	-	-	7/15/71/71	-
39	CLA	a	835	-	-	13/39/115/115	-
39	CLA	H	309	20	-	5/24/100/115	-
39	CLA	J	316	-	-	7/17/93/115	-
39	CLA	3	320	-	-	5/15/91/115	-
49	KC2	y	314	-	-	7/15/71/71	-
39	CLA	E	312	-	-	23/39/115/115	-
39	CLA	h	201	-	-	10/27/103/115	-
39	CLA	i	101	-	-	10/39/115/115	-
39	CLA	Q	310	-	-	20/39/115/115	-
48	A86	9	303	-	-	7/34/90/90	0/3/3/3
39	CLA	y	310	-	-	7/10/86/115	-
39	CLA	A	312	-	-	15/39/115/115	-
51	A1ECV	1	318	-	3/3/17/24	6/19/117/117	-
39	CLA	W	319	-	-	8/17/93/115	-
50	A1EB1	H	301	-	-	12/42/100/100	0/3/3/3
39	CLA	1	308	-	-	6/10/86/115	-
39	CLA	I	310	-	-	10/26/102/115	-
48	A86	F	302	-	-	2/34/90/90	0/3/3/3
39	CLA	K	308	22	-	13/32/108/115	-
49	KC2	R	306	-	-	8/15/71/71	-
49	KC2	2	317	-	-	7/15/71/71	-
50	A1EB1	R	303	-	-	10/42/100/100	0/3/3/3
39	CLA	P	308	24	-	22/39/115/115	-
39	CLA	l	203	-	-	8/20/96/115	-
39	CLA	T	310	29	-	6/24/100/115	-
39	CLA	H	315	-	-	6/10/86/115	-
39	CLA	b	828	-	-	15/39/115/115	-
39	CLA	F	321	-	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	J	308	-	-	6/21/97/115	-
39	CLA	y	318	-	-	7/12/88/115	-
49	KC2	Z	310	-	-	9/15/71/71	-
48	A86	8	309	-	-	4/34/90/90	0/3/3/3
50	A1EB1	F	304	-	-	11/42/100/100	0/3/3/3
39	CLA	O	313	-	-	4/21/97/115	-
39	CLA	a	808	-	-	12/29/105/115	-
39	CLA	X	311	27	-	5/21/97/115	-
39	CLA	0	315	31	-	5/21/97/115	-
39	CLA	b	851	-	-	13/39/115/115	-
48	A86	U	206	-	-	3/34/90/90	0/3/3/3
49	KC2	R	318	-	-	7/15/71/71	-
49	KC2	L	312	-	-	8/15/71/71	-
47	SQD	4	327	-	-	17/34/54/69	0/1/1/1
49	KC2	1	312	-	-	7/15/71/71	-
39	CLA	8	312	-	-	8/15/91/115	-
47	SQD	T	321	-	-	13/31/51/69	0/1/1/1
39	CLA	k	203	-	-	9/27/103/115	-
48	A86	3	308	-	-	6/34/90/90	0/3/3/3
50	A1EB1	0	302	-	-	13/42/100/100	0/3/3/3
49	KC2	Q	315	-	-	8/15/71/71	-
43	DD6	z	305	-	-	1/26/80/80	0/3/3/3
48	A86	I	304	-	-	11/34/90/90	0/3/3/3
39	CLA	b	841	2	-	12/39/115/115	-
50	A1EB1	x	302	-	-	15/42/100/100	0/3/3/3
39	CLA	z	308	-	-	4/17/93/115	-
46	LMG	9	321	-	-	16/31/51/70	0/1/1/1
48	A86	Z	301	-	-	11/34/90/90	0/3/3/3
49	KC2	5	314	-	-	8/15/71/71	-
39	CLA	L	316	-	-	8/10/86/115	-
39	CLA	o	201	-	-	5/23/99/115	-
39	CLA	b	838	-	-	15/39/115/115	-
39	CLA	8	321	-	-	4/12/88/115	-
43	DD6	y	304	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	O	306	-	-	6/34/90/90	0/3/3/3
39	CLA	L	313	-	-	3/21/97/115	-
39	CLA	0	322	-	-	14/23/99/115	-
39	CLA	a	825	-	-	11/36/112/115	-
39	CLA	b	842	-	-	14/39/115/115	-
48	A86	J	301	-	-	2/34/90/90	0/3/3/3
39	CLA	a	831	-	-	12/39/115/115	-
41	LHG	D	301	-	-	8/39/39/53	-
39	CLA	H	307	-	-	4/15/91/115	-
43	DD6	O	305	-	-	5/26/80/80	0/3/3/3
49	KC2	L	321	-	-	7/15/71/71	-
50	A1EB1	8	308	-	-	11/42/100/100	0/3/3/3
52	A1EB4	P	319	-	-	6/38/99/103	0/3/3/3
39	CLA	b	801	-	-	10/39/115/115	-
39	CLA	A	315	-	-	8/21/97/115	-
49	KC2	M	314	-	-	7/15/71/71	-
49	KC2	9	313	-	-	6/15/71/71	-
39	CLA	C	305	-	-	17/35/111/115	-
39	CLA	W	316	24	-	3/10/86/115	-
39	CLA	a	804	-	-	18/39/115/115	-
48	A86	B	201	-	-	5/34/90/90	0/3/3/3
49	KC2	7	320	-	-	7/15/71/71	-
43	DD6	K	303	-	-	0/26/80/80	0/3/3/3
39	CLA	H	306	-	-	10/19/95/115	-
47	SQD	P	301	-	-	12/33/53/69	0/1/1/1
50	A1EB1	V	306	-	-	7/42/100/100	0/3/3/3
39	CLA	l	201	-	-	16/39/115/115	-
39	CLA	S	310	-	-	4/12/88/115	-
49	KC2	P	306	24	-	7/15/71/71	-
51	A1ECV	P	315	-	3/3/17/24	12/19/117/117	-
39	CLA	a	824	-	-	7/39/115/115	-
39	CLA	R	316	-	-	10/24/100/115	-
39	CLA	B	204	-	-	4/17/93/115	-
48	A86	6	303	-	-	2/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	P	312	-	-	7/15/71/71	-
39	CLA	a	834	-	-	6/23/99/115	-
39	CLA	Z	315	-	-	4/10/86/115	-
39	CLA	1	309	-	-	6/12/88/115	-
39	CLA	y	319	-	-	5/10/86/115	-
43	DD6	A	303	-	-	5/26/80/80	0/3/3/3
48	A86	1	306	-	-	9/34/90/90	0/3/3/3
39	CLA	0	318	-	-	3/10/86/115	-
39	CLA	a	803	-	-	17/39/115/115	-
39	CLA	T	311	-	-	5/29/105/115	-
39	CLA	J	311	-	-	12/39/115/115	-
49	KC2	X	314	46	-	7/14/70/71	-
49	KC2	1	314	-	-	11/15/71/71	-
43	DD6	V	303	-	-	0/26/80/80	0/3/3/3
39	CLA	a	847	-	-	20/39/115/115	-
39	CLA	3	314	-	-	18/39/115/115	-
39	CLA	4	316	-	-	13/39/115/115	-
39	CLA	X	316	-	-	9/18/94/115	-
48	A86	8	305	-	-	12/34/90/90	0/3/3/3
39	CLA	E	314	-	-	12/29/105/115	-
39	CLA	T	319	29	-	10/17/93/115	-
39	CLA	Z	316	-	-	8/10/86/115	-
42	BCR	l	206	-	-	6/29/63/63	0/2/2/2
39	CLA	x	307	-	-	4/10/86/115	-
50	A1EB1	V	302	-	-	12/42/100/100	0/3/3/3
49	KC2	L	315	-	-	9/15/71/71	-
39	CLA	5	308	-	-	14/39/115/115	-
48	A86	S	304	-	-	8/34/90/90	0/3/3/3
49	KC2	L	314	-	-	7/15/71/71	-
48	A86	G	301	-	-	11/34/90/90	0/3/3/3
49	KC2	P	320	-	-	9/15/71/71	-
42	BCR	m	101	-	-	9/29/63/63	0/2/2/2
47	SQD	E	320	-	-	12/30/50/69	0/1/1/1
39	CLA	Z	305	-	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	J	313	-	-	9/17/93/115	-
39	CLA	F	315	18	-	4/10/86/115	-
39	CLA	9	315	-	-	3/10/86/115	-
48	A86	Q	304	-	-	2/34/90/90	0/3/3/3
39	CLA	Z	306	-	-	9/17/93/115	-
50	A1EB1	3	324	-	-	20/42/100/100	0/3/3/3
49	KC2	z	313	-	-	6/16/59/71	-
49	KC2	P	313	24	-	10/15/71/71	-
49	KC2	9	316	35	-	9/15/71/71	-
39	CLA	D	310	47	-	19/35/111/115	-
50	A1EB1	C	302	-	-	10/42/100/100	0/3/3/3
50	A1EB1	5	302	-	-	9/42/100/100	0/3/3/3
46	LMG	4	325	-	-	16/27/47/70	0/1/1/1
39	CLA	L	310	23	-	14/39/115/115	-
39	CLA	D	312	16	-	9/27/103/115	-
50	A1EB1	Q	307	-	-	8/42/100/100	0/3/3/3
39	CLA	1	310	-	-	6/15/91/115	-
39	CLA	Z	309	-	-	2/10/86/115	-
46	LMG	l	208	49	-	15/34/54/70	0/1/1/1
51	A1ECV	y	317	-	3/3/17/24	9/19/117/117	-
50	A1EB1	h	203	-	-	10/42/100/100	0/3/3/3
48	A86	L	301	-	-	7/34/90/90	0/3/3/3
51	A1ECV	z	310	-	3/3/17/24	11/19/117/117	-
39	CLA	a	836	-	-	9/39/115/115	-
39	CLA	0	310	-	-	25/35/111/115	-
48	A86	W	303	-	-	4/34/90/90	0/3/3/3
39	CLA	4	311	-	-	19/35/111/115	-
39	CLA	3	323	-	-	11/17/93/115	-
49	KC2	6	319	-	-	11/15/71/71	-
49	KC2	P	310	46	-	8/14/70/71	-
39	CLA	1	311	-	-	7/10/86/115	-
39	CLA	j	101	-	-	19/39/115/115	-
47	SQD	D	321	-	-	16/34/54/69	0/1/1/1
39	CLA	X	308	-	-	18/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	W	304	-	-	0/34/90/90	0/3/3/3
39	CLA	U	207	-	-	17/33/109/115	-
39	CLA	x	311	-	-	2/15/91/115	-
49	KC2	0	314	46,31	-	8/14/70/71	-
49	KC2	V	315	-	-	9/15/71/71	-
39	CLA	2	307	-	-	4/10/86/115	-
39	CLA	S	319	-	-	10/24/100/115	-
48	A86	X	303	-	-	8/34/90/90	0/3/3/3
43	DD6	3	301	-	-	2/26/80/80	0/3/3/3
51	A1ECV	7	317	-	3/3/17/24	7/19/117/117	-
48	A86	6	307	-	-	10/34/90/90	0/3/3/3
43	DD6	4	308	-	-	1/26/80/80	0/3/3/3
39	CLA	F	310	-	-	7/26/102/115	-
48	A86	1	307	-	-	0/34/90/90	0/3/3/3
39	CLA	4	313	-	-	3/17/93/115	-
39	CLA	z	309	-	-	5/10/86/115	-
49	KC2	A	313	-	-	11/15/71/71	-
39	CLA	4	323	-	-	13/39/115/115	-
39	CLA	C	308	-	-	16/33/109/115	-
49	KC2	6	317	-	-	9/15/71/71	-
44	SF4	b	804	-	-	-	0/6/5/5
39	CLA	b	813	-	-	3/25/101/115	-
44	SF4	c	101	-	-	-	0/6/5/5
43	DD6	H	303	-	-	1/26/80/80	0/3/3/3
46	LMG	W	302	49	-	18/34/54/70	0/1/1/1
48	A86	3	306	-	-	8/34/90/90	0/3/3/3
51	A1ECV	7	323	-	2/2/17/24	8/19/117/117	-
48	A86	T	301	-	-	2/34/90/90	0/3/3/3
43	DD6	5	303	-	-	1/26/80/80	0/3/3/3
49	KC2	G	313	-	-	6/15/71/71	-
49	KC2	B	208	-	-	9/15/71/71	-
39	CLA	V	310	-	-	10/33/109/115	-
39	CLA	6	322	-	-	11/17/93/115	-
50	A1EB1	3	303	-	-	8/42/100/100	0/3/3/3
50	A1EB1	8	301	-	-	13/42/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	A1ECV	X	310	-	3/3/17/24	10/19/117/117	-
49	KC2	W	312	24,46	-	8/14/70/71	-
48	A86	Y	301	-	-	5/34/90/90	0/3/3/3
50	A1EB1	1	305	-	-	10/42/100/100	0/3/3/3
39	CLA	b	814	-	-	7/27/103/115	-
51	A1ECV	x	310	-	3/3/17/24	5/19/117/117	-
50	A1EB1	K	305	-	-	7/42/100/100	0/3/3/3
39	CLA	J	312	-	-	7/17/93/115	-
39	CLA	W	309	-	-	12/39/115/115	-
39	CLA	D	311	-	-	23/39/115/115	-
49	KC2	W	308	-	-	6/15/71/71	-
39	CLA	y	312	-	-	5/12/88/115	-
39	CLA	z	311	-	-	5/10/86/115	-
39	CLA	D	319	16	-	22/39/115/115	-
39	CLA	T	308	-	-	10/17/93/115	-
49	KC2	2	314	-	-	10/15/71/71	-
39	CLA	L	319	-	-	8/23/99/115	-
50	A1EB1	3	309	-	-	9/42/100/100	0/3/3/3
43	DD6	R	304	-	-	0/26/80/80	0/3/3/3
50	A1EB1	G	304	-	-	8/42/100/100	0/3/3/3
39	CLA	1	319	-	-	12/23/99/115	-
39	CLA	7	313	-	-	21/35/111/115	-
49	KC2	X	312	-	-	7/15/71/71	-
50	A1EB1	0	305	-	-	16/42/100/100	0/3/3/3
39	CLA	2	316	-	-	6/10/86/115	-
39	CLA	M	310	-	-	14/39/115/115	-
43	DD6	J	305	-	-	3/26/80/80	0/3/3/3
39	CLA	b	816	-	-	10/33/109/115	-
49	KC2	V	318	-	-	7/15/71/71	-
39	CLA	a	832	-	-	7/21/97/115	-
43	DD6	A	301	-	-	0/26/80/80	0/3/3/3
39	CLA	B	203	-	-	5/17/93/115	-
39	CLA	D	313	-	-	12/39/115/115	-
39	CLA	M	317	-	-	6/23/99/115	-
43	DD6	U	204	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	DD6	7	309	-	-	2/26/80/80	0/3/3/3
48	A86	T	306	-	-	6/34/90/90	0/3/3/3
49	KC2	5	305	27	-	7/15/71/71	-
39	CLA	T	320	-	-	10/24/100/115	-
43	DD6	1	304	-	-	4/26/80/80	0/3/3/3
39	CLA	C	304	-	-	5/13/89/115	-
51	A1ECV	L	318	-	3/3/17/24	14/19/117/117	-
39	CLA	A	306	-	-	11/35/111/115	-
39	CLA	3	316	-	-	7/21/97/115	-
48	A86	5	301	-	-	3/34/90/90	0/3/3/3
50	A1EB1	D	308	-	-	8/42/100/100	0/3/3/3
51	A1ECV	4	321	-	3/3/17/24	10/19/117/117	-
39	CLA	M	318	24	-	7/17/93/115	-
39	CLA	U	209	-	-	8/24/100/115	-
39	CLA	Z	312	-	-	4/10/86/115	-
46	LMG	7	301	49	-	23/41/61/70	0/1/1/1
39	CLA	D	317	-	-	16/39/115/115	-
48	A86	6	305	-	-	11/34/90/90	0/3/3/3
39	CLA	9	307	-	-	4/10/86/115	-
48	A86	Q	301	-	-	5/34/90/90	0/3/3/3
39	CLA	T	313	-	-	6/23/99/115	-
48	A86	8	307	-	-	12/34/90/90	0/3/3/3
39	CLA	1	317	-	-	6/10/86/115	-
39	CLA	a	826	-	-	18/39/115/115	-
39	CLA	9	308	-	-	17/27/103/115	-
39	CLA	I	301	41	-	7/24/100/115	-
39	CLA	I	315	-	-	6/24/100/115	-
47	SQD	k	205	-	-	13/33/53/69	0/1/1/1
51	A1ECV	Z	314	-	3/3/17/24	7/19/117/117	-
39	CLA	K	314	-	-	6/10/86/115	-
39	CLA	H	313	-	-	9/39/115/115	-
39	CLA	M	309	-	-	17/39/115/115	-
49	KC2	6	314	-	-	8/15/71/71	-
51	A1ECV	O	315	-	3/3/17/24	7/19/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	b	836	-	-	3/15/91/115	-
39	CLA	J	318	-	-	7/17/93/115	-
51	A1ECV	4	315	-	3/3/17/24	9/19/117/117	-
50	A1EB1	7	304	-	-	14/42/100/100	0/3/3/3
39	CLA	J	314	-	-	20/39/115/115	-
43	DD6	I	305	-	-	1/26/80/80	0/3/3/3
49	KC2	W	315	-	-	8/15/71/71	-
52	A1EB4	W	321	-	-	8/38/99/103	0/3/3/3
39	CLA	V	319	-	-	6/24/100/115	-
50	A1EB1	8	306	-	-	13/42/100/100	0/3/3/3
39	CLA	I	313	-	-	19/39/115/115	-
39	CLA	2	312	-	-	7/10/86/115	-
50	A1EB1	O	301	-	-	16/42/100/100	0/3/3/3
39	CLA	8	311	-	-	11/27/103/115	-
39	CLA	X	309	-	-	14/39/115/115	-
46	LMG	S	322	49	-	28/41/61/70	0/1/1/1
49	KC2	G	317	-	-	7/15/71/71	-
39	CLA	S	308	-	-	18/35/111/115	-
43	DD6	x	303	-	-	1/26/80/80	0/3/3/3
39	CLA	b	832	-	-	15/39/115/115	-
51	A1ECV	Y	312	-	3/3/17/24	7/19/117/117	-
39	CLA	3	322	-	-	12/23/99/115	-
48	A86	W	307	-	-	2/34/90/90	0/3/3/3
50	A1EB1	1	301	-	-	11/42/100/100	0/3/3/3
43	DD6	P	304	-	-	2/26/80/80	0/3/3/3
49	KC2	0	319	-	-	10/15/71/71	-
39	CLA	E	308	-	-	11/39/115/115	-
48	A86	8	303	-	-	6/34/90/90	0/3/3/3
48	A86	H	302	-	-	6/34/90/90	0/3/3/3
49	KC2	Y	308	-	-	9/15/71/71	-
39	CLA	U	210	-	-	9/33/109/115	-
49	KC2	O	317	46	-	7/14/70/71	-
39	CLA	o	202	-	-	5/12/88/115	-
49	KC2	S	315	28	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	L	320	-	-	10/17/93/115	-
39	CLA	a	807	1	-	13/39/115/115	-
39	CLA	L	308	-	-	15/35/111/115	-
50	A1EB1	H	304	-	-	14/42/100/100	0/3/3/3
39	CLA	o	203	12	-	7/27/103/115	-
48	A86	3	305	-	-	12/34/90/90	0/3/3/3
48	A86	Q	308	-	-	8/34/90/90	0/3/3/3
39	CLA	K	312	-	-	17/39/115/115	-
51	A1ECV	T	317	-	3/3/17/24	6/19/117/117	-
39	CLA	J	310	-	-	8/27/103/115	-
39	CLA	U	208	-	-	5/17/93/115	-
43	DD6	O	304	-	-	1/26/80/80	0/3/3/3
39	CLA	9	309	-	-	3/10/86/115	-
39	CLA	G	318	-	-	13/20/96/115	-
46	LMG	0	324	49	-	13/21/41/70	0/1/1/1
49	KC2	0	317	31	-	3/15/71/71	-
49	KC2	y	313	-	-	8/15/71/71	-
50	A1EB1	7	306	-	-	10/42/100/100	0/3/3/3
39	CLA	R	315	-	-	7/18/94/115	-
48	A86	L	307	-	-	3/34/90/90	0/3/3/3
48	A86	M	302	-	-	8/34/90/90	0/3/3/3
39	CLA	Q	312	-	-	11/39/115/115	-
50	A1EB1	G	302	-	-	8/42/100/100	0/3/3/3
50	A1EB1	V	305	-	-	12/42/100/100	0/3/3/3
39	CLA	b	822	2	-	4/21/97/115	-
49	KC2	3	321	-	-	10/15/71/71	-
49	KC2	L	317	-	-	11/15/71/71	-
49	KC2	G	315	-	-	11/15/71/71	-
39	CLA	a	809	-	-	14/36/112/115	-
39	CLA	3	313	-	-	5/25/101/115	-
49	KC2	X	306	27	-	10/15/71/71	-
51	A1ECV	5	312	27	3/3/17/24	11/19/117/117	-
39	CLA	M	321	24	-	5/17/93/115	-
52	A1EB4	R	305	-	-	10/38/99/103	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	4	305	-	-	6/34/90/90	0/3/3/3
43	DD6	D	307	-	-	2/26/80/80	0/3/3/3
47	SQD	H	318	-	-	9/33/53/69	0/1/1/1
39	CLA	b	839	-	-	4/18/94/115	-
42	BCR	l	202	-	-	4/29/63/63	0/2/2/2
47	SQD	7	302	-	-	15/34/54/69	0/1/1/1
46	LMG	F	317	49	-	20/34/54/70	0/1/1/1
48	A86	K	301	-	-	6/34/90/90	0/3/3/3
39	CLA	l	204	-	-	11/39/115/115	-
52	A1EB4	W	306	-	-	10/37/98/103	0/3/3/3
48	A86	z	303	-	-	9/34/90/90	0/3/3/3
39	CLA	O	318	-	-	6/17/93/115	-
47	SQD	9	322	-	-	10/31/51/69	0/1/1/1
48	A86	S	305	-	-	6/34/90/90	0/3/3/3
49	KC2	V	320	-	-	8/15/71/71	-
39	CLA	1	313	32	-	5/10/86/115	-
43	DD6	O	303	-	-	3/26/80/80	0/3/3/3
52	A1EB4	5	304	-	-	5/38/99/103	0/3/3/3
48	A86	J	303	-	-	6/34/90/90	0/3/3/3
39	CLA	b	840	-	-	11/39/115/115	-
39	CLA	S	320	-	-	15/39/115/115	-
49	KC2	8	314	-	-	10/15/71/71	-
52	A1EB4	X	305	-	-	10/38/99/103	0/3/3/3
39	CLA	7	318	28	-	5/17/93/115	-
39	CLA	G	310	-	-	12/39/115/115	-
42	BCR	l	207	-	-	2/29/63/63	0/2/2/2
39	CLA	E	318	17	-	10/17/93/115	-
39	CLA	E	309	-	-	7/25/101/115	-
47	SQD	F	319	-	-	13/32/52/69	0/1/1/1
47	SQD	W	301	-	-	8/22/42/69	0/1/1/1
43	DD6	E	303	-	-	1/26/80/80	0/3/3/3
39	CLA	F	314	18	-	10/27/103/115	-
49	KC2	Y	309	-	-	8/15/71/71	-
39	CLA	6	311	-	-	1/8/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	7	312	-	-	4/34/90/90	0/3/3/3
39	CLA	U	211	-	-	9/33/109/115	-
48	A86	E	304	-	-	2/34/90/90	0/3/3/3
48	A86	R	317	-	-	3/34/90/90	0/3/3/3
48	A86	9	301	-	-	9/34/90/90	0/3/3/3
49	KC2	3	315	-	-	8/15/71/71	-
39	CLA	U	213	-	-	6/10/86/115	-
52	A1EB4	T	304	-	-	9/36/97/103	0/3/3/3
40	PQN	a	839	-	-	7/23/43/43	0/2/2/2
39	CLA	z	306	-	-	4/10/86/115	-
43	DD6	B	202	-	-	3/26/80/80	0/3/3/3
43	DD6	3	304	-	-	3/26/80/80	0/3/3/3
39	CLA	D	318	-	-	16/39/115/115	-
39	CLA	a	805	-	-	11/39/115/115	-
48	A86	R	302	-	-	11/34/90/90	0/3/3/3
43	DD6	G	306	-	-	4/26/80/80	0/3/3/3
49	KC2	8	317	-	-	8/15/71/71	-
39	CLA	z	318	-	-	6/10/86/115	-
39	CLA	Z	313	-	-	6/10/86/115	-
50	A1EB1	T	302	-	-	14/42/100/100	0/3/3/3
43	DD6	A	302	-	-	0/26/80/80	0/3/3/3
43	DD6	S	306	-	-	4/26/80/80	0/3/3/3
52	A1EB4	M	305	-	-	9/39/100/103	0/3/3/3
39	CLA	U	214	-	-	4/17/93/115	-
50	A1EB1	z	302	-	-	13/42/100/100	0/3/3/3
39	CLA	a	813	1	-	4/21/97/115	-
39	CLA	b	830	-	-	13/39/115/115	-
39	CLA	5	315	-	-	5/18/94/115	-
43	DD6	A	304	-	-	3/26/80/80	0/3/3/3
39	CLA	Q	321	-	-	6/25/101/115	-
39	CLA	8	313	-	-	5/10/86/115	-
39	CLA	a	814	-	-	15/35/111/115	-
49	KC2	K	313	22	-	9/15/71/71	-
49	KC2	C	312	-	-	10/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	9	306	-	-	6/34/90/90	0/3/3/3
48	A86	6	309	-	-	13/34/90/90	0/3/3/3
39	CLA	b	818	-	-	11/27/103/115	-
48	A86	y	306	-	-	6/34/90/90	0/3/3/3
42	BCR	f	801	-	-	4/29/63/63	0/2/2/2
41	LHG	a	840	-	-	26/53/53/53	-
39	CLA	x	314	-	-	7/10/86/115	-
51	A1ECV	E	311	-	3/3/17/24	8/19/117/117	-
39	CLA	M	315	-	-	4/10/86/115	-
39	CLA	J	317	-	-	4/12/88/115	-
41	LHG	X	301	-	-	25/45/45/53	-
43	DD6	W	305	-	-	1/26/80/80	0/3/3/3
43	DD6	j	102	-	-	6/26/80/80	0/3/3/3
43	DD6	F	305	-	-	1/26/80/80	0/3/3/3
50	A1EB1	G	307	-	-	17/42/100/100	0/3/3/3
49	KC2	I	312	46	-	7/14/70/71	-
47	SQD	D	304	-	-	8/33/53/69	0/1/1/1
39	CLA	H	310	-	-	7/30/106/115	-
39	CLA	H	312	20	-	19/39/115/115	-
39	CLA	V	316	-	-	6/21/97/115	-
39	CLA	I	311	-	-	15/39/115/115	-
46	LMG	A	316	-	-	13/24/44/70	0/1/1/1
48	A86	Q	305	-	-	16/34/90/90	0/3/3/3
39	CLA	C	310	-	-	18/39/115/115	-
39	CLA	b	817	-	-	7/32/108/115	-
39	CLA	K	309	-	-	9/36/112/115	-
39	CLA	x	318	-	-	8/10/86/115	-
39	CLA	b	820	-	-	16/33/109/115	-
42	BCR	a	845	-	-	4/29/63/63	0/2/2/2
49	KC2	4	318	28	-	9/15/71/71	-
49	KC2	F	307	-	-	9/15/71/71	-
49	KC2	x	312	-	-	8/15/71/71	-
50	A1EB1	L	303	-	-	15/42/100/100	0/3/3/3
39	CLA	b	809	-	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	P	302	-	-	12/34/90/90	0/3/3/3
50	A1EB1	6	308	-	-	15/42/100/100	0/3/3/3
39	CLA	k	202	-	-	13/27/103/115	-
39	CLA	J	309	-	-	17/39/115/115	-
48	A86	L	306	-	-	12/34/90/90	0/3/3/3
39	CLA	b	810	-	-	15/39/115/115	-
39	CLA	b	811	-	-	10/39/115/115	-
51	A1ECV	9	314	-	3/3/17/24	9/19/117/117	-
39	CLA	2	308	-	-	11/17/93/115	-
39	CLA	i	103	-	-	17/39/115/115	-
49	KC2	4	320	-	-	10/15/71/71	-
51	A1ECV	R	313	-	3/3/17/24	9/19/117/117	-
39	CLA	b	815	-	-	14/39/115/115	-
39	CLA	W	318	-	-	7/23/99/115	-
50	A1EB1	2	304	-	-	16/42/100/100	0/3/3/3
39	CLA	O	314	-	-	7/27/103/115	-
39	CLA	M	308	-	-	12/39/115/115	-
39	CLA	f	803	-	-	11/27/103/115	-
52	A1EB4	P	318	-	-	9/35/96/103	0/3/3/3
50	A1EB1	3	310	-	-	11/42/100/100	0/3/3/3
49	KC2	9	311	-	-	7/15/71/71	-
49	KC2	3	318	-	-	6/15/71/71	-
39	CLA	O	311	-	-	2/12/88/115	-
42	BCR	a	844	-	-	0/29/63/63	0/2/2/2
39	CLA	7	316	-	-	10/39/115/115	-
39	CLA	A	314	-	-	17/39/115/115	-
39	CLA	K	311	-	-	14/39/115/115	-
39	CLA	b	807	-	-	14/39/115/115	-
39	CLA	6	312	-	-	8/20/96/115	-
48	A86	M	306	-	-	2/34/90/90	0/3/3/3
49	KC2	8	320	-	-	8/15/71/71	-
48	A86	0	301	-	-	4/34/90/90	0/3/3/3
39	CLA	b	825	-	-	14/39/115/115	-
50	A1EB1	y	301	-	-	11/42/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	Y	303	-	-	4/10/86/115	-
43	DD6	C	301	-	-	3/26/80/80	0/3/3/3
39	CLA	a	823	-	-	10/39/115/115	-
39	CLA	F	308	-	-	16/39/115/115	-
48	A86	k	206	-	-	5/34/90/90	0/3/3/3
39	CLA	A	311	-	-	13/39/115/115	-
39	CLA	y	315	-	-	8/10/86/115	-
39	CLA	a	829	-	-	7/29/105/115	-
49	KC2	V	314	-	-	9/15/71/71	-
49	KC2	5	313	46	-	7/14/70/71	-
39	CLA	Q	309	-	-	9/35/111/115	-
39	CLA	W	313	-	-	10/39/115/115	-
39	CLA	a	811	-	-	17/39/115/115	-
39	CLA	Y	304	-	-	9/17/93/115	-
39	CLA	o	205	-	-	12/24/100/115	-
39	CLA	8	315	-	-	3/13/89/115	-
49	KC2	S	317	-	-	7/15/71/71	-
49	KC2	X	315	-	-	8/15/71/71	-
39	CLA	S	311	-	-	13/39/115/115	-
39	CLA	5	310	27	-	6/21/97/115	-
43	DD6	T	303	-	-	1/26/80/80	0/3/3/3
39	CLA	L	311	23	-	10/24/100/115	-
39	CLA	P	316	-	-	7/23/99/115	-
39	CLA	a	838	-	-	12/39/115/115	-
39	CLA	B	209	-	-	12/29/105/115	-
39	CLA	C	311	-	-	17/39/115/115	-
49	KC2	0	316	-	-	4/15/71/71	-
49	KC2	M	313	-	-	6/15/71/71	-
50	A1EB1	2	306	-	-	16/42/100/100	0/3/3/3
39	CLA	J	307	21	-	10/20/96/115	-
39	CLA	H	316	-	-	10/17/93/115	-
39	CLA	2	309	-	-	6/17/93/115	-
51	A1ECV	0	321	48	2/2/17/24	10/19/117/117	-
51	A1ECV	z	316	-	3/3/17/24	6/19/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	DD6	a	846	-	-	5/26/80/80	0/3/3/3
39	CLA	a	812	-	-	4/15/91/115	-
39	CLA	9	320	-	-	4/10/86/115	-
39	CLA	B	206	-	-	6/12/88/115	-
49	KC2	3	317	-	-	7/15/71/71	-
39	CLA	a	816	-	-	15/39/115/115	-
39	CLA	y	307	-	-	4/10/86/115	-
48	A86	2	305	-	-	12/34/90/90	0/3/3/3
52	A1EB4	M	322	-	-	6/38/99/103	0/3/3/3
39	CLA	a	828	1	-	6/21/97/115	-
47	SQD	M	301	-	-	15/34/54/69	0/1/1/1
39	CLA	a	801	-	-	16/39/115/115	-
49	KC2	Q	313	46	-	9/14/70/71	-
39	CLA	7	321	-	-	6/10/86/115	-
39	CLA	a	817	1	-	6/15/91/115	-
39	CLA	Y	313	-	-	5/10/86/115	-
49	KC2	7	322	-	-	12/15/71/71	-
39	CLA	O	316	-	-	6/10/86/115	-
39	CLA	E	316	-	-	8/24/100/115	-
45	DGD	b	849	-	-	27/49/89/95	0/2/2/2
39	CLA	5	306	-	-	13/39/115/115	-
49	KC2	7	319	-	-	7/15/71/71	-
39	CLA	Y	302	-	-	4/10/86/115	-
39	CLA	b	826	-	-	9/39/115/115	-
39	CLA	x	306	-	-	7/15/91/115	-
46	LMG	F	320	49	-	14/29/49/70	0/1/1/1
39	CLA	K	307	-	-	14/39/115/115	-
49	KC2	4	324	-	-	8/15/71/71	-
39	CLA	4	314	-	-	10/39/115/115	-
41	LHG	a	841	39	-	13/31/31/53	-
48	A86	8	323	-	-	4/34/90/90	0/3/3/3
50	A1EB1	U	203	-	-	9/42/100/100	0/3/3/3
43	DD6	I	306	-	-	2/26/80/80	0/3/3/3
43	DD6	D	306	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	T	318	-	-	9/18/94/115	-
39	CLA	Q	311	-	-	5/17/93/115	-
43	DD6	F	303	-	-	0/26/80/80	0/3/3/3
39	CLA	x	308	-	-	2/10/86/115	-
49	KC2	4	317	-	-	5/15/71/71	-
48	A86	O	302	-	-	2/34/90/90	0/3/3/3
46	LMG	W	320	-	-	15/28/48/70	0/1/1/1
40	PQN	b	843	-	-	3/23/43/43	0/2/2/2
48	A86	x	305	-	-	8/34/90/90	0/3/3/3
39	CLA	b	819	-	-	11/32/108/115	-
39	CLA	b	833	-	-	15/39/115/115	-
39	CLA	V	311	-	-	17/39/115/115	-
39	CLA	0	311	-	-	11/27/103/115	-
39	CLA	8	318	-	-	5/10/86/115	-
39	CLA	2	310	-	-	6/12/88/115	-
39	CLA	U	215	-	-	7/10/86/115	-
48	A86	9	304	-	-	9/34/90/90	0/3/3/3
39	CLA	b	829	-	-	8/39/115/115	-
43	DD6	H	305	-	-	2/26/80/80	0/3/3/3
49	KC2	T	315	29	-	7/15/71/71	-
49	KC2	S	314	-	-	6/15/71/71	-
42	BCR	b	846	-	-	3/29/63/63	0/2/2/2
39	CLA	Q	314	-	-	6/26/102/115	-
49	KC2	X	318	-	-	7/15/71/71	-
51	A1ECV	Q	316	26	3/3/17/24	9/19/117/117	-
39	CLA	7	325	-	-	9/21/97/115	-
39	CLA	E	315	-	-	12/17/93/115	-
42	BCR	b	845	-	-	1/29/63/63	0/2/2/2
46	LMG	P	317	49	-	18/34/54/70	0/1/1/1
39	CLA	S	316	-	-	6/10/86/115	-
39	CLA	b	805	-	-	9/39/115/115	-
39	CLA	a	830	-	-	20/39/115/115	-
50	A1EB1	7	305	-	-	16/42/100/100	0/3/3/3
50	A1EB1	y	302	-	-	10/42/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	2	318	-	-	5/10/86/115	-
39	CLA	k	201	-	-	7/24/100/115	-
39	CLA	M	312	-	-	14/39/115/115	-
48	A86	2	301	-	-	3/34/90/90	0/3/3/3
43	DD6	E	305	-	-	3/26/80/80	0/3/3/3
39	CLA	b	802	-	-	6/39/115/115	-
39	CLA	a	806	-	-	17/39/115/115	-
42	BCR	a	843	-	-	0/29/63/63	0/2/2/2
39	CLA	7	314	-	-	13/29/105/115	-
50	A1EB1	9	302	-	-	18/42/100/100	0/3/3/3
42	BCR	j	103	-	-	4/29/63/63	0/2/2/2
43	DD6	x	304	-	-	0/26/80/80	0/3/3/3
49	KC2	z	315	-	-	10/15/71/71	-
43	DD6	4	307	-	-	1/26/80/80	0/3/3/3
39	CLA	C	309	-	-	13/17/93/115	-
47	SQD	D	320	39	-	11/32/52/69	0/1/1/1
50	A1EB1	7	303	-	-	17/42/100/100	0/3/3/3
49	KC2	9	318	-	-	10/15/71/71	-
39	CLA	R	307	-	-	12/39/115/115	-
39	CLA	F	312	-	-	8/39/115/115	-
39	CLA	a	820	-	-	10/23/99/115	-
49	KC2	C	313	-	-	11/15/71/71	-
39	CLA	R	311	27	-	5/21/97/115	-
39	CLA	W	311	-	-	15/39/115/115	-
39	CLA	8	310	-	-	8/15/91/115	-
48	A86	G	305	-	-	7/34/90/90	0/3/3/3
39	CLA	E	306	17	-	6/20/96/115	-
39	CLA	Y	314	-	-	8/10/86/115	-
39	CLA	x	309	-	-	4/10/86/115	-
39	CLA	F	309	-	-	6/24/100/115	-
39	CLA	A	308	-	-	9/23/99/115	-
39	CLA	Z	307	-	-	0/10/86/115	-
39	CLA	1	320	-	-	6/10/86/115	-
51	A1ECV	S	318	-	3/3/17/24	6/19/117/117	-
51	A1ECV	y	311	-	3/3/17/24	10/19/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	0	312	31	-	8/25/101/115	-
39	CLA	0	320	-	-	8/15/91/115	-
39	CLA	a	821	-	-	13/27/103/115	-
49	KC2	x	315	-	-	10/15/71/71	-
39	CLA	7	315	-	-	6/21/97/115	-
49	KC2	J	315	-	-	10/15/71/71	-
50	A1EB1	4	303	-	-	12/42/100/100	0/3/3/3
43	DD6	Z	302	-	-	2/26/80/80	0/3/3/3
39	CLA	P	309	-	-	14/39/115/115	-
48	A86	L	305	-	-	2/34/90/90	0/3/3/3
50	A1EB1	0	307	-	-	11/42/100/100	0/3/3/3
50	A1EB1	4	302	-	-	11/42/100/100	0/3/3/3
48	A86	U	202	-	-	4/34/90/90	0/3/3/3
45	DGD	C	314	-	-	15/29/69/95	0/2/2/2
51	A1ECV	G	316	-	3/3/17/24	11/19/117/117	-
39	CLA	b	812	-	-	10/39/115/115	-
50	A1EB1	x	301	-	-	14/42/100/100	0/3/3/3
39	CLA	2	319	-	-	13/17/93/115	-
50	A1EB1	4	304	-	-	9/42/100/100	0/3/3/3
39	CLA	S	313	-	-	7/39/115/115	-
47	SQD	F	318	-	-	17/37/57/69	0/1/1/1
39	CLA	O	308	-	-	4/4/80/115	-
39	CLA	K	306	-	-	13/35/111/115	-
39	CLA	Y	305	-	-	2/10/86/115	-
39	CLA	Q	317	-	-	7/17/93/115	-
39	CLA	U	201	-	-	11/17/93/115	-
43	DD6	J	304	-	-	3/26/80/80	0/3/3/3
39	CLA	E	313	-	-	13/39/115/115	-
49	KC2	I	303	-	-	7/15/71/71	-
39	CLA	A	305	13	-	6/20/96/115	-
49	KC2	R	314	46	-	7/14/70/71	-
50	A1EB1	U	205	-	-	11/42/100/100	0/3/3/3
39	CLA	I	314	-	-	14/39/115/115	-
50	A1EB1	Q	323	-	-	9/42/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	O	309	-	-	6/15/91/115	-
39	CLA	D	314	-	-	11/39/115/115	-
39	CLA	D	315	-	-	9/39/115/115	-
49	KC2	x	313	-	-	6/15/71/71	-
51	A1ECV	Z	308	-	3/3/17/24	11/19/117/117	-
49	KC2	5	311	-	-	6/15/71/71	-
51	A1ECV	M	316	-	3/3/17/24	8/19/117/117	-
48	A86	6	302	-	-	7/34/90/90	0/3/3/3
51	A1ECV	R	310	-	3/3/17/24	12/19/117/117	-
49	KC2	F	311	46	-	7/14/70/71	-
50	A1EB1	3	302	-	-	15/42/100/100	0/3/3/3
44	SF4	c	102	-	-	-	0/6/5/5
39	CLA	B	207	-	-	14/27/103/115	-
49	KC2	W	314	-	-	7/15/71/71	-
50	A1EB1	K	302	-	-	6/42/100/100	0/3/3/3
39	CLA	b	837	-	-	10/33/109/115	-
39	CLA	A	309	-	-	13/39/115/115	-
39	CLA	E	310	-	-	9/39/115/115	-
39	CLA	b	823	-	-	9/17/93/115	-
39	CLA	a	810	-	-	8/26/102/115	-
49	KC2	T	312	-	-	10/15/71/71	-
49	KC2	1	315	-	-	11/15/71/71	-
49	KC2	Z	311	-	-	10/15/71/71	-
42	BCR	i	102	-	-	4/29/63/63	0/2/2/2
43	DD6	2	303	-	-	2/26/80/80	0/3/3/3
42	BCR	b	844	-	-	6/29/63/63	0/2/2/2
49	KC2	M	311	46	-	7/14/70/71	-
48	A86	X	302	-	-	7/34/90/90	0/3/3/3
49	KC2	6	316	-	-	10/15/71/71	-
39	CLA	L	309	-	-	11/25/101/115	-
49	KC2	Q	318	26	-	6/15/71/71	-
48	A86	1	303	-	-	2/34/90/90	0/3/3/3
39	CLA	7	324	-	-	5/10/86/115	-
43	DD6	z	304	-	-	6/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LHG	j	104	-	-	22/34/34/53	-
48	A86	4	310	-	-	5/34/90/90	0/3/3/3
39	CLA	S	309	-	-	19/39/115/115	-
48	A86	4	328	-	-	15/34/90/90	0/3/3/3
50	A1EB1	V	307	-	-	12/42/100/100	0/3/3/3
51	A1ECV	Q	319	-	3/3/17/24	13/19/117/117	-
49	KC2	H	314	-	-	11/15/71/71	-
49	KC2	H	311	-	-	9/15/71/71	-
48	A86	0	304	-	-	12/34/90/90	0/3/3/3
43	DD6	7	310	-	-	4/26/80/80	0/3/3/3
48	A86	V	304	-	-	3/34/90/90	0/3/3/3
51	A1ECV	5	309	27	3/3/17/24	11/19/117/117	-
48	A86	0	308	51	-	2/34/90/90	0/3/3/3
49	KC2	8	316	-	-	11/15/71/71	-
39	CLA	a	819	-	-	11/20/96/115	-
50	A1EB1	z	301	-	-	12/34/90/100	0/3/3/3
39	CLA	C	307	-	-	12/39/115/115	-
42	BCR	b	848	-	-	1/29/63/63	0/2/2/2
39	CLA	b	806	-	-	15/39/115/115	-
39	CLA	0	313	-	-	12/27/103/115	-
48	A86	L	304	-	-	12/34/90/90	0/3/3/3
39	CLA	Y	310	-	-	4/10/86/115	-
46	LMG	I	302	-	-	23/37/57/70	0/1/1/1
48	A86	0	309	-	-	7/34/90/90	0/3/3/3
49	KC2	2	313	-	-	6/13/69/71	-
47	SQD	S	301	-	-	13/34/54/69	0/1/1/1
39	CLA	P	314	-	-	4/10/86/115	-
39	CLA	P	311	-	-	10/39/115/115	-
39	CLA	4	322	-	-	7/24/100/115	-
39	CLA	x	317	-	-	5/10/86/115	-
39	CLA	6	321	-	-	5/10/86/115	-
39	CLA	a	827	-	-	6/39/115/115	-
39	CLA	R	308	-	-	11/33/109/115	-
39	CLA	I	316	36	-	2/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	A1ECV	6	320	-	3/3/17/24	12/19/117/117	-
39	CLA	D	316	-	-	16/39/115/115	-
43	DD6	M	304	-	-	0/26/80/80	0/3/3/3
39	CLA	P	307	-	-	12/39/115/115	-
51	A1ECV	9	317	-	3/3/17/24	7/19/117/117	-
46	LMG	7	326	-	-	6/27/47/70	0/1/1/1
39	CLA	O	310	-	-	15/33/109/115	-
48	A86	7	311	-	-	3/34/90/90	0/3/3/3
39	CLA	Z	304	-	-	5/10/86/115	-
48	A86	Z	303	-	-	8/34/90/90	0/3/3/3
51	A1ECV	S	312	-	3/3/17/24	9/19/117/117	-
43	DD6	G	303	-	-	1/26/80/80	0/3/3/3
39	CLA	a	833	1	-	11/15/91/115	-
50	A1EB1	K	304	-	-	8/42/100/100	0/3/3/3
50	A1EB1	6	301	-	-	12/42/100/100	0/3/3/3
42	BCR	h	202	-	-	6/29/63/63	0/2/2/2
39	CLA	b	824	-	-	10/33/109/115	-
39	CLA	U	212	-	-	7/17/93/115	-
50	A1EB1	0	303	-	-	10/42/100/100	0/3/3/3
39	CLA	5	316	-	-	10/24/100/115	-
49	KC2	M	307	-	-	7/15/71/71	-
51	A1ECV	2	311	-	3/3/17/24	8/19/117/117	-
39	CLA	Q	320	-	-	8/18/94/115	-
51	A1ECV	x	316	-	3/3/17/24	8/19/117/117	-
43	DD6	X	304	-	-	0/26/80/80	0/3/3/3
39	CLA	2	315	-	-	5/10/86/115	-
48	A86	7	308	-	-	8/34/90/90	0/3/3/3
43	DD6	J	306	-	-	3/26/80/80	0/3/3/3
48	A86	4	306	-	-	8/34/90/90	0/3/3/3
39	CLA	G	309	-	-	15/29/105/115	-
50	A1EB1	S	303	-	-	14/42/100/100	0/3/3/3
39	CLA	V	309	-	-	11/39/115/115	-
43	DD6	I	307	-	-	1/26/80/80	0/3/3/3
49	KC2	V	308	27	-	8/15/71/71	-
39	CLA	a	802	-	-	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	H	308	-	-	7/33/109/115	-
48	A86	4	309	-	-	1/34/90/90	0/3/3/3
41	LHG	D	302	-	-	21/39/39/53	-
48	A86	8	302	-	-	8/34/90/90	0/3/3/3
48	A86	Q	302	-	-	7/34/90/90	0/3/3/3
51	A1ECV	X	313	-	3/3/17/24	7/19/117/117	-
46	LMG	4	326	49	-	23/41/61/70	0/1/1/1
50	A1EB1	T	307	-	-	6/42/100/100	0/3/3/3
39	CLA	b	831	-	-	7/21/97/115	-
39	CLA	a	815	-	-	16/39/115/115	-
39	CLA	z	317	-	-	7/12/88/115	-
39	CLA	6	315	-	-	1/10/86/115	-
39	CLA	E	307	-	-	21/39/115/115	-
39	CLA	a	822	-	-	9/39/115/115	-
48	A86	M	303	-	-	0/34/90/90	0/3/3/3
39	CLA	3	311	-	-	16/35/111/115	-
49	KC2	8	319	34	-	12/15/71/71	-
46	LMG	D	322	-	-	14/32/52/70	0/1/1/1
52	A1EB4	P	305	-	-	10/37/98/103	0/3/3/3
50	A1EB1	6	306	-	-	5/34/90/100	0/3/3/3
42	BCR	b	847	-	-	4/29/63/63	0/2/2/2
39	CLA	3	319	-	-	6/10/86/115	-
42	BCR	k	204	-	-	2/29/63/63	0/2/2/2
49	KC2	K	310	-	-	7/15/71/71	-
39	CLA	Y	311	-	-	6/10/86/115	-
39	CLA	A	307	-	-	8/33/109/115	-
46	LMG	S	321	-	-	11/27/47/70	0/1/1/1
39	CLA	E	317	-	-	8/24/100/115	-
50	A1EB1	6	304	-	-	11/39/97/100	0/3/3/3
42	BCR	b	850	-	-	6/29/63/63	0/2/2/2
43	DD6	D	303	-	-	0/26/80/80	0/3/3/3
49	KC2	R	312	-	-	8/15/71/71	-
39	CLA	b	834	-	-	7/31/107/115	-
39	CLA	z	314	-	-	5/10/86/115	-
42	BCR	f	804	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	F	316	-	-	10/23/99/115	-
48	A86	0	306	-	-	2/34/90/90	0/3/3/3
51	A1ECV	Y	306	-	3/3/17/24	9/19/117/117	-
39	CLA	B	205	-	-	5/12/88/115	-
48	A86	3	307	-	-	6/34/90/90	0/3/3/3
48	A86	D	305	-	-	8/34/90/90	0/3/3/3
48	A86	O	307	-	-	9/34/90/90	0/3/3/3
39	CLA	9	310	-	-	3/10/86/115	-
39	CLA	C	306	-	-	8/39/115/115	-
39	CLA	9	312	35	-	5/12/88/115	-
39	CLA	y	308	-	-	9/15/91/115	-
39	CLA	z	307	-	-	3/12/88/115	-
48	A86	1	302	-	-	5/34/90/90	0/3/3/3
49	KC2	G	311	19	-	9/15/71/71	-
39	CLA	8	322	-	-	4/10/86/115	-
49	KC2	T	314	-	-	7/15/71/71	-
48	A86	F	301	-	-	4/34/90/90	0/3/3/3
39	CLA	0	323	-	-	11/17/93/115	-
43	DD6	o	204	-	-	2/26/80/80	0/3/3/3
39	CLA	b	821	-	-	11/39/115/115	-
39	CLA	V	313	27	-	8/39/115/115	-
48	A86	C	303	-	-	6/34/90/90	0/3/3/3
39	CLA	W	310	-	-	16/39/115/115	-
48	A86	L	302	-	-	13/34/90/90	0/3/3/3
48	A86	T	305	-	-	6/34/90/90	0/3/3/3
50	A1EB1	G	308	-	-	10/42/100/100	0/3/3/3
39	CLA	6	318	-	-	8/10/86/115	-
48	A86	2	302	-	-	5/34/90/90	0/3/3/3
39	CLA	F	306	-	-	6/17/93/115	-
39	CLA	b	808	-	-	7/15/91/115	-
39	CLA	b	835	-	-	16/39/115/115	-
50	A1EB1	8	304	-	-	10/42/100/100	0/3/3/3
49	KC2	T	316	-	-	7/15/71/71	-
39	CLA	l	205	-	-	2/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	V	301	-	-	2/34/90/90	0/3/3/3
39	CLA	o	206	-	-	14/31/107/115	-
39	CLA	E	319	17	-	13/20/96/115	-
39	CLA	4	312	-	-	18/39/115/115	-
51	A1ECV	V	317	-	3/3/17/24	11/19/117/117	-
39	CLA	3	312	-	-	22/39/115/115	-
42	BCR	a	842	-	-	4/29/63/63	0/2/2/2

All (5834) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	M	322	A1EB4	C13-C11	-17.07	1.25	1.43
52	P	319	A1EB4	C13-C11	-17.07	1.25	1.43
52	P	318	A1EB4	C13-C11	-16.98	1.25	1.43
52	W	321	A1EB4	C13-C11	-16.67	1.25	1.43
52	T	304	A1EB4	C13-C11	-16.45	1.25	1.43
52	W	306	A1EB4	C13-C11	-16.36	1.25	1.43
52	P	305	A1EB4	C13-C11	-16.33	1.25	1.43
52	X	305	A1EB4	C13-C11	-16.31	1.26	1.43
52	R	305	A1EB4	C13-C11	-16.28	1.26	1.43
52	5	304	A1EB4	C13-C11	-16.18	1.26	1.43
52	M	305	A1EB4	C13-C11	-15.97	1.26	1.43
43	D	306	DD6	C21-C20	10.09	1.67	1.51
51	S	312	A1ECV	C3C-C4C	9.96	1.49	1.41
51	4	315	A1ECV	C3C-C4C	9.66	1.49	1.41
51	7	317	A1ECV	C3C-C4C	9.55	1.49	1.41
51	0	321	A1ECV	C3C-C4C	9.36	1.48	1.41
51	9	317	A1ECV	C3C-C4C	9.14	1.48	1.41
51	V	317	A1ECV	C3C-C4C	9.08	1.48	1.41
51	Q	319	A1ECV	C3C-C4C	9.08	1.48	1.41
43	Q	303	DD6	C29-C27	-9.03	1.25	1.42
43	F	305	DD6	C29-C27	-8.96	1.25	1.42
43	x	303	DD6	C29-C27	-8.93	1.25	1.42
43	1	304	DD6	C29-C27	-8.87	1.25	1.42
51	y	317	A1ECV	C3C-C4C	8.84	1.48	1.41
43	z	304	DD6	C29-C27	-8.82	1.25	1.42
51	4	321	A1ECV	C3C-C4C	8.81	1.48	1.41
43	D	303	DD6	C29-C27	-8.79	1.25	1.42
43	D	306	DD6	C29-C27	-8.79	1.25	1.42
51	E	311	A1ECV	C3C-C4C	8.78	1.48	1.41
43	z	305	DD6	C29-C27	-8.78	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	7	310	DD6	C29-C27	-8.74	1.25	1.42
43	4	308	DD6	C29-C27	-8.73	1.25	1.42
51	6	320	A1ECV	C3C-C4C	8.73	1.48	1.41
43	3	301	DD6	C29-C27	-8.73	1.25	1.42
43	2	303	DD6	C29-C27	-8.72	1.25	1.42
43	P	304	DD6	C29-C27	-8.71	1.25	1.42
43	I	307	DD6	C29-C27	-8.71	1.25	1.42
43	Z	302	DD6	C29-C27	-8.70	1.25	1.42
51	L	318	A1ECV	C3C-C4C	8.70	1.48	1.41
43	a	846	DD6	C29-C27	-8.70	1.25	1.42
43	E	305	DD6	C29-C27	-8.69	1.25	1.42
43	o	204	DD6	C29-C27	-8.69	1.25	1.42
51	z	316	A1ECV	C3C-C4C	8.69	1.48	1.41
43	J	305	DD6	C29-C27	-8.68	1.25	1.42
51	X	313	A1ECV	C3C-C4C	8.67	1.48	1.41
51	R	313	A1ECV	C3C-C4C	8.67	1.48	1.41
43	U	204	DD6	C29-C27	-8.65	1.25	1.42
51	9	314	A1ECV	C3C-C4C	8.65	1.48	1.41
43	O	303	DD6	C29-C27	-8.65	1.25	1.42
43	y	304	DD6	C29-C27	-8.64	1.25	1.42
43	3	304	DD6	C29-C27	-8.64	1.25	1.42
43	S	306	DD6	C29-C27	-8.64	1.25	1.42
43	x	304	DD6	C29-C27	-8.63	1.25	1.42
43	H	305	DD6	C29-C27	-8.62	1.26	1.42
43	7	309	DD6	C29-C27	-8.62	1.26	1.42
43	G	306	DD6	C29-C27	-8.61	1.26	1.42
51	W	317	A1ECV	C3C-C4C	8.61	1.48	1.41
43	y	303	DD6	C29-C27	-8.60	1.26	1.42
43	Q	306	DD6	C29-C27	-8.59	1.26	1.42
43	O	305	DD6	C29-C27	-8.59	1.26	1.42
51	R	310	A1ECV	C3C-C4C	8.58	1.48	1.41
43	B	202	DD6	C29-C27	-8.57	1.26	1.42
51	P	315	A1ECV	C3C-C4C	8.57	1.48	1.41
51	x	316	A1ECV	C3C-C4C	8.55	1.48	1.41
43	J	306	DD6	C29-C27	-8.54	1.26	1.42
43	A	302	DD6	C29-C27	-8.52	1.26	1.42
43	D	307	DD6	C29-C27	-8.52	1.26	1.42
43	V	303	DD6	C29-C27	-8.52	1.26	1.42
43	4	307	DD6	C29-C27	-8.52	1.26	1.42
43	E	302	DD6	C29-C27	-8.51	1.26	1.42
43	j	102	DD6	C29-C27	-8.50	1.26	1.42
43	A	301	DD6	C29-C27	-8.49	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	H	303	DD6	C29-C27	-8.48	1.26	1.42
43	K	303	DD6	C29-C27	-8.48	1.26	1.42
43	A	304	DD6	C29-C27	-8.48	1.26	1.42
51	Y	312	A1ECV	C3C-C4C	8.48	1.48	1.41
43	I	305	DD6	C29-C27	-8.46	1.26	1.42
43	I	306	DD6	C29-C27	-8.45	1.26	1.42
43	T	303	DD6	C29-C27	-8.43	1.26	1.42
43	A	303	DD6	C29-C27	-8.42	1.26	1.42
43	O	304	DD6	C29-C27	-8.41	1.26	1.42
51	2	311	A1ECV	C3C-C4C	8.35	1.48	1.41
43	F	303	DD6	C29-C27	-8.34	1.26	1.42
51	7	323	A1ECV	C3C-C4C	8.34	1.48	1.41
43	E	303	DD6	C29-C27	-8.34	1.26	1.42
43	C	301	DD6	C29-C27	-8.32	1.26	1.42
43	G	303	DD6	C29-C27	-8.32	1.26	1.42
51	Z	314	A1ECV	C3C-C4C	8.30	1.48	1.41
51	X	310	A1ECV	C3C-C4C	8.27	1.48	1.41
51	5	312	A1ECV	C3C-C4C	8.27	1.48	1.41
43	F	305	DD6	C30-C31	-8.26	1.25	1.42
51	Q	316	A1ECV	C3C-C4C	8.26	1.48	1.41
43	J	304	DD6	C29-C27	-8.25	1.26	1.42
51	S	318	A1ECV	C3C-C4C	8.24	1.47	1.41
51	T	317	A1ECV	C3C-C4C	8.23	1.47	1.41
51	z	310	A1ECV	C3C-C4C	8.23	1.47	1.41
43	Q	303	DD6	C30-C31	-8.22	1.25	1.42
43	M	304	DD6	C29-C27	-8.21	1.26	1.42
51	1	318	A1ECV	C3C-C4C	8.20	1.47	1.41
51	G	316	A1ECV	C3C-C4C	8.15	1.47	1.41
43	W	305	DD6	C29-C27	-8.12	1.26	1.42
51	O	315	A1ECV	C3C-C4C	8.12	1.47	1.41
43	5	303	DD6	C29-C27	-8.12	1.26	1.42
51	5	309	A1ECV	C3C-C4C	8.12	1.47	1.41
43	X	304	DD6	C29-C27	-8.08	1.27	1.42
51	x	310	A1ECV	C3C-C4C	8.08	1.47	1.41
51	M	316	A1ECV	C3C-C4C	8.07	1.47	1.41
43	R	304	DD6	C29-C27	-8.04	1.27	1.42
43	1	304	DD6	C30-C31	-8.04	1.25	1.42
51	X	313	A1ECV	C4A-C3A	8.01	1.49	1.39
43	D	303	DD6	C30-C31	-8.00	1.25	1.42
51	L	318	A1ECV	C4A-C3A	7.97	1.49	1.39
51	y	311	A1ECV	C3C-C4C	7.96	1.47	1.41
43	Z	302	DD6	C30-C31	-7.96	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	O	303	DD6	C30-C31	-7.96	1.25	1.42
43	3	304	DD6	C30-C31	-7.95	1.25	1.42
51	Z	308	A1ECV	C3C-C4C	7.95	1.47	1.41
51	Y	306	A1ECV	C3C-C4C	7.93	1.47	1.41
43	J	306	DD6	C30-C31	-7.93	1.25	1.42
43	2	303	DD6	C30-C31	-7.92	1.25	1.42
43	7	310	DD6	C30-C31	-7.91	1.25	1.42
43	D	306	DD6	C30-C31	-7.88	1.25	1.42
43	A	304	DD6	C30-C31	-7.88	1.25	1.42
51	R	313	A1ECV	C4A-C3A	7.88	1.49	1.39
43	G	306	DD6	C30-C31	-7.86	1.25	1.42
43	B	202	DD6	C30-C31	-7.86	1.25	1.42
43	4	308	DD6	C30-C31	-7.84	1.26	1.42
43	P	304	DD6	C30-C31	-7.83	1.26	1.42
43	x	303	DD6	C30-C31	-7.82	1.26	1.42
43	Q	306	DD6	C30-C31	-7.80	1.26	1.42
43	J	305	DD6	C30-C31	-7.79	1.26	1.42
51	9	314	A1ECV	C4A-C3A	7.78	1.49	1.39
43	I	307	DD6	C30-C31	-7.78	1.26	1.42
51	6	320	A1ECV	C4A-C3A	7.77	1.49	1.39
43	S	306	DD6	C30-C31	-7.76	1.26	1.42
43	z	304	DD6	C30-C31	-7.76	1.26	1.42
43	4	307	DD6	C30-C31	-7.75	1.26	1.42
51	V	317	A1ECV	C4A-C3A	7.74	1.49	1.39
43	x	304	DD6	C30-C31	-7.74	1.26	1.42
43	z	305	DD6	C30-C31	-7.72	1.26	1.42
43	y	303	DD6	C30-C31	-7.71	1.26	1.42
43	a	846	DD6	C30-C31	-7.71	1.26	1.42
43	U	204	DD6	C30-C31	-7.71	1.26	1.42
43	A	303	DD6	C30-C31	-7.71	1.26	1.42
43	E	305	DD6	C30-C31	-7.70	1.26	1.42
51	P	315	A1ECV	C4A-C3A	7.69	1.48	1.39
43	H	303	DD6	C30-C31	-7.67	1.26	1.42
51	M	316	A1ECV	C4A-C3A	7.67	1.48	1.39
43	O	305	DD6	C30-C31	-7.67	1.26	1.42
51	7	323	A1ECV	C4A-C3A	7.66	1.48	1.39
40	a	839	PQN	C3-C2	7.66	1.49	1.35
43	3	301	DD6	C30-C31	-7.65	1.26	1.42
43	o	204	DD6	C30-C31	-7.64	1.26	1.42
43	y	304	DD6	C30-C31	-7.63	1.26	1.42
43	7	309	DD6	C30-C31	-7.63	1.26	1.42
43	D	307	DD6	C30-C31	-7.61	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	E	302	DD6	C30-C31	-7.61	1.26	1.42
51	Z	314	A1ECV	C4A-C3A	7.60	1.48	1.39
43	I	305	DD6	C30-C31	-7.60	1.26	1.42
43	O	304	DD6	C30-C31	-7.59	1.26	1.42
51	Y	312	A1ECV	C4A-C3A	7.58	1.48	1.39
43	A	301	DD6	C30-C31	-7.57	1.26	1.42
43	I	306	DD6	C30-C31	-7.57	1.26	1.42
43	T	303	DD6	C30-C31	-7.57	1.26	1.42
51	x	316	A1ECV	C4A-C3A	7.57	1.48	1.39
43	C	301	DD6	C21-C20	7.56	1.63	1.51
51	O	315	A1ECV	C4A-C3A	7.56	1.48	1.39
43	H	305	DD6	C30-C31	-7.56	1.26	1.42
43	C	301	DD6	C30-C31	-7.56	1.26	1.42
51	O	315	A1ECV	OBD-CAD	7.55	1.35	1.22
51	Y	306	A1ECV	OBD-CAD	7.54	1.35	1.22
43	V	303	DD6	C30-C31	-7.54	1.26	1.42
51	2	311	A1ECV	OBD-CAD	7.53	1.35	1.22
43	E	303	DD6	C30-C31	-7.53	1.26	1.42
51	R	310	A1ECV	OBD-CAD	7.53	1.35	1.22
51	Z	308	A1ECV	C4A-C3A	7.53	1.48	1.39
51	z	316	A1ECV	C4A-C3A	7.52	1.48	1.39
51	z	316	A1ECV	OBD-CAD	7.52	1.35	1.22
51	x	316	A1ECV	OBD-CAD	7.52	1.35	1.22
51	y	317	A1ECV	C4A-C3A	7.52	1.48	1.39
43	j	102	DD6	C30-C31	-7.52	1.26	1.42
51	4	321	A1ECV	C4A-C3A	7.51	1.48	1.39
43	J	304	DD6	C30-C31	-7.51	1.26	1.42
51	2	311	A1ECV	C4A-C3A	7.51	1.48	1.39
51	y	311	A1ECV	OBD-CAD	7.51	1.35	1.22
51	x	310	A1ECV	OBD-CAD	7.50	1.35	1.22
43	M	304	DD6	C30-C31	-7.50	1.26	1.42
43	F	303	DD6	C30-C31	-7.50	1.26	1.42
51	6	320	A1ECV	OBD-CAD	7.50	1.35	1.22
51	S	318	A1ECV	C4A-C3A	7.50	1.48	1.39
51	W	317	A1ECV	C4A-C3A	7.50	1.48	1.39
51	Z	308	A1ECV	OBD-CAD	7.49	1.35	1.22
51	5	312	A1ECV	OBD-CAD	7.49	1.35	1.22
51	4	315	A1ECV	OBD-CAD	7.49	1.35	1.22
51	z	310	A1ECV	OBD-CAD	7.49	1.35	1.22
51	7	317	A1ECV	C4A-C3A	7.48	1.48	1.39
51	y	317	A1ECV	OBD-CAD	7.48	1.35	1.22
51	E	311	A1ECV	C4A-C3A	7.48	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	A	302	DD6	C30-C31	-7.48	1.26	1.42
51	1	318	A1ECV	OBD-CAD	7.48	1.35	1.22
51	X	310	A1ECV	OBD-CAD	7.47	1.35	1.22
51	Y	312	A1ECV	OBD-CAD	7.47	1.35	1.22
43	K	303	DD6	C30-C31	-7.47	1.26	1.42
51	5	309	A1ECV	C4A-C3A	7.47	1.48	1.39
51	7	317	A1ECV	OBD-CAD	7.47	1.35	1.22
51	5	309	A1ECV	OBD-CAD	7.47	1.35	1.22
51	4	321	A1ECV	OBD-CAD	7.46	1.35	1.22
51	X	310	A1ECV	C4A-C3A	7.46	1.48	1.39
51	S	312	A1ECV	C4A-C3A	7.46	1.48	1.39
51	Y	306	A1ECV	C4A-C3A	7.45	1.48	1.39
43	X	304	DD6	C30-C31	-7.45	1.26	1.42
51	S	318	A1ECV	OBD-CAD	7.44	1.35	1.22
51	S	312	A1ECV	OBD-CAD	7.43	1.35	1.22
51	Q	319	A1ECV	C4A-C3A	7.43	1.48	1.39
43	G	303	DD6	C30-C31	-7.42	1.26	1.42
51	T	317	A1ECV	C4A-C3A	7.40	1.48	1.39
51	Z	314	A1ECV	OBD-CAD	7.40	1.35	1.22
51	T	317	A1ECV	OBD-CAD	7.39	1.35	1.22
51	z	310	A1ECV	C4A-C3A	7.38	1.48	1.39
51	Q	319	A1ECV	OBD-CAD	7.38	1.35	1.22
51	4	315	A1ECV	C4A-C3A	7.37	1.48	1.39
51	x	310	A1ECV	C4A-C3A	7.37	1.48	1.39
51	L	318	A1ECV	OBD-CAD	7.37	1.35	1.22
51	Q	316	A1ECV	C4A-C3A	7.34	1.48	1.39
51	9	317	A1ECV	C4A-C3A	7.33	1.48	1.39
43	5	303	DD6	C30-C31	-7.32	1.27	1.42
43	W	305	DD6	C30-C31	-7.31	1.27	1.42
51	Q	316	A1ECV	OBD-CAD	7.31	1.35	1.22
51	E	311	A1ECV	OBD-CAD	7.31	1.35	1.22
51	G	316	A1ECV	OBD-CAD	7.31	1.35	1.22
51	1	318	A1ECV	C4A-C3A	7.29	1.48	1.39
43	R	304	DD6	C30-C31	-7.29	1.27	1.42
51	9	317	A1ECV	OBD-CAD	7.29	1.35	1.22
51	5	312	A1ECV	C4A-C3A	7.28	1.48	1.39
51	0	321	A1ECV	C4A-C3A	7.28	1.48	1.39
51	G	316	A1ECV	C4A-C3A	7.20	1.48	1.39
51	R	310	A1ECV	C4A-C3A	7.19	1.48	1.39
51	y	311	A1ECV	C4A-C3A	7.18	1.48	1.39
40	b	843	PQN	C3-C2	7.17	1.48	1.35
51	0	321	A1ECV	OBD-CAD	7.15	1.34	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	7	323	A1ECV	OBD-CAD	7.14	1.34	1.22
51	W	317	A1ECV	OBD-CAD	7.09	1.34	1.22
51	M	316	A1ECV	OBD-CAD	7.09	1.34	1.22
51	9	314	A1ECV	OBD-CAD	7.09	1.34	1.22
51	V	317	A1ECV	OBD-CAD	7.08	1.34	1.22
51	P	315	A1ECV	OBD-CAD	7.03	1.34	1.22
51	X	313	A1ECV	OBD-CAD	7.03	1.34	1.22
51	R	313	A1ECV	OBD-CAD	6.98	1.34	1.22
51	E	311	A1ECV	C4D-ND	6.09	1.40	1.35
51	E	311	A1ECV	C1A-CHA	5.99	1.49	1.39
51	S	318	A1ECV	C4D-ND	5.88	1.40	1.35
51	Y	306	A1ECV	C1A-CHA	5.86	1.48	1.39
51	5	312	A1ECV	C4D-ND	5.85	1.40	1.35
51	Q	316	A1ECV	C4D-ND	5.82	1.40	1.35
51	z	310	A1ECV	C1A-CHA	5.81	1.48	1.39
51	Z	308	A1ECV	C1A-CHA	5.81	1.48	1.39
51	x	316	A1ECV	C1A-CHA	5.80	1.48	1.39
51	9	314	A1ECV	C1A-CHA	5.78	1.48	1.39
51	O	315	A1ECV	C1A-CHA	5.77	1.48	1.39
51	X	313	A1ECV	O2-CMC	5.77	1.46	1.33
51	T	317	A1ECV	C1A-CHA	5.76	1.48	1.39
51	R	313	A1ECV	O2-CMC	5.74	1.46	1.33
51	y	317	A1ECV	C1A-CHA	5.74	1.48	1.39
51	2	311	A1ECV	C1A-CHA	5.73	1.48	1.39
51	X	310	A1ECV	C1A-CHA	5.73	1.48	1.39
51	4	321	A1ECV	C4D-ND	5.72	1.40	1.35
51	T	317	A1ECV	C4D-ND	5.71	1.40	1.35
51	5	309	A1ECV	O2-CMC	5.71	1.46	1.33
51	V	317	A1ECV	C4D-ND	5.70	1.40	1.35
51	5	312	A1ECV	O2-CMC	5.70	1.46	1.33
51	X	313	A1ECV	C1A-CHA	5.70	1.48	1.39
51	G	316	A1ECV	C4D-ND	5.70	1.40	1.35
51	y	311	A1ECV	C1A-CHA	5.70	1.48	1.39
51	Z	308	A1ECV	O2-CMC	5.69	1.45	1.33
51	Y	306	A1ECV	O2-CMC	5.69	1.45	1.33
51	x	310	A1ECV	C1A-CHA	5.68	1.48	1.39
51	9	314	A1ECV	O2-CMC	5.68	1.45	1.33
51	7	323	A1ECV	O2-CMC	5.67	1.45	1.33
51	S	312	A1ECV	O2-CMC	5.67	1.45	1.33
51	R	313	A1ECV	C1A-CHA	5.67	1.48	1.39
51	4	315	A1ECV	O2-CMC	5.66	1.45	1.33
51	y	317	A1ECV	O2-CMC	5.66	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	2	311	A1ECV	O2-CMC	5.66	1.45	1.33
51	S	318	A1ECV	C1A-CHA	5.66	1.48	1.39
51	L	318	A1ECV	O2-CMC	5.65	1.45	1.33
51	z	310	A1ECV	O2-CMC	5.65	1.45	1.33
51	7	317	A1ECV	O2-CMC	5.65	1.45	1.33
51	M	316	A1ECV	C4D-ND	5.65	1.40	1.35
51	W	317	A1ECV	C4D-ND	5.65	1.40	1.35
51	4	321	A1ECV	O2-CMC	5.65	1.45	1.33
51	E	311	A1ECV	C2A-C1A	5.64	1.51	1.41
51	x	316	A1ECV	O2-CMC	5.64	1.45	1.33
51	M	316	A1ECV	O2-CMC	5.64	1.45	1.33
51	4	321	A1ECV	C1A-CHA	5.64	1.48	1.39
51	P	315	A1ECV	O2-CMC	5.63	1.45	1.33
51	x	310	A1ECV	O2-CMC	5.63	1.45	1.33
52	P	319	A1EB4	C21-C20	5.63	1.60	1.51
51	6	320	A1ECV	O2-CMC	5.63	1.45	1.33
51	G	316	A1ECV	O2-CMC	5.63	1.45	1.33
51	L	318	A1ECV	C1A-CHA	5.62	1.48	1.39
51	Q	319	A1ECV	O2-CMC	5.62	1.45	1.33
51	X	310	A1ECV	O2-CMC	5.62	1.45	1.33
51	y	311	A1ECV	O2-CMC	5.60	1.45	1.33
51	9	317	A1ECV	C4D-ND	5.60	1.40	1.35
51	R	310	A1ECV	C4D-ND	5.59	1.40	1.35
51	P	315	A1ECV	C1A-CHA	5.59	1.48	1.39
51	Y	312	A1ECV	C1A-CHA	5.59	1.48	1.39
51	4	315	A1ECV	C1A-CHA	5.58	1.48	1.39
52	M	322	A1EB4	C21-C20	5.58	1.60	1.51
51	S	318	A1ECV	O2-CMC	5.58	1.45	1.33
51	Q	316	A1ECV	O2-CMC	5.58	1.45	1.33
51	R	310	A1ECV	O2-CMC	5.57	1.45	1.33
51	5	309	A1ECV	C1A-CHA	5.57	1.48	1.39
51	O	315	A1ECV	O2-CMC	5.56	1.45	1.33
51	W	317	A1ECV	O2-CMC	5.56	1.45	1.33
51	Q	316	A1ECV	C1A-CHA	5.56	1.48	1.39
51	1	318	A1ECV	O2-CMC	5.55	1.45	1.33
51	O	315	A1ECV	C4D-ND	5.55	1.40	1.35
51	E	311	A1ECV	O2-CMC	5.55	1.45	1.33
51	z	316	A1ECV	C1A-CHA	5.54	1.48	1.39
51	Z	314	A1ECV	C1A-CHA	5.54	1.48	1.39
51	V	317	A1ECV	C1A-CHA	5.54	1.48	1.39
51	Z	314	A1ECV	C4D-ND	5.53	1.40	1.35
51	Q	319	A1ECV	C4D-ND	5.52	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S	312	A1ECV	C1A-CHA	5.52	1.48	1.39
51	0	321	A1ECV	C4D-ND	5.51	1.40	1.35
51	z	316	A1ECV	O2-CMC	5.51	1.45	1.33
51	Y	312	A1ECV	O2-CMC	5.51	1.45	1.33
51	7	317	A1ECV	C1A-CHA	5.50	1.48	1.39
51	Z	314	A1ECV	O2-CMC	5.49	1.45	1.33
51	6	320	A1ECV	C4D-ND	5.47	1.40	1.35
51	W	317	A1ECV	C2A-C1A	5.46	1.50	1.41
51	W	317	A1ECV	C1A-CHA	5.46	1.48	1.39
51	4	315	A1ECV	C4D-ND	5.46	1.40	1.35
51	0	321	A1ECV	C1A-CHA	5.46	1.48	1.39
51	5	312	A1ECV	C1A-CHA	5.45	1.48	1.39
51	7	317	A1ECV	C4D-ND	5.43	1.40	1.35
51	1	318	A1ECV	C1A-CHA	5.43	1.48	1.39
51	6	320	A1ECV	C1A-CHA	5.43	1.48	1.39
51	Q	316	A1ECV	C2A-C1A	5.43	1.50	1.41
49	0	319	KC2	CHD-C4C	5.43	1.49	1.38
51	5	309	A1ECV	C4D-ND	5.43	1.40	1.35
51	G	316	A1ECV	C1A-CHA	5.42	1.48	1.39
51	Q	319	A1ECV	C1A-CHA	5.42	1.48	1.39
49	O	317	KC2	CHD-C4C	5.41	1.49	1.38
51	S	312	A1ECV	C4D-ND	5.41	1.40	1.35
51	M	316	A1ECV	C1A-CHA	5.40	1.48	1.39
49	T	312	KC2	CHD-C4C	5.40	1.49	1.38
51	Y	312	A1ECV	C2A-C1A	5.40	1.50	1.41
51	9	317	A1ECV	C1A-CHA	5.38	1.48	1.39
51	7	323	A1ECV	C1A-CHA	5.38	1.48	1.39
51	5	312	A1ECV	C2A-C1A	5.37	1.50	1.41
51	V	317	A1ECV	O2-CMC	5.37	1.45	1.33
51	1	318	A1ECV	C2A-C1A	5.36	1.50	1.41
51	R	313	A1ECV	C4D-ND	5.36	1.40	1.35
51	Z	314	A1ECV	C2A-C1A	5.36	1.50	1.41
51	L	318	A1ECV	C4D-ND	5.35	1.40	1.35
51	Y	312	A1ECV	C4D-ND	5.35	1.40	1.35
51	S	318	A1ECV	C2A-C1A	5.34	1.50	1.41
51	Z	308	A1ECV	C2A-C1A	5.34	1.50	1.41
51	T	317	A1ECV	O2-CMC	5.34	1.45	1.33
49	Y	308	KC2	CHD-C4C	5.32	1.49	1.38
49	6	319	KC2	CHD-C4C	5.32	1.49	1.38
51	7	323	A1ECV	C4D-ND	5.32	1.40	1.35
51	0	321	A1ECV	O2-CMC	5.32	1.45	1.33
51	5	309	A1ECV	C2A-C1A	5.31	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	P	315	A1ECV	C4D-ND	5.31	1.39	1.35
48	0	308	A86	O4-C38	5.30	1.47	1.35
51	y	317	A1ECV	C2A-C1A	5.30	1.50	1.41
51	Y	306	A1ECV	C2A-C1A	5.29	1.50	1.41
51	2	311	A1ECV	C2A-C1A	5.29	1.50	1.41
49	9	318	KC2	CHD-C4C	5.29	1.49	1.38
51	R	310	A1ECV	C1A-CHA	5.29	1.48	1.39
51	7	317	A1ECV	C2A-C1A	5.29	1.50	1.41
51	9	314	A1ECV	C2A-C1A	5.28	1.50	1.41
51	x	310	A1ECV	C2A-C1A	5.26	1.50	1.41
51	z	316	A1ECV	C2A-C1A	5.26	1.50	1.41
49	8	319	KC2	CHD-C4C	5.26	1.49	1.38
49	W	315	KC2	CHD-C4C	5.26	1.49	1.38
49	L	312	KC2	CHD-C4C	5.26	1.49	1.38
51	x	310	A1ECV	C3B-C2B	5.26	1.48	1.37
49	7	322	KC2	CHD-C4C	5.26	1.49	1.38
51	R	310	A1ECV	C2A-C1A	5.26	1.50	1.41
49	1	314	KC2	CHD-C4C	5.25	1.49	1.38
51	4	321	A1ECV	O2D-CGD	5.25	1.46	1.33
49	1	315	KC2	CHD-C4C	5.24	1.49	1.38
49	S	315	KC2	CHD-C4C	5.24	1.49	1.38
49	2	317	KC2	CHD-C4C	5.24	1.49	1.38
51	6	320	A1ECV	O2D-CGD	5.24	1.46	1.33
51	V	317	A1ECV	O2D-CGD	5.24	1.46	1.33
51	x	316	A1ECV	C2A-C1A	5.24	1.50	1.41
51	4	315	A1ECV	C2A-C1A	5.24	1.50	1.41
49	8	316	KC2	CHD-C4C	5.23	1.49	1.38
51	X	310	A1ECV	C2A-C1A	5.23	1.50	1.41
49	L	321	KC2	CHD-C4C	5.23	1.49	1.38
49	J	315	KC2	CHD-C4C	5.23	1.49	1.38
51	O	315	A1ECV	C2A-C1A	5.22	1.50	1.41
51	Q	319	A1ECV	C2A-C1A	5.22	1.50	1.41
49	F	307	KC2	CHD-C4C	5.22	1.49	1.38
51	P	315	A1ECV	C2A-C1A	5.22	1.50	1.41
49	z	312	KC2	CHD-C4C	5.22	1.49	1.38
49	y	314	KC2	CHD-C4C	5.22	1.49	1.38
51	0	321	A1ECV	O2D-CGD	5.22	1.45	1.33
49	2	314	KC2	CHD-C4C	5.22	1.49	1.38
49	K	313	KC2	CHD-C4C	5.21	1.49	1.38
51	y	317	A1ECV	O2D-CGD	5.21	1.45	1.33
49	F	311	KC2	CHD-C4C	5.21	1.49	1.38
49	Z	310	KC2	CHD-C4C	5.21	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	7	323	A1ECV	C2A-C1A	5.21	1.50	1.41
49	I	312	KC2	CHD-C4C	5.21	1.49	1.38
51	S	318	A1ECV	O2D-CGD	5.20	1.45	1.33
49	X	306	KC2	CHD-C4C	5.20	1.49	1.38
49	L	315	KC2	CHD-C4C	5.20	1.49	1.38
51	M	316	A1ECV	O2D-CGD	5.20	1.45	1.33
51	X	313	A1ECV	O2D-CGD	5.20	1.45	1.33
49	Y	309	KC2	CHD-C4C	5.19	1.49	1.38
49	P	310	KC2	CHD-C4C	5.19	1.49	1.38
51	T	317	A1ECV	C2A-C1A	5.19	1.50	1.41
51	Q	316	A1ECV	O2D-CGD	5.19	1.45	1.33
51	R	313	A1ECV	O2D-CGD	5.19	1.45	1.33
51	W	317	A1ECV	O2D-CGD	5.19	1.45	1.33
51	x	316	A1ECV	O2D-CGD	5.19	1.45	1.33
51	9	314	A1ECV	C4D-ND	5.19	1.39	1.35
51	0	321	A1ECV	C2A-C1A	5.19	1.50	1.41
51	9	317	A1ECV	C2A-C1A	5.19	1.50	1.41
49	K	310	KC2	CHD-C4C	5.18	1.49	1.38
49	3	318	KC2	CHD-C4C	5.18	1.49	1.38
49	y	313	KC2	CHD-C4C	5.18	1.49	1.38
51	P	315	A1ECV	O2D-CGD	5.18	1.45	1.33
49	M	313	KC2	CHD-C4C	5.18	1.49	1.38
51	G	316	A1ECV	O2D-CGD	5.18	1.45	1.33
48	3	305	A86	O4-C38	5.17	1.46	1.35
49	3	315	KC2	CHD-C4C	5.17	1.49	1.38
49	9	311	KC2	CHD-C4C	5.17	1.49	1.38
49	M	311	KC2	CHD-C4C	5.17	1.49	1.38
49	A	313	KC2	CHD-C4C	5.17	1.49	1.38
50	V	302	A1EB1	O4-C38	5.17	1.46	1.35
51	S	312	A1ECV	O2D-CGD	5.17	1.45	1.33
49	C	312	KC2	CHD-C4C	5.17	1.49	1.38
49	G	313	KC2	CHD-C4C	5.17	1.49	1.38
51	V	317	A1ECV	C2A-C1A	5.17	1.50	1.41
49	H	311	KC2	CHD-C4C	5.17	1.49	1.38
49	W	312	KC2	CHD-C4C	5.17	1.49	1.38
51	4	315	A1ECV	O2D-CGD	5.17	1.45	1.33
49	4	318	KC2	CHD-C4C	5.17	1.49	1.38
49	L	317	KC2	CHD-C4C	5.17	1.49	1.38
49	V	312	KC2	CHD-C4C	5.17	1.49	1.38
49	z	315	KC2	CHD-C4C	5.16	1.49	1.38
51	L	318	A1ECV	O2D-CGD	5.16	1.45	1.33
49	P	313	KC2	CHD-C4C	5.16	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	V	308	KC2	CHD-C4C	5.16	1.49	1.38
49	V	315	KC2	CHD-C4C	5.16	1.49	1.38
49	8	317	KC2	CHD-C4C	5.16	1.49	1.38
49	z	313	KC2	CHA-C4D	-5.16	1.40	1.50
49	P	306	KC2	CHD-C4C	5.16	1.49	1.38
49	P	312	KC2	CHD-C4C	5.16	1.49	1.38
49	0	314	KC2	CHD-C4C	5.16	1.49	1.38
49	x	315	KC2	CHD-C4C	5.16	1.49	1.38
49	1	312	KC2	CHD-C4C	5.16	1.49	1.38
49	6	317	KC2	CHD-C4C	5.16	1.49	1.38
51	z	310	A1ECV	O2D-CGD	5.16	1.45	1.33
49	9	316	KC2	CHD-C4C	5.16	1.49	1.38
49	x	313	KC2	CHD-C4C	5.16	1.49	1.38
49	4	317	KC2	CHD-C4C	5.16	1.49	1.38
51	G	316	A1ECV	C2A-C1A	5.15	1.50	1.41
51	M	316	A1ECV	C2A-C1A	5.15	1.50	1.41
51	X	313	A1ECV	C2A-C1A	5.15	1.50	1.41
51	y	311	A1ECV	O2D-CGD	5.15	1.45	1.33
49	R	306	KC2	CHD-C4C	5.15	1.49	1.38
49	A	310	KC2	CHD-C4C	5.15	1.49	1.38
51	X	310	A1ECV	C4D-ND	5.15	1.39	1.35
49	L	314	KC2	CHD-C4C	5.15	1.49	1.38
51	9	314	A1ECV	C2C-C1C	5.15	1.50	1.41
49	H	314	KC2	CHD-C4C	5.15	1.49	1.38
51	x	310	A1ECV	O2D-CGD	5.15	1.45	1.33
51	5	312	A1ECV	O2D-CGD	5.14	1.45	1.33
49	V	318	KC2	CHD-C4C	5.14	1.49	1.38
51	9	317	A1ECV	O2D-CGD	5.14	1.45	1.33
49	R	314	KC2	CHD-C4C	5.14	1.49	1.38
49	R	318	KC2	CHD-C4C	5.14	1.49	1.38
49	Z	311	KC2	CHD-C4C	5.14	1.49	1.38
51	2	311	A1ECV	O2D-CGD	5.14	1.45	1.33
49	8	320	KC2	CHD-C4C	5.14	1.49	1.38
49	S	317	KC2	CHD-C4C	5.13	1.49	1.38
51	9	314	A1ECV	O2D-CGD	5.13	1.45	1.33
51	X	313	A1ECV	C4D-ND	5.13	1.39	1.35
51	4	321	A1ECV	C2A-C1A	5.13	1.50	1.41
49	B	208	KC2	CHD-C4C	5.13	1.48	1.38
51	7	317	A1ECV	O2D-CGD	5.13	1.45	1.33
51	O	315	A1ECV	O2D-CGD	5.13	1.45	1.33
51	Q	316	A1ECV	C2C-C1C	5.13	1.50	1.41
51	9	317	A1ECV	O2-CMC	5.13	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	J	304	DD6	C26-C27	-5.13	1.26	1.37
49	3	321	KC2	CHD-C4C	5.13	1.48	1.38
50	T	302	A1EB1	O4-C38	5.13	1.46	1.35
51	Z	314	A1ECV	O2D-CGD	5.13	1.45	1.33
49	S	314	KC2	CHD-C4C	5.13	1.48	1.38
49	7	320	KC2	CHD-C4C	5.12	1.48	1.38
49	W	314	KC2	CHD-C4C	5.12	1.48	1.38
51	y	311	A1ECV	C2A-C1A	5.12	1.50	1.41
49	M	314	KC2	CHD-C4C	5.12	1.48	1.38
51	z	316	A1ECV	C4D-ND	5.12	1.39	1.35
50	7	303	A1EB1	O4-C38	5.12	1.46	1.35
49	T	315	KC2	CHD-C4C	5.12	1.48	1.38
49	0	317	KC2	CHD-C4C	5.12	1.48	1.38
49	X	312	KC2	CHD-C4C	5.12	1.48	1.38
49	2	313	KC2	CHD-C4C	5.12	1.48	1.38
49	G	311	KC2	CHD-C4C	5.12	1.48	1.38
51	1	318	A1ECV	C4D-ND	5.12	1.39	1.35
49	X	314	KC2	CHD-C4C	5.12	1.48	1.38
51	7	323	A1ECV	O2D-CGD	5.12	1.45	1.33
51	R	313	A1ECV	C2A-C1A	5.11	1.50	1.41
49	x	312	KC2	CHD-C4C	5.11	1.48	1.38
49	X	315	KC2	CHD-C4C	5.11	1.48	1.38
51	Z	308	A1ECV	O2D-CGD	5.11	1.45	1.33
51	S	312	A1ECV	C2A-C1A	5.11	1.50	1.41
50	G	302	A1EB1	O4-C38	5.11	1.46	1.35
51	Y	312	A1ECV	O2D-CGD	5.11	1.45	1.33
49	V	314	KC2	CHD-C4C	5.11	1.48	1.38
51	Y	306	A1ECV	O2D-CGD	5.11	1.45	1.33
51	x	310	A1ECV	C2C-C1C	5.10	1.50	1.41
49	T	316	KC2	CHD-C4C	5.10	1.48	1.38
49	X	318	KC2	CHD-C4C	5.10	1.48	1.38
49	7	319	KC2	CHD-C4C	5.10	1.48	1.38
49	y	316	KC2	CHD-C4C	5.10	1.48	1.38
49	6	314	KC2	CHD-C4C	5.10	1.48	1.38
49	5	314	KC2	CHD-C4C	5.10	1.48	1.38
50	z	302	A1EB1	O4-C38	5.10	1.46	1.35
48	3	308	A86	O4-C38	5.10	1.46	1.35
49	5	311	KC2	CHD-C4C	5.09	1.48	1.38
49	C	313	KC2	CHD-C4C	5.09	1.48	1.38
49	P	320	KC2	CHD-C4C	5.09	1.48	1.38
49	5	313	KC2	CHD-C4C	5.09	1.48	1.38
48	7	312	A86	O4-C38	5.09	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	X	310	A1ECV	O2D-CGD	5.09	1.45	1.33
51	z	310	A1ECV	C4D-ND	5.09	1.39	1.35
50	6	304	A1EB1	O4-C38	5.08	1.46	1.35
49	Q	318	KC2	CHD-C4C	5.08	1.48	1.38
51	Z	308	A1ECV	C2C-C1C	5.08	1.50	1.41
49	0	316	KC2	CHD-C4C	5.08	1.48	1.38
51	x	310	A1ECV	C4D-ND	5.07	1.39	1.35
51	6	320	A1ECV	C2A-C1A	5.07	1.50	1.41
49	G	317	KC2	CHD-C4C	5.07	1.48	1.38
50	R	303	A1EB1	O4-C38	5.07	1.46	1.35
48	y	306	A86	O4-C38	5.07	1.46	1.35
50	Q	307	A1EB1	O4-C38	5.07	1.46	1.35
49	4	324	KC2	CHD-C4C	5.07	1.48	1.38
49	5	305	KC2	CHD-C4C	5.07	1.48	1.38
50	E	301	A1EB1	O4-C38	5.06	1.46	1.35
49	4	320	KC2	CHD-C4C	5.06	1.48	1.38
51	E	311	A1ECV	O2D-CGD	5.06	1.45	1.33
49	Q	315	KC2	CHD-C4C	5.06	1.48	1.38
49	9	313	KC2	CHD-C4C	5.06	1.48	1.38
51	T	317	A1ECV	O2D-CGD	5.05	1.45	1.33
51	L	318	A1ECV	C2A-C1A	5.05	1.50	1.41
51	x	316	A1ECV	C4D-ND	5.05	1.39	1.35
49	I	303	KC2	CHD-C4C	5.05	1.48	1.38
51	z	316	A1ECV	O2D-CGD	5.05	1.45	1.33
51	1	318	A1ECV	C2C-C1C	5.05	1.50	1.41
48	7	307	A86	O4-C38	5.05	1.46	1.35
51	y	317	A1ECV	C4D-ND	5.05	1.39	1.35
48	0	301	A86	O4-C38	5.05	1.46	1.35
50	1	305	A1EB1	O4-C38	5.04	1.46	1.35
51	z	310	A1ECV	C2A-C1A	5.04	1.50	1.41
51	1	318	A1ECV	O2D-CGD	5.04	1.45	1.33
49	3	317	KC2	CHD-C4C	5.04	1.48	1.38
48	4	310	A86	O4-C38	5.03	1.46	1.35
50	G	307	A1EB1	O4-C38	5.03	1.46	1.35
50	3	302	A1EB1	O4-C38	5.03	1.46	1.35
51	Q	319	A1ECV	O2D-CGD	5.03	1.45	1.33
50	7	305	A1EB1	O4-C38	5.03	1.46	1.35
49	M	307	KC2	CHD-C4C	5.03	1.48	1.38
49	V	320	KC2	CHD-C4C	5.02	1.48	1.38
50	F	304	A1EB1	O4-C38	5.02	1.46	1.35
43	1	304	DD6	C21-C20	5.02	1.59	1.51
48	E	304	A86	O4-C38	5.02	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	G	315	KC2	CHD-C4C	5.01	1.48	1.38
51	z	310	A1ECV	C2C-C1C	5.01	1.50	1.41
51	y	311	A1ECV	C2C-C1C	5.01	1.50	1.41
51	5	309	A1ECV	O2D-CGD	5.01	1.45	1.33
49	6	316	KC2	CHD-C4C	5.01	1.48	1.38
48	G	305	A86	O4-C38	5.00	1.46	1.35
50	L	303	A1EB1	O4-C38	5.00	1.46	1.35
49	T	314	KC2	CHD-C4C	5.00	1.48	1.38
50	8	306	A1EB1	O4-C38	4.99	1.46	1.35
50	8	304	A1EB1	O4-C38	4.98	1.46	1.35
48	V	301	A86	O4-C38	4.97	1.46	1.35
51	z	316	A1ECV	C2C-C1C	4.97	1.49	1.41
51	S	312	A1ECV	C2C-C1C	4.96	1.49	1.41
50	V	305	A1EB1	O4-C38	4.95	1.46	1.35
51	2	311	A1ECV	C4D-ND	4.95	1.39	1.35
49	8	314	KC2	CHD-C4C	4.95	1.48	1.38
48	9	303	A86	O4-C38	4.95	1.46	1.35
51	E	311	A1ECV	C2A-C3A	4.94	1.47	1.40
49	R	312	KC2	CHD-C4C	4.94	1.48	1.38
50	6	308	A1EB1	O4-C38	4.94	1.46	1.35
49	0	319	KC2	MG-ND	-4.94	1.96	2.05
50	H	301	A1EB1	O4-C38	4.93	1.46	1.35
50	D	308	A1EB1	O4-C38	4.93	1.46	1.35
51	4	315	A1ECV	C2C-C1C	4.93	1.49	1.41
48	P	302	A86	O4-C38	4.92	1.46	1.35
51	Z	308	A1ECV	C2A-C3A	4.92	1.47	1.40
51	x	316	A1ECV	C3B-C2B	4.92	1.47	1.37
51	R	310	A1ECV	O2D-CGD	4.92	1.45	1.33
51	y	317	A1ECV	C3B-C2B	4.92	1.47	1.37
51	2	311	A1ECV	C2C-C1C	4.90	1.49	1.41
51	R	313	A1ECV	C2C-C1C	4.90	1.49	1.41
51	Y	306	A1ECV	C2A-C3A	4.90	1.47	1.40
51	Z	314	A1ECV	C3B-C2B	4.89	1.47	1.37
49	W	308	KC2	CHD-C4C	4.89	1.48	1.38
50	3	324	A1EB1	O4-C38	4.89	1.46	1.35
51	E	311	A1ECV	C2C-C1C	4.89	1.49	1.41
48	0	304	A86	O4-C38	4.89	1.46	1.35
49	Q	313	KC2	CHD-C4C	4.89	1.48	1.38
48	W	303	A86	O4-C38	4.89	1.46	1.35
40	b	843	PQN	C10-C5	4.88	1.48	1.40
51	6	320	A1ECV	C3B-C2B	4.88	1.47	1.37
51	Q	316	A1ECV	CHC-C1C	4.88	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	O	306	A86	O4-C38	4.88	1.46	1.35
51	z	316	A1ECV	C3B-C2B	4.87	1.47	1.37
48	M	302	A86	O4-C38	4.87	1.46	1.35
51	1	318	A1ECV	C3B-C2B	4.87	1.47	1.37
40	a	839	PQN	C10-C5	4.87	1.48	1.40
50	x	301	A1EB1	O4-C38	4.87	1.46	1.35
51	y	311	A1ECV	C4D-ND	4.86	1.39	1.35
51	Y	306	A1ECV	C3B-C2B	4.86	1.47	1.37
51	Z	308	A1ECV	C3B-C2B	4.86	1.47	1.37
51	7	317	A1ECV	C2C-C1C	4.86	1.49	1.41
48	x	305	A86	O4-C38	4.86	1.46	1.35
50	0	307	A1EB1	O4-C38	4.85	1.46	1.35
50	S	302	A1EB1	O4-C38	4.85	1.46	1.35
51	x	316	A1ECV	C2A-C3A	4.85	1.47	1.40
48	J	301	A86	O4-C38	4.85	1.46	1.35
48	8	303	A86	O4-C38	4.85	1.46	1.35
51	S	318	A1ECV	C3B-C2B	4.85	1.47	1.37
50	h	203	A1EB1	O4-C38	4.84	1.46	1.35
51	Z	308	A1ECV	C4D-ND	4.83	1.39	1.35
50	K	304	A1EB1	O4-C38	4.83	1.46	1.35
51	G	316	A1ECV	C3B-C2B	4.83	1.47	1.37
49	z	313	KC2	CHD-C4C	4.83	1.48	1.38
51	2	311	A1ECV	C2A-C3A	4.83	1.47	1.40
48	B	201	A86	O4-C38	4.83	1.46	1.35
48	5	301	A86	O4-C38	4.83	1.46	1.35
48	6	309	A86	O4-C38	4.83	1.46	1.35
51	Y	306	A1ECV	C2C-C1C	4.83	1.49	1.41
48	U	206	A86	O4-C38	4.82	1.46	1.35
48	F	302	A86	O4-C38	4.82	1.46	1.35
48	G	301	A86	O4-C38	4.82	1.46	1.35
48	1	306	A86	O4-C38	4.82	1.46	1.35
50	0	303	A1EB1	O4-C38	4.82	1.46	1.35
51	y	311	A1ECV	C3B-C2B	4.82	1.47	1.37
48	T	305	A86	O4-C38	4.82	1.46	1.35
48	J	303	A86	O4-C38	4.81	1.46	1.35
48	H	302	A86	O4-C38	4.81	1.46	1.35
48	1	307	A86	O4-C38	4.81	1.46	1.35
48	L	304	A86	O4-C38	4.81	1.46	1.35
48	F	301	A86	O4-C38	4.80	1.46	1.35
51	9	314	A1ECV	CHC-C1C	4.80	1.47	1.39
51	X	310	A1ECV	C3B-C2B	4.80	1.47	1.37
48	7	311	A86	O4-C38	4.80	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	y	317	A1ECV	C2A-C3A	4.80	1.47	1.40
52	5	304	A1EB4	O4-C38	4.80	1.46	1.35
48	S	305	A86	O4-C38	4.80	1.46	1.35
51	P	315	A1ECV	C3B-C2B	4.80	1.47	1.37
50	8	308	A1EB1	O4-C38	4.80	1.46	1.35
48	k	206	A86	O4-C38	4.80	1.46	1.35
48	L	301	A86	O4-C38	4.79	1.46	1.35
51	Z	314	A1ECV	C2C-C1C	4.79	1.49	1.41
51	5	309	A1ECV	C3B-C2B	4.79	1.47	1.37
48	3	307	A86	O4-C38	4.79	1.46	1.35
51	Y	306	A1ECV	C4D-ND	4.79	1.39	1.35
50	y	302	A1EB1	O4-C38	4.79	1.46	1.35
48	C	303	A86	O4-C38	4.79	1.46	1.35
50	7	304	A1EB1	O4-C38	4.79	1.46	1.35
48	S	304	A86	O4-C38	4.79	1.46	1.35
50	K	302	A1EB1	O4-C38	4.79	1.46	1.35
50	z	301	A1EB1	O4-C38	4.79	1.46	1.35
48	L	305	A86	O4-C38	4.79	1.46	1.35
48	L	306	A86	O4-C38	4.78	1.46	1.35
51	7	323	A1ECV	C2C-C1C	4.78	1.49	1.41
51	z	310	A1ECV	C3B-C2B	4.78	1.47	1.37
48	4	306	A86	O4-C38	4.78	1.46	1.35
50	6	301	A1EB1	O4-C38	4.78	1.46	1.35
50	4	303	A1EB1	O4-C38	4.78	1.46	1.35
48	8	302	A86	O4-C38	4.78	1.46	1.35
50	9	302	A1EB1	O4-C38	4.77	1.46	1.35
51	Q	319	A1ECV	C3B-C2B	4.77	1.47	1.37
50	6	306	A1EB1	O4-C38	4.77	1.46	1.35
48	Y	301	A86	O4-C38	4.77	1.46	1.35
50	4	301	A1EB1	O4-C38	4.77	1.46	1.35
52	M	305	A1EB4	O4-C38	4.77	1.46	1.35
51	2	311	A1ECV	C3B-C2B	4.77	1.47	1.37
51	Y	312	A1ECV	C3B-C2B	4.77	1.47	1.37
49	X	306	KC2	MG-ND	-4.77	1.96	2.05
48	8	307	A86	O4-C38	4.77	1.46	1.35
50	G	308	A1EB1	O4-C38	4.76	1.46	1.35
48	Q	308	A86	O4-C38	4.76	1.46	1.35
48	W	304	A86	O4-C38	4.76	1.46	1.35
51	9	317	A1ECV	C3B-C2B	4.76	1.47	1.37
48	L	302	A86	O4-C38	4.76	1.46	1.35
50	O	301	A1EB1	O4-C38	4.76	1.45	1.35
51	7	323	A1ECV	C3B-C2B	4.76	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	9	306	A86	O4-C38	4.76	1.45	1.35
48	Q	305	A86	O4-C38	4.76	1.45	1.35
51	V	317	A1ECV	C3B-C2B	4.76	1.46	1.37
48	z	303	A86	O4-C38	4.76	1.45	1.35
50	1	301	A1EB1	O4-C38	4.76	1.45	1.35
48	L	307	A86	O4-C38	4.75	1.45	1.35
50	3	310	A1EB1	O4-C38	4.75	1.45	1.35
51	O	315	A1ECV	CHC-C1C	4.75	1.47	1.39
48	1	302	A86	O4-C38	4.75	1.45	1.35
48	I	304	A86	O4-C38	4.75	1.45	1.35
50	7	306	A1EB1	O4-C38	4.75	1.45	1.35
50	K	305	A1EB1	O4-C38	4.75	1.45	1.35
50	0	302	A1EB1	O4-C38	4.75	1.45	1.35
50	2	306	A1EB1	O4-C38	4.75	1.45	1.35
48	2	302	A86	O4-C38	4.75	1.45	1.35
48	6	305	A86	O4-C38	4.75	1.45	1.35
50	3	309	A1EB1	O4-C38	4.75	1.45	1.35
48	R	302	A86	O4-C38	4.74	1.45	1.35
48	Z	301	A86	O4-C38	4.74	1.45	1.35
48	X	302	A86	O4-C38	4.74	1.45	1.35
50	5	302	A1EB1	O4-C38	4.74	1.45	1.35
51	R	310	A1ECV	C3B-C2B	4.74	1.46	1.37
48	U	202	A86	O4-C38	4.74	1.45	1.35
48	Q	302	A86	O4-C38	4.74	1.45	1.35
50	4	304	A1EB1	O4-C38	4.74	1.45	1.35
49	Q	313	KC2	MG-ND	-4.74	1.96	2.05
48	8	323	A86	O4-C38	4.74	1.45	1.35
48	M	306	A86	O4-C38	4.74	1.45	1.35
50	V	306	A1EB1	O4-C38	4.74	1.45	1.35
48	0	309	A86	O4-C38	4.74	1.45	1.35
51	y	311	A1ECV	C2A-C3A	4.74	1.46	1.40
50	V	307	A1EB1	O4-C38	4.73	1.45	1.35
51	S	312	A1ECV	CHC-C1C	4.73	1.47	1.39
51	4	321	A1ECV	C3B-C2B	4.73	1.46	1.37
50	4	302	A1EB1	O4-C38	4.73	1.45	1.35
48	S	307	A86	O4-C38	4.73	1.45	1.35
48	2	301	A86	O4-C38	4.73	1.45	1.35
50	0	305	A1EB1	O4-C38	4.73	1.45	1.35
48	Q	301	A86	O4-C38	4.73	1.45	1.35
52	T	304	A1EB4	O4-C38	4.73	1.45	1.35
48	8	309	A86	O4-C38	4.73	1.45	1.35
48	O	302	A86	O4-C38	4.73	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	P	303	A86	O4-C38	4.73	1.45	1.35
48	M	303	A86	O4-C38	4.72	1.45	1.35
50	U	205	A1EB1	O4-C38	4.72	1.45	1.35
51	L	318	A1ECV	CHB-C1B	4.72	1.48	1.39
48	7	308	A86	O4-C38	4.72	1.45	1.35
51	O	315	A1ECV	C3B-C2B	4.72	1.46	1.37
48	K	301	A86	O4-C38	4.72	1.45	1.35
48	V	304	A86	O4-C38	4.72	1.45	1.35
51	5	312	A1ECV	C2C-C1C	4.72	1.49	1.41
48	X	303	A86	O4-C38	4.72	1.45	1.35
50	2	304	A1EB1	O4-C38	4.72	1.45	1.35
49	1	312	KC2	MG-ND	-4.72	1.96	2.05
50	3	303	A1EB1	O4-C38	4.72	1.45	1.35
51	5	312	A1ECV	C3B-C2B	4.72	1.46	1.37
51	0	321	A1ECV	C2C-C1C	4.72	1.49	1.41
50	J	302	A1EB1	O4-C38	4.71	1.45	1.35
50	G	304	A1EB1	O4-C38	4.71	1.45	1.35
48	6	307	A86	O4-C38	4.71	1.45	1.35
52	R	305	A1EB4	O4-C38	4.71	1.45	1.35
48	T	306	A86	O4-C38	4.71	1.45	1.35
51	R	313	A1ECV	CHC-C1C	4.71	1.47	1.39
48	Z	303	A86	O4-C38	4.70	1.45	1.35
48	1	303	A86	O4-C38	4.70	1.45	1.35
48	4	309	A86	O4-C38	4.70	1.45	1.35
48	8	305	A86	O4-C38	4.70	1.45	1.35
51	R	313	A1ECV	C3B-C2B	4.70	1.46	1.37
48	4	328	A86	O4-C38	4.70	1.45	1.35
50	y	301	A1EB1	O4-C38	4.70	1.45	1.35
50	x	302	A1EB1	O4-C38	4.70	1.45	1.35
51	4	315	A1ECV	C3B-C2B	4.69	1.46	1.37
48	W	307	A86	O4-C38	4.69	1.45	1.35
50	H	304	A1EB1	O4-C38	4.69	1.45	1.35
48	3	306	A86	O4-C38	4.69	1.45	1.35
48	6	303	A86	O4-C38	4.68	1.45	1.35
48	4	305	A86	O4-C38	4.68	1.45	1.35
49	G	315	KC2	MG-ND	-4.68	1.96	2.05
51	7	317	A1ECV	CHC-C1C	4.68	1.47	1.39
51	9	314	A1ECV	C3B-C2B	4.68	1.46	1.37
50	8	301	A1EB1	O4-C38	4.68	1.45	1.35
48	9	305	A86	O4-C38	4.68	1.45	1.35
51	M	316	A1ECV	C2C-C1C	4.68	1.49	1.41
51	M	316	A1ECV	C3B-C2B	4.68	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	W	321	A1EB4	O4-C38	4.68	1.45	1.35
51	X	313	A1ECV	C3B-C2B	4.67	1.46	1.37
51	1	318	A1ECV	CHC-C1C	4.67	1.47	1.39
50	C	302	A1EB1	O4-C38	4.67	1.45	1.35
51	x	310	A1ECV	CHC-C1C	4.66	1.47	1.39
51	Z	314	A1ECV	CHC-C1C	4.66	1.47	1.39
48	T	301	A86	O4-C38	4.66	1.45	1.35
51	z	310	A1ECV	CHC-C1C	4.66	1.47	1.39
48	y	305	A86	O4-C38	4.66	1.45	1.35
48	9	304	A86	O4-C38	4.66	1.45	1.35
49	9	318	KC2	MG-ND	-4.66	1.96	2.05
50	S	303	A1EB1	O4-C38	4.66	1.45	1.35
50	U	203	A1EB1	O4-C38	4.66	1.45	1.35
48	Q	304	A86	O4-C38	4.65	1.45	1.35
48	D	305	A86	O4-C38	4.65	1.45	1.35
49	O	317	KC2	MG-ND	-4.65	1.96	2.05
48	2	305	A86	O4-C38	4.65	1.45	1.35
48	R	317	A86	O4-C38	4.65	1.45	1.35
48	O	307	A86	O4-C38	4.65	1.45	1.35
49	Y	308	KC2	MG-ND	-4.65	1.96	2.05
48	6	302	A86	O4-C38	4.65	1.45	1.35
51	4	315	A1ECV	CHC-C1C	4.65	1.47	1.39
48	0	306	A86	O4-C38	4.64	1.45	1.35
51	S	312	A1ECV	C3B-C2B	4.64	1.46	1.37
49	6	319	KC2	MG-ND	-4.64	1.96	2.05
48	9	301	A86	O4-C38	4.64	1.45	1.35
51	7	317	A1ECV	C3B-C2B	4.64	1.46	1.37
48	R	301	A86	O4-C38	4.63	1.45	1.35
49	R	306	KC2	MG-ND	-4.63	1.96	2.05
49	L	312	KC2	MG-ND	-4.63	1.96	2.05
51	P	315	A1ECV	CHC-C1C	4.63	1.47	1.39
51	7	323	A1ECV	CHC-C1C	4.62	1.47	1.39
52	P	319	A1EB4	O4-C38	4.62	1.45	1.35
51	T	317	A1ECV	C3B-C2B	4.62	1.46	1.37
51	x	310	A1ECV	C2A-C3A	4.62	1.46	1.40
49	P	313	KC2	MG-ND	-4.62	1.96	2.05
51	G	316	A1ECV	CHC-C1C	4.62	1.47	1.39
51	2	311	A1ECV	CHC-C1C	4.62	1.47	1.39
51	G	316	A1ECV	C2C-C1C	4.61	1.49	1.41
50	Q	323	A1EB1	O4-C38	4.61	1.45	1.35
51	5	312	A1ECV	CHC-C1C	4.61	1.47	1.39
51	W	317	A1ECV	C3B-C2B	4.61	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	X	313	A1ECV	CHB-C4A	4.60	1.47	1.39
50	T	307	A1EB1	O4-C38	4.60	1.45	1.35
52	M	322	A1EB4	O4-C38	4.60	1.45	1.35
52	P	305	A1EB4	O4-C38	4.60	1.45	1.35
51	W	317	A1ECV	C2A-C3A	4.60	1.46	1.40
49	A	310	KC2	MG-ND	-4.59	1.96	2.05
52	W	306	A1EB4	O4-C38	4.59	1.45	1.35
52	X	305	A1EB4	O4-C38	4.59	1.45	1.35
51	X	313	A1ECV	C2C-C1C	4.59	1.49	1.41
51	Q	316	A1ECV	C3B-C2B	4.59	1.46	1.37
49	0	319	KC2	MG-NB	-4.59	1.96	2.05
51	X	310	A1ECV	C2C-C1C	4.58	1.49	1.41
51	y	311	A1ECV	CHC-C1C	4.58	1.47	1.39
51	S	318	A1ECV	C2C-C1C	4.58	1.49	1.41
51	P	315	A1ECV	C2C-C1C	4.58	1.49	1.41
51	5	309	A1ECV	CHC-C1C	4.58	1.47	1.39
51	S	318	A1ECV	C2A-C3A	4.58	1.46	1.40
49	8	314	KC2	MG-ND	-4.58	1.96	2.05
51	X	313	A1ECV	C2A-C3A	4.57	1.46	1.40
49	y	314	KC2	MG-ND	-4.57	1.96	2.05
51	9	314	A1ECV	C2A-C3A	4.57	1.46	1.40
51	X	313	A1ECV	CHC-C1C	4.57	1.47	1.39
51	T	317	A1ECV	C2A-C3A	4.57	1.46	1.40
51	M	316	A1ECV	CHC-C1C	4.56	1.47	1.39
52	P	318	A1EB4	O4-C38	4.55	1.45	1.35
51	Y	312	A1ECV	C2A-C3A	4.55	1.46	1.40
51	R	313	A1ECV	CHB-C4A	4.55	1.47	1.39
51	X	310	A1ECV	C2A-C3A	4.55	1.46	1.40
43	O	304	DD6	C21-C20	4.55	1.59	1.51
51	z	316	A1ECV	CHC-C1C	4.54	1.47	1.39
49	9	313	KC2	MG-ND	-4.54	1.96	2.05
51	z	316	A1ECV	C2A-C3A	4.54	1.46	1.40
49	L	321	KC2	MG-ND	-4.54	1.96	2.05
51	W	317	A1ECV	C2C-C1C	4.53	1.49	1.41
49	9	316	KC2	MG-ND	-4.53	1.96	2.05
51	1	318	A1ECV	C2A-C3A	4.53	1.46	1.40
51	0	321	A1ECV	C3B-C2B	4.53	1.46	1.37
49	3	315	KC2	MG-ND	-4.52	1.96	2.05
51	W	317	A1ECV	CHC-C1C	4.52	1.47	1.39
51	V	317	A1ECV	CHC-C1C	4.51	1.47	1.39
51	Q	316	A1ECV	C2A-C3A	4.51	1.46	1.40
51	L	318	A1ECV	CHB-C4A	4.51	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	Q	313	KC2	MG-NB	-4.50	1.96	2.05
51	R	310	A1ECV	CHC-C1C	4.50	1.47	1.39
49	H	311	KC2	MG-ND	-4.50	1.96	2.05
49	W	315	KC2	MG-ND	-4.50	1.96	2.05
51	5	312	A1ECV	CHB-C1B	4.50	1.47	1.39
51	S	318	A1ECV	CHC-C1C	4.50	1.46	1.39
51	Z	308	A1ECV	CHC-C1C	4.50	1.46	1.39
49	x	315	KC2	MG-ND	-4.49	1.96	2.05
51	O	315	A1ECV	C2A-C3A	4.49	1.46	1.40
51	L	318	A1ECV	C3B-C2B	4.49	1.46	1.37
49	3	317	KC2	MG-ND	-4.49	1.96	2.05
51	E	311	A1ECV	C3B-C2B	4.49	1.46	1.37
51	X	310	A1ECV	CHC-C1C	4.48	1.46	1.39
49	R	314	KC2	MG-ND	-4.48	1.96	2.05
49	1	315	KC2	MG-ND	-4.48	1.96	2.05
51	9	314	A1ECV	CHB-C4A	4.48	1.46	1.39
49	P	306	KC2	MG-ND	-4.47	1.96	2.05
51	Y	306	A1ECV	CHC-C1C	4.47	1.46	1.39
50	3	310	A1EB1	O6-C42	4.47	1.46	1.33
46	0	324	LMG	O7-C10	4.47	1.45	1.35
51	5	309	A1ECV	C2C-C1C	4.47	1.49	1.41
49	W	308	KC2	MG-ND	-4.47	1.96	2.05
49	5	311	KC2	MG-ND	-4.46	1.96	2.05
51	6	320	A1ECV	CHC-C1C	4.46	1.46	1.39
49	8	319	KC2	MG-ND	-4.46	1.96	2.05
51	y	317	A1ECV	C2C-C1C	4.46	1.49	1.41
49	G	311	KC2	MG-ND	-4.46	1.97	2.05
49	2	313	KC2	MG-ND	-4.46	1.97	2.05
49	4	324	KC2	MG-ND	-4.45	1.97	2.05
51	z	310	A1ECV	C2A-C3A	4.45	1.46	1.40
49	I	303	KC2	MG-ND	-4.45	1.97	2.05
50	3	324	A1EB1	O6-C42	4.45	1.46	1.33
49	9	311	KC2	MG-ND	-4.45	1.97	2.05
49	X	314	KC2	MG-ND	-4.45	1.97	2.05
49	z	312	KC2	MG-ND	-4.44	1.97	2.05
49	3	321	KC2	MG-ND	-4.44	1.97	2.05
51	y	317	A1ECV	CHC-C1C	4.44	1.46	1.39
50	6	301	A1EB1	O6-C42	4.44	1.46	1.33
49	4	317	KC2	MG-ND	-4.44	1.97	2.05
51	0	321	A1ECV	C2A-C3A	4.44	1.46	1.40
49	V	320	KC2	MG-ND	-4.44	1.97	2.05
51	T	317	A1ECV	CHC-C1C	4.43	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	1	314	KC2	MG-ND	-4.43	1.97	2.05
49	V	318	KC2	MG-ND	-4.43	1.97	2.05
49	Q	315	KC2	MG-ND	-4.43	1.97	2.05
49	L	315	KC2	MG-ND	-4.42	1.97	2.05
49	5	313	KC2	MG-ND	-4.42	1.97	2.05
51	E	311	A1ECV	CHB-C1B	4.42	1.47	1.39
51	Y	312	A1ECV	CHB-C1B	4.42	1.47	1.39
49	6	316	KC2	MG-ND	-4.42	1.97	2.05
49	P	312	KC2	MG-ND	-4.42	1.97	2.05
49	R	312	KC2	MG-ND	-4.41	1.97	2.05
51	9	317	A1ECV	C2C-C1C	4.41	1.48	1.41
51	x	316	A1ECV	CHC-C1C	4.41	1.46	1.39
51	Z	314	A1ECV	C2A-C3A	4.41	1.46	1.40
51	x	316	A1ECV	C2C-C1C	4.41	1.48	1.41
50	8	306	A1EB1	O6-C42	4.40	1.46	1.33
49	T	314	KC2	MG-ND	-4.40	1.97	2.05
49	S	314	KC2	MG-ND	-4.40	1.97	2.05
49	M	314	KC2	MG-ND	-4.40	1.97	2.05
49	8	320	KC2	MG-ND	-4.40	1.97	2.05
51	G	316	A1ECV	CHB-C1B	4.40	1.47	1.39
49	T	312	KC2	MG-ND	-4.40	1.97	2.05
49	7	320	KC2	MG-ND	-4.39	1.97	2.05
49	3	318	KC2	MG-ND	-4.39	1.97	2.05
49	F	311	KC2	MG-ND	-4.39	1.97	2.05
51	4	321	A1ECV	CHC-C1C	4.39	1.46	1.39
51	V	317	A1ECV	C2C-C1C	4.39	1.48	1.41
49	V	308	KC2	MG-ND	-4.39	1.97	2.05
49	Y	309	KC2	MG-ND	-4.39	1.97	2.05
50	0	307	A1EB1	O6-C42	4.38	1.46	1.33
49	L	317	KC2	MG-ND	-4.38	1.97	2.05
49	5	314	KC2	MG-ND	-4.38	1.97	2.05
49	6	314	KC2	MG-ND	-4.38	1.97	2.05
49	K	313	KC2	MG-ND	-4.38	1.97	2.05
51	Q	319	A1ECV	C2A-C3A	4.38	1.46	1.40
49	I	312	KC2	MG-ND	-4.38	1.97	2.05
49	7	322	KC2	MG-ND	-4.38	1.97	2.05
49	K	310	KC2	MG-ND	-4.38	1.97	2.05
51	T	317	A1ECV	CHB-C4A	4.38	1.46	1.39
51	E	311	A1ECV	CHC-C1C	4.38	1.46	1.39
51	T	317	A1ECV	C2C-C1C	4.38	1.48	1.41
46	F	320	LMG	O8-C28	4.38	1.46	1.33
49	G	317	KC2	MG-ND	-4.37	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	V	315	KC2	MG-ND	-4.37	1.97	2.05
49	A	313	KC2	MG-ND	-4.37	1.97	2.05
49	M	313	KC2	CHC-C1C	4.37	1.49	1.39
49	0	319	KC2	CHC-C1C	4.37	1.49	1.39
51	S	318	A1ECV	CHB-C1B	4.37	1.47	1.39
50	G	304	A1EB1	O6-C42	4.37	1.46	1.33
49	M	307	KC2	MG-ND	-4.36	1.97	2.05
49	y	316	KC2	MG-ND	-4.36	1.97	2.05
51	7	317	A1ECV	C2A-C3A	4.36	1.46	1.40
49	0	316	KC2	MG-ND	-4.36	1.97	2.05
49	0	317	KC2	MG-ND	-4.36	1.97	2.05
50	Q	323	A1EB1	O6-C42	4.36	1.46	1.33
51	9	317	A1ECV	CHC-C1C	4.36	1.46	1.39
49	R	318	KC2	MG-ND	-4.35	1.97	2.05
49	0	319	KC2	CHC-C4B	4.35	1.46	1.38
49	7	319	KC2	MG-ND	-4.35	1.97	2.05
49	T	315	KC2	MG-ND	-4.35	1.97	2.05
49	C	312	KC2	MG-ND	-4.35	1.97	2.05
50	3	303	A1EB1	O6-C42	4.35	1.46	1.33
50	K	302	A1EB1	O6-C42	4.34	1.46	1.33
49	G	313	KC2	MG-ND	-4.34	1.97	2.05
49	P	320	KC2	MG-ND	-4.34	1.97	2.05
50	x	302	A1EB1	O6-C42	4.34	1.46	1.33
49	H	314	KC2	MG-ND	-4.34	1.97	2.05
49	Q	318	KC2	MG-ND	-4.34	1.97	2.05
49	x	313	KC2	MG-ND	-4.34	1.97	2.05
51	Y	312	A1ECV	C2C-C1C	4.34	1.48	1.41
49	X	315	KC2	MG-ND	-4.34	1.97	2.05
49	X	318	KC2	MG-ND	-4.33	1.97	2.05
49	V	314	KC2	MG-ND	-4.33	1.97	2.05
49	Y	308	KC2	MG-NB	-4.33	1.97	2.05
50	D	308	A1EB1	O6-C42	4.33	1.46	1.33
50	7	304	A1EB1	O6-C42	4.33	1.46	1.33
49	2	317	KC2	MG-ND	-4.33	1.97	2.05
49	B	208	KC2	MG-ND	-4.33	1.97	2.05
49	W	314	KC2	MG-ND	-4.33	1.97	2.05
49	3	317	KC2	CHC-C4B	4.33	1.46	1.38
49	P	310	KC2	MG-ND	-4.33	1.97	2.05
49	x	312	KC2	MG-ND	-4.33	1.97	2.05
49	Z	310	KC2	MG-ND	-4.33	1.97	2.05
49	J	315	KC2	MG-ND	-4.33	1.97	2.05
49	T	316	KC2	MG-ND	-4.33	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	K	305	A1EB1	O6-C42	4.33	1.46	1.33
49	M	313	KC2	CHC-C4B	4.33	1.46	1.38
49	8	316	KC2	MG-ND	-4.33	1.97	2.05
49	S	315	KC2	CHC-C1C	4.32	1.49	1.39
39	Z	313	CLA	C1D-ND	4.32	1.43	1.37
49	0	314	KC2	MG-ND	-4.32	1.97	2.05
50	V	305	A1EB1	O6-C42	4.32	1.46	1.33
49	C	313	KC2	MG-ND	-4.32	1.97	2.05
49	8	317	KC2	MG-ND	-4.32	1.97	2.05
49	W	312	KC2	MG-ND	-4.32	1.97	2.05
49	y	313	KC2	MG-ND	-4.32	1.97	2.05
50	H	301	A1EB1	O6-C42	4.32	1.46	1.33
49	Z	311	KC2	MG-ND	-4.32	1.97	2.05
51	7	323	A1ECV	CHB-C1B	4.32	1.47	1.39
49	4	318	KC2	MG-ND	-4.32	1.97	2.05
50	1	305	A1EB1	O6-C42	4.31	1.45	1.33
51	0	321	A1ECV	CHC-C1C	4.31	1.46	1.39
49	M	313	KC2	MG-ND	-4.31	1.97	2.05
50	z	302	A1EB1	O6-C42	4.31	1.45	1.33
49	V	312	KC2	MG-ND	-4.31	1.97	2.05
49	O	317	KC2	MG-NB	-4.31	1.97	2.05
49	z	315	KC2	MG-ND	-4.31	1.97	2.05
49	S	315	KC2	MG-ND	-4.31	1.97	2.05
50	S	302	A1EB1	O6-C42	4.31	1.45	1.33
49	z	313	KC2	CHC-C4B	4.31	1.46	1.38
51	R	313	A1ECV	C2A-C3A	4.31	1.46	1.40
51	5	309	A1ECV	C2A-C3A	4.31	1.46	1.40
50	4	302	A1EB1	O6-C42	4.31	1.45	1.33
50	6	308	A1EB1	O6-C42	4.31	1.45	1.33
52	P	319	A1EB4	O3-C39	4.31	1.45	1.33
51	4	315	A1ECV	C2A-C3A	4.31	1.46	1.40
50	1	301	A1EB1	O6-C42	4.31	1.45	1.33
49	5	305	KC2	MG-ND	-4.31	1.97	2.05
49	Y	308	KC2	CHC-C1C	4.31	1.49	1.39
51	Y	312	A1ECV	CHC-C1C	4.30	1.46	1.39
50	4	303	A1EB1	O6-C42	4.30	1.45	1.33
49	8	314	KC2	CHC-C4B	4.30	1.46	1.38
49	7	320	KC2	CHC-C1C	4.30	1.49	1.39
50	2	306	A1EB1	O6-C42	4.30	1.45	1.33
50	V	307	A1EB1	O6-C42	4.30	1.45	1.33
50	3	309	A1EB1	O6-C42	4.30	1.45	1.33
50	E	301	A1EB1	O6-C42	4.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	1	312	KC2	MG-NB	-4.30	1.97	2.05
49	M	311	KC2	MG-ND	-4.30	1.97	2.05
50	Q	307	A1EB1	O6-C42	4.30	1.45	1.33
50	T	307	A1EB1	O6-C42	4.30	1.45	1.33
49	V	314	KC2	CHC-C1C	4.30	1.49	1.39
49	3	318	KC2	CHC-C1C	4.29	1.49	1.39
49	S	317	KC2	MG-ND	-4.29	1.97	2.05
50	S	303	A1EB1	O6-C42	4.29	1.45	1.33
49	X	306	KC2	CHC-C1C	4.29	1.49	1.39
49	3	317	KC2	CHC-C1C	4.29	1.49	1.39
50	2	304	A1EB1	O6-C42	4.29	1.45	1.33
50	K	304	A1EB1	O6-C42	4.29	1.45	1.33
51	5	309	A1ECV	CHB-C1B	4.29	1.47	1.39
49	4	320	KC2	MG-ND	-4.29	1.97	2.05
50	U	203	A1EB1	O6-C42	4.29	1.45	1.33
51	4	321	A1ECV	C2A-C3A	4.29	1.46	1.40
46	M	319	LMG	O8-C28	4.29	1.45	1.33
51	Q	319	A1ECV	CHC-C1C	4.28	1.46	1.39
49	X	312	KC2	MG-ND	-4.28	1.97	2.05
46	Q	322	LMG	O8-C28	4.28	1.45	1.33
49	L	314	KC2	MG-ND	-4.28	1.97	2.05
50	x	301	A1EB1	O6-C42	4.28	1.45	1.33
50	7	306	A1EB1	O6-C42	4.28	1.45	1.33
49	F	307	KC2	MG-ND	-4.28	1.97	2.05
50	T	302	A1EB1	O6-C42	4.28	1.45	1.33
51	4	321	A1ECV	C2C-C1C	4.28	1.48	1.41
52	W	321	A1EB4	O3-C39	4.28	1.45	1.33
50	y	302	A1EB1	O6-C42	4.28	1.45	1.33
51	P	315	A1ECV	C2A-C3A	4.27	1.46	1.40
50	0	305	A1EB1	O6-C42	4.27	1.45	1.33
50	8	301	A1EB1	O6-C42	4.27	1.45	1.33
51	6	320	A1ECV	C2C-C1C	4.27	1.48	1.41
49	2	314	KC2	MG-ND	-4.27	1.97	2.05
52	M	322	A1EB4	O3-C39	4.27	1.45	1.33
49	z	313	KC2	CHC-C1C	4.27	1.49	1.39
49	Y	308	KC2	CHC-C4B	4.27	1.46	1.38
50	G	302	A1EB1	O6-C42	4.27	1.45	1.33
49	6	317	KC2	MG-ND	-4.27	1.97	2.05
52	T	304	A1EB4	O3-C39	4.27	1.45	1.33
50	8	304	A1EB1	O6-C42	4.27	1.45	1.33
50	7	305	A1EB1	O6-C42	4.27	1.45	1.33
50	y	301	A1EB1	O6-C42	4.27	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	X	305	A1EB4	O3-C39	4.27	1.45	1.33
51	R	310	A1ECV	C2C-C1C	4.27	1.48	1.41
50	3	302	A1EB1	O6-C42	4.26	1.45	1.33
39	a	801	CLA	C4D-ND	-4.26	1.31	1.37
51	7	323	A1ECV	C2A-C3A	4.26	1.46	1.40
50	F	304	A1EB1	O6-C42	4.26	1.45	1.33
49	P	306	KC2	MG-NB	-4.26	1.97	2.05
49	6	316	KC2	CHC-C4B	4.26	1.46	1.38
50	5	302	A1EB1	O6-C42	4.26	1.45	1.33
50	C	302	A1EB1	O6-C42	4.26	1.45	1.33
51	E	311	A1ECV	CHB-C4A	4.26	1.46	1.39
50	L	303	A1EB1	O6-C42	4.26	1.45	1.33
52	5	304	A1EB4	O3-C39	4.25	1.45	1.33
50	H	304	A1EB1	O6-C42	4.25	1.45	1.33
50	G	307	A1EB1	O6-C42	4.25	1.45	1.33
50	O	301	A1EB1	O6-C42	4.25	1.45	1.33
51	Z	314	A1ECV	CHB-C1B	4.25	1.47	1.39
51	R	310	A1ECV	C2A-C3A	4.25	1.46	1.40
50	G	308	A1EB1	O6-C42	4.25	1.45	1.33
50	8	308	A1EB1	O6-C42	4.25	1.45	1.33
50	9	302	A1EB1	O6-C42	4.25	1.45	1.33
49	6	319	KC2	CHC-C1C	4.25	1.48	1.39
49	X	312	KC2	CHC-C1C	4.25	1.48	1.39
50	0	302	A1EB1	O6-C42	4.24	1.45	1.33
52	P	305	A1EB4	O3-C39	4.24	1.45	1.33
49	8	317	KC2	CHC-C1C	4.24	1.48	1.39
49	9	318	KC2	CHC-C1C	4.24	1.48	1.39
49	9	318	KC2	MG-NB	-4.24	1.97	2.05
49	8	314	KC2	CHC-C1C	4.24	1.48	1.39
51	9	317	A1ECV	CHB-C1B	4.24	1.47	1.39
49	0	317	KC2	CHC-C1C	4.24	1.48	1.39
49	6	316	KC2	CHC-C1C	4.24	1.48	1.39
51	O	315	A1ECV	C2C-C1C	4.24	1.48	1.41
50	4	304	A1EB1	O6-C42	4.24	1.45	1.33
52	R	305	A1EB4	O3-C39	4.24	1.45	1.33
49	X	306	KC2	MG-NB	-4.24	1.97	2.05
49	X	306	KC2	CHC-C4B	4.24	1.46	1.38
49	A	310	KC2	MG-NB	-4.24	1.97	2.05
52	W	306	A1EB4	O3-C39	4.23	1.45	1.33
49	7	320	KC2	CHC-C4B	4.23	1.46	1.38
50	4	301	A1EB1	O6-C42	4.23	1.45	1.33
49	6	319	KC2	MG-NB	-4.23	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	H	314	KC2	CHC-C1C	4.22	1.48	1.39
49	G	315	KC2	CHC-C4B	4.22	1.46	1.38
50	6	304	A1EB1	O6-C42	4.22	1.45	1.33
49	y	314	KC2	CHC-C1C	4.22	1.48	1.39
49	G	315	KC2	MG-NB	-4.22	1.97	2.05
50	R	303	A1EB1	O6-C42	4.22	1.45	1.33
50	7	303	A1EB1	O6-C42	4.22	1.45	1.33
49	W	315	KC2	CHC-C1C	4.22	1.48	1.39
49	5	313	KC2	MG-NB	-4.22	1.97	2.05
51	S	312	A1ECV	C2A-C3A	4.22	1.46	1.40
50	0	303	A1EB1	O6-C42	4.22	1.45	1.33
49	M	314	KC2	CHC-C1C	4.21	1.48	1.39
49	P	312	KC2	MG-NB	-4.21	1.97	2.05
51	V	317	A1ECV	C2A-C3A	4.21	1.46	1.40
51	0	321	A1ECV	CHB-C1B	4.21	1.47	1.39
50	U	205	A1EB1	O6-C42	4.21	1.45	1.33
49	L	312	KC2	MG-NB	-4.21	1.97	2.05
49	S	314	KC2	CHC-C1C	4.21	1.48	1.39
49	9	318	KC2	CHC-C4B	4.21	1.46	1.38
50	V	302	A1EB1	O6-C42	4.21	1.45	1.33
49	8	317	KC2	CHC-C4B	4.21	1.46	1.38
50	h	203	A1EB1	O6-C42	4.21	1.45	1.33
51	6	320	A1ECV	CHB-C1B	4.21	1.47	1.39
49	9	311	KC2	CHC-C1C	4.21	1.48	1.39
51	6	320	A1ECV	CHB-C4A	4.20	1.46	1.39
49	9	316	KC2	CHC-C1C	4.20	1.48	1.39
49	W	315	KC2	CHC-C4B	4.20	1.46	1.38
49	L	314	KC2	CHC-C1C	4.20	1.48	1.39
51	4	321	A1ECV	CHB-C1B	4.20	1.47	1.39
49	6	319	KC2	CHC-C4B	4.20	1.46	1.38
49	y	314	KC2	MG-NB	-4.20	1.97	2.05
51	P	315	A1ECV	CHB-C1B	4.20	1.47	1.39
43	J	304	DD6	C21-C20	4.20	1.58	1.51
51	5	312	A1ECV	C2A-C3A	4.20	1.46	1.40
49	R	306	KC2	CHC-C1C	4.19	1.48	1.39
49	4	318	KC2	CHC-C1C	4.19	1.48	1.39
49	1	312	KC2	CHC-C4B	4.19	1.46	1.38
49	X	314	KC2	MG-NB	-4.19	1.97	2.05
49	S	314	KC2	MG-NB	-4.19	1.97	2.05
49	A	310	KC2	CHC-C4B	4.19	1.46	1.38
49	8	314	KC2	MG-NB	-4.19	1.97	2.05
51	S	318	A1ECV	CHB-C4A	4.19	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	x	313	KC2	CHC-C1C	4.19	1.48	1.39
50	J	302	A1EB1	O6-C42	4.19	1.45	1.33
51	0	321	A1ECV	CHB-C4A	4.19	1.46	1.39
51	O	315	A1ECV	CHB-C4A	4.18	1.46	1.39
49	V	315	KC2	CHC-C1C	4.18	1.48	1.39
51	O	315	A1ECV	CHB-C1B	4.18	1.47	1.39
51	G	316	A1ECV	C2A-C3A	4.18	1.46	1.40
46	P	317	LMG	O8-C28	4.18	1.45	1.33
49	A	310	KC2	CHC-C1C	4.18	1.48	1.39
51	L	318	A1ECV	C2A-C3A	4.18	1.46	1.40
49	J	315	KC2	CHC-C1C	4.18	1.48	1.39
46	F	317	LMG	O8-C28	4.18	1.45	1.33
49	x	315	KC2	CHC-C1C	4.18	1.48	1.39
49	6	317	KC2	CHC-C1C	4.18	1.48	1.39
49	1	312	KC2	CHC-C1C	4.17	1.48	1.39
46	W	302	LMG	O8-C28	4.17	1.45	1.33
49	X	314	KC2	CHC-C1C	4.17	1.48	1.39
49	5	313	KC2	CHC-C1C	4.17	1.48	1.39
49	R	306	KC2	MG-NB	-4.17	1.97	2.05
49	1	315	KC2	CHC-C1C	4.17	1.48	1.39
49	x	315	KC2	MG-NB	-4.17	1.97	2.05
49	Y	309	KC2	CHC-C1C	4.17	1.48	1.39
49	0	317	KC2	CHC-C4B	4.17	1.46	1.38
49	X	315	KC2	CHC-C1C	4.16	1.48	1.39
49	1	315	KC2	MG-NB	-4.16	1.97	2.05
49	3	318	KC2	CHC-C4B	4.16	1.46	1.38
49	M	314	KC2	CHC-C4B	4.16	1.46	1.38
49	X	318	KC2	CHC-C1C	4.16	1.48	1.39
49	3	315	KC2	CHC-C1C	4.16	1.48	1.39
49	K	313	KC2	CHC-C1C	4.16	1.48	1.39
49	O	317	KC2	CHC-C4B	4.16	1.46	1.38
49	G	315	KC2	CHC-C1C	4.16	1.48	1.39
51	V	317	A1ECV	CHB-C1B	4.16	1.47	1.39
49	L	314	KC2	CHC-C4B	4.16	1.46	1.38
49	R	314	KC2	CHC-C1C	4.16	1.48	1.39
51	M	316	A1ECV	CHB-C4A	4.16	1.46	1.39
49	9	311	KC2	CHC-C4B	4.15	1.46	1.38
49	R	306	KC2	CHC-C4B	4.15	1.46	1.38
49	y	314	KC2	CHC-C4B	4.15	1.46	1.38
49	Y	309	KC2	CHC-C4B	4.15	1.46	1.38
49	C	312	KC2	CHC-C1C	4.15	1.48	1.39
49	8	316	KC2	CHC-C1C	4.15	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	V	317	A1ECV	CHB-C4A	4.15	1.46	1.39
49	P	313	KC2	CHC-C1C	4.15	1.48	1.39
51	R	313	A1ECV	CHB-C1B	4.15	1.47	1.39
51	1	318	A1ECV	CHB-C1B	4.15	1.47	1.39
49	1	314	KC2	CHC-C1C	4.15	1.48	1.39
49	R	318	KC2	CHC-C1C	4.15	1.48	1.39
49	x	312	KC2	CHC-C1C	4.15	1.48	1.39
49	W	308	KC2	CHC-C1C	4.15	1.48	1.39
49	9	313	KC2	MG-NB	-4.15	1.97	2.05
49	Z	310	KC2	CHC-C1C	4.15	1.48	1.39
49	T	316	KC2	CHC-C1C	4.14	1.48	1.39
49	S	315	KC2	CHC-C4B	4.14	1.46	1.38
49	T	314	KC2	CHC-C1C	4.14	1.48	1.39
51	M	316	A1ECV	CHB-C1B	4.14	1.47	1.39
49	V	318	KC2	CHC-C1C	4.14	1.48	1.39
49	4	317	KC2	CHC-C1C	4.14	1.48	1.39
49	R	314	KC2	MG-NB	-4.14	1.97	2.05
49	W	315	KC2	MG-NB	-4.14	1.97	2.05
46	4	326	LMG	O8-C28	4.14	1.45	1.33
49	8	319	KC2	CHC-C1C	4.14	1.48	1.39
51	L	318	A1ECV	C2C-C1C	4.14	1.48	1.41
49	x	315	KC2	CHC-C4B	4.13	1.46	1.38
49	8	320	KC2	CHC-C1C	4.13	1.48	1.39
46	7	301	LMG	O8-C28	4.13	1.45	1.33
49	z	315	KC2	CHC-C1C	4.13	1.48	1.39
49	P	313	KC2	CHC-C4B	4.13	1.46	1.38
49	S	314	KC2	CHC-C4B	4.13	1.46	1.38
49	V	314	KC2	CHC-C4B	4.13	1.46	1.38
51	6	320	A1ECV	C2A-C3A	4.13	1.46	1.40
46	0	324	LMG	O8-C28	4.13	1.45	1.33
52	P	318	A1EB4	O3-C39	4.13	1.45	1.33
51	7	323	A1ECV	CHB-C4A	4.13	1.46	1.39
49	L	317	KC2	CHC-C1C	4.13	1.48	1.39
49	W	314	KC2	CHC-C1C	4.13	1.48	1.39
49	1	315	KC2	CHC-C4B	4.13	1.46	1.38
49	z	312	KC2	CHC-C4B	4.13	1.46	1.38
49	P	320	KC2	CHC-C1C	4.12	1.48	1.39
49	L	321	KC2	CHC-C1C	4.12	1.48	1.39
49	z	312	KC2	CHC-C1C	4.12	1.48	1.39
51	P	315	A1ECV	CHB-C4A	4.12	1.46	1.39
49	Z	311	KC2	CHC-C1C	4.12	1.48	1.39
51	z	316	A1ECV	CHB-C1B	4.12	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	M	307	KC2	CHC-C1C	4.12	1.48	1.39
49	8	320	KC2	CHC-C4B	4.12	1.46	1.38
49	V	318	KC2	CHC-C4B	4.12	1.46	1.38
49	V	312	KC2	CHC-C1C	4.12	1.48	1.39
49	L	321	KC2	MG-NB	-4.12	1.97	2.05
52	M	305	A1EB4	O3-C39	4.12	1.45	1.33
49	P	313	KC2	MG-NB	-4.12	1.97	2.05
49	C	313	KC2	CHC-C1C	4.12	1.48	1.39
51	y	317	A1ECV	CHB-C1B	4.12	1.47	1.39
50	V	306	A1EB1	O6-C42	4.11	1.45	1.33
39	0	311	CLA	C1D-ND	4.11	1.42	1.37
49	K	310	KC2	MG-NB	-4.11	1.97	2.05
49	X	314	KC2	CHC-C4B	4.11	1.46	1.38
51	9	317	A1ECV	C2A-C3A	4.11	1.46	1.40
46	P	317	LMG	O7-C10	4.11	1.45	1.34
49	O	317	KC2	CHC-C1C	4.11	1.48	1.39
49	x	312	KC2	CHC-C4B	4.11	1.46	1.38
49	T	315	KC2	CHC-C1C	4.11	1.48	1.39
49	R	314	KC2	CHC-C4B	4.11	1.46	1.38
49	2	314	KC2	CHC-C1C	4.11	1.48	1.39
49	V	315	KC2	CHC-C4B	4.11	1.46	1.38
49	6	317	KC2	CHC-C4B	4.11	1.46	1.38
49	F	307	KC2	CHC-C1C	4.11	1.48	1.39
49	7	322	KC2	CHC-C1C	4.11	1.48	1.39
51	x	310	A1ECV	CHB-C1B	4.11	1.47	1.39
49	5	313	KC2	CHC-C4B	4.11	1.46	1.38
49	9	311	KC2	MG-NB	-4.10	1.97	2.05
46	l	208	LMG	O8-C28	4.10	1.45	1.33
49	7	319	KC2	CHC-C1C	4.10	1.48	1.39
49	z	313	KC2	MG-NB	-4.10	1.97	2.05
49	8	319	KC2	MG-NB	-4.10	1.97	2.05
49	W	308	KC2	CHC-C4B	4.10	1.46	1.38
51	x	316	A1ECV	CHB-C1B	4.10	1.47	1.39
49	A	313	KC2	CHC-C1C	4.09	1.48	1.39
49	M	311	KC2	CHC-C1C	4.09	1.48	1.39
49	V	318	KC2	MG-NB	-4.09	1.97	2.05
46	l	208	LMG	O7-C10	4.09	1.45	1.34
46	W	302	LMG	O7-C10	4.09	1.45	1.34
49	5	314	KC2	CHC-C1C	4.09	1.48	1.39
51	Q	316	A1ECV	CHB-C1B	4.09	1.47	1.39
49	P	312	KC2	CHC-C1C	4.09	1.48	1.39
51	x	316	A1ECV	CHB-C4A	4.09	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	J	312	CLA	C1D-ND	4.09	1.42	1.37
39	0	318	CLA	C1D-ND	4.09	1.42	1.37
49	y	313	KC2	CHC-C1C	4.09	1.48	1.39
49	Y	309	KC2	MG-NB	-4.09	1.97	2.05
49	4	317	KC2	MG-NB	-4.09	1.97	2.05
49	P	310	KC2	CHC-C1C	4.09	1.48	1.39
49	H	314	KC2	CHC-C4B	4.09	1.46	1.38
49	H	311	KC2	CHC-C1C	4.08	1.48	1.39
49	L	321	KC2	CHC-C4B	4.08	1.46	1.38
49	0	314	KC2	CHC-C1C	4.08	1.48	1.39
49	X	312	KC2	CHC-C4B	4.08	1.46	1.38
49	3	315	KC2	MG-NB	-4.08	1.97	2.05
49	1	314	KC2	CHC-C4B	4.08	1.46	1.38
49	9	316	KC2	CHC-C4B	4.08	1.46	1.38
49	4	318	KC2	CHC-C4B	4.08	1.46	1.38
49	J	315	KC2	MG-NB	-4.08	1.97	2.05
51	R	310	A1ECV	CHB-C1B	4.08	1.47	1.39
49	C	312	KC2	CHC-C4B	4.08	1.46	1.38
49	L	312	KC2	CHC-C1C	4.08	1.48	1.39
49	K	313	KC2	CHC-C4B	4.08	1.46	1.38
49	3	315	KC2	CHC-C4B	4.08	1.46	1.38
49	Q	318	KC2	CHC-C1C	4.08	1.48	1.39
49	B	208	KC2	CHC-C1C	4.07	1.48	1.39
49	J	315	KC2	CHC-C4B	4.07	1.46	1.38
51	Y	306	A1ECV	CHB-C4A	4.07	1.46	1.39
49	4	324	KC2	CHC-C1C	4.07	1.48	1.39
49	T	312	KC2	MG-NB	-4.07	1.97	2.05
49	8	316	KC2	CHC-C4B	4.07	1.46	1.38
49	7	322	KC2	MG-NB	-4.07	1.97	2.05
49	x	313	KC2	CHC-C4B	4.07	1.46	1.38
49	z	315	KC2	CHC-C4B	4.07	1.46	1.38
49	4	320	KC2	CHC-C1C	4.07	1.48	1.39
49	R	312	KC2	CHC-C1C	4.07	1.48	1.39
49	4	324	KC2	MG-NB	-4.07	1.97	2.05
49	W	312	KC2	CHC-C1C	4.07	1.48	1.39
46	M	319	LMG	O7-C10	4.07	1.45	1.34
49	2	317	KC2	MG-NB	-4.07	1.97	2.05
51	L	318	A1ECV	CHC-C1C	4.07	1.46	1.39
49	7	322	KC2	CHC-C4B	4.07	1.46	1.38
49	R	318	KC2	MG-NB	-4.07	1.97	2.05
49	1	314	KC2	MG-NB	-4.07	1.97	2.05
49	R	318	KC2	CHC-C4B	4.06	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	G	311	KC2	MG-NB	-4.06	1.97	2.05
49	T	314	KC2	CHC-C4B	4.06	1.46	1.38
49	8	319	KC2	CHC-C4B	4.06	1.46	1.38
49	G	313	KC2	CHC-C1C	4.06	1.48	1.39
49	L	317	KC2	CHC-C4B	4.06	1.46	1.38
49	X	318	KC2	CHC-C4B	4.06	1.46	1.38
49	P	306	KC2	CHC-C1C	4.06	1.48	1.39
49	T	316	KC2	CHC-C4B	4.06	1.46	1.38
49	G	317	KC2	CHC-C1C	4.06	1.48	1.39
39	S	310	CLA	C1D-ND	4.06	1.42	1.37
49	W	314	KC2	CHC-C4B	4.06	1.46	1.38
39	a	813	CLA	C1D-ND	4.06	1.42	1.37
46	S	322	LMG	O8-C28	4.06	1.45	1.33
49	H	311	KC2	MG-NB	-4.06	1.97	2.05
49	X	318	KC2	MG-NB	-4.05	1.97	2.05
39	4	323	CLA	C1D-ND	4.05	1.42	1.37
46	Q	322	LMG	O7-C10	4.05	1.45	1.34
51	4	321	A1ECV	CHB-C4A	4.05	1.46	1.39
39	a	831	CLA	C1D-ND	4.05	1.42	1.37
49	G	311	KC2	CHC-C1C	4.05	1.48	1.39
49	M	313	KC2	MG-NB	-4.05	1.97	2.05
49	C	313	KC2	CHC-C4B	4.05	1.46	1.38
49	T	315	KC2	CHC-C4B	4.05	1.46	1.38
49	L	315	KC2	CHC-C1C	4.05	1.48	1.39
49	y	313	KC2	CHC-C4B	4.05	1.46	1.38
49	H	311	KC2	CHC-C4B	4.05	1.46	1.38
49	2	314	KC2	CHC-C4B	4.05	1.46	1.38
49	T	312	KC2	CHC-C1C	4.05	1.48	1.39
51	M	316	A1ECV	C2A-C3A	4.05	1.46	1.40
49	X	315	KC2	MG-NB	-4.05	1.97	2.05
39	x	317	CLA	C1D-ND	4.04	1.42	1.37
49	K	313	KC2	MG-NB	-4.04	1.97	2.05
49	y	316	KC2	CHC-C1C	4.04	1.48	1.39
49	5	305	KC2	CHC-C1C	4.04	1.48	1.39
49	4	318	KC2	MG-NB	-4.04	1.97	2.05
49	z	312	KC2	MG-NB	-4.04	1.97	2.05
39	7	325	CLA	C1D-ND	4.04	1.42	1.37
49	T	316	KC2	MG-NB	-4.04	1.97	2.05
51	S	312	A1ECV	CHD-C4C	4.04	1.46	1.39
49	Q	318	KC2	CHC-C4B	4.04	1.46	1.38
49	Z	310	KC2	CHC-C4B	4.04	1.46	1.38
49	V	320	KC2	CHC-C1C	4.04	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	8	320	KC2	MG-NB	-4.04	1.97	2.05
49	S	317	KC2	CHC-C1C	4.04	1.48	1.39
49	4	317	KC2	CHC-C4B	4.03	1.46	1.38
49	9	316	KC2	MG-NB	-4.03	1.97	2.05
49	4	320	KC2	CHC-C4B	4.03	1.46	1.38
49	V	308	KC2	CHC-C1C	4.03	1.48	1.39
49	y	316	KC2	CHC-C4B	4.03	1.46	1.38
49	R	312	KC2	CHC-C4B	4.03	1.46	1.38
39	O	316	CLA	C1D-ND	4.03	1.42	1.37
49	2	313	KC2	MG-NB	-4.03	1.97	2.05
49	P	312	KC2	CHC-C4B	4.03	1.46	1.38
39	b	851	CLA	C1D-ND	4.03	1.42	1.37
39	F	306	CLA	C1D-ND	4.03	1.42	1.37
48	E	304	A86	C30-C29	-4.03	1.25	1.32
51	y	317	A1ECV	CHB-C4A	4.03	1.46	1.39
49	M	311	KC2	MG-NB	-4.03	1.97	2.05
49	W	314	KC2	MG-NB	-4.02	1.97	2.05
49	L	315	KC2	MG-NB	-4.02	1.97	2.05
49	5	314	KC2	MG-NB	-4.02	1.97	2.05
51	9	317	A1ECV	CHD-C4C	4.02	1.46	1.39
39	F	315	CLA	C1D-ND	4.02	1.42	1.37
49	8	316	KC2	MG-NB	-4.02	1.97	2.05
49	P	306	KC2	CHC-C4B	4.02	1.46	1.38
49	S	317	KC2	CHC-C4B	4.02	1.46	1.38
49	3	321	KC2	MG-NB	-4.02	1.97	2.05
51	2	311	A1ECV	CHB-C4A	4.02	1.46	1.39
49	0	316	KC2	CHC-C1C	4.02	1.48	1.39
49	M	314	KC2	MG-NB	-4.02	1.97	2.05
49	L	317	KC2	MG-NB	-4.02	1.97	2.05
49	x	313	KC2	MG-NB	-4.02	1.97	2.05
49	6	314	KC2	CHC-C1C	4.02	1.48	1.39
49	W	308	KC2	MG-NB	-4.02	1.97	2.05
49	2	314	KC2	MG-NB	-4.02	1.97	2.05
39	P	314	CLA	C1D-ND	4.01	1.42	1.37
49	3	317	KC2	MG-NB	-4.01	1.97	2.05
49	F	307	KC2	CHC-C4B	4.01	1.46	1.38
49	G	317	KC2	CHC-C4B	4.01	1.46	1.38
49	H	314	KC2	MG-NB	-4.01	1.97	2.05
49	7	319	KC2	CHC-C4B	4.01	1.46	1.38
51	T	317	A1ECV	CHB-C1B	4.01	1.46	1.39
49	X	315	KC2	CHC-C4B	4.01	1.46	1.38
49	V	312	KC2	CHC-C4B	4.01	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	6	314	KC2	MG-NB	-4.01	1.97	2.05
51	Z	308	A1ECV	CHB-C4A	4.01	1.46	1.39
49	A	313	KC2	CHC-C4B	4.01	1.46	1.38
51	Y	306	A1ECV	CHB-C1B	4.01	1.46	1.39
49	K	310	KC2	CHC-C1C	4.01	1.48	1.39
49	Z	311	KC2	CHC-C4B	4.01	1.46	1.38
39	L	320	CLA	C1D-ND	4.01	1.42	1.37
39	8	310	CLA	C1D-ND	4.01	1.42	1.37
49	V	314	KC2	MG-NB	-4.01	1.97	2.05
49	Z	311	KC2	MG-NB	-4.01	1.97	2.05
39	B	207	CLA	C1D-ND	4.01	1.42	1.37
51	Z	308	A1ECV	CHB-C1B	4.01	1.46	1.39
39	8	311	CLA	C1D-ND	4.00	1.42	1.37
49	I	303	KC2	MG-NB	-4.00	1.97	2.05
49	R	312	KC2	MG-NB	-4.00	1.97	2.05
46	4	326	LMG	O7-C10	4.00	1.45	1.34
49	7	320	KC2	MG-NB	-4.00	1.97	2.05
51	5	309	A1ECV	CHB-C4A	4.00	1.46	1.39
49	2	317	KC2	CHC-C1C	4.00	1.48	1.39
51	R	313	A1ECV	CHD-C4C	4.00	1.46	1.39
49	F	311	KC2	CHC-C1C	4.00	1.48	1.39
49	M	307	KC2	CHC-C4B	4.00	1.46	1.38
39	W	319	CLA	C1D-ND	4.00	1.42	1.37
49	A	313	KC2	MG-NB	-4.00	1.97	2.05
39	O	311	CLA	C1D-ND	4.00	1.42	1.37
49	P	310	KC2	CHC-C4B	4.00	1.46	1.38
49	0	314	KC2	CHC-C4B	4.00	1.46	1.38
49	5	311	KC2	MG-NB	-3.99	1.97	2.05
39	C	309	CLA	C1D-ND	3.99	1.42	1.37
49	W	312	KC2	CHC-C4B	3.99	1.46	1.38
49	P	320	KC2	CHC-C4B	3.99	1.46	1.38
39	z	317	CLA	C1D-ND	3.99	1.42	1.37
49	6	316	KC2	MG-NB	-3.99	1.97	2.05
39	3	312	CLA	C1D-ND	3.99	1.42	1.37
49	I	312	KC2	CHC-C1C	3.99	1.48	1.39
49	2	313	KC2	CHC-C1C	3.99	1.48	1.39
49	C	312	KC2	MG-NB	-3.99	1.97	2.05
49	B	208	KC2	CHC-C4B	3.99	1.46	1.38
49	5	314	KC2	CHC-C4B	3.99	1.46	1.38
46	7	301	LMG	O7-C10	3.99	1.45	1.34
51	Q	316	A1ECV	CHC-C4B	3.99	1.46	1.39
39	J	313	CLA	C1D-ND	3.99	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	P	310	KC2	MG-NB	-3.99	1.97	2.05
48	T	301	A86	C30-C29	-3.98	1.25	1.32
49	0	317	KC2	MG-NB	-3.98	1.97	2.05
49	3	321	KC2	CHC-C1C	3.98	1.48	1.39
39	1	310	CLA	C1D-ND	3.98	1.42	1.37
49	I	312	KC2	MG-NB	-3.98	1.97	2.05
49	V	312	KC2	MG-NB	-3.98	1.97	2.05
51	W	317	A1ECV	CHB-C1B	3.98	1.46	1.39
49	x	312	KC2	MG-NB	-3.98	1.97	2.05
49	4	320	KC2	MG-NB	-3.98	1.97	2.05
39	Z	315	CLA	C1D-ND	3.98	1.42	1.37
49	B	208	KC2	MG-NB	-3.98	1.97	2.05
39	b	839	CLA	C1D-ND	3.98	1.42	1.37
39	M	321	CLA	C1D-ND	3.98	1.42	1.37
49	I	303	KC2	CHC-C1C	3.98	1.48	1.39
51	Q	319	A1ECV	C2C-C1C	3.98	1.48	1.41
39	S	320	CLA	C1D-ND	3.98	1.42	1.37
51	X	310	A1ECV	CHB-C4A	3.97	1.46	1.39
49	V	308	KC2	MG-NB	-3.97	1.97	2.05
49	3	318	KC2	MG-NB	-3.97	1.97	2.05
39	J	316	CLA	C1D-ND	3.97	1.42	1.37
39	T	320	CLA	C1D-ND	3.97	1.42	1.37
39	S	309	CLA	C1D-ND	3.97	1.42	1.37
49	W	312	KC2	MG-NB	-3.97	1.97	2.05
49	X	312	KC2	MG-NB	-3.97	1.97	2.05
49	4	324	KC2	CHC-C4B	3.97	1.46	1.38
49	T	314	KC2	MG-NB	-3.97	1.97	2.05
39	0	313	CLA	C1D-ND	3.97	1.42	1.37
49	0	314	KC2	MG-NB	-3.97	1.97	2.05
49	0	316	KC2	CHC-C4B	3.97	1.46	1.38
49	6	317	KC2	MG-NB	-3.97	1.97	2.05
49	M	311	KC2	CHC-C4B	3.97	1.46	1.38
39	A	314	CLA	C1D-ND	3.97	1.42	1.37
49	Z	310	KC2	MG-NB	-3.97	1.97	2.05
49	F	311	KC2	MG-NB	-3.97	1.97	2.05
49	5	311	KC2	CHC-C1C	3.96	1.48	1.39
39	a	824	CLA	C1D-ND	3.96	1.42	1.37
49	L	312	KC2	CHC-C4B	3.96	1.46	1.38
39	x	306	CLA	C1D-ND	3.96	1.42	1.37
51	G	316	A1ECV	CHC-C4B	3.96	1.46	1.39
39	8	322	CLA	C1D-ND	3.96	1.42	1.37
39	1	309	CLA	C1D-ND	3.96	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	320	CLA	C1D-ND	3.96	1.42	1.37
49	C	313	KC2	MG-NB	-3.96	1.97	2.05
39	1	319	CLA	C1D-ND	3.96	1.42	1.37
49	V	315	KC2	MG-NB	-3.96	1.97	2.05
51	7	317	A1ECV	CHB-C1B	3.96	1.46	1.39
39	J	317	CLA	C1D-ND	3.96	1.42	1.37
51	2	311	A1ECV	CHB-C1B	3.96	1.46	1.39
39	a	836	CLA	C1D-ND	3.96	1.42	1.37
39	B	209	CLA	C1D-ND	3.96	1.42	1.37
39	Y	305	CLA	C1D-ND	3.95	1.42	1.37
51	y	317	A1ECV	CHD-C1D	3.95	1.46	1.39
49	y	316	KC2	MG-NB	-3.95	1.98	2.05
46	S	322	LMG	O7-C10	3.95	1.45	1.34
49	Q	315	KC2	MG-NB	-3.95	1.98	2.05
39	P	311	CLA	C1D-ND	3.95	1.42	1.37
51	X	310	A1ECV	CHB-C1B	3.95	1.46	1.39
39	T	313	CLA	C1D-ND	3.95	1.42	1.37
49	6	314	KC2	CHC-C4B	3.95	1.46	1.38
49	z	315	KC2	MG-NB	-3.95	1.98	2.05
39	Q	317	CLA	C1D-ND	3.95	1.42	1.37
39	6	310	CLA	C1D-ND	3.95	1.42	1.37
49	G	317	KC2	MG-NB	-3.95	1.98	2.05
49	Q	318	KC2	MG-NB	-3.95	1.98	2.05
49	y	313	KC2	MG-NB	-3.95	1.98	2.05
39	y	312	CLA	C1D-ND	3.95	1.42	1.37
49	G	313	KC2	MG-NB	-3.95	1.98	2.05
39	D	309	CLA	C1D-ND	3.95	1.42	1.37
39	J	308	CLA	C1D-ND	3.95	1.42	1.37
39	Y	310	CLA	C1D-ND	3.95	1.42	1.37
39	Z	309	CLA	C1D-ND	3.94	1.42	1.37
39	B	205	CLA	C1D-ND	3.94	1.42	1.37
39	E	312	CLA	C1D-ND	3.94	1.42	1.37
39	O	312	CLA	C1D-ND	3.94	1.42	1.37
49	G	313	KC2	CHC-C4B	3.94	1.46	1.38
39	A	308	CLA	C1D-ND	3.94	1.42	1.37
39	1	317	CLA	C1D-ND	3.94	1.42	1.37
51	y	311	A1ECV	CHB-C1B	3.94	1.46	1.39
49	0	316	KC2	MG-NB	-3.94	1.98	2.05
49	F	307	KC2	MG-NB	-3.94	1.98	2.05
39	1	308	CLA	C1D-ND	3.94	1.42	1.37
39	8	318	CLA	C1D-ND	3.94	1.42	1.37
49	M	307	KC2	MG-NB	-3.94	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	P	320	KC2	MG-NB	-3.94	1.98	2.05
51	S	318	A1ECV	CHD-C1D	3.94	1.46	1.39
39	E	309	CLA	C1D-ND	3.94	1.42	1.37
39	L	310	CLA	C1D-ND	3.94	1.42	1.37
39	b	815	CLA	C1D-ND	3.94	1.42	1.37
49	3	321	KC2	CHC-C4B	3.94	1.46	1.38
46	F	317	LMG	O7-C10	3.94	1.45	1.34
39	f	802	CLA	C1D-ND	3.94	1.42	1.37
39	4	319	CLA	C1D-ND	3.93	1.42	1.37
39	y	319	CLA	C1D-ND	3.93	1.42	1.37
39	H	307	CLA	C1D-ND	3.93	1.42	1.37
39	6	313	CLA	C1D-ND	3.93	1.42	1.37
51	P	315	A1ECV	CHC-C4B	3.93	1.46	1.39
51	6	320	A1ECV	CHD-C1D	3.93	1.46	1.39
39	U	212	CLA	C1D-ND	3.93	1.42	1.37
39	z	306	CLA	C1D-ND	3.93	1.42	1.37
39	Z	305	CLA	C1D-ND	3.93	1.42	1.37
39	2	307	CLA	C1D-ND	3.93	1.42	1.37
39	9	319	CLA	C1D-ND	3.93	1.42	1.37
39	P	316	CLA	C1D-ND	3.93	1.42	1.37
39	T	309	CLA	C1D-ND	3.93	1.42	1.37
51	Z	314	A1ECV	CHB-C4A	3.93	1.46	1.39
51	X	313	A1ECV	CHB-C1B	3.93	1.46	1.39
39	S	316	CLA	C1D-ND	3.93	1.42	1.37
50	7	303	A1EB1	C30-C29	-3.93	1.25	1.32
49	8	317	KC2	MG-NB	-3.93	1.98	2.05
39	8	321	CLA	C1D-ND	3.93	1.42	1.37
39	A	307	CLA	C1D-ND	3.93	1.42	1.37
39	a	828	CLA	C1D-ND	3.93	1.42	1.37
39	b	825	CLA	C1D-ND	3.93	1.42	1.37
39	9	315	CLA	C1D-ND	3.93	1.42	1.37
39	z	311	CLA	C1D-ND	3.93	1.42	1.37
39	a	833	CLA	C1D-ND	3.92	1.42	1.37
39	x	307	CLA	C1D-ND	3.92	1.42	1.37
39	2	310	CLA	C1D-ND	3.92	1.42	1.37
39	C	308	CLA	C1D-ND	3.92	1.42	1.37
39	L	319	CLA	C1D-ND	3.92	1.42	1.37
39	y	318	CLA	C1D-ND	3.92	1.42	1.37
39	x	311	CLA	C1D-ND	3.92	1.42	1.37
49	S	315	KC2	MG-NB	-3.92	1.98	2.05
39	Y	313	CLA	C1D-ND	3.92	1.42	1.37
39	a	822	CLA	C1D-ND	3.92	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	5	305	KC2	CHC-C4B	3.92	1.46	1.38
51	7	317	A1ECV	CHD-C4C	3.92	1.46	1.39
51	S	312	A1ECV	CHB-C4A	3.92	1.46	1.39
49	L	315	KC2	CHC-C4B	3.92	1.46	1.38
39	a	807	CLA	C1D-ND	3.92	1.42	1.37
39	Y	304	CLA	C1D-ND	3.92	1.42	1.37
49	K	310	KC2	CHC-C4B	3.92	1.46	1.38
39	U	215	CLA	C1D-ND	3.92	1.42	1.37
39	0	322	CLA	C1D-ND	3.92	1.42	1.37
51	W	317	A1ECV	CHB-C4A	3.92	1.46	1.39
49	7	319	KC2	MG-NB	-3.91	1.98	2.05
49	S	317	KC2	MG-NB	-3.91	1.98	2.05
39	E	318	CLA	C1D-ND	3.91	1.42	1.37
39	Y	302	CLA	C1D-ND	3.91	1.42	1.37
49	G	311	KC2	CHC-C4B	3.91	1.46	1.38
39	a	821	CLA	C1D-ND	3.91	1.42	1.37
39	6	322	CLA	C1D-ND	3.91	1.42	1.37
39	b	835	CLA	C1D-ND	3.91	1.42	1.37
39	1	316	CLA	C1D-ND	3.91	1.42	1.37
39	Y	307	CLA	C1D-ND	3.91	1.42	1.37
39	a	830	CLA	C1D-ND	3.91	1.42	1.37
39	W	318	CLA	C1D-ND	3.91	1.42	1.37
39	J	307	CLA	C1D-ND	3.91	1.42	1.37
39	K	309	CLA	C1D-ND	3.91	1.42	1.37
39	M	318	CLA	C1D-ND	3.91	1.42	1.37
39	2	315	CLA	C1D-ND	3.91	1.42	1.37
51	4	315	A1ECV	CHD-C4C	3.90	1.46	1.39
51	O	315	A1ECV	CHC-C4B	3.90	1.46	1.39
51	9	317	A1ECV	CHB-C4A	3.90	1.46	1.39
39	3	323	CLA	C1D-ND	3.90	1.42	1.37
39	I	313	CLA	C1D-ND	3.90	1.42	1.37
51	9	314	A1ECV	CHB-C1B	3.90	1.46	1.39
49	2	313	KC2	CHC-C4B	3.90	1.46	1.38
39	b	817	CLA	C1D-ND	3.90	1.42	1.37
39	K	306	CLA	C1D-ND	3.90	1.42	1.37
39	M	310	CLA	C1D-ND	3.90	1.42	1.37
39	Z	312	CLA	C1D-ND	3.90	1.42	1.37
49	V	320	KC2	CHC-C4B	3.90	1.46	1.38
39	H	316	CLA	C1D-ND	3.90	1.42	1.37
39	z	308	CLA	C1D-ND	3.90	1.42	1.37
39	b	819	CLA	C1D-ND	3.90	1.42	1.37
39	o	205	CLA	C1D-ND	3.90	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	C	304	CLA	C1D-ND	3.90	1.42	1.37
39	C	305	CLA	C1D-ND	3.90	1.42	1.37
39	S	308	CLA	C1D-ND	3.90	1.42	1.37
39	o	202	CLA	C1D-ND	3.90	1.42	1.37
39	3	319	CLA	C1D-ND	3.90	1.42	1.37
51	S	312	A1ECV	CHB-C1B	3.90	1.46	1.39
39	E	315	CLA	C1D-ND	3.90	1.42	1.37
39	z	314	CLA	C1D-ND	3.90	1.42	1.37
39	9	307	CLA	C1D-ND	3.90	1.42	1.37
39	y	309	CLA	C1D-ND	3.90	1.42	1.37
39	0	310	CLA	C1D-ND	3.89	1.42	1.37
39	Y	311	CLA	C1D-ND	3.89	1.42	1.37
49	5	311	KC2	CHC-C4B	3.89	1.45	1.38
39	T	319	CLA	C1D-ND	3.89	1.42	1.37
39	z	318	CLA	C1D-ND	3.89	1.42	1.37
39	D	318	CLA	C1D-ND	3.89	1.42	1.37
39	V	316	CLA	C1D-ND	3.89	1.42	1.37
39	7	313	CLA	C1D-ND	3.89	1.42	1.37
39	L	308	CLA	C1D-ND	3.89	1.42	1.37
49	V	308	KC2	CHC-C4B	3.89	1.45	1.38
46	F	320	LMG	O7-C10	3.89	1.45	1.34
39	7	321	CLA	C1D-ND	3.89	1.42	1.37
39	F	312	CLA	C1D-ND	3.89	1.42	1.37
39	b	820	CLA	C1D-ND	3.89	1.42	1.37
39	U	214	CLA	C1D-ND	3.89	1.42	1.37
51	z	316	A1ECV	CHB-C4A	3.89	1.46	1.39
51	5	309	A1ECV	CHC-C4B	3.89	1.46	1.39
49	T	312	KC2	CHC-C4B	3.88	1.45	1.38
39	6	312	CLA	C1D-ND	3.88	1.42	1.37
39	a	808	CLA	C1D-ND	3.88	1.42	1.37
39	2	318	CLA	C1D-ND	3.88	1.42	1.37
39	a	820	CLA	C1D-ND	3.88	1.42	1.37
39	A	315	CLA	C1D-ND	3.88	1.42	1.37
49	9	313	KC2	CHC-C1C	3.88	1.48	1.39
39	b	823	CLA	C1D-ND	3.88	1.42	1.37
39	X	311	CLA	C1D-ND	3.88	1.42	1.37
39	5	316	CLA	C1D-ND	3.88	1.42	1.37
49	Q	315	KC2	CHC-C4B	3.88	1.45	1.38
39	a	837	CLA	C1D-ND	3.88	1.42	1.37
39	L	309	CLA	C1D-ND	3.88	1.42	1.37
39	3	320	CLA	C1D-ND	3.88	1.42	1.37
39	l	203	CLA	C1D-ND	3.88	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Q	310	CLA	C1D-ND	3.88	1.42	1.37
49	2	317	KC2	CHC-C4B	3.88	1.45	1.38
39	h	201	CLA	C1D-ND	3.88	1.42	1.37
39	a	811	CLA	C1D-ND	3.88	1.42	1.37
39	A	305	CLA	C1D-ND	3.88	1.42	1.37
51	X	313	A1ECV	CHD-C4C	3.88	1.45	1.39
39	z	307	CLA	C1D-ND	3.88	1.42	1.37
39	x	314	CLA	C1D-ND	3.87	1.42	1.37
39	a	829	CLA	C1D-ND	3.87	1.42	1.37
39	0	323	CLA	C1D-ND	3.87	1.42	1.37
51	5	312	A1ECV	CHC-C4B	3.87	1.46	1.39
49	I	312	KC2	CHC-C4B	3.87	1.45	1.38
51	z	310	A1ECV	CHB-C4A	3.87	1.45	1.39
39	Q	321	CLA	C1D-ND	3.87	1.42	1.37
39	R	316	CLA	C1D-ND	3.87	1.42	1.37
39	9	309	CLA	C1D-ND	3.87	1.42	1.37
39	I	308	CLA	C1D-ND	3.87	1.42	1.37
39	y	307	CLA	C1D-ND	3.87	1.42	1.37
39	E	317	CLA	C1D-ND	3.87	1.42	1.37
39	T	311	CLA	C1D-ND	3.87	1.42	1.37
51	S	318	A1ECV	CHC-C4B	3.87	1.46	1.39
39	A	311	CLA	C1D-ND	3.87	1.42	1.37
39	P	309	CLA	C1D-ND	3.87	1.42	1.37
39	V	319	CLA	C1D-ND	3.87	1.42	1.37
39	I	314	CLA	C1D-ND	3.87	1.42	1.37
51	z	310	A1ECV	CHB-C1B	3.87	1.46	1.39
51	4	321	A1ECV	CHD-C1D	3.87	1.46	1.39
39	b	810	CLA	C1D-ND	3.87	1.42	1.37
39	b	841	CLA	C1D-ND	3.86	1.42	1.37
39	o	203	CLA	C1D-ND	3.86	1.42	1.37
39	J	310	CLA	C1D-ND	3.86	1.42	1.37
39	W	313	CLA	C1D-ND	3.86	1.42	1.37
39	X	307	CLA	C1D-ND	3.86	1.42	1.37
39	E	319	CLA	C1D-ND	3.86	1.42	1.37
39	0	320	CLA	C1D-ND	3.86	1.42	1.37
39	G	310	CLA	C1D-ND	3.86	1.42	1.37
39	Q	312	CLA	C1D-ND	3.86	1.42	1.37
39	U	209	CLA	C1D-ND	3.86	1.42	1.37
39	4	311	CLA	C1D-ND	3.86	1.42	1.37
39	H	309	CLA	C1D-ND	3.86	1.42	1.37
49	Q	313	KC2	CHC-C1C	3.86	1.48	1.39
51	7	317	A1ECV	CHB-C4A	3.86	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Z	306	CLA	C1D-ND	3.86	1.42	1.37
49	V	320	KC2	MG-NB	-3.86	1.98	2.05
39	S	313	CLA	C1D-ND	3.86	1.42	1.37
39	1	311	CLA	C1D-ND	3.85	1.42	1.37
39	Y	314	CLA	C1D-ND	3.85	1.42	1.37
39	D	315	CLA	C1D-ND	3.85	1.42	1.37
39	3	311	CLA	C1D-ND	3.85	1.42	1.37
51	Z	308	A1ECV	CHD-C1D	3.85	1.46	1.39
39	a	835	CLA	C1D-ND	3.85	1.42	1.37
39	b	828	CLA	C1D-ND	3.85	1.42	1.37
39	F	309	CLA	C1D-ND	3.85	1.42	1.37
39	o	201	CLA	C1D-ND	3.85	1.42	1.37
51	y	311	A1ECV	CHB-C4A	3.85	1.45	1.39
39	6	311	CLA	C1D-ND	3.85	1.42	1.37
39	a	810	CLA	C1D-ND	3.85	1.42	1.37
39	E	307	CLA	C1D-ND	3.85	1.42	1.37
39	X	317	CLA	C1D-ND	3.85	1.42	1.37
39	Y	303	CLA	C1D-ND	3.85	1.42	1.37
39	Q	320	CLA	C1D-ND	3.84	1.42	1.37
39	I	315	CLA	C1D-ND	3.84	1.42	1.37
49	L	314	KC2	MG-NB	-3.84	1.98	2.05
39	5	307	CLA	C1D-ND	3.84	1.42	1.37
51	7	323	A1ECV	CHC-C4B	3.84	1.46	1.39
39	b	837	CLA	C1D-ND	3.84	1.42	1.37
39	y	308	CLA	C1D-ND	3.84	1.42	1.37
39	6	321	CLA	C1D-ND	3.84	1.42	1.37
39	b	803	CLA	C1D-ND	3.84	1.42	1.37
39	i	103	CLA	C1D-ND	3.84	1.42	1.37
39	P	308	CLA	C1D-ND	3.84	1.42	1.37
39	y	315	CLA	C1D-ND	3.84	1.42	1.37
39	Z	304	CLA	C1D-ND	3.84	1.42	1.37
51	Q	319	A1ECV	CHB-C1B	3.84	1.46	1.39
49	T	315	KC2	MG-NB	-3.84	1.98	2.05
39	B	204	CLA	C1D-ND	3.84	1.42	1.37
39	M	309	CLA	C1D-ND	3.84	1.42	1.37
39	7	324	CLA	C1D-ND	3.84	1.42	1.37
39	b	834	CLA	C1D-ND	3.84	1.42	1.37
39	b	838	CLA	C1D-ND	3.84	1.42	1.37
39	2	309	CLA	C1D-ND	3.84	1.42	1.37
39	a	832	CLA	C1D-ND	3.84	1.42	1.37
39	j	101	CLA	C1D-ND	3.84	1.42	1.37
51	9	314	A1ECV	CHD-C4C	3.84	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	f	803	CLA	C1D-ND	3.84	1.42	1.37
39	5	310	CLA	C1D-ND	3.84	1.42	1.37
51	4	315	A1ECV	CHB-C1B	3.83	1.46	1.39
39	E	310	CLA	C1D-ND	3.83	1.42	1.37
39	3	316	CLA	C1D-ND	3.83	1.42	1.37
39	F	316	CLA	C1D-ND	3.83	1.42	1.37
39	W	316	CLA	C1D-ND	3.83	1.42	1.37
39	3	322	CLA	C1D-ND	3.83	1.42	1.37
39	b	802	CLA	C1D-ND	3.83	1.42	1.37
39	I	316	CLA	C1D-ND	3.83	1.42	1.37
39	D	319	CLA	C1D-ND	3.83	1.42	1.37
39	H	306	CLA	C1D-ND	3.83	1.42	1.37
39	K	308	CLA	C1D-ND	3.83	1.42	1.37
51	x	310	A1ECV	CHD-C1D	3.83	1.46	1.39
51	Y	306	A1ECV	CHD-C1D	3.83	1.46	1.39
39	K	307	CLA	C1D-ND	3.83	1.42	1.37
39	F	314	CLA	C1D-ND	3.83	1.42	1.37
49	F	311	KC2	CHC-C4B	3.83	1.45	1.38
39	C	307	CLA	C1D-ND	3.83	1.42	1.37
39	x	318	CLA	C1D-ND	3.83	1.42	1.37
39	H	308	CLA	C1D-ND	3.83	1.42	1.37
39	b	814	CLA	C1D-ND	3.82	1.42	1.37
39	4	322	CLA	C1D-ND	3.82	1.42	1.37
51	V	317	A1ECV	CHD-C1D	3.82	1.46	1.39
50	L	303	A1EB1	C30-C29	-3.82	1.25	1.32
39	A	306	CLA	C1D-ND	3.82	1.42	1.37
39	G	318	CLA	C1D-ND	3.82	1.42	1.37
39	6	315	CLA	C1D-ND	3.82	1.42	1.37
39	b	818	CLA	C1D-ND	3.82	1.42	1.37
39	4	312	CLA	C1D-ND	3.82	1.42	1.37
39	9	320	CLA	C1D-ND	3.82	1.42	1.37
39	K	311	CLA	C1D-ND	3.82	1.42	1.37
39	V	311	CLA	C1D-ND	3.82	1.42	1.37
51	X	310	A1ECV	CHD-C1D	3.82	1.46	1.39
39	D	317	CLA	C1D-ND	3.82	1.42	1.37
39	E	314	CLA	C1D-ND	3.82	1.42	1.37
39	U	211	CLA	C1D-ND	3.82	1.42	1.37
39	a	806	CLA	C1D-ND	3.82	1.42	1.37
39	V	310	CLA	C1D-ND	3.82	1.42	1.37
39	D	314	CLA	C1D-ND	3.82	1.42	1.37
39	D	312	CLA	C1D-ND	3.81	1.42	1.37
39	R	315	CLA	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	k	203	CLA	C1D-ND	3.81	1.42	1.37
51	Z	314	A1ECV	CHC-C4B	3.81	1.46	1.39
39	a	816	CLA	C1D-ND	3.81	1.42	1.37
51	7	323	A1ECV	CHD-C4C	3.81	1.45	1.39
39	o	206	CLA	C1D-ND	3.81	1.42	1.37
39	R	308	CLA	C1D-ND	3.81	1.42	1.37
39	3	314	CLA	C1D-ND	3.81	1.42	1.37
39	a	825	CLA	C1D-ND	3.81	1.42	1.37
39	J	311	CLA	C1D-ND	3.81	1.42	1.37
39	O	318	CLA	C1D-ND	3.81	1.42	1.37
39	3	313	CLA	C1D-ND	3.81	1.42	1.37
39	U	210	CLA	C1D-ND	3.81	1.42	1.37
39	7	315	CLA	C1D-ND	3.81	1.42	1.37
39	a	847	CLA	C1D-ND	3.81	1.42	1.37
48	1	307	A86	C30-C29	-3.81	1.25	1.32
51	T	317	A1ECV	CHD-C1D	3.81	1.46	1.39
51	4	321	A1ECV	CHD-C4C	3.81	1.45	1.39
39	F	310	CLA	C1D-ND	3.81	1.42	1.37
39	J	314	CLA	C1D-ND	3.81	1.42	1.37
39	W	310	CLA	C1D-ND	3.81	1.42	1.37
51	x	316	A1ECV	CHD-C1D	3.81	1.46	1.39
51	z	316	A1ECV	CHD-C1D	3.81	1.46	1.39
39	K	314	CLA	C1D-ND	3.81	1.42	1.37
51	Q	319	A1ECV	CHD-C1D	3.81	1.46	1.39
39	4	313	CLA	C1D-ND	3.81	1.42	1.37
49	I	303	KC2	CHC-C4B	3.80	1.45	1.38
39	Z	307	CLA	C1D-ND	3.80	1.42	1.37
39	2	316	CLA	C1D-ND	3.80	1.42	1.37
39	b	842	CLA	C1D-ND	3.80	1.42	1.37
51	Y	312	A1ECV	CHB-C4A	3.80	1.45	1.39
49	Q	315	KC2	CHC-C1C	3.80	1.47	1.39
39	a	817	CLA	C1D-ND	3.80	1.42	1.37
39	b	822	CLA	C1D-ND	3.80	1.42	1.37
39	Q	321	CLA	C4B-NB	3.80	1.42	1.37
39	W	311	CLA	C1D-ND	3.80	1.42	1.37
39	2	308	CLA	C1D-ND	3.80	1.42	1.37
39	U	208	CLA	C1D-ND	3.80	1.42	1.37
39	M	315	CLA	C1D-ND	3.80	1.42	1.37
39	l	201	CLA	C1D-ND	3.79	1.42	1.37
39	S	319	CLA	C1D-ND	3.79	1.42	1.37
51	0	321	A1ECV	CHD-C4C	3.79	1.45	1.39
39	F	321	CLA	C1D-ND	3.79	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	6	318	CLA	C1D-ND	3.79	1.42	1.37
39	E	316	CLA	C1D-ND	3.79	1.42	1.37
39	a	838	CLA	C1D-ND	3.79	1.42	1.37
39	b	832	CLA	C1D-ND	3.79	1.42	1.37
39	7	314	CLA	C1D-ND	3.79	1.42	1.37
51	M	316	A1ECV	CHD-C4C	3.79	1.45	1.39
39	a	805	CLA	C1D-ND	3.79	1.42	1.37
39	a	815	CLA	C1D-ND	3.79	1.42	1.37
39	I	310	CLA	C1D-ND	3.79	1.42	1.37
39	T	313	CLA	C4B-NB	3.79	1.42	1.37
39	I	309	CLA	C1D-ND	3.79	1.42	1.37
39	G	312	CLA	C1D-ND	3.79	1.42	1.37
39	L	316	CLA	C1D-ND	3.78	1.42	1.37
39	9	310	CLA	C1D-ND	3.78	1.42	1.37
51	x	310	A1ECV	CHB-C4A	3.78	1.45	1.39
51	y	311	A1ECV	CHD-C1D	3.78	1.46	1.39
39	b	821	CLA	C1D-ND	3.78	1.42	1.37
39	b	809	CLA	C1D-ND	3.78	1.42	1.37
39	a	818	CLA	C1D-ND	3.78	1.42	1.37
39	b	808	CLA	C1D-ND	3.78	1.42	1.37
39	E	306	CLA	C1D-ND	3.78	1.42	1.37
39	G	314	CLA	C1D-ND	3.78	1.42	1.37
51	E	311	A1ECV	CHD-C4C	3.78	1.45	1.39
51	1	318	A1ECV	CHB-C4A	3.78	1.45	1.39
39	L	311	CLA	C1D-ND	3.78	1.42	1.37
39	x	309	CLA	C1D-ND	3.78	1.42	1.37
51	2	311	A1ECV	CHD-C1D	3.78	1.46	1.39
39	i	101	CLA	C1D-ND	3.78	1.42	1.37
39	D	310	CLA	C1D-ND	3.78	1.42	1.37
39	X	309	CLA	C1D-ND	3.78	1.42	1.37
51	R	310	A1ECV	CHD-C1D	3.77	1.46	1.39
39	a	802	CLA	C1D-ND	3.77	1.42	1.37
39	A	309	CLA	C1D-ND	3.77	1.42	1.37
39	8	312	CLA	C1D-ND	3.77	1.42	1.37
39	z	309	CLA	C1D-ND	3.77	1.42	1.37
39	D	313	CLA	C1D-ND	3.77	1.42	1.37
39	b	840	CLA	C1D-ND	3.77	1.42	1.37
39	E	308	CLA	C1D-ND	3.77	1.42	1.37
39	8	313	CLA	C1D-ND	3.77	1.42	1.37
39	X	308	CLA	C1D-ND	3.77	1.42	1.37
51	Q	316	A1ECV	CHD-C1D	3.76	1.46	1.39
39	T	310	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	8	315	CLA	C1D-ND	3.76	1.42	1.37
39	K	312	CLA	C1D-ND	3.76	1.42	1.37
51	2	311	A1ECV	CHC-C4B	3.76	1.46	1.39
39	a	812	CLA	C1D-ND	3.76	1.42	1.37
51	Q	316	A1ECV	CHB-C4A	3.76	1.45	1.39
39	a	809	CLA	C1D-ND	3.76	1.42	1.37
51	R	313	A1ECV	CHC-C4B	3.75	1.46	1.39
39	M	317	CLA	C1D-ND	3.75	1.42	1.37
39	E	313	CLA	C1D-ND	3.75	1.42	1.37
39	L	313	CLA	C1D-ND	3.75	1.42	1.37
39	R	311	CLA	C1D-ND	3.75	1.42	1.37
49	Q	313	KC2	CHC-C4B	3.75	1.45	1.38
39	T	318	CLA	C1D-ND	3.75	1.42	1.37
39	F	308	CLA	C1D-ND	3.75	1.42	1.37
51	R	310	A1ECV	CHC-C4B	3.75	1.46	1.39
51	x	310	A1ECV	CHC-C4B	3.75	1.46	1.39
39	b	836	CLA	C1D-ND	3.75	1.42	1.37
39	Z	316	CLA	C1D-ND	3.75	1.42	1.37
39	M	312	CLA	C1D-ND	3.74	1.42	1.37
51	R	310	A1ECV	CHD-C4C	3.74	1.45	1.39
39	1	313	CLA	C1D-ND	3.74	1.42	1.37
50	G	304	A1EB1	C30-C29	-3.74	1.25	1.32
51	1	318	A1ECV	CHC-C4B	3.74	1.46	1.39
39	R	307	CLA	C1D-ND	3.74	1.42	1.37
51	4	315	A1ECV	CHB-C4A	3.74	1.45	1.39
39	R	309	CLA	C1D-ND	3.74	1.42	1.37
51	5	312	A1ECV	CHD-C1D	3.74	1.46	1.39
39	H	313	CLA	C1D-ND	3.74	1.42	1.37
51	z	310	A1ECV	CHD-C1D	3.74	1.46	1.39
39	b	811	CLA	C1D-ND	3.73	1.42	1.37
39	a	823	CLA	C1D-ND	3.73	1.42	1.37
39	k	201	CLA	C1D-ND	3.73	1.42	1.37
39	b	830	CLA	C1D-ND	3.73	1.42	1.37
39	a	834	CLA	C1D-ND	3.73	1.42	1.37
51	M	316	A1ECV	CHD-C1D	3.73	1.46	1.39
51	1	318	A1ECV	CHD-C1D	3.73	1.46	1.39
39	O	314	CLA	C1D-ND	3.73	1.42	1.37
51	Q	319	A1ECV	CHD-C4C	3.73	1.45	1.39
51	9	314	A1ECV	CHC-C4B	3.73	1.46	1.39
39	F	313	CLA	C1D-ND	3.73	1.42	1.37
50	7	305	A1EB1	C30-C29	-3.73	1.25	1.32
50	S	302	A1EB1	C30-C29	-3.72	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	b	816	CLA	C1D-ND	3.72	1.42	1.37
39	V	309	CLA	C1D-ND	3.72	1.42	1.37
39	5	306	CLA	C1D-ND	3.72	1.42	1.37
51	6	320	A1ECV	CHC-C4B	3.72	1.46	1.39
51	Y	306	A1ECV	CHC-C4B	3.72	1.46	1.39
39	b	841	CLA	C4B-NB	3.72	1.42	1.37
39	U	213	CLA	C1D-ND	3.72	1.42	1.37
51	W	317	A1ECV	CHC-C4B	3.72	1.46	1.39
51	x	316	A1ECV	CHC-C4B	3.72	1.46	1.39
39	W	309	CLA	C1D-ND	3.72	1.42	1.37
39	a	804	CLA	C1D-ND	3.71	1.42	1.37
39	C	311	CLA	C1D-ND	3.71	1.42	1.37
51	Q	319	A1ECV	CHB-C4A	3.71	1.45	1.39
39	b	806	CLA	C1D-ND	3.71	1.42	1.37
39	x	308	CLA	C1D-ND	3.71	1.42	1.37
51	W	317	A1ECV	CHD-C1D	3.71	1.46	1.39
39	O	311	CLA	C4B-NB	3.71	1.42	1.37
39	I	311	CLA	C1D-ND	3.71	1.42	1.37
39	b	812	CLA	C1D-ND	3.70	1.42	1.37
39	b	805	CLA	C1D-ND	3.70	1.42	1.37
39	D	316	CLA	C1D-ND	3.70	1.42	1.37
50	F	304	A1EB1	C30-C29	-3.70	1.25	1.32
39	a	827	CLA	C1D-ND	3.70	1.42	1.37
49	O	317	KC2	CHD-C1D	3.70	1.47	1.39
50	S	303	A1EB1	C30-C29	-3.69	1.25	1.32
48	K	301	A86	C30-C29	-3.69	1.25	1.32
51	M	316	A1ECV	CHC-C4B	3.69	1.46	1.39
48	7	307	A86	C30-C29	-3.69	1.25	1.32
52	P	318	A1EB4	C30-C29	-3.69	1.25	1.32
51	L	318	A1ECV	CHD-C1D	3.69	1.46	1.39
39	O	310	CLA	C1D-ND	3.69	1.42	1.37
39	4	314	CLA	C1D-ND	3.69	1.42	1.37
50	3	302	A1EB1	C30-C29	-3.69	1.25	1.32
51	S	312	A1ECV	CHC-C4B	3.69	1.46	1.39
51	Z	308	A1ECV	CHC-C4B	3.69	1.46	1.39
51	y	311	A1ECV	CHC-C4B	3.69	1.46	1.39
50	E	301	A1EB1	C30-C29	-3.69	1.25	1.32
39	y	309	CLA	C4B-NB	3.69	1.42	1.37
39	a	814	CLA	C1D-ND	3.68	1.42	1.37
39	b	826	CLA	C1D-ND	3.68	1.42	1.37
39	O	313	CLA	C1D-ND	3.68	1.42	1.37
51	y	317	A1ECV	CHC-C4B	3.68	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	9	313	KC2	CHC-C4B	3.68	1.45	1.38
39	l	205	CLA	C1D-ND	3.68	1.42	1.37
48	0	301	A86	C30-C29	-3.68	1.25	1.32
51	X	310	A1ECV	CHC-C4B	3.68	1.46	1.39
48	9	303	A86	C30-C29	-3.67	1.25	1.32
48	P	302	A86	C30-C29	-3.67	1.25	1.32
39	B	206	CLA	C1D-ND	3.67	1.42	1.37
51	5	312	A1ECV	CHB-C4A	3.67	1.45	1.39
39	y	310	CLA	C1D-ND	3.67	1.42	1.37
48	G	305	A86	C30-C29	-3.66	1.25	1.32
51	z	310	A1ECV	CHC-C4B	3.66	1.46	1.39
51	7	317	A1ECV	CHC-C4B	3.66	1.46	1.39
51	V	317	A1ECV	CHD-C4C	3.66	1.45	1.39
39	a	803	CLA	C1D-ND	3.66	1.42	1.37
39	U	207	CLA	C1D-ND	3.66	1.42	1.37
51	Y	312	A1ECV	CHD-C1D	3.66	1.46	1.39
51	W	317	A1ECV	CHD-C4C	3.65	1.45	1.39
39	J	309	CLA	C1D-ND	3.65	1.42	1.37
50	6	308	A1EB1	C30-C29	-3.64	1.25	1.32
49	0	319	KC2	CHD-C1D	3.64	1.47	1.39
39	C	306	CLA	C1D-ND	3.64	1.42	1.37
49	5	305	KC2	MG-NB	-3.64	1.98	2.05
51	4	315	A1ECV	CHC-C4B	3.64	1.46	1.39
51	4	321	A1ECV	CHC-C4B	3.64	1.46	1.39
51	V	317	A1ECV	CHC-C4B	3.64	1.46	1.39
39	b	827	CLA	C1D-ND	3.64	1.42	1.37
39	5	308	CLA	C1D-ND	3.64	1.42	1.37
39	Q	321	CLA	C3B-C4B	3.63	1.51	1.42
51	Y	312	A1ECV	CHC-C4B	3.63	1.46	1.39
39	b	824	CLA	C1D-ND	3.63	1.42	1.37
48	S	307	A86	C30-C29	-3.63	1.25	1.32
50	Q	307	A1EB1	C30-C29	-3.63	1.25	1.32
51	4	315	A1ECV	CHD-C1D	3.63	1.46	1.39
51	G	316	A1ECV	CHD-C1D	3.62	1.46	1.39
39	b	813	CLA	C1D-ND	3.62	1.42	1.37
39	4	316	CLA	C1D-ND	3.62	1.42	1.37
50	R	303	A1EB1	C30-C29	-3.62	1.25	1.32
50	V	305	A1EB1	C30-C29	-3.62	1.25	1.32
51	Z	314	A1ECV	CHD-C1D	3.62	1.46	1.39
50	0	303	A1EB1	C30-C29	-3.62	1.25	1.32
51	X	313	A1ECV	CHC-C4B	3.62	1.46	1.39
39	H	310	CLA	C1D-ND	3.61	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	K	302	A1EB1	C30-C29	-3.61	1.25	1.32
39	0	315	CLA	C1D-ND	3.61	1.42	1.37
39	I	301	CLA	C1D-ND	3.61	1.42	1.37
39	A	312	CLA	C1D-ND	3.61	1.42	1.37
51	P	315	A1ECV	CHD-C1D	3.61	1.46	1.39
39	H	315	CLA	C1D-ND	3.61	1.42	1.37
39	M	308	CLA	C1D-ND	3.61	1.42	1.37
51	6	320	A1ECV	CHD-C4C	3.61	1.45	1.39
48	P	303	A86	C30-C29	-3.61	1.26	1.32
49	Y	308	KC2	CHD-C1D	3.61	1.47	1.39
39	k	202	CLA	C1D-ND	3.60	1.42	1.37
51	R	313	A1ECV	CHD-C1D	3.60	1.46	1.39
51	5	312	A1ECV	CHD-C4C	3.60	1.45	1.39
49	z	313	KC2	CHD-C1D	3.60	1.47	1.39
50	7	306	A1EB1	C30-C29	-3.60	1.26	1.32
51	R	310	A1ECV	CHB-C4A	3.59	1.45	1.39
51	S	312	A1ECV	CHD-C1D	3.59	1.46	1.39
39	7	316	CLA	C1D-ND	3.59	1.42	1.37
39	X	316	CLA	C1D-ND	3.59	1.42	1.37
39	2	312	CLA	C1D-ND	3.59	1.42	1.37
51	7	317	A1ECV	CHD-C1D	3.59	1.46	1.39
49	9	318	KC2	CHD-C1D	3.59	1.47	1.39
39	T	313	CLA	C3B-C4B	3.59	1.51	1.42
39	2	319	CLA	C1D-ND	3.59	1.42	1.37
48	T	306	A86	C30-C29	-3.59	1.26	1.32
52	W	321	A1EB4	C30-C29	-3.59	1.26	1.32
39	D	311	CLA	C1D-ND	3.58	1.42	1.37
48	L	305	A86	C30-C29	-3.58	1.26	1.32
50	4	304	A1EB1	C30-C29	-3.58	1.26	1.32
48	5	301	A86	C30-C29	-3.58	1.26	1.32
51	z	316	A1ECV	CHC-C4B	3.58	1.46	1.39
51	G	316	A1ECV	CHB-C4A	3.57	1.45	1.39
39	a	819	CLA	C1D-ND	3.57	1.42	1.37
50	6	304	A1EB1	C30-C29	-3.57	1.26	1.32
48	X	303	A86	C30-C29	-3.57	1.26	1.32
48	8	307	A86	C30-C29	-3.57	1.26	1.32
39	b	831	CLA	C1D-ND	3.57	1.42	1.37
39	J	317	CLA	C4B-NB	3.57	1.42	1.37
39	Q	317	CLA	C4B-NB	3.57	1.42	1.37
39	x	318	CLA	C4B-NB	3.56	1.42	1.37
48	M	303	A86	C30-C29	-3.56	1.26	1.32
39	a	826	CLA	C1D-ND	3.56	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	T	308	CLA	C1D-ND	3.56	1.42	1.37
48	O	307	A86	C30-C29	-3.56	1.26	1.32
50	G	307	A1EB1	C30-C29	-3.56	1.26	1.32
51	X	313	A1ECV	CHD-C1D	3.56	1.46	1.39
39	b	829	CLA	C1D-ND	3.56	1.42	1.37
39	S	311	CLA	C1D-ND	3.56	1.42	1.37
39	b	807	CLA	C1D-ND	3.55	1.42	1.37
48	Q	302	A86	C30-C29	-3.55	1.26	1.32
49	T	312	KC2	CHD-C1D	3.55	1.47	1.39
39	4	322	CLA	C4B-NB	3.55	1.42	1.37
39	a	837	CLA	C4B-NB	3.54	1.42	1.37
39	8	312	CLA	C4B-NB	3.54	1.42	1.37
50	U	203	A1EB1	C30-C29	-3.54	1.26	1.32
49	L	312	KC2	CHD-C1D	3.54	1.47	1.39
50	z	302	A1EB1	C30-C29	-3.54	1.26	1.32
39	B	203	CLA	C1D-ND	3.54	1.42	1.37
39	Y	307	CLA	C4B-NB	3.54	1.42	1.37
49	y	314	KC2	CHD-C1D	3.54	1.47	1.39
49	3	315	KC2	CHD-C1D	3.54	1.47	1.39
39	T	309	CLA	C4B-NB	3.54	1.42	1.37
48	Q	301	A86	C30-C29	-3.53	1.26	1.32
49	2	317	KC2	CHD-C1D	3.53	1.47	1.39
39	X	308	CLA	C4B-NB	3.53	1.42	1.37
48	0	309	A86	C30-C29	-3.53	1.26	1.32
49	6	319	KC2	CHD-C1D	3.53	1.47	1.39
51	5	309	A1ECV	CHD-C1D	3.53	1.46	1.39
50	G	302	A1EB1	C30-C29	-3.53	1.26	1.32
39	9	308	CLA	C1D-ND	3.53	1.42	1.37
39	1	311	CLA	C4B-NB	3.53	1.42	1.37
39	b	833	CLA	C4B-NB	3.53	1.42	1.37
49	1	312	KC2	CHD-C1D	3.53	1.47	1.39
39	C	305	CLA	C4B-NB	3.52	1.42	1.37
39	U	213	CLA	C4B-NB	3.52	1.42	1.37
48	7	312	A86	C30-C29	-3.52	1.26	1.32
48	W	304	A86	C30-C29	-3.52	1.26	1.32
49	A	310	KC2	CHD-C1D	3.52	1.47	1.39
39	Y	313	CLA	C4B-NB	3.52	1.42	1.37
51	0	321	A1ECV	CHD-C1D	3.52	1.46	1.39
48	B	201	A86	C30-C29	-3.52	1.26	1.32
50	y	302	A1EB1	C30-C29	-3.52	1.26	1.32
52	M	322	A1EB4	C30-C29	-3.52	1.26	1.32
49	z	312	KC2	CHD-C1D	3.51	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	318	CLA	C1D-ND	3.51	1.42	1.37
51	S	318	A1ECV	CHD-C4C	3.51	1.45	1.39
39	B	209	CLA	C4B-NB	3.51	1.42	1.37
39	U	201	CLA	C1D-ND	3.51	1.42	1.37
39	I	301	CLA	C4B-NB	3.51	1.42	1.37
51	Z	314	A1ECV	CHD-C4C	3.51	1.45	1.39
49	S	315	KC2	CHD-C1D	3.51	1.47	1.39
39	b	823	CLA	C4B-NB	3.51	1.42	1.37
39	D	314	CLA	C4B-NB	3.51	1.42	1.37
39	8	310	CLA	C4B-NB	3.50	1.42	1.37
51	E	311	A1ECV	CHC-C4B	3.50	1.46	1.39
39	K	306	CLA	C4B-NB	3.50	1.42	1.37
50	K	305	A1EB1	C30-C29	-3.50	1.26	1.32
51	T	317	A1ECV	CHD-C4C	3.50	1.45	1.39
39	C	310	CLA	C1D-ND	3.50	1.42	1.37
39	H	312	CLA	C1D-ND	3.50	1.42	1.37
39	O	310	CLA	C4B-NB	3.50	1.42	1.37
49	8	319	KC2	CHD-C1D	3.50	1.47	1.39
39	U	212	CLA	C4B-NB	3.50	1.42	1.37
48	M	306	A86	C30-C29	-3.50	1.26	1.32
51	5	309	A1ECV	CHD-C4C	3.49	1.45	1.39
48	L	304	A86	C30-C29	-3.49	1.26	1.32
51	z	316	A1ECV	CHD-C4C	3.49	1.45	1.39
52	P	319	A1EB4	C30-C29	-3.49	1.26	1.32
52	X	305	A1EB4	C30-C29	-3.49	1.26	1.32
39	l	203	CLA	C4B-NB	3.49	1.42	1.37
39	J	318	CLA	C1D-ND	3.49	1.42	1.37
49	9	316	KC2	CHD-C1D	3.49	1.47	1.39
49	9	311	KC2	CHD-C1D	3.49	1.47	1.39
49	1	314	KC2	CHD-C1D	3.49	1.47	1.39
39	2	318	CLA	C4B-NB	3.49	1.42	1.37
49	P	313	KC2	CHD-C1D	3.48	1.47	1.39
39	8	321	CLA	C4B-NB	3.48	1.42	1.37
39	S	309	CLA	C4B-NB	3.48	1.42	1.37
39	2	308	CLA	C4B-NB	3.48	1.42	1.37
50	9	302	A1EB1	C30-C29	-3.48	1.26	1.32
39	9	315	CLA	C4B-NB	3.48	1.42	1.37
49	L	321	KC2	CHD-C1D	3.48	1.47	1.39
39	O	314	CLA	C4B-NB	3.48	1.42	1.37
51	O	315	A1ECV	CHD-C1D	3.48	1.45	1.39
39	b	805	CLA	C4B-NB	3.48	1.42	1.37
49	3	318	KC2	CHD-C1D	3.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	311	CLA	C4B-NB	3.48	1.42	1.37
49	7	322	KC2	CHD-C1D	3.48	1.47	1.39
49	X	306	KC2	CHD-C1D	3.47	1.47	1.39
49	4	318	KC2	CHD-C1D	3.47	1.47	1.39
39	Q	314	CLA	C1D-ND	3.47	1.42	1.37
39	0	318	CLA	C4B-NB	3.47	1.42	1.37
39	6	322	CLA	C4B-NB	3.47	1.42	1.37
39	U	215	CLA	C4B-NB	3.47	1.42	1.37
49	F	311	KC2	CHD-C1D	3.47	1.47	1.39
48	8	323	A86	C30-C29	-3.47	1.26	1.32
49	F	307	KC2	CHD-C1D	3.47	1.47	1.39
39	l	204	CLA	C1D-ND	3.47	1.42	1.37
49	W	312	KC2	CHD-C1D	3.47	1.47	1.39
39	P	311	CLA	C4B-NB	3.47	1.42	1.37
52	T	304	A1EB4	C30-C29	-3.46	1.26	1.32
39	S	311	CLA	C4B-NB	3.46	1.42	1.37
48	L	307	A86	C30-C29	-3.46	1.26	1.32
39	2	319	CLA	C4B-NB	3.46	1.42	1.37
39	8	318	CLA	C4B-NB	3.46	1.42	1.37
39	R	316	CLA	C4B-NB	3.46	1.42	1.37
39	0	320	CLA	C4B-NB	3.46	1.42	1.37
48	U	206	A86	C30-C29	-3.46	1.26	1.32
39	z	317	CLA	C4B-NB	3.46	1.42	1.37
51	1	318	A1ECV	CHD-C4C	3.45	1.45	1.39
49	8	316	KC2	CHD-C1D	3.45	1.47	1.39
50	4	303	A1EB1	C30-C29	-3.45	1.26	1.32
49	7	320	KC2	CHD-C1D	3.45	1.47	1.39
49	K	313	KC2	CHD-C1D	3.45	1.47	1.39
39	4	313	CLA	C4B-NB	3.45	1.42	1.37
39	b	834	CLA	C4B-NB	3.45	1.42	1.37
39	J	318	CLA	C4B-NB	3.45	1.42	1.37
49	I	312	KC2	CHD-C1D	3.45	1.47	1.39
49	A	313	KC2	CHD-C1D	3.45	1.47	1.39
50	3	309	A1EB1	C30-C29	-3.45	1.26	1.32
39	y	318	CLA	C4B-NB	3.45	1.42	1.37
49	V	308	KC2	CHD-C1D	3.45	1.47	1.39
49	V	318	KC2	CHD-C1D	3.45	1.47	1.39
39	O	311	CLA	C3B-C4B	3.45	1.50	1.42
49	0	314	KC2	CHD-C1D	3.45	1.47	1.39
48	3	307	A86	C30-C29	-3.45	1.26	1.32
49	R	306	KC2	CHD-C1D	3.45	1.47	1.39
49	1	315	KC2	CHD-C1D	3.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	Y	309	KC2	CHD-C1D	3.45	1.47	1.39
39	C	309	CLA	C4B-NB	3.45	1.42	1.37
51	E	311	A1ECV	CHD-C1D	3.45	1.45	1.39
39	y	310	CLA	C4B-NB	3.45	1.42	1.37
49	x	315	KC2	CHD-C1D	3.44	1.47	1.39
39	H	315	CLA	C4B-NB	3.44	1.42	1.37
39	b	839	CLA	C4B-NB	3.44	1.42	1.37
49	W	315	KC2	CHD-C1D	3.44	1.47	1.39
39	B	203	CLA	C4B-NB	3.44	1.42	1.37
39	z	306	CLA	C4B-NB	3.44	1.42	1.37
48	O	302	A86	C30-C29	-3.44	1.26	1.32
39	a	815	CLA	C4B-NB	3.44	1.42	1.37
39	7	321	CLA	C4B-NB	3.44	1.42	1.37
39	5	307	CLA	C4B-NB	3.44	1.42	1.37
49	J	315	KC2	CHD-C1D	3.44	1.47	1.39
39	A	315	CLA	C4B-NB	3.44	1.42	1.37
48	9	306	A86	C30-C29	-3.44	1.26	1.32
49	P	310	KC2	CHD-C1D	3.44	1.47	1.39
48	M	302	A86	C30-C29	-3.44	1.26	1.32
51	Q	319	A1ECV	CHC-C4B	3.44	1.45	1.39
48	4	310	A86	C30-C29	-3.44	1.26	1.32
39	a	827	CLA	C4B-NB	3.43	1.42	1.37
39	Q	312	CLA	C4B-NB	3.43	1.42	1.37
39	V	316	CLA	C4B-NB	3.43	1.42	1.37
39	0	322	CLA	C4B-NB	3.43	1.42	1.37
49	2	313	KC2	CHD-C1D	3.43	1.47	1.39
39	Y	303	CLA	C4B-NB	3.43	1.42	1.37
39	z	311	CLA	C4B-NB	3.43	1.42	1.37
39	J	312	CLA	C4B-NB	3.43	1.42	1.37
39	T	318	CLA	C4B-NB	3.43	1.42	1.37
39	z	314	CLA	C4B-NB	3.43	1.42	1.37
39	I	309	CLA	C4B-NB	3.43	1.42	1.37
48	J	303	A86	C30-C29	-3.43	1.26	1.32
39	7	325	CLA	C4B-NB	3.43	1.42	1.37
39	Z	316	CLA	C4B-NB	3.43	1.42	1.37
49	G	313	KC2	CHD-C1D	3.43	1.47	1.39
49	Z	310	KC2	CHD-C1D	3.43	1.47	1.39
39	f	802	CLA	C4B-NB	3.43	1.42	1.37
39	H	308	CLA	C4B-NB	3.43	1.42	1.37
39	b	801	CLA	C4D-ND	-3.43	1.33	1.37
39	a	833	CLA	C4B-NB	3.43	1.42	1.37
39	b	830	CLA	C4B-NB	3.43	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	4	312	CLA	C4B-NB	3.43	1.42	1.37
49	Z	311	KC2	CHD-C1D	3.42	1.47	1.39
39	E	315	CLA	C4B-NB	3.42	1.42	1.37
49	K	310	KC2	CHD-C1D	3.42	1.47	1.39
39	b	836	CLA	C4B-NB	3.42	1.42	1.37
39	D	310	CLA	C4B-NB	3.42	1.42	1.37
39	Z	315	CLA	C4B-NB	3.42	1.42	1.37
49	4	317	KC2	CHD-C1D	3.42	1.47	1.39
50	h	203	A1EB1	C30-C29	-3.42	1.26	1.32
39	E	314	CLA	C4B-NB	3.42	1.42	1.37
39	G	309	CLA	C1D-ND	3.42	1.42	1.37
39	D	318	CLA	C4B-NB	3.42	1.42	1.37
39	0	310	CLA	C4B-NB	3.42	1.42	1.37
51	9	314	A1ECV	CHD-C1D	3.42	1.45	1.39
49	M	311	KC2	CHD-C1D	3.42	1.47	1.39
39	x	307	CLA	C4B-NB	3.42	1.42	1.37
49	2	314	KC2	CHD-C1D	3.42	1.47	1.39
49	x	312	KC2	CHD-C1D	3.42	1.47	1.39
39	x	317	CLA	C4B-NB	3.41	1.42	1.37
39	D	309	CLA	C4B-NB	3.41	1.42	1.37
39	J	307	CLA	C4B-NB	3.41	1.42	1.37
39	1	320	CLA	C4B-NB	3.41	1.42	1.37
48	G	301	A86	C30-C29	-3.41	1.26	1.32
51	O	315	A1ECV	CHD-C4C	3.41	1.45	1.39
39	1	308	CLA	C4B-NB	3.41	1.42	1.37
39	Q	311	CLA	C4B-NB	3.41	1.42	1.37
51	P	315	A1ECV	CHD-C4C	3.41	1.45	1.39
49	5	314	KC2	CHD-C1D	3.41	1.47	1.39
39	Q	309	CLA	C4B-NB	3.41	1.42	1.37
39	Y	310	CLA	C4B-NB	3.41	1.42	1.37
51	Y	312	A1ECV	CHD-C4C	3.41	1.45	1.39
39	L	310	CLA	C4B-NB	3.41	1.42	1.37
39	X	317	CLA	C4B-NB	3.41	1.42	1.37
49	y	316	KC2	CHD-C1D	3.41	1.47	1.39
48	W	303	A86	C30-C29	-3.41	1.26	1.32
51	T	317	A1ECV	CHC-C4B	3.41	1.45	1.39
39	K	307	CLA	C4B-NB	3.41	1.42	1.37
39	8	322	CLA	C4B-NB	3.41	1.42	1.37
51	Q	316	A1ECV	CHD-C4C	3.41	1.45	1.39
39	D	311	CLA	C4B-NB	3.41	1.42	1.37
49	z	315	KC2	CHD-C1D	3.41	1.47	1.39
39	H	306	CLA	C4B-NB	3.41	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Q	304	A86	C30-C29	-3.41	1.26	1.32
49	H	311	KC2	CHD-C1D	3.41	1.47	1.39
49	7	319	KC2	CHD-C1D	3.41	1.47	1.39
39	B	205	CLA	C4B-NB	3.41	1.42	1.37
39	J	310	CLA	C4B-NB	3.41	1.42	1.37
39	X	309	CLA	C4B-NB	3.41	1.42	1.37
39	a	830	CLA	C4B-NB	3.40	1.42	1.37
49	X	315	KC2	CHD-C1D	3.40	1.47	1.39
39	U	208	CLA	C4B-NB	3.40	1.42	1.37
39	3	319	CLA	C4B-NB	3.40	1.42	1.37
39	Z	305	CLA	C4B-NB	3.40	1.42	1.37
39	E	312	CLA	C4B-NB	3.40	1.42	1.37
48	3	308	A86	C30-C29	-3.40	1.26	1.32
39	T	319	CLA	C4B-NB	3.40	1.42	1.37
51	L	318	A1ECV	CHD-C4C	3.40	1.45	1.39
39	A	306	CLA	C4B-NB	3.40	1.42	1.37
39	x	309	CLA	C4B-NB	3.40	1.42	1.37
39	6	318	CLA	C4B-NB	3.40	1.42	1.37
39	z	308	CLA	C4B-NB	3.40	1.42	1.37
39	Y	314	CLA	C4B-NB	3.40	1.42	1.37
49	H	314	KC2	CHD-C1D	3.40	1.47	1.39
48	R	301	A86	C30-C29	-3.40	1.26	1.32
39	4	323	CLA	C4B-NB	3.40	1.42	1.37
39	b	816	CLA	C4B-NB	3.40	1.42	1.37
49	V	315	KC2	CHD-C1D	3.40	1.47	1.39
39	2	307	CLA	C4B-NB	3.40	1.42	1.37
39	a	814	CLA	C4B-NB	3.40	1.42	1.37
39	b	851	CLA	C4B-NB	3.40	1.42	1.37
39	Q	309	CLA	C1D-ND	3.40	1.42	1.37
39	O	316	CLA	C4B-NB	3.40	1.42	1.37
49	L	317	KC2	CHD-C1D	3.39	1.47	1.39
39	3	313	CLA	C4B-NB	3.39	1.42	1.37
49	P	312	KC2	CHD-C1D	3.39	1.47	1.39
39	A	307	CLA	C4B-NB	3.39	1.42	1.37
39	L	316	CLA	C4B-NB	3.39	1.42	1.37
39	3	322	CLA	C4B-NB	3.39	1.42	1.37
49	x	313	KC2	CHD-C1D	3.39	1.47	1.39
39	a	820	CLA	C4B-NB	3.39	1.42	1.37
51	z	310	A1ECV	CHD-C4C	3.39	1.45	1.39
39	1	317	CLA	C4B-NB	3.39	1.42	1.37
50	D	308	A1EB1	C30-C29	-3.39	1.26	1.32
49	y	313	KC2	CHD-C1D	3.39	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	y	307	CLA	C4B-NB	3.39	1.42	1.37
39	L	308	CLA	C4B-NB	3.39	1.42	1.37
50	0	305	A1EB1	C30-C29	-3.39	1.26	1.32
51	L	318	A1ECV	CHC-C4B	3.39	1.45	1.39
49	V	312	KC2	CHD-C1D	3.39	1.47	1.39
39	F	312	CLA	C4B-NB	3.39	1.41	1.37
39	O	308	CLA	C1D-ND	3.39	1.41	1.37
39	7	313	CLA	C4B-NB	3.39	1.41	1.37
39	y	319	CLA	C4B-NB	3.39	1.41	1.37
39	k	202	CLA	C4B-NB	3.39	1.41	1.37
39	3	320	CLA	C4B-NB	3.39	1.41	1.37
50	x	302	A1EB1	C30-C29	-3.39	1.26	1.32
39	S	310	CLA	C4B-NB	3.39	1.41	1.37
39	x	311	CLA	C4B-NB	3.39	1.41	1.37
49	5	313	KC2	CHD-C1D	3.39	1.47	1.39
49	Q	318	KC2	CHD-C1D	3.38	1.47	1.39
49	M	314	KC2	CHD-C1D	3.38	1.47	1.39
39	4	311	CLA	C4B-NB	3.38	1.41	1.37
39	6	312	CLA	C4B-NB	3.38	1.41	1.37
49	V	314	KC2	CHD-C1D	3.38	1.47	1.39
39	a	829	CLA	C4B-NB	3.38	1.41	1.37
49	X	314	KC2	CHD-C1D	3.38	1.47	1.39
49	6	314	KC2	CHD-C1D	3.38	1.47	1.39
39	O	318	CLA	C4B-NB	3.38	1.41	1.37
39	U	214	CLA	C4B-NB	3.38	1.41	1.37
49	B	208	KC2	CHD-C1D	3.38	1.47	1.39
39	b	820	CLA	C4B-NB	3.38	1.41	1.37
39	R	315	CLA	C4B-NB	3.38	1.41	1.37
39	x	314	CLA	C4B-NB	3.38	1.41	1.37
52	P	305	A1EB4	C30-C29	-3.38	1.26	1.32
49	R	314	KC2	CHD-C1D	3.38	1.47	1.39
39	k	203	CLA	C4B-NB	3.38	1.41	1.37
39	V	319	CLA	C4B-NB	3.38	1.41	1.37
39	J	314	CLA	C4B-NB	3.38	1.41	1.37
39	T	311	CLA	C4B-NB	3.38	1.41	1.37
39	A	305	CLA	C4B-NB	3.38	1.41	1.37
39	5	316	CLA	C4B-NB	3.38	1.41	1.37
49	X	312	KC2	CHD-C1D	3.37	1.47	1.39
39	a	817	CLA	C4B-NB	3.37	1.41	1.37
39	b	821	CLA	C4B-NB	3.37	1.41	1.37
39	9	319	CLA	C4B-NB	3.37	1.41	1.37
48	4	309	A86	C30-C29	-3.37	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	8	305	A86	C30-C29	-3.37	1.26	1.32
39	1	310	CLA	C4B-NB	3.37	1.41	1.37
39	3	312	CLA	C4B-NB	3.37	1.41	1.37
39	x	306	CLA	C4B-NB	3.37	1.41	1.37
49	P	320	KC2	CHD-C1D	3.37	1.47	1.39
39	A	312	CLA	C4B-NB	3.37	1.41	1.37
39	S	316	CLA	C4B-NB	3.37	1.41	1.37
39	U	207	CLA	C4B-NB	3.37	1.41	1.37
39	H	307	CLA	C4B-NB	3.37	1.41	1.37
39	y	308	CLA	C4B-NB	3.37	1.41	1.37
39	E	319	CLA	C4B-NB	3.37	1.41	1.37
39	L	320	CLA	C4B-NB	3.37	1.41	1.37
48	1	302	A86	C30-C29	-3.37	1.26	1.32
49	Q	315	KC2	CHD-C1D	3.37	1.47	1.39
39	M	312	CLA	C4B-NB	3.37	1.41	1.37
48	C	303	A86	C30-C29	-3.37	1.26	1.32
49	T	315	KC2	CHD-C1D	3.37	1.47	1.39
52	M	305	A1EB4	C30-C29	-3.37	1.26	1.32
39	b	817	CLA	C4B-NB	3.37	1.41	1.37
51	X	310	A1ECV	CHD-C4C	3.37	1.45	1.39
49	P	306	KC2	CHD-C1D	3.37	1.47	1.39
51	x	316	A1ECV	CHD-C4C	3.37	1.45	1.39
39	a	847	CLA	C4B-NB	3.37	1.41	1.37
39	f	803	CLA	C4B-NB	3.37	1.41	1.37
39	F	321	CLA	C4B-NB	3.37	1.41	1.37
50	5	302	A1EB1	C30-C29	-3.37	1.26	1.32
49	4	324	KC2	CHD-C1D	3.37	1.47	1.39
39	b	814	CLA	C4B-NB	3.37	1.41	1.37
39	b	822	CLA	C4B-NB	3.37	1.41	1.37
39	3	323	CLA	C4B-NB	3.37	1.41	1.37
48	R	317	A86	C30-C29	-3.37	1.26	1.32
50	T	302	A1EB1	C30-C29	-3.36	1.26	1.32
39	a	819	CLA	C4B-NB	3.36	1.41	1.37
39	b	842	CLA	C4B-NB	3.36	1.41	1.37
39	Y	302	CLA	C4B-NB	3.36	1.41	1.37
39	a	824	CLA	C4B-NB	3.36	1.41	1.37
39	S	319	CLA	C4B-NB	3.36	1.41	1.37
49	4	320	KC2	CHD-C1D	3.36	1.46	1.39
39	A	308	CLA	C4B-NB	3.36	1.41	1.37
48	W	307	A86	C30-C29	-3.36	1.26	1.32
49	5	311	KC2	CHD-C1D	3.36	1.46	1.39
39	P	307	CLA	C1D-ND	3.36	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S	317	KC2	CHD-C1D	3.36	1.46	1.39
39	Y	305	CLA	C4B-NB	3.36	1.41	1.37
39	6	310	CLA	C4B-NB	3.36	1.41	1.37
39	L	319	CLA	C4B-NB	3.36	1.41	1.37
39	P	314	CLA	C4B-NB	3.36	1.41	1.37
39	Z	312	CLA	C4B-NB	3.36	1.41	1.37
39	6	321	CLA	C4B-NB	3.36	1.41	1.37
39	W	313	CLA	C4B-NB	3.36	1.41	1.37
49	C	313	KC2	CHD-C1D	3.36	1.46	1.39
39	b	808	CLA	C4B-NB	3.36	1.41	1.37
39	Z	306	CLA	C4B-NB	3.36	1.41	1.37
39	J	313	CLA	C4B-NB	3.35	1.41	1.37
39	U	210	CLA	C4B-NB	3.35	1.41	1.37
39	1	316	CLA	C4B-NB	3.35	1.41	1.37
49	3	321	KC2	CHD-C1D	3.35	1.46	1.39
49	V	320	KC2	CHD-C1D	3.35	1.46	1.39
39	a	810	CLA	C4B-NB	3.35	1.41	1.37
49	W	314	KC2	CHD-C1D	3.35	1.46	1.39
49	0	317	KC2	CHD-C1D	3.35	1.46	1.39
39	7	315	CLA	C4B-NB	3.35	1.41	1.37
39	D	317	CLA	C4B-NB	3.35	1.41	1.37
39	V	309	CLA	C4B-NB	3.35	1.41	1.37
39	3	316	CLA	C4B-NB	3.35	1.41	1.37
39	0	311	CLA	C4D-ND	-3.35	1.33	1.37
49	S	314	KC2	CHD-C1D	3.35	1.46	1.39
39	F	314	CLA	C4B-NB	3.35	1.41	1.37
39	b	828	CLA	C4B-NB	3.34	1.41	1.37
39	I	311	CLA	C4B-NB	3.34	1.41	1.37
49	M	313	KC2	CHD-C1D	3.34	1.46	1.39
49	X	318	KC2	CHD-C1D	3.34	1.46	1.39
49	0	316	KC2	CHD-C1D	3.34	1.46	1.39
39	l	204	CLA	C4B-NB	3.34	1.41	1.37
39	3	314	CLA	C4B-NB	3.34	1.41	1.37
39	Y	304	CLA	C4B-NB	3.34	1.41	1.37
39	A	314	CLA	C4B-NB	3.34	1.41	1.37
39	Q	314	CLA	C4B-NB	3.34	1.41	1.37
39	5	315	CLA	C4B-NB	3.34	1.41	1.37
39	5	315	CLA	C1D-ND	3.34	1.41	1.37
39	I	316	CLA	C4B-NB	3.34	1.41	1.37
39	G	312	CLA	C4B-NB	3.34	1.41	1.37
39	9	312	CLA	C1D-ND	3.34	1.41	1.37
49	G	317	KC2	CHD-C1D	3.34	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	C	304	CLA	C4B-NB	3.34	1.41	1.37
39	T	320	CLA	C4B-NB	3.34	1.41	1.37
39	M	309	CLA	C4B-NB	3.34	1.41	1.37
39	b	819	CLA	C4B-NB	3.34	1.41	1.37
39	S	320	CLA	C4B-NB	3.34	1.41	1.37
51	9	317	A1ECV	CHD-C1D	3.34	1.45	1.39
39	R	309	CLA	C4B-NB	3.33	1.41	1.37
50	8	301	A1EB1	C30-C29	-3.33	1.26	1.32
39	2	315	CLA	C4B-NB	3.33	1.41	1.37
39	i	103	CLA	C4B-NB	3.33	1.41	1.37
39	5	308	CLA	C4B-NB	3.33	1.41	1.37
39	Z	304	CLA	C4B-NB	3.33	1.41	1.37
49	8	317	KC2	CHD-C1D	3.33	1.46	1.39
39	E	306	CLA	C4B-NB	3.33	1.41	1.37
39	X	316	CLA	C4B-NB	3.33	1.41	1.37
51	G	316	A1ECV	CHD-C4C	3.33	1.45	1.39
39	F	316	CLA	C4B-NB	3.33	1.41	1.37
39	b	833	CLA	C1D-ND	3.33	1.41	1.37
39	Q	310	CLA	C4B-NB	3.33	1.41	1.37
39	0	312	CLA	C1D-ND	3.33	1.41	1.37
39	Z	307	CLA	C4B-NB	3.33	1.41	1.37
49	L	314	KC2	CHD-C1D	3.33	1.46	1.39
39	M	317	CLA	C4B-NB	3.33	1.41	1.37
49	G	311	KC2	CHD-C1D	3.33	1.46	1.39
39	a	825	CLA	C4B-NB	3.33	1.41	1.37
39	7	314	CLA	C4B-NB	3.33	1.41	1.37
39	7	324	CLA	C4B-NB	3.33	1.41	1.37
39	F	310	CLA	C4B-NB	3.33	1.41	1.37
39	x	308	CLA	C4B-NB	3.33	1.41	1.37
49	T	316	KC2	CHD-C1D	3.33	1.46	1.39
39	y	312	CLA	C4B-NB	3.33	1.41	1.37
39	a	808	CLA	C4B-NB	3.32	1.41	1.37
39	O	309	CLA	C4B-NB	3.32	1.41	1.37
39	5	306	CLA	C4B-NB	3.32	1.41	1.37
39	2	312	CLA	C4B-NB	3.32	1.41	1.37
39	K	314	CLA	C4B-NB	3.32	1.41	1.37
39	W	318	CLA	C4B-NB	3.32	1.41	1.37
48	7	308	A86	C30-C29	-3.32	1.26	1.32
39	a	812	CLA	C4B-NB	3.32	1.41	1.37
39	a	809	CLA	C4B-NB	3.32	1.41	1.37
39	o	205	CLA	C4B-NB	3.32	1.41	1.37
49	5	305	KC2	CHD-C1D	3.32	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B	204	CLA	C4B-NB	3.32	1.41	1.37
39	V	311	CLA	C4B-NB	3.32	1.41	1.37
49	6	317	KC2	CHD-C1D	3.32	1.46	1.39
39	4	319	CLA	C4B-NB	3.32	1.41	1.37
49	C	312	KC2	CHD-C1D	3.32	1.46	1.39
50	4	301	A1EB1	C30-C29	-3.32	1.26	1.32
49	8	320	KC2	CHD-C1D	3.32	1.46	1.39
39	I	314	CLA	C4B-NB	3.32	1.41	1.37
52	W	306	A1EB4	C30-C29	-3.32	1.26	1.32
49	L	315	KC2	CHD-C1D	3.31	1.46	1.39
39	D	319	CLA	C4B-NB	3.31	1.41	1.37
39	a	838	CLA	C4B-NB	3.31	1.41	1.37
39	G	310	CLA	C4B-NB	3.31	1.41	1.37
39	9	309	CLA	C4B-NB	3.31	1.41	1.37
39	h	201	CLA	C4B-NB	3.31	1.41	1.37
39	F	315	CLA	C4B-NB	3.31	1.41	1.37
39	J	308	CLA	C4B-NB	3.31	1.41	1.37
39	1	309	CLA	C4B-NB	3.31	1.41	1.37
39	3	311	CLA	C4B-NB	3.31	1.41	1.37
39	z	309	CLA	C4B-NB	3.31	1.41	1.37
39	G	309	CLA	C4B-NB	3.31	1.41	1.37
39	W	311	CLA	C4B-NB	3.31	1.41	1.37
39	Z	309	CLA	C4B-NB	3.31	1.41	1.37
39	X	307	CLA	C4B-NB	3.31	1.41	1.37
39	0	311	CLA	C4B-NB	3.31	1.41	1.37
39	1	319	CLA	C4B-NB	3.31	1.41	1.37
39	b	841	CLA	C3B-C4B	3.31	1.50	1.42
39	0	313	CLA	C4B-NB	3.31	1.41	1.37
39	H	316	CLA	C4B-NB	3.31	1.41	1.37
39	2	316	CLA	C4B-NB	3.31	1.41	1.37
39	l	201	CLA	C4B-NB	3.31	1.41	1.37
48	F	301	A86	C30-C29	-3.31	1.26	1.32
39	K	308	CLA	C4B-NB	3.31	1.41	1.37
39	b	827	CLA	C4B-NB	3.30	1.41	1.37
39	O	308	CLA	C4B-NB	3.30	1.41	1.37
39	T	310	CLA	C4B-NB	3.30	1.41	1.37
48	V	301	A86	C30-C29	-3.30	1.26	1.32
39	J	316	CLA	C4B-NB	3.30	1.41	1.37
39	X	311	CLA	C4B-NB	3.30	1.41	1.37
49	6	316	KC2	CHD-C1D	3.30	1.46	1.39
39	b	825	CLA	C4B-NB	3.30	1.41	1.37
48	D	305	A86	C30-C29	-3.30	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	a	835	CLA	C4B-NB	3.30	1.41	1.37
39	b	810	CLA	C4B-NB	3.30	1.41	1.37
39	L	311	CLA	C4B-NB	3.30	1.41	1.37
39	0	323	CLA	C4B-NB	3.30	1.41	1.37
39	o	201	CLA	C4B-NB	3.30	1.41	1.37
39	O	312	CLA	C4B-NB	3.30	1.41	1.37
39	4	314	CLA	C4B-NB	3.30	1.41	1.37
39	8	315	CLA	C4B-NB	3.30	1.41	1.37
39	b	835	CLA	C4B-NB	3.30	1.41	1.37
39	o	203	CLA	C4B-NB	3.30	1.41	1.37
39	C	311	CLA	C4B-NB	3.30	1.41	1.37
39	9	312	CLA	C4B-NB	3.30	1.41	1.37
39	o	206	CLA	C4B-NB	3.30	1.41	1.37
39	E	310	CLA	C4B-NB	3.30	1.41	1.37
39	H	313	CLA	C4B-NB	3.30	1.41	1.37
39	P	316	CLA	C4B-NB	3.30	1.41	1.37
50	8	304	A1EB1	C30-C29	-3.30	1.26	1.32
39	C	306	CLA	C4B-NB	3.30	1.41	1.37
39	C	308	CLA	C4B-NB	3.30	1.41	1.37
39	R	311	CLA	C4B-NB	3.30	1.41	1.37
50	2	304	A1EB1	C30-C29	-3.29	1.26	1.32
39	R	308	CLA	C4B-NB	3.29	1.41	1.37
39	7	316	CLA	C4B-NB	3.29	1.41	1.37
39	I	313	CLA	C4B-NB	3.29	1.41	1.37
39	6	313	CLA	C4B-NB	3.29	1.41	1.37
39	E	316	CLA	C4B-NB	3.29	1.41	1.37
49	M	307	KC2	CHD-C1D	3.29	1.46	1.39
39	F	309	CLA	C4B-NB	3.29	1.41	1.37
51	7	323	A1ECV	CHD-C1D	3.29	1.45	1.39
49	R	318	KC2	CHD-C1D	3.29	1.46	1.39
51	y	317	A1ECV	CHD-C4C	3.29	1.45	1.39
39	F	313	CLA	C4B-NB	3.29	1.41	1.37
39	a	832	CLA	C4B-NB	3.29	1.41	1.37
39	k	201	CLA	C4B-NB	3.29	1.41	1.37
39	a	807	CLA	C4B-NB	3.29	1.41	1.37
39	E	309	CLA	C4B-NB	3.29	1.41	1.37
48	k	206	A86	C30-C29	-3.29	1.26	1.32
50	V	302	A1EB1	C30-C29	-3.29	1.26	1.32
39	a	818	CLA	C4B-NB	3.29	1.41	1.37
48	y	305	A86	C30-C29	-3.28	1.26	1.32
39	a	801	CLA	C1D-ND	3.28	1.41	1.37
39	a	816	CLA	C4B-NB	3.28	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	9	305	A86	C30-C29	-3.28	1.26	1.32
39	J	311	CLA	C4B-NB	3.28	1.41	1.37
39	B	207	CLA	C4B-NB	3.28	1.41	1.37
48	6	305	A86	C30-C29	-3.28	1.26	1.32
39	J	309	CLA	C4B-NB	3.28	1.41	1.37
48	V	304	A86	C30-C29	-3.28	1.26	1.32
39	H	309	CLA	C4B-NB	3.28	1.41	1.37
39	y	315	CLA	C4B-NB	3.28	1.41	1.37
39	2	310	CLA	C4B-NB	3.28	1.41	1.37
48	4	306	A86	C30-C29	-3.28	1.26	1.32
48	8	302	A86	C30-C29	-3.28	1.26	1.32
39	b	829	CLA	C4B-NB	3.27	1.41	1.37
39	H	310	CLA	C4B-NB	3.27	1.41	1.37
39	M	318	CLA	C4B-NB	3.27	1.41	1.37
39	1	313	CLA	C4B-NB	3.27	1.41	1.37
39	9	320	CLA	C4B-NB	3.27	1.41	1.37
48	X	302	A86	C30-C29	-3.27	1.26	1.32
39	S	308	CLA	C4B-NB	3.27	1.41	1.37
50	V	306	A1EB1	C30-C29	-3.27	1.26	1.32
39	W	309	CLA	C4B-NB	3.27	1.41	1.37
39	G	314	CLA	C4B-NB	3.27	1.41	1.37
51	2	311	A1ECV	CHD-C4C	3.27	1.44	1.39
39	b	838	CLA	C4B-NB	3.27	1.41	1.37
48	9	301	A86	C30-C29	-3.26	1.26	1.32
48	1	303	A86	C30-C29	-3.26	1.26	1.32
39	b	826	CLA	C4D-ND	-3.26	1.33	1.37
39	H	312	CLA	C4B-NB	3.26	1.41	1.37
39	M	321	CLA	C4B-NB	3.26	1.41	1.37
49	T	314	KC2	CHD-C1D	3.26	1.46	1.39
39	W	310	CLA	C4B-NB	3.26	1.41	1.37
39	9	308	CLA	C4B-NB	3.26	1.41	1.37
49	9	313	KC2	CHD-C1D	3.26	1.46	1.39
39	U	211	CLA	C4B-NB	3.26	1.41	1.37
48	S	305	A86	C30-C29	-3.26	1.26	1.32
39	E	318	CLA	C4B-NB	3.26	1.41	1.37
39	6	311	CLA	C4B-NB	3.26	1.41	1.37
39	M	310	CLA	C4B-NB	3.26	1.41	1.37
39	9	307	CLA	C4B-NB	3.26	1.41	1.37
50	3	303	A1EB1	C30-C29	-3.25	1.26	1.32
39	T	309	CLA	C3B-C4B	3.25	1.50	1.42
39	z	307	CLA	C4B-NB	3.25	1.41	1.37
39	5	310	CLA	C4B-NB	3.25	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	I	303	KC2	CHD-C1D	3.25	1.46	1.39
39	b	824	CLA	C4B-NB	3.25	1.41	1.37
39	o	202	CLA	C4B-NB	3.25	1.41	1.37
39	D	316	CLA	C4B-NB	3.25	1.41	1.37
39	E	317	CLA	C4B-NB	3.25	1.41	1.37
39	M	315	CLA	C4B-NB	3.25	1.41	1.37
49	3	317	KC2	CHD-C1D	3.25	1.46	1.39
49	W	308	KC2	CHD-C1D	3.25	1.46	1.39
39	L	313	CLA	C4B-NB	3.25	1.41	1.37
39	O	309	CLA	C1D-ND	3.24	1.41	1.37
48	Q	308	A86	C30-C29	-3.24	1.26	1.32
48	y	306	A86	C30-C29	-3.24	1.26	1.32
39	W	319	CLA	C4B-NB	3.24	1.41	1.37
39	F	306	CLA	C4B-NB	3.24	1.41	1.37
39	U	209	CLA	C4B-NB	3.24	1.41	1.37
49	G	315	KC2	CHD-C1D	3.24	1.46	1.39
39	a	828	CLA	C4B-NB	3.24	1.41	1.37
39	b	811	CLA	C4B-NB	3.24	1.41	1.37
39	b	818	CLA	C4B-NB	3.24	1.41	1.37
39	6	315	CLA	C4B-NB	3.24	1.41	1.37
39	I	315	CLA	C4B-NB	3.24	1.41	1.37
39	D	315	CLA	C4B-NB	3.24	1.41	1.37
39	b	833	CLA	C4D-ND	-3.24	1.33	1.37
51	9	317	A1ECV	CHC-C4B	3.24	1.45	1.39
39	b	809	CLA	C4B-NB	3.24	1.41	1.37
39	a	831	CLA	C4B-NB	3.23	1.41	1.37
39	0	312	CLA	C4D-ND	-3.23	1.33	1.37
48	0	308	A86	C30-C29	-3.23	1.26	1.32
39	V	313	CLA	C1D-ND	3.23	1.41	1.37
39	a	802	CLA	C4B-NB	3.23	1.41	1.37
39	a	836	CLA	C4B-NB	3.23	1.41	1.37
39	O	313	CLA	C4B-NB	3.23	1.41	1.37
50	V	307	A1EB1	C30-C29	-3.23	1.26	1.32
39	b	812	CLA	C4B-NB	3.23	1.41	1.37
39	E	307	CLA	C4B-NB	3.23	1.41	1.37
39	z	318	CLA	C4B-NB	3.23	1.41	1.37
49	R	312	KC2	CHD-C1D	3.23	1.46	1.39
39	a	803	CLA	C4B-NB	3.23	1.41	1.37
39	Q	320	CLA	C4B-NB	3.23	1.41	1.37
48	F	302	A86	C30-C29	-3.22	1.26	1.32
51	y	311	A1ECV	CHD-C4C	3.22	1.44	1.39
39	P	307	CLA	C4B-NB	3.22	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	b	813	CLA	C4B-NB	3.22	1.41	1.37
51	x	310	A1ECV	CHD-C4C	3.22	1.44	1.39
48	1	306	A86	C30-C29	-3.22	1.26	1.32
39	a	826	CLA	C4B-NB	3.22	1.41	1.37
39	8	313	CLA	C4B-NB	3.22	1.41	1.37
39	b	832	CLA	C4B-NB	3.22	1.41	1.37
39	E	308	CLA	C4B-NB	3.22	1.41	1.37
39	a	811	CLA	C4B-NB	3.22	1.41	1.37
39	Q	311	CLA	C1D-ND	3.22	1.41	1.37
39	a	822	CLA	C4B-NB	3.21	1.41	1.37
48	Z	301	A86	C30-C29	-3.21	1.26	1.32
39	R	307	CLA	C4B-NB	3.21	1.41	1.37
39	V	310	CLA	C4B-NB	3.21	1.41	1.37
39	F	308	CLA	C4B-NB	3.21	1.41	1.37
39	M	308	CLA	C4B-NB	3.21	1.41	1.37
39	b	840	CLA	C4B-NB	3.21	1.41	1.37
39	O	314	CLA	C3B-C4B	3.21	1.50	1.42
49	8	314	KC2	CHD-C1D	3.21	1.46	1.39
39	b	803	CLA	C4B-NB	3.21	1.41	1.37
49	z	313	KC2	CHA-CBD	-3.21	1.49	1.54
39	b	802	CLA	C4D-ND	-3.21	1.33	1.37
39	a	821	CLA	C4B-NB	3.20	1.41	1.37
39	P	309	CLA	C4B-NB	3.20	1.41	1.37
39	9	310	CLA	C4B-NB	3.20	1.41	1.37
39	X	308	CLA	C3B-C4B	3.20	1.50	1.42
39	b	826	CLA	C4B-NB	3.20	1.41	1.37
39	A	309	CLA	C4B-NB	3.20	1.41	1.37
51	Y	306	A1ECV	CHD-C4C	3.20	1.44	1.39
47	D	304	SQD	O48-C23	3.20	1.42	1.33
39	S	309	CLA	C3B-C4B	3.19	1.50	1.42
39	b	831	CLA	C4B-NB	3.19	1.41	1.37
47	M	301	SQD	O48-C23	3.19	1.42	1.33
39	D	313	CLA	C4B-NB	3.19	1.41	1.37
48	2	302	A86	C30-C29	-3.19	1.26	1.32
39	G	318	CLA	C4B-NB	3.19	1.41	1.37
39	B	206	CLA	C4B-NB	3.19	1.41	1.37
39	7	318	CLA	C4B-NB	3.19	1.41	1.37
39	D	312	CLA	C4B-NB	3.19	1.41	1.37
39	I	310	CLA	C4B-NB	3.18	1.41	1.37
39	4	316	CLA	C4B-NB	3.18	1.41	1.37
50	T	307	A1EB1	C30-C29	-3.18	1.26	1.32
48	7	311	A86	C30-C29	-3.18	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	4	312	CLA	C3B-C4B	3.18	1.50	1.42
47	4	327	SQD	O48-C23	3.17	1.42	1.33
39	C	310	CLA	C4B-NB	3.17	1.41	1.37
50	2	306	A1EB1	C30-C29	-3.17	1.26	1.32
47	E	320	SQD	O48-C23	3.17	1.42	1.33
47	H	318	SQD	O48-C23	3.17	1.42	1.33
39	K	309	CLA	C4B-NB	3.17	1.41	1.37
39	2	309	CLA	C4B-NB	3.17	1.41	1.37
39	B	207	CLA	C3B-C4B	3.17	1.50	1.42
39	T	308	CLA	C4D-ND	-3.17	1.33	1.37
50	H	301	A1EB1	C30-C29	-3.17	1.26	1.32
39	L	309	CLA	C4B-NB	3.17	1.41	1.37
39	8	311	CLA	C4D-ND	-3.17	1.33	1.37
47	7	302	SQD	O48-C23	3.17	1.42	1.33
39	a	823	CLA	C4B-NB	3.17	1.41	1.37
39	l	205	CLA	C4D-ND	-3.16	1.33	1.37
39	P	308	CLA	C4B-NB	3.16	1.41	1.37
39	l	205	CLA	C4B-NB	3.16	1.41	1.37
39	K	312	CLA	C4B-NB	3.16	1.41	1.37
47	S	301	SQD	O48-C23	3.16	1.42	1.33
39	I	308	CLA	C4B-NB	3.16	1.41	1.37
39	K	311	CLA	C4B-NB	3.16	1.41	1.37
48	H	302	A86	C30-C29	-3.16	1.26	1.32
39	b	833	CLA	C3B-C4B	3.15	1.50	1.42
50	8	306	A1EB1	C30-C29	-3.15	1.26	1.32
52	R	305	A1EB4	C30-C29	-3.15	1.26	1.32
48	4	305	A86	C30-C29	-3.15	1.26	1.32
39	a	825	CLA	C3B-C4B	3.15	1.50	1.42
39	a	806	CLA	C4B-NB	3.15	1.41	1.37
48	6	309	A86	C30-C29	-3.15	1.26	1.32
39	7	314	CLA	C3B-C4B	3.15	1.50	1.42
47	F	319	SQD	O48-C23	3.14	1.42	1.33
49	Q	313	KC2	CHD-C1D	3.14	1.46	1.39
39	W	316	CLA	C4B-NB	3.14	1.41	1.37
47	F	318	SQD	O48-C23	3.14	1.42	1.33
52	5	304	A1EB4	C30-C29	-3.14	1.26	1.32
39	Q	311	CLA	C4D-ND	-3.14	1.33	1.37
39	a	837	CLA	C3B-C4B	3.14	1.50	1.42
39	b	802	CLA	C4B-NB	3.14	1.41	1.37
50	8	308	A1EB1	C30-C29	-3.14	1.26	1.32
47	9	322	SQD	O48-C23	3.14	1.42	1.33
39	Q	312	CLA	C3B-C4B	3.14	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	9	304	A86	C30-C29	-3.13	1.26	1.32
50	J	302	A1EB1	C30-C29	-3.13	1.26	1.32
39	a	813	CLA	C4B-NB	3.13	1.41	1.37
47	D	320	SQD	O48-C23	3.13	1.42	1.33
47	k	205	SQD	O48-C23	3.13	1.42	1.33
39	a	824	CLA	C3B-C4B	3.13	1.50	1.42
39	j	101	CLA	C4B-NB	3.13	1.41	1.37
39	x	307	CLA	C3B-C4B	3.13	1.50	1.42
39	2	308	CLA	C3B-C4B	3.12	1.50	1.42
48	O	306	A86	C30-C29	-3.12	1.26	1.32
47	D	321	SQD	O48-C23	3.12	1.42	1.33
39	U	212	CLA	C3B-C4B	3.12	1.50	1.42
39	b	815	CLA	C4B-NB	3.12	1.41	1.37
39	I	314	CLA	C4D-ND	-3.12	1.33	1.37
39	U	208	CLA	C3B-C4B	3.12	1.50	1.42
50	x	301	A1EB1	C30-C29	-3.12	1.26	1.32
39	a	802	CLA	C3B-C4B	3.12	1.50	1.42
39	S	313	CLA	C4B-NB	3.12	1.41	1.37
39	I	301	CLA	C3B-C4B	3.12	1.50	1.42
48	0	304	A86	C30-C29	-3.11	1.26	1.32
39	7	314	CLA	C4D-ND	-3.11	1.33	1.37
51	Z	308	A1ECV	CHD-C4C	3.11	1.44	1.39
51	0	321	A1ECV	CHC-C4B	3.11	1.45	1.39
48	2	301	A86	C30-C29	-3.11	1.26	1.32
39	R	307	CLA	C3B-C4B	3.10	1.50	1.42
39	S	311	CLA	C3B-C4B	3.10	1.50	1.42
48	U	202	A86	C30-C29	-3.10	1.26	1.32
39	A	311	CLA	C4B-NB	3.10	1.41	1.37
48	6	302	A86	C30-C29	-3.10	1.26	1.32
50	6	301	A1EB1	C30-C29	-3.10	1.26	1.32
39	C	307	CLA	C4B-NB	3.10	1.41	1.37
39	I	309	CLA	C3B-C4B	3.09	1.50	1.42
50	U	205	A1EB1	C30-C29	-3.09	1.26	1.32
39	5	307	CLA	C3B-C4B	3.09	1.50	1.42
39	a	804	CLA	C4B-NB	3.09	1.41	1.37
39	O	310	CLA	C4D-ND	-3.09	1.33	1.37
39	i	101	CLA	C4B-NB	3.09	1.41	1.37
50	C	302	A1EB1	C30-C29	-3.09	1.26	1.32
39	J	314	CLA	C3B-C4B	3.08	1.50	1.42
39	i	101	CLA	C4D-ND	-3.08	1.33	1.37
39	E	313	CLA	C4D-ND	-3.08	1.33	1.37
39	b	813	CLA	CAB-C3B	-3.08	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	X	307	CLA	C3B-C4B	3.08	1.50	1.42
39	Y	307	CLA	C3B-C4B	3.08	1.50	1.42
50	O	301	A1EB1	C30-C29	-3.08	1.26	1.32
39	b	806	CLA	C4B-NB	3.08	1.41	1.37
39	f	803	CLA	C3B-C4B	3.08	1.50	1.42
39	a	816	CLA	C3B-C4B	3.08	1.50	1.42
39	0	315	CLA	C4B-NB	3.08	1.41	1.37
39	a	834	CLA	C4B-NB	3.07	1.41	1.37
48	T	305	A86	C30-C29	-3.07	1.26	1.32
39	b	805	CLA	C3B-C4B	3.07	1.50	1.42
39	B	207	CLA	C4D-ND	-3.07	1.33	1.37
39	y	309	CLA	C3B-C4B	3.07	1.49	1.42
39	9	308	CLA	C3B-C4B	3.07	1.49	1.42
39	a	820	CLA	C3B-C4B	3.07	1.49	1.42
48	R	302	A86	C30-C29	-3.07	1.26	1.32
48	8	303	A86	C30-C29	-3.07	1.26	1.32
39	3	313	CLA	C4D-ND	-3.07	1.33	1.37
39	b	837	CLA	C4D-ND	-3.07	1.33	1.37
39	0	310	CLA	C3B-C4B	3.06	1.49	1.42
39	b	818	CLA	C3B-C4B	3.06	1.49	1.42
39	b	808	CLA	C3B-C4B	3.06	1.49	1.42
47	T	321	SQD	O48-C23	3.06	1.42	1.33
39	J	310	CLA	C3B-C4B	3.06	1.49	1.42
39	P	311	CLA	C3B-C4B	3.06	1.49	1.42
50	6	306	A1EB1	C30-C29	-3.06	1.26	1.32
39	A	305	CLA	C3B-C4B	3.06	1.49	1.42
50	0	307	A1EB1	C30-C29	-3.06	1.26	1.32
39	B	205	CLA	C3B-C4B	3.05	1.49	1.42
39	b	837	CLA	C4B-NB	3.05	1.41	1.37
39	a	834	CLA	C4D-ND	-3.05	1.33	1.37
39	2	309	CLA	C4D-ND	-3.05	1.33	1.37
39	Z	313	CLA	C4D-ND	-3.05	1.33	1.37
48	6	303	A86	C30-C29	-3.05	1.26	1.32
39	a	823	CLA	C3B-C4B	3.05	1.49	1.42
39	0	315	CLA	C3B-C4B	3.05	1.49	1.42
39	3	319	CLA	C3B-C4B	3.05	1.49	1.42
39	V	310	CLA	C3B-C4B	3.05	1.49	1.42
39	9	310	CLA	C3B-C4B	3.05	1.49	1.42
39	a	805	CLA	C4B-NB	3.05	1.41	1.37
39	f	802	CLA	C4D-ND	-3.05	1.33	1.37
39	a	803	CLA	C3B-C4B	3.05	1.49	1.42
39	A	315	CLA	C3B-C4B	3.05	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	3	324	A1EB1	C30-C29	-3.05	1.26	1.32
48	J	301	A86	C30-C29	-3.05	1.26	1.32
39	X	311	CLA	C3B-C4B	3.05	1.49	1.42
39	b	807	CLA	C4D-ND	-3.04	1.33	1.37
39	Q	310	CLA	C4D-ND	-3.04	1.33	1.37
48	8	309	A86	C30-C29	-3.04	1.26	1.32
47	P	301	SQD	O48-C23	3.04	1.42	1.33
39	8	311	CLA	C3B-C4B	3.04	1.49	1.42
39	8	311	CLA	C4B-NB	3.04	1.41	1.37
39	4	322	CLA	C3B-C4B	3.04	1.49	1.42
39	B	203	CLA	C3B-C4B	3.04	1.49	1.42
39	8	310	CLA	C3B-C4B	3.04	1.49	1.42
39	b	814	CLA	C3B-C4B	3.03	1.49	1.42
50	K	304	A1EB1	C30-C29	-3.03	1.26	1.32
50	z	301	A1EB1	C30-C29	-3.03	1.26	1.32
39	b	837	CLA	C3B-C4B	3.03	1.49	1.42
39	E	313	CLA	C3B-C4B	3.03	1.49	1.42
39	4	323	CLA	C4D-ND	-3.03	1.33	1.37
39	a	810	CLA	C3B-C4B	3.03	1.49	1.42
39	F	308	CLA	C4D-ND	-3.03	1.33	1.37
39	4	311	CLA	C4D-ND	-3.03	1.33	1.37
48	3	305	A86	C30-C29	-3.03	1.26	1.32
39	b	807	CLA	C3B-C4B	3.03	1.49	1.42
39	o	205	CLA	C3B-C4B	3.03	1.49	1.42
39	z	317	CLA	C3B-C4B	3.03	1.49	1.42
39	3	313	CLA	C3B-C4B	3.03	1.49	1.42
39	0	312	CLA	C4B-NB	3.03	1.41	1.37
39	b	827	CLA	C4D-ND	-3.02	1.33	1.37
50	0	302	A1EB1	C30-C29	-3.02	1.26	1.32
39	U	213	CLA	C3B-C4B	3.02	1.49	1.42
39	b	807	CLA	C4B-NB	3.02	1.41	1.37
50	3	310	A1EB1	C30-C29	-3.02	1.26	1.32
39	l	204	CLA	C4D-ND	-3.02	1.33	1.37
39	9	307	CLA	C4D-ND	-3.02	1.33	1.37
39	L	320	CLA	C4D-ND	-3.02	1.33	1.37
39	P	309	CLA	C4D-ND	-3.02	1.33	1.37
39	S	320	CLA	C4D-ND	-3.02	1.33	1.37
39	O	318	CLA	C3B-C4B	3.02	1.49	1.42
39	l	201	CLA	C4D-ND	-3.02	1.33	1.37
39	a	829	CLA	C3B-C4B	3.02	1.49	1.42
39	W	309	CLA	C3B-C4B	3.02	1.49	1.42
39	F	314	CLA	C3B-C4B	3.02	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	T	308	CLA	C4B-NB	3.01	1.41	1.37
39	l	205	CLA	C3B-C4B	3.01	1.49	1.42
48	0	306	A86	C30-C29	-3.01	1.26	1.32
39	R	311	CLA	C3B-C4B	3.01	1.49	1.42
39	D	315	CLA	C3B-C4B	3.01	1.49	1.42
39	a	811	CLA	C3B-C4B	3.01	1.49	1.42
48	z	303	A86	C30-C29	-3.01	1.26	1.32
50	Q	323	A1EB1	C30-C29	-3.01	1.26	1.32
39	4	312	CLA	C4D-ND	-3.01	1.33	1.37
39	0	320	CLA	C3B-C4B	3.01	1.49	1.42
39	E	314	CLA	C3B-C4B	3.01	1.49	1.42
39	V	313	CLA	C4B-NB	3.01	1.41	1.37
39	E	312	CLA	C3B-C4B	3.01	1.49	1.42
39	b	817	CLA	C3B-C4B	3.01	1.49	1.42
39	O	314	CLA	C4D-ND	-3.01	1.33	1.37
39	7	313	CLA	C4D-ND	-3.01	1.33	1.37
39	H	313	CLA	C4D-ND	-3.01	1.33	1.37
39	J	314	CLA	C4D-ND	-3.01	1.33	1.37
48	Q	305	A86	C30-C29	-3.00	1.27	1.32
48	Z	303	A86	C30-C29	-3.00	1.27	1.32
48	Y	301	A86	C30-C29	-3.00	1.27	1.32
39	a	823	CLA	C4D-ND	-3.00	1.33	1.37
39	z	307	CLA	C3B-C4B	3.00	1.49	1.42
39	f	802	CLA	C3B-C4B	3.00	1.49	1.42
48	x	305	A86	C30-C29	-3.00	1.27	1.32
39	b	815	CLA	C3B-C4B	3.00	1.49	1.42
39	8	322	CLA	C4D-ND	-3.00	1.33	1.37
39	A	309	CLA	C3B-C4B	2.99	1.49	1.42
39	P	307	CLA	C4D-ND	-2.99	1.33	1.37
39	L	309	CLA	C3B-C4B	2.99	1.49	1.42
39	U	210	CLA	C3B-C4B	2.99	1.49	1.42
39	7	313	CLA	C3B-C4B	2.99	1.49	1.42
50	7	304	A1EB1	C30-C29	-2.99	1.27	1.32
39	M	308	CLA	C4D-ND	-2.99	1.33	1.37
39	y	308	CLA	C3B-C4B	2.99	1.49	1.42
39	Z	313	CLA	C4B-NB	2.99	1.41	1.37
39	9	320	CLA	C3B-C4B	2.99	1.49	1.42
39	V	310	CLA	C4D-ND	-2.99	1.33	1.37
39	W	313	CLA	C3B-C4B	2.99	1.49	1.42
39	J	311	CLA	C3B-C4B	2.99	1.49	1.42
39	b	836	CLA	C3B-C4B	2.99	1.49	1.42
39	R	309	CLA	C3B-C4B	2.99	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	D	311	CLA	C3B-C4B	2.99	1.49	1.42
39	D	317	CLA	C3B-C4B	2.99	1.49	1.42
50	4	302	A1EB1	C30-C29	-2.99	1.27	1.32
39	C	311	CLA	C4D-ND	-2.99	1.33	1.37
39	Q	310	CLA	C3B-C4B	2.99	1.49	1.42
39	F	321	CLA	C3B-C4B	2.99	1.49	1.42
39	8	318	CLA	C3B-C4B	2.99	1.49	1.42
39	I	315	CLA	C3B-C4B	2.98	1.49	1.42
39	y	310	CLA	C3B-C4B	2.98	1.49	1.42
39	4	311	CLA	C3B-C4B	2.98	1.49	1.42
39	b	824	CLA	C3B-C4B	2.98	1.49	1.42
39	B	203	CLA	C4D-ND	-2.98	1.33	1.37
49	Q	313	KC2	C4B-NB	-2.98	1.34	1.37
39	L	311	CLA	C3B-C4B	2.98	1.49	1.42
39	W	311	CLA	C4D-ND	-2.98	1.33	1.37
39	3	314	CLA	C3B-C4B	2.98	1.49	1.42
39	I	316	CLA	C3B-C4B	2.98	1.49	1.42
48	I	304	A86	C30-C29	-2.98	1.27	1.32
39	x	318	CLA	C3B-C4B	2.98	1.49	1.42
39	G	318	CLA	C4D-ND	-2.98	1.33	1.37
39	F	308	CLA	C3B-C4B	2.98	1.49	1.42
39	B	209	CLA	C3B-C4B	2.98	1.49	1.42
39	O	310	CLA	C3B-C4B	2.98	1.49	1.42
39	4	314	CLA	C3B-C4B	2.98	1.49	1.42
39	a	805	CLA	C4D-ND	-2.98	1.33	1.37
47	D	304	SQD	O47-C7	2.98	1.42	1.34
39	x	309	CLA	C3B-C4B	2.98	1.49	1.42
39	a	824	CLA	C4D-ND	-2.97	1.33	1.37
39	3	311	CLA	C4D-ND	-2.97	1.33	1.37
39	a	805	CLA	C3B-C4B	2.97	1.49	1.42
39	b	838	CLA	C3B-C4B	2.97	1.49	1.42
39	l	204	CLA	C3B-C4B	2.97	1.49	1.42
50	1	305	A1EB1	C30-C29	-2.97	1.27	1.32
39	C	304	CLA	C3B-C4B	2.97	1.49	1.42
39	E	307	CLA	C3B-C4B	2.97	1.49	1.42
39	x	317	CLA	C3B-C4B	2.97	1.49	1.42
39	k	202	CLA	C4D-ND	-2.97	1.33	1.37
39	3	322	CLA	C3B-C4B	2.97	1.49	1.42
39	A	307	CLA	C4D-ND	-2.97	1.33	1.37
39	M	310	CLA	C4D-ND	-2.97	1.33	1.37
39	b	842	CLA	C4D-ND	-2.97	1.33	1.37
39	5	306	CLA	C3B-C4B	2.97	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	E	306	CLA	C3B-C4B	2.97	1.49	1.42
39	X	309	CLA	C3B-C4B	2.97	1.49	1.42
39	6	322	CLA	C3B-C4B	2.97	1.49	1.42
39	E	315	CLA	C3B-C4B	2.97	1.49	1.42
39	1	311	CLA	C3B-C4B	2.97	1.49	1.42
39	S	313	CLA	C4D-ND	-2.97	1.33	1.37
39	0	323	CLA	C3B-C4B	2.97	1.49	1.42
39	D	311	CLA	C4D-ND	-2.97	1.33	1.37
39	3	311	CLA	C3B-C4B	2.97	1.49	1.42
39	G	310	CLA	C3B-C4B	2.96	1.49	1.42
39	O	308	CLA	C4D-ND	-2.96	1.33	1.37
39	T	310	CLA	C4D-ND	-2.96	1.33	1.37
39	z	318	CLA	C3B-C4B	2.96	1.49	1.42
39	W	311	CLA	C3B-C4B	2.96	1.49	1.42
39	B	204	CLA	C3B-C4B	2.96	1.49	1.42
39	E	319	CLA	C3B-C4B	2.96	1.49	1.42
39	l	203	CLA	C3B-C4B	2.96	1.49	1.42
39	a	813	CLA	C4D-ND	-2.96	1.33	1.37
50	G	308	A1EB1	C30-C29	-2.96	1.27	1.32
50	y	301	A1EB1	C30-C29	-2.96	1.27	1.32
39	J	309	CLA	C3B-C4B	2.96	1.49	1.42
39	9	308	CLA	C4D-ND	-2.96	1.33	1.37
39	2	319	CLA	C4D-ND	-2.96	1.33	1.37
39	j	101	CLA	C3B-C4B	2.96	1.49	1.42
39	H	313	CLA	C3B-C4B	2.96	1.49	1.42
39	V	316	CLA	C3B-C4B	2.96	1.49	1.42
39	U	211	CLA	C3B-C4B	2.96	1.49	1.42
39	U	215	CLA	C3B-C4B	2.96	1.49	1.42
39	O	313	CLA	C3B-C4B	2.96	1.49	1.42
39	a	819	CLA	C3B-C4B	2.96	1.49	1.42
39	A	311	CLA	C3B-C4B	2.96	1.49	1.42
39	Y	310	CLA	C3B-C4B	2.96	1.49	1.42
39	V	313	CLA	C4D-ND	-2.96	1.33	1.37
39	D	314	CLA	C3B-C4B	2.96	1.49	1.42
39	F	310	CLA	C3B-C4B	2.96	1.49	1.42
39	b	816	CLA	C3B-C4B	2.96	1.49	1.42
39	a	814	CLA	C3B-C4B	2.96	1.49	1.42
39	a	817	CLA	C3B-C4B	2.95	1.49	1.42
39	6	315	CLA	C3B-C4B	2.95	1.49	1.42
39	E	314	CLA	C4D-ND	-2.95	1.33	1.37
39	a	833	CLA	C3B-C4B	2.95	1.49	1.42
39	6	310	CLA	C3B-C4B	2.95	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	K	312	CLA	C3B-C4B	2.95	1.49	1.42
39	a	815	CLA	C3B-C4B	2.95	1.49	1.42
39	E	307	CLA	C4D-ND	-2.95	1.33	1.37
39	U	211	CLA	C4D-ND	-2.95	1.33	1.37
39	P	309	CLA	C3B-C4B	2.95	1.49	1.42
39	Q	311	CLA	C3B-C4B	2.95	1.49	1.42
39	I	311	CLA	C3B-C4B	2.95	1.49	1.42
39	6	313	CLA	C3B-C4B	2.95	1.49	1.42
39	A	312	CLA	C3B-C4B	2.95	1.49	1.42
39	Q	309	CLA	C3B-C4B	2.95	1.49	1.42
39	b	815	CLA	C4D-ND	-2.95	1.33	1.37
39	b	839	CLA	C3B-C4B	2.95	1.49	1.42
39	0	313	CLA	C3B-C4B	2.95	1.49	1.42
39	b	828	CLA	C3B-C4B	2.95	1.49	1.42
39	b	809	CLA	C3B-C4B	2.95	1.49	1.42
39	k	201	CLA	C3B-C4B	2.95	1.49	1.42
39	x	306	CLA	C3B-C4B	2.95	1.49	1.42
39	y	307	CLA	C3B-C4B	2.95	1.49	1.42
39	k	202	CLA	C3B-C4B	2.95	1.49	1.42
39	y	318	CLA	C3B-C4B	2.95	1.49	1.42
39	Z	312	CLA	C3B-C4B	2.95	1.49	1.42
48	4	328	A86	C30-C29	-2.94	1.27	1.32
39	o	206	CLA	C3B-C4B	2.94	1.49	1.42
39	1	319	CLA	C3B-C4B	2.94	1.49	1.42
39	I	314	CLA	C3B-C4B	2.94	1.49	1.42
39	A	307	CLA	C3B-C4B	2.94	1.49	1.42
39	H	309	CLA	C4D-ND	-2.94	1.33	1.37
39	J	318	CLA	C3B-C4B	2.94	1.49	1.42
39	E	310	CLA	C3B-C4B	2.94	1.49	1.42
39	a	803	CLA	C4D-ND	-2.94	1.33	1.37
39	a	812	CLA	C3B-C4B	2.94	1.49	1.42
39	7	316	CLA	C3B-C4B	2.94	1.49	1.42
39	z	309	CLA	C3B-C4B	2.94	1.49	1.42
39	D	313	CLA	C3B-C4B	2.94	1.49	1.42
39	L	320	CLA	C3B-C4B	2.94	1.49	1.42
39	M	308	CLA	C3B-C4B	2.94	1.49	1.42
39	a	809	CLA	C4D-ND	-2.94	1.33	1.37
39	5	310	CLA	C3B-C4B	2.94	1.49	1.42
39	0	318	CLA	C3B-C4B	2.94	1.49	1.42
39	G	312	CLA	C4D-ND	-2.94	1.33	1.37
39	5	308	CLA	C3B-C4B	2.94	1.49	1.42
39	o	201	CLA	C4D-ND	-2.94	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	b	832	CLA	C3B-C4B	2.94	1.49	1.42
39	U	207	CLA	C3B-C4B	2.94	1.49	1.42
39	o	203	CLA	C3B-C4B	2.93	1.49	1.42
39	Y	311	CLA	C3B-C4B	2.93	1.49	1.42
39	b	816	CLA	C4D-ND	-2.93	1.33	1.37
39	H	308	CLA	C3B-C4B	2.93	1.49	1.42
39	5	308	CLA	C4D-ND	-2.93	1.33	1.37
39	2	312	CLA	C3B-C4B	2.93	1.49	1.42
39	a	807	CLA	C4D-ND	-2.93	1.33	1.37
39	a	811	CLA	C4D-ND	-2.93	1.33	1.37
39	R	307	CLA	C4D-ND	-2.93	1.33	1.37
39	7	324	CLA	C3B-C4B	2.93	1.49	1.42
39	z	314	CLA	C3B-C4B	2.93	1.49	1.42
39	6	311	CLA	C3B-C4B	2.93	1.49	1.42
48	3	306	A86	C30-C29	-2.93	1.27	1.32
39	i	103	CLA	C3B-C4B	2.93	1.49	1.42
39	R	308	CLA	C3B-C4B	2.93	1.49	1.42
50	1	301	A1EB1	C30-C29	-2.93	1.27	1.32
39	W	309	CLA	C4D-ND	-2.93	1.33	1.37
39	S	316	CLA	C3B-C4B	2.93	1.49	1.42
39	Y	314	CLA	C3B-C4B	2.93	1.49	1.42
39	Z	304	CLA	C3B-C4B	2.93	1.49	1.42
39	J	310	CLA	C4D-ND	-2.93	1.33	1.37
39	3	316	CLA	C3B-C4B	2.93	1.49	1.42
39	K	312	CLA	C4D-ND	-2.93	1.33	1.37
39	L	311	CLA	C4D-ND	-2.93	1.33	1.37
39	T	311	CLA	C4D-ND	-2.93	1.33	1.37
39	1	308	CLA	C3B-C4B	2.93	1.49	1.42
39	b	835	CLA	C3B-C4B	2.93	1.49	1.42
39	3	320	CLA	C3B-C4B	2.93	1.49	1.42
39	A	312	CLA	C4D-ND	-2.92	1.33	1.37
39	G	314	CLA	C3B-C4B	2.92	1.49	1.42
39	b	829	CLA	C3B-C4B	2.92	1.49	1.42
39	h	201	CLA	C3B-C4B	2.92	1.49	1.42
39	E	316	CLA	C3B-C4B	2.92	1.49	1.42
39	a	813	CLA	C3B-C4B	2.92	1.49	1.42
39	P	307	CLA	C3B-C4B	2.92	1.49	1.42
39	3	323	CLA	C3B-C4B	2.92	1.49	1.42
39	Z	316	CLA	C3B-C4B	2.92	1.49	1.42
39	E	317	CLA	C3B-C4B	2.92	1.49	1.42
39	Y	305	CLA	C3B-C4B	2.92	1.49	1.42
39	b	803	CLA	C3B-C4B	2.92	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	R	315	CLA	C3B-C4B	2.92	1.49	1.42
39	U	214	CLA	C3B-C4B	2.92	1.49	1.42
39	b	803	CLA	C4D-ND	-2.92	1.33	1.37
39	3	312	CLA	C4D-ND	-2.92	1.33	1.37
39	b	806	CLA	C1B-C2B	2.92	1.50	1.43
39	V	309	CLA	C3B-C4B	2.92	1.49	1.42
39	4	319	CLA	C3B-C4B	2.92	1.49	1.42
39	E	308	CLA	C4D-ND	-2.92	1.33	1.37
39	o	202	CLA	C3B-C4B	2.92	1.49	1.42
39	A	308	CLA	C3B-C4B	2.92	1.49	1.42
39	C	311	CLA	C3B-C4B	2.92	1.49	1.42
39	U	210	CLA	C4D-ND	-2.92	1.33	1.37
39	H	306	CLA	C3B-C4B	2.92	1.49	1.42
39	9	315	CLA	C3B-C4B	2.92	1.49	1.42
47	F	318	SQD	O47-C7	2.92	1.42	1.34
39	b	840	CLA	C3B-C4B	2.92	1.49	1.42
39	k	203	CLA	C3B-C4B	2.92	1.49	1.42
39	o	201	CLA	C3B-C4B	2.92	1.49	1.42
39	F	313	CLA	C3B-C4B	2.92	1.49	1.42
39	K	306	CLA	C4D-ND	-2.92	1.33	1.37
39	1	317	CLA	C3B-C4B	2.92	1.49	1.42
39	b	821	CLA	C4D-ND	-2.92	1.33	1.37
39	7	318	CLA	C3B-C4B	2.92	1.49	1.42
39	7	321	CLA	C3B-C4B	2.92	1.49	1.42
39	K	308	CLA	C4D-ND	-2.92	1.33	1.37
39	y	312	CLA	C3B-C4B	2.92	1.49	1.42
39	F	310	CLA	C4D-ND	-2.91	1.33	1.37
39	a	819	CLA	C4D-ND	-2.91	1.33	1.37
39	a	818	CLA	C3B-C4B	2.91	1.49	1.42
39	b	851	CLA	C3B-C4B	2.91	1.49	1.42
48	2	305	A86	C30-C29	-2.91	1.27	1.32
39	Y	303	CLA	C3B-C4B	2.91	1.49	1.42
39	L	316	CLA	C3B-C4B	2.91	1.49	1.42
39	X	316	CLA	C3B-C4B	2.91	1.49	1.42
39	Z	313	CLA	C1B-C2B	2.91	1.50	1.43
39	a	818	CLA	C4D-ND	-2.91	1.33	1.37
39	T	311	CLA	C3B-C4B	2.91	1.49	1.42
39	Z	305	CLA	C3B-C4B	2.91	1.49	1.42
47	D	320	SQD	O47-C7	2.91	1.42	1.34
39	a	815	CLA	C4D-ND	-2.91	1.33	1.37
39	A	309	CLA	C4D-ND	-2.91	1.33	1.37
39	J	309	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	k	205	SQD	O47-C7	2.91	1.42	1.34
39	C	307	CLA	C4D-ND	-2.91	1.33	1.37
39	b	822	CLA	C4D-ND	-2.91	1.33	1.37
39	k	203	CLA	C4D-ND	-2.91	1.33	1.37
39	E	318	CLA	C3B-C4B	2.91	1.49	1.42
39	H	310	CLA	C3B-C4B	2.91	1.49	1.42
39	o	206	CLA	C4D-ND	-2.91	1.33	1.37
39	Q	314	CLA	C4D-ND	-2.91	1.33	1.37
39	J	307	CLA	C3B-C4B	2.91	1.49	1.42
39	1	310	CLA	C3B-C4B	2.91	1.49	1.42
39	Y	302	CLA	C3B-C4B	2.91	1.49	1.42
39	x	308	CLA	C3B-C4B	2.91	1.49	1.42
39	a	820	CLA	C4D-ND	-2.91	1.33	1.37
39	K	308	CLA	C3B-C4B	2.91	1.49	1.42
39	J	308	CLA	C3B-C4B	2.90	1.49	1.42
39	U	209	CLA	C3B-C4B	2.90	1.49	1.42
39	b	822	CLA	C3B-C4B	2.90	1.49	1.42
39	D	312	CLA	C4D-ND	-2.90	1.33	1.37
39	0	310	CLA	C4D-ND	-2.90	1.33	1.37
39	2	308	CLA	C4D-ND	-2.90	1.33	1.37
39	U	201	CLA	C4D-ND	-2.90	1.33	1.37
39	b	842	CLA	C3B-C4B	2.90	1.49	1.42
39	D	316	CLA	C3B-C4B	2.90	1.49	1.42
39	F	309	CLA	C3B-C4B	2.90	1.49	1.42
39	S	308	CLA	C3B-C4B	2.90	1.49	1.42
39	b	829	CLA	C4D-ND	-2.90	1.33	1.37
39	J	313	CLA	C3B-C4B	2.90	1.49	1.42
39	1	320	CLA	C3B-C4B	2.90	1.49	1.42
39	M	309	CLA	C3B-C4B	2.90	1.49	1.42
39	M	310	CLA	C3B-C4B	2.90	1.49	1.42
39	Z	307	CLA	C3B-C4B	2.90	1.49	1.42
39	7	321	CLA	C4D-ND	-2.90	1.33	1.37
39	b	826	CLA	C3B-C4B	2.90	1.49	1.42
39	1	316	CLA	C3B-C4B	2.90	1.49	1.42
39	D	310	CLA	C4D-ND	-2.90	1.33	1.37
39	P	314	CLA	C3B-C4B	2.90	1.49	1.42
39	b	809	CLA	C4D-ND	-2.90	1.33	1.37
39	b	840	CLA	C4D-ND	-2.90	1.33	1.37
39	L	310	CLA	C4D-ND	-2.90	1.33	1.37
39	1	308	CLA	C4D-ND	-2.90	1.33	1.37
39	9	312	CLA	C4D-ND	-2.90	1.33	1.37
48	L	301	A86	C30-C29	-2.90	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	J	312	CLA	C3B-C4B	2.90	1.49	1.42
39	C	306	CLA	C3B-C4B	2.90	1.49	1.42
39	z	306	CLA	C3B-C4B	2.90	1.49	1.42
39	S	313	CLA	C3B-C4B	2.90	1.49	1.42
39	a	809	CLA	C3B-C4B	2.90	1.49	1.42
39	A	314	CLA	C3B-C4B	2.90	1.49	1.42
39	Q	314	CLA	C3B-C4B	2.90	1.49	1.42
39	S	309	CLA	C4D-ND	-2.90	1.33	1.37
39	Q	312	CLA	C4D-ND	-2.90	1.33	1.37
39	8	312	CLA	C3B-C4B	2.90	1.49	1.42
39	a	828	CLA	C3B-C4B	2.90	1.49	1.42
39	V	311	CLA	C3B-C4B	2.90	1.49	1.42
39	a	812	CLA	C4D-ND	-2.89	1.33	1.37
39	b	805	CLA	C4D-ND	-2.89	1.33	1.37
39	1	320	CLA	C4D-ND	-2.89	1.33	1.37
39	K	311	CLA	C3B-C4B	2.89	1.49	1.42
39	3	312	CLA	C3B-C4B	2.89	1.49	1.42
47	F	319	SQD	O47-C7	2.89	1.42	1.34
39	b	839	CLA	C4D-ND	-2.89	1.33	1.37
39	Q	320	CLA	C3B-C4B	2.89	1.49	1.42
39	I	301	CLA	C4D-ND	-2.89	1.33	1.37
39	8	322	CLA	C3B-C4B	2.89	1.49	1.42
39	l	201	CLA	C3B-C4B	2.89	1.49	1.42
39	C	306	CLA	C4D-ND	-2.89	1.33	1.37
39	G	310	CLA	C4D-ND	-2.89	1.33	1.37
39	B	204	CLA	C4D-ND	-2.89	1.33	1.37
39	Q	321	CLA	C4D-ND	-2.89	1.33	1.37
39	Z	316	CLA	C4D-ND	-2.89	1.33	1.37
39	0	322	CLA	C3B-C4B	2.89	1.49	1.42
39	a	835	CLA	C3B-C4B	2.89	1.49	1.42
39	a	835	CLA	C4D-ND	-2.89	1.33	1.37
39	A	311	CLA	C4D-ND	-2.89	1.33	1.37
39	b	823	CLA	C3B-C4B	2.89	1.49	1.42
39	b	810	CLA	C3B-C4B	2.89	1.49	1.42
39	5	306	CLA	C4D-ND	-2.89	1.33	1.37
39	x	318	CLA	C4D-ND	-2.89	1.33	1.37
39	K	307	CLA	C3B-C4B	2.89	1.49	1.42
39	M	315	CLA	C3B-C4B	2.89	1.49	1.42
39	a	816	CLA	C4D-ND	-2.89	1.33	1.37
39	b	818	CLA	C4D-ND	-2.89	1.33	1.37
39	J	317	CLA	C3B-C4B	2.89	1.49	1.42
39	H	309	CLA	C3B-C4B	2.89	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	9	319	CLA	C3B-C4B	2.89	1.49	1.42
39	b	819	CLA	C4D-ND	-2.88	1.33	1.37
39	H	307	CLA	C3B-C4B	2.88	1.49	1.42
39	D	318	CLA	C3B-C4B	2.88	1.49	1.42
39	b	810	CLA	C4D-ND	-2.88	1.33	1.37
39	F	313	CLA	C4D-ND	-2.88	1.33	1.37
39	L	313	CLA	C3B-C4B	2.88	1.49	1.42
39	9	309	CLA	C3B-C4B	2.88	1.49	1.42
39	O	308	CLA	C3B-C4B	2.88	1.49	1.42
39	9	310	CLA	C4D-ND	-2.88	1.33	1.37
39	h	201	CLA	C4D-ND	-2.88	1.33	1.37
39	6	312	CLA	C3B-C4B	2.88	1.49	1.42
39	6	310	CLA	C4D-ND	-2.88	1.33	1.37
39	C	309	CLA	C3B-C4B	2.88	1.49	1.42
39	L	319	CLA	C3B-C4B	2.88	1.49	1.42
39	O	312	CLA	C3B-C4B	2.88	1.49	1.42
39	b	836	CLA	C4D-ND	-2.88	1.33	1.37
39	l	203	CLA	C4D-ND	-2.88	1.33	1.37
39	E	312	CLA	C4D-ND	-2.88	1.33	1.37
39	z	318	CLA	C4D-ND	-2.88	1.33	1.37
39	F	306	CLA	C3B-C4B	2.88	1.49	1.42
39	6	312	CLA	C4D-ND	-2.88	1.33	1.37
39	4	316	CLA	C3B-C4B	2.88	1.49	1.42
39	6	311	CLA	C4D-ND	-2.87	1.33	1.37
39	y	319	CLA	C4D-ND	-2.87	1.33	1.37
39	7	315	CLA	C3B-C4B	2.87	1.49	1.42
39	b	825	CLA	C3B-C4B	2.87	1.49	1.42
39	z	306	CLA	C4D-ND	-2.87	1.33	1.37
39	T	319	CLA	C3B-C4B	2.87	1.49	1.42
39	G	309	CLA	C4D-ND	-2.87	1.33	1.37
39	F	312	CLA	C3B-C4B	2.87	1.49	1.42
49	T	315	KC2	CBA-CGA	-2.87	1.41	1.48
39	U	201	CLA	C4B-NB	2.87	1.41	1.37
39	C	308	CLA	C3B-C4B	2.87	1.49	1.42
39	F	316	CLA	C3B-C4B	2.87	1.49	1.42
39	D	318	CLA	C4D-ND	-2.87	1.33	1.37
39	R	309	CLA	C4D-ND	-2.87	1.33	1.37
39	b	823	CLA	C4D-ND	-2.87	1.33	1.37
39	U	208	CLA	C4D-ND	-2.87	1.33	1.37
39	G	318	CLA	C3B-C4B	2.87	1.49	1.42
39	V	313	CLA	C3B-C4B	2.87	1.49	1.42
39	o	205	CLA	C4D-ND	-2.87	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	D	319	CLA	C3B-C4B	2.87	1.49	1.42
49	R	318	KC2	CBA-CGA	-2.87	1.41	1.48
39	D	312	CLA	C3B-C4B	2.87	1.49	1.42
39	9	312	CLA	C3B-C4B	2.87	1.49	1.42
39	a	817	CLA	C4D-ND	-2.87	1.33	1.37
39	0	322	CLA	C4D-ND	-2.87	1.33	1.37
39	L	310	CLA	C3B-C4B	2.87	1.49	1.42
39	Y	304	CLA	C3B-C4B	2.87	1.49	1.42
39	C	305	CLA	C3B-C4B	2.87	1.49	1.42
39	Z	315	CLA	C3B-C4B	2.87	1.49	1.42
39	F	306	CLA	C4D-ND	-2.86	1.33	1.37
39	1	309	CLA	C4D-ND	-2.86	1.33	1.37
39	a	822	CLA	C3B-C4B	2.86	1.49	1.42
39	8	315	CLA	C3B-C4B	2.86	1.49	1.42
39	a	808	CLA	C3B-C4B	2.86	1.49	1.42
39	Q	317	CLA	C3B-C4B	2.86	1.49	1.42
39	5	315	CLA	C3B-C4B	2.86	1.49	1.42
39	9	307	CLA	C3B-C4B	2.86	1.49	1.42
39	a	832	CLA	C4D-ND	-2.86	1.33	1.37
39	I	308	CLA	C4D-ND	-2.86	1.33	1.37
39	Y	303	CLA	C4D-ND	-2.86	1.33	1.37
39	E	313	CLA	C4B-NB	2.86	1.41	1.37
39	D	316	CLA	C4D-ND	-2.86	1.33	1.37
39	H	308	CLA	C4D-ND	-2.86	1.33	1.37
39	8	312	CLA	C4D-ND	-2.86	1.33	1.37
39	2	307	CLA	C3B-C4B	2.86	1.49	1.42
39	7	316	CLA	C4D-ND	-2.86	1.33	1.37
39	I	311	CLA	C4D-ND	-2.86	1.33	1.37
39	y	319	CLA	C3B-C4B	2.86	1.49	1.42
39	6	318	CLA	C3B-C4B	2.86	1.49	1.42
39	T	320	CLA	C4D-ND	-2.86	1.33	1.37
47	D	321	SQD	O47-C7	2.86	1.42	1.34
39	L	308	CLA	C3B-C4B	2.86	1.49	1.42
39	b	834	CLA	C3B-C4B	2.86	1.49	1.42
39	H	312	CLA	C3B-C4B	2.86	1.49	1.42
39	T	319	CLA	C4D-ND	-2.86	1.33	1.37
39	y	308	CLA	C4D-ND	-2.86	1.33	1.37
39	O	316	CLA	C3B-C4B	2.86	1.49	1.42
39	W	310	CLA	C3B-C4B	2.86	1.49	1.42
39	y	315	CLA	C3B-C4B	2.86	1.49	1.42
39	Z	309	CLA	C1B-C2B	2.86	1.50	1.43
39	x	311	CLA	C3B-C4B	2.86	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	a	827	CLA	CMB-C2B	-2.86	1.44	1.50
39	8	313	CLA	C3B-C4B	2.86	1.49	1.42
39	b	835	CLA	C4D-ND	-2.86	1.33	1.37
39	R	316	CLA	C4D-ND	-2.86	1.33	1.37
39	i	101	CLA	C3B-C4B	2.86	1.49	1.42
39	O	309	CLA	C3B-C4B	2.86	1.49	1.42
39	x	314	CLA	C3B-C4B	2.86	1.49	1.42
39	V	319	CLA	C3B-C4B	2.86	1.49	1.42
39	a	804	CLA	C4D-ND	-2.86	1.33	1.37
39	a	806	CLA	C4D-ND	-2.86	1.33	1.37
39	1	309	CLA	C3B-C4B	2.86	1.49	1.42
39	2	318	CLA	C3B-C4B	2.86	1.49	1.42
39	I	313	CLA	C4D-ND	-2.86	1.33	1.37
39	5	316	CLA	C3B-C4B	2.85	1.49	1.42
39	U	207	CLA	C4D-ND	-2.85	1.33	1.37
39	a	807	CLA	C3B-C4B	2.85	1.49	1.42
39	G	312	CLA	C3B-C4B	2.85	1.49	1.42
39	H	316	CLA	C3B-C4B	2.85	1.49	1.42
39	a	806	CLA	C3B-C4B	2.85	1.49	1.42
39	P	316	CLA	C3B-C4B	2.85	1.49	1.42
39	B	206	CLA	C4D-ND	-2.85	1.33	1.37
39	5	307	CLA	C4D-ND	-2.85	1.33	1.37
39	4	323	CLA	C3B-C4B	2.85	1.49	1.42
39	2	315	CLA	C3B-C4B	2.85	1.49	1.42
39	y	312	CLA	C4D-ND	-2.85	1.33	1.37
39	z	307	CLA	C4D-ND	-2.85	1.33	1.37
39	S	320	CLA	C3B-C4B	2.85	1.49	1.42
39	2	309	CLA	C3B-C4B	2.85	1.49	1.42
39	K	307	CLA	C4D-ND	-2.85	1.33	1.37
39	L	308	CLA	C4D-ND	-2.85	1.33	1.37
39	O	309	CLA	C4D-ND	-2.85	1.33	1.37
39	I	310	CLA	C3B-C4B	2.85	1.49	1.42
39	6	321	CLA	C3B-C4B	2.85	1.49	1.42
39	E	309	CLA	C3B-C4B	2.85	1.49	1.42
39	G	309	CLA	C3B-C4B	2.85	1.49	1.42
39	E	318	CLA	C4D-ND	-2.85	1.33	1.37
39	C	310	CLA	C3B-C4B	2.85	1.49	1.42
39	V	319	CLA	C4D-ND	-2.85	1.33	1.37
39	1	319	CLA	C4D-ND	-2.85	1.33	1.37
39	M	317	CLA	C3B-C4B	2.85	1.49	1.42
39	a	827	CLA	C4D-ND	-2.85	1.33	1.37
39	X	309	CLA	C4D-ND	-2.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	V	315	KC2	CBA-CGA	-2.85	1.41	1.48
39	I	315	CLA	C4D-ND	-2.85	1.33	1.37
39	9	312	CLA	C1B-C2B	2.84	1.50	1.43
39	a	826	CLA	C4D-ND	-2.84	1.33	1.37
39	b	821	CLA	C3B-C4B	2.84	1.49	1.42
39	W	316	CLA	C3B-C4B	2.84	1.49	1.42
39	V	316	CLA	C4D-ND	-2.84	1.33	1.37
48	L	306	A86	C30-C29	-2.84	1.27	1.32
39	I	313	CLA	C3B-C4B	2.84	1.49	1.42
39	V	309	CLA	C4D-ND	-2.84	1.33	1.37
39	9	319	CLA	C4D-ND	-2.84	1.33	1.37
47	H	318	SQD	O47-C7	2.84	1.42	1.34
39	z	311	CLA	C3B-C4B	2.84	1.49	1.42
39	a	826	CLA	C3B-C4B	2.84	1.49	1.42
39	L	319	CLA	C4D-ND	-2.84	1.33	1.37
39	0	311	CLA	C3B-C4B	2.84	1.49	1.42
39	2	310	CLA	C3B-C4B	2.84	1.49	1.42
39	K	311	CLA	C4D-ND	-2.84	1.33	1.37
51	y	317	A1ECV	C3D-C2D	2.84	1.46	1.37
39	z	311	CLA	C4D-ND	-2.84	1.33	1.37
39	C	307	CLA	C3B-C4B	2.84	1.49	1.42
39	b	827	CLA	C3B-C4B	2.84	1.49	1.42
39	R	308	CLA	C4D-ND	-2.84	1.33	1.37
47	9	322	SQD	O47-C7	2.84	1.42	1.34
39	a	847	CLA	C4D-ND	-2.84	1.33	1.37
39	o	202	CLA	C4D-ND	-2.84	1.33	1.37
39	T	313	CLA	C4D-ND	-2.84	1.33	1.37
39	X	311	CLA	C4D-ND	-2.84	1.33	1.37
39	Y	314	CLA	C4D-ND	-2.84	1.33	1.37
50	H	304	A1EB1	C30-C29	-2.84	1.27	1.32
39	I	309	CLA	C4D-ND	-2.83	1.33	1.37
39	j	101	CLA	C4D-ND	-2.83	1.33	1.37
39	D	315	CLA	C4D-ND	-2.83	1.33	1.37
39	3	314	CLA	C4D-ND	-2.83	1.33	1.37
39	2	315	CLA	C4D-ND	-2.83	1.33	1.37
39	R	311	CLA	C4D-ND	-2.83	1.33	1.37
39	b	802	CLA	C3B-C4B	2.83	1.49	1.42
39	b	811	CLA	C4D-ND	-2.83	1.33	1.37
39	S	308	CLA	C4D-ND	-2.83	1.33	1.37
39	K	309	CLA	C4D-ND	-2.83	1.33	1.37
39	x	306	CLA	C4D-ND	-2.83	1.33	1.37
39	9	315	CLA	C4D-ND	-2.83	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	313	CLA	C3B-C4B	2.83	1.49	1.42
39	a	837	CLA	C4D-ND	-2.83	1.33	1.37
39	A	308	CLA	C4D-ND	-2.83	1.33	1.37
39	D	313	CLA	C4D-ND	-2.83	1.33	1.37
39	4	319	CLA	C4D-ND	-2.83	1.33	1.37
47	M	301	SQD	O47-C7	2.83	1.42	1.34
39	F	309	CLA	C4D-ND	-2.83	1.33	1.37
39	0	315	CLA	C4D-ND	-2.83	1.33	1.37
39	2	316	CLA	C3B-C4B	2.83	1.49	1.42
48	6	307	A86	C30-C29	-2.83	1.27	1.32
39	y	315	CLA	C4D-ND	-2.83	1.33	1.37
39	K	314	CLA	C3B-C4B	2.83	1.49	1.42
39	f	803	CLA	C4D-ND	-2.83	1.33	1.37
39	Q	317	CLA	C4D-ND	-2.83	1.33	1.37
39	2	316	CLA	C4D-ND	-2.83	1.33	1.37
39	H	316	CLA	C4D-ND	-2.82	1.33	1.37
39	J	318	CLA	C4D-ND	-2.82	1.33	1.37
39	W	316	CLA	C4D-ND	-2.82	1.33	1.37
39	y	310	CLA	C4D-ND	-2.82	1.33	1.37
47	E	320	SQD	O47-C7	2.82	1.42	1.34
39	7	318	CLA	C4D-ND	-2.82	1.33	1.37
39	z	308	CLA	C3B-C4B	2.82	1.49	1.42
39	S	320	CLA	C1B-C2B	2.82	1.49	1.43
39	4	313	CLA	C3B-C4B	2.82	1.49	1.42
39	Z	304	CLA	C4D-ND	-2.82	1.33	1.37
39	T	318	CLA	C3B-C4B	2.82	1.49	1.42
39	a	830	CLA	C3B-C4B	2.82	1.49	1.42
39	i	103	CLA	C4D-ND	-2.82	1.33	1.37
39	E	315	CLA	C4D-ND	-2.82	1.33	1.37
39	R	316	CLA	C3B-C4B	2.82	1.49	1.42
39	S	310	CLA	C3B-C4B	2.82	1.49	1.42
39	a	828	CLA	C4D-ND	-2.82	1.33	1.37
39	K	306	CLA	C3B-C4B	2.82	1.49	1.42
39	b	830	CLA	C4D-ND	-2.82	1.33	1.37
39	S	319	CLA	C3B-C4B	2.82	1.49	1.42
39	W	319	CLA	C3B-C4B	2.82	1.49	1.42
39	J	316	CLA	C3B-C4B	2.82	1.49	1.42
39	P	314	CLA	C4D-ND	-2.82	1.33	1.37
39	b	819	CLA	C3B-C4B	2.82	1.49	1.42
39	J	308	CLA	C4D-ND	-2.82	1.33	1.37
39	L	309	CLA	C4D-ND	-2.82	1.33	1.37
39	4	314	CLA	C4D-ND	-2.82	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	M	315	CLA	C4D-ND	-2.81	1.33	1.37
39	M	318	CLA	C4D-ND	-2.81	1.33	1.37
39	Q	320	CLA	C4D-ND	-2.81	1.33	1.37
39	X	307	CLA	C4D-ND	-2.81	1.33	1.37
39	8	310	CLA	C4D-ND	-2.81	1.33	1.37
49	G	313	KC2	CBA-CGA	-2.81	1.42	1.48
39	b	812	CLA	C4D-ND	-2.81	1.33	1.37
39	C	309	CLA	C4D-ND	-2.81	1.33	1.37
39	a	821	CLA	C1B-C2B	2.81	1.49	1.43
39	b	830	CLA	C3B-C4B	2.81	1.49	1.42
39	a	829	CLA	C4D-ND	-2.81	1.33	1.37
39	b	820	CLA	C3B-C4B	2.81	1.49	1.42
39	B	206	CLA	C3B-C4B	2.81	1.49	1.42
39	6	322	CLA	C4D-ND	-2.81	1.33	1.37
51	Z	308	A1ECV	C3D-C2D	2.81	1.46	1.37
47	P	301	SQD	O47-C7	2.81	1.42	1.34
39	H	312	CLA	C4D-ND	-2.81	1.33	1.37
39	1	310	CLA	C4D-ND	-2.81	1.33	1.37
39	x	308	CLA	C4D-ND	-2.81	1.33	1.37
39	6	313	CLA	C4D-ND	-2.81	1.33	1.37
49	X	318	KC2	CBA-CGA	-2.81	1.42	1.48
39	b	812	CLA	C3B-C4B	2.81	1.49	1.42
39	A	306	CLA	C3B-C4B	2.81	1.49	1.42
39	a	814	CLA	C4D-ND	-2.81	1.33	1.37
39	T	310	CLA	C3B-C4B	2.81	1.49	1.42
39	H	315	CLA	C3B-C4B	2.81	1.49	1.42
39	1	317	CLA	C4D-ND	-2.81	1.33	1.37
49	9	313	KC2	C4B-NB	-2.81	1.34	1.37
39	D	310	CLA	C3B-C4B	2.81	1.49	1.42
39	7	325	CLA	C1B-C2B	2.81	1.49	1.43
39	b	834	CLA	C4D-ND	-2.81	1.33	1.37
39	b	838	CLA	C4D-ND	-2.81	1.33	1.37
39	J	317	CLA	C4D-ND	-2.81	1.33	1.37
39	k	201	CLA	C4D-ND	-2.81	1.33	1.37
39	x	314	CLA	C4D-ND	-2.81	1.33	1.37
39	K	309	CLA	C3B-C4B	2.81	1.49	1.42
49	V	320	KC2	CBA-CGA	-2.81	1.42	1.48
39	C	304	CLA	C4D-ND	-2.80	1.33	1.37
39	J	311	CLA	C4D-ND	-2.80	1.33	1.37
39	a	810	CLA	C4D-ND	-2.80	1.33	1.37
39	8	321	CLA	C4D-ND	-2.80	1.33	1.37
49	A	313	KC2	CBA-CGA	-2.80	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	V	318	KC2	CBA-CGA	-2.80	1.42	1.48
47	4	327	SQD	O47-C7	2.80	1.42	1.34
39	8	321	CLA	C3B-C4B	2.80	1.49	1.42
39	O	318	CLA	C4D-ND	-2.80	1.33	1.37
39	1	311	CLA	C4D-ND	-2.80	1.33	1.37
39	5	310	CLA	C4D-ND	-2.80	1.33	1.37
39	7	325	CLA	C4D-ND	-2.80	1.33	1.37
49	H	314	KC2	CBA-CGA	-2.80	1.42	1.48
39	b	831	CLA	C4D-ND	-2.80	1.33	1.37
39	W	318	CLA	C3B-C4B	2.80	1.49	1.42
39	F	316	CLA	C4D-ND	-2.80	1.33	1.37
39	J	313	CLA	C4D-ND	-2.80	1.33	1.37
39	8	313	CLA	C4D-ND	-2.80	1.33	1.37
49	4	324	KC2	CBA-CGA	-2.80	1.42	1.48
39	8	315	CLA	C4D-ND	-2.80	1.33	1.37
51	Y	306	A1ECV	C3D-C2D	2.80	1.46	1.37
49	P	312	KC2	CBA-CGA	-2.80	1.42	1.48
39	L	313	CLA	C4D-ND	-2.80	1.33	1.37
39	1	313	CLA	C3B-C4B	2.80	1.49	1.42
49	M	313	KC2	CBA-CGA	-2.80	1.42	1.48
39	a	831	CLA	C3B-C4B	2.80	1.49	1.42
39	W	310	CLA	C4D-ND	-2.80	1.33	1.37
39	Z	306	CLA	C4D-ND	-2.80	1.33	1.37
39	2	319	CLA	C3B-C4B	2.80	1.49	1.42
39	E	319	CLA	C4D-ND	-2.80	1.33	1.37
39	U	212	CLA	C4D-ND	-2.80	1.33	1.37
39	M	312	CLA	C3B-C4B	2.80	1.49	1.42
39	a	808	CLA	C4D-ND	-2.80	1.33	1.37
39	3	322	CLA	C4D-ND	-2.80	1.33	1.37
39	2	310	CLA	C4D-ND	-2.80	1.33	1.37
47	T	321	SQD	O47-C7	2.80	1.42	1.34
39	E	308	CLA	C3B-C4B	2.80	1.49	1.42
49	L	315	KC2	CBA-CGA	-2.80	1.42	1.48
39	H	310	CLA	C4D-ND	-2.80	1.33	1.37
39	b	808	CLA	C4D-ND	-2.80	1.33	1.37
39	M	312	CLA	C4D-ND	-2.80	1.33	1.37
39	x	311	CLA	C4D-ND	-2.80	1.33	1.37
39	b	828	CLA	C4D-ND	-2.79	1.33	1.37
39	Z	305	CLA	C4D-ND	-2.79	1.33	1.37
39	b	820	CLA	C4D-ND	-2.79	1.33	1.37
39	b	851	CLA	C4D-ND	-2.79	1.33	1.37
39	6	318	CLA	C4D-ND	-2.79	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	3	316	CLA	C4D-ND	-2.79	1.33	1.37
49	R	312	KC2	CBA-CGA	-2.79	1.42	1.48
39	Z	306	CLA	C3B-C4B	2.79	1.49	1.42
39	Q	309	CLA	C4D-ND	-2.79	1.33	1.37
39	0	320	CLA	C4D-ND	-2.79	1.33	1.37
39	5	316	CLA	C4D-ND	-2.79	1.33	1.37
39	x	307	CLA	C4D-ND	-2.79	1.33	1.37
49	V	312	KC2	CBA-CGA	-2.79	1.42	1.48
39	0	313	CLA	C4D-ND	-2.79	1.33	1.37
39	A	306	CLA	C4D-ND	-2.79	1.33	1.37
39	b	831	CLA	C3B-C4B	2.79	1.49	1.42
39	b	801	CLA	C1D-ND	2.79	1.41	1.37
39	F	315	CLA	C3B-C4B	2.79	1.49	1.42
39	a	821	CLA	C4D-ND	-2.79	1.33	1.37
39	a	830	CLA	C4D-ND	-2.79	1.33	1.37
39	E	306	CLA	C4D-ND	-2.79	1.33	1.37
39	P	308	CLA	C4D-ND	-2.79	1.33	1.37
39	T	318	CLA	C4D-ND	-2.79	1.33	1.37
39	b	824	CLA	C4D-ND	-2.79	1.33	1.37
39	D	309	CLA	C3B-C4B	2.79	1.49	1.42
49	V	314	KC2	CBA-CGA	-2.79	1.42	1.48
39	S	316	CLA	C4D-ND	-2.79	1.33	1.37
39	z	314	CLA	C4D-ND	-2.79	1.33	1.37
39	b	814	CLA	C4D-ND	-2.78	1.33	1.37
39	C	308	CLA	C4D-ND	-2.78	1.33	1.37
49	8	314	KC2	CBA-CGA	-2.78	1.42	1.48
39	F	321	CLA	C4D-ND	-2.78	1.33	1.37
39	K	314	CLA	C4D-ND	-2.78	1.33	1.37
39	b	841	CLA	C4D-ND	-2.78	1.33	1.37
39	Z	309	CLA	C3B-C4B	2.78	1.49	1.42
39	O	313	CLA	C4D-ND	-2.78	1.33	1.37
39	U	215	CLA	C4D-ND	-2.78	1.33	1.37
49	T	312	KC2	CBA-CGA	-2.78	1.42	1.48
39	a	847	CLA	C3B-C4B	2.78	1.49	1.42
39	C	305	CLA	C4D-ND	-2.78	1.33	1.37
39	9	309	CLA	C4D-ND	-2.78	1.33	1.37
49	F	307	KC2	CBA-CGA	-2.78	1.42	1.48
39	U	214	CLA	C4D-ND	-2.78	1.33	1.37
39	V	311	CLA	C4D-ND	-2.78	1.33	1.37
39	W	318	CLA	C4D-ND	-2.78	1.33	1.37
39	T	309	CLA	C4D-ND	-2.78	1.33	1.37
47	S	301	SQD	O47-C7	2.78	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	y	311	A1ECV	C3D-C2D	2.78	1.46	1.37
49	W	315	KC2	CBA-CGA	-2.78	1.42	1.48
39	4	316	CLA	C4D-ND	-2.78	1.33	1.37
49	7	319	KC2	CBA-CGA	-2.78	1.42	1.48
39	E	316	CLA	C4D-ND	-2.78	1.33	1.37
42	m	101	BCR	C30-C25	-2.78	1.49	1.53
51	x	316	A1ECV	C3D-C2D	2.78	1.46	1.37
39	a	802	CLA	C4D-ND	-2.78	1.33	1.37
49	W	314	KC2	CBA-CGA	-2.78	1.42	1.48
39	z	311	CLA	C1B-C2B	2.78	1.49	1.43
39	1	316	CLA	C4D-ND	-2.78	1.33	1.37
39	6	321	CLA	C4D-ND	-2.78	1.33	1.37
39	S	311	CLA	C4D-ND	-2.78	1.33	1.37
39	Z	315	CLA	C4D-ND	-2.78	1.33	1.37
39	M	321	CLA	C1B-C2B	2.78	1.49	1.43
49	9	313	KC2	CBA-CGA	-2.78	1.42	1.48
39	y	307	CLA	C4D-ND	-2.77	1.33	1.37
49	C	312	KC2	CBA-CGA	-2.77	1.42	1.48
39	6	315	CLA	C4D-ND	-2.77	1.33	1.37
39	z	309	CLA	C4D-ND	-2.77	1.33	1.37
39	Y	302	CLA	C4D-ND	-2.77	1.33	1.37
39	O	308	CLA	C1B-C2B	2.77	1.49	1.43
39	1	313	CLA	C1B-C2B	2.77	1.49	1.43
51	x	310	A1ECV	C3D-C2D	2.77	1.46	1.37
39	P	311	CLA	C4D-ND	-2.77	1.33	1.37
39	Y	307	CLA	C1B-C2B	2.77	1.49	1.43
39	D	317	CLA	C4D-ND	-2.77	1.33	1.37
39	Y	305	CLA	C4D-ND	-2.77	1.33	1.37
49	K	310	KC2	CBA-CGA	-2.77	1.42	1.48
39	D	314	CLA	C4D-ND	-2.77	1.33	1.37
39	W	319	CLA	C4D-ND	-2.77	1.33	1.37
39	a	827	CLA	C3B-C4B	2.77	1.49	1.42
39	Q	309	CLA	C1B-C2B	2.77	1.49	1.43
49	1	314	KC2	CBA-CGA	-2.77	1.42	1.48
39	H	307	CLA	C4D-ND	-2.77	1.33	1.37
39	5	315	CLA	CMD-C2D	-2.77	1.44	1.50
51	z	310	A1ECV	C3D-C2D	2.77	1.46	1.37
49	V	308	KC2	CBA-CGA	-2.77	1.42	1.48
39	3	323	CLA	C4D-ND	-2.77	1.33	1.37
39	2	310	CLA	C1B-C2B	2.76	1.49	1.43
49	7	322	KC2	CBA-CGA	-2.76	1.42	1.48
39	A	305	CLA	C4D-ND	-2.76	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	313	CLA	C4D-ND	-2.76	1.33	1.37
39	7	315	CLA	C4D-ND	-2.76	1.33	1.37
47	W	301	SQD	O47-C7	2.76	1.42	1.34
39	b	832	CLA	C4D-ND	-2.76	1.33	1.37
39	E	317	CLA	C4D-ND	-2.76	1.33	1.37
49	T	314	KC2	CBA-CGA	-2.76	1.42	1.48
39	H	306	CLA	C4D-ND	-2.76	1.33	1.37
39	4	313	CLA	C4D-ND	-2.76	1.33	1.37
49	0	319	KC2	CBA-CGA	-2.76	1.42	1.48
49	3	315	KC2	CBA-CGA	-2.76	1.42	1.48
49	5	311	KC2	CBA-CGA	-2.76	1.42	1.48
39	B	205	CLA	C4D-ND	-2.76	1.33	1.37
39	X	308	CLA	C4D-ND	-2.76	1.33	1.37
39	G	318	CLA	C1B-C2B	2.76	1.49	1.43
39	0	318	CLA	C4D-ND	-2.76	1.33	1.37
49	2	314	KC2	CBA-CGA	-2.76	1.42	1.48
39	a	834	CLA	C3B-C4B	2.76	1.49	1.42
39	W	319	CLA	C1B-C2B	2.76	1.49	1.43
39	8	312	CLA	C1B-C2B	2.76	1.49	1.43
51	z	316	A1ECV	C3D-C2D	2.76	1.46	1.37
39	b	817	CLA	C4D-ND	-2.76	1.33	1.37
39	1	313	CLA	C4D-ND	-2.76	1.33	1.37
49	z	313	KC2	CBA-CGA	-2.76	1.42	1.48
39	E	309	CLA	C4D-ND	-2.76	1.33	1.37
49	L	312	KC2	C4B-NB	-2.76	1.34	1.37
49	9	318	KC2	CBA-CGA	-2.76	1.42	1.48
39	a	836	CLA	C3B-C4B	2.75	1.49	1.42
39	3	320	CLA	C4D-ND	-2.75	1.33	1.37
49	X	312	KC2	CBA-CGA	-2.75	1.42	1.48
49	x	315	KC2	CBA-CGA	-2.75	1.42	1.48
39	M	321	CLA	C4D-ND	-2.75	1.33	1.37
39	2	307	CLA	C4D-ND	-2.75	1.33	1.37
49	P	320	KC2	CBA-CGA	-2.75	1.42	1.48
49	8	317	KC2	CBA-CGA	-2.75	1.42	1.48
39	3	320	CLA	C1B-C2B	2.75	1.49	1.43
49	1	315	KC2	CBA-CGA	-2.75	1.42	1.48
39	M	318	CLA	C3B-C4B	2.75	1.49	1.42
39	X	317	CLA	C3B-C4B	2.75	1.49	1.42
49	4	320	KC2	CBA-CGA	-2.75	1.42	1.48
39	B	209	CLA	C4D-ND	-2.75	1.33	1.37
39	M	317	CLA	C4D-ND	-2.75	1.33	1.37
49	6	317	KC2	CBA-CGA	-2.75	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	C	308	CLA	C1B-C2B	2.75	1.49	1.43
39	I	310	CLA	C4D-ND	-2.75	1.33	1.37
49	Z	310	KC2	CBA-CGA	-2.75	1.42	1.48
39	9	320	CLA	C4D-ND	-2.75	1.33	1.37
39	b	806	CLA	C4D-ND	-2.75	1.33	1.37
39	o	203	CLA	C4D-ND	-2.75	1.33	1.37
39	C	310	CLA	C4D-ND	-2.75	1.33	1.37
49	9	311	KC2	CBA-CGA	-2.75	1.42	1.48
49	Y	308	KC2	CBA-CGA	-2.75	1.42	1.48
39	2	315	CLA	C1B-C2B	2.75	1.49	1.43
39	F	313	CLA	C1B-C2B	2.75	1.49	1.43
39	H	315	CLA	C1B-C2B	2.75	1.49	1.43
39	K	314	CLA	C1B-C2B	2.75	1.49	1.43
39	O	312	CLA	C4D-ND	-2.75	1.33	1.37
39	M	321	CLA	C3B-C4B	2.75	1.49	1.42
39	Z	315	CLA	C1B-C2B	2.75	1.49	1.43
39	Y	304	CLA	C4D-ND	-2.74	1.33	1.37
49	0	316	KC2	CBA-CGA	-2.74	1.42	1.48
39	b	811	CLA	C3B-C4B	2.74	1.49	1.42
39	Z	309	CLA	C4D-ND	-2.74	1.33	1.37
39	b	813	CLA	C4D-ND	-2.74	1.33	1.37
39	U	201	CLA	C1B-C2B	2.74	1.49	1.43
39	Y	314	CLA	C1B-C2B	2.74	1.49	1.43
39	2	319	CLA	C1B-C2B	2.74	1.49	1.43
39	U	214	CLA	C1B-C2B	2.74	1.49	1.43
49	I	303	KC2	CBA-CGA	-2.74	1.42	1.48
49	y	313	KC2	CBA-CGA	-2.74	1.42	1.48
49	4	318	KC2	CBA-CGA	-2.74	1.42	1.48
39	a	821	CLA	C3B-C4B	2.74	1.49	1.42
49	A	310	KC2	CBA-CGA	-2.74	1.42	1.48
49	W	308	KC2	CBA-CGA	-2.74	1.42	1.48
49	z	315	KC2	CBA-CGA	-2.74	1.42	1.48
39	7	325	CLA	C3B-C4B	2.74	1.49	1.42
39	I	316	CLA	C4D-ND	-2.74	1.33	1.37
49	y	316	KC2	CBA-CGA	-2.74	1.42	1.48
39	a	825	CLA	C4D-ND	-2.74	1.33	1.37
39	a	801	CLA	C4B-NB	2.74	1.41	1.37
49	5	314	KC2	CBA-CGA	-2.74	1.42	1.48
39	a	833	CLA	C4D-ND	-2.74	1.33	1.37
39	J	312	CLA	C4D-ND	-2.74	1.33	1.37
49	R	306	KC2	CBA-CGA	-2.74	1.42	1.48
49	7	320	KC2	CBA-CGA	-2.74	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	y	315	CLA	C1B-C2B	2.74	1.49	1.43
39	a	822	CLA	C4D-ND	-2.74	1.33	1.37
49	4	317	KC2	CBA-CGA	-2.74	1.42	1.48
39	a	838	CLA	C4D-ND	-2.74	1.33	1.37
39	Z	307	CLA	C1B-C2B	2.74	1.49	1.43
39	P	316	CLA	C4D-ND	-2.74	1.33	1.37
39	z	308	CLA	C4D-ND	-2.74	1.33	1.37
39	F	315	CLA	C1B-C2B	2.74	1.49	1.43
49	8	316	KC2	CBA-CGA	-2.74	1.42	1.48
49	z	312	KC2	CBA-CGA	-2.74	1.42	1.48
39	Y	310	CLA	C4D-ND	-2.74	1.33	1.37
39	a	804	CLA	C3B-C4B	2.74	1.49	1.42
48	S	304	A86	C30-C29	-2.73	1.27	1.32
49	M	307	KC2	CBA-CGA	-2.73	1.42	1.48
49	8	320	KC2	CBA-CGA	-2.73	1.42	1.48
39	6	322	CLA	C1B-C2B	2.73	1.49	1.43
39	8	318	CLA	C4D-ND	-2.73	1.33	1.37
39	F	312	CLA	C1B-C2B	2.73	1.49	1.43
49	y	314	KC2	CBA-CGA	-2.73	1.42	1.48
39	Z	312	CLA	C4D-ND	-2.73	1.33	1.37
39	J	307	CLA	C1B-C2B	2.73	1.49	1.43
49	3	317	KC2	CBA-CGA	-2.73	1.42	1.48
39	b	810	CLA	C1B-C2B	2.73	1.49	1.43
39	z	317	CLA	C4D-ND	-2.73	1.33	1.37
49	H	311	KC2	CBA-CGA	-2.73	1.42	1.48
39	U	209	CLA	C4D-ND	-2.73	1.33	1.37
39	x	311	CLA	C1B-C2B	2.73	1.49	1.43
49	S	317	KC2	CBA-CGA	-2.73	1.42	1.48
39	P	308	CLA	C3B-C4B	2.73	1.49	1.42
49	9	316	KC2	CBA-CGA	-2.73	1.42	1.48
49	6	316	KC2	CBA-CGA	-2.73	1.42	1.48
49	Q	315	KC2	CBA-CGA	-2.73	1.42	1.48
39	O	311	CLA	C4D-ND	-2.73	1.33	1.37
39	C	311	CLA	C1B-C2B	2.73	1.49	1.43
39	G	314	CLA	C4D-ND	-2.73	1.33	1.37
39	J	316	CLA	C1B-C2B	2.73	1.49	1.43
49	P	306	KC2	CBA-CGA	-2.73	1.42	1.48
49	K	313	KC2	CBA-CGA	-2.73	1.42	1.48
49	X	315	KC2	CBA-CGA	-2.73	1.42	1.48
49	L	314	KC2	CBA-CGA	-2.72	1.42	1.48
49	S	314	KC2	CBA-CGA	-2.72	1.42	1.48
49	8	319	KC2	CBA-CGA	-2.72	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	a	847	CLA	C1B-C2B	2.72	1.49	1.43
39	L	308	CLA	C1B-C2B	2.72	1.49	1.43
39	Z	306	CLA	C1B-C2B	2.72	1.49	1.43
39	b	801	CLA	MG-NB	-2.72	2.00	2.05
49	2	313	KC2	CBA-CGA	-2.72	1.42	1.48
39	y	318	CLA	C4D-ND	-2.72	1.33	1.37
47	7	302	SQD	O47-C7	2.72	1.42	1.34
39	x	314	CLA	C1B-C2B	2.72	1.49	1.43
49	x	313	KC2	CBA-CGA	-2.72	1.42	1.48
39	0	322	CLA	C1B-C2B	2.72	1.49	1.43
39	9	309	CLA	C1B-C2B	2.72	1.49	1.43
39	a	831	CLA	C4D-ND	-2.72	1.33	1.37
39	F	314	CLA	C4D-ND	-2.72	1.33	1.37
39	U	213	CLA	C4D-ND	-2.72	1.33	1.37
39	B	203	CLA	C1B-C2B	2.72	1.49	1.43
49	L	321	KC2	CBA-CGA	-2.72	1.42	1.48
39	J	316	CLA	C4D-ND	-2.72	1.33	1.37
49	Z	311	KC2	CBA-CGA	-2.72	1.42	1.48
39	Z	305	CLA	C1B-C2B	2.72	1.49	1.43
39	K	311	CLA	C1B-C2B	2.72	1.49	1.43
39	F	312	CLA	C4D-ND	-2.72	1.34	1.37
39	L	316	CLA	C4D-ND	-2.72	1.34	1.37
39	2	318	CLA	C4D-ND	-2.72	1.34	1.37
49	G	317	KC2	CBA-CGA	-2.72	1.42	1.48
39	K	307	CLA	C1B-C2B	2.72	1.49	1.43
49	1	312	KC2	CBA-CGA	-2.72	1.42	1.48
39	2	312	CLA	C4D-ND	-2.72	1.34	1.37
39	3	322	CLA	C1B-C2B	2.72	1.49	1.43
49	T	316	KC2	CBA-CGA	-2.72	1.42	1.48
39	Z	307	CLA	C4D-ND	-2.72	1.34	1.37
49	3	318	KC2	CBA-CGA	-2.72	1.42	1.48
49	0	317	KC2	CBA-CGA	-2.72	1.42	1.48
39	E	315	CLA	C1B-C2B	2.72	1.49	1.43
39	T	308	CLA	C3B-C4B	2.72	1.49	1.42
39	a	836	CLA	C4D-ND	-2.72	1.34	1.37
39	X	317	CLA	C4D-ND	-2.72	1.34	1.37
39	a	813	CLA	C1B-C2B	2.72	1.49	1.43
39	W	313	CLA	C4D-ND	-2.71	1.34	1.37
39	P	308	CLA	C1B-C2B	2.71	1.49	1.43
39	y	312	CLA	C1B-C2B	2.71	1.49	1.43
39	F	306	CLA	C1B-C2B	2.71	1.49	1.43
39	6	318	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	L	312	KC2	CBA-CGA	-2.71	1.42	1.48
39	D	319	CLA	C4D-ND	-2.71	1.34	1.37
39	a	831	CLA	C1B-C2B	2.71	1.49	1.43
39	H	307	CLA	C1B-C2B	2.71	1.49	1.43
39	8	315	CLA	C1B-C2B	2.71	1.49	1.43
39	T	310	CLA	C1B-C2B	2.71	1.49	1.43
49	Y	309	KC2	CBA-CGA	-2.71	1.42	1.48
39	O	312	CLA	C1B-C2B	2.71	1.49	1.43
49	x	312	KC2	CBA-CGA	-2.71	1.42	1.48
42	m	101	BCR	C1-C6	-2.71	1.50	1.53
39	A	315	CLA	C4D-ND	-2.71	1.34	1.37
39	E	310	CLA	C4D-ND	-2.71	1.34	1.37
39	J	311	CLA	C1B-C2B	2.71	1.49	1.43
39	F	316	CLA	C1B-C2B	2.71	1.49	1.43
39	J	307	CLA	C4D-ND	-2.71	1.34	1.37
39	S	308	CLA	C1B-C2B	2.71	1.49	1.43
39	Z	312	CLA	C1B-C2B	2.71	1.49	1.43
39	J	312	CLA	C1B-C2B	2.71	1.49	1.43
39	O	316	CLA	C1B-C2B	2.71	1.49	1.43
39	7	316	CLA	C1B-C2B	2.71	1.49	1.43
39	7	318	CLA	C1B-C2B	2.71	1.49	1.43
39	T	318	CLA	C1B-C2B	2.71	1.49	1.43
39	4	323	CLA	C1B-C2B	2.71	1.49	1.43
39	a	838	CLA	C3B-C4B	2.71	1.49	1.42
39	a	804	CLA	C1B-C2B	2.71	1.49	1.43
39	3	312	CLA	C1B-C2B	2.70	1.49	1.43
39	z	309	CLA	C1B-C2B	2.70	1.49	1.43
39	H	315	CLA	C4D-ND	-2.70	1.34	1.37
49	G	315	KC2	CBA-CGA	-2.70	1.42	1.48
39	E	308	CLA	C1B-C2B	2.70	1.49	1.43
39	8	310	CLA	C1B-C2B	2.70	1.49	1.43
49	6	319	KC2	CBA-CGA	-2.70	1.42	1.48
39	6	315	CLA	C1B-C2B	2.70	1.49	1.43
49	C	313	KC2	CBA-CGA	-2.70	1.42	1.48
49	J	315	KC2	CBA-CGA	-2.70	1.42	1.48
51	2	311	A1ECV	C3D-C2D	2.70	1.46	1.37
39	C	305	CLA	C1B-C2B	2.70	1.49	1.43
39	W	316	CLA	C1B-C2B	2.70	1.49	1.43
39	H	313	CLA	C1B-C2B	2.70	1.49	1.43
39	6	311	CLA	C1B-C2B	2.70	1.49	1.43
39	P	307	CLA	C1B-C2B	2.70	1.49	1.43
51	E	311	A1ECV	C4D-CHA	2.70	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	D	306	DD6	O1-C20	-2.70	1.42	1.46
49	G	311	KC2	CBA-CGA	-2.70	1.42	1.48
39	1	316	CLA	C1B-C2B	2.70	1.49	1.43
51	Q	319	A1ECV	C3D-C2D	2.70	1.46	1.37
39	a	822	CLA	C1B-C2B	2.70	1.49	1.43
39	A	314	CLA	C1B-C2B	2.70	1.49	1.43
39	C	310	CLA	C1B-C2B	2.70	1.49	1.43
51	T	317	A1ECV	C3D-C2D	2.70	1.46	1.37
51	1	318	A1ECV	C3D-C2D	2.70	1.46	1.37
39	S	313	CLA	C1B-C2B	2.70	1.49	1.43
39	5	306	CLA	C1B-C2B	2.70	1.49	1.43
39	8	313	CLA	C1B-C2B	2.70	1.49	1.43
49	P	313	KC2	CBA-CGA	-2.70	1.42	1.48
39	b	851	CLA	C1B-C2B	2.69	1.49	1.43
39	x	317	CLA	C4D-ND	-2.69	1.34	1.37
51	V	317	A1ECV	C3D-C2D	2.69	1.46	1.37
39	a	820	CLA	C1B-C2B	2.69	1.49	1.43
39	5	316	CLA	C1B-C2B	2.69	1.49	1.43
39	a	830	CLA	C1B-C2B	2.69	1.49	1.43
39	0	318	CLA	C1B-C2B	2.69	1.49	1.43
39	x	308	CLA	C1B-C2B	2.69	1.49	1.43
51	6	320	A1ECV	C3D-C2D	2.69	1.46	1.37
39	B	206	CLA	C1B-C2B	2.69	1.49	1.43
39	y	318	CLA	C1B-C2B	2.69	1.49	1.43
39	Y	304	CLA	C1B-C2B	2.69	1.49	1.43
39	x	309	CLA	C4D-ND	-2.69	1.34	1.37
39	H	306	CLA	C1B-C2B	2.69	1.49	1.43
49	Q	318	KC2	CBA-CGA	-2.69	1.42	1.48
39	S	310	CLA	C1B-C2B	2.69	1.49	1.43
51	E	311	A1ECV	C3D-C2D	2.69	1.46	1.37
39	Y	311	CLA	C1B-C2B	2.69	1.49	1.43
39	Z	304	CLA	C1B-C2B	2.69	1.49	1.43
39	2	307	CLA	C1B-C2B	2.69	1.49	1.43
39	4	319	CLA	C1B-C2B	2.69	1.49	1.43
39	1	317	CLA	C1B-C2B	2.69	1.49	1.43
39	3	314	CLA	C1B-C2B	2.69	1.49	1.43
39	y	307	CLA	C1B-C2B	2.69	1.49	1.43
39	i	101	CLA	C1B-C2B	2.69	1.49	1.43
39	F	315	CLA	C4D-ND	-2.69	1.34	1.37
49	2	317	KC2	CBA-CGA	-2.69	1.42	1.48
39	A	314	CLA	C4D-ND	-2.69	1.34	1.37
39	K	309	CLA	C1B-C2B	2.69	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	324	CLA	C4D-ND	-2.69	1.34	1.37
39	L	316	CLA	C1B-C2B	2.69	1.49	1.43
49	X	306	KC2	CBA-CGA	-2.69	1.42	1.48
51	Q	316	A1ECV	C3D-C2D	2.68	1.46	1.37
49	L	317	KC2	CBA-CGA	-2.68	1.42	1.48
39	k	202	CLA	C1B-C2B	2.68	1.49	1.43
39	1	310	CLA	C1B-C2B	2.68	1.49	1.43
39	x	306	CLA	C1B-C2B	2.68	1.49	1.43
39	H	312	CLA	C1B-C2B	2.68	1.49	1.43
39	T	320	CLA	C3B-C4B	2.68	1.49	1.42
39	V	319	CLA	C1B-C2B	2.68	1.49	1.43
39	L	319	CLA	C1B-C2B	2.68	1.49	1.43
39	O	313	CLA	C1B-C2B	2.68	1.49	1.43
39	C	309	CLA	C1B-C2B	2.68	1.49	1.43
39	Y	303	CLA	C1B-C2B	2.68	1.49	1.43
39	M	315	CLA	C1B-C2B	2.68	1.49	1.43
39	9	319	CLA	C1B-C2B	2.68	1.49	1.43
39	H	316	CLA	C1B-C2B	2.68	1.49	1.43
39	M	308	CLA	C1B-C2B	2.68	1.49	1.43
39	8	321	CLA	C1B-C2B	2.68	1.49	1.43
39	3	323	CLA	C1B-C2B	2.68	1.49	1.43
39	7	321	CLA	C1B-C2B	2.68	1.49	1.43
39	I	308	CLA	C1B-C2B	2.68	1.49	1.43
39	E	317	CLA	C1B-C2B	2.68	1.49	1.43
39	Y	302	CLA	C1B-C2B	2.68	1.49	1.43
39	P	314	CLA	C1B-C2B	2.68	1.49	1.43
39	h	201	CLA	C1B-C2B	2.68	1.49	1.43
39	a	832	CLA	C1B-C2B	2.68	1.49	1.43
39	4	316	CLA	C1B-C2B	2.68	1.49	1.43
39	z	314	CLA	C1B-C2B	2.68	1.49	1.43
39	z	317	CLA	C1B-C2B	2.68	1.49	1.43
39	X	316	CLA	C1B-C2B	2.68	1.49	1.43
39	4	314	CLA	C1B-C2B	2.67	1.49	1.43
39	1	319	CLA	C1B-C2B	2.67	1.49	1.43
39	A	312	CLA	C1B-C2B	2.67	1.49	1.43
39	D	318	CLA	C1B-C2B	2.67	1.49	1.43
39	b	834	CLA	C1B-C2B	2.67	1.49	1.43
39	7	313	CLA	C1B-C2B	2.67	1.49	1.43
39	Y	310	CLA	C1B-C2B	2.67	1.49	1.43
39	4	313	CLA	C1B-C2B	2.67	1.49	1.43
49	S	315	KC2	CBA-CGA	-2.67	1.42	1.48
39	E	310	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	x	317	CLA	C1B-C2B	2.67	1.49	1.43
39	z	306	CLA	C1B-C2B	2.67	1.49	1.43
39	D	311	CLA	C1B-C2B	2.67	1.49	1.43
39	Z	316	CLA	C1B-C2B	2.67	1.49	1.43
39	X	309	CLA	C1B-C2B	2.67	1.49	1.43
39	b	830	CLA	CMB-C2B	-2.67	1.45	1.50
39	M	318	CLA	C1B-C2B	2.67	1.49	1.43
49	6	314	KC2	CBA-CGA	-2.67	1.42	1.48
39	1	308	CLA	C1B-C2B	2.67	1.49	1.43
39	b	806	CLA	C3B-C4B	2.67	1.49	1.42
39	R	307	CLA	C1B-C2B	2.67	1.49	1.43
51	L	318	A1ECV	C3D-C2D	2.67	1.46	1.37
39	I	308	CLA	C3B-C4B	2.67	1.49	1.42
39	b	813	CLA	C4B-C3B	2.67	1.49	1.43
39	K	306	CLA	C1B-C2B	2.67	1.49	1.43
39	2	312	CLA	C1B-C2B	2.67	1.49	1.43
39	l	205	CLA	C1B-C2B	2.67	1.49	1.43
39	3	311	CLA	C1B-C2B	2.67	1.49	1.43
39	H	310	CLA	C1B-C2B	2.66	1.49	1.43
39	a	809	CLA	C1B-C2B	2.66	1.49	1.43
39	b	835	CLA	C1B-C2B	2.66	1.49	1.43
39	0	320	CLA	C1B-C2B	2.66	1.49	1.43
39	3	319	CLA	C4D-ND	-2.66	1.34	1.37
39	S	319	CLA	C4D-ND	-2.66	1.34	1.37
39	X	316	CLA	CMD-C2D	-2.66	1.45	1.50
39	8	311	CLA	C1B-C2B	2.66	1.49	1.43
39	6	310	CLA	C1B-C2B	2.66	1.49	1.43
39	b	816	CLA	C1B-C2B	2.66	1.49	1.43
39	J	313	CLA	C1B-C2B	2.66	1.49	1.43
39	Q	317	CLA	C1B-C2B	2.66	1.49	1.43
39	T	320	CLA	C1B-C2B	2.66	1.49	1.43
51	Y	312	A1ECV	C3D-C2D	2.66	1.46	1.37
49	5	305	KC2	CBA-CGA	-2.65	1.42	1.48
39	F	309	CLA	C1B-C2B	2.65	1.49	1.43
39	Q	320	CLA	C1B-C2B	2.65	1.49	1.43
39	l	201	CLA	C1B-C2B	2.65	1.49	1.43
39	A	307	CLA	C1B-C2B	2.65	1.49	1.43
39	S	311	CLA	C1B-C2B	2.65	1.49	1.43
49	I	312	KC2	C4A-C3A	-2.65	1.39	1.44
39	a	834	CLA	C1B-C2B	2.65	1.49	1.43
39	D	309	CLA	C4D-ND	-2.65	1.34	1.37
49	M	314	KC2	CBA-CGA	-2.65	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	z	308	CLA	C1B-C2B	2.65	1.49	1.43
39	S	316	CLA	C1B-C2B	2.65	1.49	1.43
39	M	309	CLA	C1B-C2B	2.65	1.49	1.43
39	a	806	CLA	C1B-C2B	2.65	1.49	1.43
49	F	311	KC2	C4A-C3A	-2.65	1.39	1.44
39	o	206	CLA	C1B-C2B	2.65	1.49	1.43
39	1	320	CLA	C1B-C2B	2.65	1.49	1.43
39	I	310	CLA	C1B-C2B	2.65	1.49	1.43
39	a	808	CLA	C1B-C2B	2.65	1.49	1.43
39	8	322	CLA	C1B-C2B	2.65	1.49	1.43
49	0	319	KC2	C4B-NB	-2.65	1.34	1.37
39	Y	307	CLA	C4D-ND	-2.65	1.34	1.37
39	E	314	CLA	C1B-C2B	2.65	1.49	1.43
39	I	313	CLA	C1B-C2B	2.65	1.49	1.43
39	E	306	CLA	C1B-C2B	2.65	1.49	1.43
39	U	213	CLA	C1B-C2B	2.65	1.49	1.43
39	D	314	CLA	C1B-C2B	2.64	1.49	1.43
39	5	310	CLA	C1B-C2B	2.64	1.49	1.43
39	J	308	CLA	C1B-C2B	2.64	1.49	1.43
39	8	318	CLA	C1B-C2B	2.64	1.49	1.43
39	b	823	CLA	C1B-C2B	2.64	1.49	1.43
39	6	321	CLA	C1B-C2B	2.64	1.49	1.43
39	y	309	CLA	C4D-ND	-2.64	1.34	1.37
39	V	311	CLA	C1B-C2B	2.64	1.49	1.43
39	C	306	CLA	C1B-C2B	2.64	1.49	1.43
39	L	313	CLA	C1B-C2B	2.64	1.49	1.43
39	b	824	CLA	C1B-C2B	2.64	1.49	1.43
39	b	808	CLA	C1B-C2B	2.64	1.49	1.43
39	I	311	CLA	C1B-C2B	2.64	1.49	1.43
51	5	312	A1ECV	C3D-C2D	2.64	1.46	1.37
39	D	319	CLA	C1B-C2B	2.64	1.49	1.43
39	b	842	CLA	C1B-C2B	2.64	1.49	1.43
39	y	308	CLA	C1B-C2B	2.64	1.49	1.43
39	U	212	CLA	C1B-C2B	2.64	1.49	1.43
39	W	310	CLA	C1B-C2B	2.64	1.49	1.43
39	D	317	CLA	C1B-C2B	2.64	1.49	1.43
39	R	309	CLA	C1B-C2B	2.64	1.49	1.43
39	b	839	CLA	C1B-C2B	2.64	1.49	1.43
39	f	803	CLA	C1B-C2B	2.64	1.49	1.43
39	R	316	CLA	C1B-C2B	2.64	1.49	1.43
39	3	316	CLA	C1B-C2B	2.64	1.49	1.43
39	b	817	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	b	822	CLA	C1B-C2B	2.64	1.49	1.43
39	T	319	CLA	C1B-C2B	2.64	1.49	1.43
39	5	315	CLA	C1B-C2B	2.64	1.49	1.43
39	y	309	CLA	C1B-C2B	2.64	1.49	1.43
39	a	832	CLA	C3B-C4B	2.63	1.48	1.42
51	X	310	A1ECV	C3D-C2D	2.63	1.46	1.37
39	0	313	CLA	C1B-C2B	2.63	1.49	1.43
39	z	307	CLA	C1B-C2B	2.63	1.49	1.43
39	k	203	CLA	C1B-C2B	2.63	1.49	1.43
39	1	311	CLA	C1B-C2B	2.63	1.49	1.43
39	I	315	CLA	C1B-C2B	2.63	1.49	1.43
39	S	310	CLA	C4D-ND	-2.63	1.34	1.37
39	B	205	CLA	C1B-C2B	2.63	1.49	1.43
39	b	825	CLA	C4D-ND	-2.63	1.34	1.37
39	6	312	CLA	C1B-C2B	2.63	1.49	1.43
39	C	307	CLA	C1B-C2B	2.63	1.49	1.43
51	R	313	A1ECV	C3D-C2D	2.63	1.46	1.37
39	b	811	CLA	C1B-C2B	2.63	1.49	1.43
49	1	312	KC2	C4B-NB	-2.63	1.34	1.37
39	F	321	CLA	C1B-C2B	2.63	1.49	1.43
39	H	308	CLA	C1B-C2B	2.63	1.49	1.43
39	Q	311	CLA	C1B-C2B	2.63	1.49	1.43
39	Q	314	CLA	C1B-C2B	2.63	1.49	1.43
39	b	827	CLA	C1B-C2B	2.62	1.49	1.43
39	x	309	CLA	C1B-C2B	2.62	1.49	1.43
39	0	323	CLA	C4D-ND	-2.62	1.34	1.37
39	a	819	CLA	C1B-C2B	2.62	1.49	1.43
39	a	837	CLA	C1B-C2B	2.62	1.49	1.43
49	A	313	KC2	C4B-NB	-2.62	1.34	1.37
39	Y	305	CLA	C1B-C2B	2.62	1.49	1.43
39	6	313	CLA	C1B-C2B	2.62	1.49	1.43
39	a	829	CLA	C1B-C2B	2.62	1.49	1.43
39	o	201	CLA	C1B-C2B	2.62	1.49	1.43
39	P	316	CLA	C1B-C2B	2.62	1.49	1.43
39	Y	311	CLA	C4D-ND	-2.62	1.34	1.37
39	b	832	CLA	C1B-C2B	2.62	1.49	1.43
39	L	310	CLA	C1B-C2B	2.62	1.49	1.43
39	z	318	CLA	C1B-C2B	2.62	1.49	1.43
43	P	304	DD6	O1-C20	-2.62	1.42	1.46
39	A	309	CLA	C1B-C2B	2.62	1.49	1.43
39	I	314	CLA	C1B-C2B	2.62	1.49	1.43
39	y	310	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	W	317	A1ECV	C3D-C2D	2.62	1.46	1.37
39	T	311	CLA	C1B-C2B	2.62	1.49	1.43
39	U	211	CLA	C1B-C2B	2.62	1.49	1.43
39	5	308	CLA	C1B-C2B	2.62	1.49	1.43
39	b	807	CLA	CMC-C2C	-2.62	1.45	1.50
39	E	318	CLA	C1B-C2B	2.62	1.49	1.43
39	Q	312	CLA	C1B-C2B	2.62	1.49	1.43
39	I	309	CLA	C1B-C2B	2.62	1.49	1.43
39	V	316	CLA	C1B-C2B	2.62	1.49	1.43
39	X	317	CLA	C1B-C2B	2.62	1.49	1.43
39	b	809	CLA	C1B-C2B	2.61	1.49	1.43
39	F	308	CLA	C1B-C2B	2.61	1.49	1.43
51	9	314	A1ECV	C3D-C2D	2.61	1.46	1.37
39	o	202	CLA	C1B-C2B	2.61	1.49	1.43
39	o	205	CLA	C1B-C2B	2.61	1.49	1.43
39	O	309	CLA	C1B-C2B	2.61	1.49	1.43
39	0	315	CLA	C1B-C2B	2.61	1.49	1.43
39	b	815	CLA	C1B-C2B	2.61	1.49	1.43
51	G	316	A1ECV	C3D-C2D	2.61	1.46	1.37
51	4	315	A1ECV	C3D-C2D	2.61	1.46	1.37
39	j	101	CLA	C1B-C2B	2.61	1.49	1.43
39	R	315	CLA	C1B-C2B	2.61	1.49	1.43
39	W	318	CLA	C1B-C2B	2.61	1.49	1.43
39	M	310	CLA	C1B-C2B	2.61	1.49	1.43
51	7	317	A1ECV	C3D-C2D	2.61	1.45	1.37
39	a	836	CLA	C1B-C2B	2.61	1.49	1.43
39	2	318	CLA	C1B-C2B	2.61	1.49	1.43
51	X	313	A1ECV	C3D-C2D	2.61	1.45	1.37
39	H	309	CLA	C1B-C2B	2.61	1.49	1.43
39	a	814	CLA	C1B-C2B	2.61	1.49	1.43
39	o	203	CLA	C1B-C2B	2.61	1.49	1.43
39	D	316	CLA	C1B-C2B	2.61	1.49	1.43
39	G	310	CLA	C1B-C2B	2.61	1.49	1.43
39	9	310	CLA	C1B-C2B	2.61	1.49	1.43
39	2	309	CLA	C1B-C2B	2.61	1.49	1.43
39	K	308	CLA	C1B-C2B	2.61	1.49	1.43
39	G	312	CLA	C1B-C2B	2.61	1.49	1.43
39	L	320	CLA	C1B-C2B	2.61	1.49	1.43
49	Q	315	KC2	C4B-NB	-2.61	1.34	1.37
49	5	311	KC2	C4B-NB	-2.61	1.34	1.37
49	6	319	KC2	C4B-NB	-2.60	1.34	1.37
39	L	311	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	I	316	CLA	C1B-C2B	2.60	1.49	1.43
39	V	309	CLA	C1B-C2B	2.60	1.49	1.43
39	9	308	CLA	C1B-C2B	2.60	1.49	1.43
51	O	315	A1ECV	C3D-C2D	2.60	1.45	1.37
49	O	317	KC2	C4B-NB	-2.60	1.34	1.37
51	M	316	A1ECV	C3D-C2D	2.60	1.45	1.37
39	D	313	CLA	C1B-C2B	2.60	1.49	1.43
39	G	314	CLA	C1B-C2B	2.60	1.49	1.43
39	R	315	CLA	C4D-ND	-2.60	1.34	1.37
49	2	313	KC2	C4B-NB	-2.60	1.34	1.37
39	b	812	CLA	C1B-C2B	2.60	1.49	1.43
39	A	315	CLA	C1B-C2B	2.60	1.49	1.43
49	I	303	KC2	C4A-C3A	-2.60	1.39	1.44
39	3	319	CLA	C1B-C2B	2.60	1.49	1.43
39	Y	313	CLA	C1B-C2B	2.60	1.49	1.43
49	X	306	KC2	C4B-NB	-2.60	1.34	1.37
39	R	311	CLA	C1B-C2B	2.60	1.49	1.43
39	D	315	CLA	C1B-C2B	2.59	1.49	1.43
39	U	209	CLA	C1B-C2B	2.59	1.49	1.43
39	4	322	CLA	C4D-ND	-2.59	1.34	1.37
51	S	312	A1ECV	C3D-C2D	2.59	1.45	1.37
39	R	308	CLA	C1B-C2B	2.59	1.49	1.43
39	X	307	CLA	C1B-C2B	2.59	1.49	1.43
39	b	820	CLA	C1B-C2B	2.59	1.49	1.43
39	a	807	CLA	C1B-C2B	2.59	1.49	1.43
49	3	318	KC2	C4B-NB	-2.59	1.34	1.37
50	V	307	A1EB1	O1-C20	-2.59	1.42	1.46
39	b	838	CLA	C1B-C2B	2.59	1.49	1.43
39	O	314	CLA	CHC-C1C	2.59	1.43	1.38
39	b	803	CLA	C1B-C2B	2.59	1.49	1.43
39	M	309	CLA	C4D-ND	-2.59	1.34	1.37
39	W	309	CLA	C1B-C2B	2.59	1.49	1.43
49	z	313	KC2	MG-ND	-2.59	2.00	2.05
39	U	215	CLA	C1B-C2B	2.58	1.49	1.43
39	E	316	CLA	C1B-C2B	2.58	1.49	1.43
39	G	309	CLA	C1B-C2B	2.58	1.49	1.43
39	U	201	CLA	C3B-C4B	2.58	1.48	1.42
39	O	316	CLA	C4D-ND	-2.58	1.34	1.37
39	a	812	CLA	C1B-C2B	2.58	1.49	1.43
39	a	838	CLA	C1B-C2B	2.58	1.49	1.43
39	D	312	CLA	C1B-C2B	2.58	1.49	1.43
39	E	319	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	X	311	CLA	C1B-C2B	2.58	1.49	1.43
39	A	308	CLA	C1B-C2B	2.58	1.49	1.43
39	4	312	CLA	CHC-C1C	2.58	1.43	1.38
39	K	312	CLA	C1B-C2B	2.58	1.49	1.43
39	2	316	CLA	C1B-C2B	2.58	1.49	1.43
39	a	835	CLA	C1B-C2B	2.58	1.49	1.43
39	7	315	CLA	C1B-C2B	2.58	1.49	1.43
43	4	308	DD6	O1-C20	-2.58	1.42	1.46
49	4	318	KC2	C4B-NB	-2.58	1.34	1.37
39	I	301	CLA	C1B-C2B	2.58	1.49	1.43
39	U	207	CLA	C1B-C2B	2.58	1.49	1.43
39	X	308	CLA	CHC-C1C	2.57	1.43	1.38
39	P	309	CLA	C1B-C2B	2.57	1.49	1.43
49	A	310	KC2	C4B-NB	-2.57	1.34	1.37
39	U	201	CLA	CMD-C2D	-2.57	1.45	1.50
39	0	312	CLA	C3B-C4B	2.57	1.48	1.42
39	M	312	CLA	C1B-C2B	2.57	1.49	1.43
51	4	321	A1ECV	C3D-C2D	2.57	1.45	1.37
39	b	828	CLA	C1B-C2B	2.57	1.49	1.43
39	a	817	CLA	C1B-C2B	2.57	1.49	1.43
39	a	811	CLA	C1B-C2B	2.57	1.49	1.43
39	a	815	CLA	C1B-C2B	2.57	1.49	1.43
39	b	819	CLA	C1B-C2B	2.57	1.49	1.43
39	F	310	CLA	C1B-C2B	2.57	1.49	1.43
39	4	312	CLA	C1B-C2B	2.56	1.49	1.43
39	7	314	CLA	C1B-C2B	2.56	1.49	1.43
49	R	318	KC2	C4B-NB	-2.56	1.34	1.37
39	9	307	CLA	C1B-C2B	2.56	1.49	1.43
51	R	310	A1ECV	C3D-C2D	2.56	1.45	1.37
39	A	305	CLA	C1B-C2B	2.56	1.49	1.43
51	P	315	A1ECV	C3D-C2D	2.56	1.45	1.37
49	Q	313	KC2	C1C-C2C	-2.56	1.39	1.44
39	0	310	CLA	C1B-C2B	2.56	1.49	1.43
39	b	813	CLA	C1B-C2B	2.56	1.49	1.43
39	l	203	CLA	C1B-C2B	2.56	1.49	1.43
39	b	825	CLA	C1B-C2B	2.56	1.49	1.43
43	A	303	DD6	O1-C20	-2.56	1.42	1.46
39	M	317	CLA	C1B-C2B	2.56	1.49	1.43
39	a	805	CLA	C1B-C2B	2.56	1.49	1.43
39	b	805	CLA	C1B-C2B	2.55	1.49	1.43
39	E	309	CLA	C1B-C2B	2.55	1.49	1.43
49	B	208	KC2	CBA-CGA	-2.55	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S	318	A1ECV	C3D-C2D	2.55	1.45	1.37
49	3	315	KC2	C4B-NB	-2.55	1.34	1.37
39	a	818	CLA	C1B-C2B	2.55	1.49	1.43
49	S	315	KC2	C4A-C3A	-2.55	1.39	1.44
49	T	312	KC2	C4B-NB	-2.55	1.34	1.37
39	J	317	CLA	C1B-C2B	2.55	1.49	1.43
39	F	314	CLA	C1B-C2B	2.55	1.49	1.43
39	O	318	CLA	C1B-C2B	2.55	1.49	1.43
49	3	321	KC2	C4B-NB	-2.55	1.34	1.37
49	B	208	KC2	C4A-C3A	-2.55	1.39	1.44
39	3	313	CLA	C1B-C2B	2.55	1.49	1.43
51	Z	314	A1ECV	C3D-C2D	2.54	1.45	1.37
39	a	826	CLA	C1B-C2B	2.54	1.49	1.43
51	9	317	A1ECV	C3D-C2D	2.54	1.45	1.37
39	1	309	CLA	C1B-C2B	2.54	1.49	1.43
39	x	307	CLA	C1B-C2B	2.54	1.49	1.43
49	J	315	KC2	C4B-NB	-2.54	1.34	1.37
48	9	301	A86	O1-C20	-2.54	1.42	1.46
39	4	311	CLA	C1B-C2B	2.54	1.49	1.43
39	f	802	CLA	C1B-C2B	2.54	1.49	1.43
39	W	311	CLA	C1B-C2B	2.54	1.49	1.43
39	D	309	CLA	C1B-C2B	2.53	1.49	1.43
48	2	301	A86	O1-C20	-2.53	1.42	1.46
49	G	315	KC2	C4B-NB	-2.53	1.34	1.37
49	8	319	KC2	C4B-NB	-2.53	1.34	1.37
49	Q	313	KC2	C4A-C3A	-2.53	1.39	1.44
49	V	318	KC2	C4B-NB	-2.53	1.34	1.37
39	a	810	CLA	C1B-C2B	2.53	1.49	1.43
49	W	312	KC2	C4B-NB	-2.53	1.34	1.37
39	C	304	CLA	C1B-C2B	2.53	1.49	1.43
50	3	303	A1EB1	O1-C20	-2.53	1.42	1.46
49	T	316	KC2	C4B-NB	-2.53	1.34	1.37
43	2	303	DD6	O1-C20	-2.53	1.42	1.46
39	T	308	CLA	C1B-C2B	2.53	1.49	1.43
39	2	308	CLA	C1B-C2B	2.53	1.49	1.43
39	J	314	CLA	C1B-C2B	2.52	1.49	1.43
49	Y	308	KC2	C4B-NB	-2.52	1.34	1.37
49	R	306	KC2	C4B-NB	-2.52	1.34	1.37
49	z	313	KC2	C4B-NB	-2.52	1.34	1.37
39	B	204	CLA	C1B-C2B	2.52	1.49	1.43
49	G	311	KC2	C4B-NB	-2.52	1.34	1.37
49	2	314	KC2	C4B-NB	-2.52	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	9	316	KC2	C4B-NB	-2.52	1.34	1.37
39	b	807	CLA	C1B-C2B	2.52	1.49	1.43
49	S	315	KC2	C4B-NB	-2.52	1.34	1.37
51	S	312	A1ECV	C3C-C2C	2.52	1.46	1.42
49	P	312	KC2	C4B-NB	-2.51	1.34	1.37
39	P	311	CLA	C1B-C2B	2.51	1.49	1.43
39	9	315	CLA	C1B-C2B	2.51	1.49	1.43
49	4	324	KC2	C4A-C3A	-2.51	1.39	1.44
49	G	317	KC2	C4A-C3A	-2.51	1.39	1.44
49	y	314	KC2	C4B-NB	-2.51	1.34	1.37
49	2	317	KC2	C4B-NB	-2.51	1.34	1.37
39	a	828	CLA	C1B-C2B	2.51	1.49	1.43
51	5	309	A1ECV	C3D-C2D	2.51	1.45	1.37
39	J	309	CLA	C1B-C2B	2.51	1.49	1.43
39	a	833	CLA	C1B-C2B	2.51	1.49	1.43
39	b	818	CLA	C1B-C2B	2.51	1.49	1.43
39	b	829	CLA	C1B-C2B	2.51	1.49	1.43
49	0	314	KC2	C4B-NB	-2.51	1.34	1.37
49	9	311	KC2	C4B-NB	-2.51	1.34	1.37
51	0	321	A1ECV	C3D-C2D	2.50	1.45	1.37
39	X	316	CLA	C4D-ND	-2.50	1.34	1.37
49	W	314	KC2	C4B-NB	-2.50	1.34	1.37
49	3	318	KC2	C4A-C3A	-2.50	1.39	1.44
49	T	315	KC2	C4B-NB	-2.50	1.34	1.37
39	J	310	CLA	C1B-C2B	2.50	1.49	1.43
49	K	313	KC2	C4A-C3A	-2.50	1.39	1.44
39	b	814	CLA	C1B-C2B	2.50	1.49	1.43
39	a	823	CLA	C1B-C2B	2.50	1.49	1.43
39	B	207	CLA	C1B-C2B	2.50	1.49	1.43
49	V	320	KC2	C4A-C3A	-2.50	1.39	1.44
43	Z	302	DD6	O1-C20	-2.50	1.42	1.46
39	3	313	CLA	CHC-C1C	2.50	1.43	1.38
39	a	803	CLA	C1B-C2B	2.50	1.49	1.43
39	T	309	CLA	CHC-C1C	2.49	1.43	1.38
52	W	321	A1EB4	C32-C31	-2.49	1.50	1.54
39	b	826	CLA	C1B-C2B	2.49	1.49	1.43
39	W	313	CLA	C1B-C2B	2.49	1.49	1.43
50	U	205	A1EB1	O1-C20	-2.48	1.42	1.46
39	b	833	CLA	C1B-C2B	2.48	1.49	1.43
39	a	825	CLA	C1B-C2B	2.48	1.49	1.43
48	7	307	A86	O1-C20	-2.48	1.42	1.46
39	b	821	CLA	CMB-C2B	-2.48	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	J	318	CLA	C1B-C2B	2.48	1.49	1.43
49	8	317	KC2	C4B-NB	-2.48	1.34	1.37
49	G	317	KC2	C4B-NB	-2.48	1.34	1.37
49	H	311	KC2	C4B-NB	-2.48	1.34	1.37
49	7	320	KC2	C4B-NB	-2.48	1.34	1.37
39	S	319	CLA	C1B-C2B	2.48	1.49	1.43
39	A	311	CLA	C1B-C2B	2.48	1.49	1.43
39	B	209	CLA	C1B-C2B	2.47	1.49	1.43
39	a	801	CLA	C1B-C2B	2.47	1.49	1.43
39	O	309	CLA	CMD-C2D	-2.47	1.45	1.50
49	P	310	KC2	C4B-NB	-2.47	1.34	1.37
49	7	319	KC2	C4B-NB	-2.47	1.34	1.37
43	R	304	DD6	C26-C27	-2.47	1.31	1.37
49	R	314	KC2	C4B-NB	-2.47	1.34	1.37
43	C	301	DD6	O1-C20	-2.47	1.42	1.46
49	L	321	KC2	C4B-NB	-2.47	1.34	1.37
49	M	307	KC2	C4B-NB	-2.47	1.34	1.37
49	K	313	KC2	C4B-NB	-2.46	1.34	1.37
49	8	314	KC2	C4B-NB	-2.46	1.34	1.37
49	4	317	KC2	C4B-NB	-2.46	1.34	1.37
50	G	304	A1EB1	O1-C20	-2.46	1.42	1.46
39	U	210	CLA	C1B-C2B	2.46	1.49	1.43
39	5	307	CLA	C1B-C2B	2.46	1.49	1.43
39	O	311	CLA	C1B-C2B	2.46	1.49	1.43
49	H	314	KC2	C4B-NB	-2.46	1.34	1.37
39	T	313	CLA	C1B-C2B	2.46	1.49	1.43
39	y	319	CLA	C1B-C2B	2.46	1.49	1.43
49	3	315	KC2	C4A-C3A	-2.46	1.39	1.44
51	7	323	A1ECV	C3D-C2D	2.46	1.45	1.37
39	J	314	CLA	CHC-C1C	2.45	1.43	1.38
39	i	103	CLA	C1B-C2B	2.45	1.49	1.43
39	b	841	CLA	C1B-C2B	2.45	1.49	1.43
49	M	307	KC2	C4A-C3A	-2.45	1.39	1.44
39	5	315	CLA	C4D-ND	-2.45	1.34	1.37
39	a	813	CLA	CMC-C2C	-2.45	1.45	1.50
49	2	313	KC2	C4A-C3A	-2.45	1.39	1.44
51	S	318	A1ECV	C4D-CHA	2.45	1.47	1.41
39	a	802	CLA	C1B-C2B	2.45	1.49	1.43
49	K	310	KC2	C4B-NB	-2.45	1.34	1.37
49	W	315	KC2	C4B-NB	-2.45	1.34	1.37
49	x	315	KC2	C4B-NB	-2.45	1.34	1.37
39	L	309	CLA	C1B-C2B	2.45	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	a	801	CLA	C3B-C4B	2.45	1.48	1.42
39	b	801	CLA	C3B-C4B	2.45	1.48	1.42
39	E	312	CLA	C1B-C2B	2.45	1.49	1.43
49	L	317	KC2	C4B-NB	-2.45	1.34	1.37
49	M	311	KC2	C4B-NB	-2.45	1.34	1.37
49	L	315	KC2	C4B-NB	-2.45	1.34	1.37
39	D	310	CLA	CMB-C2B	-2.45	1.45	1.50
48	V	301	A86	O1-C20	-2.45	1.42	1.46
39	b	837	CLA	C1B-C2B	2.45	1.49	1.43
39	0	323	CLA	C1B-C2B	2.45	1.49	1.43
49	X	314	KC2	C4B-NB	-2.45	1.34	1.37
39	7	314	CLA	CHC-C1C	2.44	1.43	1.38
49	9	318	KC2	C4B-NB	-2.44	1.34	1.37
39	b	831	CLA	C1B-C2B	2.44	1.49	1.43
39	R	307	CLA	CHC-C1C	2.44	1.43	1.38
39	b	807	CLA	CHC-C1C	2.44	1.43	1.38
49	x	313	KC2	C4B-NB	-2.44	1.34	1.37
48	W	304	A86	O1-C20	-2.44	1.42	1.46
39	x	318	CLA	C1B-C2B	2.44	1.49	1.43
49	0	314	KC2	C4A-C3A	-2.44	1.39	1.44
49	F	311	KC2	C4B-NB	-2.44	1.34	1.37
49	P	313	KC2	C4B-NB	-2.44	1.34	1.37
48	L	302	A86	O1-C20	-2.44	1.42	1.46
39	Q	310	CLA	C1B-C2B	2.44	1.49	1.43
49	G	313	KC2	C4A-C3A	-2.44	1.39	1.44
49	P	306	KC2	C4A-C3A	-2.44	1.39	1.44
49	P	306	KC2	C4B-NB	-2.44	1.34	1.37
49	S	314	KC2	C4B-NB	-2.44	1.34	1.37
49	3	321	KC2	CBA-CGA	-2.43	1.42	1.48
49	4	324	KC2	C4B-NB	-2.43	1.34	1.37
51	V	317	A1ECV	C4D-CHA	2.43	1.47	1.41
49	V	308	KC2	C4B-NB	-2.43	1.34	1.37
49	W	308	KC2	C4B-NB	-2.43	1.34	1.37
49	I	312	KC2	C4B-NB	-2.43	1.34	1.37
39	4	322	CLA	C1B-C2B	2.43	1.49	1.43
48	9	303	A86	O1-C20	-2.43	1.42	1.46
39	V	313	CLA	C1B-C2B	2.43	1.49	1.43
49	X	318	KC2	C4B-NB	-2.43	1.34	1.37
49	G	313	KC2	C4B-NB	-2.43	1.34	1.37
49	1	315	KC2	C4B-NB	-2.43	1.34	1.37
39	a	825	CLA	CHC-C1C	2.43	1.43	1.38
49	P	306	KC2	C1B-NB	-2.43	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	V	315	KC2	C4B-NB	-2.43	1.34	1.37
51	4	315	A1ECV	C3C-C2C	2.43	1.46	1.42
43	J	304	DD6	O1-C20	-2.43	1.42	1.46
50	G	302	A1EB1	O1-C20	-2.43	1.42	1.46
39	a	816	CLA	CMB-C2B	-2.43	1.45	1.50
49	0	317	KC2	C4B-NB	-2.43	1.34	1.37
39	U	208	CLA	C1B-C2B	2.43	1.49	1.43
39	b	826	CLA	CMD-C2D	-2.43	1.45	1.50
43	F	305	DD6	O1-C20	-2.42	1.42	1.46
39	b	818	CLA	CHC-C1C	2.42	1.43	1.38
49	5	313	KC2	C4B-NB	-2.42	1.34	1.37
39	T	309	CLA	C1B-C2B	2.42	1.49	1.43
50	3	302	A1EB1	O1-C20	-2.42	1.42	1.46
51	T	317	A1ECV	C4D-CHA	2.42	1.47	1.41
39	E	313	CLA	C1B-C2B	2.42	1.49	1.43
48	1	302	A86	O1-C20	-2.42	1.42	1.46
39	5	307	CLA	CHC-C1C	2.42	1.43	1.38
49	I	303	KC2	C4B-NB	-2.42	1.34	1.37
51	5	312	A1ECV	C4D-CHA	2.42	1.47	1.41
39	k	201	CLA	C1B-C2B	2.42	1.48	1.43
49	X	312	KC2	C4A-C3A	-2.42	1.39	1.44
45	C	314	DGD	O1G-C1G	-2.42	1.39	1.45
49	F	307	KC2	C4B-NB	-2.42	1.34	1.37
39	V	310	CLA	C1B-C2B	2.42	1.48	1.43
50	2	304	A1EB1	O1-C20	-2.42	1.42	1.46
49	A	313	KC2	C4A-C3A	-2.42	1.39	1.44
48	K	301	A86	O1-C20	-2.42	1.42	1.46
50	y	301	A1EB1	O1-C20	-2.41	1.42	1.46
39	a	802	CLA	CHC-C1C	2.41	1.43	1.38
39	V	310	CLA	CHC-C1C	2.41	1.43	1.38
39	2	308	CLA	CHC-C1C	2.41	1.43	1.38
51	W	317	A1ECV	C4D-CHA	2.41	1.47	1.41
49	V	312	KC2	C4B-NB	-2.41	1.34	1.37
49	Q	313	KC2	C1D-ND	-2.41	1.34	1.37
49	6	317	KC2	C4B-NB	-2.41	1.34	1.37
39	I	309	CLA	CHC-C1C	2.41	1.43	1.38
39	b	840	CLA	C1B-C2B	2.41	1.48	1.43
50	R	303	A1EB1	O1-C20	-2.41	1.42	1.46
48	x	305	A86	O1-C20	-2.40	1.42	1.46
51	Q	319	A1ECV	C4D-CHA	2.40	1.47	1.41
51	7	317	A1ECV	C3C-C2C	2.40	1.46	1.42
49	P	320	KC2	C4B-NB	-2.40	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S	317	KC2	C4B-NB	-2.40	1.34	1.37
49	y	313	KC2	C4B-NB	-2.40	1.34	1.37
49	F	307	KC2	C4A-C3A	-2.40	1.39	1.44
49	1	314	KC2	C4B-NB	-2.40	1.34	1.37
49	V	314	KC2	C4B-NB	-2.40	1.34	1.37
49	8	317	KC2	C4A-C3A	-2.40	1.39	1.44
39	b	826	CLA	CHC-C1C	2.40	1.43	1.38
50	K	302	A1EB1	O1-C20	-2.40	1.42	1.46
43	R	304	DD6	O1-C20	-2.40	1.42	1.46
48	M	303	A86	O1-C20	-2.40	1.42	1.46
48	V	304	A86	O1-C20	-2.40	1.42	1.46
49	5	314	KC2	C4B-NB	-2.40	1.34	1.37
39	x	307	CLA	CHC-C1C	2.40	1.43	1.38
49	M	314	KC2	C4A-C3A	-2.39	1.39	1.44
49	X	315	KC2	C4B-NB	-2.39	1.34	1.37
49	0	319	KC2	C4A-C3A	-2.39	1.39	1.44
49	7	322	KC2	C4B-NB	-2.39	1.34	1.37
39	b	801	CLA	CMD-C2D	-2.39	1.45	1.50
48	7	311	A86	O1-C20	-2.39	1.42	1.46
49	Y	309	KC2	C4B-NB	-2.39	1.34	1.37
39	J	309	CLA	CHC-C1C	2.39	1.43	1.38
49	C	313	KC2	C4B-NB	-2.39	1.34	1.37
49	0	316	KC2	C4B-NB	-2.39	1.34	1.37
48	8	302	A86	O1-C20	-2.39	1.42	1.46
48	T	301	A86	O1-C20	-2.39	1.42	1.46
50	4	302	A1EB1	O1-C20	-2.39	1.42	1.46
39	b	808	CLA	CHC-C1C	2.39	1.43	1.38
49	C	312	KC2	C4B-NB	-2.39	1.34	1.37
49	W	308	KC2	C4A-C3A	-2.39	1.39	1.44
39	a	824	CLA	C1B-C2B	2.39	1.48	1.43
39	b	837	CLA	CHC-C1C	2.39	1.43	1.38
39	A	311	CLA	CHC-C1C	2.39	1.43	1.38
51	0	321	A1ECV	C4D-CHA	2.39	1.47	1.41
49	V	314	KC2	C4A-C3A	-2.38	1.40	1.44
49	4	320	KC2	C4B-NB	-2.38	1.34	1.37
39	0	312	CLA	C1B-C2B	2.38	1.48	1.43
49	R	306	KC2	C4A-C3A	-2.38	1.40	1.44
51	Q	316	A1ECV	C4D-CHA	2.38	1.47	1.41
49	M	314	KC2	C4B-NB	-2.38	1.34	1.37
39	S	309	CLA	CHC-C1C	2.38	1.43	1.38
49	6	314	KC2	C4A-C3A	-2.38	1.40	1.44
48	T	305	A86	O1-C20	-2.38	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	4	309	A86	O1-C20	-2.38	1.42	1.46
39	l	204	CLA	CHC-C1C	2.38	1.43	1.38
39	P	307	CLA	CMD-C2D	-2.38	1.45	1.50
49	y	316	KC2	C4A-C3A	-2.38	1.40	1.44
49	8	316	KC2	C4B-NB	-2.38	1.34	1.37
39	7	324	CLA	C1B-C2B	2.38	1.48	1.43
51	O	315	A1ECV	C4D-CHA	2.38	1.47	1.41
39	b	805	CLA	CHC-C1C	2.38	1.43	1.38
49	0	317	KC2	C4A-C3A	-2.38	1.40	1.44
49	P	320	KC2	C4A-C3A	-2.38	1.40	1.44
49	5	311	KC2	C1C-C2C	-2.38	1.40	1.44
50	E	301	A1EB1	O1-C20	-2.38	1.42	1.46
39	9	320	CLA	CHC-C1C	2.38	1.43	1.38
48	0	308	A86	O1-C20	-2.38	1.42	1.46
49	B	208	KC2	C4B-NB	-2.38	1.34	1.37
49	Q	318	KC2	C4A-C3A	-2.37	1.40	1.44
39	A	306	CLA	C1B-C2B	2.37	1.48	1.43
49	O	317	KC2	C4A-C3A	-2.37	1.40	1.44
49	V	320	KC2	C4B-NB	-2.37	1.34	1.37
39	D	310	CLA	C1B-C2B	2.37	1.48	1.43
49	Z	311	KC2	C4B-NB	-2.37	1.34	1.37
39	a	824	CLA	CHC-C1C	2.37	1.43	1.38
48	L	301	A86	O1-C20	-2.37	1.42	1.46
48	6	303	A86	O1-C20	-2.37	1.42	1.46
39	l	204	CLA	C1B-C2B	2.37	1.48	1.43
49	V	308	KC2	C4A-C3A	-2.37	1.40	1.44
39	Q	321	CLA	C1B-C2B	2.37	1.48	1.43
48	P	303	A86	O1-C20	-2.37	1.42	1.46
49	R	312	KC2	C4B-NB	-2.37	1.34	1.37
49	z	312	KC2	C4B-NB	-2.37	1.34	1.37
43	7	310	DD6	O1-C20	-2.37	1.42	1.46
48	Y	301	A86	O1-C20	-2.37	1.42	1.46
49	M	313	KC2	C4B-NB	-2.37	1.34	1.37
49	x	312	KC2	C4B-NB	-2.37	1.34	1.37
39	b	821	CLA	C1B-C2B	2.36	1.48	1.43
49	V	315	KC2	C4A-C3A	-2.36	1.40	1.44
49	8	320	KC2	C4B-NB	-2.36	1.34	1.37
49	6	316	KC2	C4B-NB	-2.36	1.34	1.37
49	4	318	KC2	C4A-C3A	-2.36	1.40	1.44
48	E	304	A86	O1-C20	-2.36	1.42	1.46
39	9	310	CLA	CHC-C1C	2.36	1.43	1.38
49	L	314	KC2	C4A-C3A	-2.36	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	X	314	KC2	C4A-C3A	-2.36	1.40	1.44
52	T	304	A1EB4	O1-C20	-2.36	1.42	1.46
49	J	315	KC2	C4A-C3A	-2.36	1.40	1.44
48	Q	301	A86	O1-C20	-2.36	1.42	1.46
49	0	316	KC2	C4A-C3A	-2.36	1.40	1.44
48	9	305	A86	O1-C20	-2.36	1.42	1.46
39	O	310	CLA	C1B-C2B	2.35	1.48	1.43
49	0	319	KC2	C1D-ND	-2.35	1.34	1.37
39	b	833	CLA	CHC-C1C	2.35	1.43	1.38
39	a	832	CLA	CMB-C2B	-2.35	1.45	1.50
49	1	315	KC2	C4A-C3A	-2.35	1.40	1.44
49	V	318	KC2	C4A-C3A	-2.35	1.40	1.44
50	G	307	A1EB1	O1-C20	-2.35	1.42	1.46
39	D	311	CLA	CHC-C1C	2.35	1.43	1.38
39	3	319	CLA	CHC-C1C	2.35	1.43	1.38
48	Q	304	A86	O1-C20	-2.35	1.42	1.46
39	U	201	CLA	MG-NB	-2.35	2.01	2.05
48	Q	302	A86	O1-C20	-2.35	1.42	1.46
48	J	301	A86	O1-C20	-2.35	1.42	1.46
49	Z	310	KC2	C4B-NB	-2.35	1.34	1.37
46	I	302	LMG	C7-C8	2.34	1.57	1.50
48	2	302	A86	O1-C20	-2.34	1.42	1.46
39	J	310	CLA	CHC-C1C	2.34	1.43	1.38
49	P	310	KC2	C4A-C3A	-2.34	1.40	1.44
49	5	313	KC2	C4A-C3A	-2.34	1.40	1.44
49	3	317	KC2	C4B-NB	-2.34	1.34	1.37
49	3	317	KC2	C4A-C3A	-2.34	1.40	1.44
51	G	316	A1ECV	C4D-CHA	2.34	1.47	1.41
39	b	816	CLA	CHC-C1C	2.34	1.43	1.38
49	L	317	KC2	C4A-C3A	-2.34	1.40	1.44
49	M	311	KC2	C4A-C3A	-2.34	1.40	1.44
49	M	313	KC2	C4A-C3A	-2.34	1.40	1.44
49	X	306	KC2	C4A-C3A	-2.34	1.40	1.44
48	1	303	A86	O1-C20	-2.34	1.42	1.46
39	9	320	CLA	C1B-C2B	2.34	1.48	1.43
51	M	316	A1ECV	C4D-CHA	2.34	1.47	1.41
49	R	314	KC2	C4A-C3A	-2.34	1.40	1.44
39	V	313	CLA	CMD-C2D	-2.34	1.45	1.50
49	8	320	KC2	C4A-C3A	-2.33	1.40	1.44
39	D	309	CLA	CMB-C2B	-2.33	1.45	1.50
39	b	816	CLA	CMD-C2D	-2.33	1.45	1.50
39	b	824	CLA	CHC-C1C	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	9	316	KC2	C4A-C3A	-2.33	1.40	1.44
50	K	304	A1EB1	O1-C20	-2.33	1.42	1.46
39	W	311	CLA	CHC-C1C	2.33	1.43	1.38
39	b	831	CLA	CMD-C2D	-2.33	1.45	1.50
49	7	322	KC2	C4A-C3A	-2.33	1.40	1.44
51	4	321	A1ECV	C4D-CHA	2.33	1.47	1.41
39	J	311	CLA	CHC-C1C	2.33	1.43	1.38
39	Q	321	CLA	CHC-C1C	2.33	1.43	1.38
39	a	838	CLA	CMB-C2B	-2.33	1.45	1.50
49	6	314	KC2	C4B-NB	-2.33	1.34	1.37
39	X	307	CLA	CHC-C1C	2.33	1.43	1.38
49	4	320	KC2	C4A-C3A	-2.33	1.40	1.44
51	P	315	A1ECV	C4D-CHA	2.33	1.47	1.41
39	2	316	CLA	CHC-C1C	2.33	1.43	1.38
39	B	203	CLA	CHC-C1C	2.33	1.43	1.38
49	T	314	KC2	C4B-NB	-2.33	1.34	1.37
51	X	313	A1ECV	C4D-CHA	2.33	1.47	1.41
49	H	311	KC2	C4A-C3A	-2.33	1.40	1.44
39	0	315	CLA	CHC-C1C	2.33	1.43	1.38
39	O	314	CLA	C1B-C2B	2.33	1.48	1.43
48	8	303	A86	O1-C20	-2.33	1.42	1.46
48	6	307	A86	O1-C20	-2.33	1.42	1.46
39	b	802	CLA	C1B-C2B	2.33	1.48	1.43
49	P	313	KC2	C4A-C3A	-2.33	1.40	1.44
48	U	202	A86	O1-C20	-2.33	1.42	1.46
39	a	823	CLA	CHC-C1C	2.32	1.43	1.38
39	Z	313	CLA	C3B-C4B	2.32	1.48	1.42
50	J	302	A1EB1	O1-C20	-2.32	1.42	1.46
49	L	312	KC2	C4A-C3A	-2.32	1.40	1.44
39	B	204	CLA	CHC-C1C	2.32	1.43	1.38
49	A	310	KC2	C4A-C3A	-2.32	1.40	1.44
39	7	324	CLA	CMB-C2B	-2.32	1.45	1.50
39	L	309	CLA	CHC-C1C	2.32	1.43	1.38
52	M	322	A1EB4	C32-C31	-2.32	1.50	1.54
39	b	813	CLA	CHC-C1C	2.32	1.43	1.38
52	P	319	A1EB4	C32-C31	-2.32	1.50	1.54
39	U	207	CLA	CHC-C1C	2.32	1.43	1.38
49	V	312	KC2	C4A-C3A	-2.32	1.40	1.44
49	T	312	KC2	C4A-C3A	-2.31	1.40	1.44
49	5	305	KC2	C4A-C3A	-2.31	1.40	1.44
48	F	302	A86	O1-C20	-2.31	1.42	1.46
50	T	307	A1EB1	O1-C20	-2.31	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	U	210	CLA	CHC-C1C	2.31	1.43	1.38
39	D	317	CLA	CHC-C1C	2.31	1.43	1.38
39	G	310	CLA	CHC-C1C	2.31	1.43	1.38
49	X	306	KC2	C1B-NB	-2.31	1.34	1.37
43	O	303	DD6	O1-C20	-2.31	1.42	1.46
39	G	318	CLA	CMC-C2C	-2.31	1.45	1.50
51	y	317	A1ECV	C4D-CHA	2.31	1.47	1.41
39	U	215	CLA	CHC-C1C	2.31	1.43	1.38
39	F	310	CLA	CHC-C1C	2.31	1.43	1.38
39	0	311	CLA	C1B-C2B	2.31	1.48	1.43
49	Q	318	KC2	C4B-NB	-2.31	1.34	1.37
39	a	811	CLA	CHC-C1C	2.30	1.43	1.38
39	A	307	CLA	CHC-C1C	2.30	1.43	1.38
39	R	309	CLA	CHC-C1C	2.30	1.43	1.38
49	T	312	KC2	C1C-C2C	-2.30	1.40	1.44
48	y	305	A86	O1-C20	-2.30	1.42	1.46
51	6	320	A1ECV	C4D-CHA	2.30	1.47	1.41
49	W	312	KC2	C4A-C3A	-2.30	1.40	1.44
39	9	308	CLA	CHC-C1C	2.30	1.43	1.38
39	O	318	CLA	CHC-C1C	2.30	1.43	1.38
39	2	312	CLA	CMD-C2D	-2.30	1.45	1.50
43	H	305	DD6	C26-C27	-2.30	1.32	1.37
49	6	316	KC2	C4A-C3A	-2.30	1.40	1.44
50	R	303	A1EB1	C32-C31	-2.30	1.50	1.54
51	9	314	A1ECV	C3C-C2C	2.30	1.46	1.42
51	x	316	A1ECV	C4D-CHA	2.30	1.47	1.41
39	5	308	CLA	CHC-C1C	2.30	1.43	1.38
39	Q	310	CLA	CHC-C1C	2.30	1.43	1.38
39	z	307	CLA	CHC-C1C	2.30	1.43	1.38
39	4	322	CLA	CMB-C2B	-2.30	1.45	1.50
48	6	302	A86	O1-C20	-2.30	1.42	1.46
49	z	315	KC2	C4B-NB	-2.30	1.35	1.37
39	a	829	CLA	CHC-C1C	2.30	1.43	1.38
39	b	838	CLA	CHC-C1C	2.30	1.43	1.38
49	C	313	KC2	C4A-C3A	-2.30	1.40	1.44
39	b	801	CLA	C4B-NB	2.30	1.40	1.37
49	8	319	KC2	C4A-C3A	-2.30	1.40	1.44
39	b	809	CLA	CHC-C1C	2.30	1.43	1.38
39	H	313	CLA	CHC-C1C	2.30	1.43	1.38
39	S	319	CLA	CMB-C2B	-2.30	1.45	1.50
39	a	815	CLA	CHC-C1C	2.29	1.43	1.38
39	O	313	CLA	CHC-C1C	2.29	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	0	310	CLA	CHC-C1C	2.29	1.43	1.38
39	a	801	CLA	CMB-C2B	-2.29	1.45	1.50
39	A	312	CLA	CHC-C1C	2.29	1.43	1.38
39	E	312	CLA	CHC-C1C	2.29	1.43	1.38
39	X	309	CLA	CHC-C1C	2.29	1.43	1.38
50	x	301	A1EB1	O1-C20	-2.29	1.42	1.46
39	O	310	CLA	CMB-C2B	-2.29	1.45	1.50
48	J	303	A86	O1-C20	-2.29	1.42	1.46
39	Y	305	CLA	CHC-C1C	2.29	1.43	1.38
49	T	315	KC2	C4A-C3A	-2.29	1.40	1.44
39	f	803	CLA	CHC-C1C	2.29	1.43	1.38
48	8	309	A86	O1-C20	-2.29	1.42	1.46
49	L	315	KC2	C1C-C2C	-2.29	1.40	1.44
39	H	310	CLA	CMD-C2D	-2.29	1.45	1.50
39	P	309	CLA	CHC-C1C	2.29	1.43	1.38
49	S	317	KC2	C4A-C3A	-2.29	1.40	1.44
39	H	308	CLA	CHC-C1C	2.29	1.43	1.38
39	a	801	CLA	CMD-C2D	-2.29	1.46	1.50
48	0	301	A86	O1-C20	-2.29	1.42	1.46
49	X	312	KC2	C4B-NB	-2.29	1.35	1.37
51	Z	308	A1ECV	C4D-CHA	2.29	1.47	1.41
39	T	311	CLA	CHC-C1C	2.28	1.43	1.38
39	B	206	CLA	CMD-C2D	-2.28	1.46	1.50
49	x	315	KC2	C4A-C3A	-2.28	1.40	1.44
51	R	313	A1ECV	C4D-CHA	2.28	1.47	1.41
51	x	310	A1ECV	C4D-CHA	2.28	1.47	1.41
51	Y	312	A1ECV	C4D-CHA	2.28	1.47	1.41
39	R	311	CLA	CHC-C1C	2.28	1.43	1.38
39	E	318	CLA	CHC-C1C	2.28	1.43	1.38
39	I	301	CLA	CHC-C1C	2.28	1.43	1.38
39	6	311	CLA	CHC-C1C	2.28	1.43	1.38
39	b	830	CLA	CMD-C2D	-2.28	1.46	1.50
39	D	315	CLA	CHC-C1C	2.28	1.43	1.38
39	E	307	CLA	CHC-C1C	2.28	1.43	1.38
49	5	305	KC2	C4B-NB	-2.28	1.35	1.37
39	b	813	CLA	CMD-C2D	-2.28	1.46	1.50
39	9	308	CLA	CMD-C2D	-2.28	1.46	1.50
49	R	318	KC2	C4A-C3A	-2.28	1.40	1.44
51	Z	314	A1ECV	C4D-CHA	2.28	1.47	1.41
39	A	309	CLA	CHC-C1C	2.28	1.43	1.38
39	y	308	CLA	CHC-C1C	2.28	1.43	1.38
49	y	316	KC2	C4B-NB	-2.28	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	L	318	A1ECV	C4D-CHA	2.28	1.47	1.41
51	9	317	A1ECV	C4D-CHA	2.28	1.47	1.41
48	R	301	A86	O1-C20	-2.28	1.43	1.46
39	a	812	CLA	CHC-C1C	2.28	1.43	1.38
39	S	311	CLA	CHC-C1C	2.28	1.43	1.38
39	W	309	CLA	CHC-C1C	2.28	1.43	1.38
39	X	311	CLA	CHC-C1C	2.28	1.43	1.38
49	G	311	KC2	C4A-C3A	-2.28	1.40	1.44
49	G	315	KC2	C4A-C3A	-2.28	1.40	1.44
39	k	201	CLA	CHC-C1C	2.28	1.43	1.38
48	Z	301	A86	O1-C20	-2.28	1.43	1.46
39	f	802	CLA	CHC-C1C	2.28	1.43	1.38
39	B	207	CLA	CHC-C1C	2.28	1.43	1.38
49	H	314	KC2	C4A-C3A	-2.28	1.40	1.44
43	X	304	DD6	O1-C20	-2.27	1.43	1.46
49	z	315	KC2	C4A-C3A	-2.27	1.40	1.44
39	Q	311	CLA	CHC-C1C	2.27	1.43	1.38
39	5	306	CLA	CHC-C1C	2.27	1.43	1.38
49	6	319	KC2	C4A-C3A	-2.27	1.40	1.44
39	o	206	CLA	CHC-C1C	2.27	1.43	1.38
39	C	311	CLA	CHC-C1C	2.27	1.43	1.38
51	9	314	A1ECV	C4D-CHA	2.27	1.47	1.41
39	b	802	CLA	CHC-C1C	2.27	1.43	1.38
39	a	828	CLA	CHC-C1C	2.27	1.43	1.38
39	C	306	CLA	CHC-C1C	2.27	1.43	1.38
39	O	311	CLA	CHC-C1C	2.27	1.43	1.38
48	1	307	A86	O1-C20	-2.27	1.43	1.46
39	0	320	CLA	CHC-C1C	2.27	1.43	1.38
49	5	314	KC2	C4A-C3A	-2.27	1.40	1.44
39	a	814	CLA	CHC-C1C	2.27	1.43	1.38
39	D	316	CLA	CHC-C1C	2.27	1.43	1.38
39	O	309	CLA	MG-NB	-2.27	2.01	2.05
39	5	315	CLA	MG-NB	-2.27	2.01	2.05
51	R	313	A1ECV	C3C-C2C	2.27	1.46	1.42
49	Q	315	KC2	C1C-C2C	-2.27	1.40	1.44
39	b	810	CLA	CHC-C1C	2.27	1.43	1.38
39	E	310	CLA	CHC-C1C	2.27	1.43	1.38
49	X	315	KC2	C4A-C3A	-2.27	1.40	1.44
39	b	801	CLA	CMB-C2B	-2.27	1.46	1.50
39	D	319	CLA	CHC-C1C	2.27	1.43	1.38
39	I	316	CLA	CHC-C1C	2.27	1.43	1.38
39	T	313	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	3	314	CLA	CHC-C1C	2.27	1.43	1.38
39	8	313	CLA	CHC-C1C	2.27	1.43	1.38
39	6	310	CLA	CHC-C1C	2.27	1.43	1.38
39	l	203	CLA	CMB-C2B	-2.27	1.46	1.50
39	M	310	CLA	CHC-C1C	2.27	1.43	1.38
39	Q	320	CLA	CHC-C1C	2.27	1.43	1.38
39	U	213	CLA	CHC-C1C	2.27	1.43	1.38
39	1	316	CLA	CHC-C1C	2.27	1.43	1.38
48	O	302	A86	O1-C20	-2.27	1.43	1.46
39	D	313	CLA	CHC-C1C	2.27	1.43	1.38
39	O	312	CLA	CHC-C1C	2.26	1.43	1.38
39	U	208	CLA	CHC-C1C	2.26	1.43	1.38
49	9	313	KC2	C4A-C3A	-2.26	1.40	1.44
39	b	831	CLA	MG-NB	-2.26	2.01	2.05
48	O	306	A86	O1-C20	-2.26	1.43	1.46
39	b	830	CLA	C1B-C2B	2.26	1.48	1.43
39	4	311	CLA	CHC-C1C	2.26	1.43	1.38
39	4	314	CLA	CHC-C1C	2.26	1.43	1.38
39	b	836	CLA	CHC-C1C	2.26	1.43	1.38
39	i	103	CLA	CHC-C1C	2.26	1.43	1.38
48	L	302	A86	C30-C29	-2.26	1.28	1.32
51	5	309	A1ECV	C4D-CHA	2.26	1.46	1.41
39	V	311	CLA	CHC-C1C	2.26	1.43	1.38
39	x	309	CLA	CHC-C1C	2.26	1.43	1.38
39	x	318	CLA	CHC-C1C	2.26	1.43	1.38
39	k	202	CLA	CHC-C1C	2.26	1.43	1.38
39	A	306	CLA	CMB-C2B	-2.26	1.46	1.50
39	0	311	CLA	CMB-C2B	-2.26	1.46	1.50
50	Q	307	A1EB1	O1-C20	-2.26	1.43	1.46
39	z	314	CLA	CHC-C1C	2.26	1.43	1.38
39	o	201	CLA	CHC-C1C	2.26	1.43	1.38
39	I	314	CLA	CHC-C1C	2.26	1.43	1.38
51	y	311	A1ECV	C4D-CHA	2.26	1.46	1.41
39	4	319	CLA	CHC-C1C	2.26	1.43	1.38
51	Y	306	A1ECV	C4D-CHA	2.26	1.46	1.41
39	Z	305	CLA	CHC-C1C	2.26	1.43	1.38
39	a	826	CLA	CHC-C1C	2.26	1.43	1.38
39	L	311	CLA	CHC-C1C	2.26	1.43	1.38
39	U	211	CLA	CHC-C1C	2.26	1.43	1.38
39	5	310	CLA	CHC-C1C	2.26	1.43	1.38
39	z	309	CLA	CHC-C1C	2.26	1.43	1.38
49	L	315	KC2	C4A-C3A	-2.26	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	a	820	CLA	CMD-C2D	-2.26	1.46	1.50
39	M	308	CLA	CHC-C1C	2.26	1.43	1.38
51	x	310	A1ECV	C3C-C2C	2.26	1.46	1.42
51	7	323	A1ECV	C4D-CHA	2.26	1.46	1.41
39	b	814	CLA	CHC-C1C	2.25	1.43	1.38
49	L	321	KC2	C4A-C3A	-2.25	1.40	1.44
39	b	832	CLA	CHC-C1C	2.25	1.43	1.38
39	b	840	CLA	CHC-C1C	2.25	1.43	1.38
39	V	309	CLA	CHC-C1C	2.25	1.43	1.38
39	E	307	CLA	C1B-C2B	2.25	1.48	1.43
49	0	319	KC2	C1B-NB	-2.25	1.35	1.37
39	I	313	CLA	CHC-C1C	2.25	1.43	1.38
39	a	835	CLA	CHC-C1C	2.25	1.43	1.38
39	Z	312	CLA	CHC-C1C	2.25	1.43	1.38
39	K	307	CLA	CHC-C1C	2.25	1.43	1.38
49	O	317	KC2	C1C-C2C	-2.25	1.40	1.44
39	0	312	CLA	MG-NB	-2.25	2.01	2.05
49	5	311	KC2	C4A-C3A	-2.25	1.40	1.44
45	C	314	DGD	O2G-C2G	-2.25	1.41	1.46
39	K	308	CLA	CHC-C1C	2.25	1.43	1.38
39	b	841	CLA	CMB-C2B	-2.25	1.46	1.50
39	l	205	CLA	CHC-C1C	2.25	1.43	1.38
48	L	306	A86	O1-C20	-2.25	1.43	1.46
39	3	311	CLA	CHC-C1C	2.25	1.43	1.38
49	G	311	KC2	C1C-C2C	-2.25	1.40	1.44
39	b	815	CLA	CHC-C1C	2.25	1.43	1.38
39	C	305	CLA	CHC-C1C	2.25	1.43	1.38
39	I	311	CLA	CHC-C1C	2.25	1.43	1.38
39	Y	303	CLA	CHC-C1C	2.25	1.43	1.38
51	2	311	A1ECV	C4D-CHA	2.25	1.46	1.41
39	R	316	CLA	CMB-C2B	-2.24	1.46	1.50
39	J	318	CLA	CHC-C1C	2.24	1.43	1.38
49	1	312	KC2	C4A-C3A	-2.24	1.40	1.44
47	W	301	SQD	O2-C2	-2.24	1.37	1.43
39	8	312	CLA	CHC-C1C	2.24	1.43	1.38
39	D	318	CLA	CHC-C1C	2.24	1.43	1.38
39	7	316	CLA	CHC-C1C	2.24	1.43	1.38
39	W	316	CLA	CHC-C1C	2.24	1.43	1.38
49	Q	313	KC2	C1B-NB	-2.24	1.35	1.37
39	0	313	CLA	CHC-C1C	2.24	1.43	1.38
39	7	315	CLA	CHC-C1C	2.24	1.43	1.38
39	b	836	CLA	CMB-C2B	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	R	308	CLA	CHC-C1C	2.24	1.43	1.38
39	z	306	CLA	CHC-C1C	2.24	1.43	1.38
48	3	308	A86	O1-C20	-2.24	1.43	1.46
39	D	312	CLA	CHC-C1C	2.24	1.43	1.38
49	T	316	KC2	C4A-C3A	-2.24	1.40	1.44
39	a	819	CLA	CHC-C1C	2.24	1.43	1.38
39	F	321	CLA	CHC-C1C	2.24	1.43	1.38
39	6	321	CLA	CHC-C1C	2.24	1.43	1.38
39	b	817	CLA	CHC-C1C	2.24	1.43	1.38
39	O	308	CLA	C4C-C3C	2.24	1.48	1.45
39	E	316	CLA	CHC-C1C	2.24	1.43	1.38
39	8	318	CLA	CHC-C1C	2.24	1.43	1.38
41	a	840	LHG	O7-C5	-2.24	1.41	1.46
39	b	831	CLA	CHC-C1C	2.24	1.43	1.38
39	G	314	CLA	CHC-C1C	2.24	1.43	1.38
39	K	311	CLA	CHC-C1C	2.24	1.43	1.38
39	M	315	CLA	CHC-C1C	2.24	1.43	1.38
47	T	321	SQD	O2-C2	-2.23	1.37	1.43
39	H	310	CLA	CHC-C1C	2.23	1.43	1.38
48	L	307	A86	O1-C20	-2.23	1.43	1.46
51	z	310	A1ECV	C4D-CHA	2.23	1.46	1.41
39	P	307	CLA	CHC-C1C	2.23	1.43	1.38
39	z	318	CLA	CHC-C1C	2.23	1.43	1.38
51	X	310	A1ECV	C4D-CHA	2.23	1.46	1.41
39	1	320	CLA	CHC-C1C	2.23	1.43	1.38
39	b	819	CLA	CHC-C1C	2.23	1.43	1.38
39	7	313	CLA	CHC-C1C	2.23	1.43	1.38
39	b	836	CLA	C1B-C2B	2.23	1.48	1.43
39	G	309	CLA	CMD-C2D	-2.23	1.46	1.50
39	b	803	CLA	CHC-C1C	2.23	1.43	1.38
51	R	310	A1ECV	C4D-CHA	2.23	1.46	1.41
39	Z	304	CLA	CHC-C1C	2.23	1.43	1.38
39	a	824	CLA	CMC-C2C	-2.23	1.46	1.50
39	I	315	CLA	CHC-C1C	2.23	1.43	1.38
39	b	801	CLA	MG-ND	-2.23	2.01	2.05
39	B	209	CLA	CMB-C2B	-2.23	1.46	1.50
47	D	320	SQD	O2-C2	-2.23	1.37	1.43
39	9	307	CLA	CMB-C2B	-2.23	1.46	1.50
39	F	314	CLA	CHC-C1C	2.23	1.43	1.38
49	W	314	KC2	C4A-C3A	-2.23	1.40	1.44
39	b	826	CLA	MG-NB	-2.23	2.01	2.05
39	7	321	CLA	CHC-C1C	2.23	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	324	CLA	CHC-C1C	2.22	1.43	1.38
39	9	315	CLA	CHC-C1C	2.22	1.43	1.38
39	V	313	CLA	CMB-C2B	-2.22	1.46	1.50
39	b	828	CLA	CHC-C1C	2.22	1.43	1.38
39	b	834	CLA	CHC-C1C	2.22	1.43	1.38
39	E	317	CLA	CHC-C1C	2.22	1.43	1.38
39	E	319	CLA	CHC-C1C	2.22	1.43	1.38
48	M	306	A86	O1-C20	-2.22	1.43	1.46
39	x	306	CLA	CHC-C1C	2.22	1.43	1.38
45	b	849	DGD	O2G-C2G	-2.22	1.41	1.46
39	G	309	CLA	MG-NB	-2.22	2.01	2.05
39	a	810	CLA	CHC-C1C	2.22	1.43	1.38
39	F	316	CLA	CHC-C1C	2.22	1.43	1.38
39	A	315	CLA	CHC-C1C	2.22	1.43	1.38
39	9	319	CLA	CHC-C1C	2.22	1.43	1.38
49	W	315	KC2	C4A-C3A	-2.22	1.40	1.44
39	A	308	CLA	CHC-C1C	2.22	1.43	1.38
39	a	816	CLA	CHC-C1C	2.22	1.43	1.38
39	0	323	CLA	CHC-C1C	2.22	1.43	1.38
51	1	318	A1ECV	C4D-CHA	2.22	1.46	1.41
39	a	827	CLA	MG-NB	-2.22	2.01	2.05
49	K	310	KC2	C4A-C3A	-2.22	1.40	1.44
39	8	315	CLA	CHC-C1C	2.22	1.43	1.38
39	y	312	CLA	CHC-C1C	2.22	1.43	1.38
39	D	314	CLA	CMB-C2B	-2.22	1.46	1.50
39	a	816	CLA	MG-NB	-2.22	2.01	2.05
39	L	316	CLA	CHC-C1C	2.22	1.43	1.38
51	4	315	A1ECV	C4D-CHA	2.22	1.46	1.41
39	b	801	CLA	CMC-C2C	-2.22	1.46	1.50
39	j	101	CLA	CHC-C1C	2.22	1.43	1.38
39	b	839	CLA	CHC-C1C	2.22	1.43	1.38
39	G	312	CLA	CHC-C1C	2.22	1.43	1.38
39	a	818	CLA	CHC-C1C	2.22	1.43	1.38
39	9	312	CLA	CHC-C1C	2.22	1.43	1.38
39	S	309	CLA	CMD-C2D	-2.22	1.46	1.50
49	S	314	KC2	C4A-C3A	-2.22	1.40	1.44
39	1	317	CLA	CHC-C1C	2.21	1.43	1.38
39	6	315	CLA	CHC-C1C	2.21	1.43	1.38
45	b	849	DGD	O1G-C1G	-2.21	1.40	1.45
39	E	315	CLA	CHC-C1C	2.21	1.43	1.38
49	P	312	KC2	C4A-C3A	-2.21	1.40	1.44
39	G	318	CLA	CMD-C2D	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Q	309	CLA	CMD-C2D	-2.21	1.46	1.50
39	b	812	CLA	CMB-C2B	-2.21	1.46	1.50
49	4	317	KC2	C4A-C3A	-2.21	1.40	1.44
51	Q	316	A1ECV	C3C-C2C	2.21	1.46	1.42
39	a	822	CLA	CHC-C1C	2.21	1.43	1.38
39	F	309	CLA	CHC-C1C	2.21	1.43	1.38
39	6	312	CLA	CHC-C1C	2.21	1.43	1.38
49	y	314	KC2	C4A-C3A	-2.21	1.40	1.44
49	Z	311	KC2	C4A-C3A	-2.21	1.40	1.44
47	P	301	SQD	O2-C2	-2.21	1.37	1.43
49	2	317	KC2	C4A-C3A	-2.21	1.40	1.44
43	U	204	DD6	O1-C20	-2.21	1.43	1.46
48	U	206	A86	O1-C20	-2.21	1.43	1.46
39	J	317	CLA	CMB-C2B	-2.21	1.46	1.50
39	F	313	CLA	CMD-C2D	-2.21	1.46	1.50
39	b	835	CLA	CHC-C1C	2.21	1.43	1.38
39	H	307	CLA	CHC-C1C	2.21	1.43	1.38
49	Y	309	KC2	C4A-C3A	-2.21	1.40	1.44
49	8	316	KC2	C4A-C3A	-2.21	1.40	1.44
39	W	310	CLA	CHC-C1C	2.21	1.43	1.38
39	4	322	CLA	CHC-C1C	2.21	1.43	1.38
39	o	203	CLA	CHC-C1C	2.21	1.43	1.38
39	E	307	CLA	MG-NB	-2.21	2.01	2.05
48	D	305	A86	O1-C20	-2.21	1.43	1.46
39	W	313	CLA	CMB-C2B	-2.21	1.46	1.50
41	a	841	LHG	O7-C5	-2.21	1.41	1.46
39	8	321	CLA	CHC-C1C	2.21	1.43	1.38
39	b	834	CLA	CMD-C2D	-2.21	1.46	1.50
39	L	320	CLA	CHC-C1C	2.21	1.43	1.38
39	1	308	CLA	CHC-C1C	2.21	1.43	1.38
39	H	315	CLA	CMD-C2D	-2.21	1.46	1.50
39	x	309	CLA	CMD-C2D	-2.21	1.46	1.50
39	L	319	CLA	CHC-C1C	2.21	1.43	1.38
39	I	310	CLA	CHC-C1C	2.21	1.43	1.38
39	H	312	CLA	CMD-C2D	-2.21	1.46	1.50
39	Q	312	CLA	CHC-C1C	2.21	1.43	1.38
39	y	318	CLA	CHC-C1C	2.21	1.43	1.38
39	B	206	CLA	CHC-C1C	2.21	1.43	1.38
39	b	829	CLA	CHC-C1C	2.20	1.43	1.38
39	7	318	CLA	CHC-C1C	2.20	1.43	1.38
39	a	837	CLA	CHC-C1C	2.20	1.43	1.38
39	b	840	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	k	203	CLA	CHC-C1C	2.20	1.43	1.38
39	E	314	CLA	CHC-C1C	2.20	1.43	1.38
39	y	319	CLA	CHC-C1C	2.20	1.43	1.38
39	a	830	CLA	CHC-C1C	2.20	1.43	1.38
39	4	316	CLA	CMD-C2D	-2.20	1.46	1.50
39	Y	310	CLA	CHC-C1C	2.20	1.43	1.38
39	Y	311	CLA	CHC-C1C	2.20	1.43	1.38
39	7	318	CLA	CMD-C2D	-2.20	1.46	1.50
39	4	323	CLA	CHC-C1C	2.20	1.43	1.38
39	a	826	CLA	CMD-C2D	-2.20	1.46	1.50
39	a	801	CLA	MG-NB	-2.20	2.01	2.05
39	2	315	CLA	CHC-C1C	2.20	1.43	1.38
39	T	308	CLA	MG-NB	-2.20	2.01	2.05
39	M	318	CLA	CMB-C2B	-2.20	1.46	1.50
39	Q	314	CLA	CHC-C1C	2.20	1.43	1.38
39	1	310	CLA	CHC-C1C	2.20	1.43	1.38
39	Z	315	CLA	CHC-C1C	2.20	1.43	1.38
51	9	317	A1ECV	C3C-C2C	2.20	1.46	1.42
49	7	319	KC2	C4A-C3A	-2.20	1.40	1.44
39	J	313	CLA	CHC-C1C	2.20	1.43	1.38
47	E	320	SQD	O2-C2	-2.20	1.37	1.43
39	3	322	CLA	CHC-C1C	2.20	1.43	1.38
51	7	317	A1ECV	C4D-CHA	2.20	1.46	1.41
47	D	304	SQD	O2-C2	-2.20	1.37	1.43
39	L	313	CLA	CHC-C1C	2.20	1.43	1.38
39	x	311	CLA	CHC-C1C	2.20	1.43	1.38
39	J	308	CLA	CHC-C1C	2.20	1.43	1.38
48	W	307	A86	O1-C20	-2.20	1.43	1.46
39	a	838	CLA	CMD-C2D	-2.20	1.46	1.50
39	6	318	CLA	CHC-C1C	2.20	1.43	1.38
39	S	309	CLA	CMB-C2B	-2.19	1.46	1.50
48	F	302	A86	C32-C31	-2.19	1.50	1.54
39	O	310	CLA	CHC-C1C	2.19	1.43	1.38
50	3	309	A1EB1	O1-C20	-2.19	1.43	1.46
39	H	309	CLA	CHC-C1C	2.19	1.43	1.38
49	I	312	KC2	C1C-C2C	-2.19	1.40	1.44
39	a	806	CLA	CHC-C1C	2.19	1.43	1.38
39	b	812	CLA	CHC-C1C	2.19	1.43	1.38
39	z	311	CLA	CHC-C1C	2.19	1.43	1.38
39	F	306	CLA	CHC-C1C	2.19	1.43	1.38
39	y	310	CLA	CMD-C2D	-2.19	1.46	1.50
39	Z	307	CLA	CHC-C1C	2.19	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	U	212	CLA	CHC-C1C	2.19	1.43	1.38
51	y	311	A1ECV	C3C-C2C	2.19	1.46	1.42
49	2	314	KC2	C4A-C3A	-2.19	1.40	1.44
39	A	305	CLA	CHC-C1C	2.19	1.43	1.38
39	b	825	CLA	CMD-C2D	-2.19	1.46	1.50
39	b	820	CLA	CMB-C2B	-2.19	1.46	1.50
39	M	317	CLA	CMB-C2B	-2.19	1.46	1.50
39	i	101	CLA	CHC-C1C	2.19	1.43	1.38
39	I	309	CLA	CMD-C2D	-2.19	1.46	1.50
39	K	312	CLA	CHC-C1C	2.19	1.43	1.38
39	y	310	CLA	CHC-C1C	2.19	1.43	1.38
39	4	316	CLA	CHC-C1C	2.19	1.43	1.38
49	C	312	KC2	C4A-C3A	-2.19	1.40	1.44
51	z	310	A1ECV	C3C-C2C	2.19	1.46	1.42
39	a	809	CLA	CHC-C1C	2.19	1.43	1.38
39	E	309	CLA	CHC-C1C	2.19	1.43	1.38
49	9	318	KC2	C4A-C3A	-2.19	1.40	1.44
39	h	201	CLA	CHC-C1C	2.19	1.43	1.38
51	S	312	A1ECV	C4D-CHA	2.19	1.46	1.41
43	U	204	DD6	C36-C31	-2.19	1.32	1.34
39	Y	302	CLA	CHC-C1C	2.18	1.43	1.38
49	L	314	KC2	C4B-NB	-2.18	1.35	1.37
39	9	320	CLA	CMB-C2B	-2.18	1.46	1.50
49	3	318	KC2	C1B-NB	-2.18	1.35	1.37
47	F	318	SQD	O2-C2	-2.18	1.37	1.43
50	1	305	A1EB1	O1-C20	-2.18	1.43	1.46
39	a	833	CLA	CHC-C1C	2.18	1.43	1.38
39	V	316	CLA	CHC-C1C	2.18	1.43	1.38
47	M	301	SQD	O2-C2	-2.18	1.37	1.43
39	L	310	CLA	CHC-C1C	2.18	1.43	1.38
39	C	310	CLA	CHC-C1C	2.18	1.43	1.38
39	S	319	CLA	CHC-C1C	2.18	1.43	1.38
49	7	320	KC2	C4A-C3A	-2.18	1.40	1.44
39	J	318	CLA	CMD-C2D	-2.18	1.46	1.50
39	E	313	CLA	CHC-C1C	2.18	1.43	1.38
49	V	308	KC2	C1C-C2C	-2.18	1.40	1.44
39	O	308	CLA	CHC-C1C	2.18	1.43	1.38
39	y	315	CLA	CHC-C1C	2.18	1.43	1.38
39	a	827	CLA	C1B-C2B	2.18	1.48	1.43
39	b	806	CLA	CHC-C1C	2.18	1.43	1.38
43	7	309	DD6	O1-C20	-2.18	1.43	1.46
48	F	301	A86	O1-C20	-2.18	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	S	311	CLA	CMD-C2D	-2.18	1.46	1.50
49	2	317	KC2	C1C-C2C	-2.18	1.40	1.44
39	b	821	CLA	MG-NB	-2.18	2.01	2.05
39	a	816	CLA	C1B-C2B	2.18	1.48	1.43
48	8	307	A86	O1-C20	-2.18	1.43	1.46
49	I	303	KC2	C1C-C2C	-2.18	1.40	1.44
49	Z	310	KC2	C4A-C3A	-2.18	1.40	1.44
49	Y	308	KC2	C4A-C3A	-2.18	1.40	1.44
39	b	836	CLA	MG-NB	-2.18	2.01	2.05
49	x	313	KC2	C4A-C3A	-2.18	1.40	1.44
51	z	316	A1ECV	C3C-C2C	2.18	1.46	1.42
39	1	313	CLA	CHC-C1C	2.18	1.42	1.38
39	0	322	CLA	CHC-C1C	2.18	1.42	1.38
47	F	319	SQD	O2-C2	-2.18	1.37	1.43
39	b	822	CLA	CHC-C1C	2.18	1.42	1.38
39	H	315	CLA	CHC-C1C	2.18	1.42	1.38
47	9	322	SQD	O2-C2	-2.18	1.37	1.43
51	z	316	A1ECV	C4D-CHA	2.18	1.46	1.41
43	x	304	DD6	O1-C20	-2.18	1.43	1.46
39	x	317	CLA	CHC-C1C	2.18	1.42	1.38
43	J	305	DD6	O1-C20	-2.18	1.43	1.46
43	T	303	DD6	O1-C20	-2.18	1.43	1.46
43	W	305	DD6	O1-C20	-2.18	1.43	1.46
39	X	316	CLA	MG-NB	-2.18	2.01	2.05
39	S	316	CLA	CHC-C1C	2.17	1.42	1.38
39	1	309	CLA	CHC-C1C	2.17	1.42	1.38
39	3	320	CLA	CHC-C1C	2.17	1.42	1.38
39	X	308	CLA	C1B-C2B	2.17	1.48	1.43
49	F	311	KC2	C1C-C2C	-2.17	1.40	1.44
51	4	321	A1ECV	C3C-C2C	2.17	1.46	1.42
39	M	312	CLA	CMB-C2B	-2.17	1.46	1.50
39	a	813	CLA	CHC-C1C	2.17	1.42	1.38
39	b	821	CLA	CHC-C1C	2.17	1.42	1.38
47	k	205	SQD	O2-C2	-2.17	1.37	1.43
49	G	317	KC2	C1C-C2C	-2.17	1.40	1.44
39	3	312	CLA	CHC-C1C	2.17	1.42	1.38
43	5	303	DD6	O1-C20	-2.17	1.43	1.46
39	V	319	CLA	CHC-C1C	2.17	1.42	1.38
39	9	307	CLA	MG-NB	-2.17	2.01	2.05
39	2	312	CLA	CHC-C1C	2.17	1.42	1.38
39	Q	310	CLA	CMD-C2D	-2.17	1.46	1.50
39	0	311	CLA	MG-NB	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	F	308	CLA	CHC-C1C	2.17	1.42	1.38
39	F	313	CLA	CHC-C1C	2.17	1.42	1.38
39	Y	314	CLA	CHC-C1C	2.17	1.42	1.38
39	X	316	CLA	CHC-C1C	2.17	1.42	1.38
39	3	323	CLA	CHC-C1C	2.17	1.42	1.38
39	5	315	CLA	CHC-C1C	2.17	1.42	1.38
39	S	309	CLA	MG-NB	-2.17	2.01	2.05
49	9	313	KC2	C1C-C2C	-2.17	1.40	1.44
39	b	822	CLA	CMD-C2D	-2.17	1.46	1.50
39	H	306	CLA	CHC-C1C	2.17	1.42	1.38
39	P	314	CLA	CHC-C1C	2.17	1.42	1.38
43	M	304	DD6	O1-C20	-2.17	1.43	1.46
39	b	840	CLA	CMC-C2C	-2.17	1.46	1.50
39	a	808	CLA	CHC-C1C	2.17	1.42	1.38
39	S	309	CLA	C1B-C2B	2.17	1.48	1.43
39	b	824	CLA	CMD-C2D	-2.17	1.46	1.50
39	F	316	CLA	CMD-C2D	-2.17	1.46	1.50
39	9	307	CLA	CHC-C1C	2.17	1.42	1.38
49	G	315	KC2	C1D-ND	-2.16	1.35	1.37
39	b	806	CLA	CMD-C2D	-2.16	1.46	1.50
39	C	310	CLA	CMD-C2D	-2.16	1.46	1.50
39	1	311	CLA	CHC-C1C	2.16	1.42	1.38
39	Y	313	CLA	CHC-C1C	2.16	1.42	1.38
51	1	318	A1ECV	C3C-C2C	2.16	1.46	1.42
39	W	318	CLA	CMB-C2B	-2.16	1.46	1.50
48	8	323	A86	O1-C20	-2.16	1.43	1.46
39	2	318	CLA	CHC-C1C	2.16	1.42	1.38
47	7	302	SQD	O2-C2	-2.16	1.37	1.43
39	b	829	CLA	CMD-C2D	-2.16	1.46	1.50
39	C	304	CLA	CHC-C1C	2.16	1.42	1.38
49	9	311	KC2	C4A-C3A	-2.16	1.40	1.44
39	x	314	CLA	CHC-C1C	2.16	1.42	1.38
39	P	316	CLA	CMB-C2B	-2.16	1.46	1.50
39	a	847	CLA	CHC-C1C	2.16	1.42	1.38
39	y	307	CLA	CHC-C1C	2.16	1.42	1.38
39	a	818	CLA	CMB-C2B	-2.16	1.46	1.50
50	V	302	A1EB1	O1-C20	-2.16	1.43	1.46
39	8	322	CLA	CHC-C1C	2.16	1.42	1.38
39	W	318	CLA	CHC-C1C	2.16	1.42	1.38
39	a	803	CLA	CMB-C2B	-2.16	1.46	1.50
39	D	310	CLA	MG-NB	-2.16	2.01	2.05
39	3	316	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	a	803	CLA	CMD-C2D	-2.16	1.46	1.50
39	W	309	CLA	CMD-C2D	-2.16	1.46	1.50
39	0	323	CLA	CMB-C2B	-2.16	1.46	1.50
39	Q	317	CLA	CHC-C1C	2.16	1.42	1.38
39	0	318	CLA	CHC-C1C	2.16	1.42	1.38
39	a	817	CLA	CMD-C2D	-2.16	1.46	1.50
47	S	301	SQD	O3-C3	-2.16	1.37	1.43
39	V	313	CLA	CMC-C2C	-2.16	1.46	1.50
49	y	313	KC2	C4A-C3A	-2.16	1.40	1.44
39	J	312	CLA	CHC-C1C	2.16	1.42	1.38
43	G	306	DD6	O1-C20	-2.16	1.43	1.46
43	K	303	DD6	O1-C20	-2.16	1.43	1.46
48	H	302	A86	O1-C20	-2.16	1.43	1.46
39	b	827	CLA	CHC-C1C	2.16	1.42	1.38
39	b	813	CLA	MG-NB	-2.15	2.01	2.05
39	S	320	CLA	CHC-C1C	2.15	1.42	1.38
39	E	307	CLA	CMB-C2B	-2.15	1.46	1.50
39	3	313	CLA	MG-NB	-2.15	2.01	2.05
39	O	309	CLA	CHC-C1C	2.15	1.42	1.38
39	W	313	CLA	CHC-C1C	2.15	1.42	1.38
43	y	304	DD6	O1-C20	-2.15	1.43	1.46
49	A	313	KC2	C1C-C2C	-2.15	1.40	1.44
49	R	312	KC2	C1D-ND	-2.15	1.35	1.37
39	H	316	CLA	CHC-C1C	2.15	1.42	1.38
39	E	306	CLA	CHC-C1C	2.15	1.42	1.38
39	Z	313	CLA	CMB-C2B	-2.15	1.46	1.50
47	H	318	SQD	O2-C2	-2.15	1.37	1.43
48	L	304	A86	O1-C20	-2.15	1.43	1.46
39	b	842	CLA	CHC-C1C	2.15	1.42	1.38
39	o	202	CLA	CHC-C1C	2.15	1.42	1.38
43	E	302	DD6	O1-C20	-2.15	1.43	1.46
39	z	308	CLA	CHC-C1C	2.15	1.42	1.38
39	a	826	CLA	MG-NB	-2.15	2.01	2.05
39	b	829	CLA	MG-NB	-2.15	2.01	2.05
49	R	312	KC2	C4A-C3A	-2.15	1.40	1.44
39	y	319	CLA	CMB-C2B	-2.15	1.46	1.50
39	X	317	CLA	MG-NB	-2.15	2.01	2.05
43	H	303	DD6	O1-C20	-2.15	1.43	1.46
39	T	308	CLA	CMB-C2B	-2.15	1.46	1.50
39	F	312	CLA	CMB-C2B	-2.15	1.46	1.50
39	K	314	CLA	CMB-C2B	-2.15	1.46	1.50
49	T	315	KC2	C1C-C2C	-2.15	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	A	314	CLA	CHC-C1C	2.15	1.42	1.38
39	6	322	CLA	CHC-C1C	2.15	1.42	1.38
39	b	830	CLA	MG-NB	-2.15	2.01	2.05
49	z	312	KC2	C1C-C2C	-2.15	1.40	1.44
39	8	310	CLA	CHC-C1C	2.15	1.42	1.38
43	B	202	DD6	O1-C20	-2.15	1.43	1.46
39	a	817	CLA	CHC-C1C	2.14	1.42	1.38
39	5	316	CLA	CHC-C1C	2.14	1.42	1.38
48	3	307	A86	O1-C20	-2.14	1.43	1.46
49	x	312	KC2	C4A-C3A	-2.14	1.40	1.44
39	C	307	CLA	CHC-C1C	2.14	1.42	1.38
47	4	327	SQD	O2-C2	-2.14	1.37	1.43
39	l	203	CLA	CHC-C1C	2.14	1.42	1.38
39	S	313	CLA	CHC-C1C	2.14	1.42	1.38
39	2	315	CLA	CMD-C2D	-2.14	1.46	1.50
39	0	312	CLA	CMD-C2D	-2.14	1.46	1.50
39	9	320	CLA	MG-NB	-2.14	2.01	2.05
39	C	309	CLA	CHC-C1C	2.14	1.42	1.38
39	T	319	CLA	CHC-C1C	2.14	1.42	1.38
39	K	309	CLA	CHC-C1C	2.14	1.42	1.38
39	a	834	CLA	MG-NB	-2.14	2.01	2.05
39	P	307	CLA	MG-NB	-2.14	2.01	2.05
39	T	318	CLA	CMD-C2D	-2.14	1.46	1.50
43	Q	306	DD6	O1-C20	-2.14	1.43	1.46
39	E	308	CLA	CHC-C1C	2.14	1.42	1.38
39	b	811	CLA	CMC-C2C	-2.14	1.46	1.50
39	2	307	CLA	CHC-C1C	2.14	1.42	1.38
39	0	312	CLA	CMB-C2B	-2.14	1.46	1.50
49	C	312	KC2	C1C-C2C	-2.14	1.40	1.44
39	2	309	CLA	CHC-C1C	2.14	1.42	1.38
39	2	310	CLA	CHC-C1C	2.14	1.42	1.38
39	b	823	CLA	CHC-C1C	2.14	1.42	1.38
39	a	825	CLA	CMC-C2C	-2.13	1.46	1.50
39	i	103	CLA	MG-NB	-2.13	2.01	2.05
43	D	307	DD6	O1-C20	-2.13	1.43	1.46
48	X	303	A86	O1-C20	-2.13	1.43	1.46
39	l	205	CLA	CMD-C2D	-2.13	1.46	1.50
39	T	308	CLA	CMD-C2D	-2.13	1.46	1.50
49	K	310	KC2	C1C-C2C	-2.13	1.40	1.44
39	T	310	CLA	CHC-C1C	2.13	1.42	1.38
39	a	847	CLA	CMB-C2B	-2.13	1.46	1.50
39	z	317	CLA	CHC-C1C	2.13	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	b	811	CLA	CMD-C2D	-2.13	1.46	1.50
39	b	802	CLA	MG-NB	-2.13	2.01	2.05
39	X	308	CLA	MG-NB	-2.13	2.01	2.05
39	a	807	CLA	CMD-C2D	-2.13	1.46	1.50
49	7	319	KC2	C1C-C2C	-2.13	1.40	1.44
39	R	315	CLA	CHC-C1C	2.13	1.42	1.38
49	S	315	KC2	C1B-NB	-2.13	1.35	1.37
49	1	314	KC2	C4A-C3A	-2.13	1.40	1.44
47	D	321	SQD	O2-C2	-2.13	1.38	1.43
39	U	209	CLA	CHC-C1C	2.13	1.42	1.38
39	G	309	CLA	CMB-C2B	-2.13	1.46	1.50
39	b	837	CLA	MG-NB	-2.13	2.01	2.05
39	a	828	CLA	MG-NB	-2.13	2.01	2.05
39	Y	304	CLA	CHC-C1C	2.13	1.42	1.38
49	z	312	KC2	C4A-C3A	-2.13	1.40	1.44
51	7	323	A1ECV	C3C-C2C	2.13	1.46	1.42
39	2	309	CLA	MG-NB	-2.13	2.01	2.05
39	K	314	CLA	CHC-C1C	2.13	1.42	1.38
47	S	301	SQD	O2-C2	-2.13	1.38	1.43
49	H	314	KC2	C1C-C2C	-2.13	1.40	1.44
39	a	807	CLA	CHC-C1C	2.13	1.42	1.38
39	O	313	CLA	CMD-C2D	-2.13	1.46	1.50
39	7	324	CLA	MG-NB	-2.13	2.01	2.05
49	3	321	KC2	O2A-CGA	2.13	1.35	1.30
39	S	308	CLA	CHC-C1C	2.12	1.42	1.38
39	E	312	CLA	CMB-C2B	-2.12	1.46	1.50
39	2	309	CLA	CMD-C2D	-2.12	1.46	1.50
39	F	308	CLA	CMD-C2D	-2.12	1.46	1.50
39	J	307	CLA	CHC-C1C	2.12	1.42	1.38
49	R	312	KC2	C1C-C2C	-2.12	1.40	1.44
39	G	318	CLA	CHC-C1C	2.12	1.42	1.38
39	M	317	CLA	CHC-C1C	2.12	1.42	1.38
39	1	309	CLA	MG-NB	-2.12	2.01	2.05
43	4	307	DD6	O1-C20	-2.12	1.43	1.46
49	8	314	KC2	C1D-ND	-2.12	1.35	1.37
39	L	308	CLA	CMB-C2B	-2.12	1.46	1.50
39	b	820	CLA	MG-NB	-2.12	2.01	2.05
39	H	306	CLA	CMC-C2C	-2.12	1.46	1.50
39	a	801	CLA	CMC-C2C	-2.12	1.46	1.50
49	Q	315	KC2	C4A-C3A	-2.12	1.40	1.44
39	H	312	CLA	MG-NB	-2.12	2.01	2.05
49	P	312	KC2	C1C-C2C	-2.12	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	l	203	CLA	MG-NB	-2.12	2.01	2.05
39	y	319	CLA	MG-NB	-2.12	2.01	2.05
39	b	824	CLA	CMC-C2C	-2.12	1.46	1.50
39	0	315	CLA	CMD-C2D	-2.12	1.46	1.50
39	x	318	CLA	CMB-C2B	-2.12	1.46	1.50
43	3	301	DD6	O1-C20	-2.12	1.43	1.46
39	b	801	CLA	C1B-C2B	2.12	1.48	1.43
39	a	831	CLA	CHC-C1C	2.12	1.42	1.38
39	1	319	CLA	CHC-C1C	2.12	1.42	1.38
39	b	827	CLA	MG-NB	-2.12	2.01	2.05
39	X	317	CLA	CMB-C2B	-2.12	1.46	1.50
39	G	309	CLA	CHC-C1C	2.11	1.42	1.38
49	L	312	KC2	C1B-NB	-2.11	1.35	1.37
39	6	311	CLA	CMD-C2D	-2.11	1.46	1.50
39	a	804	CLA	MG-NB	-2.11	2.01	2.05
39	A	306	CLA	MG-NB	-2.11	2.01	2.05
49	P	306	KC2	C1C-C2C	-2.11	1.40	1.44
48	W	307	A86	C32-C31	-2.11	1.51	1.54
39	2	312	CLA	MG-NB	-2.11	2.01	2.05
39	b	831	CLA	CMB-C2B	-2.11	1.46	1.50
39	H	309	CLA	CMD-C2D	-2.11	1.46	1.50
39	2	318	CLA	CMB-C2B	-2.11	1.46	1.50
39	F	312	CLA	CHC-C1C	2.11	1.42	1.38
39	U	207	CLA	CMD-C2D	-2.11	1.46	1.50
39	S	319	CLA	MG-NB	-2.11	2.01	2.05
49	G	313	KC2	C1C-C2C	-2.11	1.40	1.44
39	C	308	CLA	CHC-C1C	2.11	1.42	1.38
39	4	313	CLA	CHC-C1C	2.11	1.42	1.38
39	E	314	CLA	CMD-C2D	-2.11	1.46	1.50
39	Q	320	CLA	CMD-C2D	-2.11	1.46	1.50
39	3	323	CLA	CMC-C2C	-2.11	1.46	1.50
39	D	311	CLA	CMC-C2C	-2.11	1.46	1.50
50	h	203	A1EB1	O1-C20	-2.11	1.43	1.46
39	O	316	CLA	CHC-C1C	2.11	1.42	1.38
39	7	325	CLA	CHC-C1C	2.11	1.42	1.38
43	z	304	DD6	C36-C31	-2.11	1.32	1.34
39	M	309	CLA	CHC-C1C	2.11	1.42	1.38
39	Y	307	CLA	CHC-C1C	2.11	1.42	1.38
39	M	317	CLA	CMD-C2D	-2.11	1.46	1.50
39	Q	314	CLA	CMD-C2D	-2.11	1.46	1.50
39	a	836	CLA	CHC-C1C	2.11	1.42	1.38
43	I	305	DD6	O1-C20	-2.11	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	1	314	KC2	C1C-C2C	-2.11	1.40	1.44
39	a	818	CLA	MG-NB	-2.11	2.01	2.05
39	x	308	CLA	CHC-C1C	2.11	1.42	1.38
39	R	315	CLA	CMD-C2D	-2.11	1.46	1.50
49	6	317	KC2	C4A-C3A	-2.11	1.40	1.44
50	Q	307	A1EB1	C13-C11	-2.11	1.45	1.49
39	Q	310	CLA	MG-NB	-2.11	2.01	2.05
39	3	313	CLA	CMC-C2C	-2.11	1.46	1.50
47	k	205	SQD	O4-C4	-2.11	1.38	1.43
39	5	316	CLA	CMB-C2B	-2.11	1.46	1.50
39	b	840	CLA	MG-NB	-2.11	2.01	2.05
39	E	316	CLA	CMD-C2D	-2.10	1.46	1.50
39	O	314	CLA	CMC-C2C	-2.10	1.46	1.50
51	L	318	A1ECV	C1D-ND	2.10	1.37	1.35
39	x	318	CLA	MG-NB	-2.10	2.01	2.05
39	l	204	CLA	CMB-C2B	-2.10	1.46	1.50
52	P	318	A1EB4	C32-C31	-2.10	1.51	1.54
51	Z	308	A1ECV	C3C-C2C	2.10	1.46	1.42
49	2	313	KC2	C1C-C2C	-2.10	1.40	1.44
47	T	321	SQD	O4-C4	-2.10	1.38	1.43
39	a	834	CLA	CHC-C1C	2.10	1.42	1.38
39	A	307	CLA	CMD-C2D	-2.10	1.46	1.50
49	M	311	KC2	C1C-C2C	-2.10	1.40	1.44
39	M	312	CLA	CHC-C1C	2.10	1.42	1.38
43	A	301	DD6	O1-C20	-2.10	1.43	1.46
39	9	309	CLA	CHC-C1C	2.10	1.42	1.38
39	R	316	CLA	CHC-C1C	2.10	1.42	1.38
39	b	814	CLA	CMB-C2B	-2.10	1.46	1.50
39	S	311	CLA	MG-NB	-2.10	2.01	2.05
47	7	302	SQD	O4-C4	-2.10	1.38	1.43
39	A	305	CLA	CMB-C2B	-2.10	1.46	1.50
49	4	320	KC2	C1C-C2C	-2.10	1.40	1.44
49	8	314	KC2	C4A-C3A	-2.10	1.40	1.44
39	A	308	CLA	MG-NB	-2.10	2.01	2.05
39	L	309	CLA	CMD-C2D	-2.10	1.46	1.50
43	a	846	DD6	O1-C20	-2.10	1.43	1.46
39	b	837	CLA	CMC-C2C	-2.10	1.46	1.50
39	b	851	CLA	CHC-C1C	2.10	1.42	1.38
47	D	304	SQD	O4-C4	-2.10	1.38	1.43
47	4	327	SQD	O4-C4	-2.10	1.38	1.43
39	b	812	CLA	MG-NB	-2.09	2.01	2.05
49	1	312	KC2	C1C-C2C	-2.09	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Z	303	A86	O1-C20	-2.09	1.43	1.46
39	O	310	CLA	MG-NB	-2.09	2.01	2.05
39	X	317	CLA	CMD-C2D	-2.09	1.46	1.50
39	h	201	CLA	CMD-C2D	-2.09	1.46	1.50
39	b	811	CLA	CHC-C1C	2.09	1.42	1.38
39	b	825	CLA	CHC-C1C	2.09	1.42	1.38
39	b	825	CLA	CMB-C2B	-2.09	1.46	1.50
39	b	826	CLA	CMC-C2C	-2.09	1.46	1.50
48	9	304	A86	O1-C20	-2.09	1.43	1.46
39	a	821	CLA	CMB-C2B	-2.09	1.46	1.50
47	W	301	SQD	O4-C4	-2.09	1.38	1.43
47	4	327	SQD	O3-C3	-2.09	1.38	1.43
39	W	310	CLA	CMD-C2D	-2.09	1.46	1.50
49	2	317	KC2	C1B-NB	-2.09	1.35	1.37
39	B	209	CLA	CMD-C2D	-2.09	1.46	1.50
39	a	835	CLA	CMB-C2B	-2.09	1.46	1.50
39	Z	316	CLA	CHC-C1C	2.09	1.42	1.38
39	i	101	CLA	MG-NB	-2.09	2.01	2.05
49	T	314	KC2	C4A-C3A	-2.09	1.40	1.44
49	3	315	KC2	C1C-C2C	-2.09	1.40	1.44
39	D	313	CLA	CMD-C2D	-2.09	1.46	1.50
39	2	319	CLA	CMD-C2D	-2.09	1.46	1.50
49	T	314	KC2	C1C-C2C	-2.09	1.40	1.44
39	Z	309	CLA	CHC-C1C	2.09	1.42	1.38
39	a	838	CLA	MG-NB	-2.09	2.01	2.05
39	a	820	CLA	CHC-C1C	2.09	1.42	1.38
39	K	306	CLA	CHC-C1C	2.09	1.42	1.38
48	0	306	A86	O1-C20	-2.09	1.43	1.46
39	J	318	CLA	MG-NB	-2.09	2.01	2.05
49	4	318	KC2	C1C-C2C	-2.09	1.40	1.44
39	a	815	CLA	CMC-C2C	-2.09	1.46	1.50
39	2	316	CLA	MG-NB	-2.09	2.01	2.05
39	b	813	CLA	CMB-C2B	-2.09	1.46	1.50
39	J	309	CLA	MG-NB	-2.09	2.01	2.05
39	5	316	CLA	MG-NB	-2.09	2.01	2.05
39	E	313	CLA	CMB-C2B	-2.09	1.46	1.50
47	D	320	SQD	O4-C4	-2.09	1.38	1.43
39	a	804	CLA	CHC-C1C	2.09	1.42	1.38
42	m	101	BCR	C38-C26	-2.09	1.47	1.50
39	P	316	CLA	CHC-C1C	2.09	1.42	1.38
39	P	311	CLA	CMB-C2B	-2.09	1.46	1.50
39	A	306	CLA	CHC-C1C	2.09	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	k	201	CLA	CMB-C2B	-2.09	1.46	1.50
47	H	318	SQD	O4-C4	-2.09	1.38	1.43
39	K	308	CLA	MG-NB	-2.09	2.01	2.05
39	b	819	CLA	CMB-C2B	-2.09	1.46	1.50
39	G	310	CLA	CMC-C2C	-2.09	1.46	1.50
39	B	209	CLA	CHC-C1C	2.09	1.42	1.38
39	B	205	CLA	CHC-C1C	2.09	1.42	1.38
39	L	313	CLA	CMD-C2D	-2.08	1.46	1.50
39	W	319	CLA	CMB-C2B	-2.08	1.46	1.50
39	9	308	CLA	MG-NB	-2.08	2.01	2.05
39	I	308	CLA	CHC-C1C	2.08	1.42	1.38
49	M	307	KC2	C1C-C2C	-2.08	1.40	1.44
43	V	303	DD6	O1-C20	-2.08	1.43	1.46
39	1	313	CLA	CMB-C2B	-2.08	1.46	1.50
39	F	308	CLA	MG-NB	-2.08	2.01	2.05
39	J	314	CLA	MG-NB	-2.08	2.01	2.05
39	Q	317	CLA	CMB-C2B	-2.08	1.46	1.50
39	P	308	CLA	CHC-C1C	2.08	1.42	1.38
39	X	317	CLA	CHC-C1C	2.08	1.42	1.38
39	F	315	CLA	CHC-C1C	2.08	1.42	1.38
39	C	310	CLA	MG-NB	-2.08	2.01	2.05
39	Q	309	CLA	MG-NB	-2.08	2.01	2.05
39	J	316	CLA	CHC-C1C	2.08	1.42	1.38
39	B	207	CLA	MG-NB	-2.08	2.01	2.05
39	V	310	CLA	MG-NB	-2.08	2.01	2.05
51	X	313	A1ECV	C3C-C2C	2.08	1.46	1.42
39	R	315	CLA	MG-NB	-2.08	2.01	2.05
39	O	311	CLA	CMB-C2B	-2.08	1.46	1.50
43	A	302	DD6	O1-C20	-2.08	1.43	1.46
39	b	829	CLA	CMB-C2B	-2.08	1.46	1.50
39	a	808	CLA	CMB-C2B	-2.08	1.46	1.50
39	a	828	CLA	CMB-C2B	-2.08	1.46	1.50
39	R	311	CLA	CMD-C2D	-2.08	1.46	1.50
39	7	325	CLA	CMB-C2B	-2.08	1.46	1.50
49	S	317	KC2	C1C-C2C	-2.08	1.40	1.44
39	M	308	CLA	CMD-C2D	-2.08	1.46	1.50
49	F	307	KC2	C1C-C2C	-2.08	1.40	1.44
39	b	842	CLA	MG-NB	-2.08	2.01	2.05
39	C	304	CLA	CMB-C2B	-2.08	1.46	1.50
39	U	207	CLA	MG-NB	-2.08	2.01	2.05
47	T	321	SQD	O3-C3	-2.08	1.38	1.43
39	0	312	CLA	CMC-C2C	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	9	315	CLA	CMB-C2B	-2.08	1.46	1.50
48	L	305	A86	O1-C20	-2.08	1.43	1.46
39	C	306	CLA	MG-NB	-2.08	2.01	2.05
39	b	840	CLA	CMB-C2B	-2.08	1.46	1.50
47	M	301	SQD	O4-C4	-2.08	1.38	1.43
39	H	313	CLA	CMC-C2C	-2.08	1.46	1.50
39	y	309	CLA	CMD-C2D	-2.08	1.46	1.50
39	a	817	CLA	MG-NB	-2.08	2.01	2.05
39	b	851	CLA	CMD-C2D	-2.08	1.46	1.50
39	D	317	CLA	CMC-C2C	-2.08	1.46	1.50
39	M	312	CLA	CMD-C2D	-2.08	1.46	1.50
39	Y	313	CLA	CMB-C2B	-2.08	1.46	1.50
39	H	315	CLA	MG-NB	-2.08	2.01	2.05
39	I	308	CLA	MG-NB	-2.08	2.01	2.05
39	A	305	CLA	CMD-C2D	-2.07	1.46	1.50
39	Z	313	CLA	CHC-C4B	-2.07	1.34	1.39
39	E	308	CLA	MG-NB	-2.07	2.01	2.05
39	a	811	CLA	CMC-C2C	-2.07	1.46	1.50
43	z	304	DD6	O1-C20	-2.07	1.43	1.46
50	3	310	A1EB1	O1-C20	-2.07	1.43	1.46
49	L	321	KC2	C1C-C2C	-2.07	1.40	1.44
39	B	206	CLA	MG-NB	-2.07	2.01	2.05
39	E	313	CLA	MG-NB	-2.07	2.01	2.05
49	V	320	KC2	C1C-C2C	-2.07	1.40	1.44
39	D	309	CLA	MG-NB	-2.07	2.01	2.05
39	Q	311	CLA	MG-NB	-2.07	2.01	2.05
39	4	322	CLA	MG-NB	-2.07	2.01	2.05
39	J	310	CLA	CMB-C2B	-2.07	1.46	1.50
39	a	847	CLA	MG-NB	-2.07	2.01	2.05
39	Q	314	CLA	MG-NB	-2.07	2.01	2.05
39	U	208	CLA	MG-NB	-2.07	2.01	2.05
49	0	314	KC2	C1C-C2C	-2.07	1.40	1.44
51	x	310	A1ECV	C4B-C3B	2.07	1.48	1.45
43	Q	303	DD6	C36-C31	-2.07	1.32	1.34
47	P	301	SQD	O4-C4	-2.07	1.38	1.43
39	Z	306	CLA	CHC-C1C	2.07	1.42	1.38
39	k	201	CLA	MG-NB	-2.07	2.01	2.05
39	W	309	CLA	MG-NB	-2.07	2.01	2.05
49	9	313	KC2	C1D-ND	-2.07	1.35	1.37
39	l	201	CLA	CHC-C1C	2.07	1.42	1.38
47	W	301	SQD	O3-C3	-2.07	1.38	1.43
39	I	310	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	W	312	KC2	C1C-C2C	-2.07	1.40	1.44
39	T	320	CLA	MG-NB	-2.07	2.01	2.05
39	T	309	CLA	CMD-C2D	-2.07	1.46	1.50
39	1	313	CLA	CMD-C2D	-2.07	1.46	1.50
49	P	306	KC2	C1B-C2B	-2.07	1.41	1.45
39	M	321	CLA	CMB-C2B	-2.07	1.46	1.50
39	4	322	CLA	CMD-C2D	-2.07	1.46	1.50
39	a	805	CLA	MG-NB	-2.07	2.01	2.05
39	C	307	CLA	MG-NB	-2.07	2.01	2.05
39	1	309	CLA	CMD-C2D	-2.07	1.46	1.50
47	9	322	SQD	O4-C4	-2.07	1.38	1.43
39	R	307	CLA	CMD-C2D	-2.07	1.46	1.50
39	a	827	CLA	CMD-C2D	-2.07	1.46	1.50
51	T	317	A1ECV	C3C-C2C	2.07	1.46	1.42
39	x	309	CLA	MG-NB	-2.07	2.01	2.05
49	7	322	KC2	C1C-C2C	-2.07	1.40	1.44
49	y	313	KC2	C1C-C2C	-2.07	1.40	1.44
39	l	204	CLA	MG-NB	-2.07	2.01	2.05
39	4	311	CLA	CMB-C2B	-2.07	1.46	1.50
39	b	819	CLA	MG-NB	-2.07	2.01	2.05
39	6	321	CLA	MG-NB	-2.07	2.01	2.05
50	7	304	A1EB1	O1-C20	-2.07	1.43	1.46
49	P	313	KC2	C1D-ND	-2.07	1.35	1.37
39	a	828	CLA	CMD-C2D	-2.07	1.46	1.50
39	A	308	CLA	CMD-C2D	-2.07	1.46	1.50
39	E	306	CLA	CMD-C2D	-2.07	1.46	1.50
39	K	306	CLA	CMB-C2B	-2.07	1.46	1.50
39	T	320	CLA	CMB-C2B	-2.07	1.46	1.50
39	5	306	CLA	CMD-C2D	-2.07	1.46	1.50
49	H	311	KC2	C1C-C2C	-2.07	1.40	1.44
43	Z	302	DD6	C21-C20	-2.07	1.48	1.51
39	A	312	CLA	MG-NB	-2.07	2.01	2.05
39	D	311	CLA	CMD-C2D	-2.07	1.46	1.50
39	l	205	CLA	MG-NB	-2.06	2.01	2.05
39	S	310	CLA	CHC-C1C	2.06	1.42	1.38
49	4	324	KC2	C1C-C2C	-2.06	1.40	1.44
39	a	824	CLA	MG-NB	-2.06	2.01	2.05
39	H	316	CLA	CMB-C2B	-2.06	1.46	1.50
49	P	310	KC2	C1C-C2C	-2.06	1.40	1.44
39	7	316	CLA	MG-NB	-2.06	2.01	2.05
39	b	820	CLA	CHC-C1C	2.06	1.42	1.38
39	i	103	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Q	312	CLA	CMC-C2C	-2.06	1.46	1.50
39	b	816	CLA	MG-NB	-2.06	2.01	2.05
39	1	309	CLA	CMB-C2B	-2.06	1.46	1.50
39	a	827	CLA	CMC-C2C	-2.06	1.46	1.50
39	0	310	CLA	CMD-C2D	-2.06	1.46	1.50
49	R	318	KC2	C1C-C2C	-2.06	1.40	1.44
39	J	313	CLA	CMD-C2D	-2.06	1.46	1.50
39	z	306	CLA	MG-NB	-2.06	2.01	2.05
39	C	308	CLA	CMD-C2D	-2.06	1.46	1.50
39	L	313	CLA	MG-NB	-2.06	2.01	2.05
39	V	309	CLA	MG-NB	-2.06	2.01	2.05
39	W	316	CLA	MG-NB	-2.06	2.01	2.05
49	0	316	KC2	C1C-C2C	-2.06	1.40	1.44
39	A	311	CLA	MG-NB	-2.06	2.01	2.05
39	D	312	CLA	MG-NB	-2.06	2.01	2.05
39	E	315	CLA	CMB-C2B	-2.06	1.46	1.50
39	R	308	CLA	MG-NB	-2.06	2.01	2.05
49	L	321	KC2	C1B-NB	-2.06	1.35	1.37
39	4	311	CLA	MG-NB	-2.06	2.01	2.05
48	Q	305	A86	O1-C20	-2.06	1.43	1.46
49	9	313	KC2	C1B-NB	-2.06	1.35	1.37
39	0	310	CLA	CMB-C2B	-2.06	1.46	1.50
39	y	308	CLA	CMD-C2D	-2.06	1.46	1.50
39	b	815	CLA	MG-NB	-2.06	2.01	2.05
39	S	313	CLA	MG-NB	-2.06	2.01	2.05
39	b	818	CLA	CMC-C2C	-2.06	1.46	1.50
39	S	308	CLA	CMD-C2D	-2.06	1.46	1.50
39	V	319	CLA	CMD-C2D	-2.06	1.46	1.50
39	6	312	CLA	MG-NB	-2.06	2.01	2.05
39	a	832	CLA	MG-NB	-2.06	2.01	2.05
39	a	835	CLA	MG-NB	-2.06	2.01	2.05
39	F	316	CLA	MG-NB	-2.06	2.01	2.05
39	L	309	CLA	MG-NB	-2.06	2.01	2.05
43	O	304	DD6	O1-C20	-2.06	1.43	1.46
39	Q	311	CLA	CMD-C2D	-2.05	1.46	1.50
39	Y	313	CLA	MG-NB	-2.05	2.01	2.05
39	J	310	CLA	MG-NB	-2.05	2.01	2.05
39	D	314	CLA	CHC-C1C	2.05	1.42	1.38
43	E	303	DD6	O1-C20	-2.05	1.43	1.46
39	3	316	CLA	MG-NB	-2.05	2.01	2.05
47	S	301	SQD	O4-C4	-2.05	1.38	1.43
50	8	301	A1EB1	C32-C31	-2.05	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	k	202	CLA	MG-NB	-2.05	2.01	2.05
49	V	315	KC2	C1B-NB	-2.05	1.35	1.37
43	J	306	DD6	O1-C20	-2.05	1.43	1.46
43	I	306	DD6	O1-C20	-2.05	1.43	1.46
39	U	210	CLA	CMB-C2B	-2.05	1.46	1.50
39	6	315	CLA	CMD-C2D	-2.05	1.46	1.50
47	F	318	SQD	O3-C3	-2.05	1.38	1.43
39	P	308	CLA	MG-NB	-2.05	2.01	2.05
39	1	308	CLA	MG-NB	-2.05	2.01	2.05
39	a	804	CLA	CMD-C2D	-2.05	1.46	1.50
39	l	201	CLA	MG-NB	-2.05	2.01	2.05
39	K	307	CLA	CMD-C2D	-2.05	1.46	1.50
39	7	316	CLA	CMD-C2D	-2.05	1.46	1.50
39	8	315	CLA	CMD-C2D	-2.05	1.46	1.50
39	T	318	CLA	CHC-C1C	2.05	1.42	1.38
47	7	302	SQD	O3-C3	-2.05	1.38	1.43
43	2	303	DD6	C21-C20	-2.05	1.48	1.51
47	F	319	SQD	O3-C3	-2.05	1.38	1.43
39	a	814	CLA	CMC-C2C	-2.05	1.46	1.50
39	b	815	CLA	CMC-C2C	-2.05	1.46	1.50
39	a	807	CLA	MG-NB	-2.05	2.01	2.05
39	E	314	CLA	CMC-C2C	-2.05	1.46	1.50
39	G	314	CLA	CMD-C2D	-2.05	1.46	1.50
48	k	206	A86	O1-C20	-2.05	1.43	1.46
39	B	207	CLA	CMB-C2B	-2.05	1.46	1.50
39	U	213	CLA	CMD-C2D	-2.05	1.46	1.50
39	5	316	CLA	CMD-C2D	-2.05	1.46	1.50
51	S	318	A1ECV	C1D-ND	2.05	1.37	1.35
39	H	310	CLA	MG-NB	-2.05	2.01	2.05
39	a	824	CLA	CMB-C2B	-2.05	1.46	1.50
39	a	847	CLA	CMD-C2D	-2.05	1.46	1.50
49	V	312	KC2	C1C-C2C	-2.05	1.40	1.44
39	b	835	CLA	CMD-C2D	-2.05	1.46	1.50
39	b	842	CLA	CMD-C2D	-2.05	1.46	1.50
39	F	308	CLA	CMB-C2B	-2.05	1.46	1.50
39	3	316	CLA	CMD-C2D	-2.05	1.46	1.50
39	Z	307	CLA	CMD-C2D	-2.05	1.46	1.50
39	V	313	CLA	CHC-C1C	2.05	1.42	1.38
39	a	817	CLA	CMB-C2B	-2.05	1.46	1.50
47	D	304	SQD	O3-C3	-2.05	1.38	1.43
39	a	803	CLA	MG-NB	-2.05	2.01	2.05
39	M	317	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	H	318	SQD	O3-C3	-2.05	1.38	1.43
39	4	323	CLA	CMB-C2B	-2.05	1.46	1.50
39	S	320	CLA	MG-NB	-2.05	2.01	2.05
49	P	313	KC2	C1B-NB	-2.05	1.35	1.37
47	9	322	SQD	O3-C3	-2.05	1.38	1.43
39	9	312	CLA	CMB-C2B	-2.05	1.46	1.50
39	b	833	CLA	MG-NB	-2.05	2.01	2.05
39	E	310	CLA	CMD-C2D	-2.05	1.46	1.50
39	B	204	CLA	MG-NB	-2.05	2.01	2.05
39	H	309	CLA	MG-NB	-2.05	2.01	2.05
39	U	210	CLA	MG-NB	-2.05	2.01	2.05
39	7	315	CLA	MG-NB	-2.05	2.01	2.05
49	1	315	KC2	C1C-C2C	-2.05	1.40	1.44
39	a	806	CLA	CMD-C2D	-2.05	1.46	1.50
39	S	319	CLA	CMD-C2D	-2.04	1.46	1.50
39	H	312	CLA	CHC-C1C	2.04	1.42	1.38
49	5	313	KC2	C1C-C2C	-2.04	1.40	1.44
39	a	809	CLA	CMD-C2D	-2.04	1.46	1.50
47	M	301	SQD	O3-C3	-2.04	1.38	1.43
49	K	313	KC2	C1C-C2C	-2.04	1.40	1.44
51	E	311	A1ECV	C3C-C2C	2.04	1.46	1.42
39	1	310	CLA	MG-NB	-2.04	2.01	2.05
39	E	309	CLA	CMB-C2B	-2.04	1.46	1.50
39	S	320	CLA	CMB-C2B	-2.04	1.46	1.50
39	U	210	CLA	CMD-C2D	-2.04	1.46	1.50
39	0	322	CLA	CMD-C2D	-2.04	1.46	1.50
39	O	314	CLA	MG-NB	-2.04	2.01	2.05
39	9	312	CLA	CMD-C2D	-2.04	1.46	1.50
39	M	308	CLA	MG-NB	-2.04	2.01	2.05
39	V	311	CLA	MG-NB	-2.04	2.01	2.05
39	Y	303	CLA	MG-NB	-2.04	2.01	2.05
43	y	303	DD6	O1-C20	-2.04	1.43	1.46
49	L	317	KC2	C1C-C2C	-2.04	1.40	1.44
39	7	313	CLA	MG-NB	-2.04	2.01	2.05
39	a	814	CLA	CMD-C2D	-2.04	1.46	1.50
39	T	320	CLA	CHC-C1C	2.04	1.42	1.38
39	F	309	CLA	MG-NB	-2.04	2.01	2.05
39	Z	304	CLA	MG-NB	-2.04	2.01	2.05
39	R	316	CLA	MG-NB	-2.04	2.01	2.05
39	k	201	CLA	CMD-C2D	-2.04	1.46	1.50
39	1	311	CLA	CMD-C2D	-2.04	1.46	1.50
39	L	308	CLA	CHC-C1C	2.04	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	a	820	CLA	MG-NB	-2.04	2.01	2.05
39	U	211	CLA	MG-NB	-2.04	2.01	2.05
47	E	320	SQD	O3-C3	-2.04	1.38	1.43
46	7	326	LMG	O7-C8	-2.04	1.41	1.46
39	b	826	CLA	CMB-C2B	-2.04	1.46	1.50
47	F	318	SQD	O4-C4	-2.04	1.38	1.43
39	a	818	CLA	CMD-C2D	-2.04	1.46	1.50
39	Q	311	CLA	CMC-C2C	-2.04	1.46	1.50
39	9	310	CLA	MG-NB	-2.04	2.01	2.05
39	O	312	CLA	CMD-C2D	-2.04	1.46	1.50
39	Q	321	CLA	CMC-C2C	-2.04	1.46	1.50
39	a	827	CLA	C1B-NB	-2.04	1.35	1.37
39	b	822	CLA	CMB-C2B	-2.04	1.46	1.50
39	b	832	CLA	CMD-C2D	-2.04	1.46	1.50
39	a	806	CLA	MG-NB	-2.04	2.01	2.05
39	P	309	CLA	MG-NB	-2.04	2.01	2.05
48	8	305	A86	O1-C20	-2.04	1.43	1.46
39	D	314	CLA	CMD-C2D	-2.04	1.46	1.50
39	T	310	CLA	CMD-C2D	-2.04	1.46	1.50
49	Z	310	KC2	C1C-C2C	-2.04	1.40	1.44
43	x	303	DD6	O1-C20	-2.04	1.43	1.46
47	F	319	SQD	O4-C4	-2.04	1.38	1.43
39	0	322	CLA	CMB-C2B	-2.04	1.46	1.50
51	Q	316	A1ECV	C4B-C3B	2.04	1.48	1.45
49	6	314	KC2	C1C-C2C	-2.04	1.40	1.44
39	a	812	CLA	MG-NB	-2.04	2.01	2.05
39	L	316	CLA	MG-NB	-2.04	2.01	2.05
39	V	310	CLA	CMD-C2D	-2.04	1.46	1.50
39	7	315	CLA	CMD-C2D	-2.04	1.46	1.50
39	a	805	CLA	CHC-C1C	2.04	1.42	1.38
39	B	203	CLA	MG-NB	-2.04	2.01	2.05
39	T	311	CLA	MG-NB	-2.04	2.01	2.05
39	o	205	CLA	CHC-C1C	2.04	1.42	1.38
39	C	304	CLA	MG-NB	-2.04	2.01	2.05
39	E	309	CLA	MG-NB	-2.04	2.01	2.05
39	8	311	CLA	MG-NB	-2.03	2.01	2.05
39	Y	302	CLA	MG-NB	-2.03	2.01	2.05
39	b	808	CLA	CMD-C2D	-2.03	1.46	1.50
39	4	323	CLA	MG-NB	-2.03	2.01	2.05
39	5	307	CLA	MG-NB	-2.03	2.01	2.05
39	b	803	CLA	CMD-C2D	-2.03	1.46	1.50
50	6	308	A1EB1	O1-C20	-2.03	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	a	822	CLA	MG-NB	-2.03	2.01	2.05
39	W	310	CLA	MG-NB	-2.03	2.01	2.05
39	x	307	CLA	CMD-C2D	-2.03	1.46	1.50
39	W	311	CLA	MG-NB	-2.03	2.01	2.05
39	8	322	CLA	MG-NB	-2.03	2.01	2.05
39	j	101	CLA	CMD-C2D	-2.03	1.46	1.50
39	K	312	CLA	CMD-C2D	-2.03	1.46	1.50
39	9	315	CLA	MG-NB	-2.03	2.01	2.05
39	Z	306	CLA	MG-NB	-2.03	2.01	2.05
39	b	837	CLA	CMD-C2D	-2.03	1.46	1.50
39	0	323	CLA	CMD-C2D	-2.03	1.46	1.50
39	6	321	CLA	CMB-C2B	-2.03	1.46	1.50
49	y	316	KC2	C1C-C2C	-2.03	1.40	1.44
39	f	802	CLA	MG-NB	-2.03	2.01	2.05
39	4	312	CLA	MG-NB	-2.03	2.01	2.05
39	D	312	CLA	CMD-C2D	-2.03	1.46	1.50
39	E	315	CLA	CMD-C2D	-2.03	1.46	1.50
49	P	320	KC2	C1C-C2C	-2.03	1.40	1.44
39	E	316	CLA	MG-NB	-2.03	2.01	2.05
39	z	318	CLA	MG-NB	-2.03	2.01	2.05
39	a	807	CLA	CMB-C2B	-2.03	1.46	1.50
39	4	312	CLA	CMD-C2D	-2.03	1.46	1.50
39	o	202	CLA	MG-NB	-2.03	2.01	2.05
47	D	321	SQD	O4-C4	-2.03	1.38	1.43
39	a	811	CLA	MG-NB	-2.03	2.01	2.05
39	8	313	CLA	MG-NB	-2.03	2.01	2.05
43	G	303	DD6	O1-C20	-2.03	1.43	1.46
39	b	814	CLA	CMD-C2D	-2.03	1.46	1.50
49	5	314	KC2	C1C-C2C	-2.03	1.40	1.44
51	Z	314	A1ECV	C1D-ND	2.03	1.37	1.35
39	D	309	CLA	CHC-C1C	2.03	1.42	1.38
47	D	321	SQD	O3-C3	-2.03	1.38	1.43
39	L	310	CLA	MG-NB	-2.03	2.01	2.05
39	M	318	CLA	MG-NB	-2.03	2.01	2.05
39	6	315	CLA	MG-NB	-2.03	2.01	2.05
47	k	205	SQD	O3-C3	-2.03	1.38	1.43
39	6	313	CLA	CHC-C1C	2.03	1.42	1.38
39	b	833	CLA	CMB-C2B	-2.03	1.46	1.50
39	I	314	CLA	CMC-C2C	-2.03	1.46	1.50
39	V	316	CLA	MG-NB	-2.03	2.01	2.05
39	M	310	CLA	MG-NB	-2.03	2.01	2.05
39	Z	305	CLA	MG-NB	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	W	313	CLA	CMD-C2D	-2.03	1.46	1.50
39	4	314	CLA	CMD-C2D	-2.03	1.46	1.50
49	B	208	KC2	C1C-C2C	-2.03	1.40	1.44
39	b	839	CLA	CMB-C2B	-2.03	1.46	1.50
39	3	312	CLA	CMD-C2D	-2.03	1.46	1.50
51	O	315	A1ECV	C1D-ND	2.03	1.37	1.35
39	4	314	CLA	MG-NB	-2.03	2.01	2.05
39	C	306	CLA	CMD-C2D	-2.03	1.46	1.50
39	I	310	CLA	CMD-C2D	-2.03	1.46	1.50
50	V	305	A1EB1	O1-C20	-2.03	1.43	1.46
39	a	823	CLA	MG-NB	-2.03	2.01	2.05
39	E	318	CLA	MG-NB	-2.03	2.01	2.05
39	6	318	CLA	MG-NB	-2.03	2.01	2.05
49	R	314	KC2	C1C-C2C	-2.03	1.40	1.44
39	D	310	CLA	CHC-C1C	2.03	1.42	1.38
39	W	318	CLA	MG-NB	-2.03	2.01	2.05
39	9	309	CLA	CMD-C2D	-2.03	1.46	1.50
39	G	310	CLA	MG-NB	-2.03	2.01	2.05
39	a	837	CLA	CMB-C2B	-2.03	1.46	1.50
39	o	205	CLA	CMD-C2D	-2.03	1.46	1.50
39	T	310	CLA	CMC-C2C	-2.03	1.46	1.50
49	X	318	KC2	C4A-C3A	-2.03	1.40	1.44
42	m	101	BCR	C33-C5	-2.03	1.47	1.50
39	H	308	CLA	MG-NB	-2.03	2.01	2.05
49	X	314	KC2	C1C-C2C	-2.03	1.40	1.44
39	a	834	CLA	CMD-C2D	-2.03	1.46	1.50
39	2	308	CLA	CMD-C2D	-2.03	1.46	1.50
47	P	301	SQD	O3-C3	-2.03	1.38	1.43
39	a	833	CLA	CMB-C2B	-2.02	1.46	1.50
39	F	313	CLA	CMB-C2B	-2.02	1.46	1.50
39	R	307	CLA	MG-NB	-2.02	2.01	2.05
49	2	314	KC2	C1C-C2C	-2.02	1.40	1.44
43	3	304	DD6	O1-C20	-2.02	1.43	1.46
49	1	312	KC2	C1B-NB	-2.02	1.35	1.37
39	a	819	CLA	MG-NB	-2.02	2.01	2.05
39	Z	307	CLA	MG-NB	-2.02	2.01	2.05
39	l	201	CLA	CMB-C2B	-2.02	1.46	1.50
39	A	312	CLA	CMC-C2C	-2.02	1.46	1.50
39	8	321	CLA	MG-NB	-2.02	2.01	2.05
39	O	312	CLA	MG-NB	-2.02	2.01	2.05
39	a	802	CLA	CMD-C2D	-2.02	1.46	1.50
39	k	202	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	T	310	CLA	MG-NB	-2.02	2.01	2.05
39	5	308	CLA	MG-NB	-2.02	2.01	2.05
39	O	318	CLA	MG-NB	-2.02	2.01	2.05
39	y	312	CLA	MG-NB	-2.02	2.01	2.05
39	Q	309	CLA	CMB-C2B	-2.02	1.46	1.50
39	W	316	CLA	CMD-C2D	-2.02	1.46	1.50
39	a	808	CLA	MG-NB	-2.02	2.01	2.05
39	z	314	CLA	MG-NB	-2.02	2.01	2.05
39	o	201	CLA	CMB-C2B	-2.02	1.46	1.50
39	S	313	CLA	CMD-C2D	-2.02	1.46	1.50
39	U	209	CLA	CMD-C2D	-2.02	1.46	1.50
39	V	309	CLA	CMB-C2B	-2.02	1.46	1.50
39	V	311	CLA	CMD-C2D	-2.02	1.46	1.50
39	3	322	CLA	CMD-C2D	-2.02	1.46	1.50
51	y	317	A1ECV	C4B-C3B	2.02	1.48	1.45
39	x	314	CLA	MG-NB	-2.02	2.01	2.05
39	S	313	CLA	CMC-C2C	-2.02	1.46	1.50
39	y	309	CLA	CHC-C1C	2.02	1.42	1.38
39	1	319	CLA	MG-NB	-2.02	2.01	2.05
39	H	306	CLA	CMD-C2D	-2.02	1.46	1.50
39	I	311	CLA	CMC-C2C	-2.02	1.46	1.50
39	b	802	CLA	CMD-C2D	-2.02	1.46	1.50
39	T	308	CLA	CMC-C2C	-2.02	1.46	1.50
39	o	201	CLA	MG-NB	-2.02	2.01	2.05
39	L	311	CLA	MG-NB	-2.02	2.01	2.05
39	a	821	CLA	CMC-C2C	-2.02	1.46	1.50
39	0	311	CLA	CMC-C2C	-2.02	1.46	1.50
39	I	301	CLA	CMB-C2B	-2.02	1.46	1.50
41	X	301	LHG	O7-C5	-2.02	1.41	1.46
39	b	828	CLA	CMD-C2D	-2.02	1.46	1.50
47	D	320	SQD	O3-C3	-2.02	1.38	1.43
39	R	316	CLA	CMD-C2D	-2.02	1.46	1.50
39	S	310	CLA	MG-NB	-2.02	2.01	2.05
47	E	320	SQD	O4-C4	-2.02	1.38	1.43
48	I	304	A86	O1-C20	-2.02	1.43	1.46
39	A	306	CLA	CMD-C2D	-2.02	1.46	1.50
39	P	314	CLA	CMD-C2D	-2.02	1.46	1.50
39	x	308	CLA	CMD-C2D	-2.02	1.46	1.50
39	b	811	CLA	MG-NB	-2.02	2.01	2.05
39	E	312	CLA	MG-NB	-2.02	2.01	2.05
39	9	309	CLA	MG-NB	-2.02	2.01	2.05
39	F	321	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	6	312	CLA	CMD-C2D	-2.02	1.46	1.50
39	b	825	CLA	MG-NB	-2.02	2.01	2.05
39	3	311	CLA	MG-NB	-2.02	2.01	2.05
39	O	310	CLA	CMD-C2D	-2.02	1.46	1.50
39	b	805	CLA	CMD-C2D	-2.02	1.46	1.50
39	A	309	CLA	CMD-C2D	-2.02	1.46	1.50
39	Q	314	CLA	CMB-C2B	-2.02	1.46	1.50
49	V	315	KC2	C1C-C2C	-2.02	1.40	1.44
39	a	803	CLA	CHC-C1C	2.02	1.42	1.38
39	A	307	CLA	MG-NB	-2.02	2.01	2.05
39	U	209	CLA	MG-NB	-2.02	2.01	2.05
39	K	306	CLA	MG-NB	-2.02	2.01	2.05
39	Z	313	CLA	MG-NB	-2.02	2.01	2.05
49	0	317	KC2	C1B-NB	-2.02	1.35	1.37
39	b	820	CLA	CMD-C2D	-2.02	1.46	1.50
39	D	317	CLA	CMD-C2D	-2.02	1.46	1.50
39	K	308	CLA	CMD-C2D	-2.02	1.46	1.50
49	z	315	KC2	C1C-C2C	-2.02	1.40	1.44
39	F	313	CLA	MG-NB	-2.02	2.01	2.05
39	7	318	CLA	CMC-C2C	-2.01	1.46	1.50
39	y	307	CLA	CMD-C2D	-2.01	1.46	1.50
48	B	201	A86	O1-C20	-2.01	1.43	1.46
39	M	312	CLA	MG-NB	-2.01	2.01	2.05
39	a	831	CLA	CMD-C2D	-2.01	1.46	1.50
39	b	839	CLA	CMC-C2C	-2.01	1.46	1.50
39	G	310	CLA	CMD-C2D	-2.01	1.46	1.50
39	4	323	CLA	CMD-C2D	-2.01	1.46	1.50
39	9	310	CLA	CMC-C2C	-2.01	1.46	1.50
39	2	315	CLA	CMC-C2C	-2.01	1.46	1.50
41	j	104	LHG	P-O6	2.01	1.67	1.59
51	2	311	A1ECV	C3C-C2C	2.01	1.46	1.42
49	8	319	KC2	C1C-C2C	-2.01	1.40	1.44
39	G	310	CLA	CMB-C2B	-2.01	1.46	1.50
39	K	306	CLA	CMD-C2D	-2.01	1.46	1.50
39	2	319	CLA	CHC-C1C	2.01	1.42	1.38
39	J	317	CLA	MG-NB	-2.01	2.01	2.05
39	i	103	CLA	CMD-C2D	-2.01	1.46	1.50
43	I	307	DD6	O1-C20	-2.01	1.43	1.46
39	Z	315	CLA	MG-NB	-2.01	2.01	2.05
39	a	836	CLA	MG-NB	-2.01	2.01	2.05
39	b	812	CLA	CMD-C2D	-2.01	1.46	1.50
39	J	317	CLA	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	6	319	KC2	C1D-ND	-2.01	1.35	1.37
39	3	322	CLA	MG-NB	-2.01	2.01	2.05
39	a	815	CLA	CMB-C2B	-2.01	1.46	1.50
39	R	311	CLA	CMC-C2C	-2.01	1.46	1.50
49	x	312	KC2	C1C-C2C	-2.01	1.40	1.44
39	4	316	CLA	MG-NB	-2.01	2.01	2.05
39	z	311	CLA	MG-NB	-2.01	2.01	2.05
39	L	309	CLA	CMB-C2B	-2.01	1.46	1.50
39	L	311	CLA	CMD-C2D	-2.01	1.46	1.50
39	Y	307	CLA	CMB-C2B	-2.01	1.46	1.50
39	E	306	CLA	CMB-C2B	-2.01	1.46	1.50
39	1	319	CLA	CMB-C2B	-2.01	1.46	1.50
39	2	310	CLA	MG-NB	-2.01	2.01	2.05
39	a	821	CLA	CHC-C1C	2.01	1.42	1.38
39	a	805	CLA	CMD-C2D	-2.01	1.46	1.50
39	J	311	CLA	CMD-C2D	-2.01	1.46	1.50
39	O	309	CLA	CMC-C2C	-2.01	1.46	1.50
39	W	310	CLA	CMB-C2B	-2.01	1.46	1.50
39	4	313	CLA	CMB-C2B	-2.01	1.46	1.50
39	U	215	CLA	MG-NB	-2.01	2.01	2.05
39	C	307	CLA	CMD-C2D	-2.01	1.46	1.50
39	U	214	CLA	CMD-C2D	-2.01	1.46	1.50
39	a	823	CLA	CMD-C2D	-2.01	1.46	1.50
39	E	314	CLA	CMB-C2B	-2.01	1.46	1.50
39	P	314	CLA	CMC-C2C	-2.01	1.46	1.50
49	Q	318	KC2	C1C-C2C	-2.01	1.40	1.44
39	K	307	CLA	MG-NB	-2.01	2.01	2.05
39	K	312	CLA	MG-NB	-2.01	2.01	2.05
39	5	306	CLA	MG-NB	-2.01	2.01	2.05
39	b	811	CLA	CMB-C2B	-2.01	1.46	1.50
39	B	204	CLA	CMD-C2D	-2.01	1.46	1.50
39	J	307	CLA	CMD-C2D	-2.01	1.46	1.50
39	U	201	CLA	CMB-C2B	-2.01	1.46	1.50
39	U	212	CLA	CMB-C2B	-2.01	1.46	1.50
39	W	309	CLA	CMB-C2B	-2.01	1.46	1.50
39	3	311	CLA	CMB-C2B	-2.01	1.46	1.50
39	y	315	CLA	CMD-C2D	-2.01	1.46	1.50
39	8	315	CLA	MG-NB	-2.01	2.01	2.05
49	W	308	KC2	C1C-C2C	-2.01	1.40	1.44
39	M	321	CLA	CHC-C1C	2.01	1.42	1.38
39	Z	304	CLA	CMD-C2D	-2.01	1.46	1.50
39	U	201	CLA	MG-ND	-2.01	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	4	319	CLA	MG-NB	-2.01	2.01	2.05
39	a	810	CLA	CMB-C2B	-2.01	1.46	1.50
39	b	807	CLA	CMD-C2D	-2.01	1.46	1.50
39	D	315	CLA	CMB-C2B	-2.01	1.46	1.50
39	V	319	CLA	CMB-C2B	-2.01	1.46	1.50
39	X	308	CLA	CMB-C2B	-2.01	1.46	1.50
39	C	308	CLA	MG-NB	-2.01	2.01	2.05
39	z	308	CLA	MG-NB	-2.01	2.01	2.05
39	a	804	CLA	CMB-C2B	-2.01	1.46	1.50
39	a	810	CLA	CMD-C2D	-2.01	1.46	1.50
39	H	312	CLA	CMB-C2B	-2.01	1.46	1.50
39	M	310	CLA	CMD-C2D	-2.01	1.46	1.50
39	a	838	CLA	CHC-C1C	2.01	1.42	1.38
49	O	317	KC2	C1B-NB	-2.01	1.35	1.37
39	2	308	CLA	CMB-C2B	-2.01	1.46	1.50
39	y	308	CLA	MG-NB	-2.01	2.01	2.05
39	a	812	CLA	CMB-C2B	-2.01	1.46	1.50
39	1	319	CLA	CMD-C2D	-2.01	1.46	1.50
39	2	309	CLA	CMB-C2B	-2.01	1.46	1.50
39	D	311	CLA	MG-NB	-2.01	2.01	2.05
39	I	313	CLA	MG-NB	-2.01	2.01	2.05
49	R	306	KC2	C1C-C2C	-2.01	1.40	1.44
39	a	803	CLA	CMC-C2C	-2.01	1.46	1.50
39	O	313	CLA	MG-NB	-2.01	2.01	2.05
39	I	314	CLA	MG-NB	-2.01	2.01	2.05
39	F	306	CLA	CMC-C2C	-2.01	1.46	1.50
39	P	308	CLA	CMD-C2D	-2.01	1.46	1.50
39	4	311	CLA	CMD-C2D	-2.01	1.46	1.50
50	F	304	A1EB1	O1-C20	-2.01	1.43	1.46
39	0	322	CLA	MG-NB	-2.01	2.01	2.05
39	8	312	CLA	MG-NB	-2.01	2.01	2.05
39	T	313	CLA	CMB-C2B	-2.01	1.46	1.50
39	M	315	CLA	MG-NB	-2.01	2.01	2.05
39	6	310	CLA	MG-NB	-2.01	2.01	2.05
39	3	314	CLA	MG-NB	-2.00	2.01	2.05
39	0	322	CLA	CMC-C2C	-2.00	1.46	1.50
49	X	315	KC2	C1C-C2C	-2.00	1.40	1.44
49	8	316	KC2	C1C-C2C	-2.00	1.40	1.44
46	W	320	LMG	O7-C8	-2.00	1.41	1.46
39	k	202	CLA	CMB-C2B	-2.00	1.46	1.50
51	6	320	A1ECV	C4B-C3B	2.00	1.48	1.45
39	8	311	CLA	CHC-C1C	2.00	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	E	307	CLA	CMD-C2D	-2.00	1.46	1.50
39	E	318	CLA	CMD-C2D	-2.00	1.46	1.50
39	J	316	CLA	CMD-C2D	-2.00	1.46	1.50
39	M	309	CLA	CMD-C2D	-2.00	1.46	1.50
39	4	316	CLA	CMC-C2C	-2.00	1.46	1.50
39	X	309	CLA	CMD-C2D	-2.00	1.46	1.50
39	6	318	CLA	CMD-C2D	-2.00	1.46	1.50
50	8	308	A1EB1	O1-C20	-2.00	1.43	1.46
39	3	323	CLA	MG-NB	-2.00	2.01	2.05
51	V	317	A1ECV	C3C-C2C	2.00	1.46	1.42
39	k	203	CLA	CMB-C2B	-2.00	1.46	1.50
39	E	312	CLA	CMD-C2D	-2.00	1.46	1.50
39	J	312	CLA	CMD-C2D	-2.00	1.46	1.50
39	S	320	CLA	CMD-C2D	-2.00	1.46	1.50
39	U	214	CLA	CMB-C2B	-2.00	1.46	1.50
39	0	313	CLA	CMC-C2C	-2.00	1.46	1.50
39	J	312	CLA	MG-NB	-2.00	2.01	2.05
49	9	311	KC2	C1C-C2C	-2.00	1.40	1.44
39	a	820	CLA	CMB-C2B	-2.00	1.46	1.50
39	E	316	CLA	CMB-C2B	-2.00	1.46	1.50
39	U	208	CLA	CMD-C2D	-2.00	1.46	1.50
39	b	851	CLA	MG-NB	-2.00	2.01	2.05
39	P	316	CLA	MG-NB	-2.00	2.01	2.05
43	E	305	DD6	O1-C20	-2.00	1.43	1.46
50	7	305	A1EB1	O1-C20	-2.00	1.43	1.46
39	f	803	CLA	CMD-C2D	-2.00	1.46	1.50
39	7	313	CLA	CMB-C2B	-2.00	1.46	1.50
39	2	307	CLA	CMD-C2D	-2.00	1.46	1.50
39	2	312	CLA	CMB-C2B	-2.00	1.46	1.50
39	7	314	CLA	MG-NB	-2.00	2.01	2.05
39	h	201	CLA	MG-NB	-2.00	2.01	2.05
39	y	307	CLA	MG-NB	-2.00	2.01	2.05
49	z	313	KC2	C3D-C4D	2.00	1.42	1.38
39	a	830	CLA	CMB-C2B	-2.00	1.46	1.50
39	A	312	CLA	CMD-C2D	-2.00	1.46	1.50
39	H	316	CLA	CMD-C2D	-2.00	1.46	1.50
39	U	208	CLA	CMB-C2B	-2.00	1.46	1.50
39	I	314	CLA	CMD-C2D	-2.00	1.46	1.50
48	3	306	A86	O1-C20	-2.00	1.43	1.46
39	o	203	CLA	CMD-C2D	-2.00	1.46	1.50
39	E	319	CLA	CMB-C2B	-2.00	1.46	1.50
39	T	319	CLA	CMB-C2B	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	321	CLA	MG-NB	-2.00	2.01	2.05
39	0	311	CLA	CHC-C1C	2.00	1.42	1.38
50	O	301	A1EB1	O1-C20	-2.00	1.43	1.46
49	9	316	KC2	C1C-C2C	-2.00	1.40	1.44
49	6	319	KC2	C1C-C2C	-2.00	1.40	1.44
39	a	824	CLA	CMD-C2D	-2.00	1.46	1.50
39	D	316	CLA	CMD-C2D	-2.00	1.46	1.50
39	z	309	CLA	CMD-C2D	-2.00	1.46	1.50

All (9304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	303	DD6	O1-C20-C21	17.30	135.78	115.06
43	Z	302	DD6	O1-C20-C21	17.29	135.77	115.06
43	F	305	DD6	O1-C20-C21	13.19	130.87	115.06
43	D	303	DD6	O1-C20-C21	12.88	130.49	115.06
52	M	322	A1EB4	O1-C20-C21	12.53	130.07	115.06
52	P	319	A1EB4	O1-C20-C21	12.50	130.04	115.06
43	3	304	DD6	O1-C20-C19	-12.37	104.09	113.38
51	E	311	A1ECV	O2D-CGD-CBD	11.00	124.93	111.00
51	9	314	A1ECV	C1D-C2D-C3D	-10.99	98.21	108.46
43	Z	302	DD6	O1-C20-C19	-10.94	105.17	113.38
43	2	303	DD6	O1-C20-C19	-10.89	105.20	113.38
51	7	323	A1ECV	C1D-C2D-C3D	-10.80	98.38	108.46
51	X	313	A1ECV	C1D-C2D-C3D	-10.77	98.41	108.46
51	E	311	A1ECV	C1D-C2D-C3D	-10.75	98.42	108.46
51	P	315	A1ECV	C1D-C2D-C3D	-10.73	98.45	108.46
51	O	315	A1ECV	C1D-C2D-C3D	-10.72	98.46	108.46
51	Y	312	A1ECV	C1D-C2D-C3D	-10.69	98.48	108.46
51	z	310	A1ECV	C1D-C2D-C3D	-10.69	98.48	108.46
51	Z	314	A1ECV	C1D-C2D-C3D	-10.67	98.51	108.46
51	Y	306	A1ECV	C1D-C2D-C3D	-10.65	98.52	108.46
51	Z	308	A1ECV	C1D-C2D-C3D	-10.64	98.53	108.46
51	1	318	A1ECV	C1D-C2D-C3D	-10.61	98.56	108.46
51	y	311	A1ECV	C1D-C2D-C3D	-10.59	98.58	108.46
51	R	313	A1ECV	C1D-C2D-C3D	-10.58	98.58	108.46
51	G	316	A1ECV	C1D-C2D-C3D	-10.55	98.61	108.46
51	L	318	A1ECV	C1D-C2D-C3D	-10.55	98.62	108.46
51	z	316	A1ECV	C1D-C2D-C3D	-10.53	98.63	108.46
51	x	316	A1ECV	C1D-C2D-C3D	-10.51	98.65	108.46
51	M	316	A1ECV	C1D-C2D-C3D	-10.51	98.65	108.46
51	2	311	A1ECV	C1D-C2D-C3D	-10.51	98.65	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	x	310	A1ECV	C1D-C2D-C3D	-10.48	98.68	108.46
51	5	309	A1ECV	C1D-C2D-C3D	-10.46	98.70	108.46
51	y	317	A1ECV	C1D-C2D-C3D	-10.46	98.70	108.46
51	S	312	A1ECV	C1D-C2D-C3D	-10.46	98.70	108.46
43	A	303	DD6	O1-C20-C19	-10.45	105.53	113.38
51	4	315	A1ECV	C1D-C2D-C3D	-10.45	98.71	108.46
51	7	317	A1ECV	C1D-C2D-C3D	-10.44	98.72	108.46
51	W	317	A1ECV	C1D-C2D-C3D	-10.41	98.75	108.46
51	Q	319	A1ECV	C1D-C2D-C3D	-10.39	98.77	108.46
51	Q	316	A1ECV	C1D-C2D-C3D	-10.36	98.79	108.46
51	X	310	A1ECV	C1D-C2D-C3D	-10.32	98.83	108.46
51	T	317	A1ECV	C1D-C2D-C3D	-10.25	98.90	108.46
51	R	310	A1ECV	C1D-C2D-C3D	-10.22	98.92	108.46
51	V	317	A1ECV	C1D-C2D-C3D	-10.20	98.94	108.46
51	6	320	A1ECV	C1D-C2D-C3D	-10.20	98.94	108.46
51	R	310	A1ECV	O2D-CGD-CBD	10.14	123.84	111.00
51	9	317	A1ECV	C1D-C2D-C3D	-10.12	99.02	108.46
51	5	312	A1ECV	C1D-C2D-C3D	-10.09	99.05	108.46
51	4	321	A1ECV	C1D-C2D-C3D	-10.04	99.09	108.46
51	S	318	A1ECV	C1D-C2D-C3D	-9.95	99.18	108.46
43	1	304	DD6	O1-C20-C19	-9.95	105.91	113.38
51	0	321	A1ECV	C1D-C2D-C3D	-9.87	99.24	108.46
43	3	304	DD6	O1-C20-C21	9.66	126.63	115.06
51	7	323	A1ECV	O2D-CGD-CBD	9.56	123.11	111.00
43	D	306	DD6	O1-C20-C21	9.13	126.00	115.06
43	C	301	DD6	O1-C20-C21	9.07	125.92	115.06
43	Z	302	DD6	C14-C13-C11	-8.98	111.60	125.53
43	2	303	DD6	C14-C13-C11	-8.96	111.62	125.53
51	5	309	A1ECV	O2D-CGD-CBD	8.88	122.25	111.00
51	z	316	A1ECV	O2D-CGD-CBD	8.76	122.09	111.00
43	P	304	DD6	O1-C20-C19	-8.68	106.86	113.38
43	7	310	DD6	O1-C20-C21	8.68	125.45	115.06
51	X	310	A1ECV	O2D-CGD-CBD	8.45	121.71	111.00
43	A	303	DD6	O1-C20-C21	8.45	125.18	115.06
51	Y	312	A1ECV	O2D-CGD-CBD	8.44	121.69	111.00
51	X	310	A1ECV	CMD-C2D-C1D	8.35	140.51	124.73
48	D	305	A86	O1-C20-C19	-8.30	107.14	113.38
51	S	312	A1ECV	O2D-CGD-CBD	8.29	121.50	111.00
39	2	319	CLA	C4A-NA-C1A	8.27	110.43	106.71
51	4	321	A1ECV	CMD-C2D-C1D	8.26	140.34	124.73
51	Z	314	A1ECV	CMD-C2D-C1D	8.26	140.34	124.73
51	S	318	A1ECV	CMD-C2D-C1D	8.24	140.30	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	4	315	A1ECV	O2D-CGD-CBD	8.23	121.43	111.00
51	R	310	A1ECV	CMD-C2D-C1D	8.22	140.26	124.73
51	5	309	A1ECV	CMD-C2D-C1D	8.20	140.22	124.73
51	1	318	A1ECV	O2D-CGD-CBD	8.20	121.38	111.00
51	7	317	A1ECV	O2D-CGD-CBD	8.20	121.38	111.00
51	6	320	A1ECV	CMD-C2D-C1D	8.19	140.20	124.73
43	Q	303	DD6	O1-C20-C21	8.17	124.85	115.06
51	9	317	A1ECV	O2D-CGD-CBD	8.16	121.33	111.00
51	P	315	A1ECV	CMD-C2D-C1D	8.16	140.14	124.73
43	1	304	DD6	O1-C20-C21	8.15	124.82	115.06
43	Q	303	DD6	O1-C20-C19	-8.13	107.27	113.38
51	S	312	A1ECV	CMD-C2D-C1D	8.12	140.06	124.73
51	7	323	A1ECV	CMD-C2D-C1D	8.09	140.02	124.73
51	Z	314	A1ECV	O2D-CGD-CBD	8.09	121.25	111.00
51	M	316	A1ECV	CMD-C2D-C1D	8.06	139.95	124.73
39	Z	313	CLA	C4A-NA-C1A	8.06	110.33	106.71
51	Y	312	A1ECV	CMD-C2D-C1D	8.05	139.93	124.73
51	1	318	A1ECV	CMD-C2D-C1D	8.04	139.91	124.73
51	9	314	A1ECV	CMD-C2D-C1D	8.04	139.91	124.73
51	X	313	A1ECV	CMD-C2D-C1D	8.02	139.88	124.73
51	T	317	A1ECV	O2D-CGD-CBD	8.02	121.15	111.00
51	2	311	A1ECV	CMD-C2D-C1D	8.01	139.87	124.73
51	T	317	A1ECV	CMD-C2D-C1D	8.00	139.84	124.73
51	O	315	A1ECV	CMD-C2D-C1D	7.99	139.81	124.73
51	z	316	A1ECV	CMD-C2D-C1D	7.98	139.81	124.73
51	Q	316	A1ECV	CMD-C2D-C1D	7.98	139.80	124.73
43	P	304	DD6	O1-C20-C21	7.98	124.62	115.06
51	z	310	A1ECV	CMD-C2D-C1D	7.98	139.79	124.73
51	4	315	A1ECV	CMD-C2D-C1D	7.97	139.79	124.73
51	G	316	A1ECV	CMD-C2D-C1D	7.97	139.79	124.73
43	J	304	DD6	O1-C20-C19	-7.97	107.40	113.38
51	L	318	A1ECV	CMD-C2D-C1D	7.97	139.78	124.73
51	7	317	A1ECV	CMD-C2D-C1D	7.95	139.74	124.73
51	Y	306	A1ECV	CMD-C2D-C1D	7.94	139.73	124.73
51	x	316	A1ECV	CMD-C2D-C1D	7.94	139.73	124.73
51	y	311	A1ECV	CMD-C2D-C1D	7.93	139.70	124.73
51	y	317	A1ECV	CMD-C2D-C1D	7.92	139.69	124.73
51	R	313	A1ECV	O2D-CGD-CBD	7.91	121.02	111.00
51	5	312	A1ECV	CMD-C2D-C1D	7.91	139.67	124.73
51	Z	308	A1ECV	CMD-C2D-C1D	7.89	139.64	124.73
51	W	317	A1ECV	CMD-C2D-C1D	7.88	139.61	124.73
43	1	304	DD6	C21-C20-C19	7.87	123.14	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	R	313	A1ECV	CMD-C2D-C1D	7.87	139.60	124.73
51	0	321	A1ECV	O2D-CGD-CBD	7.87	120.97	111.00
51	Q	319	A1ECV	CMD-C2D-C1D	7.87	139.59	124.73
48	4	328	A86	O1-C20-C19	-7.86	107.47	113.38
51	x	310	A1ECV	CMD-C2D-C1D	7.86	139.58	124.73
39	Q	311	CLA	C4A-NA-C1A	7.85	110.24	106.71
39	b	811	CLA	C4A-NA-C1A	7.85	110.23	106.71
39	b	807	CLA	C4A-NA-C1A	7.80	110.21	106.71
49	P	306	KC2	CHB-C1B-NB	7.79	131.61	124.45
51	Y	306	A1ECV	O2D-CGD-CBD	7.78	120.85	111.00
49	M	313	KC2	CHB-C1B-NB	7.77	131.59	124.45
43	7	310	DD6	C21-C20-C15	-7.76	109.25	122.26
51	Z	308	A1ECV	O2D-CGD-CBD	7.76	120.83	111.00
51	y	311	A1ECV	O2D-CGD-CBD	7.74	120.80	111.00
51	V	317	A1ECV	O2D-CGD-CBD	7.71	120.77	111.00
48	8	305	A86	C4-C5-C6	-7.69	116.33	127.31
51	2	311	A1ECV	O2D-CGD-CBD	7.66	120.70	111.00
51	z	310	A1ECV	C2A-CAA-CBA	-7.63	111.42	128.63
39	I	311	CLA	C4A-NA-C1A	7.63	110.14	106.71
51	V	317	A1ECV	CMD-C2D-C1D	7.63	139.13	124.73
48	2	305	A86	C25-C26-C27	-7.60	116.46	127.31
43	C	301	DD6	C21-C20-C15	-7.59	109.54	122.26
51	X	313	A1ECV	O2D-CGD-CBD	7.58	120.60	111.00
51	9	314	A1ECV	O2D-CGD-CBD	7.57	120.59	111.00
39	L	320	CLA	C4A-NA-C1A	7.55	110.10	106.71
51	6	320	A1ECV	O2D-CGD-CBD	7.55	120.56	111.00
39	A	314	CLA	C4A-NA-C1A	7.54	110.10	106.71
39	Z	316	CLA	C4A-NA-C1A	7.54	110.10	106.71
51	x	310	A1ECV	O2D-CGD-CBD	7.54	120.55	111.00
50	G	308	A1EB1	O1-C20-C19	-7.53	107.72	113.38
51	G	316	A1ECV	O2D-CGD-CBD	7.49	120.49	111.00
43	2	303	DD6	C9-C10-C11	-7.46	116.66	127.31
39	9	312	CLA	C4A-NA-C1A	7.44	110.05	106.71
43	Z	302	DD6	C9-C10-C11	-7.44	116.69	127.31
43	1	304	DD6	C21-C20-C15	-7.44	109.80	122.26
51	O	315	A1ECV	O2D-CGD-CBD	7.43	120.41	111.00
39	5	310	CLA	C4A-NA-C1A	7.41	110.04	106.71
39	Y	314	CLA	C4A-NA-C1A	7.41	110.04	106.71
49	R	314	KC2	CHB-C1B-NB	7.41	131.26	124.45
39	C	310	CLA	C4A-NA-C1A	7.40	110.03	106.71
49	Q	313	KC2	CHB-C1B-NB	7.39	131.24	124.45
49	S	315	KC2	CHB-C1B-NB	7.39	131.24	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	T	318	CLA	C4A-NA-C1A	7.38	110.02	106.71
49	5	313	KC2	CHB-C1B-NB	7.38	131.23	124.45
51	0	321	A1ECV	CMD-C2D-C1D	7.37	138.66	124.73
39	F	315	CLA	C4A-NA-C1A	7.37	110.02	106.71
51	9	317	A1ECV	CMD-C2D-C1D	7.37	138.65	124.73
49	X	314	KC2	CHB-C1B-NB	7.36	131.22	124.45
39	a	808	CLA	C4A-NA-C1A	7.35	110.01	106.71
39	M	312	CLA	C4A-NA-C1A	7.33	110.00	106.71
49	X	312	KC2	CHB-C1B-NB	7.32	131.18	124.45
48	V	301	A86	O1-C20-C19	-7.32	107.88	113.38
39	b	833	CLA	C4A-NA-C1A	7.32	110.00	106.71
51	y	317	A1ECV	O2D-CGD-CBD	7.31	120.26	111.00
49	P	312	KC2	CHB-C1B-NB	7.31	131.17	124.45
49	8	316	KC2	CHB-C1B-NB	7.30	131.17	124.45
49	4	318	KC2	CHB-C1B-NB	7.30	131.16	124.45
39	G	314	CLA	C4A-NA-C1A	7.30	109.99	106.71
39	x	308	CLA	C4A-NA-C1A	7.29	109.98	106.71
49	V	314	KC2	CHB-C1B-NB	7.28	131.15	124.45
39	J	316	CLA	C4A-NA-C1A	7.28	109.98	106.71
51	z	310	A1ECV	O2D-CGD-CBD	7.27	120.21	111.00
39	b	808	CLA	C4A-NA-C1A	7.27	109.97	106.71
39	a	813	CLA	C4A-NA-C1A	7.26	109.97	106.71
48	3	306	A86	O1-C20-C19	-7.26	107.93	113.38
39	8	312	CLA	C4A-NA-C1A	7.25	109.97	106.71
51	x	316	A1ECV	O2D-CGD-CBD	7.25	120.19	111.00
48	O	306	A86	O1-C20-C19	-7.25	107.94	113.38
39	8	311	CLA	C4A-NA-C1A	7.25	109.97	106.71
51	E	311	A1ECV	CMD-C2D-C1D	7.25	138.41	124.73
39	a	801	CLA	C4A-NA-C1A	7.24	109.96	106.71
49	K	310	KC2	CHB-C1B-NB	7.24	131.10	124.45
49	2	317	KC2	CHB-C1B-NB	7.23	131.10	124.45
39	F	314	CLA	C4A-NA-C1A	7.23	109.96	106.71
39	R	309	CLA	C4A-NA-C1A	7.23	109.96	106.71
39	8	322	CLA	C4A-NA-C1A	7.22	109.95	106.71
39	S	310	CLA	C4A-NA-C1A	7.21	109.95	106.71
39	Q	309	CLA	C4A-NA-C1A	7.21	109.95	106.71
48	9	306	A86	O1-C20-C19	-7.20	107.97	113.38
50	0	307	A1EB1	O1-C20-C19	-7.20	107.97	113.38
39	M	321	CLA	C4A-NA-C1A	7.20	109.94	106.71
49	W	314	KC2	CHB-C1B-NB	7.19	131.06	124.45
39	0	322	CLA	C4A-NA-C1A	7.19	109.94	106.71
49	X	318	KC2	CHB-C1B-NB	7.18	131.06	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	H	310	CLA	C4A-NA-C1A	7.18	109.93	106.71
51	Q	319	A1ECV	O2D-CGD-CBD	7.17	120.09	111.00
39	E	317	CLA	C4A-NA-C1A	7.17	109.93	106.71
39	R	316	CLA	C4A-NA-C1A	7.17	109.93	106.71
49	7	319	KC2	CHB-C1B-NB	7.16	131.04	124.45
39	3	323	CLA	C4A-NA-C1A	7.16	109.92	106.71
39	5	308	CLA	C4A-NA-C1A	7.15	109.92	106.71
49	T	314	KC2	CHB-C1B-NB	7.15	131.02	124.45
39	M	318	CLA	C4A-NA-C1A	7.14	109.92	106.71
49	C	312	KC2	CHB-C1B-NB	7.14	131.02	124.45
39	P	307	CLA	C4A-NA-C1A	7.14	109.92	106.71
39	J	318	CLA	C4A-NA-C1A	7.14	109.92	106.71
39	L	319	CLA	C4A-NA-C1A	7.14	109.91	106.71
49	z	315	KC2	CHB-C1B-NB	7.13	131.01	124.45
39	H	306	CLA	C4A-NA-C1A	7.13	109.91	106.71
49	6	316	KC2	CHB-C1B-NB	7.12	131.00	124.45
39	S	319	CLA	C4A-NA-C1A	7.12	109.91	106.71
39	C	308	CLA	C4A-NA-C1A	7.12	109.91	106.71
49	4	317	KC2	CHB-C1B-NB	7.12	130.99	124.45
39	D	309	CLA	C4A-NA-C1A	7.11	109.90	106.71
49	3	317	KC2	CHB-C1B-NB	7.11	130.99	124.45
49	1	315	KC2	CHB-C1B-NB	7.10	130.98	124.45
39	9	309	CLA	C4A-NA-C1A	7.10	109.90	106.71
39	E	316	CLA	C4A-NA-C1A	7.10	109.90	106.71
49	V	315	KC2	CHB-C1B-NB	7.10	130.98	124.45
49	T	316	KC2	CHB-C1B-NB	7.10	130.97	124.45
49	0	317	KC2	CHB-C1B-NB	7.09	130.97	124.45
39	F	310	CLA	C4A-NA-C1A	7.09	109.89	106.71
49	Z	310	KC2	CHB-C1B-NB	7.09	130.97	124.45
39	U	201	CLA	C4A-NA-C1A	7.09	109.89	106.71
39	3	322	CLA	C4A-NA-C1A	7.09	109.89	106.71
49	F	307	KC2	CHB-C1B-NB	7.08	130.96	124.45
39	2	310	CLA	C4A-NA-C1A	7.08	109.89	106.71
39	J	307	CLA	C4A-NA-C1A	7.07	109.89	106.71
39	b	819	CLA	C4A-NA-C1A	7.07	109.88	106.71
39	U	213	CLA	C4A-NA-C1A	7.07	109.88	106.71
49	3	318	KC2	CHB-C1B-NB	7.07	130.95	124.45
39	b	823	CLA	C4A-NA-C1A	7.06	109.88	106.71
39	D	317	CLA	C4A-NA-C1A	7.06	109.88	106.71
39	x	311	CLA	C4A-NA-C1A	7.06	109.88	106.71
39	O	308	CLA	CAC-C3C-C4C	7.06	133.97	124.81
49	3	321	KC2	CHC-C4B-NB	7.05	130.94	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	L	304	A86	O1-C20-C19	-7.05	108.08	113.38
39	L	316	CLA	C4A-NA-C1A	7.05	109.88	106.71
49	2	314	KC2	CHB-C1B-NB	7.05	130.93	124.45
48	L	302	A86	C3-C2-C1	-7.05	117.25	127.31
39	C	311	CLA	C4A-NA-C1A	7.04	109.87	106.71
49	6	317	KC2	CHB-C1B-NB	7.04	130.93	124.45
49	4	320	KC2	CHB-C1B-NB	7.04	130.92	124.45
39	P	316	CLA	C4A-NA-C1A	7.04	109.87	106.71
48	S	304	A86	O1-C20-C19	-7.04	108.10	113.38
39	o	206	CLA	C4A-NA-C1A	7.03	109.87	106.71
39	7	325	CLA	C4A-NA-C1A	7.03	109.86	106.71
49	0	314	KC2	CHB-C1B-NB	7.03	130.91	124.45
49	L	317	KC2	CHB-C1B-NB	7.03	130.91	124.45
49	W	312	KC2	CHB-C1B-NB	7.03	130.91	124.45
49	S	314	KC2	CHB-C1B-NB	7.02	130.91	124.45
39	3	320	CLA	C4A-NA-C1A	7.02	109.86	106.71
49	H	314	KC2	CHB-C1B-NB	7.02	130.91	124.45
39	H	316	CLA	C4A-NA-C1A	7.02	109.86	106.71
49	V	318	KC2	CHB-C1B-NB	7.02	130.90	124.45
39	M	309	CLA	C4A-NA-C1A	7.02	109.86	106.71
49	G	311	KC2	CHB-C1B-NB	7.01	130.90	124.45
39	V	311	CLA	C4A-NA-C1A	7.01	109.86	106.71
49	L	315	KC2	CHB-C1B-NB	7.00	130.89	124.45
39	a	821	CLA	C4A-NA-C1A	7.00	109.85	106.71
39	b	817	CLA	C4A-NA-C1A	7.00	109.85	106.71
39	6	322	CLA	C4A-NA-C1A	7.00	109.85	106.71
43	3	304	DD6	C9-C10-C11	-6.99	117.33	127.31
49	P	310	KC2	CHB-C1B-NB	6.99	130.88	124.45
49	G	315	KC2	CHB-C1B-NB	6.99	130.88	124.45
39	a	836	CLA	C4A-NA-C1A	6.99	109.85	106.71
50	0	303	A1EB1	O1-C20-C19	-6.99	108.13	113.38
49	9	313	KC2	CHB-C1B-NB	6.99	130.88	124.45
39	T	319	CLA	C4A-NA-C1A	6.99	109.85	106.71
49	x	313	KC2	CHB-C1B-NB	6.99	130.87	124.45
39	7	321	CLA	C4A-NA-C1A	6.98	109.85	106.71
49	L	314	KC2	CHB-C1B-NB	6.98	130.87	124.45
39	E	310	CLA	C4A-NA-C1A	6.98	109.84	106.71
49	y	313	KC2	CHB-C1B-NB	6.98	130.87	124.45
39	a	814	CLA	C4A-NA-C1A	6.98	109.84	106.71
49	M	311	KC2	CHB-C1B-NB	6.97	130.86	124.45
48	E	304	A86	O1-C20-C19	-6.97	108.14	113.38
39	D	318	CLA	C4A-NA-C1A	6.97	109.84	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	y	315	CLA	C4A-NA-C1A	6.97	109.84	106.71
49	S	317	KC2	CHB-C1B-NB	6.97	130.86	124.45
49	X	315	KC2	CHB-C1B-NB	6.97	130.86	124.45
49	Z	311	KC2	CHB-C1B-NB	6.97	130.86	124.45
39	B	203	CLA	C4A-NA-C1A	6.96	109.84	106.71
39	G	309	CLA	C4A-NA-C1A	6.96	109.83	106.71
39	O	313	CLA	C4A-NA-C1A	6.96	109.83	106.71
39	X	317	CLA	C4A-NA-C1A	6.96	109.83	106.71
49	8	317	KC2	CHB-C1B-NB	6.95	130.84	124.45
49	P	320	KC2	CHB-C1B-NB	6.95	130.84	124.45
39	z	317	CLA	C4A-NA-C1A	6.95	109.83	106.71
49	G	317	KC2	CHB-C1B-NB	6.95	130.84	124.45
51	L	318	A1ECV	O2D-CGD-CBD	6.95	119.80	111.00
49	V	308	KC2	CHB-C1B-NB	6.95	130.84	124.45
49	R	318	KC2	CHB-C1B-NB	6.95	130.84	124.45
39	L	310	CLA	C4A-NA-C1A	6.95	109.83	106.71
39	O	316	CLA	C4A-NA-C1A	6.95	109.83	106.71
39	E	315	CLA	C4A-NA-C1A	6.94	109.83	106.71
39	a	829	CLA	C4A-NA-C1A	6.94	109.82	106.71
39	K	312	CLA	C4A-NA-C1A	6.94	109.82	106.71
48	D	305	A86	C25-C26-C27	-6.93	117.41	127.31
49	Y	309	KC2	CHB-C1B-NB	6.93	130.82	124.45
39	A	309	CLA	C4A-NA-C1A	6.93	109.82	106.71
39	y	309	CLA	C4A-NA-C1A	6.93	109.82	106.71
39	T	311	CLA	C4A-NA-C1A	6.93	109.82	106.71
39	X	309	CLA	C4A-NA-C1A	6.93	109.82	106.71
39	b	827	CLA	C4A-NA-C1A	6.93	109.82	106.71
49	4	324	KC2	CHB-C1B-NB	6.92	130.81	124.45
39	O	309	CLA	C4A-NA-C1A	6.92	109.82	106.71
39	D	311	CLA	C4A-NA-C1A	6.91	109.81	106.71
39	F	312	CLA	C4A-NA-C1A	6.91	109.81	106.71
39	K	306	CLA	C4A-NA-C1A	6.91	109.81	106.71
49	M	307	KC2	CHB-C1B-NB	6.91	130.80	124.45
39	a	833	CLA	C4A-NA-C1A	6.91	109.81	106.71
49	x	312	KC2	CHB-C1B-NB	6.90	130.80	124.45
49	y	316	KC2	CHB-C1B-NB	6.90	130.80	124.45
49	6	314	KC2	CHB-C1B-NB	6.90	130.80	124.45
43	P	304	DD6	C4-C5-C6	-6.90	117.46	127.31
49	7	320	KC2	CHB-C1B-NB	6.90	130.79	124.45
49	V	312	KC2	CHB-C1B-NB	6.90	130.79	124.45
43	P	304	DD6	C3-C2-C1	-6.90	117.47	127.31
39	R	315	CLA	C4A-NA-C1A	6.90	109.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	S	320	CLA	C4A-NA-C1A	6.90	109.81	106.71
49	2	313	KC2	CHC-C4B-NB	6.90	130.79	124.45
39	H	313	CLA	C4A-NA-C1A	6.90	109.81	106.71
39	5	316	CLA	C4A-NA-C1A	6.90	109.81	106.71
49	C	313	KC2	CHB-C1B-NB	6.89	130.79	124.45
39	a	825	CLA	C4A-NA-C1A	6.89	109.80	106.71
49	Q	318	KC2	CHB-C1B-NB	6.88	130.78	124.45
49	T	312	KC2	CHB-C1B-NB	6.88	130.78	124.45
49	5	314	KC2	CHB-C1B-NB	6.88	130.78	124.45
39	1	319	CLA	C4A-NA-C1A	6.88	109.80	106.71
39	o	201	CLA	C4A-NA-C1A	6.88	109.80	106.71
39	Z	306	CLA	C4A-NA-C1A	6.88	109.80	106.71
43	3	304	DD6	C4-C5-C6	-6.87	117.50	127.31
39	E	314	CLA	C4A-NA-C1A	6.87	109.79	106.71
39	Q	312	CLA	C4A-NA-C1A	6.87	109.79	106.71
39	a	838	CLA	C4A-NA-C1A	6.86	109.79	106.71
49	W	308	KC2	CHB-C1B-NB	6.86	130.76	124.45
39	7	324	CLA	C4A-NA-C1A	6.86	109.79	106.71
39	T	320	CLA	C4A-NA-C1A	6.86	109.79	106.71
39	b	830	CLA	C4A-NA-C1A	6.86	109.79	106.71
39	a	835	CLA	C4A-NA-C1A	6.85	109.79	106.71
39	2	312	CLA	C4A-NA-C1A	6.85	109.79	106.71
49	R	312	KC2	CHB-C1B-NB	6.85	130.75	124.45
39	Q	314	CLA	C4A-NA-C1A	6.85	109.79	106.71
39	7	316	CLA	C4A-NA-C1A	6.85	109.78	106.71
39	b	822	CLA	C4A-NA-C1A	6.85	109.78	106.71
39	U	214	CLA	C4A-NA-C1A	6.85	109.78	106.71
39	a	831	CLA	C4A-NA-C1A	6.84	109.78	106.71
39	3	312	CLA	C4A-NA-C1A	6.84	109.78	106.71
39	b	840	CLA	C4A-NA-C1A	6.84	109.78	106.71
39	1	310	CLA	C4A-NA-C1A	6.84	109.78	106.71
39	4	316	CLA	C4A-NA-C1A	6.84	109.78	106.71
39	a	834	CLA	C4A-NA-C1A	6.84	109.78	106.71
39	4	322	CLA	C4A-NA-C1A	6.84	109.78	106.71
39	a	805	CLA	C4A-NA-C1A	6.84	109.78	106.71
39	x	317	CLA	C4A-NA-C1A	6.84	109.78	106.71
39	Y	304	CLA	C4A-NA-C1A	6.84	109.78	106.71
39	Y	311	CLA	C4A-NA-C1A	6.84	109.78	106.71
39	l	203	CLA	C4A-NA-C1A	6.83	109.78	106.71
39	O	318	CLA	C4A-NA-C1A	6.83	109.78	106.71
39	9	319	CLA	C4A-NA-C1A	6.83	109.78	106.71
49	K	313	KC2	CHB-C1B-NB	6.83	130.73	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	z	311	CLA	C4A-NA-C1A	6.83	109.78	106.71
39	6	313	CLA	C4A-NA-C1A	6.83	109.78	106.71
39	S	311	CLA	C4A-NA-C1A	6.82	109.77	106.71
39	3	314	CLA	C4A-NA-C1A	6.82	109.77	106.71
39	b	806	CLA	C4A-NA-C1A	6.82	109.77	106.71
39	P	311	CLA	C4A-NA-C1A	6.82	109.77	106.71
39	h	201	CLA	C4A-NA-C1A	6.82	109.77	106.71
39	U	207	CLA	C4A-NA-C1A	6.82	109.77	106.71
49	G	313	KC2	CHB-C1B-NB	6.82	130.72	124.45
39	J	311	CLA	C4A-NA-C1A	6.82	109.77	106.71
39	K	307	CLA	C4A-NA-C1A	6.82	109.77	106.71
39	x	314	CLA	C4A-NA-C1A	6.81	109.77	106.71
48	F	301	A86	O1-C20-C19	-6.81	108.26	113.38
49	B	208	KC2	CHB-C1B-NB	6.81	130.71	124.45
49	J	315	KC2	CHB-C1B-NB	6.81	130.71	124.45
39	0	313	CLA	C4A-NA-C1A	6.81	109.77	106.71
39	4	314	CLA	C4A-NA-C1A	6.81	109.77	106.71
39	X	311	CLA	C4A-NA-C1A	6.81	109.77	106.71
39	o	202	CLA	C4A-NA-C1A	6.80	109.76	106.71
39	J	317	CLA	C4A-NA-C1A	6.80	109.76	106.71
39	M	310	CLA	C4A-NA-C1A	6.80	109.76	106.71
39	F	313	CLA	C4A-NA-C1A	6.80	109.76	106.71
39	5	306	CLA	C4A-NA-C1A	6.80	109.76	106.71
49	I	312	KC2	CHB-C1B-NB	6.79	130.70	124.45
39	I	315	CLA	C4A-NA-C1A	6.79	109.76	106.71
49	F	311	KC2	CHB-C1B-NB	6.79	130.69	124.45
49	P	313	KC2	CHB-C1B-NB	6.79	130.69	124.45
39	M	317	CLA	C4A-NA-C1A	6.79	109.76	106.71
39	W	318	CLA	C4A-NA-C1A	6.79	109.76	106.71
39	3	316	CLA	C4A-NA-C1A	6.79	109.76	106.71
39	A	312	CLA	C4A-NA-C1A	6.78	109.75	106.71
49	z	313	KC2	CHB-C1B-NB	6.78	130.68	124.45
49	5	311	KC2	CHB-C1B-NB	6.78	130.68	124.45
39	T	310	CLA	C4A-NA-C1A	6.78	109.75	106.71
39	V	319	CLA	C4A-NA-C1A	6.78	109.75	106.71
39	R	307	CLA	C4A-NA-C1A	6.77	109.75	106.71
39	8	321	CLA	C4A-NA-C1A	6.77	109.75	106.71
49	3	315	KC2	CHB-C1B-NB	6.77	130.68	124.45
39	E	308	CLA	C4A-NA-C1A	6.77	109.75	106.71
49	1	314	KC2	CHB-C1B-NB	6.77	130.68	124.45
39	a	822	CLA	C4A-NA-C1A	6.77	109.75	106.71
39	a	818	CLA	C4A-NA-C1A	6.76	109.75	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	X	316	CLA	C4A-NA-C1A	6.76	109.75	106.71
39	y	318	CLA	C4A-NA-C1A	6.76	109.75	106.71
49	2	313	KC2	CHB-C1B-NB	6.76	130.67	124.45
39	H	307	CLA	C4A-NA-C1A	6.76	109.75	106.71
39	B	205	CLA	C4A-NA-C1A	6.76	109.74	106.71
51	P	315	A1ECV	O2D-CGD-CBD	6.76	119.56	111.00
39	a	817	CLA	C4A-NA-C1A	6.76	109.74	106.71
39	F	306	CLA	C4A-NA-C1A	6.76	109.74	106.71
39	P	308	CLA	C4A-NA-C1A	6.76	109.74	106.71
39	I	314	CLA	C4A-NA-C1A	6.76	109.74	106.71
39	Z	309	CLA	C4A-NA-C1A	6.76	109.74	106.71
52	P	318	A1EB4	C9-C10-C11	-6.75	118.88	127.00
48	3	307	A86	C25-C26-C27	-6.75	117.68	127.31
39	K	309	CLA	C4A-NA-C1A	6.75	109.74	106.71
39	8	315	CLA	C4A-NA-C1A	6.75	109.74	106.71
49	V	320	KC2	CHB-C1B-NB	6.75	130.65	124.45
39	b	803	CLA	C4A-NA-C1A	6.75	109.74	106.71
39	a	830	CLA	C4A-NA-C1A	6.74	109.74	106.71
39	j	101	CLA	C4A-NA-C1A	6.74	109.74	106.71
39	E	306	CLA	C4A-NA-C1A	6.74	109.74	106.71
39	Y	310	CLA	C4A-NA-C1A	6.74	109.74	106.71
39	6	315	CLA	C4A-NA-C1A	6.74	109.74	106.71
39	F	309	CLA	C4A-NA-C1A	6.74	109.74	106.71
39	U	211	CLA	C4A-NA-C1A	6.74	109.73	106.71
39	0	312	CLA	C4A-NA-C1A	6.74	109.73	106.71
39	x	306	CLA	C4A-NA-C1A	6.74	109.73	106.71
39	b	814	CLA	C4A-NA-C1A	6.73	109.73	106.71
39	b	838	CLA	C4A-NA-C1A	6.73	109.73	106.71
49	8	320	KC2	CHB-C1B-NB	6.73	130.64	124.45
39	a	847	CLA	C4A-NA-C1A	6.73	109.73	106.71
39	b	834	CLA	C4A-NA-C1A	6.73	109.73	106.71
39	o	205	CLA	C4A-NA-C1A	6.73	109.73	106.71
39	F	321	CLA	C4A-NA-C1A	6.73	109.73	106.71
49	8	314	KC2	CHB-C1B-NB	6.73	130.64	124.45
48	L	302	A86	C40-C32-C31	6.73	116.49	110.47
39	D	313	CLA	C4A-NA-C1A	6.72	109.73	106.71
39	U	212	CLA	C4A-NA-C1A	6.72	109.73	106.71
49	9	311	KC2	CHB-C1B-NB	6.72	130.63	124.45
39	P	314	CLA	C4A-NA-C1A	6.72	109.73	106.71
39	U	215	CLA	C4A-NA-C1A	6.72	109.73	106.71
49	7	322	KC2	CHB-C1B-NB	6.72	130.63	124.45
39	a	819	CLA	C4A-NA-C1A	6.72	109.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	G	312	CLA	C4A-NA-C1A	6.72	109.72	106.71
39	2	307	CLA	C4A-NA-C1A	6.71	109.72	106.71
39	J	313	CLA	C4A-NA-C1A	6.71	109.72	106.71
39	6	312	CLA	C4A-NA-C1A	6.71	109.72	106.71
39	H	315	CLA	C4A-NA-C1A	6.71	109.72	106.71
39	1	316	CLA	C4A-NA-C1A	6.71	109.72	106.71
39	S	313	CLA	C4A-NA-C1A	6.70	109.72	106.71
39	2	316	CLA	C4A-NA-C1A	6.70	109.72	106.71
39	7	314	CLA	C4A-NA-C1A	6.70	109.72	106.71
39	Q	320	CLA	C4A-NA-C1A	6.70	109.72	106.71
39	b	825	CLA	C4A-NA-C1A	6.69	109.72	106.71
39	R	311	CLA	C4A-NA-C1A	6.69	109.72	106.71
39	V	309	CLA	C4A-NA-C1A	6.69	109.71	106.71
39	1	308	CLA	C4A-NA-C1A	6.69	109.71	106.71
39	4	319	CLA	C4A-NA-C1A	6.69	109.71	106.71
39	a	815	CLA	C4A-NA-C1A	6.69	109.71	106.71
39	b	820	CLA	C4A-NA-C1A	6.69	109.71	106.71
39	k	203	CLA	C4A-NA-C1A	6.69	109.71	106.71
39	J	312	CLA	C4A-NA-C1A	6.69	109.71	106.71
48	T	306	A86	O1-C20-C19	-6.69	108.36	113.38
49	z	312	KC2	CHB-C1B-NB	6.69	130.60	124.45
39	Z	307	CLA	C4A-NA-C1A	6.68	109.71	106.71
39	L	313	CLA	C4A-NA-C1A	6.68	109.71	106.71
49	R	306	KC2	CHB-C1B-NB	6.68	130.59	124.45
39	a	832	CLA	C4A-NA-C1A	6.68	109.71	106.71
39	M	308	CLA	C4A-NA-C1A	6.68	109.71	106.71
39	4	313	CLA	C4A-NA-C1A	6.68	109.71	106.71
39	k	202	CLA	C4A-NA-C1A	6.67	109.71	106.71
39	6	318	CLA	C4A-NA-C1A	6.67	109.71	106.71
39	o	203	CLA	C4A-NA-C1A	6.67	109.70	106.71
39	X	307	CLA	C4A-NA-C1A	6.67	109.70	106.71
39	z	309	CLA	C4A-NA-C1A	6.67	109.70	106.71
39	Z	304	CLA	C4A-NA-C1A	6.67	109.70	106.71
49	M	314	KC2	CHB-C1B-NB	6.67	130.58	124.45
49	Q	315	KC2	CHB-C1B-NB	6.67	130.58	124.45
49	A	313	KC2	CHB-C1B-NB	6.66	130.58	124.45
39	K	314	CLA	C4A-NA-C1A	6.66	109.70	106.71
39	W	319	CLA	C4A-NA-C1A	6.66	109.70	106.71
39	b	832	CLA	C4A-NA-C1A	6.66	109.70	106.71
39	U	209	CLA	C4A-NA-C1A	6.66	109.70	106.71
39	2	315	CLA	C4A-NA-C1A	6.66	109.70	106.71
49	8	319	KC2	CHB-C1B-NB	6.66	130.57	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	a	804	CLA	C4A-NA-C1A	6.66	109.70	106.71
39	z	308	CLA	C4A-NA-C1A	6.66	109.70	106.71
39	F	308	CLA	C4A-NA-C1A	6.65	109.70	106.71
49	H	311	KC2	CHB-C1B-NB	6.65	130.56	124.45
39	F	316	CLA	C4A-NA-C1A	6.65	109.69	106.71
39	W	311	CLA	C4A-NA-C1A	6.65	109.69	106.71
39	Z	315	CLA	C4A-NA-C1A	6.65	109.69	106.71
39	M	315	CLA	C4A-NA-C1A	6.65	109.69	106.71
39	P	309	CLA	C4A-NA-C1A	6.65	109.69	106.71
48	I	304	A86	O1-C20-C19	-6.64	108.39	113.38
39	a	806	CLA	C4A-NA-C1A	6.64	109.69	106.71
39	V	313	CLA	C4A-NA-C1A	6.64	109.69	106.71
51	Q	316	A1ECV	O2D-CGD-CBD	6.64	119.41	111.00
39	W	313	CLA	C4A-NA-C1A	6.64	109.69	106.71
39	b	810	CLA	C4A-NA-C1A	6.64	109.69	106.71
39	Y	302	CLA	C4A-NA-C1A	6.64	109.69	106.71
39	a	827	CLA	C4A-NA-C1A	6.63	109.69	106.71
39	Q	317	CLA	C4A-NA-C1A	6.63	109.69	106.71
48	T	301	A86	O1-C20-C19	-6.63	108.40	113.38
39	E	319	CLA	C4A-NA-C1A	6.63	109.69	106.71
39	y	310	CLA	C4A-NA-C1A	6.62	109.68	106.71
48	6	309	A86	O1-C20-C19	-6.62	108.41	113.38
49	W	315	KC2	CHB-C1B-NB	6.62	130.54	124.45
39	7	315	CLA	C4A-NA-C1A	6.62	109.68	106.71
39	y	307	CLA	C4A-NA-C1A	6.62	109.68	106.71
49	Q	313	KC2	CHC-C4B-NB	6.62	130.53	124.45
39	z	314	CLA	C4A-NA-C1A	6.62	109.68	106.71
39	I	309	CLA	C4A-NA-C1A	6.61	109.68	106.71
39	a	837	CLA	C4A-NA-C1A	6.61	109.68	106.71
39	I	308	CLA	C4A-NA-C1A	6.61	109.68	106.71
49	5	305	KC2	CHC-C4B-NB	6.61	130.53	124.45
49	K	310	KC2	CHC-C4B-NB	6.61	130.53	124.45
39	D	316	CLA	C4A-NA-C1A	6.60	109.67	106.71
39	V	316	CLA	C4A-NA-C1A	6.60	109.67	106.71
43	D	303	DD6	C3-C2-C1	-6.60	117.89	127.31
39	I	301	CLA	C4A-NA-C1A	6.60	109.67	106.71
39	y	312	CLA	C4A-NA-C1A	6.60	109.67	106.71
39	x	309	CLA	C4A-NA-C1A	6.59	109.67	106.71
49	X	306	KC2	CHB-C1B-NB	6.59	130.51	124.45
39	3	313	CLA	C4A-NA-C1A	6.59	109.67	106.71
48	J	303	A86	O1-C20-C19	-6.58	108.44	113.38
39	4	323	CLA	C4A-NA-C1A	6.58	109.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	C	305	CLA	C4A-NA-C1A	6.57	109.66	106.71
39	2	318	CLA	C4A-NA-C1A	6.57	109.66	106.71
39	O	312	CLA	C4A-NA-C1A	6.57	109.66	106.71
49	I	303	KC2	CHC-C4B-NB	6.57	130.49	124.45
39	L	309	CLA	C4A-NA-C1A	6.57	109.66	106.71
39	i	103	CLA	C4A-NA-C1A	6.56	109.66	106.71
39	T	308	CLA	C4A-NA-C1A	6.56	109.66	106.71
39	b	801	CLA	C4A-NA-C1A	6.56	109.66	106.71
49	9	316	KC2	CHB-C1B-NB	6.56	130.48	124.45
39	0	320	CLA	C4A-NA-C1A	6.56	109.65	106.71
50	0	302	A1EB1	C17-C16-C15	6.56	115.85	109.16
39	b	842	CLA	C4A-NA-C1A	6.56	109.65	106.71
39	H	312	CLA	C4A-NA-C1A	6.55	109.65	106.71
39	K	311	CLA	C4A-NA-C1A	6.55	109.65	106.71
51	5	312	A1ECV	O2D-CGD-CBD	6.55	119.29	111.00
39	b	841	CLA	C4A-NA-C1A	6.54	109.65	106.71
48	L	302	A86	O1-C20-C19	-6.54	108.47	113.38
39	b	824	CLA	C4A-NA-C1A	6.54	109.64	106.71
49	L	321	KC2	CHB-C1B-NB	6.53	130.46	124.45
39	a	807	CLA	C4A-NA-C1A	6.53	109.64	106.71
39	C	307	CLA	C4A-NA-C1A	6.53	109.64	106.71
39	J	308	CLA	C4A-NA-C1A	6.53	109.64	106.71
39	1	317	CLA	C4A-NA-C1A	6.53	109.64	106.71
39	b	829	CLA	C4A-NA-C1A	6.53	109.64	106.71
42	a	845	BCR	C24-C23-C22	-6.52	116.38	126.23
39	C	306	CLA	C4A-NA-C1A	6.52	109.64	106.71
39	3	319	CLA	C4A-NA-C1A	6.52	109.64	106.71
48	B	201	A86	O1-C20-C19	-6.52	108.48	113.38
39	A	315	CLA	C4A-NA-C1A	6.52	109.64	106.71
48	L	307	A86	O1-C20-C19	-6.52	108.49	113.38
39	W	309	CLA	C4A-NA-C1A	6.52	109.64	106.71
39	0	318	CLA	C4A-NA-C1A	6.51	109.63	106.71
39	Y	313	CLA	C4A-NA-C1A	6.51	109.63	106.71
49	x	315	KC2	CHB-C1B-NB	6.51	130.44	124.45
49	W	312	KC2	CHC-C4B-NB	6.51	130.43	124.45
39	D	319	CLA	C4A-NA-C1A	6.50	109.63	106.71
39	b	851	CLA	C4A-NA-C1A	6.50	109.63	106.71
39	i	101	CLA	C4A-NA-C1A	6.50	109.63	106.71
39	H	308	CLA	C4A-NA-C1A	6.50	109.63	106.71
39	z	318	CLA	C4A-NA-C1A	6.50	109.63	106.71
49	5	311	KC2	CHC-C4B-NB	6.50	130.43	124.45
49	P	310	KC2	CHC-C4B-NB	6.50	130.43	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	J	310	CLA	C4A-NA-C1A	6.49	109.63	106.71
49	V	318	KC2	CHC-C4B-NB	6.49	130.42	124.45
39	b	813	CLA	C4A-NA-C1A	6.49	109.62	106.71
49	5	305	KC2	CHB-C1B-NB	6.49	130.42	124.45
39	b	839	CLA	C4A-NA-C1A	6.49	109.62	106.71
39	z	306	CLA	C4A-NA-C1A	6.49	109.62	106.71
49	0	316	KC2	CHB-C1B-NB	6.49	130.42	124.45
39	Z	312	CLA	C4A-NA-C1A	6.49	109.62	106.71
39	6	321	CLA	C4A-NA-C1A	6.48	109.62	106.71
51	W	317	A1ECV	O2D-CGD-CBD	6.48	119.21	111.00
39	A	306	CLA	C4A-NA-C1A	6.48	109.62	106.71
39	H	309	CLA	C4A-NA-C1A	6.48	109.62	106.71
39	a	812	CLA	C4A-NA-C1A	6.48	109.62	106.71
39	G	310	CLA	C4A-NA-C1A	6.48	109.62	106.71
48	2	305	A86	C4-C5-C6	-6.48	118.06	127.31
48	L	302	A86	C28-C27-C26	-6.48	113.85	122.92
42	i	102	BCR	C24-C23-C22	-6.48	116.45	126.23
39	b	835	CLA	C4A-NA-C1A	6.47	109.62	106.71
39	5	315	CLA	C4A-NA-C1A	6.47	109.62	106.71
39	1	313	CLA	C4A-NA-C1A	6.47	109.62	106.71
49	Z	311	KC2	CHC-C4B-NB	6.47	130.40	124.45
51	M	316	A1ECV	O2D-CGD-CBD	6.47	119.19	111.00
39	k	201	CLA	C4A-NA-C1A	6.47	109.61	106.71
49	A	310	KC2	CHB-C1B-NB	6.47	130.40	124.45
49	2	314	KC2	CHC-C4B-NB	6.46	130.40	124.45
48	G	301	A86	C17-C16-C15	6.46	115.76	109.16
39	b	812	CLA	C4A-NA-C1A	6.46	109.61	106.71
39	a	803	CLA	C4A-NA-C1A	6.46	109.61	106.71
39	D	312	CLA	C4A-NA-C1A	6.46	109.61	106.71
49	V	320	KC2	CHC-C4B-NB	6.46	130.39	124.45
49	4	324	KC2	CHC-C4B-NB	6.46	130.39	124.45
39	7	318	CLA	C4A-NA-C1A	6.45	109.61	106.71
39	6	310	CLA	C4A-NA-C1A	6.45	109.61	106.71
50	0	303	A1EB1	C17-C16-C15	6.45	115.74	109.16
49	V	308	KC2	CHC-C4B-NB	6.45	130.38	124.45
49	L	315	KC2	CHC-C4B-NB	6.45	130.38	124.45
39	Z	305	CLA	C4A-NA-C1A	6.45	109.60	106.71
49	T	316	KC2	CHC-C4B-NB	6.44	130.37	124.45
48	O	307	A86	C17-C16-C15	6.44	115.73	109.16
49	P	312	KC2	CHC-C4B-NB	6.44	130.37	124.45
39	W	310	CLA	C4A-NA-C1A	6.43	109.60	106.71
50	V	302	A1EB1	C21-C20-C19	6.43	121.52	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	a	809	CLA	C4A-NA-C1A	6.43	109.60	106.71
39	9	308	CLA	C4A-NA-C1A	6.43	109.60	106.71
43	C	301	DD6	O1-C20-C19	-6.43	108.55	113.38
49	V	312	KC2	CHC-C4B-NB	6.43	130.36	124.45
39	Y	307	CLA	C4A-NA-C1A	6.43	109.60	106.71
39	E	312	CLA	C4A-NA-C1A	6.42	109.59	106.71
39	C	309	CLA	C4A-NA-C1A	6.41	109.59	106.71
39	z	307	CLA	C4A-NA-C1A	6.41	109.59	106.71
51	4	321	A1ECV	O2D-CGD-CBD	6.41	119.12	111.00
43	J	304	DD6	O1-C20-C21	6.41	122.74	115.06
48	7	312	A86	O1-C20-C19	-6.41	108.57	113.38
39	8	318	CLA	C4A-NA-C1A	6.41	109.59	106.71
49	I	303	KC2	O2D-CGD-CBD	6.41	122.65	111.27
39	a	824	CLA	C4A-NA-C1A	6.41	109.59	106.71
39	b	828	CLA	C4A-NA-C1A	6.41	109.59	106.71
39	L	308	CLA	C4A-NA-C1A	6.41	109.59	106.71
49	y	314	KC2	CHB-C1B-NB	6.40	130.34	124.45
48	0	308	A86	O1-C20-C21	-6.40	107.38	115.06
39	3	311	CLA	C4A-NA-C1A	6.40	109.58	106.71
49	Y	308	KC2	CHB-C1B-NB	6.40	130.34	124.45
49	R	318	KC2	CHC-C4B-NB	6.40	130.34	124.45
39	b	809	CLA	C4A-NA-C1A	6.40	109.58	106.71
49	W	308	KC2	CHC-C4B-NB	6.40	130.33	124.45
49	z	315	KC2	CHC-C4B-NB	6.40	130.33	124.45
39	Y	305	CLA	C4A-NA-C1A	6.39	109.58	106.71
49	M	311	KC2	CHC-C4B-NB	6.39	130.33	124.45
39	a	826	CLA	C4A-NA-C1A	6.39	109.58	106.71
49	2	317	KC2	CHC-C4B-NB	6.39	130.33	124.45
39	4	311	CLA	C4A-NA-C1A	6.39	109.58	106.71
39	Y	303	CLA	C4A-NA-C1A	6.39	109.58	106.71
39	f	803	CLA	C4A-NA-C1A	6.38	109.58	106.71
39	S	308	CLA	C4A-NA-C1A	6.38	109.58	106.71
51	S	312	A1ECV	C2A-CAA-CBA	-6.38	114.24	128.63
49	0	314	KC2	CHC-C4B-NB	6.38	130.32	124.45
49	I	303	KC2	CHB-C1B-NB	6.38	130.32	124.45
48	O	306	A86	C25-C26-C27	-6.38	118.21	127.31
39	0	323	CLA	C4A-NA-C1A	6.38	109.57	106.71
39	J	309	CLA	C4A-NA-C1A	6.37	109.57	106.71
39	O	311	CLA	C4A-NA-C1A	6.37	109.57	106.71
39	1	311	CLA	C4A-NA-C1A	6.37	109.57	106.71
49	5	314	KC2	CHC-C4B-NB	6.37	130.31	124.45
39	y	308	CLA	C4A-NA-C1A	6.37	109.57	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	a	810	CLA	C4A-NA-C1A	6.36	109.57	106.71
49	0	316	KC2	CHC-C4B-NB	6.36	130.30	124.45
49	x	313	KC2	CHC-C4B-NB	6.36	130.30	124.45
49	G	311	KC2	CHC-C4B-NB	6.36	130.30	124.45
49	X	318	KC2	CHC-C4B-NB	6.36	130.30	124.45
48	L	306	A86	C4-C5-C6	-6.36	118.23	127.31
49	R	312	KC2	CHC-C4B-NB	6.36	130.30	124.45
49	L	317	KC2	CHC-C4B-NB	6.36	130.30	124.45
39	l	204	CLA	C4A-NA-C1A	6.35	109.56	106.71
39	9	310	CLA	C4A-NA-C1A	6.35	109.56	106.71
39	D	315	CLA	C4A-NA-C1A	6.35	109.56	106.71
39	O	310	CLA	C4A-NA-C1A	6.35	109.56	106.71
49	B	208	KC2	CHC-C4B-NB	6.35	130.29	124.45
39	E	309	CLA	C4A-NA-C1A	6.35	109.56	106.71
51	S	318	A1ECV	O2D-CGD-CBD	6.35	119.04	111.00
49	6	314	KC2	CHC-C4B-NB	6.35	130.28	124.45
49	P	320	KC2	CHC-C4B-NB	6.34	130.28	124.45
49	4	320	KC2	CHC-C4B-NB	6.34	130.28	124.45
49	Z	310	KC2	CHC-C4B-NB	6.34	130.28	124.45
39	b	818	CLA	C4A-NA-C1A	6.34	109.56	106.71
49	M	307	KC2	CHC-C4B-NB	6.34	130.28	124.45
39	a	828	CLA	C4A-NA-C1A	6.34	109.56	106.71
43	G	306	DD6	C9-C10-C11	-6.34	118.27	127.31
49	H	311	KC2	CHC-C4B-NB	6.34	130.28	124.45
49	S	317	KC2	CHC-C4B-NB	6.33	130.27	124.45
39	S	316	CLA	C4A-NA-C1A	6.33	109.55	106.71
39	8	313	CLA	C4A-NA-C1A	6.33	109.55	106.71
50	D	308	A1EB1	O1-C20-C19	-6.33	108.63	113.38
43	D	306	DD6	C3-C2-C1	-6.33	118.28	127.31
39	9	315	CLA	C4A-NA-C1A	6.33	109.55	106.71
39	8	310	CLA	C4A-NA-C1A	6.32	109.55	106.71
39	D	314	CLA	C4A-NA-C1A	6.32	109.55	106.71
50	U	203	A1EB1	C17-C16-C15	6.32	115.61	109.16
39	a	802	CLA	C4A-NA-C1A	6.32	109.55	106.71
39	E	318	CLA	C4A-NA-C1A	6.32	109.55	106.71
43	1	304	DD6	C9-C10-C11	-6.31	118.31	127.31
48	S	307	A86	O1-C20-C19	-6.31	108.64	113.38
49	6	319	KC2	CHB-C1B-NB	6.30	130.25	124.45
49	X	315	KC2	CHC-C4B-NB	6.30	130.24	124.45
39	2	309	CLA	C4A-NA-C1A	6.30	109.54	106.71
48	U	206	A86	O1-C20-C19	-6.30	108.65	113.38
39	2	308	CLA	C4A-NA-C1A	6.29	109.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	C	313	KC2	CHC-C4B-NB	6.29	130.23	124.45
39	0	315	CLA	C4A-NA-C1A	6.29	109.53	106.71
39	R	308	CLA	C4A-NA-C1A	6.28	109.53	106.71
39	x	318	CLA	C4A-NA-C1A	6.28	109.53	106.71
48	Z	303	A86	C3-C2-C1	-6.28	118.34	127.31
50	K	305	A1EB1	C17-C16-C15	6.28	115.57	109.16
49	y	316	KC2	CHC-C4B-NB	6.28	130.22	124.45
49	z	313	KC2	CHD-C1D-ND	6.27	130.90	124.26
49	T	315	KC2	CHB-C1B-NB	6.27	130.22	124.45
48	J	301	A86	O1-C20-C19	-6.26	108.68	113.38
39	4	312	CLA	C4A-NA-C1A	6.26	109.52	106.71
39	b	816	CLA	C4A-NA-C1A	6.26	109.52	106.71
39	G	318	CLA	C4A-NA-C1A	6.26	109.52	106.71
39	O	308	CLA	C4A-NA-C1A	6.26	109.52	106.71
48	G	305	A86	O1-C20-C19	-6.26	108.68	113.38
39	y	319	CLA	C4A-NA-C1A	6.25	109.52	106.71
39	B	204	CLA	C4A-NA-C1A	6.25	109.52	106.71
39	f	802	CLA	C4A-NA-C1A	6.25	109.52	106.71
39	I	313	CLA	C4A-NA-C1A	6.25	109.52	106.71
50	D	308	A1EB1	C17-C16-C15	6.25	115.53	109.16
49	F	307	KC2	CHC-C4B-NB	6.24	130.19	124.45
49	W	314	KC2	CHC-C4B-NB	6.24	130.19	124.45
49	I	312	KC2	CHC-C4B-NB	6.24	130.19	124.45
50	Q	323	A1EB1	C25-C26-C27	-6.23	118.39	127.26
50	Q	323	A1EB1	C3-C2-C1	-6.23	118.42	127.31
43	F	305	DD6	C3-C2-C1	-6.23	118.42	127.31
49	6	317	KC2	CHC-C4B-NB	6.22	130.17	124.45
49	G	313	KC2	CHC-C4B-NB	6.22	130.17	124.45
49	y	313	KC2	CHC-C4B-NB	6.22	130.17	124.45
39	b	837	CLA	C4A-NA-C1A	6.22	109.50	106.71
49	8	319	KC2	CHC-C4B-NB	6.22	130.17	124.45
48	8	305	A86	C25-C26-C27	-6.21	118.44	127.31
49	F	311	KC2	CHC-C4B-NB	6.21	130.16	124.45
48	6	305	A86	O1-C20-C19	-6.21	108.72	113.38
49	Q	315	KC2	CHC-C4B-NB	6.21	130.16	124.45
49	Q	318	KC2	CHC-C4B-NB	6.21	130.16	124.45
39	a	811	CLA	C4A-NA-C1A	6.21	109.50	106.71
39	B	206	CLA	C4A-NA-C1A	6.21	109.50	106.71
39	W	316	CLA	C4A-NA-C1A	6.20	109.49	106.71
39	I	310	CLA	C4A-NA-C1A	6.20	109.49	106.71
49	S	314	KC2	CHC-C4B-NB	6.19	130.15	124.45
39	C	304	CLA	C4A-NA-C1A	6.19	109.49	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Q	308	A86	O1-C20-C19	-6.18	108.74	113.38
49	7	319	KC2	CHC-C4B-NB	6.17	130.13	124.45
43	3	304	DD6	C15-C14-C13	-6.17	112.95	125.99
49	R	314	KC2	CHC-C4B-NB	6.17	130.12	124.45
49	L	312	KC2	CHB-C1B-NB	6.17	130.12	124.45
49	X	312	KC2	CHC-C4B-NB	6.17	130.12	124.45
39	1	320	CLA	C4A-NA-C1A	6.17	109.48	106.71
49	9	318	KC2	CHB-C1B-NB	6.17	130.12	124.45
49	G	315	KC2	CHC-C4B-NB	6.16	130.12	124.45
49	G	317	KC2	CHC-C4B-NB	6.16	130.12	124.45
49	8	320	KC2	CHC-C4B-NB	6.16	130.12	124.45
43	A	303	DD6	C3-C2-C1	-6.16	118.51	127.31
39	b	821	CLA	C4A-NA-C1A	6.16	109.47	106.71
49	Y	309	KC2	CHC-C4B-NB	6.16	130.11	124.45
49	7	322	KC2	CHC-C4B-NB	6.16	130.11	124.45
48	4	310	A86	O1-C20-C19	-6.16	108.76	113.38
49	H	314	KC2	CHC-C4B-NB	6.15	130.11	124.45
49	9	311	KC2	CHC-C4B-NB	6.15	130.11	124.45
49	T	312	KC2	CHC-C4B-NB	6.15	130.11	124.45
43	x	304	DD6	C3-C2-C1	-6.15	118.53	127.31
49	L	314	KC2	CHC-C4B-NB	6.15	130.10	124.45
39	D	310	CLA	C4A-NA-C1A	6.15	109.47	106.71
49	X	314	KC2	CHC-C4B-NB	6.14	130.10	124.45
49	9	316	KC2	CHC-C4B-NB	6.14	130.10	124.45
39	b	836	CLA	C4A-NA-C1A	6.14	109.47	106.71
39	A	305	CLA	C4A-NA-C1A	6.14	109.47	106.71
48	Q	308	A86	C17-C16-C15	6.14	115.42	109.16
48	E	304	A86	O4-C38-C39	6.14	122.38	111.09
48	8	307	A86	C25-C26-C27	-6.14	118.55	127.31
49	A	313	KC2	CHC-C4B-NB	6.14	130.09	124.45
50	3	310	A1EB1	O1-C20-C19	-6.13	108.78	113.38
48	P	302	A86	C4-C5-C6	-6.12	118.57	127.31
39	b	815	CLA	C4A-NA-C1A	6.12	109.46	106.71
39	b	831	CLA	C4A-NA-C1A	6.11	109.45	106.71
39	B	207	CLA	C4A-NA-C1A	6.11	109.45	106.71
43	1	304	DD6	C4-C5-C6	-6.11	118.59	127.31
48	x	305	A86	O1-C20-C19	-6.11	108.79	113.38
39	6	311	CLA	C4A-NA-C1A	6.11	109.45	106.71
49	J	315	KC2	CHC-C4B-NB	6.10	130.06	124.45
48	2	301	A86	O1-C20-C19	-6.10	108.80	113.38
49	8	316	KC2	CHC-C4B-NB	6.10	130.06	124.45
48	D	305	A86	C33-C32-C31	6.10	115.14	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	l	201	CLA	C4A-NA-C1A	6.10	109.45	106.71
49	5	313	KC2	CHC-C4B-NB	6.10	130.06	124.45
48	y	306	A86	O1-C20-C19	-6.10	108.80	113.38
39	a	816	CLA	C4A-NA-C1A	6.09	109.44	106.71
39	B	209	CLA	C4A-NA-C1A	6.09	109.44	106.71
39	9	307	CLA	C4A-NA-C1A	6.09	109.44	106.71
49	8	314	KC2	CHC-C4B-NB	6.09	130.05	124.45
49	4	318	KC2	CHC-C4B-NB	6.08	130.04	124.45
43	J	305	DD6	O1-C20-C21	6.08	122.34	115.06
49	L	321	KC2	CHC-C4B-NB	6.07	130.03	124.45
49	1	312	KC2	CHB-C1B-NB	6.07	130.03	124.45
49	T	314	KC2	CHC-C4B-NB	6.07	130.03	124.45
39	T	309	CLA	C4A-NA-C1A	6.07	109.43	106.71
39	A	307	CLA	C4A-NA-C1A	6.06	109.43	106.71
39	I	316	CLA	C4A-NA-C1A	6.06	109.43	106.71
49	1	314	KC2	CHC-C4B-NB	6.06	130.02	124.45
39	l	205	CLA	C4A-NA-C1A	6.05	109.43	106.71
39	U	208	CLA	C4A-NA-C1A	6.05	109.43	106.71
49	y	314	KC2	CHC-C4B-NB	6.04	130.01	124.45
39	E	313	CLA	C4A-NA-C1A	6.04	109.42	106.71
49	C	312	KC2	CHC-C4B-NB	6.03	130.00	124.45
43	O	303	DD6	C3-C2-C1	-6.03	118.70	127.31
52	W	321	A1EB4	C21-C20-C19	6.03	121.06	114.28
51	4	315	A1ECV	C2A-CAA-CBA	-6.03	115.03	128.63
39	L	311	CLA	C4A-NA-C1A	6.03	109.42	106.71
52	M	322	A1EB4	O1-C20-C19	-6.03	108.86	113.38
48	B	201	A86	C25-C26-C27	-6.02	118.72	127.31
39	a	820	CLA	C4A-NA-C1A	6.01	109.41	106.71
48	B	201	A86	C3-C2-C1	-6.01	118.73	127.31
49	K	313	KC2	CHC-C4B-NB	6.01	129.97	124.45
43	x	303	DD6	C3-C2-C1	-6.00	118.75	127.31
39	A	311	CLA	C4A-NA-C1A	5.99	109.40	106.71
43	3	301	DD6	C3-C2-C1	-5.99	118.76	127.31
39	Q	321	CLA	C4A-NA-C1A	5.99	109.40	106.71
39	A	308	CLA	C4A-NA-C1A	5.98	109.39	106.71
39	K	308	CLA	C4A-NA-C1A	5.98	109.39	106.71
49	4	317	KC2	CHC-C4B-NB	5.98	129.95	124.45
39	E	307	CLA	C4A-NA-C1A	5.97	109.39	106.71
42	b	846	BCR	C24-C23-C22	-5.97	117.22	126.23
39	O	314	CLA	C4A-NA-C1A	5.96	109.39	106.71
39	0	310	CLA	C4A-NA-C1A	5.96	109.39	106.71
39	1	309	CLA	C4A-NA-C1A	5.96	109.39	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	S	303	A1EB1	C3-C2-C1	-5.96	118.81	127.31
50	K	305	A1EB1	O1-C20-C19	-5.95	108.91	113.38
48	X	302	A86	C25-C26-C27	-5.95	118.83	127.31
52	P	319	A1EB4	O1-C20-C19	-5.94	108.92	113.38
48	R	302	A86	O4-C38-C39	5.94	122.02	111.09
43	4	308	DD6	C3-C2-C1	-5.93	118.84	127.31
49	O	317	KC2	CHB-C1B-NB	5.93	129.91	124.45
39	a	823	CLA	C4A-NA-C1A	5.93	109.37	106.71
48	1	302	A86	O1-C20-C19	-5.93	108.93	113.38
49	x	312	KC2	CHC-C4B-NB	5.92	129.90	124.45
49	6	316	KC2	CHC-C4B-NB	5.92	129.89	124.45
43	z	305	DD6	C3-C2-C1	-5.91	118.87	127.31
49	T	315	KC2	CHC-C4B-NB	5.91	129.88	124.45
48	9	304	A86	O1-C20-C21	-5.91	107.98	115.06
39	V	310	CLA	C4A-NA-C1A	5.90	109.36	106.71
51	R	310	A1ECV	C2A-CAA-CBA	-5.90	115.33	128.63
49	3	317	KC2	CHC-C4B-NB	5.90	129.87	124.45
49	R	306	KC2	CHC-C4B-NB	5.89	129.87	124.45
50	F	304	A1EB1	C4-C5-C6	-5.89	118.91	127.31
49	3	315	KC2	CHC-C4B-NB	5.89	129.87	124.45
39	5	307	CLA	C4A-NA-C1A	5.89	109.35	106.71
43	1	304	DD6	C14-C13-C11	-5.88	116.40	125.53
43	A	303	DD6	C9-C10-C11	-5.88	118.91	127.31
49	x	315	KC2	CHC-C4B-NB	5.88	129.85	124.45
51	x	310	A1ECV	C2A-CAA-CBA	-5.87	115.39	128.63
48	L	307	A86	C17-C16-C15	5.87	115.15	109.16
49	M	313	KC2	CHC-C4B-NB	5.86	129.84	124.45
43	y	304	DD6	C3-C2-C1	-5.86	118.95	127.31
39	x	307	CLA	C4A-NA-C1A	5.85	109.34	106.71
48	O	307	A86	O1-C20-C19	-5.85	108.98	113.38
49	P	306	KC2	CHC-C4B-NB	5.85	129.83	124.45
49	X	306	KC2	CHC-C4B-NB	5.84	129.82	124.45
39	T	313	CLA	C4A-NA-C1A	5.84	109.33	106.71
50	6	304	A1EB1	O4-C38-C39	5.84	121.84	111.09
48	T	306	A86	C17-C16-C15	5.84	115.12	109.16
48	G	301	A86	C25-C26-C27	-5.84	118.98	127.31
48	6	303	A86	O1-C20-C19	-5.83	109.00	113.38
39	0	311	CLA	C4A-NA-C1A	5.83	109.33	106.71
49	P	313	KC2	CHC-C4B-NB	5.83	129.81	124.45
48	W	303	A86	C25-C26-C27	-5.83	118.99	127.31
49	1	315	KC2	CHC-C4B-NB	5.83	129.81	124.45
42	f	801	BCR	C24-C23-C22	-5.81	117.45	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Q	302	A86	O1-C20-C19	-5.80	109.02	113.38
49	A	310	KC2	CHC-C4B-NB	5.80	129.78	124.45
52	P	318	A1EB4	C3-C2-C1	-5.80	119.03	127.31
48	0	306	A86	C17-C16-C15	5.80	115.08	109.16
48	7	307	A86	O1-C20-C19	-5.80	109.03	113.38
43	J	305	DD6	C3-C2-C1	-5.79	119.04	127.31
48	L	305	A86	O1-C20-C21	-5.79	108.12	115.06
39	J	314	CLA	C4A-NA-C1A	5.79	109.31	106.71
39	U	210	CLA	C4A-NA-C1A	5.79	109.31	106.71
49	3	321	KC2	CHB-C1B-NB	5.78	129.77	124.45
49	M	314	KC2	CHC-C4B-NB	5.78	129.77	124.45
48	8	307	A86	C3-C2-C1	-5.78	119.06	127.31
39	Q	310	CLA	C4A-NA-C1A	5.78	109.30	106.71
49	V	314	KC2	CHC-C4B-NB	5.77	129.76	124.45
50	8	304	A1EB1	C17-C16-C15	5.77	115.05	109.16
48	8	309	A86	C3-C2-C1	-5.77	119.08	127.31
48	P	302	A86	C25-C26-C27	-5.76	119.08	127.31
50	h	203	A1EB1	O1-C20-C21	-5.75	108.17	115.06
49	6	319	KC2	CHC-C4B-NB	5.74	129.73	124.45
50	L	303	A1EB1	O4-C38-C39	5.74	121.65	111.09
49	0	319	KC2	CHB-C1B-NB	5.74	129.73	124.45
48	M	302	A86	C25-C26-C27	-5.71	119.16	127.31
48	1	303	A86	O1-C20-C21	-5.71	108.22	115.06
48	6	302	A86	O1-C20-C19	-5.70	109.10	113.38
49	0	317	KC2	CHC-C4B-NB	5.70	129.69	124.45
50	T	307	A1EB1	C4-C5-C6	-5.70	119.18	127.31
50	3	324	A1EB1	C3-C4-C5	-5.70	111.81	123.47
39	b	826	CLA	C4A-NA-C1A	5.69	109.26	106.71
43	T	303	DD6	O1-C20-C19	-5.68	109.11	113.38
48	9	306	A86	C17-C16-C15	5.68	114.96	109.16
50	F	304	A1EB1	O4-C38-C39	5.68	121.54	111.09
49	Y	308	KC2	CHC-C4B-NB	5.68	129.67	124.45
39	b	805	CLA	C4A-NA-C1A	5.67	109.26	106.71
48	2	302	A86	O1-C20-C19	-5.67	109.12	113.38
48	0	309	A86	O1-C20-C19	-5.67	109.12	113.38
48	T	305	A86	O1-C20-C19	-5.66	109.13	113.38
49	V	315	KC2	CHC-C4B-NB	5.66	129.66	124.45
48	6	307	A86	C4-C5-C6	-5.66	119.23	127.31
49	8	316	KC2	O2D-CGD-CBD	5.66	121.32	111.27
49	W	315	KC2	CHC-C4B-NB	5.65	129.65	124.45
49	F	311	KC2	O2D-CGD-CBD	5.65	121.31	111.27
49	I	312	KC2	O2D-CGD-CBD	5.65	121.31	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	7	311	A86	C33-C32-C31	5.64	114.69	109.21
49	8	317	KC2	CHC-C4B-NB	5.63	129.63	124.45
49	G	317	KC2	O2D-CGD-CBD	5.63	121.27	111.27
50	8	304	A1EB1	O4-C38-C39	5.63	121.44	111.09
49	7	320	KC2	CHC-C4B-NB	5.62	129.62	124.45
39	7	313	CLA	C4A-NA-C1A	5.60	109.22	106.71
49	V	320	KC2	O2D-CGD-CBD	5.60	121.22	111.27
50	D	308	A1EB1	C3-C2-C1	-5.60	119.32	127.31
51	y	311	A1ECV	C2A-CAA-CBA	-5.59	116.02	128.63
42	f	804	BCR	C11-C10-C9	-5.59	119.33	127.31
48	P	302	A86	O4-C38-C39	5.59	121.37	111.09
43	J	306	DD6	C9-C10-C11	-5.59	119.34	127.31
48	2	301	A86	O1-C20-C21	-5.58	108.37	115.06
50	H	301	A1EB1	O1-C20-C19	-5.58	109.19	113.38
48	8	323	A86	C3-C2-C1	-5.58	119.34	127.31
50	H	301	A1EB1	O4-C38-C39	5.58	121.36	111.09
50	y	302	A1EB1	O1-C20-C19	-5.58	109.19	113.38
48	5	301	A86	C25-C26-C27	-5.58	119.35	127.31
39	X	308	CLA	C4A-NA-C1A	5.57	109.21	106.71
48	V	301	A86	O4-C38-C39	5.57	121.33	111.09
50	R	303	A1EB1	O1-C20-C19	-5.56	109.20	113.38
48	L	302	A86	C25-C26-C27	5.55	135.23	127.31
48	O	302	A86	C21-C20-C19	5.54	120.52	114.28
48	Q	305	A86	O1-C20-C19	-5.54	109.22	113.38
49	1	312	KC2	CHC-C4B-NB	5.53	129.54	124.45
50	0	305	A1EB1	C25-C26-C27	-5.53	119.38	127.26
49	9	318	KC2	CHC-C4B-NB	5.53	129.54	124.45
50	8	306	A1EB1	O4-C38-C39	5.53	121.26	111.09
50	V	305	A1EB1	O4-C38-C39	5.52	121.25	111.09
48	9	301	A86	O1-C20-C21	-5.52	108.44	115.06
48	D	305	A86	C3-C2-C1	-5.52	119.43	127.31
43	7	310	DD6	C3-C2-C1	-5.52	119.44	127.31
48	X	302	A86	C4-C5-C6	-5.52	119.44	127.31
50	1	305	A1EB1	C21-C20-C19	5.52	120.48	114.28
48	W	304	A86	O1-C20-C19	-5.51	109.24	113.38
49	z	312	KC2	CHC-C4B-NB	5.51	129.52	124.45
50	6	308	A1EB1	O4-C38-C39	5.50	121.21	111.09
50	T	302	A1EB1	C33-C32-C31	5.50	114.56	109.21
50	7	303	A1EB1	O4-C38-C39	5.50	121.20	111.09
39	9	320	CLA	C4A-NA-C1A	5.50	109.18	106.71
52	M	322	A1EB4	O1-C15-C14	-5.50	110.14	115.71
43	G	306	DD6	C4-C5-C6	-5.50	119.47	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	J	306	DD6	C21-C20-C19	5.49	120.45	114.28
52	P	319	A1EB4	O1-C15-C14	-5.49	110.15	115.71
48	7	307	A86	O4-C38-C39	5.49	121.18	111.09
48	y	306	A86	O4-C38-C39	5.48	121.18	111.09
48	3	307	A86	C3-C2-C1	-5.48	119.49	127.31
48	L	306	A86	C25-C26-C27	-5.48	119.49	127.31
50	1	305	A1EB1	O4-C38-C39	5.47	121.16	111.09
50	8	306	A1EB1	C3-C2-C1	-5.47	119.50	127.31
48	L	302	A86	C25-C24-C1	-5.47	111.04	126.42
39	S	309	CLA	C4A-NA-C1A	5.47	109.17	106.71
52	M	305	A1EB4	C21-C20-C19	5.47	120.43	114.28
48	R	317	A86	C33-C32-C31	5.47	114.52	109.21
48	6	307	A86	C25-C26-C27	-5.46	119.51	127.31
48	0	306	A86	O1-C20-C19	-5.46	109.28	113.38
50	y	301	A1EB1	C3-C2-C1	-5.46	119.52	127.31
52	P	318	A1EB4	C21-C20-C19	5.46	120.42	114.28
50	D	308	A1EB1	O4-C38-C39	5.45	121.12	111.09
48	4	305	A86	O1-C20-C19	-5.45	109.29	113.38
50	5	302	A1EB1	C25-C26-C27	-5.44	119.51	127.26
42	l	202	BCR	C7-C8-C9	-5.44	118.01	126.23
48	1	302	A86	C4-C5-C6	-5.43	119.56	127.31
48	y	306	A86	C17-C16-C15	5.43	114.70	109.16
49	3	318	KC2	CHC-C4B-NB	5.43	129.44	124.45
48	G	305	A86	C17-C16-C15	5.43	114.70	109.16
43	Q	303	DD6	C9-C10-C11	-5.42	119.57	127.31
52	T	304	A1EB4	C21-C20-C19	5.42	120.38	114.28
48	O	302	A86	C4-C5-C6	-5.41	119.58	127.31
50	S	302	A1EB1	O4-C38-C39	5.41	121.04	111.09
50	8	304	A1EB1	C4-C5-C6	-5.41	119.59	127.31
50	2	304	A1EB1	C3-C2-C1	-5.41	119.60	127.31
50	O	301	A1EB1	C3-C2-C1	-5.40	119.60	127.31
48	Q	301	A86	C17-C16-C15	5.40	114.67	109.16
48	7	311	A86	O1-C20-C21	-5.40	108.59	115.06
48	Q	304	A86	O1-C20-C19	-5.39	109.33	113.38
49	9	313	KC2	CHC-C4B-NB	5.39	129.41	124.45
49	S	315	KC2	CHC-C4B-NB	5.39	129.40	124.45
43	4	307	DD6	C3-C2-C1	-5.38	119.63	127.31
48	5	301	A86	C4-C5-C6	-5.38	119.63	127.31
48	4	310	A86	C17-C16-C15	5.38	114.65	109.16
46	0	324	LMG	O7-C10-C11	5.38	120.99	111.09
50	1	305	A1EB1	C17-C16-C15	5.38	114.65	109.16
50	3	310	A1EB1	C4-C5-C6	-5.37	119.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	x	301	A1EB1	O4-C38-C39	5.37	120.97	111.09
48	S	305	A86	C3-C2-C1	-5.37	119.64	127.31
48	3	306	A86	C4-C5-C6	-5.37	119.65	127.31
42	k	204	BCR	C11-C10-C9	-5.36	119.66	127.31
48	Q	301	A86	O1-C20-C19	-5.36	109.36	113.38
50	J	302	A1EB1	C4-C5-C6	-5.36	119.67	127.31
43	D	306	DD6	O1-C20-C19	-5.36	109.36	113.38
42	i	102	BCR	C3-C4-C5	-5.35	104.52	114.08
49	z	313	KC2	CHC-C4B-NB	5.35	129.37	124.45
48	O	302	A86	O1-C20-C19	-5.35	109.36	113.38
50	K	302	A1EB1	C33-C32-C31	5.35	114.41	109.21
50	2	306	A1EB1	C33-C32-C31	5.34	114.41	109.21
48	P	303	A86	O1-C20-C19	-5.34	109.37	113.38
48	M	303	A86	O1-C20-C19	-5.34	109.37	113.38
43	C	301	DD6	C21-C20-C19	5.33	120.28	114.28
50	J	302	A1EB1	C25-C26-C27	-5.33	119.67	127.26
50	0	305	A1EB1	C3-C2-C1	-5.33	119.71	127.31
50	6	308	A1EB1	C4-C5-C6	-5.33	119.71	127.31
49	L	312	KC2	CHC-C4B-NB	5.32	129.35	124.45
48	U	202	A86	C4-C5-C6	-5.32	119.71	127.31
48	8	305	A86	O1-C20-C19	-5.32	109.38	113.38
48	3	308	A86	O4-C38-C39	5.32	120.88	111.09
43	I	307	DD6	C9-C10-C11	-5.32	119.72	127.31
48	H	302	A86	C17-C16-C15	5.31	114.58	109.16
43	3	304	DD6	C21-C20-C19	5.31	120.25	114.28
49	O	317	KC2	CHC-C4B-NB	5.31	129.33	124.45
42	a	845	BCR	C16-C17-C18	-5.31	119.73	127.31
49	0	319	KC2	CHC-C4B-NB	5.31	129.33	124.45
42	f	801	BCR	C16-C17-C18	-5.31	119.74	127.31
49	4	324	KC2	O2D-CGD-CBD	5.30	120.69	111.27
48	9	306	A86	C21-C20-C19	5.29	120.24	114.28
48	8	309	A86	O1-C20-C19	-5.29	109.41	113.38
48	4	309	A86	O1-C20-C19	-5.29	109.41	113.38
50	G	308	A1EB1	C17-C16-C15	5.29	114.56	109.16
50	2	306	A1EB1	C4-C5-C6	-5.29	119.77	127.31
50	7	305	A1EB1	C4-C5-C6	-5.28	119.77	127.31
49	0	319	KC2	C1D-ND-C4D	5.28	110.08	106.33
48	2	302	A86	C3-C2-C1	-5.28	119.78	127.31
39	b	802	CLA	C4A-NA-C1A	5.28	109.08	106.71
48	1	306	A86	C4-C5-C6	-5.28	119.78	127.31
49	P	313	KC2	CHD-C1D-ND	5.28	129.84	124.26
48	9	304	A86	C3-C2-C1	-5.27	119.78	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	6	308	A1EB1	C36-C31-C32	5.27	124.92	119.70
48	y	306	A86	C4-C5-C6	-5.26	119.80	127.31
48	1	307	A86	C4-C5-C6	-5.26	119.81	127.31
43	j	102	DD6	C4-C5-C6	-5.25	119.81	127.31
48	W	303	A86	C4-C5-C6	-5.25	119.82	127.31
50	6	301	A1EB1	C4-C5-C6	-5.25	119.82	127.31
48	R	301	A86	O1-C20-C21	-5.24	108.77	115.06
50	0	307	A1EB1	C17-C16-C15	5.24	114.51	109.16
50	K	305	A1EB1	C21-C20-C19	5.24	120.17	114.28
43	3	304	DD6	C21-C20-C15	-5.22	113.50	122.26
43	y	303	DD6	C3-C2-C1	-5.22	119.86	127.31
48	M	302	A86	C17-C16-C15	5.22	114.49	109.16
48	G	305	A86	O4-C38-C39	5.22	120.70	111.09
50	7	305	A1EB1	C17-C16-C15	5.21	114.48	109.16
50	S	303	A1EB1	O1-C20-C19	-5.21	109.47	113.38
42	b	847	BCR	C15-C14-C13	-5.21	119.88	127.31
48	O	306	A86	C3-C2-C1	-5.21	119.88	127.31
50	0	307	A1EB1	C21-C20-C19	5.20	120.13	114.28
48	1	306	A86	O1-C20-C19	-5.20	109.48	113.38
48	9	303	A86	O1-C20-C19	-5.20	109.48	113.38
48	8	309	A86	C25-C26-C27	-5.19	119.90	127.31
49	7	319	KC2	O2D-CGD-CBD	5.19	120.50	111.27
50	L	303	A1EB1	O1-C20-C19	-5.19	109.48	113.38
51	G	316	A1ECV	C2A-CAA-CBA	-5.19	116.92	128.63
52	X	305	A1EB4	C21-C20-C19	5.19	120.11	114.28
50	x	301	A1EB1	C25-C26-C27	-5.18	119.88	127.26
47	E	320	SQD	C1-O5-C5	5.18	123.86	113.69
49	W	308	KC2	CHD-C1D-ND	5.17	129.74	124.26
50	U	203	A1EB1	C21-C20-C19	5.17	120.09	114.28
48	F	302	A86	O1-C20-C19	-5.16	109.50	113.38
48	3	308	A86	O1-C20-C21	-5.16	108.88	115.06
48	4	310	A86	O4-C38-C39	5.15	120.56	111.09
48	R	302	A86	C3-C2-C1	-5.14	119.97	127.31
48	U	206	A86	C4-C5-C6	-5.14	119.97	127.31
50	6	304	A1EB1	C4-C5-C6	-5.14	119.97	127.31
48	Z	301	A86	C3-C2-C1	-5.14	119.98	127.31
48	0	304	A86	O4-C38-C39	5.13	120.53	111.09
49	K	313	KC2	O2D-CGD-CBD	5.13	120.39	111.27
50	H	301	A1EB1	C4-C5-C6	-5.12	120.00	127.31
50	x	302	A1EB1	C4-C5-C6	-5.12	120.00	127.31
51	O	315	A1ECV	C2A-CAA-CBA	-5.12	117.08	128.63
43	4	308	DD6	O1-C20-C21	-5.12	108.92	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	y	305	A86	C4-C5-C6	-5.12	120.01	127.31
50	6	304	A1EB1	O1-C20-C19	-5.12	109.54	113.38
48	3	308	A86	C3-C2-C1	-5.11	120.01	127.31
50	7	305	A1EB1	C25-C26-C27	-5.11	119.98	127.26
49	V	315	KC2	O2D-CGD-CBD	5.10	120.33	111.27
42	a	845	BCR	C11-C10-C9	-5.10	120.04	127.31
48	H	302	A86	O1-C20-C19	-5.10	109.55	113.38
48	7	308	A86	C3-C2-C1	-5.09	120.05	127.31
49	5	311	KC2	CHD-C1D-ND	5.09	129.64	124.26
43	S	306	DD6	C3-C2-C1	-5.09	120.05	127.31
48	4	306	A86	C25-C26-C27	-5.07	120.07	127.31
43	B	202	DD6	C4-C5-C6	-5.07	120.07	127.31
48	1	303	A86	C3-C2-C1	-5.07	120.07	127.31
49	W	315	KC2	O2D-CGD-CBD	5.07	120.28	111.27
48	6	302	A86	C4-C5-C6	-5.07	120.08	127.31
48	7	312	A86	O4-C38-C39	5.06	120.41	111.09
47	D	320	SQD	O9-S-C6	5.06	112.96	106.94
48	3	308	A86	C33-C32-C31	5.06	114.13	109.21
51	1	318	A1ECV	C2A-CAA-CBA	-5.06	117.22	128.63
52	P	319	A1EB4	C3-C2-C1	-5.06	120.09	127.31
50	V	307	A1EB1	O1-C20-C19	-5.05	109.59	113.38
50	0	303	A1EB1	C25-C26-C27	-5.05	120.06	127.26
50	4	304	A1EB1	C3-C2-C1	-5.05	120.10	127.31
50	4	304	A1EB1	O1-C20-C19	-5.05	109.59	113.38
50	y	301	A1EB1	O1-C20-C19	-5.05	109.59	113.38
50	Q	307	A1EB1	O1-C20-C21	-5.05	109.00	115.06
43	7	309	DD6	C3-C2-C1	-5.05	120.11	127.31
50	x	302	A1EB1	C25-C26-C27	-5.04	120.08	127.26
43	J	306	DD6	C3-C2-C1	-5.04	120.11	127.31
42	b	846	BCR	C7-C8-C9	-5.04	118.62	126.23
52	5	304	A1EB4	C21-C20-C19	5.04	119.95	114.28
48	x	305	A86	C33-C32-C31	5.03	114.10	109.21
43	4	307	DD6	C21-C20-C19	5.03	119.94	114.28
52	R	305	A1EB4	C21-C20-C19	5.02	119.93	114.28
49	R	312	KC2	CHD-C1D-ND	5.02	129.57	124.26
49	4	324	KC2	CHD-C1D-ND	5.02	129.57	124.26
48	0	301	A86	O1-C20-C19	-5.02	109.61	113.38
50	0	302	A1EB1	C21-C20-C19	5.02	119.93	114.28
48	G	301	A86	C3-C2-C1	-5.02	120.15	127.31
52	W	306	A1EB4	C21-C20-C19	5.02	119.92	114.28
50	R	303	A1EB1	C17-C16-C15	5.01	114.27	109.16
42	a	845	BCR	C20-C21-C22	-5.01	120.16	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	M	322	A1EB4	C3-C2-C1	-5.01	120.16	127.31
52	P	305	A1EB4	C21-C20-C19	5.01	119.91	114.28
52	W	321	A1EB4	C3-C2-C1	-5.01	120.17	127.31
48	V	304	A86	O1-C20-C21	-5.01	109.06	115.06
50	F	304	A1EB1	C36-C31-C32	5.00	124.66	119.70
42	b	845	BCR	C15-C14-C13	-5.00	120.17	127.31
42	i	102	BCR	C20-C21-C22	-5.00	120.17	127.31
48	L	307	A86	C25-C26-C27	-5.00	120.17	127.31
50	U	205	A1EB1	C4-C5-C6	-5.00	120.18	127.31
50	G	302	A1EB1	O1-C20-C19	-5.00	109.63	113.38
49	V	320	KC2	CHD-C1D-ND	5.00	129.54	124.26
49	6	314	KC2	CHD-C1D-ND	4.99	129.54	124.26
49	M	307	KC2	CHD-C1D-ND	4.99	129.54	124.26
48	V	301	A86	O1-C15-C14	-4.99	103.20	113.21
50	9	302	A1EB1	C4-C5-C6	-4.98	120.21	127.31
48	0	306	A86	C21-C20-C19	4.97	119.88	114.28
50	7	305	A1EB1	C21-C20-C19	4.97	119.87	114.28
48	8	302	A86	C4-C5-C6	-4.97	120.22	127.31
50	U	205	A1EB1	O1-C20-C19	-4.97	109.65	113.38
48	I	304	A86	C17-C16-C15	4.97	114.23	109.16
50	L	303	A1EB1	C4-C5-C6	-4.96	120.22	127.31
49	B	208	KC2	O2D-CGD-CBD	4.96	120.09	111.27
48	J	301	A86	O4-C38-C39	4.96	120.21	111.09
43	J	305	DD6	C9-C10-C11	-4.96	120.23	127.31
50	D	308	A1EB1	C21-C20-C19	4.96	119.86	114.28
43	R	304	DD6	C21-C20-C19	4.96	119.86	114.28
43	A	304	DD6	C4-C5-C6	-4.96	120.23	127.31
48	S	307	A86	C17-C16-C15	4.96	114.22	109.16
48	R	302	A86	C4-C5-C6	-4.95	120.24	127.31
49	G	315	KC2	CHD-C1D-ND	4.95	129.50	124.26
52	M	305	A1EB4	O4-C38-C42	4.95	120.20	111.09
50	7	305	A1EB1	C36-C31-C32	4.95	124.61	119.70
48	2	305	A86	C4-C3-C2	-4.94	113.34	123.47
43	A	302	DD6	C21-C20-C19	4.94	119.84	114.28
48	M	302	A86	C4-C5-C6	-4.94	120.25	127.31
43	a	846	DD6	C9-C10-C11	-4.94	120.26	127.31
42	f	804	BCR	C15-C14-C13	-4.94	120.26	127.31
50	z	302	A1EB1	C3-C2-C1	-4.94	120.26	127.31
48	S	307	A86	C25-C26-C27	-4.94	120.27	127.31
48	1	307	A86	C25-C26-C27	-4.93	120.27	127.31
49	F	311	KC2	CHD-C1D-ND	4.93	129.48	124.26
48	U	206	A86	O4-C38-C39	4.93	120.16	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	I	312	KC2	CHD-C1D-ND	4.93	129.47	124.26
43	y	304	DD6	C21-C20-C19	4.93	119.82	114.28
50	8	304	A1EB1	C21-C20-C19	4.93	119.82	114.28
49	2	313	KC2	CHD-C1D-ND	4.92	129.47	124.26
48	G	305	A86	C4-C5-C6	-4.92	120.29	127.31
50	4	302	A1EB1	O1-C20-C19	-4.92	109.69	113.38
43	7	309	DD6	C21-C20-C19	4.91	119.81	114.28
48	9	301	A86	C21-C20-C19	4.91	119.80	114.28
48	y	306	A86	C25-C26-C27	-4.91	120.30	127.31
50	7	304	A1EB1	C3-C2-C1	-4.91	120.30	127.31
50	G	308	A1EB1	C28-C27-C26	-4.91	118.51	124.93
50	4	302	A1EB1	C3-C2-C1	-4.91	120.31	127.31
49	I	303	KC2	CHD-C1D-ND	4.90	129.45	124.26
52	P	319	A1EB4	O4-C38-C42	4.90	120.11	111.09
49	z	313	KC2	O2D-CGD-CBD	4.90	119.67	111.49
48	S	305	A86	C25-C26-C27	-4.90	120.31	127.31
48	T	306	A86	C3-C2-C1	-4.90	120.31	127.31
48	L	302	A86	C33-C32-C31	-4.90	104.45	109.21
52	M	322	A1EB4	O4-C38-C42	4.90	120.10	111.09
48	U	206	A86	C17-C16-C15	4.90	114.16	109.16
49	x	312	KC2	O2D-CGD-CBD	4.90	119.97	111.27
49	T	312	KC2	O2D-CGD-CBD	4.89	119.97	111.27
51	0	321	A1ECV	C2A-CAA-CBA	-4.89	117.60	128.63
43	z	304	DD6	C3-C2-C1	-4.89	120.33	127.31
49	T	314	KC2	CHD-C1D-ND	4.89	129.43	124.26
50	3	309	A1EB1	C4-C5-C6	-4.89	120.34	127.31
50	7	306	A1EB1	C3-C2-C1	-4.89	120.34	127.31
43	O	304	DD6	C3-C2-C1	-4.88	120.34	127.31
49	Q	318	KC2	O2D-CGD-CBD	4.88	119.94	111.27
43	J	304	DD6	C4-C5-C6	-4.88	120.35	127.31
48	Q	301	A86	C3-C2-C1	-4.88	120.35	127.31
49	z	312	KC2	O2D-CGD-CBD	4.88	119.94	111.27
48	Q	308	A86	C21-C20-C19	4.88	119.77	114.28
50	z	302	A1EB1	C33-C32-C31	4.88	113.95	109.21
50	V	302	A1EB1	O4-C38-C39	4.87	120.06	111.09
43	D	306	DD6	C4-C5-C6	-4.87	120.36	127.31
43	o	204	DD6	C21-C20-C19	4.87	119.76	114.28
43	X	304	DD6	C21-C20-C19	4.87	119.76	114.28
48	8	323	A86	C25-C26-C27	-4.87	120.36	127.31
43	Q	306	DD6	C21-C20-C19	4.87	119.75	114.28
48	V	304	A86	O4-C38-C39	4.86	120.04	111.09
51	9	314	A1ECV	C2A-CAA-CBA	-4.86	117.66	128.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	5	302	A1EB1	C21-C20-C19	4.86	119.75	114.28
48	O	306	A86	O4-C38-C39	4.86	120.03	111.09
48	0	309	A86	C3-C2-C1	-4.86	120.37	127.31
48	L	301	A86	O1-C20-C19	-4.86	109.73	113.38
48	8	309	A86	O1-C20-C21	-4.86	109.23	115.06
50	6	306	A1EB1	C3-C2-C1	-4.86	120.38	127.31
49	G	317	KC2	CHD-C1D-ND	4.86	129.40	124.26
52	W	321	A1EB4	C9-C10-C11	-4.85	121.17	127.00
50	3	324	A1EB1	C21-C20-C19	4.85	119.74	114.28
43	I	306	DD6	C21-C20-C19	4.85	119.73	114.28
48	T	305	A86	O4-C38-C39	4.85	120.01	111.09
43	H	305	DD6	C21-C20-C19	4.85	119.73	114.28
50	4	304	A1EB1	C36-C31-C32	4.85	124.50	119.70
50	8	308	A1EB1	O4-C38-C39	4.84	120.00	111.09
48	G	301	A86	C33-C32-C31	4.84	113.92	109.21
43	3	301	DD6	C21-C20-C19	4.84	119.73	114.28
49	M	314	KC2	CHD-C1D-ND	4.84	129.38	124.26
48	8	302	A86	O4-C38-C39	4.83	119.98	111.09
48	8	303	A86	C25-C26-C27	-4.83	120.41	127.31
42	l	207	BCR	C24-C23-C22	-4.83	118.93	126.23
42	b	850	BCR	C16-C17-C18	-4.83	120.42	127.31
43	T	303	DD6	C21-C20-C19	4.83	119.71	114.28
48	4	310	A86	C21-C20-C19	4.83	119.71	114.28
50	4	302	A1EB1	C4-C5-C6	-4.83	120.42	127.31
48	L	306	A86	O4-C38-C39	4.83	119.97	111.09
48	L	305	A86	C3-C2-C1	-4.82	120.42	127.31
52	T	304	A1EB4	C3-C2-C1	-4.82	120.42	127.31
43	J	305	DD6	C21-C20-C15	-4.82	114.18	122.26
48	V	301	A86	C21-C20-C19	4.82	119.70	114.28
51	0	321	A1ECV	O2-CMC-O1	-4.82	114.02	123.45
43	5	303	DD6	C21-C20-C19	4.82	119.70	114.28
43	O	304	DD6	O1-C20-C21	4.82	120.83	115.06
52	T	304	A1EB4	O4-C38-C42	4.82	119.95	111.09
50	8	301	A1EB1	C25-C26-C27	-4.82	120.40	127.26
49	3	317	KC2	CHD-C1D-ND	4.82	129.36	124.26
43	x	304	DD6	C21-C20-C19	4.82	119.70	114.28
48	5	301	A86	C3-C2-C1	-4.81	120.44	127.31
48	8	323	A86	C21-C20-C19	4.81	119.69	114.28
49	9	313	KC2	CHD-C1D-ND	4.81	129.35	124.26
48	8	305	A86	C8-C6-C5	4.81	126.31	118.94
48	8	302	A86	O1-C20-C21	-4.80	109.30	115.06
43	V	303	DD6	C21-C20-C19	4.80	119.68	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	X	312	KC2	O2D-CGD-CBD	4.80	119.80	111.27
48	C	303	A86	C3-C2-C1	-4.80	120.46	127.31
50	7	306	A1EB1	O1-C20-C19	-4.80	109.78	113.38
43	a	846	DD6	C3-C2-C1	-4.79	120.47	127.31
50	8	306	A1EB1	C25-C26-C27	-4.79	120.43	127.26
42	b	846	BCR	C11-C10-C9	-4.79	120.47	127.31
43	E	305	DD6	C21-C20-C19	4.79	119.67	114.28
48	3	307	A86	C4-C5-C6	-4.79	120.47	127.31
52	T	304	A1EB4	C20-O1-C15	4.79	64.85	61.17
49	X	318	KC2	O2D-CGD-CBD	4.79	119.78	111.27
48	3	307	A86	O4-C38-C39	4.79	119.90	111.09
50	3	324	A1EB1	O4-C38-C39	4.79	119.90	111.09
48	G	301	A86	O4-C38-C39	4.78	119.89	111.09
48	4	328	A86	C17-C16-C15	4.78	114.04	109.16
48	2	302	A86	O4-C38-C39	4.78	119.89	111.09
51	z	316	A1ECV	C2A-CAA-CBA	-4.78	117.84	128.63
43	z	304	DD6	C21-C20-C19	4.78	119.66	114.28
48	D	305	A86	O4-C38-C39	4.78	119.88	111.09
43	F	303	DD6	C21-C20-C19	4.78	119.66	114.28
48	z	303	A86	C25-C26-C27	-4.78	120.49	127.31
49	4	317	KC2	O2D-CGD-CBD	4.78	119.76	111.27
43	A	301	DD6	C21-C20-C19	4.78	119.65	114.28
48	M	306	A86	C4-C5-C6	-4.77	120.50	127.31
48	4	328	A86	C3-C2-C1	-4.77	120.50	127.31
50	L	303	A1EB1	C36-C31-C32	4.77	124.43	119.70
49	8	314	KC2	CHD-C1D-ND	4.77	129.31	124.26
48	8	302	A86	O1-C20-C19	-4.77	109.80	113.38
51	Q	319	A1ECV	C2A-CAA-CBA	-4.77	117.88	128.63
49	9	318	KC2	O2D-CGD-CBD	4.77	119.74	111.27
49	6	317	KC2	O2D-CGD-CBD	4.77	119.74	111.27
48	S	307	A86	C4-C5-C6	-4.77	120.51	127.31
49	R	312	KC2	O2D-CGD-CBD	4.76	119.73	111.27
48	6	302	A86	C25-C26-C27	-4.76	120.52	127.31
43	E	305	DD6	C4-C5-C6	-4.76	120.52	127.31
50	7	304	A1EB1	C25-C26-C27	-4.76	120.48	127.26
48	y	306	A86	C3-C2-C1	-4.76	120.52	127.31
48	Q	302	A86	C21-C20-C19	4.76	119.63	114.28
48	K	301	A86	C3-C2-C1	-4.76	120.52	127.31
47	F	318	SQD	O7-S-C6	4.75	112.59	106.94
50	3	303	A1EB1	O1-C20-C21	-4.75	109.36	115.06
49	Q	318	KC2	CHD-C1D-ND	4.75	129.28	124.26
49	M	311	KC2	O2D-CGD-CBD	4.75	119.71	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	B	201	A86	O4-C38-C39	4.75	119.82	111.09
49	K	310	KC2	O2D-CGD-CBD	4.75	119.70	111.27
51	0	321	A1ECV	O2-CMC-C2C	4.75	123.66	112.27
47	E	320	SQD	O5-C5-C4	4.74	118.31	109.69
49	9	316	KC2	O2D-CGD-CBD	4.74	119.69	111.27
43	J	306	DD6	O1-C20-C19	-4.74	109.82	113.38
49	Q	315	KC2	CHD-C1D-ND	4.74	129.27	124.26
50	G	308	A1EB1	C4-C5-C6	-4.74	120.55	127.31
50	6	308	A1EB1	C33-C32-C31	4.74	113.81	109.21
48	0	304	A86	C3-C2-C1	-4.74	120.55	127.31
49	B	208	KC2	CHD-C1D-ND	4.73	129.27	124.26
49	G	313	KC2	CHD-C1D-ND	4.73	129.27	124.26
49	6	316	KC2	CHD-C1D-ND	4.73	129.27	124.26
50	T	302	A1EB1	C3-C2-C1	-4.73	120.55	127.31
50	h	203	A1EB1	C3-C2-C1	-4.73	120.55	127.31
43	O	303	DD6	C21-C20-C19	4.73	119.61	114.28
48	L	304	A86	C21-C20-C19	4.73	119.60	114.28
49	9	311	KC2	O2D-CGD-CBD	4.73	119.67	111.27
49	4	320	KC2	CHD-C1D-ND	4.73	129.26	124.26
48	R	301	A86	C4-C5-C6	-4.73	120.56	127.31
50	y	302	A1EB1	C25-C26-C27	-4.73	120.53	127.26
49	C	312	KC2	O2D-CGD-CBD	4.72	119.66	111.27
43	G	306	DD6	C21-C20-C19	4.72	119.59	114.28
50	J	302	A1EB1	C28-C27-C26	-4.72	118.76	124.93
48	S	304	A86	O4-C38-C39	4.72	119.78	111.09
50	V	305	A1EB1	C3-C2-C1	-4.72	120.58	127.31
48	L	301	A86	C3-C2-C1	-4.72	120.58	127.31
43	E	303	DD6	C21-C20-C19	4.72	119.58	114.28
50	8	304	A1EB1	O1-C20-C19	-4.72	109.84	113.38
49	7	320	KC2	O2D-CGD-CBD	4.71	119.64	111.27
48	0	309	A86	O4-C38-C39	4.71	119.76	111.09
42	a	843	BCR	C16-C17-C18	-4.71	120.59	127.31
49	S	317	KC2	CHD-C1D-ND	4.71	129.24	124.26
49	L	315	KC2	O2D-CGD-CBD	4.71	119.64	111.27
50	7	305	A1EB1	O4-C38-C39	4.71	119.75	111.09
48	O	306	A86	C17-C16-C15	4.71	113.97	109.16
48	3	308	A86	C41-C32-C31	-4.71	106.26	110.47
49	H	314	KC2	O2D-CGD-CBD	4.71	119.63	111.27
49	9	313	KC2	O2D-CGD-CBD	4.71	119.63	111.27
50	K	302	A1EB1	O4-C38-C39	4.71	119.75	111.09
49	4	318	KC2	O2D-CGD-CBD	4.70	119.63	111.27
48	J	303	A86	O4-C38-C39	4.70	119.74	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	y	306	A86	C21-C20-C19	4.70	119.57	114.28
50	S	303	A1EB1	O4-C38-C39	4.70	119.73	111.09
50	0	307	A1EB1	C25-C26-C27	-4.70	120.57	127.26
48	O	307	A86	C33-C32-C31	4.69	113.77	109.21
50	y	302	A1EB1	O4-C38-C39	4.69	119.72	111.09
49	5	311	KC2	O2D-CGD-CBD	4.69	119.61	111.27
50	8	306	A1EB1	C21-C20-C19	4.69	119.56	114.28
48	H	302	A86	C33-C32-C31	4.69	113.77	109.21
48	Q	305	A86	O4-C38-C39	4.69	119.72	111.09
49	T	315	KC2	CHD-C1D-ND	4.69	129.22	124.26
50	3	303	A1EB1	C25-C26-C27	-4.69	120.59	127.26
48	Y	301	A86	O1-C20-C19	-4.69	109.86	113.38
51	4	321	A1ECV	C2A-CAA-CBA	-4.68	118.07	128.63
43	A	301	DD6	C3-C2-C1	-4.68	120.63	127.31
50	5	302	A1EB1	C3-C2-C1	-4.68	120.63	127.31
48	3	305	A86	C4-C5-C6	-4.68	120.63	127.31
49	L	315	KC2	CHD-C1D-ND	4.68	129.21	124.26
49	5	305	KC2	CHD-C1D-ND	4.68	129.21	124.26
49	5	314	KC2	CHD-C1D-ND	4.68	129.21	124.26
48	8	323	A86	O4-C38-C39	4.68	119.70	111.09
52	5	304	A1EB4	O1-C20-C19	-4.68	109.87	113.38
48	Z	303	A86	C21-C20-C19	4.68	119.54	114.28
49	V	308	KC2	CHD-C1D-ND	4.67	129.21	124.26
50	z	302	A1EB1	C36-C31-C32	4.67	124.33	119.70
43	4	308	DD6	C21-C20-C19	4.67	119.53	114.28
49	T	316	KC2	O2D-CGD-CBD	4.67	119.56	111.27
48	U	202	A86	C33-C32-C31	4.67	113.75	109.21
49	V	315	KC2	CHD-C1D-ND	4.67	129.20	124.26
48	L	305	A86	C36-C31-C32	4.66	124.33	119.70
49	7	319	KC2	CHD-C1D-ND	4.66	129.19	124.26
48	4	310	A86	C4-C5-C6	-4.66	120.65	127.31
50	5	302	A1EB1	O4-C38-C39	4.66	119.67	111.09
48	6	303	A86	C3-C2-C1	-4.66	120.66	127.31
49	z	313	KC2	C4B-CHC-C1C	-4.66	116.00	126.06
49	O	317	KC2	C1D-ND-C4D	4.66	109.65	106.33
49	C	313	KC2	CHD-C1D-ND	4.66	129.19	124.26
42	b	845	BCR	C11-C10-C9	-4.66	120.66	127.31
49	x	313	KC2	O2D-CGD-CBD	4.66	119.54	111.27
43	D	303	DD6	O1-C20-C19	-4.66	109.88	113.38
48	I	304	A86	O4-C38-C39	4.66	119.66	111.09
49	W	314	KC2	O2D-CGD-CBD	4.66	119.54	111.27
49	1	315	KC2	O2D-CGD-CBD	4.65	119.53	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	8	320	KC2	CHD-C1D-ND	4.65	129.18	124.26
49	2	314	KC2	O2D-CGD-CBD	4.65	119.53	111.27
48	T	301	A86	C3-C2-C1	-4.65	120.67	127.31
49	y	313	KC2	O2D-CGD-CBD	4.65	119.53	111.27
50	G	304	A1EB1	O1-C20-C19	-4.65	109.89	113.38
50	4	301	A1EB1	O4-C38-C39	4.65	119.64	111.09
43	J	305	DD6	C4-C5-C6	-4.65	120.68	127.31
48	1	303	A86	C25-C26-C27	-4.64	120.68	127.31
48	U	206	A86	C3-C2-C1	-4.64	120.68	127.31
50	J	302	A1EB1	O4-C38-C39	4.64	119.63	111.09
48	J	301	A86	C4-C5-C6	-4.64	120.69	127.31
43	x	303	DD6	C21-C20-C19	4.64	119.50	114.28
49	8	317	KC2	O2D-CGD-CBD	4.64	119.51	111.27
50	6	304	A1EB1	C21-C20-C19	4.63	119.49	114.28
48	1	303	A86	C4-C5-C6	-4.63	120.70	127.31
50	S	302	A1EB1	C4-C5-C6	-4.63	120.70	127.31
49	0	317	KC2	CHD-C1D-ND	4.63	129.16	124.26
50	z	302	A1EB1	C25-C26-C27	-4.63	120.67	127.26
50	U	203	A1EB1	C4-C5-C6	-4.63	120.70	127.31
49	y	316	KC2	CHD-C1D-ND	4.63	129.16	124.26
50	6	301	A1EB1	O4-C38-C39	4.63	119.60	111.09
48	T	306	A86	C21-C20-C19	4.62	119.48	114.28
48	7	312	A86	C3-C2-C1	-4.62	120.71	127.31
49	X	314	KC2	CHD-C1D-ND	4.62	129.15	124.26
49	8	320	KC2	O2D-CGD-CBD	4.62	119.48	111.27
49	X	318	KC2	CHD-C1D-ND	4.62	129.15	124.26
50	0	302	A1EB1	O4-C38-C39	4.62	119.59	111.09
49	G	311	KC2	CHD-C1D-ND	4.62	129.15	124.26
49	0	314	KC2	CHD-C1D-ND	4.62	129.15	124.26
48	V	301	A86	C4-C5-C6	-4.62	120.71	127.31
43	J	306	DD6	C14-C13-C11	-4.62	118.36	125.53
48	0	309	A86	C36-C31-C32	4.62	124.28	119.70
42	b	846	BCR	C16-C17-C18	-4.61	120.72	127.31
50	K	304	A1EB1	C4-C5-C6	-4.61	120.72	127.31
42	a	844	BCR	C16-C17-C18	-4.61	120.73	127.31
50	x	301	A1EB1	C3-C2-C1	-4.61	120.73	127.31
48	z	303	A86	C3-C2-C1	-4.61	120.73	127.31
50	3	310	A1EB1	C3-C2-C1	-4.61	120.73	127.31
49	z	315	KC2	CHD-C1D-ND	4.61	129.14	124.26
49	y	314	KC2	O2D-CGD-CBD	4.61	119.46	111.27
48	X	302	A86	C3-C2-C1	-4.61	120.73	127.31
48	Q	308	A86	C3-C2-C1	-4.61	120.73	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	8	307	A86	O4-C38-C39	4.61	119.57	111.09
49	H	311	KC2	CHD-C1D-ND	4.61	129.13	124.26
50	K	305	A1EB1	C4-C5-C6	-4.61	120.73	127.31
49	P	320	KC2	CHD-C1D-ND	4.61	129.13	124.26
48	0	304	A86	C4-C5-C6	-4.61	120.74	127.31
50	E	301	A1EB1	C4-C5-C6	-4.60	120.74	127.31
50	9	302	A1EB1	C36-C31-C32	4.60	124.26	119.70
49	5	313	KC2	O2D-CGD-CBD	4.60	119.44	111.27
43	Q	303	DD6	C3-C2-C1	-4.60	120.74	127.31
43	H	303	DD6	O1-C20-C19	-4.60	109.93	113.38
48	O	306	A86	C4-C5-C6	-4.60	120.75	127.31
48	O	307	A86	C25-C26-C27	-4.60	120.75	127.31
49	1	312	KC2	O2D-CGD-CBD	4.60	119.44	111.27
48	0	309	A86	C21-C20-C19	4.60	119.45	114.28
48	F	302	A86	O4-C38-C39	4.60	119.54	111.09
49	X	314	KC2	O2D-CGD-CBD	4.59	119.43	111.27
49	5	314	KC2	O2D-CGD-CBD	4.59	119.43	111.27
49	R	314	KC2	CHD-C1D-ND	4.59	129.12	124.26
50	6	304	A1EB1	C36-C31-C32	4.59	124.25	119.70
42	a	842	BCR	C16-C17-C18	-4.59	120.76	127.31
48	0	308	A86	C3-C2-C1	-4.59	120.76	127.31
49	S	314	KC2	O2D-CGD-CBD	4.59	119.42	111.27
49	1	314	KC2	O2D-CGD-CBD	4.59	119.42	111.27
49	7	320	KC2	CHD-C1D-ND	4.59	129.11	124.26
49	5	313	KC2	CHD-C1D-ND	4.59	129.11	124.26
48	G	301	A86	C21-C20-C19	4.58	119.44	114.28
49	Z	311	KC2	CHD-C1D-ND	4.58	129.11	124.26
50	2	304	A1EB1	O4-C38-C39	4.58	119.52	111.09
49	R	318	KC2	CHD-C1D-ND	4.58	129.11	124.26
50	Q	307	A1EB1	C36-C31-C32	4.58	124.24	119.70
43	I	305	DD6	C21-C20-C19	4.58	119.43	114.28
48	T	301	A86	C4-C5-C6	-4.58	120.77	127.31
49	S	317	KC2	O2D-CGD-CBD	4.58	119.41	111.27
50	O	301	A1EB1	C21-C20-C19	4.58	119.43	114.28
48	M	306	A86	O4-C38-C39	4.58	119.51	111.09
42	b	845	BCR	C7-C8-C9	-4.58	119.32	126.23
52	P	319	A1EB4	C21-C20-C15	-4.58	114.58	122.32
50	8	308	A1EB1	C4-C5-C6	-4.58	120.78	127.31
48	8	307	A86	O1-C20-C21	-4.58	109.57	115.06
50	z	302	A1EB1	C21-C20-C19	4.58	119.43	114.28
43	B	202	DD6	C3-C2-C1	-4.57	120.78	127.31
48	0	309	A86	C25-C26-C27	-4.57	120.78	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	302	A86	C21-C20-C19	4.57	119.42	114.28
48	U	202	A86	O4-C38-C39	4.57	119.49	111.09
49	R	314	KC2	O2D-CGD-CBD	4.57	119.38	111.27
43	G	303	DD6	C21-C20-C19	4.56	119.42	114.28
48	Q	305	A86	C21-C20-C19	4.56	119.42	114.28
48	k	206	A86	O4-C38-C39	4.56	119.48	111.09
49	A	310	KC2	CHD-C1D-ND	4.56	129.09	124.26
49	X	315	KC2	CHD-C1D-ND	4.56	129.09	124.26
48	L	301	A86	O4-C38-C39	4.56	119.48	111.09
50	3	302	A1EB1	O1-C20-C21	-4.56	109.59	115.06
42	b	850	BCR	C20-C21-C22	-4.56	120.80	127.31
48	X	303	A86	C36-C31-C32	4.56	124.22	119.70
49	3	315	KC2	CHD-C1D-ND	4.56	129.08	124.26
43	H	303	DD6	C21-C20-C19	4.56	119.41	114.28
52	W	321	A1EB4	O1-C20-C19	-4.56	109.96	113.38
48	4	310	A86	C25-C26-C27	-4.56	120.81	127.31
49	1	312	KC2	CHD-C1D-ND	4.56	129.08	124.26
48	4	328	A86	O4-C38-C39	4.56	119.47	111.09
48	Z	303	A86	C17-C16-C15	4.56	113.81	109.16
50	U	205	A1EB1	O1-C15-C14	-4.55	104.07	113.21
48	2	301	A86	C3-C2-C1	-4.55	120.81	127.31
48	8	303	A86	O4-C38-C39	4.55	119.46	111.09
48	9	305	A86	O4-C38-C39	4.55	119.46	111.09
43	D	307	DD6	C4-C5-C6	-4.55	120.82	127.31
49	V	314	KC2	CHD-C1D-ND	4.55	129.07	124.26
48	G	305	A86	C21-C20-C19	4.55	119.40	114.28
48	T	305	A86	O1-C20-C21	-4.55	109.61	115.06
49	x	312	KC2	CHD-C1D-ND	4.55	129.07	124.26
50	G	304	A1EB1	O1-C15-C14	-4.55	104.09	113.21
49	S	315	KC2	O2D-CGD-CBD	4.54	119.34	111.27
48	L	307	A86	O4-C38-C39	4.54	119.45	111.09
48	U	202	A86	O1-C20-C19	-4.54	109.97	113.38
52	M	322	A1EB4	C21-C20-C15	-4.54	114.64	122.32
50	V	307	A1EB1	O1-C15-C14	-4.54	104.10	113.21
49	1	312	KC2	C1D-ND-C4D	4.54	109.56	106.33
50	7	303	A1EB1	C36-C31-C32	4.54	124.20	119.70
50	0	305	A1EB1	O4-C38-C39	4.54	119.44	111.09
48	T	305	A86	C3-C2-C1	-4.54	120.83	127.31
48	L	307	A86	C3-C2-C1	-4.54	120.83	127.31
48	S	307	A86	C36-C31-C32	4.54	124.20	119.70
48	z	303	A86	O4-C38-C39	4.54	119.44	111.09
49	6	317	KC2	CHD-C1D-ND	4.54	129.06	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	R	302	A86	C34-O4-C38	-4.53	109.45	117.90
49	3	318	KC2	O2D-CGD-CBD	4.53	119.32	111.27
48	4	306	A86	C3-C2-C1	-4.53	120.84	127.31
48	W	307	A86	O4-C38-C39	4.53	119.43	111.09
50	1	301	A1EB1	C21-C20-C19	4.53	119.38	114.28
50	6	308	A1EB1	C21-C20-C19	4.53	119.38	114.28
49	Y	309	KC2	O2D-CGD-CBD	4.53	119.32	111.27
43	H	305	DD6	C9-C10-C11	-4.53	120.85	127.31
48	L	302	A86	O1-C15-C14	-4.53	104.12	113.21
48	9	301	A86	C4-C5-C6	-4.53	120.85	127.31
48	Q	302	A86	O4-C38-C39	4.53	119.42	111.09
49	P	310	KC2	O2D-CGD-CBD	4.53	119.31	111.27
49	M	307	KC2	O2D-CGD-CBD	4.52	119.30	111.27
49	L	314	KC2	CHD-C1D-ND	4.52	129.04	124.26
51	7	317	A1ECV	C2A-CAA-CBA	-4.52	118.44	128.63
49	A	313	KC2	O2D-CGD-CBD	4.52	119.30	111.27
48	3	306	A86	O4-C38-C39	4.52	119.40	111.09
43	o	204	DD6	C9-C10-C11	-4.52	120.86	127.31
50	4	303	A1EB1	C4-C5-C6	-4.52	120.86	127.31
49	R	306	KC2	CHD-C1D-ND	4.52	129.04	124.26
48	W	307	A86	O1-C20-C21	-4.52	109.64	115.06
48	0	306	A86	C4-C5-C6	-4.52	120.86	127.31
49	P	310	KC2	CHD-C1D-ND	4.51	129.04	124.26
50	R	303	A1EB1	C3-C2-C1	-4.51	120.87	127.31
43	o	204	DD6	C14-C13-C11	-4.51	118.53	125.53
42	i	102	BCR	C16-C17-C18	-4.51	120.87	127.31
48	0	301	A86	C3-C2-C1	-4.51	120.88	127.31
48	6	307	A86	O4-C38-C39	4.51	119.38	111.09
52	W	321	A1EB4	O4-C38-C42	4.51	119.38	111.09
50	0	307	A1EB1	O4-C38-C39	4.51	119.38	111.09
48	Q	305	A86	C4-C5-C6	-4.51	120.88	127.31
49	L	317	KC2	CHD-C1D-ND	4.50	129.03	124.26
48	0	308	A86	C23-C16-C22	-4.50	100.73	107.37
48	L	304	A86	C33-C32-C31	4.50	113.59	109.21
48	6	305	A86	O4-C38-C39	4.50	119.37	111.09
50	U	205	A1EB1	O4-C38-C39	4.50	119.37	111.09
48	9	306	A86	O4-C38-C39	4.50	119.37	111.09
49	X	306	KC2	C1D-ND-C4D	4.50	109.53	106.33
50	0	307	A1EB1	C3-C2-C1	-4.50	120.89	127.31
49	W	312	KC2	O2D-CGD-CBD	4.50	119.27	111.27
48	8	307	A86	C36-C31-C32	4.50	124.16	119.70
49	K	313	KC2	CHD-C1D-ND	4.50	129.02	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	K	301	A86	O4-C38-C39	4.50	119.37	111.09
49	3	317	KC2	O2D-CGD-CBD	4.50	119.26	111.27
43	B	202	DD6	C14-C13-C11	-4.50	118.55	125.53
50	G	304	A1EB1	C4-C5-C6	-4.50	120.89	127.31
52	P	318	A1EB4	O4-C38-C42	4.50	119.36	111.09
48	Z	303	A86	O4-C38-C39	4.50	119.36	111.09
49	L	317	KC2	O2D-CGD-CBD	4.50	119.26	111.27
48	6	309	A86	C3-C2-C1	-4.50	120.89	127.31
49	0	314	KC2	O2D-CGD-CBD	4.49	119.25	111.27
49	C	312	KC2	CHD-C1D-ND	4.49	129.01	124.26
48	2	305	A86	C21-C20-C19	4.49	119.34	114.28
50	G	302	A1EB1	C3-C2-C1	-4.49	120.90	127.31
48	O	302	A86	O4-C38-C39	4.49	119.36	111.09
48	0	306	A86	C3-C2-C1	-4.49	120.90	127.31
43	B	202	DD6	C21-C20-C19	4.49	119.33	114.28
49	y	313	KC2	CHD-C1D-ND	4.49	129.01	124.26
48	1	303	A86	O4-C38-C39	4.49	119.35	111.09
49	S	314	KC2	CHD-C1D-ND	4.49	129.01	124.26
48	1	307	A86	O1-C20-C21	-4.49	109.68	115.06
49	W	312	KC2	CHD-C1D-ND	4.49	129.01	124.26
50	4	303	A1EB1	O4-C38-C39	4.49	119.34	111.09
48	4	309	A86	C4-C5-C6	-4.48	120.91	127.31
48	3	308	A86	C36-C31-C32	4.48	124.15	119.70
43	Z	302	DD6	C21-C20-C15	-4.48	114.75	122.26
48	W	304	A86	C3-C2-C1	-4.48	120.91	127.31
50	V	305	A1EB1	C36-C31-C32	4.48	124.14	119.70
50	y	301	A1EB1	O1-C15-C14	-4.48	104.22	113.21
50	O	301	A1EB1	O4-C38-C39	4.48	119.33	111.09
50	R	303	A1EB1	C36-C31-C32	4.48	124.14	119.70
48	F	302	A86	C4-C5-C6	-4.48	120.92	127.31
48	8	303	A86	C4-C5-C6	-4.48	120.92	127.31
49	9	316	KC2	CHD-C1D-ND	4.48	129.00	124.26
50	Q	307	A1EB1	C3-C2-C1	-4.48	120.92	127.31
50	0	305	A1EB1	C21-C20-C19	4.48	119.31	114.28
49	P	306	KC2	CHD-C1D-ND	4.48	129.00	124.26
50	V	307	A1EB1	O4-C38-C39	4.48	119.32	111.09
49	0	319	KC2	O2D-CGD-CBD	4.47	119.22	111.27
48	Y	301	A86	O4-C38-C39	4.47	119.32	111.09
48	3	306	A86	C21-C20-C19	4.47	119.31	114.28
48	6	303	A86	O4-C38-C39	4.47	119.32	111.09
50	3	309	A1EB1	C25-C26-C27	-4.47	120.89	127.26
43	y	303	DD6	C21-C20-C19	4.47	119.31	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	H	311	KC2	O2D-CGD-CBD	4.47	119.21	111.27
48	S	307	A86	O4-C38-C39	4.47	119.31	111.09
49	Q	313	KC2	CHD-C1D-ND	4.47	128.99	124.26
49	M	311	KC2	CHD-C1D-ND	4.47	128.99	124.26
49	2	314	KC2	CHD-C1D-ND	4.47	128.99	124.26
48	Q	302	A86	C4-C5-C6	-4.47	120.93	127.31
50	S	303	A1EB1	C36-C31-C32	4.47	124.13	119.70
49	W	314	KC2	CHD-C1D-ND	4.47	128.99	124.26
50	K	304	A1EB1	O4-C38-C39	4.47	119.31	111.09
52	M	305	A1EB4	O1-C20-C19	-4.46	110.03	113.38
50	K	302	A1EB1	C40-C32-C31	-4.46	106.48	110.47
50	G	302	A1EB1	C4-C5-C6	-4.46	120.94	127.31
43	H	305	DD6	C4-C5-C6	-4.46	120.94	127.31
49	0	316	KC2	CHD-C1D-ND	4.46	128.98	124.26
49	8	317	KC2	CHD-C1D-ND	4.46	128.98	124.26
49	T	314	KC2	O2D-CGD-CBD	4.46	119.19	111.27
48	L	304	A86	O4-C38-C39	4.46	119.29	111.09
48	O	306	A86	O1-C15-C14	-4.46	104.26	113.21
48	0	301	A86	C36-C31-C32	4.46	124.12	119.70
49	0	316	KC2	O2D-CGD-CBD	4.46	119.19	111.27
49	C	313	KC2	O2D-CGD-CBD	4.46	119.19	111.27
48	0	304	A86	C25-C26-C27	-4.46	120.95	127.31
47	S	301	SQD	O7-S-C6	4.46	112.23	106.94
49	M	313	KC2	O2D-CGD-CBD	4.46	119.19	111.27
48	R	301	A86	O4-C38-C39	4.46	119.29	111.09
49	K	310	KC2	CHD-C1D-ND	4.45	128.97	124.26
49	X	315	KC2	O2D-CGD-CBD	4.45	119.18	111.27
50	z	301	A1EB1	O4-C38-C39	4.45	119.28	111.09
49	8	319	KC2	CHD-C1D-ND	4.45	128.97	124.26
50	y	301	A1EB1	O4-C38-C39	4.45	119.28	111.09
49	L	312	KC2	O2D-CGD-CBD	4.45	119.18	111.27
52	M	322	A1EB4	C20-O1-C15	4.45	64.59	61.17
43	2	303	DD6	C21-C20-C15	-4.45	114.80	122.26
48	L	302	A86	C21-C20-C19	4.45	119.28	114.28
50	V	307	A1EB1	C4-C5-C6	-4.45	120.96	127.31
49	3	321	KC2	CHD-C1D-ND	4.45	128.97	124.26
50	y	302	A1EB1	C36-C31-C32	4.45	124.11	119.70
49	W	308	KC2	O2D-CGD-CBD	4.45	119.17	111.27
49	V	318	KC2	O2D-CGD-CBD	4.44	119.17	111.27
50	x	302	A1EB1	C3-C2-C1	-4.44	120.97	127.31
50	3	309	A1EB1	O1-C20-C21	-4.44	109.73	115.06
48	C	303	A86	O4-C38-C39	4.44	119.26	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	306	A86	C3-C2-C1	-4.44	120.97	127.31
52	W	321	A1EB4	C4-C5-C6	-4.44	120.97	127.31
50	L	303	A1EB1	C21-C20-C19	4.44	119.28	114.28
43	E	302	DD6	C4-C5-C6	-4.44	120.97	127.31
48	H	302	A86	O4-C38-C39	4.44	119.26	111.09
48	T	306	A86	O4-C38-C39	4.44	119.26	111.09
48	8	323	A86	O1-C20-C21	-4.44	109.74	115.06
42	b	844	BCR	C20-C21-C22	-4.44	120.97	127.31
48	2	305	A86	C25-C24-C1	-4.44	113.95	126.42
43	D	303	DD6	C4-C5-C6	-4.44	120.98	127.31
49	P	312	KC2	O2D-CGD-CBD	4.44	119.15	111.27
48	Z	301	A86	O4-C38-C39	4.44	119.25	111.09
50	V	306	A1EB1	O4-C38-C39	4.44	119.25	111.09
47	M	301	SQD	O7-S-C6	4.43	112.21	106.94
48	Q	301	A86	C4-C5-C6	-4.43	120.98	127.31
48	7	312	A86	C21-C20-C19	4.43	119.27	114.28
48	J	303	A86	C4-C5-C6	-4.43	120.98	127.31
48	R	317	A86	C3-C2-C1	-4.43	120.98	127.31
49	3	318	KC2	CHD-C1D-ND	4.43	128.95	124.26
50	9	302	A1EB1	C25-C26-C27	-4.43	120.95	127.26
43	W	305	DD6	C21-C20-C19	4.43	119.26	114.28
48	1	302	A86	O1-C15-C14	-4.43	104.32	113.21
49	4	317	KC2	CHD-C1D-ND	4.43	128.95	124.26
48	9	304	A86	O4-C38-C39	4.43	119.24	111.09
52	P	319	A1EB4	C20-O1-C15	4.43	64.57	61.17
48	8	309	A86	O4-C38-C39	4.43	119.23	111.09
50	3	303	A1EB1	O4-C38-C39	4.42	119.23	111.09
43	P	304	DD6	C21-C20-C15	-4.42	114.85	122.26
48	C	303	A86	C4-C5-C6	-4.42	121.00	127.31
48	L	305	A86	C25-C26-C27	-4.42	121.00	127.31
49	x	313	KC2	CHD-C1D-ND	4.42	128.94	124.26
50	6	304	A1EB1	C33-C32-C31	4.42	113.51	109.21
48	M	302	A86	C3-C2-C1	-4.42	121.00	127.31
48	U	202	A86	C3-C2-C1	-4.42	121.00	127.31
48	B	201	A86	C33-C32-C31	4.42	113.51	109.21
49	6	319	KC2	O2D-CGD-CBD	4.42	119.12	111.27
43	D	307	DD6	O1-C20-C19	-4.42	110.06	113.38
49	Y	309	KC2	CHD-C1D-ND	4.42	128.94	124.26
42	l	206	BCR	C7-C8-C9	-4.42	119.56	126.23
48	B	201	A86	C36-C31-C32	4.42	124.08	119.70
48	6	305	A86	C21-C20-C19	4.42	119.25	114.28
49	A	310	KC2	O2D-CGD-CBD	4.42	119.12	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	Q	323	A1EB1	O4-C38-C39	4.42	119.21	111.09
50	8	301	A1EB1	O4-C38-C39	4.41	119.21	111.09
50	4	304	A1EB1	O4-C38-C39	4.41	119.21	111.09
48	2	301	A86	O4-C38-C39	4.41	119.21	111.09
49	7	322	KC2	CHD-C1D-ND	4.41	128.93	124.26
50	y	301	A1EB1	C25-C26-C27	-4.41	120.97	127.26
49	Q	315	KC2	O2D-CGD-CBD	4.41	119.11	111.27
50	S	302	A1EB1	C21-C20-C19	4.41	119.24	114.28
48	K	301	A86	O1-C20-C19	-4.41	110.07	113.38
49	V	312	KC2	CHD-C1D-ND	4.41	128.93	124.26
42	f	801	BCR	C20-C21-C22	-4.41	121.02	127.31
50	V	307	A1EB1	C21-C20-C19	4.41	119.24	114.28
42	b	844	BCR	C15-C14-C13	-4.41	121.02	127.31
48	0	309	A86	C33-C32-C31	4.41	113.49	109.21
49	J	315	KC2	O2D-CGD-CBD	4.40	119.09	111.27
48	7	308	A86	C25-C26-C27	-4.40	121.03	127.31
48	R	317	A86	O4-C38-C39	4.40	119.19	111.09
50	h	203	A1EB1	O4-C38-C39	4.40	119.19	111.09
49	X	312	KC2	CHD-C1D-ND	4.40	128.92	124.26
50	4	302	A1EB1	C21-C20-C19	4.40	119.23	114.28
48	W	304	A86	O1-C20-C21	-4.40	109.78	115.06
50	G	302	A1EB1	C36-C31-C32	4.40	124.06	119.70
48	R	302	A86	C25-C26-C27	-4.40	121.03	127.31
49	Z	310	KC2	O2D-CGD-CBD	4.40	119.08	111.27
50	4	304	A1EB1	C33-C32-C31	4.40	113.48	109.21
43	Q	306	DD6	C3-C2-C1	-4.40	121.04	127.31
50	U	203	A1EB1	O4-C38-C39	4.39	119.17	111.09
43	B	202	DD6	C9-C10-C11	-4.39	121.04	127.31
49	J	315	KC2	CHD-C1D-ND	4.39	128.91	124.26
48	R	317	A86	C4-C5-C6	-4.39	121.04	127.31
49	Y	308	KC2	O2D-CGD-CBD	4.39	119.07	111.27
48	J	303	A86	C3-C2-C1	-4.39	121.04	127.31
50	1	301	A1EB1	C4-C5-C6	-4.39	121.04	127.31
49	V	314	KC2	O2D-CGD-CBD	4.39	119.07	111.27
48	Q	304	A86	O4-C38-C39	4.39	119.17	111.09
48	L	301	A86	C25-C26-C27	-4.39	121.05	127.31
50	T	302	A1EB1	C21-C20-C19	4.39	119.22	114.28
48	X	303	A86	O4-C38-C39	4.39	119.17	111.09
48	M	306	A86	C3-C2-C1	-4.39	121.05	127.31
49	V	308	KC2	O2D-CGD-CBD	4.39	119.07	111.27
49	Z	310	KC2	CHD-C1D-ND	4.39	128.90	124.26
49	V	318	KC2	CHD-C1D-ND	4.39	128.90	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	0	317	KC2	O2D-CGD-CBD	4.39	119.06	111.27
48	P	303	A86	O1-C20-C21	-4.39	109.80	115.06
50	0	302	A1EB1	O1-C20-C19	-4.39	110.09	113.38
50	3	309	A1EB1	O4-C38-C39	4.39	119.16	111.09
48	8	305	A86	O4-C38-C39	4.38	119.16	111.09
50	4	302	A1EB1	O4-C38-C39	4.38	119.16	111.09
50	9	302	A1EB1	O1-C20-C19	-4.38	110.09	113.38
49	6	319	KC2	C1D-ND-C4D	4.38	109.45	106.33
50	V	302	A1EB1	C3-C2-C1	-4.38	121.06	127.31
48	3	305	A86	C3-C2-C1	-4.38	121.06	127.31
50	G	302	A1EB1	C21-C20-C19	4.38	119.21	114.28
48	8	309	A86	C4-C5-C6	-4.38	121.06	127.31
48	9	306	A86	C3-C2-C1	-4.38	121.06	127.31
49	Y	308	KC2	C1D-ND-C4D	4.38	109.45	106.33
50	x	302	A1EB1	O4-C38-C39	4.38	119.14	111.09
48	Z	303	A86	O1-C20-C19	-4.38	110.09	113.38
51	R	313	A1ECV	C2A-CAA-CBA	-4.37	118.77	128.63
50	2	306	A1EB1	O4-C38-C39	4.37	119.14	111.09
48	1	302	A86	O4-C38-C39	4.37	119.13	111.09
50	G	304	A1EB1	C21-C20-C19	4.37	119.20	114.28
48	6	307	A86	O1-C20-C21	-4.37	109.82	115.06
49	W	315	KC2	CHD-C1D-ND	4.37	128.88	124.26
50	1	301	A1EB1	O4-C38-C39	4.37	119.13	111.09
49	G	311	KC2	O2D-CGD-CBD	4.37	119.03	111.27
49	M	314	KC2	O2D-CGD-CBD	4.37	119.03	111.27
48	L	304	A86	C25-C26-C27	-4.37	121.08	127.31
43	D	306	DD6	C14-C13-C11	-4.37	118.75	125.53
42	b	848	BCR	C16-C17-C18	-4.37	121.08	127.31
50	0	303	A1EB1	C21-C20-C19	4.37	119.19	114.28
48	x	305	A86	C3-C2-C1	-4.37	121.08	127.31
50	8	308	A1EB1	C3-C2-C1	-4.37	121.08	127.31
43	J	304	DD6	C21-C20-C19	4.37	119.19	114.28
48	9	301	A86	O4-C38-C39	4.36	119.12	111.09
48	M	302	A86	C21-C20-C19	4.36	119.19	114.28
48	Q	301	A86	C21-C20-C19	4.36	119.19	114.28
48	6	309	A86	O4-C38-C39	4.36	119.12	111.09
50	G	304	A1EB1	O4-C38-C39	4.36	119.12	111.09
48	8	302	A86	C3-C2-C1	-4.36	121.08	127.31
48	2	305	A86	C-C1-C2	-4.36	116.81	122.92
48	M	303	A86	C4-C5-C6	-4.36	121.09	127.31
49	O	317	KC2	O2D-CGD-CBD	4.36	119.01	111.27
49	F	307	KC2	CHD-C1D-ND	4.36	128.87	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	0	307	A1EB1	C28-C27-C26	-4.36	119.24	124.93
48	Z	301	A86	O1-C20-C21	-4.35	109.84	115.06
48	Z	301	A86	C25-C26-C27	-4.35	121.10	127.31
49	2	317	KC2	CHD-C1D-ND	4.35	128.87	124.26
50	6	306	A1EB1	O4-C38-C39	4.35	119.10	111.09
48	6	309	A86	C17-C16-C15	4.35	113.60	109.16
48	L	302	A86	O4-C38-C39	4.35	119.09	111.09
50	D	308	A1EB1	C25-C26-C27	-4.35	121.07	127.26
42	f	804	BCR	C7-C8-C9	-4.35	119.67	126.23
50	V	306	A1EB1	C3-C2-C1	-4.35	121.11	127.31
48	I	304	A86	C3-C2-C1	-4.34	121.11	127.31
48	S	307	A86	C21-C20-C19	4.34	119.17	114.28
49	8	316	KC2	CHD-C1D-ND	4.34	128.85	124.26
43	H	305	DD6	O1-C20-C19	-4.34	110.12	113.38
42	b	846	BCR	C33-C5-C6	-4.34	119.65	124.53
49	V	312	KC2	O2D-CGD-CBD	4.34	118.98	111.27
48	Q	308	A86	O4-C38-C39	4.34	119.08	111.09
52	R	305	A1EB4	C20-O1-C15	4.34	64.50	61.17
49	T	316	KC2	CHD-C1D-ND	4.34	128.85	124.26
50	z	301	A1EB1	C4-C5-C6	-4.34	121.12	127.31
48	O	307	A86	O4-C38-C39	4.34	119.07	111.09
49	2	313	KC2	O2D-CGD-CBD	4.34	118.98	111.27
43	P	304	DD6	C-C1-C2	-4.34	116.85	122.92
50	7	306	A1EB1	C21-C20-C19	4.34	119.16	114.28
50	3	303	A1EB1	C3-C2-C1	-4.34	121.12	127.31
48	B	201	A86	C21-C20-C19	4.34	119.16	114.28
50	K	305	A1EB1	O4-C38-C39	4.33	119.06	111.09
50	F	304	A1EB1	C33-C32-C31	4.33	113.42	109.21
49	Z	311	KC2	O2D-CGD-CBD	4.33	118.97	111.27
42	b	847	BCR	C11-C10-C9	-4.33	121.13	127.31
50	G	308	A1EB1	O4-C38-C39	4.33	119.06	111.09
49	0	319	KC2	C4B-CHC-C1C	-4.33	116.71	126.06
49	P	312	KC2	CHD-C1D-ND	4.33	128.84	124.26
48	W	304	A86	O4-C38-C39	4.33	119.06	111.09
48	7	308	A86	O4-C38-C39	4.33	119.05	111.09
50	0	302	A1EB1	C3-C2-C1	-4.33	121.14	127.31
50	0	307	A1EB1	C4-C5-C6	-4.33	121.14	127.31
48	R	317	A86	C21-C20-C19	4.33	119.15	114.28
48	S	307	A86	C3-C2-C1	-4.33	121.14	127.31
43	E	302	DD6	O1-C20-C19	-4.33	110.13	113.38
43	U	204	DD6	C21-C20-C19	4.32	119.14	114.28
49	4	318	KC2	CHD-C1D-ND	4.32	128.83	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	H	302	A86	C21-C20-C19	4.32	119.14	114.28
50	T	302	A1EB1	O4-C38-C39	4.32	119.04	111.09
48	F	301	A86	O4-C38-C39	4.32	119.04	111.09
48	Q	302	A86	C17-C16-C15	4.32	113.57	109.16
52	P	318	A1EB4	O1-C15-C14	-4.32	111.33	115.71
50	0	303	A1EB1	O4-C38-C39	4.32	119.04	111.09
49	G	315	KC2	O2D-CGD-CBD	4.32	118.94	111.27
49	1	315	KC2	CHD-C1D-ND	4.32	128.83	124.26
50	U	203	A1EB1	O1-C20-C19	-4.32	110.14	113.38
48	1	307	A86	C3-C2-C1	-4.32	121.15	127.31
49	9	311	KC2	CHD-C1D-ND	4.32	128.83	124.26
51	6	320	A1ECV	C2A-CAA-CBA	-4.32	118.90	128.63
50	C	302	A1EB1	O4-C38-C39	4.32	119.03	111.09
50	7	306	A1EB1	O4-C38-C39	4.31	119.03	111.09
42	k	204	BCR	C16-C17-C18	-4.31	121.15	127.31
42	b	844	BCR	C16-C17-C18	-4.31	121.15	127.31
50	V	305	A1EB1	C21-C20-C19	4.31	119.13	114.28
43	7	310	DD6	C4-C5-C6	-4.31	121.16	127.31
48	9	306	A86	C4-C5-C6	-4.31	121.16	127.31
49	P	320	KC2	O2D-CGD-CBD	4.31	118.93	111.27
48	V	304	A86	O1-C20-C19	-4.31	110.14	113.38
50	x	301	A1EB1	C4-C5-C6	-4.31	121.16	127.31
48	9	301	A86	C25-C26-C27	-4.31	121.16	127.31
52	P	305	A1EB4	O4-C38-C42	4.31	119.01	111.09
43	z	305	DD6	C21-C20-C19	4.31	119.12	114.28
48	W	304	A86	C4-C5-C6	-4.31	121.17	127.31
49	2	317	KC2	O2D-CGD-CBD	4.30	118.92	111.27
50	6	308	A1EB1	O1-C20-C19	-4.30	110.15	113.38
51	5	312	A1ECV	C2A-CAA-CBA	-4.30	118.93	128.63
50	z	302	A1EB1	O4-C38-C39	4.30	119.00	111.09
52	P	305	A1EB4	C9-C10-C11	-4.30	121.83	127.00
48	k	206	A86	C33-C32-C31	4.30	113.39	109.21
43	E	303	DD6	O1-C20-C19	-4.30	110.15	113.38
48	L	305	A86	O4-C38-C39	4.30	119.00	111.09
52	W	306	A1EB4	C9-C10-C11	-4.30	121.84	127.00
52	W	306	A1EB4	O4-C38-C42	4.30	119.00	111.09
50	y	302	A1EB1	C4-C5-C6	-4.30	121.18	127.31
48	0	306	A86	O4-C38-C39	4.30	118.99	111.09
48	6	302	A86	O4-C38-C39	4.29	118.99	111.09
50	4	301	A1EB1	C25-C26-C27	-4.29	121.15	127.26
48	Z	303	A86	C33-C32-C31	4.29	113.38	109.21
48	M	306	A86	C21-C20-C19	4.29	119.11	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	L	312	KC2	C1D-ND-C4D	4.29	109.38	106.33
50	3	302	A1EB1	O1-C20-C19	-4.29	110.16	113.38
50	7	303	A1EB1	C3-C2-C1	-4.29	121.19	127.31
48	2	305	A86	O4-C38-C39	4.29	118.98	111.09
42	l	207	BCR	C20-C21-C22	-4.29	121.19	127.31
50	7	305	A1EB1	C28-C27-C26	-4.29	119.33	124.93
43	F	303	DD6	O1-C20-C19	-4.29	110.16	113.38
48	U	202	A86	C25-C26-C27	-4.29	121.19	127.31
48	Y	301	A86	C3-C2-C1	-4.29	121.19	127.31
48	Z	301	A86	C4-C5-C6	-4.29	121.19	127.31
48	V	301	A86	C17-C16-C15	4.29	113.53	109.16
51	L	318	A1ECV	CMB-C2B-C1B	4.29	132.82	124.73
49	9	318	KC2	C1D-ND-C4D	4.28	109.38	106.33
48	7	308	A86	C21-C20-C19	4.28	119.10	114.28
50	7	304	A1EB1	O4-C38-C39	4.28	118.97	111.09
43	2	303	DD6	C3-C2-C1	-4.28	121.20	127.31
52	W	321	A1EB4	O1-C15-C14	-4.28	111.37	115.71
50	L	303	A1EB1	C3-C2-C1	-4.28	121.20	127.31
49	z	312	KC2	CHD-C1D-ND	4.28	128.79	124.26
46	l	208	LMG	O7-C10-C11	4.28	120.72	111.50
50	1	301	A1EB1	C3-C2-C1	-4.28	121.21	127.31
50	G	302	A1EB1	O1-C15-C14	-4.27	104.63	113.21
51	X	310	A1ECV	C2A-CAA-CBA	-4.27	119.00	128.63
50	G	302	A1EB1	O4-C38-C39	4.27	118.95	111.09
48	4	305	A86	O4-C38-C39	4.27	118.95	111.09
48	9	303	A86	C21-C20-C19	4.27	119.08	114.28
48	Q	304	A86	C3-C2-C1	-4.27	121.22	127.31
49	6	316	KC2	O2D-CGD-CBD	4.27	118.86	111.27
50	3	310	A1EB1	O4-C38-C39	4.27	118.94	111.09
48	7	311	A86	O1-C20-C19	-4.27	110.17	113.38
48	4	306	A86	O4-C38-C39	4.27	118.94	111.09
48	3	307	A86	O1-C20-C19	-4.27	110.18	113.38
48	x	305	A86	O4-C38-C39	4.27	118.94	111.09
49	S	315	KC2	CHD-C1D-ND	4.27	128.77	124.26
48	2	301	A86	C21-C20-C19	4.27	119.08	114.28
50	x	302	A1EB1	C21-C20-C19	4.26	119.08	114.28
52	5	304	A1EB4	C20-O1-C15	4.26	64.45	61.17
50	V	307	A1EB1	C25-C26-C27	-4.26	121.19	127.26
49	H	314	KC2	CHD-C1D-ND	4.26	128.77	124.26
50	4	301	A1EB1	C21-C20-C19	4.26	119.07	114.28
47	D	321	SQD	O7-S-C6	4.26	112.00	106.94
48	8	303	A86	O1-C20-C21	-4.26	109.95	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	4	304	A1EB1	C21-C20-C19	4.26	119.07	114.28
50	6	306	A1EB1	C4-C5-C6	-4.26	121.23	127.31
48	1	307	A86	O4-C38-C39	4.26	118.92	111.09
49	4	320	KC2	O2D-CGD-CBD	4.26	118.83	111.27
48	1	306	A86	O4-C38-C39	4.26	118.92	111.09
50	K	302	A1EB1	C4-C5-C6	-4.26	121.24	127.31
48	y	305	A86	O1-C20-C21	-4.25	109.96	115.06
50	H	304	A1EB1	O4-C38-C39	4.25	118.92	111.09
48	S	305	A86	O4-C38-C39	4.25	118.92	111.09
50	0	305	A1EB1	C4-C5-C6	-4.25	121.24	127.31
43	Z	302	DD6	C3-C2-C1	-4.25	121.24	127.31
50	R	303	A1EB1	O1-C15-C14	-4.25	104.68	113.21
52	M	322	A1EB4	C9-C10-C11	-4.25	121.90	127.00
48	7	307	A86	O1-C15-C14	-4.25	104.69	113.21
48	T	301	A86	O1-C15-C14	-4.25	104.69	113.21
43	U	204	DD6	C3-C2-C1	-4.25	121.25	127.31
52	X	305	A1EB4	C20-O1-C15	4.24	64.43	61.17
48	z	303	A86	C4-C5-C6	-4.24	121.25	127.31
49	L	312	KC2	CHD-C1D-ND	4.24	128.75	124.26
52	P	319	A1EB4	C9-C10-C11	-4.24	121.90	127.00
49	1	314	KC2	CHD-C1D-ND	4.24	128.75	124.26
49	3	315	KC2	O2D-CGD-CBD	4.24	118.81	111.27
52	5	304	A1EB4	O4-C38-C42	4.24	118.89	111.09
50	2	304	A1EB1	C36-C31-C32	4.24	123.90	119.70
48	P	303	A86	O4-C38-C39	4.24	118.89	111.09
50	Q	307	A1EB1	O4-C38-C39	4.24	118.89	111.09
48	6	303	A86	C21-C20-C19	4.24	119.05	114.28
50	6	306	A1EB1	C25-C26-C27	-4.24	121.26	127.31
50	3	302	A1EB1	C3-C2-C1	-4.24	121.26	127.31
52	M	305	A1EB4	C20-O1-C15	4.24	64.43	61.17
50	H	301	A1EB1	C25-C26-C27	-4.24	121.23	127.26
50	H	301	A1EB1	C21-C20-C19	4.24	119.05	114.28
48	Q	301	A86	O4-C38-C39	4.24	118.88	111.09
42	j	103	BCR	C15-C14-C13	-4.24	121.27	127.31
50	E	301	A1EB1	O4-C38-C39	4.23	118.88	111.09
43	j	102	DD6	C21-C20-C19	4.23	119.04	114.28
48	X	302	A86	C21-C20-C19	4.23	119.04	114.28
49	A	313	KC2	CHD-C1D-ND	4.23	128.74	124.26
47	D	320	SQD	O7-S-C6	4.23	111.97	106.94
48	4	309	A86	O4-C38-C39	4.23	118.88	111.09
48	P	302	A86	C21-C20-C19	4.23	119.04	114.28
49	x	315	KC2	CHD-C1D-ND	4.23	128.74	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	E	304	A86	O1-C15-C14	-4.23	104.72	113.21
51	9	317	A1ECV	O2-CMC-O1	-4.23	115.18	123.45
48	y	305	A86	O4-C38-C39	4.23	118.87	111.09
49	R	306	KC2	C1D-ND-C4D	4.23	109.34	106.33
50	T	302	A1EB1	C41-C32-C31	-4.23	106.69	110.47
50	J	302	A1EB1	C36-C31-C32	4.23	123.89	119.70
48	0	301	A86	O4-C38-C39	4.23	118.86	111.09
50	Q	307	A1EB1	C21-C20-C19	4.23	119.03	114.28
49	X	306	KC2	CHD-C1D-ND	4.22	128.73	124.26
48	9	305	A86	C3-C2-C1	-4.22	121.28	127.31
43	D	307	DD6	C21-C20-C19	4.22	119.03	114.28
43	J	304	DD6	C21-C20-C15	-4.22	115.19	122.26
48	2	302	A86	C4-C5-C6	-4.22	121.29	127.31
43	K	303	DD6	C21-C20-C19	4.22	119.03	114.28
50	G	307	A1EB1	O4-C38-C39	4.22	118.85	111.09
50	2	304	A1EB1	O1-C20-C21	-4.22	110.00	115.06
47	T	321	SQD	C1-O5-C5	4.22	121.97	113.69
42	b	844	BCR	C24-C23-C22	-4.22	119.86	126.23
48	F	301	A86	C12-C11-C13	4.22	123.10	116.02
48	L	306	A86	O1-C20-C21	-4.21	110.01	115.06
48	I	304	A86	C21-C20-C19	4.21	119.02	114.28
46	7	301	LMG	O7-C10-C11	4.21	120.58	111.50
50	5	302	A1EB1	C4-C5-C6	-4.21	121.30	127.31
51	R	310	A1ECV	O2D-CGD-O1D	-4.21	115.61	123.84
47	D	304	SQD	C1-O5-C5	4.21	121.95	113.69
50	7	305	A1EB1	O1-C20-C19	-4.21	110.22	113.38
42	b	848	BCR	C33-C5-C6	-4.21	119.80	124.53
50	T	307	A1EB1	O1-C20-C19	-4.21	110.22	113.38
50	K	302	A1EB1	C21-C20-C19	4.21	119.01	114.28
50	7	306	A1EB1	C33-C32-C31	4.21	113.30	109.21
52	W	306	A1EB4	C20-O1-C15	4.21	64.40	61.17
48	5	301	A86	O4-C38-C39	4.21	118.83	111.09
48	T	306	A86	C25-C26-C27	-4.21	121.31	127.31
48	D	305	A86	C41-C32-C31	-4.20	106.71	110.47
48	L	307	A86	O1-C20-C21	-4.20	110.02	115.06
48	F	301	A86	C3-C2-C1	-4.20	121.31	127.31
48	z	303	A86	C21-C20-C19	4.20	119.01	114.28
41	a	840	LHG	O4-P-O5	4.20	133.02	112.24
48	9	303	A86	O4-C38-C39	4.20	118.82	111.09
49	y	314	KC2	CHD-C1D-ND	4.20	128.70	124.26
48	4	305	A86	C4-C5-C6	-4.20	121.32	127.31
50	4	303	A1EB1	C21-C20-C19	4.20	119.00	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	D	303	DD6	C21-C20-C15	-4.20	115.23	122.26
48	k	206	A86	C21-C20-C19	4.20	119.00	114.28
50	H	301	A1EB1	C28-C27-C26	-4.20	119.44	124.93
49	T	312	KC2	CHD-C1D-ND	4.20	128.70	124.26
41	X	301	LHG	O4-P-O5	4.20	132.98	112.24
48	x	305	A86	O1-C15-C14	-4.20	104.79	113.21
41	D	301	LHG	O4-P-O5	4.19	132.97	112.24
46	4	326	LMG	O7-C10-C11	4.19	120.54	111.50
49	1	312	KC2	C4B-CHC-C1C	-4.19	117.02	126.06
50	3	303	A1EB1	C28-C27-C26	-4.19	119.45	124.93
49	P	306	KC2	O2D-CGD-CBD	4.19	118.71	111.27
43	I	305	DD6	O1-C20-C19	-4.19	110.24	113.38
42	h	202	BCR	C39-C30-C25	-4.19	103.51	110.30
48	0	309	A86	C4-C5-C6	-4.19	121.34	127.31
43	J	304	DD6	C37-C36-C31	-4.19	118.66	124.35
48	W	303	A86	C3-C2-C1	-4.18	121.34	127.31
50	H	304	A1EB1	C4-C5-C6	-4.18	121.34	127.31
50	3	310	A1EB1	C28-C27-C26	-4.18	119.46	124.93
50	4	302	A1EB1	O1-C15-C14	-4.18	104.81	113.21
48	8	302	A86	C25-C26-C27	-4.18	121.34	127.31
50	3	302	A1EB1	C36-C31-C32	4.18	123.85	119.70
50	G	307	A1EB1	C21-C20-C19	4.18	118.98	114.28
50	K	304	A1EB1	C28-C27-C26	-4.18	119.47	124.93
43	O	304	DD6	C9-C10-C11	-4.18	121.35	127.31
48	1	303	A86	C21-C20-C19	4.18	118.98	114.28
43	o	204	DD6	C3-C2-C1	-4.18	121.35	127.31
49	M	313	KC2	CHD-C1D-ND	4.18	128.68	124.26
49	8	314	KC2	O2D-CGD-CBD	4.18	118.69	111.27
49	L	321	KC2	CHD-C1D-ND	4.18	128.68	124.26
52	W	321	A1EB4	C20-O1-C15	4.18	64.38	61.17
50	3	302	A1EB1	O4-C38-C39	4.18	118.77	111.09
52	P	305	A1EB4	C20-O1-C15	4.18	64.38	61.17
48	k	206	A86	C4-C5-C6	-4.18	121.35	127.31
42	b	844	BCR	C3-C4-C5	-4.18	106.62	114.08
43	Q	303	DD6	C25-C26-C27	-4.17	114.46	126.58
42	a	844	BCR	C15-C14-C13	-4.17	121.36	127.31
43	I	307	DD6	O1-C20-C19	-4.17	110.25	113.38
50	3	303	A1EB1	O1-C20-C19	-4.17	110.25	113.38
49	I	303	KC2	C4B-CHC-C1C	-4.17	117.06	126.06
48	8	305	A86	C21-C20-C19	4.17	118.97	114.28
41	H	317	LHG	O4-P-O5	4.17	132.85	112.24
50	C	302	A1EB1	C21-C20-C19	4.17	118.97	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	R	317	A86	C25-C26-C27	-4.17	121.36	127.31
50	y	302	A1EB1	C21-C20-C19	4.17	118.97	114.28
48	1	307	A86	C36-C31-C32	4.17	123.83	119.70
41	D	302	LHG	O4-P-O5	4.17	132.84	112.24
41	j	104	LHG	O4-P-O5	4.17	132.84	112.24
47	H	318	SQD	O47-C7-C8	4.17	120.48	111.50
43	J	306	DD6	C4-C5-C6	-4.16	121.37	127.31
43	F	305	DD6	C37-C36-C31	-4.16	118.69	124.35
42	a	845	BCR	C7-C8-C9	-4.16	119.94	126.23
50	2	304	A1EB1	C25-C26-C27	-4.16	121.33	127.26
49	5	305	KC2	O2D-CGD-CBD	4.16	118.66	111.27
48	6	305	A86	C33-C32-C31	4.16	113.25	109.21
43	D	303	DD6	C9-C10-C11	-4.16	121.38	127.31
50	R	303	A1EB1	C21-C20-C19	4.16	118.96	114.28
50	3	303	A1EB1	C21-C20-C19	4.16	118.95	114.28
48	T	301	A86	O4-C38-C39	4.16	118.73	111.09
48	Q	301	A86	C25-C26-C27	-4.15	121.38	127.31
48	W	307	A86	C4-C5-C6	-4.15	121.39	127.31
52	M	322	A1EB4	C4-C5-C6	-4.15	121.39	127.31
48	4	306	A86	C4-C5-C6	-4.14	121.40	127.31
49	T	315	KC2	O2D-CGD-CBD	4.14	118.63	111.27
48	H	302	A86	O1-C15-C14	-4.14	104.90	113.21
50	3	302	A1EB1	C21-C20-C19	4.14	118.94	114.28
51	X	313	A1ECV	C2A-CAA-CBA	-4.13	119.31	128.63
48	8	307	A86	C4-C5-C6	-4.13	121.41	127.31
48	P	303	A86	C4-C5-C6	-4.13	121.42	127.31
48	Q	304	A86	C21-C20-C19	4.13	118.92	114.28
43	I	307	DD6	C14-C13-C11	-4.13	119.12	125.53
52	P	319	A1EB4	C4-C5-C6	-4.13	121.42	127.31
42	l	207	BCR	C16-C17-C18	-4.13	121.42	127.31
50	C	302	A1EB1	C4-C5-C6	-4.12	121.42	127.31
46	M	319	LMG	O7-C10-C11	4.12	120.38	111.50
48	M	303	A86	O4-C38-C39	4.12	118.67	111.09
52	T	304	A1EB4	C36-C31-C32	4.12	123.78	119.70
48	W	303	A86	O4-C38-C39	4.12	118.67	111.09
43	1	304	DD6	C3-C2-C1	-4.12	121.43	127.31
43	G	303	DD6	C4-C5-C6	-4.12	121.43	127.31
46	Q	322	LMG	O7-C10-C11	4.12	120.38	111.50
50	L	303	A1EB1	C33-C32-C31	4.12	113.21	109.21
50	R	303	A1EB1	C25-C26-C27	-4.12	121.40	127.26
51	7	323	A1ECV	C2A-CAA-CBA	-4.12	119.35	128.63
48	E	304	A86	C36-C31-C32	4.11	123.78	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	P	303	A86	C3-C2-C1	-4.11	121.44	127.31
49	3	321	KC2	O2D-CGD-CBD	4.11	118.58	111.27
48	Q	301	A86	O1-C20-C21	-4.11	110.13	115.06
43	K	303	DD6	C4-C5-C6	-4.11	121.44	127.31
52	X	305	A1EB4	O1-C20-C19	-4.11	110.29	113.38
49	R	318	KC2	O2D-CGD-CBD	4.11	118.57	111.27
49	L	321	KC2	O2D-CGD-CBD	4.11	118.57	111.27
48	T	305	A86	C21-C20-C19	4.11	118.90	114.28
50	7	303	A1EB1	C21-C20-C19	4.11	118.90	114.28
48	G	301	A86	O1-C20-C19	-4.11	110.30	113.38
48	Z	301	A86	O1-C20-C19	-4.11	110.30	113.38
50	6	301	A1EB1	C3-C2-C1	-4.11	121.45	127.31
48	Y	301	A86	C4-C5-C6	-4.11	121.45	127.31
50	T	302	A1EB1	C25-C26-C27	-4.10	121.41	127.26
48	8	303	A86	O1-C20-C19	-4.10	110.30	113.38
49	8	319	KC2	O2D-CGD-CBD	4.10	118.56	111.27
49	L	314	KC2	O2D-CGD-CBD	4.10	118.56	111.27
42	l	202	BCR	C38-C26-C25	-4.10	119.92	124.53
51	2	311	A1ECV	C2A-CAA-CBA	-4.10	119.39	128.63
48	W	307	A86	C3-C2-C1	-4.10	121.47	127.31
48	7	311	A86	O4-C38-C39	4.10	118.62	111.09
48	9	303	A86	O1-C15-C14	-4.09	104.99	113.21
50	U	205	A1EB1	C21-C20-C19	4.09	118.89	114.28
48	T	301	A86	O1-C20-C21	-4.09	110.15	115.06
50	J	302	A1EB1	C3-C2-C1	-4.09	121.47	127.31
39	G	314	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
43	2	303	DD6	C4-C5-C6	-4.09	121.47	127.31
52	R	305	A1EB4	O4-C38-C42	4.09	118.61	111.09
40	b	843	PQN	C11-C12-C13	-4.09	119.98	126.79
48	8	305	A86	C33-C32-C31	4.09	113.19	109.21
48	4	309	A86	C21-C20-C19	4.09	118.88	114.28
49	X	306	KC2	C1D-CHD-C4C	-4.09	116.64	126.34
43	7	310	DD6	C9-C10-C11	-4.09	121.47	127.31
48	8	303	A86	C3-C2-C1	-4.09	121.47	127.31
48	0	308	A86	C3-C4-C5	-4.09	115.10	123.47
48	7	307	A86	C36-C31-C32	4.09	123.75	119.70
43	Z	302	DD6	C4-C5-C6	-4.08	121.48	127.31
49	6	314	KC2	O2D-CGD-CBD	4.08	118.52	111.27
48	Z	303	A86	C4-C5-C6	-4.08	121.48	127.31
48	M	303	A86	C3-C2-C1	-4.08	121.49	127.31
50	V	306	A1EB1	C4-C5-C6	-4.08	121.49	127.31
50	L	303	A1EB1	C25-C26-C27	-4.08	121.45	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	Q	307	A1EB1	C4-C5-C6	-4.08	121.49	127.31
49	9	318	KC2	C1D-CHD-C4C	-4.08	116.66	126.34
43	G	306	DD6	C14-C13-C11	-4.08	119.20	125.53
51	9	317	A1ECV	C2A-CAA-CBA	-4.08	119.43	128.63
39	B	207	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
49	A	310	KC2	C1D-ND-C4D	4.08	109.23	106.33
49	x	315	KC2	C4B-CHC-C1C	-4.08	117.27	126.06
49	6	319	KC2	C4B-CHC-C1C	-4.07	117.27	126.06
48	2	301	A86	C4-C5-C6	-4.07	121.50	127.31
49	G	313	KC2	O2D-CGD-CBD	4.07	118.50	111.27
49	6	319	KC2	CHD-C1D-ND	4.07	128.57	124.26
42	b	847	BCR	C3-C4-C5	-4.07	106.81	114.08
48	X	303	A86	C21-C20-C19	4.07	118.86	114.28
43	R	304	DD6	C9-C10-C11	-4.07	121.50	127.31
48	9	305	A86	O1-C20-C21	-4.07	110.18	115.06
50	8	301	A1EB1	C3-C2-C1	-4.07	121.50	127.31
51	V	317	A1ECV	C2A-CAA-CBA	-4.07	119.45	128.63
50	7	304	A1EB1	C21-C20-C19	4.07	118.86	114.28
49	L	321	KC2	C4B-CHC-C1C	-4.07	117.28	126.06
49	9	316	KC2	C4B-CHC-C1C	-4.07	117.28	126.06
52	5	304	A1EB4	C9-C10-C11	-4.07	122.11	127.00
48	x	305	A86	C25-C26-C27	-4.07	121.51	127.31
46	W	302	LMG	O7-C10-C11	4.07	120.26	111.50
49	Q	313	KC2	C4B-CHC-C1C	-4.06	117.29	126.06
48	9	304	A86	C25-C26-C27	-4.06	121.51	127.31
50	7	304	A1EB1	O1-C20-C19	-4.06	110.33	113.38
48	2	302	A86	C33-C32-C31	4.06	113.16	109.21
47	E	320	SQD	O7-S-C6	4.06	111.77	106.94
49	T	314	KC2	C1D-CHD-C4C	-4.06	116.71	126.34
43	1	304	DD6	C20-C19-C18	-4.06	104.72	112.75
48	Q	302	A86	C3-C2-C1	-4.06	121.52	127.31
49	5	305	KC2	C4B-CHC-C1C	-4.06	117.31	126.06
46	P	317	LMG	O7-C10-C11	4.06	120.24	111.50
52	R	305	A1EB4	O1-C20-C19	-4.05	110.34	113.38
50	G	307	A1EB1	C4-C5-C6	-4.05	121.53	127.31
49	8	319	KC2	C4B-CHC-C1C	-4.05	117.32	126.06
48	6	303	A86	O1-C15-C14	-4.05	105.08	113.21
49	A	310	KC2	C4B-CHC-C1C	-4.05	117.32	126.06
52	M	305	A1EB4	C3-C2-C1	-4.05	121.53	127.31
50	z	301	A1EB1	C21-C20-C19	4.05	118.83	114.28
43	I	305	DD6	C9-C10-C11	-4.05	121.54	127.31
48	J	303	A86	O1-C15-C14	-4.04	105.09	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	8	308	A1EB1	C21-C20-C19	4.04	118.83	114.28
51	7	323	A1ECV	O2-CMC-C2C	4.04	121.97	112.27
49	y	314	KC2	C4B-CHC-C1C	-4.04	117.34	126.06
48	O	307	A86	C36-C31-C32	4.04	123.71	119.70
49	Y	308	KC2	C4B-CHC-C1C	-4.04	117.34	126.06
47	T	321	SQD	O9-S-C6	4.04	111.74	106.94
50	T	307	A1EB1	O4-C38-C39	4.04	118.52	111.09
48	X	303	A86	C3-C2-C1	-4.04	121.55	127.31
50	6	306	A1EB1	C21-C20-C19	4.04	118.82	114.28
48	5	301	A86	C36-C31-C32	4.04	123.70	119.70
50	5	302	A1EB1	C34-O4-C38	-4.04	110.37	117.90
43	E	302	DD6	C21-C20-C19	4.04	118.82	114.28
48	L	301	A86	C4-C5-C6	-4.03	121.55	127.31
51	R	313	A1ECV	O2-CMC-C2C	4.03	121.95	112.27
51	S	318	A1ECV	O2-CMC-C2C	4.03	121.95	112.27
48	L	307	A86	O1-C15-C14	-4.03	105.12	113.21
49	R	306	KC2	C4B-CHC-C1C	-4.03	117.36	126.06
50	V	305	A1EB1	C33-C32-C31	4.03	113.13	109.21
48	L	307	A86	C21-C20-C19	4.03	118.81	114.28
49	Y	308	KC2	C1D-CHD-C4C	-4.03	116.78	126.34
43	A	303	DD6	C-C1-C2	-4.03	117.28	122.92
50	x	301	A1EB1	C28-C27-C26	-4.03	119.67	124.93
43	U	204	DD6	C37-C36-C31	-4.03	118.88	124.35
48	L	306	A86	C9-C8-C6	-4.02	115.11	126.42
50	8	308	A1EB1	C25-C26-C27	-4.02	121.53	127.26
43	j	102	DD6	C9-C10-C11	-4.02	121.57	127.31
46	F	320	LMG	O7-C10-C11	4.02	120.16	111.50
46	S	322	LMG	O7-C10-C11	4.02	120.16	111.50
49	Q	313	KC2	C1D-CHD-C4C	-4.02	116.81	126.34
49	2	317	KC2	C4B-CHC-C1C	-4.02	117.39	126.06
48	U	206	A86	O1-C15-C14	-4.02	105.14	113.21
48	W	303	A86	C21-C20-C19	4.02	118.80	114.28
49	4	324	KC2	C4B-CHC-C1C	-4.02	117.39	126.06
52	R	305	A1EB4	C9-C10-C11	-4.02	122.17	127.00
49	3	315	KC2	C4B-CHC-C1C	-4.02	117.39	126.06
50	V	306	A1EB1	C25-C26-C27	-4.02	121.54	127.26
49	G	311	KC2	C1D-CHD-C4C	-4.02	116.81	126.34
52	P	318	A1EB4	C20-O1-C15	4.02	64.26	61.17
48	6	309	A86	C36-C31-C32	4.02	123.68	119.70
50	3	302	A1EB1	C4-C5-C6	-4.02	121.58	127.31
49	P	313	KC2	C2D-C1D-ND	-4.02	107.54	110.23
48	H	302	A86	C3-C2-C1	-4.01	121.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	y	316	KC2	O2D-CGD-CBD	4.01	118.40	111.27
50	7	303	A1EB1	C25-C26-C27	-4.01	121.54	127.26
41	a	841	LHG	O4-P-O5	4.01	132.07	112.24
48	Q	302	A86	O1-C15-C14	-4.01	105.16	113.21
39	0	323	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
49	X	306	KC2	C4B-CHC-C1C	-4.01	117.41	126.06
48	7	307	A86	C25-C26-C27	-4.01	121.59	127.31
50	4	301	A1EB1	C34-O4-C38	-4.01	110.43	117.90
48	O	302	A86	O1-C15-C14	-4.00	105.18	113.21
48	4	309	A86	O1-C20-C21	-4.00	110.26	115.06
50	K	302	A1EB1	C3-C2-C1	-4.00	121.60	127.31
49	8	314	KC2	C1D-CHD-C4C	-4.00	116.85	126.34
49	J	315	KC2	C4B-CHC-C1C	-4.00	117.43	126.06
49	P	306	KC2	C4B-CHC-C1C	-4.00	117.43	126.06
43	I	307	DD6	C4-C5-C6	-4.00	121.61	127.31
50	3	309	A1EB1	C33-C32-C31	4.00	113.09	109.21
48	C	303	A86	C21-C20-C19	4.00	118.78	114.28
48	4	310	A86	C3-C2-C1	-4.00	121.61	127.31
50	7	306	A1EB1	C36-C31-C32	3.99	123.66	119.70
51	Z	314	A1ECV	C2A-CAA-CBA	-3.99	119.62	128.63
49	7	322	KC2	C4B-CHC-C1C	-3.99	117.45	126.06
43	Q	303	DD6	C21-C20-C15	-3.99	115.57	122.26
48	O	302	A86	C33-C32-C31	3.99	113.09	109.21
50	S	303	A1EB1	C21-C20-C19	3.99	118.77	114.28
39	O	308	CLA	CAC-C3C-C2C	-3.99	120.70	127.53
49	x	315	KC2	O2D-CGD-CBD	3.99	118.36	111.27
43	X	304	DD6	C9-C10-C11	-3.99	121.62	127.31
48	L	307	A86	C36-C31-C32	3.99	123.65	119.70
47	9	322	SQD	O7-S-C6	3.99	111.68	106.94
49	6	319	KC2	C1D-CHD-C4C	-3.98	116.89	126.34
43	4	308	DD6	C15-C14-C13	-3.98	117.57	125.99
43	E	305	DD6	O1-C20-C19	-3.98	110.39	113.38
48	D	305	A86	O1-C20-C21	-3.98	110.28	115.06
48	Y	301	A86	O1-C20-C21	-3.98	110.29	115.06
42	b	847	BCR	C16-C17-C18	-3.98	121.63	127.31
49	7	322	KC2	O2D-CGD-CBD	3.98	118.34	111.27
48	6	309	A86	C25-C26-C27	-3.98	121.63	127.31
49	9	311	KC2	C4B-CHC-C1C	-3.98	117.47	126.06
49	9	316	KC2	C1D-ND-C4D	3.98	109.16	106.33
48	5	301	A86	C33-C32-C31	3.98	113.08	109.21
47	4	327	SQD	O47-C7-C8	3.98	120.07	111.50
48	L	305	A86	C4-C5-C6	-3.98	121.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	O	317	KC2	C1D-CHD-C4C	-3.98	116.91	126.34
50	H	304	A1EB1	C21-C20-C19	3.98	118.75	114.28
48	3	305	A86	O4-C38-C39	3.98	118.40	111.09
49	A	313	KC2	C1D-CHD-C4C	-3.97	116.91	126.34
46	F	317	LMG	O7-C10-C11	3.97	120.06	111.50
50	F	304	A1EB1	C21-C20-C19	3.97	118.75	114.28
48	P	302	A86	C33-C32-C31	3.97	113.07	109.21
49	1	315	KC2	C4B-CHC-C1C	-3.97	117.49	126.06
48	S	304	A86	C4-C5-C6	-3.97	121.64	127.31
48	Q	301	A86	O1-C15-C14	-3.97	105.24	113.21
43	z	304	DD6	C37-C36-C31	-3.97	118.95	124.35
48	J	301	A86	O1-C15-C14	-3.97	105.24	113.21
49	T	312	KC2	C4B-CHC-C1C	-3.97	117.50	126.06
48	L	302	A86	C3-C4-C5	-3.97	115.34	123.47
50	Q	323	A1EB1	C21-C20-C19	3.97	118.75	114.28
51	S	312	A1ECV	O2-CMC-O1	-3.97	115.69	123.45
48	3	305	A86	C21-C20-C19	3.97	118.74	114.28
49	X	314	KC2	C4B-CHC-C1C	-3.96	117.51	126.06
43	Z	302	DD6	C19-C18-C17	-3.96	103.12	110.77
49	R	314	KC2	C4B-CHC-C1C	-3.96	117.51	126.06
49	1	312	KC2	C1D-CHD-C4C	-3.96	116.94	126.34
48	F	302	A86	C21-C20-C19	3.96	118.74	114.28
48	V	304	A86	C21-C20-C19	3.96	118.74	114.28
50	y	302	A1EB1	C3-C2-C1	-3.96	121.66	127.31
47	D	320	SQD	C1-O5-C5	3.96	121.47	113.69
50	2	306	A1EB1	C28-C27-C26	-3.96	119.75	124.93
48	F	301	A86	C21-C20-C19	3.96	118.74	114.28
48	9	303	A86	C3-C2-C1	-3.96	121.66	127.31
50	K	305	A1EB1	C3-C2-C1	-3.96	121.66	127.31
49	W	308	KC2	C4B-CHC-C1C	-3.96	117.51	126.06
48	J	301	A86	C21-C20-C19	3.96	118.73	114.28
50	K	304	A1EB1	C21-C20-C19	3.96	118.73	114.28
50	Q	307	A1EB1	C25-C26-C27	-3.96	121.62	127.26
50	y	301	A1EB1	C21-C20-C19	3.96	118.73	114.28
48	x	305	A86	O1-C20-C21	-3.96	110.31	115.06
43	2	303	DD6	C19-C18-C17	-3.96	103.13	110.77
42	a	843	BCR	C11-C10-C9	-3.96	121.66	127.31
48	7	311	A86	C25-C26-C27	-3.96	121.66	127.31
48	4	328	A86	C21-C20-C19	3.96	118.73	114.28
50	G	308	A1EB1	C25-C26-C27	-3.96	121.63	127.26
49	3	321	KC2	C4B-CHC-C1C	-3.95	117.53	126.06
52	X	305	A1EB4	O4-C38-C42	3.95	118.36	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	y	314	KC2	C1D-CHD-C4C	-3.95	116.96	126.34
42	b	850	BCR	C15-C14-C13	-3.95	121.67	127.31
43	F	305	DD6	C21-C20-C15	-3.95	115.63	122.26
50	4	301	A1EB1	C28-C27-C26	-3.95	119.76	124.93
42	a	845	BCR	C15-C14-C13	-3.95	121.67	127.31
50	2	304	A1EB1	C33-C32-C31	3.95	113.05	109.21
49	W	308	KC2	C1D-CHD-C4C	-3.95	116.97	126.34
49	2	313	KC2	C4B-CHC-C1C	-3.95	117.53	126.06
48	W	303	A86	C36-C31-C32	3.95	123.62	119.70
48	Q	302	A86	O1-C20-C21	-3.95	110.32	115.06
49	B	208	KC2	C4B-CHC-C1C	-3.95	117.54	126.06
49	H	311	KC2	C4B-CHC-C1C	-3.95	117.54	126.06
43	O	304	DD6	C37-C36-C31	-3.95	118.98	124.35
48	4	306	A86	C21-C20-C19	3.95	118.72	114.28
50	y	301	A1EB1	C17-C16-C15	3.95	113.19	109.16
42	b	848	BCR	C15-C14-C13	-3.95	121.67	127.31
48	9	301	A86	C3-C2-C1	-3.95	121.67	127.31
43	D	306	DD6	C37-C36-C31	-3.95	118.98	124.35
39	9	308	CLA	CAA-C2A-C3A	-3.95	101.97	112.78
49	S	315	KC2	CHB-C1B-C2B	-3.95	117.20	125.48
42	i	102	BCR	C15-C14-C13	-3.95	121.68	127.31
48	6	303	A86	O1-C20-C21	-3.95	110.33	115.06
43	A	302	DD6	O1-C20-C19	-3.95	110.42	113.38
49	9	318	KC2	C4B-CHC-C1C	-3.95	117.55	126.06
49	x	315	KC2	C1D-CHD-C4C	-3.95	116.98	126.34
49	z	313	KC2	CBD-CHA-C4D	3.95	108.84	105.72
47	W	301	SQD	O8-S-C6	3.95	112.03	105.74
50	O	301	A1EB1	C25-C26-C27	-3.94	121.64	127.26
48	M	302	A86	O4-C38-C39	3.94	118.35	111.09
49	5	313	KC2	C4B-CHC-C1C	-3.94	117.55	126.06
49	T	315	KC2	C1D-CHD-C4C	-3.94	116.98	126.34
50	1	301	A1EB1	C25-C26-C27	-3.94	121.64	127.26
48	Q	308	A86	C4-C5-C6	-3.94	121.68	127.31
48	0	308	A86	C25-C26-C27	-3.94	121.68	127.31
42	b	846	BCR	C15-C14-C13	-3.94	121.69	127.31
43	A	302	DD6	C4-C5-C6	-3.94	121.69	127.31
52	P	305	A1EB4	C3-C2-C1	-3.94	121.69	127.31
49	S	314	KC2	C4B-CHC-C1C	-3.94	117.57	126.06
48	8	307	A86	O1-C20-C19	-3.94	110.42	113.38
50	3	309	A1EB1	C28-C27-C26	-3.94	119.78	124.93
49	O	317	KC2	C2D-C1D-ND	-3.94	107.59	110.23
48	J	303	A86	C17-C16-C15	3.93	113.18	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	P	312	KC2	C4B-CHC-C1C	-3.93	117.57	126.06
50	3	324	A1EB1	C28-C27-C26	-3.93	119.79	124.93
48	7	312	A86	C4-C5-C6	-3.93	121.70	127.31
49	4	317	KC2	C4B-CHC-C1C	-3.93	117.57	126.06
50	8	301	A1EB1	C21-C20-C19	3.93	118.70	114.28
49	A	310	KC2	C1D-CHD-C4C	-3.93	117.01	126.34
50	K	302	A1EB1	O1-C20-C21	-3.93	110.35	115.06
50	V	306	A1EB1	C21-C20-C19	3.93	118.70	114.28
49	R	306	KC2	O2D-CGD-CBD	3.93	118.25	111.27
48	M	302	A86	C36-C31-C32	3.93	123.59	119.70
49	X	315	KC2	C4B-CHC-C1C	-3.93	117.58	126.06
50	1	301	A1EB1	C28-C27-C26	-3.93	119.80	124.93
49	V	312	KC2	C4B-CHC-C1C	-3.93	117.58	126.06
49	I	312	KC2	C4B-CHC-C1C	-3.93	117.58	126.06
49	z	312	KC2	C4B-CHC-C1C	-3.93	117.58	126.06
50	4	301	A1EB1	C3-C2-C1	-3.93	121.71	127.31
52	W	306	A1EB4	C3-C2-C1	-3.93	121.71	127.31
43	A	303	DD6	C4-C5-C6	-3.93	121.71	127.31
49	V	308	KC2	C4B-CHC-C1C	-3.92	117.59	126.06
50	2	304	A1EB1	C21-C20-C19	3.92	118.69	114.28
43	O	305	DD6	C21-C20-C19	3.92	118.69	114.28
48	G	305	A86	C3-C2-C1	-3.92	121.72	127.31
50	9	302	A1EB1	O4-C38-C39	3.92	118.30	111.09
48	M	303	A86	O1-C20-C21	-3.92	110.36	115.06
48	U	202	A86	O1-C20-C21	-3.92	110.36	115.06
50	2	304	A1EB1	C4-C5-C6	-3.92	121.72	127.31
50	4	303	A1EB1	C34-O4-C38	-3.92	110.59	117.90
49	P	320	KC2	C4B-CHC-C1C	-3.92	117.61	126.06
51	Y	306	A1ECV	C2A-CAA-CBA	-3.92	119.80	128.63
43	Q	303	DD6	C25-C24-C1	-3.92	115.41	126.42
48	3	305	A86	C33-C32-C31	3.92	113.02	109.21
49	R	306	KC2	C1D-CHD-C4C	-3.92	117.05	126.34
43	M	304	DD6	C4-C5-C6	-3.91	121.72	127.31
49	G	313	KC2	C4B-CHC-C1C	-3.91	117.62	126.06
50	Q	323	A1EB1	C3-C4-C5	-3.91	115.46	123.47
48	0	304	A86	C21-C20-C19	3.91	118.68	114.28
48	E	304	A86	C33-C32-C31	3.91	113.01	109.21
48	O	307	A86	C3-C2-C1	-3.91	121.73	127.31
48	L	304	A86	C4-C5-C6	-3.91	121.73	127.31
49	Y	309	KC2	C4B-CHC-C1C	-3.91	117.62	126.06
49	5	314	KC2	C4B-CHC-C1C	-3.91	117.62	126.06
48	L	304	A86	C36-C31-C32	3.91	123.58	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	H	301	A1EB1	C3-C2-C1	-3.91	121.73	127.31
48	y	305	A86	O1-C20-C19	-3.91	110.44	113.38
48	K	301	A86	C25-C26-C27	-3.91	121.73	127.31
43	S	306	DD6	C4-C5-C6	-3.91	121.73	127.31
50	0	303	A1EB1	C28-C27-C26	-3.91	119.82	124.93
49	F	311	KC2	C4B-CHC-C1C	-3.91	117.63	126.06
42	a	843	BCR	C24-C23-C22	-3.91	120.33	126.23
39	L	308	CLA	CAA-C2A-C3A	-3.91	102.08	112.78
49	K	310	KC2	C4B-CHC-C1C	-3.91	117.63	126.06
50	G	308	A1EB1	C21-C20-C19	3.90	118.67	114.28
49	L	312	KC2	C1D-CHD-C4C	-3.90	117.08	126.34
50	6	308	A1EB1	C3-C2-C1	-3.90	121.74	127.31
50	7	303	A1EB1	C10-C9-C8	-3.90	111.03	123.22
49	3	321	KC2	CHC-C4B-C3B	-3.90	118.58	125.26
49	M	314	KC2	C4B-CHC-C1C	-3.90	117.64	126.06
49	X	318	KC2	C4B-CHC-C1C	-3.90	117.64	126.06
49	V	320	KC2	C4B-CHC-C1C	-3.90	117.64	126.06
43	E	305	DD6	C9-C10-C11	-3.90	121.74	127.31
47	7	302	SQD	O7-S-C6	3.90	111.58	106.94
48	Y	301	A86	C21-C20-C19	3.90	118.67	114.28
49	G	311	KC2	C4B-CHC-C1C	-3.90	117.64	126.06
50	2	306	A1EB1	C21-C20-C19	3.90	118.67	114.28
49	9	311	KC2	C1D-CHD-C4C	-3.90	117.09	126.34
49	M	307	KC2	C4B-CHC-C1C	-3.90	117.64	126.06
49	P	313	KC2	O2D-CGD-CBD	3.90	118.20	111.27
48	2	302	A86	O1-C20-C21	-3.90	110.39	115.06
48	V	301	A86	C3-C2-C1	-3.90	121.75	127.31
49	1	314	KC2	C1D-CHD-C4C	-3.90	117.09	126.34
49	z	315	KC2	O2D-CGD-CBD	3.90	118.19	111.27
49	O	317	KC2	C4B-CHC-C1C	-3.90	117.65	126.06
49	x	313	KC2	C4B-CHC-C1C	-3.90	117.65	126.06
48	X	303	A86	O1-C20-C21	-3.90	110.39	115.06
49	F	307	KC2	C4B-CHC-C1C	-3.90	117.65	126.06
50	z	302	A1EB1	C4-C5-C6	-3.90	121.75	127.31
49	G	317	KC2	C4B-CHC-C1C	-3.90	117.66	126.06
49	x	315	KC2	C1D-ND-C4D	3.90	109.10	106.33
48	J	303	A86	O1-C20-C21	-3.89	110.39	115.06
48	Q	304	A86	C36-C31-C32	3.89	123.56	119.70
49	0	316	KC2	C4B-CHC-C1C	-3.89	117.66	126.06
49	L	315	KC2	C4B-CHC-C1C	-3.89	117.66	126.06
49	L	321	KC2	C1D-ND-C4D	3.89	109.10	106.33
48	4	305	A86	C21-C20-C19	3.89	118.66	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	y	316	KC2	C4B-CHC-C1C	-3.89	117.67	126.06
48	6	302	A86	O1-C15-C14	-3.89	105.40	113.21
50	G	308	A1EB1	O1-C20-C21	-3.89	110.39	115.06
48	6	302	A86	C21-C20-C19	3.89	118.66	114.28
49	Z	311	KC2	C4B-CHC-C1C	-3.89	117.67	126.06
43	T	303	DD6	C9-C10-C11	-3.89	121.76	127.31
49	V	318	KC2	C1D-CHD-C4C	-3.89	117.12	126.34
43	A	303	DD6	C21-C20-C15	-3.89	115.75	122.26
49	Q	315	KC2	C1D-CHD-C4C	-3.89	117.12	126.34
51	L	318	A1ECV	C2A-CAA-CBA	-3.89	119.87	128.63
49	L	317	KC2	C4B-CHC-C1C	-3.89	117.68	126.06
48	X	303	A86	C25-C26-C27	-3.88	121.77	127.31
49	G	315	KC2	C1D-CHD-C4C	-3.88	117.12	126.34
49	W	315	KC2	C4B-CHC-C1C	-3.88	117.68	126.06
48	0	301	A86	C4-C5-C6	-3.88	121.77	127.31
48	7	311	A86	C3-C2-C1	-3.88	121.77	127.31
49	0	319	KC2	C1D-CHD-C4C	-3.88	117.13	126.34
43	H	305	DD6	C14-C13-C11	-3.88	119.51	125.53
49	5	305	KC2	C1D-CHD-C4C	-3.88	117.13	126.34
49	8	320	KC2	C4B-CHC-C1C	-3.88	117.69	126.06
45	C	314	DGD	O3G-C3G-C2G	-3.88	101.54	110.90
49	V	318	KC2	C4B-CHC-C1C	-3.88	117.69	126.06
45	C	314	DGD	C3D-C4D-C5D	-3.88	103.32	110.24
43	J	304	DD6	C9-C10-C11	-3.88	121.77	127.31
49	T	316	KC2	C4B-CHC-C1C	-3.88	117.69	126.06
49	2	314	KC2	C4B-CHC-C1C	-3.88	117.69	126.06
48	W	304	A86	C25-C26-C27	-3.88	121.77	127.31
48	6	302	A86	O1-C20-C21	-3.88	110.41	115.06
47	H	318	SQD	O7-S-C6	3.88	111.55	106.94
42	k	204	BCR	C20-C21-C22	-3.88	121.78	127.31
48	Q	304	A86	O1-C20-C21	-3.88	110.41	115.06
49	B	208	KC2	CBD-CHA-C1A	3.88	136.11	128.88
47	4	327	SQD	C1-O5-C5	3.88	121.30	113.69
49	9	316	KC2	C1D-CHD-C4C	-3.88	117.14	126.34
48	9	306	A86	C25-C26-C27	-3.88	121.78	127.31
49	W	315	KC2	C1D-CHD-C4C	-3.88	117.14	126.34
39	O	308	CLA	CBC-CAC-C3C	3.88	123.12	112.43
49	5	311	KC2	C4B-CHC-C1C	-3.88	117.70	126.06
49	K	313	KC2	C4B-CHC-C1C	-3.87	117.70	126.06
51	E	311	A1ECV	O2-CMC-C2C	3.87	121.56	112.27
49	Y	308	KC2	CHD-C1D-ND	3.87	128.36	124.26
49	Q	318	KC2	C4B-CHC-C1C	-3.87	117.71	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	k	205	SQD	O7-S-C6	3.87	111.54	106.94
47	F	319	SQD	O9-S-C6	3.87	111.54	106.94
42	l	202	BCR	C15-C14-C13	-3.87	121.78	127.31
49	Z	310	KC2	C4B-CHC-C1C	-3.87	117.71	126.06
43	O	305	DD6	C4-C5-C6	-3.87	121.79	127.31
49	M	307	KC2	C1D-CHD-C4C	-3.87	117.16	126.34
50	y	302	A1EB1	C28-C27-C26	-3.87	119.87	124.93
51	X	313	A1ECV	O2-CMC-C2C	3.87	121.55	112.27
50	K	305	A1EB1	C33-C32-C31	3.87	112.97	109.21
49	4	320	KC2	C4B-CHC-C1C	-3.87	117.71	126.06
43	W	305	DD6	C4-C5-C6	-3.87	121.79	127.31
48	K	301	A86	O1-C20-C21	-3.87	110.42	115.06
50	x	302	A1EB1	C28-C27-C26	-3.87	119.88	124.93
49	P	310	KC2	C4B-CHC-C1C	-3.87	117.72	126.06
49	P	313	KC2	C4B-CHC-C1C	-3.87	117.72	126.06
47	k	205	SQD	O9-S-O7	-3.87	100.57	113.95
43	P	304	DD6	C21-C20-C19	3.86	118.63	114.28
48	3	306	A86	C3-C2-C1	-3.86	121.79	127.31
49	H	311	KC2	C1D-CHD-C4C	-3.86	117.17	126.34
49	3	317	KC2	C1D-CHD-C4C	-3.86	117.17	126.34
50	T	302	A1EB1	C36-C31-C32	3.86	123.53	119.70
48	M	303	A86	C25-C26-C27	-3.86	121.80	127.31
48	6	302	A86	C3-C2-C1	-3.86	121.80	127.31
49	C	312	KC2	C1D-CHD-C4C	-3.86	117.18	126.34
50	7	306	A1EB1	C25-C26-C27	-3.86	121.76	127.26
49	W	312	KC2	C4B-CHC-C1C	-3.86	117.73	126.06
51	E	311	A1ECV	CMB-C2B-C1B	3.86	132.02	124.73
50	S	302	A1EB1	C36-C31-C32	3.86	123.53	119.70
50	G	307	A1EB1	O1-C20-C19	-3.86	110.48	113.38
52	T	304	A1EB4	C9-C10-C11	-3.86	122.36	127.00
49	R	312	KC2	C4B-CHC-C1C	-3.86	117.73	126.06
49	6	314	KC2	C4B-CHC-C1C	-3.86	117.73	126.06
48	6	305	A86	C3-C2-C1	-3.86	121.80	127.31
50	3	303	A1EB1	C4-C5-C6	-3.86	121.80	127.31
47	T	321	SQD	O9-S-O7	-3.86	100.60	113.95
50	V	302	A1EB1	C25-C26-C27	-3.86	121.77	127.26
49	M	311	KC2	C4B-CHC-C1C	-3.86	117.74	126.06
48	k	206	A86	C36-C31-C32	3.86	123.52	119.70
43	I	307	DD6	C21-C20-C19	3.86	118.62	114.28
52	M	305	A1EB4	C40-C32-C31	-3.86	107.02	110.47
49	P	313	KC2	C1D-ND-C4D	3.86	109.07	106.33
48	1	302	A86	O1-C20-C21	-3.85	110.44	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	9	306	A86	C34-O4-C38	-3.85	110.71	117.90
49	S	317	KC2	C4B-CHC-C1C	-3.85	117.74	126.06
48	X	302	A86	O4-C38-C39	3.85	118.18	111.09
49	0	314	KC2	C4B-CHC-C1C	-3.85	117.75	126.06
49	L	321	KC2	C1D-CHD-C4C	-3.85	117.20	126.34
48	L	302	A86	O1-C20-C21	-3.85	110.44	115.06
49	y	314	KC2	C1D-ND-C4D	3.85	109.07	106.33
49	S	317	KC2	C1D-CHD-C4C	-3.85	117.20	126.34
52	M	305	A1EB4	C9-C10-C11	-3.85	122.38	127.00
49	H	314	KC2	C4B-CHC-C1C	-3.85	117.75	126.06
49	z	315	KC2	C4B-CHC-C1C	-3.85	117.76	126.06
49	7	320	KC2	C1D-CHD-C4C	-3.85	117.21	126.34
49	4	320	KC2	C1D-CHD-C4C	-3.85	117.21	126.34
49	R	312	KC2	C1D-CHD-C4C	-3.84	117.22	126.34
50	C	302	A1EB1	C3-C2-C1	-3.84	121.83	127.31
48	2	305	A86	O1-C20-C19	-3.84	110.50	113.38
49	y	313	KC2	C4B-CHC-C1C	-3.84	117.77	126.06
49	8	317	KC2	C1D-CHD-C4C	-3.84	117.23	126.34
49	3	315	KC2	C1D-ND-C4D	3.84	109.06	106.33
43	A	304	DD6	C9-C10-C11	-3.84	121.83	127.31
50	h	203	A1EB1	C25-C26-C27	-3.84	121.80	127.26
43	O	303	DD6	C3-C4-C5	-3.84	115.61	123.47
49	9	318	KC2	CHD-C1D-ND	3.84	128.32	124.26
50	y	302	A1EB1	C17-C16-C15	3.84	113.08	109.16
48	8	303	A86	C21-C20-C19	3.84	118.60	114.28
49	T	315	KC2	C4B-CHC-C1C	-3.84	117.78	126.06
49	Y	309	KC2	C1D-CHD-C4C	-3.84	117.24	126.34
47	D	304	SQD	O7-S-C6	3.84	111.50	106.94
49	x	312	KC2	C1D-CHD-C4C	-3.83	117.24	126.34
49	x	313	KC2	C1D-CHD-C4C	-3.83	117.24	126.34
49	1	314	KC2	C4B-CHC-C1C	-3.83	117.79	126.06
49	z	312	KC2	C1D-CHD-C4C	-3.83	117.25	126.34
47	4	327	SQD	O7-S-C6	3.83	111.50	106.94
49	7	322	KC2	C1D-CHD-C4C	-3.83	117.25	126.34
46	M	319	LMG	O6-C5-C4	3.83	116.66	109.69
49	P	312	KC2	C1D-CHD-C4C	-3.83	117.25	126.34
49	X	314	KC2	C1D-CHD-C4C	-3.83	117.25	126.34
48	7	312	A86	C25-C26-C27	-3.83	121.84	127.31
39	3	320	CLA	O2D-CGD-O1D	-3.83	116.34	123.84
51	R	310	A1ECV	O2-CMC-C2C	3.83	121.46	112.27
51	5	309	A1ECV	C2A-CAA-CBA	-3.83	119.99	128.63
42	j	103	BCR	C16-C17-C18	-3.83	121.85	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	a	843	BCR	C15-C14-C13	-3.83	121.85	127.31
52	P	305	A1EB4	O1-C20-C19	-3.83	110.51	113.38
48	y	305	A86	C21-C20-C19	3.83	118.58	114.28
47	F	319	SQD	O9-S-O7	-3.83	100.71	113.95
49	x	312	KC2	C4B-CHC-C1C	-3.83	117.80	126.06
52	W	306	A1EB4	O1-C20-C19	-3.83	110.51	113.38
42	h	202	BCR	C15-C14-C13	-3.83	121.85	127.31
43	y	304	DD6	C15-C14-C13	-3.83	117.90	125.99
50	8	301	A1EB1	C4-C5-C6	-3.83	121.85	127.31
49	2	314	KC2	C1D-CHD-C4C	-3.82	117.27	126.34
46	0	324	LMG	C8-O7-C10	-3.82	110.77	117.90
51	S	312	A1ECV	O2-CMC-C2C	3.82	121.44	112.27
43	V	303	DD6	C3-C2-C1	-3.82	121.85	127.31
47	W	301	SQD	O9-S-O7	-3.82	100.72	113.95
51	4	315	A1ECV	O2-CMC-O1	-3.82	115.98	123.45
48	P	303	A86	C25-C26-C27	-3.82	121.86	127.31
49	L	317	KC2	C1D-CHD-C4C	-3.82	117.28	126.34
43	J	305	DD6	C21-C20-C19	3.82	118.58	114.28
49	Z	310	KC2	C1D-CHD-C4C	-3.82	117.28	126.34
49	Z	311	KC2	C1D-CHD-C4C	-3.82	117.28	126.34
49	4	318	KC2	C4B-CHC-C1C	-3.82	117.83	126.06
42	m	101	BCR	C2-C1-C6	3.82	116.36	110.48
49	R	314	KC2	C1D-CHD-C4C	-3.82	117.29	126.34
48	M	306	A86	C25-C26-C27	-3.82	121.86	127.31
50	T	307	A1EB1	C21-C20-C19	3.82	118.57	114.28
49	5	314	KC2	C1D-CHD-C4C	-3.82	117.29	126.34
47	D	304	SQD	O47-C7-C8	3.81	119.72	111.50
43	V	303	DD6	C4-C5-C6	-3.81	121.87	127.31
49	5	313	KC2	C1D-CHD-C4C	-3.81	117.29	126.34
49	6	316	KC2	C1D-CHD-C4C	-3.81	117.29	126.34
50	G	304	A1EB1	C36-C31-C32	3.81	123.48	119.70
49	M	314	KC2	C1D-CHD-C4C	-3.81	117.30	126.34
48	1	307	A86	C21-C20-C19	3.81	118.57	114.28
43	E	305	DD6	C14-C13-C11	-3.81	119.61	125.53
49	z	315	KC2	C1D-CHD-C4C	-3.81	117.30	126.34
48	W	304	A86	C33-C32-C31	3.81	112.92	109.21
43	j	102	DD6	C9-C8-C6	-3.81	115.71	126.42
49	X	312	KC2	C4B-CHC-C1C	-3.81	117.84	126.06
39	x	318	CLA	CAA-C2A-C3A	-3.81	107.21	116.10
49	8	319	KC2	C1D-CHD-C4C	-3.81	117.31	126.34
49	V	315	KC2	C4B-CHC-C1C	-3.81	117.84	126.06
49	C	313	KC2	C4B-CHC-C1C	-3.81	117.85	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	E	311	A1ECV	O2D-CGD-O1D	-3.81	116.40	123.84
43	D	303	DD6	C37-C36-C31	-3.81	119.18	124.35
50	0	302	A1EB1	C4-C5-C6	-3.80	121.88	127.31
49	V	320	KC2	CBD-CHA-C1A	3.80	135.97	128.88
49	y	316	KC2	C1D-CHD-C4C	-3.80	117.32	126.34
50	6	301	A1EB1	C21-C20-C19	3.80	118.56	114.28
49	C	313	KC2	C1D-CHD-C4C	-3.80	117.32	126.34
49	8	320	KC2	C1D-CHD-C4C	-3.80	117.32	126.34
47	P	301	SQD	O7-S-C6	3.80	111.46	106.94
49	G	317	KC2	C1D-CHD-C4C	-3.80	117.33	126.34
49	A	313	KC2	C4B-CHC-C1C	-3.80	117.86	126.06
43	7	309	DD6	C15-C14-C13	-3.80	117.96	125.99
49	R	318	KC2	C4B-CHC-C1C	-3.80	117.87	126.06
49	8	316	KC2	C4B-CHC-C1C	-3.80	117.87	126.06
42	a	844	BCR	C28-C27-C26	-3.80	107.30	114.08
43	E	303	DD6	C3-C2-C1	-3.79	121.89	127.31
48	D	305	A86	C21-C20-C19	3.79	118.55	114.28
48	O	306	A86	C21-C20-C19	3.79	118.55	114.28
48	E	304	A86	C4-C5-C6	-3.79	121.90	127.31
48	X	303	A86	C12-C11-C13	3.79	122.39	116.02
50	V	306	A1EB1	C35-C34-C33	3.79	116.49	109.88
50	7	304	A1EB1	C4-C5-C6	-3.79	121.90	127.31
49	H	314	KC2	C1D-CHD-C4C	-3.79	117.35	126.34
47	D	320	SQD	C44-O6-C1	3.79	121.14	113.74
50	O	301	A1EB1	C4-C5-C6	-3.79	121.90	127.31
48	6	307	A86	O1-C20-C19	-3.79	110.54	113.38
47	D	321	SQD	O9-S-O7	-3.79	100.84	113.95
43	A	304	DD6	C21-C20-C19	3.79	118.54	114.28
48	R	301	A86	C3-C2-C1	-3.79	121.91	127.31
49	7	319	KC2	C1D-CHD-C4C	-3.79	117.36	126.34
48	x	305	A86	C21-C20-C19	3.79	118.54	114.28
49	0	319	KC2	C2D-C1D-ND	-3.79	107.69	110.23
51	E	311	A1ECV	O2-CMC-O1	-3.79	116.05	123.45
49	6	317	KC2	C4B-CHC-C1C	-3.78	117.89	126.06
50	9	302	A1EB1	C33-C32-C31	3.78	112.89	109.21
39	b	830	CLA	CMB-C2B-C1B	-3.78	119.61	125.37
49	X	315	KC2	C1D-CHD-C4C	-3.78	117.36	126.34
49	0	314	KC2	C1D-CHD-C4C	-3.78	117.37	126.34
49	W	314	KC2	C1D-CHD-C4C	-3.78	117.37	126.34
49	1	315	KC2	C1D-CHD-C4C	-3.78	117.37	126.34
47	7	302	SQD	O47-C7-C8	3.78	119.65	111.50
49	W	315	KC2	C1D-ND-C4D	3.78	109.02	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	P	303	A86	C21-C20-C19	3.78	118.53	114.28
48	6	309	A86	C4-C3-C2	-3.78	115.73	123.47
48	8	305	A86	C3-C2-C1	-3.78	121.92	127.31
48	8	323	A86	C4-C5-C6	-3.78	121.92	127.31
47	D	304	SQD	O9-S-O7	-3.78	100.87	113.95
49	y	313	KC2	C1D-CHD-C4C	-3.78	117.38	126.34
42	b	847	BCR	C24-C23-C22	-3.78	120.53	126.23
49	z	313	KC2	C1D-CHD-C4C	-3.78	117.38	126.34
50	E	301	A1EB1	C36-C31-C32	3.78	123.44	119.70
48	F	302	A86	C17-C16-C15	3.78	113.02	109.16
48	3	306	A86	C17-C16-C15	3.78	113.02	109.16
43	W	305	DD6	C9-C10-C11	-3.78	121.92	127.31
48	J	303	A86	C21-C20-C19	3.78	118.53	114.28
49	Q	318	KC2	C1D-CHD-C4C	-3.78	117.38	126.34
47	D	321	SQD	O47-C7-C8	3.77	119.64	111.50
49	C	312	KC2	C4B-CHC-C1C	-3.77	117.92	126.06
48	T	301	A86	C21-C20-C19	3.77	118.53	114.28
47	P	301	SQD	O9-S-C6	3.77	111.42	106.94
49	L	314	KC2	C4B-CHC-C1C	-3.77	117.92	126.06
49	S	314	KC2	C1D-CHD-C4C	-3.77	117.39	126.34
48	2	302	A86	C21-C20-C19	3.77	118.52	114.28
49	P	320	KC2	C1D-CHD-C4C	-3.77	117.39	126.34
50	E	301	A1EB1	C21-C20-C19	3.77	118.52	114.28
47	D	304	SQD	O9-S-C6	3.77	111.42	106.94
49	T	314	KC2	C4B-CHC-C1C	-3.77	117.92	126.06
49	G	315	KC2	C4B-CHC-C1C	-3.77	117.93	126.06
50	x	301	A1EB1	C21-C20-C19	3.77	118.52	114.28
49	O	317	KC2	CHD-C1D-ND	3.77	128.25	124.26
48	y	306	A86	C36-C31-C32	3.77	123.44	119.70
49	V	320	KC2	C1D-CHD-C4C	-3.77	117.40	126.34
49	8	316	KC2	C1D-CHD-C4C	-3.77	117.40	126.34
49	6	314	KC2	C1D-CHD-C4C	-3.77	117.40	126.34
49	6	317	KC2	C1D-CHD-C4C	-3.77	117.40	126.34
48	0	306	A86	O1-C15-C14	-3.77	105.65	113.21
47	k	205	SQD	O47-C7-C8	3.77	119.62	111.50
49	8	314	KC2	C4B-CHC-C1C	-3.77	117.93	126.06
39	Y	311	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
50	0	305	A1EB1	C28-C27-C26	-3.76	120.01	124.93
43	x	304	DD6	C15-C14-C13	-3.76	118.04	125.99
43	H	305	DD6	C3-C2-C1	-3.76	121.94	127.31
49	3	318	KC2	C4B-CHC-C1C	-3.76	117.94	126.06
48	7	307	A86	C21-C20-C19	3.76	118.51	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	W	312	KC2	C1D-CHD-C4C	-3.76	117.42	126.34
49	P	313	KC2	C1D-CHD-C4C	-3.76	117.42	126.34
50	4	302	A1EB1	C25-C26-C27	-3.76	121.91	127.26
50	J	302	A1EB1	C21-C20-C19	3.76	118.51	114.28
49	Q	313	KC2	O2D-CGD-CBD	3.76	117.95	111.27
42	a	844	BCR	C24-C23-C22	-3.76	120.56	126.23
43	O	303	DD6	O1-C20-C21	-3.76	110.55	115.06
49	8	317	KC2	C4B-CHC-C1C	-3.76	117.95	126.06
49	R	318	KC2	C1D-CHD-C4C	-3.76	117.42	126.34
49	J	315	KC2	C1D-CHD-C4C	-3.76	117.43	126.34
48	W	304	A86	O1-C15-C14	-3.76	105.67	113.21
49	K	310	KC2	C1D-CHD-C4C	-3.76	117.43	126.34
43	C	301	DD6	C37-C36-C31	-3.76	119.24	124.35
48	4	305	A86	C3-C2-C1	-3.76	121.95	127.31
48	0	301	A86	C21-C20-C19	3.76	118.50	114.28
49	P	310	KC2	C1D-CHD-C4C	-3.76	117.43	126.34
49	7	319	KC2	C4B-CHC-C1C	-3.76	117.96	126.06
43	5	303	DD6	C9-C10-C11	-3.75	121.95	127.31
39	M	309	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
49	X	318	KC2	C1D-CHD-C4C	-3.75	117.44	126.34
48	T	306	A86	C36-C31-C32	3.75	123.42	119.70
49	8	319	KC2	C1D-ND-C4D	3.75	109.00	106.33
48	2	305	A86	C24-C1-C2	3.75	124.70	118.94
49	4	324	KC2	C1D-CHD-C4C	-3.75	117.44	126.34
48	W	304	A86	C36-C31-C32	3.75	123.42	119.70
49	K	313	KC2	C1D-CHD-C4C	-3.75	117.44	126.34
51	4	315	A1ECV	O2-CMC-C2C	3.75	121.27	112.27
43	A	302	DD6	C37-C36-C31	-3.75	119.26	124.35
48	Q	304	A86	O1-C15-C14	-3.75	105.69	113.21
43	G	303	DD6	C33-C34-C35	-3.75	105.18	110.30
50	h	203	A1EB1	C4-C5-C6	-3.75	121.97	127.31
47	H	318	SQD	O9-S-O7	-3.74	100.99	113.95
49	M	313	KC2	C1D-CHD-C4C	-3.74	117.46	126.34
50	U	203	A1EB1	C25-C26-C27	-3.74	121.93	127.26
50	J	302	A1EB1	O1-C20-C21	-3.74	110.57	115.06
49	2	317	KC2	C1D-CHD-C4C	-3.74	117.46	126.34
48	E	304	A86	C3-C2-C1	-3.74	121.97	127.31
50	S	303	A1EB1	C3-C4-C5	-3.74	115.81	123.47
49	W	314	KC2	C4B-CHC-C1C	-3.74	117.98	126.06
49	V	308	KC2	C1D-CHD-C4C	-3.74	117.46	126.34
50	G	304	A1EB1	C41-C32-C31	-3.74	107.12	110.47
50	7	304	A1EB1	O1-C20-C21	-3.74	110.57	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	O	302	A86	C17-C16-C15	3.74	112.98	109.16
47	M	301	SQD	O9-S-O7	-3.74	101.01	113.95
48	T	305	A86	O1-C15-C14	-3.74	105.71	113.21
49	3	318	KC2	CHB-C1B-C2B	-3.74	117.64	125.48
49	0	316	KC2	C1D-CHD-C4C	-3.74	117.48	126.34
49	3	321	KC2	C1D-CHD-C4C	-3.74	117.48	126.34
48	2	301	A86	C25-C26-C27	-3.73	121.98	127.31
50	5	302	A1EB1	C28-C27-C26	-3.73	120.05	124.93
48	L	306	A86	C21-C20-C19	3.73	118.48	114.28
42	a	842	BCR	C15-C14-C13	-3.73	121.99	127.31
49	M	311	KC2	C1D-CHD-C4C	-3.73	117.49	126.34
48	Z	301	A86	C21-C20-C19	3.73	118.48	114.28
48	2	302	A86	O1-C15-C14	-3.73	105.73	113.21
47	E	320	SQD	O9-S-O7	-3.73	101.05	113.95
47	F	318	SQD	O9-S-O7	-3.73	101.05	113.95
49	3	315	KC2	C1D-CHD-C4C	-3.73	117.50	126.34
49	3	318	KC2	C1D-CHD-C4C	-3.73	117.50	126.34
50	x	301	A1EB1	O1-C20-C21	-3.73	110.59	115.06
49	0	317	KC2	C1D-CHD-C4C	-3.72	117.50	126.34
43	E	302	DD6	C3-C2-C1	-3.72	121.99	127.31
49	G	313	KC2	C1D-CHD-C4C	-3.72	117.50	126.34
43	z	304	DD6	C37-C36-C35	3.72	121.25	114.36
48	M	303	A86	O1-C15-C14	-3.72	105.74	113.21
49	2	313	KC2	C1D-CHD-C4C	-3.72	117.51	126.34
48	Q	305	A86	C25-C26-C27	-3.72	122.00	127.31
50	6	304	A1EB1	C25-C26-C27	-3.72	121.96	127.26
42	a	843	BCR	C20-C21-C22	-3.72	122.00	127.31
43	a	846	DD6	C21-C20-C19	3.72	118.47	114.28
51	V	317	A1ECV	O2-CMC-C2C	3.72	121.19	112.27
50	D	308	A1EB1	C28-C27-C26	-3.72	120.07	124.93
39	y	319	CLA	CAA-C2A-C3A	-3.72	107.42	116.10
42	l	206	BCR	C38-C26-C25	-3.72	120.35	124.53
43	S	306	DD6	O1-C20-C19	-3.72	110.59	113.38
52	W	306	A1EB4	C4-C5-C6	-3.72	122.01	127.31
47	W	301	SQD	O47-C7-C8	3.72	119.51	111.50
48	S	305	A86	C21-C20-C19	3.72	118.46	114.28
50	S	303	A1EB1	C33-C32-C31	3.72	112.82	109.21
49	L	314	KC2	C1D-CHD-C4C	-3.71	117.53	126.34
48	8	302	A86	C33-C32-C31	3.71	112.82	109.21
49	V	312	KC2	C1D-CHD-C4C	-3.71	117.54	126.34
49	V	314	KC2	C1D-CHD-C4C	-3.71	117.54	126.34
43	M	304	DD6	C21-C20-C19	3.71	118.45	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	F	307	KC2	C1D-CHD-C4C	-3.71	117.54	126.34
47	7	302	SQD	O9-S-O7	-3.71	101.11	113.95
52	P	305	A1EB4	C4-C5-C6	-3.71	122.02	127.31
43	x	303	DD6	C37-C36-C31	-3.71	119.31	124.35
50	6	308	A1EB1	C40-C32-C31	-3.71	107.15	110.47
49	T	316	KC2	C1D-CHD-C4C	-3.71	117.55	126.34
49	P	306	KC2	C1D-CHD-C4C	-3.71	117.55	126.34
47	P	301	SQD	O9-S-O7	-3.71	101.12	113.95
39	D	309	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
49	5	305	KC2	CHC-C4B-C3B	-3.71	118.92	125.26
39	2	307	CLA	CAA-C2A-C3A	-3.70	107.45	116.10
39	9	315	CLA	CAA-C2A-C3A	-3.70	107.46	116.10
50	R	303	A1EB1	O4-C38-C39	3.70	117.90	111.09
42	h	202	BCR	C24-C23-C22	-3.70	120.64	126.23
39	O	314	CLA	C3B-C4B-NB	-3.70	107.08	110.52
48	Q	305	A86	C3-C2-C1	-3.70	122.03	127.31
50	S	302	A1EB1	C33-C32-C31	3.70	112.81	109.21
47	S	301	SQD	O9-S-O7	-3.70	101.15	113.95
50	U	203	A1EB1	C3-C2-C1	-3.70	122.03	127.31
50	1	305	A1EB1	O1-C20-C19	-3.70	110.61	113.38
48	H	302	A86	C4-C5-C6	-3.70	122.04	127.31
47	4	327	SQD	O9-S-O7	-3.69	101.16	113.95
48	W	304	A86	C21-C20-C19	3.69	118.44	114.28
48	L	305	A86	C21-C20-C19	3.69	118.44	114.28
42	a	844	BCR	C20-C21-C22	-3.69	122.04	127.31
43	J	305	DD6	O1-C20-C19	-3.69	110.61	113.38
49	I	303	KC2	CBD-CHA-C1A	3.69	135.76	128.88
49	0	317	KC2	C4B-CHC-C1C	-3.69	118.10	126.06
51	5	312	A1ECV	O2-CMC-C2C	3.69	121.12	112.27
48	9	303	A86	O1-C20-C21	-3.69	110.64	115.06
50	G	307	A1EB1	O1-C15-C14	-3.69	105.81	113.21
43	2	303	DD6	C37-C36-C31	-3.69	119.34	124.35
48	S	304	A86	C3-C2-C1	-3.69	122.05	127.31
43	A	303	DD6	C37-C36-C31	-3.69	119.34	124.35
48	3	307	A86	O1-C20-C21	-3.69	110.64	115.06
49	M	313	KC2	CHB-C1B-C2B	-3.69	117.75	125.48
50	1	305	A1EB1	C25-C26-C27	-3.69	122.01	127.26
48	T	305	A86	C4-C5-C6	-3.68	122.05	127.31
49	7	320	KC2	C4B-CHC-C1C	-3.68	118.11	126.06
48	F	301	A86	C25-C26-C27	-3.68	122.06	127.31
48	L	301	A86	C21-C20-C19	3.68	118.42	114.28
50	6	304	A1EB1	C3-C2-C1	-3.68	122.06	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	R	304	DD6	O1-C20-C19	-3.68	110.62	113.38
43	M	304	DD6	C9-C10-C11	-3.68	122.06	127.31
50	8	306	A1EB1	C40-C32-C31	-3.68	107.18	110.47
47	9	322	SQD	O9-S-O7	-3.68	101.21	113.95
43	Q	306	DD6	C15-C14-C13	-3.68	118.21	125.99
42	i	102	BCR	C7-C8-C9	-3.68	120.67	126.23
48	F	302	A86	O1-C15-C14	-3.68	105.83	113.21
49	F	311	KC2	C1D-CHD-C4C	-3.68	117.61	126.34
47	M	301	SQD	O9-S-C6	3.68	111.31	106.94
43	4	307	DD6	C15-C14-C13	-3.68	118.22	125.99
48	y	306	A86	C33-C32-C31	3.68	112.78	109.21
50	Q	323	A1EB1	O1-C20-C21	-3.68	110.65	115.06
49	I	303	KC2	C1D-CHD-C4C	-3.67	117.62	126.34
42	i	102	BCR	C30-C25-C26	-3.67	117.44	122.61
48	E	304	A86	O1-C20-C21	-3.67	110.65	115.06
48	9	304	A86	C4-C5-C6	-3.67	122.07	127.31
50	z	302	A1EB1	C28-C27-C26	-3.67	120.13	124.93
48	J	301	A86	O1-C20-C21	-3.67	110.66	115.06
48	G	301	A86	C4-C5-C6	-3.67	122.07	127.31
49	V	314	KC2	C4B-CHC-C1C	-3.67	118.14	126.06
50	D	308	A1EB1	C4-C5-C6	-3.67	122.07	127.31
50	h	203	A1EB1	C28-C27-C26	-3.67	120.13	124.93
49	X	312	KC2	C1D-CHD-C4C	-3.67	117.63	126.34
48	4	309	A86	C3-C2-C1	-3.67	122.07	127.31
48	4	309	A86	C25-C26-C27	-3.67	122.07	127.31
43	Z	302	DD6	C37-C36-C31	-3.67	119.36	124.35
50	S	302	A1EB1	C28-C27-C26	-3.67	120.13	124.93
50	1	305	A1EB1	C28-C27-C26	-3.67	120.14	124.93
49	I	312	KC2	C1D-CHD-C4C	-3.67	117.64	126.34
49	M	307	KC2	CBD-CHA-C1A	3.67	135.72	128.88
42	j	103	BCR	C3-C4-C5	-3.67	107.53	114.08
52	M	305	A1EB4	C4-C5-C6	-3.67	122.08	127.31
49	B	208	KC2	C1D-CHD-C4C	-3.67	117.64	126.34
50	V	306	A1EB1	C28-C27-C26	-3.67	120.14	124.93
48	M	303	A86	C21-C20-C19	3.66	118.40	114.28
48	L	304	A86	C34-O4-C38	-3.66	111.07	117.90
50	Q	307	A1EB1	C28-C27-C26	-3.66	120.14	124.93
50	6	304	A1EB1	C17-C16-C15	3.66	112.90	109.16
51	5	309	A1ECV	O2D-CGD-O1D	-3.66	116.68	123.84
50	K	305	A1EB1	C36-C31-C32	3.66	123.33	119.70
49	P	306	KC2	CHB-C1B-C2B	-3.66	117.81	125.48
49	2	317	KC2	CHC-C4B-C3B	-3.66	119.00	125.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	8	301	A1EB1	C36-C31-C32	3.66	123.32	119.70
49	S	315	KC2	C1D-CHD-C4C	-3.65	117.67	126.34
39	U	213	CLA	CAA-C2A-C3A	-3.65	107.57	116.10
49	I	312	KC2	CBD-CHA-C1A	3.65	135.69	128.88
48	H	302	A86	C40-C32-C31	-3.65	107.20	110.47
48	U	202	A86	C21-C20-C19	3.65	118.39	114.28
48	P	303	A86	O1-C15-C14	-3.65	105.88	113.21
39	b	813	CLA	C3B-C4B-NB	-3.65	107.78	110.23
48	8	302	A86	C21-C20-C19	3.65	118.39	114.28
49	0	317	KC2	CHB-C1B-C2B	-3.65	117.83	125.48
48	P	302	A86	C3-C2-C1	-3.65	122.10	127.31
48	I	304	A86	C4-C5-C6	-3.65	122.10	127.31
40	b	843	PQN	C2M-C2-C3	-3.65	118.45	124.40
48	Y	301	A86	O1-C15-C14	-3.65	105.89	113.21
50	0	303	A1EB1	C36-C31-C32	3.64	123.31	119.70
49	L	312	KC2	C4B-CHC-C1C	-3.64	118.19	126.06
39	Z	313	CLA	O2D-CGD-O1D	-3.64	116.71	123.84
51	E	311	A1ECV	O1D-CGD-CBD	-3.64	118.67	124.74
51	9	317	A1ECV	O2-CMC-C2C	3.64	121.01	112.27
49	V	315	KC2	C1D-CHD-C4C	-3.64	117.70	126.34
50	8	308	A1EB1	C40-C32-C31	-3.64	107.21	110.47
49	V	315	KC2	CHB-C1B-C2B	-3.64	117.84	125.48
48	7	308	A86	O1-C20-C21	-3.64	110.69	115.06
48	W	303	A86	C33-C32-C31	3.64	112.75	109.21
47	W	301	SQD	O7-S-C6	3.64	111.26	106.94
48	O	302	A86	C25-C26-C27	-3.64	122.12	127.31
50	G	308	A1EB1	C9-C8-C6	-3.64	116.20	126.42
43	W	305	DD6	O1-C20-C21	-3.63	110.70	115.06
49	F	311	KC2	CBD-CHA-C1A	3.63	135.66	128.88
49	I	303	KC2	CHC-C4B-C3B	-3.63	119.04	125.26
48	F	301	A86	O1-C20-C21	-3.63	110.70	115.06
49	S	315	KC2	C4B-CHC-C1C	-3.63	118.23	126.06
39	3	319	CLA	O2D-CGD-O1D	-3.63	116.75	123.84
49	4	318	KC2	CHB-C1B-C2B	-3.63	117.87	125.48
48	4	309	A86	O1-C15-C14	-3.63	105.93	113.21
47	S	301	SQD	O47-C7-C8	3.62	119.31	111.50
43	o	204	DD6	C4-C5-C6	-3.62	122.14	127.31
48	F	302	A86	C25-C26-C27	-3.62	122.14	127.31
48	7	312	A86	C17-C16-C15	3.62	112.86	109.16
50	6	301	A1EB1	O1-C20-C19	-3.62	110.66	113.38
43	A	301	DD6	C9-C10-C11	-3.62	122.14	127.31
48	7	308	A86	C12-C11-C13	3.62	122.10	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	E	320	SQD	O9-S-C6	3.62	111.24	106.94
49	H	311	KC2	C1D-ND-C4D	3.62	108.91	106.33
39	R	315	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
51	Q	316	A1ECV	O2-CMC-C2C	3.62	120.95	112.27
43	z	305	DD6	C3-C4-C5	-3.62	116.07	123.47
49	X	306	KC2	O2D-CGD-CBD	3.62	117.69	111.27
48	8	305	A86	C36-C31-C32	3.61	123.28	119.70
48	9	305	A86	C21-C20-C19	3.61	118.34	114.28
49	4	317	KC2	C1D-CHD-C4C	-3.61	117.77	126.34
48	R	301	A86	C25-C26-C27	-3.61	122.16	127.31
52	P	319	A1EB4	C34-O4-C38	-3.61	111.17	117.90
43	x	303	DD6	C37-C36-C35	3.61	121.04	114.36
50	5	302	A1EB1	O1-C20-C19	-3.60	110.67	113.38
49	5	311	KC2	C1D-CHD-C4C	-3.60	117.79	126.34
49	8	317	KC2	CHB-C1B-C2B	-3.60	117.92	125.48
42	k	204	BCR	C24-C23-C22	-3.60	120.79	126.23
48	E	304	A86	C21-C20-C19	3.60	118.33	114.28
47	F	318	SQD	O9-S-C6	3.60	111.22	106.94
43	F	303	DD6	C4-C5-C6	-3.60	122.17	127.31
49	9	313	KC2	C1D-CHD-C4C	-3.60	117.80	126.34
50	L	303	A1EB1	C28-C27-C26	-3.60	120.23	124.93
50	2	306	A1EB1	C17-C16-C15	3.60	112.83	109.16
48	F	301	A86	C4-C5-C6	-3.60	122.17	127.31
49	P	306	KC2	C1D-ND-C4D	3.60	108.89	106.33
50	J	302	A1EB1	C40-C32-C31	-3.60	107.25	110.47
49	F	311	KC2	C1D-ND-C4D	3.60	108.89	106.33
42	f	804	BCR	C28-C27-C26	-3.60	107.66	114.08
48	V	304	A86	C3-C2-C1	-3.59	122.18	127.31
50	E	301	A1EB1	O1-C20-C21	-3.59	110.75	115.06
50	F	304	A1EB1	O1-C20-C21	-3.59	110.75	115.06
50	y	301	A1EB1	C4-C5-C6	-3.59	122.18	127.31
48	L	301	A86	O1-C20-C21	-3.59	110.75	115.06
47	T	321	SQD	O7-S-C6	3.59	111.21	106.94
49	6	316	KC2	C4B-CHC-C1C	-3.59	118.31	126.06
52	M	322	A1EB4	C34-O4-C38	-3.59	111.21	117.90
49	I	312	KC2	C1D-ND-C4D	3.59	108.88	106.33
42	a	842	BCR	C3-C4-C5	-3.59	107.67	114.08
48	1	303	A86	C34-O4-C38	-3.59	111.21	117.90
43	S	306	DD6	C9-C10-C11	-3.59	122.19	127.31
48	V	301	A86	O1-C20-C21	-3.59	110.76	115.06
48	G	305	A86	C25-C26-C27	-3.58	122.19	127.31
39	Y	314	CLA	CAA-C2A-C3A	-3.58	107.74	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	y	306	A86	C41-C32-C31	-3.58	107.27	110.47
48	P	303	A86	C36-C31-C32	3.58	123.25	119.70
43	B	202	DD6	C37-C36-C31	-3.58	119.48	124.35
48	G	301	A86	C36-C31-C32	3.58	123.25	119.70
48	3	308	A86	C25-C26-C27	-3.58	122.20	127.31
48	6	307	A86	C9-C8-C6	-3.58	116.37	126.42
51	9	314	A1ECV	O2-CMC-C2C	3.58	120.85	112.27
43	3	304	DD6	C20-C19-C18	-3.58	105.67	112.75
50	1	305	A1EB1	O1-C15-C14	-3.58	106.03	113.21
42	f	801	BCR	C16-C15-C14	-3.57	116.15	123.47
43	S	306	DD6	C21-C20-C19	3.57	118.30	114.28
43	7	310	DD6	C25-C26-C27	-3.57	116.20	126.58
51	7	317	A1ECV	O2-CMC-O1	-3.57	116.46	123.45
47	9	322	SQD	O9-S-C6	3.57	111.19	106.94
39	0	323	CLA	O2D-CGD-CBD	3.57	117.61	111.27
48	Q	304	A86	C34-O4-C38	-3.57	111.24	117.90
49	L	315	KC2	C1D-CHD-C4C	-3.57	117.87	126.34
48	8	307	A86	C33-C32-C31	3.57	112.68	109.21
42	b	850	BCR	C11-C10-C9	-3.57	122.22	127.31
48	7	307	A86	C3-C2-C1	-3.57	122.22	127.31
39	x	308	CLA	CAA-C2A-C3A	-3.57	107.77	116.10
48	x	305	A86	C4-C5-C6	-3.57	122.22	127.31
51	V	317	A1ECV	O2-CMC-O1	-3.57	116.48	123.45
48	Q	308	A86	C33-C32-C31	3.56	112.67	109.21
42	b	847	BCR	C7-C8-C9	-3.56	120.85	126.23
52	M	305	A1EB4	C33-C32-C31	3.56	112.67	109.21
48	1	306	A86	C21-C20-C19	3.56	118.29	114.28
48	T	305	A86	C25-C26-C27	-3.56	122.23	127.31
48	U	206	A86	C36-C31-C32	3.56	123.23	119.70
43	P	304	DD6	C37-C36-C31	-3.56	119.51	124.35
49	9	311	KC2	C1D-ND-C4D	3.56	108.86	106.33
48	8	307	A86	C34-O4-C38	-3.56	111.26	117.90
43	I	306	DD6	O1-C20-C19	-3.56	110.71	113.38
47	9	322	SQD	O47-C7-C8	3.56	119.17	111.50
48	E	304	A86	C40-C32-C31	-3.56	107.29	110.47
50	S	302	A1EB1	C25-C26-C27	-3.56	122.20	127.26
48	C	303	A86	C25-C26-C27	-3.56	122.24	127.31
39	X	308	CLA	C3B-C4B-NB	-3.55	107.22	110.52
50	7	303	A1EB1	C12-C11-C13	3.55	121.99	116.02
48	y	305	A86	C3-C2-C1	-3.55	122.24	127.31
48	X	302	A86	C33-C32-C31	3.55	112.66	109.21
51	Q	319	A1ECV	O2-CMC-C2C	3.55	120.79	112.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	3	317	KC2	C4B-CHC-C1C	-3.55	118.40	126.06
50	8	301	A1EB1	C12-C11-C13	3.55	121.99	116.02
49	R	314	KC2	CHB-C1B-C2B	-3.55	118.03	125.48
50	8	304	A1EB1	C25-C26-C27	-3.55	122.21	127.26
48	Q	301	A86	C36-C31-C32	3.55	123.22	119.70
43	Q	303	DD6	C37-C36-C35	3.55	120.93	114.36
49	V	308	KC2	CHC-C4B-C3B	-3.55	119.19	125.26
39	1	308	CLA	CAA-C2A-C3A	-3.55	107.82	116.10
48	4	306	A86	C12-C11-C13	3.55	121.98	116.02
43	7	309	DD6	C4-C5-C6	-3.54	122.25	127.31
50	8	301	A1EB1	C28-C27-C26	-3.54	120.30	124.93
47	E	320	SQD	O47-C7-C8	3.54	119.14	111.50
51	z	316	A1ECV	O2-CMC-C2C	3.54	120.77	112.27
43	Q	303	DD6	C15-C14-C13	-3.54	118.50	125.99
48	4	305	A86	C17-C16-C15	3.54	112.78	109.16
43	O	303	DD6	C15-C14-C13	-3.54	118.50	125.99
48	U	206	A86	C21-C20-C19	3.54	118.26	114.28
49	4	324	KC2	C1D-ND-C4D	3.54	108.85	106.33
50	T	307	A1EB1	C4-C3-C2	-3.54	116.22	123.47
49	X	314	KC2	CHB-C1B-C2B	-3.54	118.06	125.48
51	z	316	A1ECV	O2-CMC-O1	-3.54	116.53	123.45
49	5	313	KC2	CHB-C1B-C2B	-3.54	118.06	125.48
48	9	301	A86	O1-C20-C19	-3.54	110.72	113.38
49	M	313	KC2	C4B-CHC-C1C	-3.54	118.42	126.06
42	h	202	BCR	C16-C17-C18	-3.54	122.26	127.31
48	Q	302	A86	C36-C31-C32	3.54	123.21	119.70
42	h	202	BCR	C28-C27-C26	-3.54	107.76	114.08
49	6	319	KC2	C2D-C1D-ND	-3.54	107.86	110.23
49	X	312	KC2	CHB-C1B-C2B	-3.53	118.07	125.48
50	3	309	A1EB1	C21-C20-C19	3.53	118.26	114.28
47	D	321	SQD	O9-S-C6	3.53	111.14	106.94
43	4	308	DD6	C37-C36-C35	3.53	120.90	114.36
47	7	302	SQD	O9-S-C6	3.53	111.14	106.94
39	Z	316	CLA	CAA-C2A-C3A	-3.53	107.86	116.10
49	1	315	KC2	C1D-ND-C4D	3.53	108.84	106.33
48	W	307	A86	C21-C20-C19	3.53	118.25	114.28
48	L	307	A86	C34-O4-C38	-3.53	111.32	117.90
42	l	206	BCR	C16-C17-C18	-3.53	122.27	127.31
49	2	317	KC2	CHB-C1B-C2B	-3.53	118.08	125.48
49	L	312	KC2	C2D-C1D-ND	-3.53	107.87	110.23
50	Q	323	A1EB1	C28-C27-C26	-3.53	120.32	124.93
48	6	307	A86	C21-C20-C19	3.53	118.25	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	Q	315	KC2	C4B-CHC-C1C	-3.53	118.45	126.06
50	h	203	A1EB1	C36-C31-C32	3.53	123.19	119.70
50	0	305	A1EB1	C17-C16-C15	3.53	112.76	109.16
42	i	102	BCR	C4-C5-C6	-3.53	117.61	122.73
50	K	304	A1EB1	C25-C26-C27	-3.53	122.24	127.26
51	Y	312	A1ECV	C2A-CAA-CBA	-3.52	120.68	128.63
48	R	301	A86	C21-C20-C19	3.52	118.25	114.28
50	S	302	A1EB1	C41-C32-C31	-3.52	107.32	110.47
49	8	316	KC2	CHB-C1B-C2B	-3.52	118.09	125.48
49	V	308	KC2	C1D-ND-C4D	3.52	108.84	106.33
49	z	312	KC2	C1D-ND-C4D	3.52	108.84	106.33
49	0	319	KC2	CHD-C1D-ND	3.52	127.99	124.26
48	2	301	A86	C34-O4-C38	-3.52	111.33	117.90
50	1	305	A1EB1	C4-C5-C6	-3.52	122.28	127.31
39	2	316	CLA	CAA-C2A-C3A	-3.52	107.89	116.10
49	4	318	KC2	C1D-CHD-C4C	-3.52	117.99	126.34
50	K	304	A1EB1	C3-C2-C1	-3.52	122.29	127.31
50	3	310	A1EB1	C28-O6-C42	3.52	123.50	115.68
43	X	304	DD6	C4-C5-C6	-3.52	122.29	127.31
48	6	305	A86	C36-C31-C32	3.51	123.18	119.70
50	2	306	A1EB1	C12-C11-C10	-3.51	114.92	123.42
47	T	321	SQD	O47-C7-C8	3.51	119.07	111.50
50	U	205	A1EB1	C3-C2-C1	-3.51	122.30	127.31
51	x	310	A1ECV	O2-CMC-C2C	3.51	120.70	112.27
50	4	303	A1EB1	C3-C2-C1	-3.51	122.30	127.31
51	z	310	A1ECV	O2-CMC-C2C	3.51	120.69	112.27
50	G	308	A1EB1	C3-C2-C1	-3.51	122.30	127.31
52	W	321	A1EB4	C25-C26-C27	-3.51	122.30	127.31
49	Q	313	KC2	CHB-C1B-C2B	-3.51	118.12	125.48
51	E	311	A1ECV	CMA-C3A-C2A	3.51	131.24	124.68
43	A	301	DD6	O1-C20-C19	-3.51	110.75	113.38
42	b	845	BCR	C24-C23-C22	-3.50	120.94	126.23
48	9	306	A86	C36-C31-C32	3.50	123.17	119.70
49	Q	313	KC2	CHC-C4B-C3B	-3.50	119.27	125.26
52	T	304	A1EB4	C33-C32-C31	3.50	112.61	109.21
43	x	304	DD6	C3-C4-C5	-3.50	116.30	123.47
50	8	304	A1EB1	C33-C32-C31	3.50	112.61	109.21
49	5	311	KC2	CHC-C4B-C3B	-3.50	119.27	125.26
43	O	305	DD6	C9-C10-C11	-3.50	122.32	127.31
50	Q	323	A1EB1	C12-C11-C13	3.50	121.90	116.02
43	E	303	DD6	C9-C10-C11	-3.50	122.32	127.31
50	y	301	A1EB1	C28-C27-C26	-3.50	120.36	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	4	307	DD6	C4-C5-C6	-3.49	122.32	127.31
49	V	320	KC2	CHC-C4B-C3B	-3.49	119.28	125.26
50	8	306	A1EB1	C28-C27-C26	-3.49	120.36	124.93
48	F	302	A86	C36-C31-C32	3.49	123.16	119.70
48	M	303	A86	C36-C31-C32	3.49	123.16	119.70
52	M	305	A1EB4	C25-C26-C27	-3.49	122.32	127.31
50	6	308	A1EB1	C25-C26-C27	-3.49	122.28	127.26
49	5	305	KC2	CBD-CHA-C1A	3.49	135.39	128.88
48	4	328	A86	C12-C11-C10	-3.49	114.97	123.42
42	a	842	BCR	C20-C21-C22	-3.49	122.33	127.31
48	I	304	A86	C25-C26-C27	-3.49	122.33	127.31
49	8	320	KC2	C1D-ND-C4D	3.49	108.81	106.33
49	Z	311	KC2	CHC-C4B-C3B	-3.49	119.29	125.26
42	a	844	BCR	C11-C10-C9	-3.49	122.33	127.31
48	L	301	A86	O1-C15-C14	-3.48	106.22	113.21
50	3	302	A1EB1	C25-C26-C27	-3.48	122.30	127.26
49	W	312	KC2	CHC-C4B-C3B	-3.48	119.30	125.26
43	Z	302	DD6	C12-C11-C10	-3.48	118.05	122.92
48	L	302	A86	C26-C25-C24	3.48	134.08	123.22
47	F	318	SQD	O47-C7-C8	3.48	119.00	111.50
50	K	304	A1EB1	O1-C20-C21	-3.48	110.89	115.06
39	1	320	CLA	CAA-C2A-C3A	-3.48	107.99	116.10
43	z	304	DD6	C3-C4-C5	-3.48	116.35	123.47
49	P	310	KC2	CHC-C4B-C3B	-3.48	119.31	125.26
43	2	303	DD6	C12-C11-C10	-3.48	118.06	122.92
49	A	313	KC2	CHC-C4B-C3B	-3.48	119.31	125.26
51	7	317	A1ECV	O2-CMC-C2C	3.47	120.61	112.27
49	L	315	KC2	CHC-C4B-C3B	-3.47	119.32	125.26
48	6	303	A86	C4-C5-C6	-3.47	122.35	127.31
49	9	313	KC2	CHB-C1B-C2B	-3.47	118.20	125.48
42	b	847	BCR	C15-C16-C17	-3.47	116.36	123.47
39	L	320	CLA	CHB-C4A-NA	3.47	129.31	124.51
50	0	303	A1EB1	C4-C5-C6	-3.47	122.36	127.31
51	5	312	A1ECV	CMB-C2B-C1B	3.47	131.28	124.73
42	l	202	BCR	C24-C23-C22	-3.47	121.00	126.23
49	M	313	KC2	C1A-NA-C4A	-3.47	105.15	106.71
49	F	307	KC2	CHB-C1B-C2B	-3.47	118.21	125.48
43	Z	302	DD6	C13-C11-C10	3.47	124.26	118.94
49	B	208	KC2	CHC-C4B-C3B	-3.47	119.33	125.26
51	2	311	A1ECV	O2-CMC-C2C	3.46	120.58	112.27
48	K	301	A86	C36-C31-C32	3.46	123.13	119.70
48	0	301	A86	C33-C32-C31	3.46	112.58	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	G	317	KC2	CBD-CHA-C1A	3.46	135.34	128.88
49	G	317	KC2	CHB-C1B-C2B	-3.46	118.22	125.48
39	T	308	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
52	P	318	A1EB4	C34-O4-C38	-3.46	111.44	117.90
46	Q	322	LMG	O1-C7-C8	-3.46	102.55	110.90
43	A	304	DD6	C3-C2-C1	-3.46	122.37	127.31
48	k	206	A86	C3-C2-C1	-3.46	122.37	127.31
49	K	310	KC2	CHC-C4B-C3B	-3.46	119.34	125.26
50	3	324	A1EB1	C40-C32-C31	-3.46	107.38	110.47
43	a	846	DD6	C4-C5-C6	-3.46	122.37	127.31
50	T	307	A1EB1	O1-C20-C21	-3.46	110.91	115.06
47	H	318	SQD	O9-S-C6	3.46	111.05	106.94
49	4	324	KC2	CHC-C4B-C3B	-3.46	119.35	125.26
39	A	306	CLA	CMB-C2B-C1B	-3.46	120.11	125.37
50	U	203	A1EB1	C36-C31-C32	3.46	123.12	119.70
50	0	302	A1EB1	C28-C27-C26	-3.45	120.42	124.93
51	G	316	A1ECV	O2-CMC-C2C	3.45	120.56	112.27
48	Q	304	A86	C4-C5-C6	-3.45	122.38	127.31
43	a	846	DD6	O1-C20-C19	-3.45	110.79	113.38
43	A	301	DD6	C15-C14-C13	-3.45	118.69	125.99
49	T	312	KC2	C1D-ND-C4D	3.45	108.79	106.33
43	D	306	DD6	C-C1-C2	-3.45	118.09	122.92
39	Y	302	CLA	CAA-C2A-C3A	-3.45	108.05	116.10
49	B	208	KC2	CHB-C1B-C2B	-3.45	118.24	125.48
51	Y	312	A1ECV	O2D-CGD-O1D	-3.45	117.09	123.84
50	3	310	A1EB1	C17-C16-C15	3.45	112.68	109.16
43	2	303	DD6	C13-C11-C10	3.45	124.23	118.94
52	X	305	A1EB4	C4-C3-C2	-3.45	116.41	123.47
42	l	207	BCR	C7-C8-C9	-3.45	121.03	126.23
50	1	301	A1EB1	O1-C20-C19	-3.45	110.79	113.38
49	2	314	KC2	CHC-C4B-C3B	-3.45	119.36	125.26
49	L	317	KC2	CHB-C1B-C2B	-3.45	118.25	125.48
48	9	301	A86	O1-C15-C14	-3.44	106.30	113.21
48	3	308	A86	C4-C5-C6	-3.44	122.39	127.31
49	3	318	KC2	C1D-ND-C4D	3.44	108.78	106.33
49	V	314	KC2	CHB-C1B-C2B	-3.44	118.26	125.48
42	l	206	BCR	C15-C14-C13	-3.44	122.40	127.31
48	F	301	A86	C10-C9-C8	-3.44	112.48	123.22
51	9	314	A1ECV	O2-CMC-O1	-3.44	116.72	123.45
48	6	305	A86	C4-C5-C6	-3.44	122.40	127.31
49	z	315	KC2	CHB-C1B-C2B	-3.44	118.27	125.48
49	7	322	KC2	C1D-ND-C4D	3.44	108.78	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	P	301	SQD	O6-C1-C2	3.44	113.67	108.30
39	F	315	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
48	U	206	A86	O1-C20-C21	-3.44	110.94	115.06
48	9	305	A86	C33-C32-C31	3.44	112.55	109.21
43	1	304	DD6	C37-C36-C31	-3.44	119.68	124.35
42	l	206	BCR	C11-C10-C9	-3.44	122.41	127.31
51	1	318	A1ECV	O2-CMC-C2C	3.43	120.51	112.27
52	W	306	A1EB4	C25-C26-C27	-3.43	122.41	127.31
48	0	301	A86	O1-C20-C21	-3.43	110.94	115.06
43	E	305	DD6	C3-C2-C1	-3.43	122.41	127.31
42	l	202	BCR	C39-C30-C25	-3.43	104.73	110.30
50	3	324	A1EB1	C4-C3-C2	3.43	130.50	123.47
49	T	312	KC2	C1D-CHD-C4C	-3.43	118.20	126.34
49	M	314	KC2	C1D-ND-C4D	3.43	108.77	106.33
50	C	302	A1EB1	C33-C32-C31	3.43	112.55	109.21
52	P	305	A1EB4	C25-C26-C27	-3.43	122.42	127.31
49	0	314	KC2	CHB-C1B-C2B	-3.43	118.29	125.48
50	4	302	A1EB1	C9-C8-C6	-3.43	116.78	126.42
49	G	315	KC2	C1D-ND-C4D	3.43	108.77	106.33
48	1	302	A86	C3-C2-C1	-3.43	122.42	127.31
50	T	307	A1EB1	O1-C15-C14	-3.43	106.34	113.21
48	3	307	A86	C36-C31-C32	3.43	123.09	119.70
49	4	317	KC2	C1D-ND-C4D	3.42	108.77	106.33
50	x	302	A1EB1	C36-C31-C32	3.42	123.09	119.70
49	V	320	KC2	C1D-ND-C4D	3.42	108.77	106.33
50	3	302	A1EB1	O1-C15-C14	-3.42	106.35	113.21
43	R	304	DD6	C4-C5-C6	-3.42	122.43	127.31
49	6	314	KC2	C1D-ND-C4D	3.42	108.76	106.33
48	8	305	A86	O1-C20-C21	-3.42	110.96	115.06
50	6	304	A1EB1	C28-C27-C26	-3.42	120.46	124.93
51	1	318	A1ECV	O2-CMC-O1	-3.42	116.77	123.45
48	U	202	A86	C36-C31-C32	3.42	123.09	119.70
47	k	205	SQD	O9-S-C6	3.42	111.00	106.94
48	8	309	A86	C21-C20-C19	3.42	118.12	114.28
49	7	320	KC2	CHB-C1B-C2B	-3.41	118.32	125.48
43	O	303	DD6	C37-C36-C31	-3.41	119.71	124.35
49	G	313	KC2	CHB-C1B-C2B	-3.41	118.32	125.48
50	2	306	A1EB1	O1-C20-C19	-3.41	110.82	113.38
49	G	313	KC2	C1D-ND-C4D	3.41	108.76	106.33
39	a	831	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
49	P	306	KC2	CBD-CHA-C1A	3.41	135.24	128.88
48	S	305	A86	C12-C11-C13	3.41	121.75	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	307	A86	C33-C32-C31	3.41	112.53	109.21
48	3	307	A86	C33-C32-C31	3.41	112.53	109.21
49	7	319	KC2	CHB-C1B-C2B	-3.41	118.33	125.48
50	7	305	A1EB1	C4-C3-C2	-3.41	116.50	123.47
42	j	103	BCR	C24-C23-C22	-3.41	121.09	126.23
48	T	305	A86	C17-C16-C15	3.41	112.64	109.16
48	3	306	A86	C25-C26-C27	-3.40	122.45	127.31
49	V	312	KC2	CHC-C4B-C3B	-3.40	119.44	125.26
43	E	302	DD6	C15-C14-C13	-3.40	118.80	125.99
47	S	301	SQD	C1-O5-C5	3.40	120.37	113.69
42	j	103	BCR	C20-C21-C22	-3.40	122.45	127.31
50	S	303	A1EB1	C17-C16-C15	3.40	112.63	109.16
47	k	205	SQD	O8-S-C6	3.40	111.16	105.74
49	I	312	KC2	CHC-C4B-C3B	-3.40	119.44	125.26
51	7	323	A1ECV	O1D-CGD-CBD	-3.40	119.08	124.74
52	T	304	A1EB4	C34-O4-C38	-3.40	111.56	117.90
49	6	317	KC2	CHB-C1B-C2B	-3.40	118.35	125.48
43	C	301	DD6	C33-C34-C35	-3.40	105.65	110.30
49	F	311	KC2	CHB-C1B-C2B	-3.40	118.35	125.48
49	I	312	KC2	CHB-C1B-C2B	-3.40	118.35	125.48
49	P	310	KC2	CHB-C1B-C2B	-3.40	118.35	125.48
49	W	312	KC2	CHB-C1B-C2B	-3.40	118.35	125.48
50	V	305	A1EB1	C12-C11-C13	3.40	121.73	116.02
48	P	302	A86	C40-C32-C31	-3.40	107.43	110.47
43	E	303	DD6	C21-C20-C15	-3.40	116.57	122.26
48	V	304	A86	O1-C15-C14	-3.40	106.39	113.21
49	V	312	KC2	CHB-C1B-C2B	-3.39	118.36	125.48
49	y	316	KC2	CHB-C1B-C2B	-3.39	118.36	125.48
47	F	319	SQD	O7-S-C6	3.39	110.97	106.94
43	H	303	DD6	C3-C2-C1	-3.39	122.47	127.31
39	U	215	CLA	CAA-C2A-C3A	-3.39	108.18	116.10
49	Q	318	KC2	CHB-C1B-C2B	-3.39	118.37	125.48
50	4	303	A1EB1	C25-C26-C27	-3.39	122.43	127.26
43	y	304	DD6	C37-C36-C31	-3.39	119.74	124.35
49	M	311	KC2	CHC-C4B-C3B	-3.39	119.46	125.26
49	Q	318	KC2	CBD-CHA-C1A	3.39	135.20	128.88
48	P	303	A86	C35-C34-C33	3.39	115.79	109.88
49	Z	310	KC2	CHB-C1B-C2B	-3.39	118.37	125.48
50	y	302	A1EB1	C33-C32-C31	3.39	112.50	109.21
43	Q	306	DD6	C37-C36-C35	3.39	120.63	114.36
49	M	311	KC2	CHB-C1B-C2B	-3.39	118.37	125.48
48	K	301	A86	C4-C5-C6	-3.39	122.47	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	G	313	KC2	CHC-C4B-C3B	-3.39	119.46	125.26
49	K	310	KC2	CHB-C1B-C2B	-3.39	118.38	125.48
49	4	320	KC2	CHB-C1B-C2B	-3.39	118.38	125.48
43	A	302	DD6	C15-C14-C13	-3.39	118.83	125.99
43	E	303	DD6	C15-C14-C13	-3.39	118.83	125.99
42	b	845	BCR	C33-C5-C6	-3.39	120.73	124.53
42	k	204	BCR	C38-C26-C25	-3.39	120.73	124.53
43	y	303	DD6	C32-C31-C36	-3.39	117.85	122.63
39	S	319	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
50	7	303	A1EB1	C28-C27-C26	-3.38	120.51	124.93
48	T	301	A86	C36-C31-C32	3.38	123.05	119.70
51	9	317	A1ECV	C4B-CHC-C1C	3.38	126.94	115.73
43	E	303	DD6	C4-C5-C6	-3.38	122.48	127.31
48	G	301	A86	C40-C32-C31	-3.38	107.44	110.47
47	F	319	SQD	O8-S-C6	3.38	111.13	105.74
49	2	314	KC2	CHB-C1B-C2B	-3.38	118.39	125.48
50	4	304	A1EB1	C3-C4-C5	-3.38	116.55	123.47
49	G	311	KC2	CHB-C1B-C2B	-3.38	118.39	125.48
49	0	314	KC2	CHC-C4B-C3B	-3.38	119.48	125.26
42	a	844	BCR	C7-C8-C9	-3.38	121.13	126.23
49	C	312	KC2	CHB-C1B-C2B	-3.38	118.39	125.48
39	O	308	CLA	CAA-C2A-C3A	-3.38	108.21	116.10
39	7	321	CLA	CAA-C2A-C3A	-3.38	108.21	116.10
50	V	302	A1EB1	O1-C20-C21	-3.38	111.01	115.06
50	E	301	A1EB1	C3-C2-C1	-3.38	122.49	127.31
42	f	804	BCR	C33-C5-C6	-3.38	120.73	124.53
49	Y	308	KC2	C2D-C1D-ND	-3.38	107.97	110.23
49	5	313	KC2	C1D-ND-C4D	3.38	108.73	106.33
49	M	307	KC2	CHB-C1B-C2B	-3.38	118.39	125.48
49	T	316	KC2	CHC-C4B-C3B	-3.38	119.48	125.26
49	6	314	KC2	CHC-C4B-C3B	-3.38	119.48	125.26
50	7	306	A1EB1	C17-C16-C15	3.38	112.61	109.16
50	8	304	A1EB1	C3-C2-C1	-3.38	122.49	127.31
49	G	311	KC2	C1D-ND-C4D	3.38	108.73	106.33
49	V	318	KC2	C1D-ND-C4D	3.38	108.73	106.33
49	V	308	KC2	CHB-C1B-C2B	-3.38	118.40	125.48
48	3	307	A86	C25-C24-C1	-3.38	116.93	126.42
48	K	301	A86	C21-C20-C19	3.38	118.08	114.28
43	H	303	DD6	C15-C14-C13	-3.38	118.86	125.99
48	V	301	A86	C25-C26-C27	-3.37	122.49	127.31
50	3	309	A1EB1	C3-C2-C1	-3.37	122.49	127.31
49	F	311	KC2	CHC-C4B-C3B	-3.37	119.49	125.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	2	313	KC2	C1D-ND-C4D	3.37	108.73	106.33
39	Y	313	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
49	S	317	KC2	CHB-C1B-C2B	-3.37	118.40	125.48
49	X	318	KC2	CHB-C1B-C2B	-3.37	118.40	125.48
50	8	308	A1EB1	C28-C27-C26	-3.37	120.52	124.93
48	P	302	A86	C36-C31-C32	3.37	123.04	119.70
49	T	316	KC2	CHB-C1B-C2B	-3.37	118.41	125.48
43	F	305	DD6	C4-C5-C6	-3.37	122.50	127.31
50	h	203	A1EB1	C12-C11-C13	3.37	121.68	116.02
49	4	324	KC2	CHB-C1B-C2B	-3.37	118.41	125.48
51	y	311	A1ECV	O2-CMC-C2C	3.37	120.35	112.27
49	Z	311	KC2	CHB-C1B-C2B	-3.37	118.42	125.48
40	a	839	PQN	C14-C13-C15	3.37	120.94	115.27
48	L	306	A86	C4-C3-C2	-3.37	116.58	123.47
50	2	304	A1EB1	C28-C27-C26	-3.37	120.53	124.93
48	4	328	A86	C10-C9-C8	-3.37	112.71	123.22
49	M	307	KC2	CHC-C4B-C3B	-3.37	119.50	125.26
49	R	318	KC2	CHC-C4B-C3B	-3.37	119.50	125.26
49	9	318	KC2	C2D-C1D-ND	-3.37	107.98	110.23
51	Z	308	A1ECV	O2-CMC-C2C	3.36	120.34	112.27
43	J	306	DD6	C37-C36-C31	-3.36	119.78	124.35
49	8	314	KC2	C1D-ND-C4D	3.36	108.72	106.33
50	6	301	A1EB1	C34-O4-C38	-3.36	111.63	117.90
48	T	301	A86	C35-C34-C33	3.36	115.74	109.88
50	2	304	A1EB1	O1-C15-C14	-3.36	106.47	113.21
49	5	314	KC2	CHC-C4B-C3B	-3.36	119.51	125.26
39	L	316	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
48	D	305	A86	C25-C24-C1	-3.36	116.98	126.42
48	0	308	A86	O1-C20-C19	-3.36	110.86	113.38
39	8	318	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
49	2	317	KC2	C1A-NA-C4A	-3.36	105.20	106.71
39	a	827	CLA	CMB-C2B-C1B	-3.36	120.25	125.37
43	F	303	DD6	C3-C2-C1	-3.36	122.52	127.31
48	6	303	A86	C17-C16-C15	3.36	112.59	109.16
50	6	301	A1EB1	C40-C32-C31	-3.36	107.47	110.47
48	7	307	A86	O1-C20-C21	-3.36	111.03	115.06
49	S	317	KC2	CHC-C4B-C3B	-3.36	119.52	125.26
50	T	302	A1EB1	C4-C5-C6	-3.36	122.52	127.31
45	b	849	DGD	O3G-C3G-C2G	-3.36	102.80	110.90
48	6	309	A86	C9-C8-C6	-3.36	116.99	126.42
49	6	316	KC2	CHB-C1B-C2B	-3.35	118.44	125.48
49	4	320	KC2	CHC-C4B-C3B	-3.35	119.52	125.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	H	314	KC2	CHB-C1B-C2B	-3.35	118.45	125.48
48	X	303	A86	C4-C5-C6	-3.35	122.52	127.31
49	3	317	KC2	CHB-C1B-C2B	-3.35	118.45	125.48
50	2	306	A1EB1	C3-C2-C1	-3.35	122.53	127.31
50	3	310	A1EB1	C25-C26-C27	-3.35	122.49	127.26
50	R	303	A1EB1	C4-C5-C6	-3.35	122.53	127.31
48	T	301	A86	C25-C26-C27	-3.35	122.53	127.31
47	D	320	SQD	O5-C5-C4	3.35	115.78	109.69
49	K	313	KC2	CHB-C1B-C2B	-3.35	118.45	125.48
48	2	302	A86	C25-C26-C27	-3.35	122.53	127.31
48	9	303	A86	C36-C31-C32	3.35	123.02	119.70
47	P	301	SQD	O47-C7-C8	3.35	118.72	111.50
49	y	316	KC2	CHC-C4B-C3B	-3.35	119.53	125.26
49	X	318	KC2	CHC-C4B-C3B	-3.35	119.53	125.26
43	I	306	DD6	C9-C10-C11	-3.35	122.53	127.31
43	y	303	DD6	C4-C5-C6	-3.35	122.53	127.31
49	X	314	KC2	C1D-ND-C4D	3.35	108.71	106.33
48	F	302	A86	O1-C20-C21	-3.35	111.04	115.06
49	K	313	KC2	C1D-ND-C4D	3.35	108.71	106.33
49	6	314	KC2	CHB-C1B-C2B	-3.35	118.46	125.48
39	b	801	CLA	C3B-C4B-NB	-3.35	107.41	110.52
43	3	301	DD6	C15-C14-C13	-3.35	118.92	125.99
43	B	202	DD6	C37-C36-C35	3.34	120.55	114.36
49	2	313	KC2	CBD-CHA-C1A	3.34	135.12	128.88
49	Q	315	KC2	CHC-C4B-C3B	-3.34	119.54	125.26
50	5	302	A1EB1	C36-C31-C32	3.34	123.01	119.70
50	Q	323	A1EB1	C4-C5-C6	-3.34	122.54	127.31
49	0	317	KC2	C1D-ND-C4D	3.34	108.71	106.33
49	C	313	KC2	CHB-C1B-C2B	-3.34	118.47	125.48
43	G	303	DD6	C3-C2-C1	-3.34	122.54	127.31
48	P	302	A86	C4-C3-C2	-3.34	116.63	123.47
47	H	318	SQD	C44-O6-C1	3.34	120.27	113.74
49	P	320	KC2	CHB-C1B-C2B	-3.34	118.47	125.48
48	L	307	A86	C3-C4-C5	-3.34	116.63	123.47
48	V	304	A86	C4-C5-C6	-3.34	122.54	127.31
52	P	318	A1EB4	C25-C26-C27	-3.34	122.55	127.31
43	F	303	DD6	C21-C20-C15	-3.34	116.67	122.26
43	4	308	DD6	C4-C5-C6	-3.34	122.55	127.31
49	W	314	KC2	CHB-C1B-C2B	-3.34	118.48	125.48
42	i	102	BCR	C27-C26-C25	-3.34	117.89	122.73
42	f	804	BCR	C16-C17-C18	-3.34	122.55	127.31
42	k	204	BCR	C33-C5-C6	-3.34	120.78	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	P	313	KC2	CHB-C1B-C2B	-3.34	118.48	125.48
49	T	314	KC2	CHB-C1B-C2B	-3.34	118.48	125.48
49	R	314	KC2	C1D-ND-C4D	3.33	108.70	106.33
49	G	317	KC2	CHC-C4B-C3B	-3.33	119.55	125.26
49	6	317	KC2	CHC-C4B-C3B	-3.33	119.56	125.26
49	T	312	KC2	CHC-C4B-C3B	-3.33	119.56	125.26
51	0	321	A1ECV	C4B-CHC-C1C	3.33	126.77	115.73
39	y	307	CLA	CAA-C2A-C3A	-3.33	108.32	116.10
43	y	304	DD6	C3-C4-C5	-3.33	116.65	123.47
39	X	316	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
43	R	304	DD6	C15-C14-C13	-3.33	118.95	125.99
49	1	315	KC2	CHB-C1B-C2B	-3.33	118.49	125.48
49	V	318	KC2	CHB-C1B-C2B	-3.33	118.49	125.48
43	Q	306	DD6	C4-C5-C6	-3.33	122.56	127.31
42	b	850	BCR	C33-C5-C6	-3.33	120.79	124.53
49	9	313	KC2	C1D-ND-C4D	3.33	108.70	106.33
50	8	306	A1EB1	C4-C5-C6	-3.33	122.56	127.31
42	f	804	BCR	C24-C23-C22	-3.33	121.21	126.23
49	Q	313	KC2	O1D-CGD-CBD	-3.33	117.67	124.48
49	S	314	KC2	C1D-ND-C4D	3.32	108.70	106.33
50	4	303	A1EB1	C28-C27-C26	-3.32	120.58	124.93
42	f	804	BCR	C20-C21-C22	-3.32	122.57	127.31
49	A	313	KC2	CHB-C1B-C2B	-3.32	118.51	125.48
39	b	836	CLA	CMB-C2B-C1B	-3.32	120.31	125.37
39	1	316	CLA	CAA-C2A-C3A	-3.32	108.35	116.10
49	G	313	KC2	CBD-CHA-C1A	3.32	135.07	128.88
48	7	311	A86	C4-C5-C6	-3.32	122.57	127.31
49	L	315	KC2	CHB-C1B-C2B	-3.32	118.51	125.48
51	x	310	A1ECV	O2-CMC-O1	-3.32	116.96	123.45
47	D	320	SQD	O9-S-O7	-3.32	102.46	113.95
49	P	312	KC2	CHB-C1B-C2B	-3.32	118.52	125.48
49	2	317	KC2	C1D-ND-C4D	3.32	108.69	106.33
43	A	302	DD6	C3-C2-C1	-3.32	122.57	127.31
49	x	313	KC2	CHC-C4B-C3B	-3.32	119.58	125.26
48	R	302	A86	C41-C32-C31	-3.32	107.50	110.47
39	7	324	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
50	J	302	A1EB1	C33-C32-C31	3.32	112.44	109.21
49	z	315	KC2	CHC-C4B-C3B	-3.32	119.58	125.26
48	8	307	A86	C25-C24-C1	-3.32	117.10	126.42
49	x	313	KC2	CHB-C1B-C2B	-3.32	118.52	125.48
49	y	316	KC2	CBD-CHA-C1A	3.32	135.06	128.88
43	A	302	DD6	C21-C20-C15	-3.32	116.70	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	T	312	KC2	CHB-C1B-C2B	-3.32	118.53	125.48
49	R	318	KC2	CHB-C1B-C2B	-3.31	118.53	125.48
49	F	307	KC2	CHC-C4B-C3B	-3.31	119.59	125.26
48	7	312	A86	C36-C31-C32	3.31	122.98	119.70
43	A	303	DD6	C33-C34-C35	-3.31	105.77	110.30
51	y	311	A1ECV	CMA-C3A-C2A	3.31	130.87	124.68
49	0	316	KC2	CHC-C4B-C3B	-3.31	119.60	125.26
49	W	308	KC2	C1D-ND-C4D	3.31	108.69	106.33
49	T	315	KC2	CHC-C4B-C3B	-3.31	119.60	125.26
51	Y	306	A1ECV	CMA-C3A-C2A	3.31	130.87	124.68
47	F	319	SQD	O47-C7-C8	3.31	118.63	111.50
49	Z	310	KC2	CHC-C4B-C3B	-3.31	119.60	125.26
42	l	202	BCR	C11-C10-C9	-3.31	122.59	127.31
49	z	315	KC2	O1D-CGD-CBD	-3.31	117.72	124.48
39	V	311	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
50	3	324	A1EB1	C3-C2-C1	-3.31	122.59	127.31
48	S	305	A86	C4-C5-C6	-3.31	122.59	127.31
50	z	301	A1EB1	C3-C2-C1	-3.30	122.59	127.31
49	M	314	KC2	CHB-C1B-C2B	-3.30	118.55	125.48
52	R	305	A1EB4	O1-C15-C14	-3.30	112.36	115.71
47	7	302	SQD	C1-O5-C5	3.30	120.17	113.69
49	Q	313	KC2	C1D-ND-C4D	3.30	108.68	106.33
49	R	312	KC2	CHC-C4B-C3B	-3.30	119.61	125.26
48	S	305	A86	C40-C32-C31	-3.30	107.52	110.47
39	7	313	CLA	CAA-C2A-C3A	-3.30	103.74	112.78
49	y	313	KC2	CHC-C4B-C3B	-3.30	119.61	125.26
50	8	301	A1EB1	C34-O4-C38	-3.30	111.75	117.90
49	C	313	KC2	CBD-CHA-C1A	3.30	135.03	128.88
49	B	208	KC2	C1D-ND-C4D	3.30	108.68	106.33
49	I	303	KC2	O1D-CGD-CBD	-3.30	117.73	124.48
50	4	303	A1EB1	C36-C31-C32	3.30	122.97	119.70
49	V	320	KC2	CHB-C1B-C2B	-3.30	118.56	125.48
49	y	313	KC2	CHB-C1B-C2B	-3.30	118.56	125.48
49	X	315	KC2	CHC-C4B-C3B	-3.30	119.62	125.26
50	V	302	A1EB1	C4-C5-C6	-3.30	122.60	127.31
49	4	317	KC2	CHB-C1B-C2B	-3.30	118.56	125.48
48	T	301	A86	C17-C16-C15	3.30	112.53	109.16
49	P	313	KC2	C4D-C3D-CAD	3.30	109.64	107.42
50	4	301	A1EB1	C12-C11-C13	3.30	121.56	116.02
49	W	308	KC2	CHC-C4B-C3B	-3.30	119.62	125.26
49	W	308	KC2	CHB-C1B-C2B	-3.29	118.57	125.48
49	L	317	KC2	CHC-C4B-C3B	-3.29	119.62	125.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	S	302	A1EB1	C35-C34-C33	3.29	115.62	109.88
49	G	317	KC2	C1D-ND-C4D	3.29	108.67	106.33
39	3	314	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
50	H	304	A1EB1	O1-C20-C21	-3.29	111.11	115.06
43	G	303	DD6	C21-C20-C15	-3.29	116.74	122.26
50	V	305	A1EB1	C25-C26-C27	-3.29	122.57	127.26
51	Q	316	A1ECV	CMA-C3A-C2A	3.29	130.84	124.68
39	2	318	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
48	M	302	A86	C33-C32-C31	3.29	112.41	109.21
49	1	314	KC2	C1D-ND-C4D	3.29	108.67	106.33
39	F	314	CLA	CHB-C4A-NA	3.29	129.06	124.51
50	8	304	A1EB1	C28-C27-C26	-3.29	120.63	124.93
49	Y	309	KC2	CHB-C1B-C2B	-3.29	118.58	125.48
49	Q	318	KC2	CHC-C4B-C3B	-3.29	119.64	125.26
43	D	307	DD6	C15-C14-C13	-3.29	119.04	125.99
43	D	307	DD6	C3-C2-C1	-3.29	122.62	127.31
48	R	317	A86	C41-C32-C31	-3.29	107.53	110.47
48	0	308	A86	O4-C38-C39	3.28	117.13	111.09
43	G	306	DD6	C3-C2-C1	-3.28	122.62	127.31
48	4	328	A86	C25-C26-C27	-3.28	122.62	127.31
47	D	320	SQD	O47-C7-C8	3.28	118.58	111.50
49	4	318	KC2	CHC-C4B-C3B	-3.28	119.64	125.26
39	a	827	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
49	S	315	KC2	C1A-NA-C4A	-3.28	105.23	106.71
52	P	318	A1EB4	C3-C4-C5	-3.28	116.75	123.47
48	Y	301	A86	C25-C26-C27	-3.28	122.62	127.31
47	T	321	SQD	O8-S-C6	3.28	110.97	105.74
39	a	833	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
39	a	822	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
49	2	313	KC2	CHB-C1B-C2B	-3.28	118.60	125.48
42	i	102	BCR	C11-C10-C9	-3.28	122.63	127.31
51	Q	316	A1ECV	O2-CMC-O1	-3.28	117.04	123.45
49	I	303	KC2	C1D-ND-C4D	3.28	108.66	106.33
49	G	311	KC2	CHC-C4B-C3B	-3.28	119.65	125.26
50	F	304	A1EB1	C4-C3-C2	-3.28	116.76	123.47
39	Z	304	CLA	CAA-C2A-C3A	-3.28	108.45	116.10
39	y	315	CLA	CAA-C2A-C3A	-3.28	108.45	116.10
49	V	308	KC2	CBD-CHA-C1A	3.28	134.99	128.88
50	6	308	A1EB1	C28-C27-C26	-3.28	120.65	124.93
39	3	323	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
50	G	307	A1EB1	O1-C20-C21	-3.27	111.13	115.06
49	X	315	KC2	CHB-C1B-C2B	-3.27	118.61	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	P	320	KC2	CHC-C4B-C3B	-3.27	119.66	125.26
43	V	303	DD6	C9-C10-C11	-3.27	122.64	127.31
49	M	307	KC2	C1D-ND-C4D	3.27	108.66	106.33
43	K	303	DD6	C9-C10-C11	-3.27	122.64	127.31
50	2	304	A1EB1	C34-O4-C38	-3.27	111.80	117.90
50	U	203	A1EB1	C35-C34-C33	3.27	115.58	109.88
43	H	303	DD6	C4-C5-C6	-3.27	122.64	127.31
49	C	313	KC2	CHC-C4B-C3B	-3.27	119.67	125.26
48	O	302	A86	C36-C31-C32	3.27	122.94	119.70
48	4	328	A86	C12-C11-C13	3.27	121.51	116.02
49	1	312	KC2	C2D-C1D-ND	-3.27	108.04	110.23
49	H	311	KC2	CHC-C4B-C3B	-3.27	119.67	125.26
48	8	305	A86	C4-C3-C2	-3.27	116.78	123.47
48	K	301	A86	O1-C15-C14	-3.26	106.66	113.21
48	T	306	A86	C3-C4-C5	-3.26	116.79	123.47
43	x	303	DD6	C4-C5-C6	-3.26	122.65	127.31
49	9	313	KC2	C4B-CHC-C1C	-3.26	119.02	126.06
39	W	318	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
52	T	304	A1EB4	O1-C15-C14	-3.26	112.41	115.71
49	5	314	KC2	C1D-ND-C4D	3.26	108.65	106.33
50	G	307	A1EB1	C36-C31-C32	3.26	122.93	119.70
43	3	304	DD6	C37-C36-C31	-3.26	119.92	124.35
42	b	850	BCR	C7-C8-C9	-3.26	121.31	126.23
49	L	314	KC2	CHB-C1B-C2B	-3.26	118.64	125.48
43	S	306	DD6	C37-C36-C31	-3.26	119.92	124.35
39	b	833	CLA	C3B-C4B-NB	-3.26	107.49	110.52
49	3	315	KC2	CHB-C1B-C2B	-3.26	118.65	125.48
43	y	303	DD6	C37-C36-C35	3.26	120.39	114.36
49	7	319	KC2	CHC-C4B-C3B	-3.26	119.69	125.26
48	O	302	A86	C35-C34-C33	3.26	115.56	109.88
50	V	307	A1EB1	C28-C27-C26	-3.26	120.67	124.93
48	X	303	A86	C10-C9-C8	-3.26	113.05	123.22
48	Z	303	A86	O1-C20-C21	-3.26	111.15	115.06
39	Z	307	CLA	CAA-C2A-C3A	-3.26	108.50	116.10
49	W	308	KC2	CBD-CHA-C1A	3.26	134.95	128.88
48	1	302	A86	C25-C26-C27	-3.26	122.66	127.31
49	X	315	KC2	C1D-ND-C4D	3.26	108.65	106.33
48	R	317	A86	C36-C31-C32	3.26	122.93	119.70
39	J	312	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
42	b	846	BCR	C29-C30-C25	3.25	115.49	110.48
39	1	320	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
39	4	312	CLA	O2D-CGD-O1D	-3.25	117.48	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	L	314	KC2	CBD-CHA-C1A	3.25	134.94	128.88
39	F	315	CLA	CAA-C2A-C3A	-3.25	108.51	116.10
50	2	306	A1EB1	C25-C26-C27	-3.25	122.63	127.26
39	a	823	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
49	V	312	KC2	CBD-CHA-C1A	3.25	134.94	128.88
43	x	303	DD6	O1-C20-C19	-3.25	110.94	113.38
52	M	322	A1EB4	C12-C11-C13	3.25	120.76	115.30
39	Q	317	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
39	0	313	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
43	J	305	DD6	C37-C36-C31	-3.25	119.93	124.35
51	P	315	A1ECV	C2A-CAA-CBA	-3.25	121.30	128.63
48	D	305	A86	C36-C31-C32	3.25	122.92	119.70
48	L	302	A86	C-C1-C2	-3.25	118.37	122.92
39	9	307	CLA	CAA-C2A-C3A	-3.25	108.52	116.10
50	7	303	A1EB1	O1-C20-C21	-3.25	111.16	115.06
43	3	304	DD6	C7-C6-C5	-3.25	118.37	122.92
50	K	302	A1EB1	O1-C20-C19	-3.25	110.94	113.38
48	0	301	A86	C41-C32-C31	-3.25	107.57	110.47
43	U	204	DD6	C4-C5-C6	-3.25	122.68	127.31
50	7	304	A1EB1	C12-C11-C13	3.25	121.47	116.02
52	P	319	A1EB4	C12-C11-C13	3.25	120.75	115.30
42	k	204	BCR	C15-C14-C13	-3.25	122.68	127.31
49	8	317	KC2	CHC-C4B-C3B	-3.24	119.71	125.26
48	X	302	A86	O1-C20-C19	-3.24	110.94	113.38
39	L	316	CLA	CAA-C2A-C3A	-3.24	108.53	116.10
48	2	301	A86	C41-C32-C31	-3.24	107.57	110.47
48	0	309	A86	C17-C16-C15	3.24	112.47	109.16
50	T	302	A1EB1	C28-C27-C26	-3.24	120.69	124.93
47	F	318	SQD	O6-C1-C2	3.24	113.36	108.30
48	6	303	A86	C25-C26-C27	-3.24	122.68	127.31
49	Y	309	KC2	C1D-ND-C4D	3.24	108.64	106.33
50	9	302	A1EB1	C21-C20-C19	3.24	117.93	114.28
49	8	316	KC2	O2D-CGD-O1D	-3.24	117.50	123.84
48	T	306	A86	O1-C20-C21	-3.24	111.17	115.06
43	z	305	DD6	C25-C24-C1	-3.24	117.31	126.42
48	R	301	A86	C34-O4-C38	-3.24	111.86	117.90
51	4	321	A1ECV	O2-CMC-C2C	3.24	120.04	112.27
48	O	307	A86	C21-C20-C19	3.24	117.92	114.28
39	z	318	CLA	CAA-C2A-C3A	-3.24	108.54	116.10
50	y	301	A1EB1	O1-C20-C21	-3.24	111.17	115.06
48	K	301	A86	C12-C11-C13	3.24	121.46	116.02
49	5	314	KC2	CHB-C1B-C2B	-3.24	118.69	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	S	305	A86	O1-C20-C21	-3.24	111.18	115.06
43	A	302	DD6	C9-C10-C11	-3.24	122.69	127.31
48	V	301	A86	C41-C32-C31	-3.24	107.58	110.47
50	K	302	A1EB1	C25-C26-C27	-3.23	122.65	127.26
49	J	315	KC2	CHB-C1B-C2B	-3.23	118.70	125.48
46	M	319	LMG	C4-C3-C2	-3.23	105.18	110.82
46	M	319	LMG	C1-O6-C5	3.23	120.03	113.69
43	5	303	DD6	C4-C5-C6	-3.23	122.70	127.31
48	L	305	A86	C33-C32-C31	3.23	112.35	109.21
42	b	846	BCR	C37-C22-C21	-3.23	118.39	122.92
49	L	317	KC2	C1D-ND-C4D	3.23	108.63	106.33
48	8	309	A86	C34-O4-C38	-3.23	111.87	117.90
43	E	302	DD6	C37-C36-C31	-3.23	119.96	124.35
49	T	312	KC2	C2D-C1D-ND	-3.23	108.07	110.23
41	a	841	LHG	O8-C23-C24	3.23	119.85	111.38
39	O	316	CLA	CAA-C2A-C3A	-3.23	108.56	116.10
48	W	307	A86	C34-O4-C38	-3.23	111.88	117.90
49	2	317	KC2	C2D-C1D-ND	-3.23	108.07	110.23
47	S	301	SQD	C44-O6-C1	3.23	120.05	113.74
42	b	846	BCR	C33-C5-C4	3.23	119.82	113.62
52	P	305	A1EB4	C33-C32-C31	3.23	112.35	109.21
42	b	848	BCR	C10-C11-C12	-3.23	113.14	123.22
48	Q	308	A86	C40-C32-C31	-3.23	107.58	110.47
50	1	305	A1EB1	C40-C32-C31	-3.23	107.58	110.47
50	H	304	A1EB1	C3-C2-C1	-3.23	122.70	127.31
48	1	302	A86	C17-C16-C15	3.23	112.46	109.16
49	y	316	KC2	C1D-ND-C4D	3.23	108.63	106.33
51	Y	306	A1ECV	O2-CMC-C2C	3.23	120.02	112.27
48	9	304	A86	C21-C20-C19	3.23	117.91	114.28
50	8	308	A1EB1	O1-C20-C21	-3.23	111.19	115.06
49	4	320	KC2	CBD-CHA-C1A	3.23	134.90	128.88
49	L	321	KC2	CHC-C4B-C3B	-3.22	119.74	125.26
39	4	319	CLA	CAA-C2A-C3A	-3.22	108.58	116.10
39	O	313	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
49	5	311	KC2	C1D-ND-C4D	3.22	108.62	106.33
39	x	314	CLA	CAA-C2A-C3A	-3.22	108.58	116.10
49	T	312	KC2	CBD-CHA-C1A	3.22	134.89	128.88
43	1	304	DD6	C37-C36-C35	3.22	120.33	114.36
49	x	312	KC2	CHB-C1B-C2B	-3.22	118.72	125.48
48	W	307	A86	C25-C26-C27	-3.22	122.71	127.31
48	T	301	A86	C40-C32-C31	-3.22	107.59	110.47
48	9	304	A86	C40-C32-C31	-3.22	107.59	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Z	301	A86	C40-C32-C31	-3.22	107.59	110.47
49	S	314	KC2	CHB-C1B-C2B	-3.22	118.72	125.48
47	T	321	SQD	O5-C5-C4	3.22	115.54	109.69
49	X	306	KC2	C2D-C1D-ND	-3.22	108.07	110.23
43	7	310	DD6	C37-C36-C31	-3.22	119.97	124.35
48	E	304	A86	C26-C25-C24	-3.22	113.17	123.22
49	0	314	KC2	CBD-CHA-C1A	3.22	134.88	128.88
48	1	302	A86	C41-C32-C31	-3.22	107.59	110.47
48	7	311	A86	O1-C15-C14	-3.22	106.75	113.21
48	M	306	A86	O1-C20-C21	-3.22	111.20	115.06
49	7	320	KC2	C1D-ND-C4D	3.22	108.62	106.33
48	2	301	A86	O1-C15-C14	-3.22	106.75	113.21
39	4	312	CLA	C3B-C4B-NB	-3.22	107.53	110.52
52	W	306	A1EB4	C12-C11-C13	3.22	120.70	115.30
43	W	305	DD6	C3-C2-C1	-3.22	122.72	127.31
51	Z	308	A1ECV	CMA-C3A-C2A	3.22	130.69	124.68
50	6	301	A1EB1	C17-C16-C15	3.22	112.44	109.16
49	8	320	KC2	CHB-C1B-C2B	-3.21	118.74	125.48
49	J	315	KC2	CHC-C4B-C3B	-3.21	119.76	125.26
49	0	317	KC2	CHC-C4B-C3B	-3.21	119.76	125.26
39	a	814	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
51	X	310	A1ECV	O2D-CGD-O1D	-3.21	117.55	123.84
49	F	307	KC2	C2D-C1D-ND	-3.21	108.08	110.23
49	9	313	KC2	CHC-C4B-C3B	-3.21	119.76	125.26
39	C	310	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
49	T	314	KC2	CHC-C4B-C3B	-3.21	119.76	125.26
39	Z	305	CLA	CAA-C2A-C3A	-3.21	108.60	116.10
49	S	317	KC2	CBD-CHA-C1A	3.21	134.87	128.88
42	a	842	BCR	C11-C10-C9	-3.21	122.73	127.31
42	a	845	BCR	C16-C15-C14	-3.21	116.90	123.47
39	E	307	CLA	CMB-C2B-C1B	-3.21	120.48	125.37
52	W	306	A1EB4	C33-C32-C31	3.21	112.33	109.21
39	V	310	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
39	x	309	CLA	CAA-C2A-C3A	-3.21	108.61	116.10
48	O	306	A86	C9-C8-C6	-3.21	117.40	126.42
49	W	314	KC2	CHC-C4B-C3B	-3.21	119.77	125.26
49	V	312	KC2	C1D-ND-C4D	3.21	108.61	106.33
49	G	315	KC2	CHB-C1B-C2B	-3.21	118.75	125.48
49	J	315	KC2	C1D-ND-C4D	3.21	108.61	106.33
49	V	318	KC2	CHC-C4B-C3B	-3.21	119.77	125.26
39	4	316	CLA	CHB-C4A-NA	3.21	128.94	124.51
42	b	845	BCR	C20-C21-C22	-3.21	122.73	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	9	302	A1EB1	C17-C16-C15	3.21	112.43	109.16
50	x	302	A1EB1	C34-O4-C38	-3.21	111.92	117.90
50	4	304	A1EB1	C25-C26-C27	-3.21	122.70	127.26
48	K	301	A86	C35-C34-C33	3.20	115.47	109.88
48	9	304	A86	C34-O4-C38	-3.20	111.93	117.90
48	B	201	A86	C17-C16-C15	3.20	112.43	109.16
49	7	322	KC2	CHC-C4B-C3B	-3.20	119.78	125.26
49	L	315	KC2	C1D-ND-C4D	3.20	108.61	106.33
43	4	308	DD6	C25-C24-C1	-3.20	117.43	126.42
39	z	306	CLA	CAA-C2A-C3A	-3.20	108.63	116.10
39	S	309	CLA	CMB-C2B-C1B	-3.20	120.50	125.37
49	3	321	KC2	C1D-ND-C4D	3.20	108.61	106.33
50	7	306	A1EB1	C3-C4-C5	-3.20	116.92	123.47
43	4	308	DD6	C32-C31-C36	-3.20	118.12	122.63
48	8	305	A86	C25-C24-C1	-3.20	117.43	126.42
39	i	103	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
48	J	303	A86	C34-O4-C38	-3.20	111.94	117.90
51	Q	316	A1ECV	CMB-C2B-C1B	3.20	130.77	124.73
39	9	309	CLA	CAA-C2A-C3A	-3.20	108.64	116.10
42	a	842	BCR	C7-C8-C9	-3.20	121.41	126.23
51	W	317	A1ECV	CMA-C3A-C2A	3.20	130.66	124.68
48	8	303	A86	O1-C15-C14	-3.19	106.80	113.21
49	F	307	KC2	C1D-ND-C4D	3.19	108.60	106.33
50	K	302	A1EB1	C34-O4-C38	-3.19	111.94	117.90
52	P	305	A1EB4	C12-C11-C13	3.19	120.66	115.30
49	6	314	KC2	CBD-CHA-C1A	3.19	134.83	128.88
51	z	310	A1ECV	O2-CMC-O1	-3.19	117.21	123.45
42	l	206	BCR	C33-C5-C6	-3.19	120.94	124.53
49	Q	318	KC2	C1D-ND-C4D	3.19	108.60	106.33
39	9	308	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
43	D	303	DD6	C-C1-C2	-3.19	118.45	122.92
48	6	305	A86	C25-C26-C27	-3.19	122.76	127.31
50	Q	323	A1EB1	C34-O4-C38	-3.19	111.95	117.90
48	3	306	A86	O1-C20-C21	-3.19	111.23	115.06
48	8	305	A86	C34-O4-C38	-3.19	111.95	117.90
49	8	319	KC2	CHC-C4B-C3B	-3.19	119.80	125.26
49	P	320	KC2	C1D-ND-C4D	3.19	108.60	106.33
48	Q	305	A86	O1-C20-C21	-3.19	111.24	115.06
48	0	308	A86	C23-C16-C17	3.19	114.52	108.98
50	4	304	A1EB1	C41-C32-C31	-3.19	107.62	110.47
39	l	203	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
48	0	308	A86	C33-C32-C31	3.18	112.31	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	6	318	CLA	CAA-C2A-C3A	-3.18	108.67	116.10
48	6	303	A86	C33-C32-C31	3.18	112.30	109.21
49	C	312	KC2	CHC-C4B-C3B	-3.18	119.81	125.26
48	2	302	A86	C17-C16-C15	3.18	112.41	109.16
39	5	315	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
48	k	206	A86	C40-C32-C31	-3.18	107.62	110.47
48	8	302	A86	O1-C15-C14	-3.18	106.83	113.21
43	U	204	DD6	C15-C14-C13	-3.18	119.27	125.99
43	O	303	DD6	C37-C36-C35	3.18	120.25	114.36
43	4	308	DD6	C3-C4-C5	-3.18	116.96	123.47
43	3	301	DD6	C25-C24-C1	-3.18	117.49	126.42
42	b	847	BCR	C20-C21-C22	-3.18	122.78	127.31
43	A	303	DD6	C21-C20-C19	3.18	117.85	114.28
48	Y	301	A86	C34-O4-C38	-3.18	111.98	117.90
49	7	322	KC2	CHB-C1B-C2B	-3.18	118.82	125.48
49	4	318	KC2	C1D-ND-C4D	3.18	108.59	106.33
42	a	844	BCR	C33-C5-C6	-3.18	120.96	124.53
50	3	302	A1EB1	C33-C32-C31	3.18	112.30	109.21
48	P	302	A86	O1-C20-C19	-3.17	111.00	113.38
39	O	308	CLA	CBD-CHA-C1A	3.17	132.51	127.43
48	T	301	A86	C34-O4-C38	-3.17	111.98	117.90
48	7	312	A86	C33-C32-C31	3.17	112.30	109.21
52	5	304	A1EB4	C12-C11-C13	3.17	120.63	115.30
49	A	313	KC2	C1D-ND-C4D	3.17	108.59	106.33
49	H	314	KC2	CHC-C4B-C3B	-3.17	119.83	125.26
43	J	305	DD6	C14-C13-C11	-3.17	120.61	125.53
48	9	301	A86	C34-O4-C38	-3.17	111.98	117.90
48	6	305	A86	C34-O4-C38	-3.17	111.98	117.90
49	V	314	KC2	C1D-ND-C4D	3.17	108.59	106.33
49	X	318	KC2	C1D-ND-C4D	3.17	108.59	106.33
42	b	845	BCR	C16-C17-C18	-3.17	122.78	127.31
49	W	315	KC2	CHB-C1B-C2B	-3.17	118.83	125.48
50	h	203	A1EB1	C21-C20-C19	3.17	117.85	114.28
50	V	305	A1EB1	C4-C5-C6	-3.17	122.79	127.31
43	A	304	DD6	C37-C36-C31	-3.17	120.04	124.35
39	S	309	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
39	A	311	CLA	C3B-C4B-NB	-3.17	107.58	110.52
43	3	301	DD6	C37-C36-C31	-3.17	120.05	124.35
49	2	313	KC2	CHC-C4B-C3B	-3.17	118.84	125.48
39	L	320	CLA	C2A-C1A-CHA	3.17	129.40	123.86
50	3	302	A1EB1	C28-C27-C26	-3.17	120.79	124.93
49	Y	309	KC2	CHC-C4B-C3B	-3.17	119.84	125.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	B	201	A86	C25-C24-C1	-3.17	117.52	126.42
43	3	301	DD6	C4-C5-C6	-3.16	122.79	127.31
48	7	308	A86	C3-C4-C5	-3.16	116.99	123.47
50	8	304	A1EB1	C40-C32-C31	-3.16	107.64	110.47
43	5	303	DD6	O1-C20-C19	-3.16	111.01	113.38
50	V	306	A1EB1	O1-C20-C19	-3.16	111.01	113.38
39	1	317	CLA	CAA-C2A-C3A	-3.16	108.72	116.10
43	I	306	DD6	C21-C20-C15	-3.16	116.96	122.26
51	x	310	A1ECV	CMA-C3A-C2A	3.16	130.59	124.68
39	2	316	CLA	C3B-C4B-NB	-3.16	107.58	110.52
48	U	202	A86	O1-C15-C14	-3.16	106.87	113.21
49	5	311	KC2	CHB-C1B-C2B	-3.16	118.85	125.48
48	0	301	A86	O1-C15-C14	-3.16	106.87	113.21
49	V	315	KC2	C1D-ND-C4D	3.16	108.58	106.33
39	U	208	CLA	C3B-C4B-NB	-3.16	107.58	110.52
49	P	320	KC2	CBD-CHA-C1A	3.16	134.77	128.88
49	1	314	KC2	CHC-C4B-C3B	-3.16	119.86	125.26
43	a	846	DD6	C15-C14-C13	-3.16	119.32	125.99
49	F	307	KC2	CBD-CHA-C1A	3.16	134.77	128.88
51	Z	308	A1ECV	C2A-CAA-CBA	-3.16	121.51	128.63
39	6	311	CLA	CAA-C2A-C3A	-3.16	108.73	116.10
43	S	306	DD6	C15-C14-C13	-3.15	119.32	125.99
49	V	315	KC2	CHC-C4B-C3B	-3.15	119.86	125.26
42	j	103	BCR	C30-C25-C26	-3.15	118.17	122.61
49	5	311	KC2	CBD-CHA-C1A	3.15	134.76	128.88
49	K	310	KC2	C1D-ND-C4D	3.15	108.58	106.33
48	B	201	A86	C3-C4-C5	-3.15	117.02	123.47
50	R	303	A1EB1	C12-C11-C13	3.15	121.32	116.02
50	x	302	A1EB1	C33-C32-C31	3.15	112.28	109.21
49	K	313	KC2	CHC-C4B-C3B	-3.15	119.87	125.26
49	P	312	KC2	CHC-C4B-C3B	-3.15	119.87	125.26
49	3	315	KC2	C2D-C1D-ND	-3.15	108.12	110.23
39	b	837	CLA	CMB-C2B-C1B	-3.15	120.57	125.37
43	7	310	DD6	C14-C13-C11	-3.15	120.64	125.53
47	T	321	SQD	C44-O6-C1	3.15	119.89	113.74
49	8	316	KC2	CHC-C4B-C3B	-3.15	119.87	125.26
51	P	315	A1ECV	O2-CMC-C2C	3.15	119.83	112.27
50	1	305	A1EB1	C4-C3-C2	-3.15	117.02	123.47
49	1	314	KC2	CHB-C1B-C2B	-3.15	118.88	125.48
42	l	206	BCR	C20-C21-C22	-3.15	122.82	127.31
43	I	306	DD6	C3-C2-C1	-3.15	122.82	127.31
39	Q	321	CLA	C3B-C4B-NB	-3.15	107.59	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	E	305	DD6	C21-C20-C15	-3.15	116.99	122.26
49	L	317	KC2	CBD-CHA-C1A	3.15	134.75	128.88
49	0	314	KC2	C1D-ND-C4D	3.15	108.57	106.33
50	T	307	A1EB1	C25-C26-C27	-3.15	122.78	127.26
39	b	818	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
49	8	319	KC2	C2D-C1D-ND	-3.15	108.12	110.23
49	3	318	KC2	CHC-C4B-C3B	-3.15	119.88	125.26
39	3	312	CLA	C1-C2-C3	-3.14	120.60	126.04
48	8	323	A86	C17-C16-C15	3.14	112.37	109.16
48	X	303	A86	C40-C32-C31	-3.14	107.66	110.47
48	W	304	A86	C34-O4-C38	-3.14	112.04	117.90
48	4	328	A86	C4-C3-C2	-3.14	117.04	123.47
39	U	210	CLA	C3B-C4B-NB	-3.14	107.60	110.52
42	l	202	BCR	C16-C17-C18	-3.14	122.83	127.31
42	h	202	BCR	C33-C5-C6	-3.14	121.00	124.53
49	R	312	KC2	CBD-CHA-C1A	3.14	134.74	128.88
39	7	314	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
51	y	317	A1ECV	O2-CMC-C2C	3.14	119.81	112.27
51	7	323	A1ECV	O2-CMC-O1	-3.14	117.31	123.45
48	O	306	A86	C9-C10-C11	-3.14	117.38	126.61
39	a	830	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
48	O	307	A86	C9-C8-C6	-3.14	117.60	126.42
49	9	316	KC2	CHC-C4B-C3B	-3.14	119.89	125.26
49	W	312	KC2	C1D-ND-C4D	3.14	108.56	106.33
42	a	842	BCR	C24-C23-C22	-3.14	121.49	126.23
46	S	322	LMG	C8-O7-C10	-3.14	110.06	117.79
39	P	314	CLA	CAA-C2A-C3A	-3.14	108.78	116.10
49	9	316	KC2	CHB-C1B-C2B	-3.14	118.90	125.48
51	M	316	A1ECV	O2-CMC-C2C	3.14	119.80	112.27
49	R	306	KC2	CHB-C1B-C2B	-3.14	118.90	125.48
39	S	311	CLA	C3B-C4B-NB	-3.14	107.61	110.52
39	I	316	CLA	CAA-C2A-C3A	-3.14	108.78	116.10
42	l	202	BCR	C33-C5-C6	-3.14	121.01	124.53
39	2	312	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
49	8	319	KC2	CHB-C1B-C2B	-3.14	118.90	125.48
49	P	312	KC2	C1D-ND-C4D	3.13	108.56	106.33
48	T	306	A86	C41-C32-C31	-3.13	107.67	110.47
46	M	319	LMG	C3-C4-C5	3.13	115.83	110.24
46	F	317	LMG	C8-O7-C10	-3.13	110.08	117.79
43	G	303	DD6	O1-C20-C19	-3.13	111.03	113.38
51	S	312	A1ECV	C4B-CHC-C1C	3.13	126.11	115.73
50	6	301	A1EB1	C33-C32-C31	3.13	112.26	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	K	302	A1EB1	O1-C15-C14	-3.13	106.92	113.21
43	J	304	DD6	C3-C2-C1	-3.13	122.84	127.31
43	4	307	DD6	C37-C36-C31	-3.13	120.09	124.35
39	H	312	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
51	4	315	A1ECV	C4B-CHC-C1C	3.13	126.10	115.73
48	x	305	A86	C41-C32-C31	-3.13	107.67	110.47
43	R	304	DD6	C3-C2-C1	-3.13	122.84	127.31
49	7	319	KC2	CBD-CHA-C1A	3.13	134.72	128.88
43	y	304	DD6	C37-C36-C35	3.13	120.15	114.36
52	T	304	A1EB4	C12-C11-C13	3.13	120.55	115.30
43	A	303	DD6	C12-C11-C10	-3.13	118.54	122.92
39	1	319	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
49	8	320	KC2	CHC-C4B-C3B	-3.13	119.91	125.26
49	y	314	KC2	C2D-C1D-ND	-3.13	108.14	110.23
49	Q	315	KC2	C1D-ND-C4D	3.13	108.56	106.33
49	7	319	KC2	C1D-ND-C4D	3.13	108.56	106.33
50	D	308	A1EB1	C36-C31-C32	3.12	122.80	119.70
48	L	307	A86	C12-C11-C13	3.12	121.27	116.02
49	0	317	KC2	CBD-CHA-C1A	3.12	134.71	128.88
48	9	305	A86	O1-C20-C19	-3.12	111.03	113.38
49	I	303	KC2	O2D-CGD-O1D	-3.12	117.73	123.84
50	1	301	A1EB1	C17-C16-C15	3.12	112.35	109.16
48	R	302	A86	C21-C20-C19	3.12	117.79	114.28
47	P	301	SQD	O8-S-C6	3.12	110.72	105.74
51	2	311	A1ECV	CMA-C3A-C2A	3.12	130.52	124.68
50	T	307	A1EB1	C28-C27-C26	-3.12	120.85	124.93
48	Q	302	A86	C25-C26-C27	-3.12	122.86	127.31
51	y	311	A1ECV	O2-CMC-O1	-3.12	117.35	123.45
49	C	313	KC2	C1D-ND-C4D	3.12	108.55	106.33
39	A	315	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
50	6	304	A1EB1	O6-C42-C44	3.12	119.56	111.38
43	I	305	DD6	C33-C34-C35	-3.12	106.03	110.30
39	b	808	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
49	P	310	KC2	C1D-ND-C4D	3.12	108.55	106.33
39	Y	305	CLA	CAA-C2A-C3A	-3.12	108.82	116.10
43	I	307	DD6	C3-C2-C1	-3.12	122.86	127.31
49	S	315	KC2	C1D-ND-C4D	3.12	108.55	106.33
49	H	311	KC2	CHB-C1B-C2B	-3.12	118.94	125.48
45	C	314	DGD	O5D-C6D-C5D	-3.12	103.28	109.05
48	7	308	A86	C10-C9-C8	-3.12	113.50	123.22
50	9	302	A1EB1	C28-C27-C26	-3.11	120.86	124.93
49	A	310	KC2	C2D-C1D-ND	-3.11	108.14	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	L	314	KC2	CHC-C4B-C3B	-3.11	119.93	125.26
43	3	301	DD6	C3-C4-C5	-3.11	117.10	123.47
49	R	318	KC2	CBD-CHA-C1A	3.11	134.69	128.88
50	0	302	A1EB1	C25-C26-C27	-3.11	122.83	127.26
49	M	311	KC2	CBD-CHA-C1A	3.11	134.69	128.88
48	7	308	A86	C34-O4-C38	-3.11	112.09	117.90
43	7	310	DD6	C25-C24-C1	-3.11	117.67	126.42
50	2	304	A1EB1	O1-C20-C19	-3.11	111.04	113.38
50	4	302	A1EB1	C34-O4-C38	-3.11	112.10	117.90
48	E	304	A86	C17-C16-C15	3.11	112.34	109.16
49	L	315	KC2	CBD-CHA-C1A	3.11	134.68	128.88
39	7	321	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
51	7	317	A1ECV	CMB-C2B-C1B	3.11	130.61	124.73
49	9	311	KC2	C2D-C1D-ND	-3.11	108.15	110.23
42	f	804	BCR	C11-C12-C13	-3.11	117.67	126.42
43	C	301	DD6	C3-C4-C5	-3.11	117.10	123.47
49	S	317	KC2	C1D-ND-C4D	3.11	108.55	106.33
49	z	315	KC2	CBD-CHA-C1A	3.11	134.68	128.88
49	9	311	KC2	CHC-C4B-C3B	-3.11	119.94	125.26
43	M	304	DD6	O1-C20-C21	-3.11	111.33	115.06
39	0	311	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
43	Q	303	DD6	C21-C20-C19	3.11	117.78	114.28
42	l	207	BCR	C15-C14-C13	-3.11	122.87	127.31
48	6	307	A86	C3-C2-C1	-3.11	122.87	127.31
51	Z	314	A1ECV	O2D-CGD-O1D	-3.11	117.76	123.84
43	z	304	DD6	C15-C14-C13	-3.11	119.42	125.99
39	Z	315	CLA	CAA-C2A-C3A	-3.11	108.85	116.10
48	S	304	A86	C21-C20-C19	3.11	117.78	114.28
49	9	311	KC2	CHB-C1B-C2B	-3.11	118.96	125.48
48	2	305	A86	C34-O4-C38	-3.11	112.11	117.90
48	Z	301	A86	O1-C15-C14	-3.11	106.98	113.21
50	F	304	A1EB1	C28-C27-C26	-3.11	120.87	124.93
39	b	825	CLA	CHB-C4A-NA	3.10	128.80	124.51
49	T	314	KC2	O1D-CGD-CBD	-3.10	118.13	124.48
48	7	312	A86	C41-C32-C31	-3.10	107.69	110.47
39	Y	310	CLA	CAA-C2A-C3A	-3.10	108.86	116.10
51	Q	319	A1ECV	CMB-C2B-C1B	3.10	130.59	124.73
50	4	301	A1EB1	C10-C9-C8	-3.10	113.54	123.22
50	G	308	A1EB1	C4-C3-C2	-3.10	117.12	123.47
49	R	312	KC2	CHB-C1B-C2B	-3.10	118.98	125.48
39	Y	303	CLA	CAA-C2A-C3A	-3.10	108.87	116.10
50	C	302	A1EB1	C41-C32-C31	-3.10	107.70	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	301	A86	C21-C20-C19	3.10	117.76	114.28
43	G	306	DD6	C9-C8-C6	-3.10	117.72	126.42
39	X	317	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
42	b	850	BCR	C28-C27-C26	-3.10	108.55	114.08
48	1	306	A86	O1-C20-C21	-3.09	111.35	115.06
48	9	305	A86	C3-C4-C5	-3.09	117.14	123.47
49	x	312	KC2	C1D-ND-C4D	3.09	108.53	106.33
47	D	321	SQD	O5-C5-C4	3.09	115.31	109.69
51	R	310	A1ECV	CMA-C3A-C2A	3.09	130.47	124.68
49	x	312	KC2	CHC-C4B-C3B	-3.09	119.97	125.26
48	T	306	A86	C4-C5-C6	-3.09	122.90	127.31
49	G	313	KC2	CHB-C4A-C3A	-3.09	120.15	124.98
50	7	305	A1EB1	O1-C20-C21	-3.09	111.35	115.06
39	K	312	CLA	CHB-C4A-NA	3.09	128.79	124.51
49	x	313	KC2	C1D-ND-C4D	3.09	108.53	106.33
48	2	302	A86	C25-C24-C1	-3.09	117.74	126.42
47	4	327	SQD	O9-S-C6	3.09	110.61	106.94
43	A	303	DD6	C24-C1-C2	3.09	123.68	118.94
43	Q	303	DD6	C32-C31-C36	-3.09	118.28	122.63
43	j	102	DD6	C3-C2-C1	-3.09	122.91	127.31
48	R	317	A86	O1-C20-C21	-3.09	111.36	115.06
49	4	324	KC2	CBD-CHA-C1A	3.09	134.63	128.88
52	T	304	A1EB4	O1-C20-C19	-3.09	111.06	113.38
50	z	302	A1EB1	C41-C32-C31	-3.08	107.71	110.47
48	L	302	A86	C17-C16-C15	3.08	112.31	109.16
48	S	304	A86	C17-C16-C15	3.08	112.31	109.16
49	K	313	KC2	C2D-C1D-ND	-3.08	108.17	110.23
43	x	304	DD6	C37-C36-C35	3.08	120.07	114.36
48	L	304	A86	O1-C20-C21	-3.08	111.36	115.06
51	7	323	A1ECV	O2D-CGD-O1D	-3.08	117.81	123.84
48	T	305	A86	C12-C11-C13	3.08	121.20	116.02
48	6	305	A86	C17-C16-C15	3.08	112.31	109.16
43	z	305	DD6	C14-C13-C11	-3.08	120.75	125.53
48	7	308	A86	C4-C5-C6	-3.08	122.91	127.31
39	V	313	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
49	z	315	KC2	C1D-ND-C4D	3.08	108.52	106.33
39	O	311	CLA	C3B-C4B-NB	-3.08	107.66	110.52
48	1	307	A86	C41-C32-C31	-3.08	107.72	110.47
43	J	305	DD6	C25-C26-C27	-3.08	117.64	126.58
39	y	309	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
43	T	303	DD6	C33-C34-C35	-3.08	106.09	110.30
48	K	301	A86	C33-C32-C31	3.08	112.20	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	Z	311	KC2	CBD-CHA-C1A	3.08	134.62	128.88
48	F	301	A86	C41-C32-C31	-3.08	107.72	110.47
48	1	302	A86	C34-O4-C38	-3.08	112.16	117.90
43	I	305	DD6	C15-C14-C13	-3.08	119.49	125.99
39	Y	310	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
43	G	306	DD6	C37-C36-C31	-3.08	120.17	124.35
50	K	305	A1EB1	C28-C27-C26	-3.07	120.91	124.93
48	y	305	A86	O1-C15-C14	-3.07	107.04	113.21
39	6	318	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
49	y	313	KC2	CBD-CHA-C1A	3.07	134.61	128.88
52	W	321	A1EB4	C34-O4-C38	-3.07	112.17	117.90
49	I	303	KC2	CHB-C1B-C2B	-3.07	119.04	125.48
49	4	320	KC2	C1D-ND-C4D	3.07	108.52	106.33
50	K	304	A1EB1	O1-C20-C19	-3.07	111.08	113.38
39	b	811	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
49	T	315	KC2	CHB-C1B-C2B	-3.07	119.04	125.48
39	K	306	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
39	2	312	CLA	CAA-C2A-C3A	-3.07	108.93	116.10
43	H	305	DD6	C37-C36-C31	-3.07	120.18	124.35
51	R	313	A1ECV	C4B-CHC-C1C	3.07	125.90	115.73
42	f	801	BCR	C3-C4-C5	-3.07	108.59	114.08
49	x	313	KC2	CBD-CHA-C1A	3.07	134.60	128.88
48	R	302	A86	O4-C38-O5	-3.07	116.86	122.96
39	8	318	CLA	CAA-C2A-C3A	-3.07	108.94	116.10
48	G	305	A86	C36-C31-C32	3.07	122.74	119.70
48	2	301	A86	C33-C32-C31	3.07	112.19	109.21
48	L	306	A86	C3-C2-C1	-3.07	122.93	127.31
48	R	302	A86	O1-C20-C21	-3.07	111.38	115.06
43	K	303	DD6	C3-C2-C1	-3.07	122.94	127.31
48	8	323	A86	C3-C4-C5	-3.07	117.19	123.47
48	K	301	A86	C34-O4-C38	-3.07	112.18	117.90
49	4	318	KC2	C1A-NA-C4A	-3.07	105.33	106.71
47	D	321	SQD	C1-O5-C5	3.06	119.70	113.69
43	O	304	DD6	C15-C14-C13	-3.06	119.51	125.99
49	X	312	KC2	CBD-CHA-C1A	3.06	134.59	128.88
50	1	305	A1EB1	C33-C32-C31	3.06	112.19	109.21
48	O	307	A86	C34-O4-C38	-3.06	112.19	117.90
51	R	313	A1ECV	O2-CMC-O1	-3.06	117.46	123.45
39	M	317	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
49	z	315	KC2	O2D-CGD-O1D	-3.06	117.85	123.84
48	4	309	A86	C35-C34-C33	3.06	115.22	109.88
49	R	318	KC2	C1D-ND-C4D	3.06	108.51	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	b	825	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
48	k	206	A86	O1-C20-C21	-3.06	111.39	115.06
39	V	316	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
49	S	314	KC2	CHC-C4B-C3B	-3.06	120.02	125.26
49	8	314	KC2	CHB-C1B-C2B	-3.06	119.06	125.48
48	M	303	A86	C17-C16-C15	3.06	112.28	109.16
43	F	303	DD6	C9-C10-C11	-3.06	122.94	127.31
50	C	302	A1EB1	C28-C27-C26	-3.06	120.93	124.93
50	U	203	A1EB1	C28-C27-C26	-3.06	120.93	124.93
39	X	308	CLA	CHB-C1B-NB	3.06	127.50	124.26
49	Q	315	KC2	CHB-C1B-C2B	-3.06	119.06	125.48
48	2	302	A86	C36-C31-C32	3.06	122.73	119.70
42	l	207	BCR	C11-C10-C9	-3.06	122.94	127.31
43	G	303	DD6	C9-C10-C11	-3.06	122.94	127.31
39	b	826	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
48	J	301	A86	C17-C16-C15	3.06	112.28	109.16
48	Q	305	A86	C17-C16-C15	3.06	112.28	109.16
49	0	316	KC2	CBD-CHA-C1A	3.06	134.58	128.88
50	V	306	A1EB1	C34-O4-C38	-3.06	112.20	117.90
48	I	304	A86	C12-C11-C13	3.06	121.16	116.02
43	y	304	DD6	C25-C24-C1	-3.06	117.83	126.42
43	A	301	DD6	C37-C36-C31	-3.06	120.19	124.35
43	3	301	DD6	C9-C10-C11	-3.06	122.95	127.31
39	9	320	CLA	CMA-C3A-C2A	-3.06	108.97	116.10
48	8	309	A86	C3-C4-C5	-3.06	117.21	123.47
49	X	312	KC2	CHC-C4B-C3B	-3.06	120.03	125.26
43	I	305	DD6	C3-C2-C1	-3.06	122.95	127.31
49	9	313	KC2	CBD-CHA-C1A	3.06	134.58	128.88
50	V	305	A1EB1	O1-C20-C21	-3.06	111.39	115.06
51	y	317	A1ECV	CMA-C3A-C2A	3.06	130.39	124.68
48	6	302	A86	C9-C8-C6	-3.05	117.84	126.42
48	P	303	A86	C33-C32-C31	3.05	112.18	109.21
39	6	312	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
43	F	303	DD6	C37-C36-C31	-3.05	120.20	124.35
39	z	314	CLA	CAA-C2A-C3A	-3.05	108.98	116.10
48	y	305	A86	C25-C26-C27	-3.05	122.95	127.31
49	5	305	KC2	CHB-C1B-C2B	-3.05	119.08	125.48
48	R	302	A86	C33-C32-C31	3.05	112.18	109.21
39	P	316	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
48	M	306	A86	C34-O4-C38	-3.05	112.21	117.90
39	Z	312	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
49	X	314	KC2	CBD-CHA-C1A	3.05	134.57	128.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B	209	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
49	8	316	KC2	CBD-CHA-C1A	3.05	134.56	128.88
47	H	318	SQD	O8-S-C6	3.05	110.60	105.74
39	j	101	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
50	S	303	A1EB1	C28-C27-C26	-3.05	120.95	124.93
48	9	303	A86	C3-C4-C5	-3.05	117.23	123.47
39	3	312	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
49	z	312	KC2	CHB-C1B-C2B	-3.05	119.09	125.48
39	A	314	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
49	L	321	KC2	C2D-C1D-ND	-3.04	108.19	110.23
39	l	201	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
43	D	307	DD6	C33-C34-C35	-3.04	106.14	110.30
39	1	309	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
51	1	318	A1ECV	CMA-C3A-C2A	3.04	130.37	124.68
39	a	835	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
50	4	304	A1EB1	C4-C5-C6	-3.04	122.97	127.31
48	O	306	A86	O1-C20-C21	-3.04	111.41	115.06
42	b	848	BCR	C21-C20-C19	-3.04	113.72	123.22
48	P	303	A86	C41-C32-C31	-3.04	107.75	110.47
50	6	304	A1EB1	C41-C32-C31	-3.04	107.75	110.47
48	4	310	A86	C33-C32-C31	3.04	112.17	109.21
49	9	316	KC2	C2D-C1D-ND	-3.04	108.19	110.23
39	b	838	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
50	4	304	A1EB1	C17-C16-C15	3.04	112.27	109.16
51	7	323	A1ECV	C4B-CHC-C1C	3.04	125.80	115.73
43	7	309	DD6	C33-C34-C35	-3.04	106.14	110.30
39	x	317	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
51	1	318	A1ECV	O2D-CGD-O1D	-3.04	117.90	123.84
46	4	326	LMG	C7-O1-C1	-3.04	107.80	113.74
51	Z	314	A1ECV	O2-CMC-O1	-3.04	117.51	123.45
48	E	304	A86	C35-C34-C33	-3.04	104.58	109.88
48	8	323	A86	C34-O4-C38	-3.04	112.24	117.90
49	M	314	KC2	CHC-C4B-C3B	-3.04	120.06	125.26
48	O	307	A86	C41-C32-C31	-3.04	107.75	110.47
49	7	322	KC2	C2D-C1D-ND	-3.04	108.20	110.23
49	4	317	KC2	CHC-C4B-C3B	-3.04	120.07	125.26
48	Z	301	A86	C33-C32-C31	3.04	112.16	109.21
49	P	313	KC2	CHC-C4B-C3B	-3.03	120.07	125.26
49	5	313	KC2	CHC-C4B-C3B	-3.03	120.07	125.26
49	5	313	KC2	CBD-CHA-C1A	3.03	134.54	128.88
43	7	310	DD6	C37-C36-C35	3.03	119.97	114.36
47	9	322	SQD	C44-O6-C1	3.03	119.66	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	L	309	CLA	CMB-C2B-C1B	-3.03	120.75	125.37
43	x	303	DD6	C3-C4-C5	-3.03	117.26	123.47
39	H	315	CLA	CAA-C2A-C3A	-3.03	109.02	116.10
46	7	301	LMG	C7-O1-C1	-3.03	107.82	113.74
39	k	202	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
42	b	847	BCR	C33-C5-C4	3.03	119.44	113.62
43	A	301	DD6	C28-C27-C29	3.03	122.84	116.84
50	V	305	A1EB1	O1-C20-C19	-3.03	111.11	113.38
43	G	306	DD6	O1-C20-C21	-3.03	111.43	115.06
39	0	320	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
42	m	101	BCR	C3-C4-C5	-3.03	108.67	114.08
42	i	102	BCR	C33-C5-C4	3.03	119.43	113.62
48	L	302	A86	C24-C1-C2	3.03	123.59	118.94
51	Q	316	A1ECV	C4B-CHC-C1C	3.03	125.76	115.73
49	R	314	KC2	CBD-CHA-C1A	3.03	134.53	128.88
49	X	314	KC2	CHC-C4B-C3B	-3.03	120.08	125.26
39	z	309	CLA	CAA-C2A-C3A	-3.03	109.04	116.10
51	E	311	A1ECV	C4B-CHC-C1C	3.03	125.75	115.73
49	R	314	KC2	CHC-C4B-C3B	-3.03	120.08	125.26
43	D	303	DD6	C15-C14-C13	-3.03	119.59	125.99
49	P	312	KC2	CBD-CHA-C1A	3.03	134.52	128.88
48	3	306	A86	C34-O4-C38	-3.03	112.26	117.90
39	1	310	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
49	7	320	KC2	CHC-C4B-C3B	-3.03	120.08	125.26
43	I	307	DD6	C33-C34-C35	-3.02	106.16	110.30
48	C	303	A86	C34-O4-C38	-3.02	112.26	117.90
48	7	311	A86	C21-C20-C19	3.02	117.68	114.28
51	z	316	A1ECV	O1D-CGD-CBD	-3.02	119.70	124.74
39	a	802	CLA	CHB-C4A-NA	3.02	128.69	124.51
43	J	306	DD6	C25-C26-C27	-3.02	117.80	126.58
39	l	204	CLA	C3B-C4B-NB	-3.02	107.71	110.52
48	X	302	A86	C41-C32-C31	-3.02	107.77	110.47
39	U	209	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
48	0	306	A86	C25-C26-C27	-3.02	123.00	127.31
43	T	303	DD6	C15-C14-C13	-3.02	119.61	125.99
48	5	301	A86	C9-C8-C6	-3.02	117.93	126.42
51	G	316	A1ECV	CMB-C2B-C1B	3.02	130.43	124.73
49	P	310	KC2	CBD-CHA-C1A	3.02	134.51	128.88
47	D	304	SQD	O5-C5-C4	3.02	115.18	109.69
46	S	322	LMG	C7-O1-C1	-3.02	107.84	113.74
48	6	309	A86	C40-C32-C31	-3.02	107.77	110.47
43	X	304	DD6	O1-C20-C19	-3.02	111.11	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	U	204	DD6	C37-C36-C35	3.02	119.94	114.36
49	2	314	KC2	C1D-ND-C4D	3.02	108.48	106.33
51	7	317	A1ECV	C4B-CHC-C1C	3.02	125.72	115.73
48	H	302	A86	C34-O4-C38	-3.02	112.28	117.90
39	S	309	CLA	CHB-C1B-NB	3.02	127.45	124.26
49	S	315	KC2	CHC-C4B-C3B	-3.02	120.10	125.26
47	E	320	SQD	C44-O6-C1	3.02	119.63	113.74
49	x	312	KC2	CBD-CHA-C1A	3.02	134.50	128.88
39	3	313	CLA	C3B-C4B-NB	-3.01	107.72	110.52
49	A	313	KC2	CBD-CHA-C1A	3.01	134.50	128.88
49	3	317	KC2	CBD-CHA-C1A	3.01	134.50	128.88
48	3	305	A86	C25-C26-C27	-3.01	123.01	127.31
50	y	301	A1EB1	C34-O4-C38	-3.01	112.28	117.90
48	5	301	A86	C35-C34-C33	-3.01	104.62	109.88
43	I	307	DD6	C4-C3-C2	-3.01	117.30	123.47
39	5	310	CLA	CHB-C4A-NA	3.01	128.68	124.51
42	l	207	BCR	C38-C26-C25	-3.01	121.14	124.53
52	5	304	A1EB4	C3-C4-C5	-3.01	117.30	123.47
39	E	317	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
39	C	311	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
39	W	316	CLA	CAA-C2A-C3A	-3.01	109.07	116.10
39	O	314	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
39	9	309	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
49	M	311	KC2	C1D-ND-C4D	3.01	108.47	106.33
51	Z	308	A1ECV	O2-CMC-O1	-3.01	117.56	123.45
39	D	318	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
50	V	307	A1EB1	C9-C8-C6	-3.01	117.96	126.42
50	2	306	A1EB1	C36-C31-C32	3.01	122.68	119.70
42	j	103	BCR	C39-C30-C25	-3.01	105.42	110.30
39	D	315	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
51	4	315	A1ECV	CMA-C3A-C2A	3.01	130.31	124.68
48	8	302	A86	C41-C32-C31	-3.01	107.78	110.47
39	b	807	CLA	CHB-C4A-NA	3.01	128.67	124.51
42	h	202	BCR	C29-C30-C25	3.01	115.11	110.48
42	l	207	BCR	C3-C4-C5	-3.01	108.71	114.08
39	D	317	CLA	CHB-C4A-NA	3.01	128.67	124.51
49	W	312	KC2	CBD-CHA-C1A	3.01	134.49	128.88
43	X	304	DD6	C15-C14-C13	-3.00	119.64	125.99
49	3	315	KC2	CHC-C4B-C3B	-3.00	120.12	125.26
45	b	849	DGD	O6D-C1D-O3G	-3.00	102.86	109.97
39	k	203	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
51	x	316	A1ECV	CMA-C3A-C2A	3.00	130.30	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	0	305	A1EB1	C34-O4-C38	-3.00	112.30	117.90
50	O	301	A1EB1	C28-C27-C26	-3.00	121.00	124.93
50	3	324	A1EB1	C12-C11-C13	3.00	121.07	116.02
49	F	307	KC2	O1D-CGD-CBD	-3.00	118.34	124.48
43	C	301	DD6	C3-C2-C1	-3.00	123.03	127.31
51	M	316	A1ECV	CMB-C2B-C1B	3.00	130.40	124.73
39	b	851	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
52	T	304	A1EB4	C21-C20-C15	-3.00	117.25	122.32
48	7	311	A86	C12-C11-C13	3.00	121.06	116.02
50	x	302	A1EB1	C40-C32-C31	-3.00	107.79	110.47
39	M	312	CLA	CHB-C4A-NA	3.00	128.66	124.51
48	z	303	A86	C34-O4-C38	-3.00	112.31	117.90
50	y	302	A1EB1	C34-O4-C38	-3.00	112.31	117.90
50	3	309	A1EB1	C36-C31-C32	3.00	122.67	119.70
39	b	831	CLA	C3B-C4B-NB	-3.00	107.74	110.52
50	8	308	A1EB1	C28-O6-C42	3.00	122.34	115.68
51	2	311	A1ECV	O2-CMC-O1	-2.99	117.59	123.45
49	H	314	KC2	C1D-ND-C4D	2.99	108.46	106.33
49	y	314	KC2	CHC-C4B-C3B	-2.99	120.14	125.26
49	5	305	KC2	C1D-ND-C4D	2.99	108.46	106.33
50	3	324	A1EB1	O6-C42-C44	2.99	121.30	111.91
51	0	321	A1ECV	CMA-C3A-C2A	2.99	130.28	124.68
39	B	204	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
48	1	302	A86	C4-C3-C2	-2.99	117.35	123.47
49	P	306	KC2	CHC-C4B-C3B	-2.99	120.14	125.26
50	K	305	A1EB1	C40-C32-C31	-2.99	107.80	110.47
39	a	802	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
50	O	301	A1EB1	O1-C20-C19	-2.99	111.14	113.38
39	O	316	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
39	y	308	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
43	a	846	DD6	C37-C36-C31	-2.99	120.29	124.35
39	0	318	CLA	CAA-C2A-C3A	-2.99	109.12	116.10
39	O	309	CLA	C3B-C4B-NB	-2.99	107.74	110.52
39	x	307	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
43	4	308	DD6	C14-C13-C11	-2.99	120.89	125.53
50	U	203	A1EB1	C34-O4-C38	-2.99	112.33	117.90
39	G	314	CLA	CHB-C4A-NA	2.99	128.64	124.51
51	2	311	A1ECV	CMB-C2B-C1B	2.99	130.37	124.73
51	Y	312	A1ECV	CMB-C2B-C1B	2.99	130.37	124.73
48	V	304	A86	C25-C26-C27	-2.99	123.05	127.31
49	x	315	KC2	C2D-C1D-ND	-2.98	108.23	110.23
48	O	306	A86	C40-C32-C31	-2.98	107.80	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	a	816	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
39	a	818	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
48	8	309	A86	C17-C16-C15	2.98	112.21	109.16
43	y	304	DD6	O1-C20-C19	-2.98	111.14	113.38
51	5	312	A1ECV	C4B-CHC-C1C	2.98	125.61	115.73
47	D	304	SQD	O6-C1-C2	2.98	112.96	108.30
39	2	308	CLA	C3B-C4B-NB	-2.98	107.75	110.52
39	9	312	CLA	CHB-C4A-NA	2.98	128.63	124.51
43	V	303	DD6	C21-C20-C15	-2.98	117.27	122.26
49	8	320	KC2	CBD-CHA-C1A	2.98	134.44	128.88
43	x	303	DD6	C15-C14-C13	-2.98	119.69	125.99
50	V	307	A1EB1	C12-C11-C13	2.98	121.03	116.02
49	F	311	KC2	CHB-C4A-C3A	-2.98	120.33	124.98
51	Z	308	A1ECV	CMB-C2B-C1B	2.98	130.35	124.73
49	x	315	KC2	CHB-C1B-C2B	-2.98	119.24	125.48
43	W	305	DD6	C33-C34-C35	-2.98	106.23	110.30
43	5	303	DD6	C15-C14-C13	-2.98	119.70	125.99
39	D	312	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
50	E	301	A1EB1	C12-C11-C13	2.98	121.02	116.02
49	0	316	KC2	C1D-ND-C4D	2.98	108.45	106.33
39	T	319	CLA	CHB-C4A-NA	2.98	128.63	124.51
39	f	802	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
50	G	307	A1EB1	C28-C27-C26	-2.97	121.04	124.93
49	V	308	KC2	C2D-C1D-ND	-2.97	108.24	110.23
51	L	318	A1ECV	O2-CMC-C2C	2.97	119.41	112.27
42	h	202	BCR	C21-C20-C19	-2.97	113.94	123.22
39	E	313	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
51	4	315	A1ECV	CMB-C2B-C1B	2.97	130.35	124.73
51	P	315	A1ECV	CMB-C2B-C1B	2.97	130.34	124.73
39	I	311	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
49	Z	311	KC2	C1D-ND-C4D	2.97	108.45	106.33
49	R	306	KC2	C2D-C1D-ND	-2.97	108.24	110.23
48	0	309	A86	O1-C20-C21	-2.97	111.50	115.06
49	y	313	KC2	C1D-ND-C4D	2.97	108.44	106.33
50	F	304	A1EB1	C25-C26-C27	-2.97	123.03	127.26
49	Q	313	KC2	CBD-CHA-C1A	2.97	134.42	128.88
49	T	316	KC2	C1D-ND-C4D	2.97	108.44	106.33
50	0	307	A1EB1	C28-O6-C42	2.97	122.28	115.68
46	l	208	LMG	O8-C28-C29	2.97	121.22	111.91
48	8	309	A86	O1-C15-C14	-2.97	107.25	113.21
48	1	306	A86	C40-C32-C31	-2.97	107.82	110.47
50	S	302	A1EB1	C3-C2-C1	-2.97	123.08	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	H	311	KC2	CBD-CHA-C1A	2.97	134.41	128.88
51	Y	306	A1ECV	CMB-C2B-C1B	2.97	130.33	124.73
39	S	309	CLA	O2D-CGD-CBD	2.97	116.54	111.27
50	U	205	A1EB1	C17-C16-C15	2.97	112.19	109.16
43	O	304	DD6	C4-C5-C6	-2.97	123.08	127.31
39	1	320	CLA	CMA-C3A-C2A	-2.97	109.18	116.10
48	R	302	A86	C9-C8-C6	-2.96	118.09	126.42
51	9	314	A1ECV	C4B-CHC-C1C	2.96	125.55	115.73
48	6	303	A86	C34-O4-C38	-2.96	112.37	117.90
39	x	318	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
50	V	307	A1EB1	O1-C20-C21	-2.96	111.50	115.06
50	8	301	A1EB1	O1-C20-C21	-2.96	111.50	115.06
50	K	304	A1EB1	C34-O4-C38	-2.96	112.37	117.90
48	6	307	A86	O1-C15-C14	-2.96	107.26	113.21
50	8	301	A1EB1	C10-C9-C8	-2.96	113.97	123.22
39	z	307	CLA	CMB-C2B-C1B	-2.96	120.86	125.37
49	8	316	KC2	C1D-ND-C4D	2.96	108.44	106.33
49	z	313	KC2	CHB-C1B-C2B	-2.96	119.27	125.48
43	I	306	DD6	C33-C34-C35	-2.96	106.25	110.30
48	4	306	A86	C10-C9-C8	-2.96	113.98	123.22
48	V	304	A86	C40-C32-C31	-2.96	107.82	110.47
48	X	302	A86	C9-C8-C6	-2.96	118.10	126.42
39	b	817	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
39	0	311	CLA	O2D-CGD-CBD	2.96	116.53	111.27
39	E	315	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
39	y	310	CLA	CAA-C2A-C3A	-2.96	109.19	116.10
39	a	815	CLA	C3B-C4B-NB	-2.96	107.77	110.52
52	T	304	A1EB4	O3-C39-C43	2.96	121.19	111.91
49	F	307	KC2	C4D-C3D-CAD	2.96	109.42	107.42
43	E	303	DD6	C37-C36-C31	-2.96	120.33	124.35
48	S	305	A86	C10-C9-C8	-2.96	113.99	123.22
49	3	317	KC2	C1D-ND-C4D	2.96	108.44	106.33
49	X	306	KC2	CHB-C1B-C2B	-2.96	119.28	125.48
39	a	808	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
39	E	316	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
43	F	303	DD6	C15-C14-C13	-2.96	119.75	125.99
48	0	301	A86	C25-C26-C27	-2.95	123.09	127.31
39	U	207	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
49	Z	310	KC2	CBD-CHA-C1A	2.95	134.39	128.88
43	K	303	DD6	C33-C34-C35	-2.95	106.26	110.30
43	A	301	DD6	C4-C5-C6	-2.95	123.09	127.31
49	L	321	KC2	CHB-C1B-C2B	-2.95	119.28	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	Q	315	KC2	CBD-CHA-C1A	2.95	134.39	128.88
49	I	312	KC2	CHB-C4A-C3A	-2.95	120.36	124.98
39	H	310	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
51	Y	312	A1ECV	CMA-C3A-C2A	2.95	130.20	124.68
49	8	317	KC2	C1D-ND-C4D	2.95	108.43	106.33
49	y	314	KC2	CHB-C1B-C2B	-2.95	119.29	125.48
51	z	316	A1ECV	C4B-CHC-C1C	2.95	125.51	115.73
49	z	312	KC2	C2D-C1D-ND	-2.95	108.25	110.23
51	Y	306	A1ECV	O2D-CGD-O1D	-2.95	118.07	123.84
50	D	308	A1EB1	C3-C4-C5	-2.95	117.43	123.47
39	a	806	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
49	A	310	KC2	CHB-C1B-C2B	-2.95	119.30	125.48
50	6	301	A1EB1	O6-C42-C44	2.95	121.16	111.91
49	K	313	KC2	CBD-CHA-C1A	2.95	134.38	128.88
50	H	301	A1EB1	C28-O6-C42	2.95	122.24	115.68
50	3	324	A1EB1	C25-C26-C27	-2.95	123.06	127.26
39	8	311	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
39	K	308	CLA	C3B-C4B-NB	-2.95	107.78	110.52
39	V	310	CLA	C3B-C4B-NB	-2.95	107.78	110.52
42	a	845	BCR	C28-C27-C26	-2.95	108.81	114.08
39	E	312	CLA	C3B-C4B-NB	-2.95	107.78	110.52
39	7	314	CLA	C3B-C4B-NB	-2.95	107.78	110.52
51	z	310	A1ECV	CMA-C3A-C2A	2.95	130.19	124.68
39	9	310	CLA	CAA-C2A-C3A	-2.94	109.23	116.10
39	F	313	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
48	8	307	A86	C41-C32-C31	-2.94	107.84	110.47
50	C	302	A1EB1	C25-C26-C27	-2.94	123.07	127.26
43	D	303	DD6	C14-C13-C11	-2.94	120.97	125.53
48	V	304	A86	C33-C32-C31	2.94	112.07	109.21
48	x	305	A86	C17-C16-C15	2.94	112.16	109.16
39	a	812	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
43	S	306	DD6	C14-C13-C11	-2.94	120.97	125.53
50	V	307	A1EB1	C34-O4-C38	-2.94	112.42	117.90
50	3	310	A1EB1	O6-C42-C44	2.94	121.13	111.91
39	D	311	CLA	C3B-C4B-NB	-2.94	107.79	110.52
39	y	315	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
39	k	201	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
39	9	307	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
39	C	305	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
50	4	302	A1EB1	C40-C32-C31	-2.94	107.84	110.47
39	C	304	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
43	4	308	DD6	C25-C26-C27	-2.94	118.06	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	S	303	A1EB1	C40-C32-C31	-2.94	107.84	110.47
39	9	315	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
48	9	304	A86	C9-C8-C6	-2.94	118.17	126.42
39	a	826	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
39	J	314	CLA	C3B-C4B-NB	-2.93	107.79	110.52
49	0	316	KC2	CHB-C1B-C2B	-2.93	119.33	125.48
48	O	302	A86	C4-C3-C2	-2.93	117.46	123.47
39	C	310	CLA	CHB-C4A-NA	2.93	128.57	124.51
48	X	303	A86	C34-O4-C38	-2.93	112.43	117.90
48	Z	301	A86	C34-O4-C38	-2.93	112.43	117.90
50	H	304	A1EB1	C28-C27-C26	-2.93	121.10	124.93
39	A	305	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
49	Z	310	KC2	C1D-ND-C4D	2.93	108.42	106.33
39	a	821	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
48	5	301	A86	O1-C20-C21	-2.93	111.54	115.06
48	D	305	A86	C12-C11-C13	2.93	120.94	116.02
48	6	302	A86	C34-O4-C38	-2.93	112.44	117.90
39	j	101	CLA	CHB-C4A-NA	2.93	128.56	124.51
49	6	317	KC2	CBD-CHA-C1A	2.93	134.34	128.88
42	a	843	BCR	C33-C5-C6	-2.93	121.24	124.53
39	a	827	CLA	CHB-C1B-NB	2.93	127.36	124.26
39	E	308	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
39	R	309	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
46	A	316	LMG	O6-C1-O1	-2.93	103.04	109.97
50	7	306	A1EB1	C40-C32-C31	-2.93	107.85	110.47
50	V	305	A1EB1	C10-C9-C8	-2.93	114.08	123.22
49	T	315	KC2	C4D-C3D-CAD	2.93	109.39	107.42
39	0	310	CLA	CAA-C2A-C3A	-2.93	104.77	112.78
48	k	206	A86	C25-C26-C27	-2.93	123.14	127.31
39	M	310	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
49	1	315	KC2	CHC-C4B-C3B	-2.92	120.25	125.26
52	X	305	A1EB4	C4-C5-C6	-2.92	123.14	127.31
48	O	302	A86	C34-O4-C38	-2.92	112.45	117.90
39	B	207	CLA	C3B-C4B-NB	-2.92	107.80	110.52
50	1	301	A1EB1	C12-C11-C13	2.92	120.93	116.02
39	7	315	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
47	F	319	SQD	O5-C5-C4	2.92	115.00	109.69
49	6	316	KC2	C1D-ND-C4D	2.92	108.41	106.33
39	b	834	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
39	P	307	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
39	S	310	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
48	L	307	A86	C10-C9-C8	-2.92	114.09	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	I	306	DD6	C14-C13-C11	-2.92	120.99	125.53
51	S	312	A1ECV	CMB-C2B-C1B	2.92	130.25	124.73
49	8	314	KC2	CHC-C4B-C3B	-2.92	120.26	125.26
50	U	205	A1EB1	C25-C26-C27	-2.92	123.10	127.26
39	D	319	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
51	Z	308	A1ECV	O2D-CGD-O1D	-2.92	118.12	123.84
48	L	306	A86	O1-C20-C19	-2.92	111.19	113.38
43	4	308	DD6	C10-C9-C8	-2.92	114.10	123.22
49	8	319	KC2	O1D-CGD-CBD	-2.92	118.51	124.48
39	9	310	CLA	CMB-C2B-C1B	-2.92	120.92	125.37
49	8	316	KC2	C1A-NA-C4A	-2.92	105.39	106.71
49	X	315	KC2	CBD-CHA-C1A	2.92	134.32	128.88
52	W	306	A1EB4	C34-O4-C38	-2.92	112.45	117.90
49	T	315	KC2	C1D-ND-C4D	2.92	108.41	106.33
49	X	312	KC2	C1D-ND-C4D	2.92	108.41	106.33
49	I	312	KC2	C2D-C1D-ND	-2.92	108.28	110.23
43	z	304	DD6	C4-C5-C6	-2.92	123.14	127.31
39	C	310	CLA	C3B-C4B-NB	-2.92	107.81	110.52
50	7	304	A1EB1	C28-C27-C26	-2.92	121.11	124.93
39	o	202	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
51	X	310	A1ECV	CMA-C3A-C2A	2.92	130.14	124.68
50	D	308	A1EB1	C41-C32-C31	-2.92	107.86	110.47
50	S	302	A1EB1	C4-C3-C2	-2.92	117.50	123.47
50	K	304	A1EB1	O1-C15-C14	-2.92	107.35	113.21
39	T	319	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
43	O	303	DD6	C25-C24-C1	-2.92	118.22	126.42
50	U	205	A1EB1	C28-C27-C26	-2.92	121.12	124.93
43	I	307	DD6	C37-C36-C31	-2.92	120.39	124.35
50	4	304	A1EB1	C34-O4-C38	-2.92	112.46	117.90
51	y	311	A1ECV	CMB-C2B-C1B	2.92	130.24	124.73
39	b	805	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
39	X	311	CLA	CHB-C4A-NA	2.92	128.54	124.51
39	1	317	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
49	V	318	KC2	C2D-C1D-ND	-2.91	108.28	110.23
43	7	310	DD6	C21-C20-C19	2.91	117.56	114.28
39	G	312	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
39	Y	305	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
39	R	311	CLA	CHB-C4A-NA	2.91	128.54	124.51
46	I	302	LMG	O6-C1-O1	-2.91	103.08	109.97
45	b	849	DGD	O5D-C6D-C5D	-2.91	103.66	109.05
42	a	843	BCR	C7-C8-C9	-2.91	121.83	126.23
39	J	314	CLA	O2D-CGD-O1D	-2.91	118.14	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	4	321	A1ECV	CMB-C2B-C1B	2.91	130.23	124.73
49	x	315	KC2	CHC-C4B-C3B	-2.91	120.28	125.26
43	G	303	DD6	C15-C14-C13	-2.91	119.84	125.99
49	P	313	KC2	O1D-CGD-CBD	-2.91	118.53	124.48
50	H	301	A1EB1	O4-C38-O5	-2.91	117.18	122.96
39	b	809	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
39	4	319	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
42	a	845	BCR	C33-C5-C6	-2.91	121.26	124.53
46	4	326	LMG	O1-C1-C2	2.91	112.85	108.30
39	1	308	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
49	2	314	KC2	CBD-CHA-C1A	2.91	134.31	128.88
50	J	302	A1EB1	C34-O4-C38	-2.91	112.47	117.90
49	G	313	KC2	C1A-NA-C4A	-2.91	105.40	106.71
39	b	811	CLA	CHB-C4A-NA	2.91	128.53	124.51
51	z	310	A1ECV	CMB-C2B-C1B	2.91	130.22	124.73
51	y	317	A1ECV	CMB-C2B-C1B	2.91	130.22	124.73
39	O	312	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
51	6	320	A1ECV	CMB-C2B-C1B	2.91	130.22	124.73
50	3	303	A1EB1	C34-O4-C38	-2.91	112.48	117.90
49	1	314	KC2	C2D-C1D-ND	-2.91	108.28	110.23
39	5	307	CLA	C3B-C4B-NB	-2.91	107.82	110.52
50	7	306	A1EB1	C4-C5-C6	-2.91	123.16	127.31
48	P	303	A86	C34-O4-C38	-2.91	112.48	117.90
48	6	309	A86	C33-C32-C31	2.91	112.04	109.21
46	7	301	LMG	O1-C1-C2	2.91	112.84	108.30
39	3	311	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
43	Q	303	DD6	C4-C5-C6	-2.91	123.16	127.31
52	P	305	A1EB4	C34-O4-C38	-2.91	112.48	117.90
39	b	823	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
39	5	308	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
39	f	803	CLA	C3B-C4B-NB	-2.91	107.82	110.52
46	S	322	LMG	O1-C1-C2	2.90	112.84	108.30
43	O	305	DD6	C14-C13-C11	-2.90	121.02	125.53
48	2	305	A86	C17-C16-C15	2.90	112.13	109.16
39	b	830	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
39	U	213	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
39	2	308	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
48	Z	303	A86	C24-C1-C2	2.90	123.40	118.94
49	V	318	KC2	CBD-CHA-C1A	2.90	134.29	128.88
50	V	307	A1EB1	C4-C3-C2	-2.90	117.53	123.47
39	0	315	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
50	J	302	A1EB1	C41-C32-C31	-2.90	107.88	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	Q	313	KC2	C2D-C1D-ND	-2.90	108.29	110.23
52	M	305	A1EB4	C12-C11-C13	2.90	120.17	115.30
39	8	313	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
39	6	315	CLA	CAA-C2A-C3A	-2.90	109.33	116.10
43	J	305	DD6	C25-C24-C1	-2.90	118.27	126.42
48	0	309	A86	C41-C32-C31	-2.90	107.88	110.47
39	H	316	CLA	CHB-C4A-NA	2.90	128.52	124.51
39	6	322	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
49	R	306	KC2	CHC-C4B-C3B	-2.90	120.30	125.26
47	4	327	SQD	C44-O6-C1	2.90	119.40	113.74
49	I	303	KC2	CHB-C4A-C3A	-2.90	120.45	124.98
39	D	315	CLA	C3B-C4B-NB	-2.90	107.83	110.52
39	9	320	CLA	C3B-C4B-NB	-2.90	107.83	110.52
39	i	101	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
39	2	319	CLA	C2A-C1A-CHA	2.90	128.93	123.86
47	F	318	SQD	O5-C5-C4	2.90	114.96	109.69
50	G	304	A1EB1	C4-C3-C2	-2.90	117.54	123.47
43	M	304	DD6	C3-C2-C1	-2.90	123.17	127.31
39	I	301	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
39	M	315	CLA	CAA-C2A-C3A	-2.90	109.34	116.10
47	P	301	SQD	C4-C3-C2	2.90	115.88	110.82
39	L	311	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
43	j	102	DD6	C4-C3-C2	-2.90	117.54	123.47
52	P	319	A1EB4	C25-C26-C27	-2.90	123.18	127.31
51	x	316	A1ECV	O2-CMC-C2C	2.90	119.22	112.27
39	a	813	CLA	CHB-C4A-NA	2.90	128.52	124.51
39	H	316	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
39	y	319	CLA	CMB-C2B-C1B	-2.89	120.96	125.37
39	H	315	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
39	a	803	CLA	C3B-C4B-NB	-2.89	107.83	110.52
39	a	824	CLA	C3B-C4B-NB	-2.89	107.83	110.52
39	Q	312	CLA	C3B-C4B-NB	-2.89	107.83	110.52
39	l	205	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
43	G	303	DD6	C37-C36-C31	-2.89	120.42	124.35
43	z	305	DD6	C15-C14-C13	-2.89	119.88	125.99
51	1	318	A1ECV	C4B-CHC-C1C	2.89	125.32	115.73
39	f	803	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
52	M	322	A1EB4	C25-C26-C27	-2.89	123.18	127.31
48	9	306	A86	C12-C11-C13	2.89	120.88	116.02
48	W	303	A86	C35-C34-C33	-2.89	104.83	109.88
39	8	322	CLA	CAA-C2A-C3A	-2.89	109.35	116.10
42	b	848	BCR	C20-C21-C22	-2.89	123.18	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	S	312	A1ECV	O1D-CGD-CBD	-2.89	119.92	124.74
49	0	317	KC2	C1A-NA-C4A	-2.89	105.41	106.71
42	k	204	BCR	C8-C7-C6	-2.89	119.08	127.20
39	7	315	CLA	C3B-C4B-NB	-2.89	107.83	110.52
51	6	320	A1ECV	O2-CMC-C2C	2.89	119.21	112.27
49	F	311	KC2	C2D-C1D-ND	-2.89	108.29	110.23
50	2	304	A1EB1	O6-C42-C44	2.89	120.98	111.91
39	a	825	CLA	CMB-C2B-C1B	-2.89	120.97	125.37
39	J	317	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
48	U	206	A86	C34-O4-C38	-2.89	112.51	117.90
39	X	316	CLA	C3B-C4B-NB	-2.89	107.83	110.52
43	J	304	DD6	C40-C32-C31	-2.89	105.88	110.47
47	P	301	SQD	O5-C5-C4	2.89	114.94	109.69
39	9	308	CLA	CHB-C4A-NA	2.89	128.50	124.51
49	G	315	KC2	CHC-C4B-C3B	-2.89	120.32	125.26
50	L	303	A1EB1	C41-C32-C31	-2.89	107.89	110.47
49	z	313	KC2	CHD-C1D-C2D	-2.89	119.08	127.24
39	3	319	CLA	CAA-C2A-C3A	-2.89	109.36	116.10
49	S	315	KC2	C2D-C1D-ND	-2.89	108.30	110.23
39	a	815	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
39	b	814	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
39	o	203	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
39	I	314	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
48	8	303	A86	C34-O4-C38	-2.88	112.52	117.90
39	3	316	CLA	CHB-C4A-NA	2.88	128.50	124.51
39	6	321	CLA	CAA-C2A-C3A	-2.88	109.37	116.10
39	b	821	CLA	C3B-C4B-NB	-2.88	107.84	110.52
39	k	202	CLA	C3B-C4B-NB	-2.88	107.84	110.52
39	W	316	CLA	CMA-C3A-C2A	-2.88	109.37	116.10
49	6	316	KC2	CBD-CHA-C1A	2.88	134.26	128.88
39	E	314	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
48	X	302	A86	C25-C24-C1	-2.88	118.32	126.42
50	6	304	A1EB1	O4-C38-O5	-2.88	117.23	122.96
43	Q	306	DD6	C37-C36-C31	-2.88	120.43	124.35
51	9	317	A1ECV	O1D-CGD-CBD	-2.88	119.94	124.74
50	T	307	A1EB1	C9-C8-C6	-2.88	118.32	126.42
50	4	301	A1EB1	O1-C20-C21	-2.88	111.60	115.06
39	b	816	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
39	H	313	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
39	W	311	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
39	I	313	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
39	2	307	CLA	O2D-CGD-O1D	-2.88	118.20	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	P	312	KC2	C2D-C1D-ND	-2.88	108.30	110.23
50	8	306	A1EB1	C3-C4-C5	-2.88	117.57	123.47
51	z	316	A1ECV	O2D-CGD-O1D	-2.88	118.20	123.84
39	C	309	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
51	x	316	A1ECV	CMB-C2B-C1B	2.88	130.17	124.73
39	G	309	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
51	S	318	A1ECV	CMA-C3A-C2A	2.88	130.07	124.68
49	L	312	KC2	CHB-C1B-C2B	-2.88	119.44	125.48
39	O	313	CLA	C3B-C4B-NB	-2.88	107.84	110.52
39	A	307	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
48	6	302	A86	C17-C16-C15	2.88	112.10	109.16
39	a	828	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
43	B	202	DD6	O1-C20-C21	-2.88	111.61	115.06
50	6	306	A1EB1	O1-C20-C21	-2.88	111.61	115.06
51	T	317	A1ECV	O1D-CGD-CBD	-2.88	119.94	124.74
39	Y	313	CLA	CAA-C2A-C3A	-2.88	109.38	116.10
39	E	316	CLA	C3B-C4B-NB	-2.88	107.84	110.52
49	B	208	KC2	CHB-C4A-C3A	-2.88	120.48	124.98
49	3	315	KC2	CBD-CHA-C1A	2.88	134.25	128.88
39	B	203	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
39	0	322	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
49	3	318	KC2	C2D-C1D-ND	-2.88	108.30	110.23
51	V	317	A1ECV	O1D-CGD-CBD	-2.88	119.95	124.74
39	F	314	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
39	8	321	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
47	W	301	SQD	O9-S-C6	2.88	110.36	106.94
47	k	205	SQD	O6-C1-C2	2.88	112.79	108.30
49	T	314	KC2	CBD-CHA-C1A	2.88	134.24	128.88
51	z	316	A1ECV	CMB-C2B-C1B	2.88	130.16	124.73
41	D	302	LHG	O8-C23-C24	2.87	120.93	111.91
39	b	840	CLA	C3B-C4B-NB	-2.87	107.85	110.52
49	4	317	KC2	C2D-C1D-ND	-2.87	108.31	110.23
50	8	304	A1EB1	C4-C3-C2	-2.87	117.59	123.47
39	b	839	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
39	F	308	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
39	7	313	CLA	C3B-C4B-NB	-2.87	107.85	110.52
43	Z	302	DD6	C37-C36-C35	2.87	119.68	114.36
49	W	314	KC2	C1D-ND-C4D	2.87	108.38	106.33
51	O	315	A1ECV	CMB-C2B-C1B	2.87	130.16	124.73
48	D	305	A86	C3-C4-C5	-2.87	117.59	123.47
39	o	202	CLA	C3B-C4B-NB	-2.87	107.85	110.52
39	2	312	CLA	C3B-C4B-NB	-2.87	107.85	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	b	824	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
39	j	101	CLA	CMB-C2B-C1B	-2.87	121.00	125.37
39	x	309	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
39	6	315	CLA	CMB-C2B-C1B	-2.87	121.00	125.37
39	a	810	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
48	y	306	A86	O4-C38-O5	-2.87	117.26	122.96
39	E	310	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
39	G	318	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
39	I	316	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
39	z	307	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
39	Y	303	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
48	4	305	A86	C41-C32-C31	-2.87	107.90	110.47
48	P	302	A86	C35-C34-C33	2.87	114.88	109.88
51	z	316	A1ECV	CMA-C3A-C2A	2.87	130.05	124.68
39	b	810	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
50	8	304	A1EB1	O4-C38-O5	-2.87	117.26	122.96
49	V	320	KC2	CHB-C4A-C3A	-2.87	120.50	124.98
39	9	308	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
42	h	202	BCR	C20-C21-C22	-2.87	123.22	127.31
52	W	321	A1EB4	C12-C11-C13	2.87	120.11	115.30
39	z	318	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
50	C	302	A1EB1	O6-C42-C44	2.87	120.90	111.91
39	O	318	CLA	CHB-C4A-NA	2.87	128.47	124.51
42	b	848	BCR	C24-C23-C22	-2.87	121.91	126.23
39	z	311	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
39	6	313	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
39	a	820	CLA	C3B-C4B-NB	-2.87	107.86	110.52
43	P	304	DD6	C9-C10-C11	-2.87	123.22	127.31
39	X	309	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
50	O	301	A1EB1	C34-O4-C38	-2.86	112.56	117.90
50	6	306	A1EB1	C34-O4-C38	-2.86	112.56	117.90
39	I	301	CLA	C3B-C4B-NB	-2.86	107.86	110.52
49	9	318	KC2	O1D-CGD-CBD	-2.86	118.62	124.48
39	J	316	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
39	Q	309	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
48	Z	303	A86	O1-C15-C14	-2.86	107.46	113.21
48	5	301	A86	C40-C32-C31	-2.86	107.91	110.47
49	3	317	KC2	C1A-NA-C4A	-2.86	105.42	106.71
48	4	306	A86	O1-C20-C21	-2.86	111.63	115.06
49	G	311	KC2	CBD-CHA-C1A	2.86	134.22	128.88
39	a	803	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
39	F	316	CLA	O2D-CGD-O1D	-2.86	118.24	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	9	308	CLA	O2D-CGD-CBD	2.86	116.35	111.27
39	b	826	CLA	C3B-C4B-NB	-2.86	107.86	110.52
43	V	303	DD6	C15-C14-C13	-2.86	119.94	125.99
50	E	301	A1EB1	O1-C15-C14	-2.86	107.47	113.21
39	a	820	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
50	J	302	A1EB1	O1-C20-C19	-2.86	111.23	113.38
39	9	320	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
49	P	306	KC2	C2D-C1D-ND	-2.86	108.31	110.23
39	2	316	CLA	CHB-C4A-NA	2.86	128.47	124.51
51	0	321	A1ECV	O1D-CGD-CBD	-2.86	119.98	124.74
39	Z	305	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
39	Z	315	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
51	S	318	A1ECV	CMB-C2B-C1B	2.86	130.13	124.73
39	G	309	CLA	C3B-C4B-NB	-2.86	107.86	110.52
43	M	304	DD6	C33-C34-C35	-2.86	106.39	110.30
39	S	316	CLA	CAA-C2A-C3A	-2.86	109.43	116.10
51	Z	314	A1ECV	C4B-CHC-C1C	2.86	125.20	115.73
39	l	204	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
39	z	306	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
49	7	322	KC2	CBD-CHA-C1A	2.86	134.21	128.88
39	2	319	CLA	CHB-C4A-NA	2.86	128.46	124.51
39	2	315	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
48	R	301	A86	O1-C20-C19	-2.86	111.24	113.38
39	K	312	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
39	9	307	CLA	C3B-C4B-NB	-2.86	107.86	110.52
43	x	304	DD6	C25-C24-C1	-2.86	118.39	126.42
51	X	310	A1ECV	CMB-C2B-C1B	2.86	130.12	124.73
39	U	210	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
43	4	307	DD6	C25-C24-C1	-2.86	118.39	126.42
49	A	313	KC2	C2D-C1D-ND	-2.86	108.32	110.23
39	b	828	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
48	5	301	A86	C9-C10-C11	-2.85	118.22	126.61
43	A	304	DD6	C14-C13-C11	-2.85	121.10	125.53
51	G	316	A1ECV	CMA-C3A-C2A	2.85	130.02	124.68
39	1	313	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
42	f	801	BCR	C28-C27-C26	-2.85	108.98	114.08
50	3	302	A1EB1	C41-C32-C31	-2.85	107.92	110.47
39	b	833	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
39	C	308	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
47	F	319	SQD	C44-O6-C1	2.85	119.31	113.74
49	W	314	KC2	CBD-CHA-C1A	2.85	134.20	128.88
39	U	211	CLA	C3B-C4B-NB	-2.85	107.87	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	P	311	CLA	CHB-C4A-NA	2.85	128.46	124.51
50	F	304	A1EB1	O4-C38-O5	-2.85	117.30	122.96
42	f	801	BCR	C20-C19-C18	-2.85	118.41	126.42
39	M	312	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
39	y	319	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
49	4	324	KC2	CHB-C4A-C3A	-2.85	120.53	124.98
43	2	303	DD6	C37-C36-C35	2.85	119.63	114.36
39	I	315	CLA	CHB-C4A-NA	2.85	128.45	124.51
49	K	310	KC2	C2D-C1D-ND	-2.85	108.32	110.23
39	1	313	CLA	CAA-C2A-C3A	-2.85	109.45	116.10
48	L	304	A86	C3-C2-C1	-2.85	123.24	127.31
49	8	319	KC2	O2D-CGD-O1D	-2.85	118.27	123.84
50	1	301	A1EB1	O6-C42-C44	2.85	120.85	111.91
39	J	310	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
39	A	312	CLA	C3B-C4B-NB	-2.85	107.87	110.52
39	W	313	CLA	CHB-C4A-NA	2.85	128.45	124.51
49	P	313	KC2	CBD-CHA-C1A	2.85	134.19	128.88
39	B	204	CLA	C3B-C4B-NB	-2.85	107.87	110.52
51	O	315	A1ECV	O2-CMC-C2C	2.85	119.10	112.27
39	a	825	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
39	D	314	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
51	9	317	A1ECV	CMB-C2B-C1B	2.84	130.10	124.73
39	h	201	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
49	z	312	KC2	CHC-C4B-C3B	-2.84	120.39	125.26
43	3	301	DD6	C25-C26-C27	-2.84	118.32	126.58
39	z	317	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
50	7	305	A1EB1	C33-C32-C31	2.84	111.97	109.21
39	y	307	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
48	7	307	A86	C17-C16-C15	2.84	112.06	109.16
39	b	838	CLA	C3B-C4B-NB	-2.84	107.88	110.52
43	o	204	DD6	C21-C20-C15	-2.84	117.50	122.26
42	b	850	BCR	C24-C23-C22	-2.84	121.94	126.23
43	J	304	DD6	C14-C13-C11	-2.84	121.12	125.53
39	U	215	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
50	8	306	A1EB1	C17-C16-C15	2.84	112.06	109.16
48	W	307	A86	C40-C32-C31	-2.84	107.93	110.47
39	A	309	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
39	G	310	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
39	a	838	CLA	CHB-C4A-NA	2.84	128.44	124.51
49	5	314	KC2	CBD-CHA-C1A	2.84	134.18	128.88
39	b	822	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
48	4	310	A86	C36-C31-C32	2.84	122.52	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	l	203	CLA	C3B-C4B-NB	-2.84	107.88	110.52
39	E	315	CLA	C3B-C4B-NB	-2.84	107.88	110.52
39	U	212	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
51	1	318	A1ECV	CMB-C2B-C1B	2.84	130.09	124.73
42	l	206	BCR	C3-C4-C5	-2.84	109.01	114.08
39	P	308	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
39	Y	302	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
39	U	201	CLA	C3B-C4B-NB	-2.84	107.88	110.52
39	H	306	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
50	z	302	A1EB1	O6-C42-C44	2.84	120.82	111.91
47	7	302	SQD	O8-S-C6	2.84	110.26	105.74
50	Q	323	A1EB1	C10-C9-C8	-2.84	114.36	123.22
39	a	813	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
39	8	310	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
51	T	317	A1ECV	O2-CMC-C2C	2.84	119.08	112.27
39	A	315	CLA	CHB-C4A-NA	2.84	128.44	124.51
50	Q	323	A1EB1	O6-C42-C44	2.84	120.81	111.91
39	L	311	CLA	C3B-C4B-NB	-2.84	107.88	110.52
39	5	315	CLA	C3B-C4B-NB	-2.84	107.88	110.52
39	M	308	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
48	V	301	A86	O4-C38-O5	-2.84	117.32	122.96
50	V	305	A1EB1	O6-C42-C44	2.84	120.81	111.91
43	M	304	DD6	C37-C36-C31	-2.84	120.49	124.35
39	Q	312	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
50	4	302	A1EB1	O1-C20-C21	-2.84	111.66	115.06
50	8	306	A1EB1	O4-C38-O5	-2.84	117.33	122.96
50	S	303	A1EB1	C41-C32-C31	-2.84	107.93	110.47
39	L	308	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
48	S	304	A86	C12-C11-C13	2.84	120.79	116.02
48	8	305	A86	C10-C9-C8	-2.84	114.36	123.22
39	a	805	CLA	CMB-C2B-C1B	-2.84	121.05	125.37
50	7	305	A1EB1	O4-C34-C35	2.84	114.66	107.59
51	4	315	A1ECV	O1D-CGD-CBD	-2.84	120.02	124.74
39	V	310	CLA	CHD-C1D-ND	-2.84	121.85	124.45
39	a	819	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
39	A	314	CLA	CHB-C4A-NA	2.84	128.43	124.51
39	W	316	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
39	2	316	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
39	b	829	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
39	O	310	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
39	y	318	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
43	x	304	DD6	C37-C36-C31	-2.83	120.50	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	E	303	DD6	C33-C34-C35	-2.83	106.42	110.30
39	b	841	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
39	W	313	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
43	1	304	DD6	C4-C3-C2	-2.83	117.67	123.47
51	Z	314	A1ECV	CMB-C2B-C1B	2.83	130.08	124.73
48	0	306	A86	C34-O4-C38	-2.83	112.62	117.90
49	S	314	KC2	CBD-CHA-C1A	2.83	134.16	128.88
43	H	303	DD6	C37-C36-C31	-2.83	120.50	124.35
50	V	305	A1EB1	O4-C38-O5	-2.83	117.33	122.96
39	a	805	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
39	J	311	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
39	K	314	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
43	X	304	DD6	C34-C35-C36	-2.83	106.21	111.85
51	5	312	A1ECV	CMA-C3A-C2A	2.83	129.98	124.68
39	o	205	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
49	1	315	KC2	C2D-C1D-ND	-2.83	108.33	110.23
51	5	309	A1ECV	CMB-C2B-C1B	2.83	130.08	124.73
50	2	306	A1EB1	O6-C42-C44	2.83	120.79	111.91
39	J	309	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
39	3	313	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
49	S	315	KC2	CBD-CHA-C1A	2.83	134.16	128.88
39	S	311	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
39	4	311	CLA	C3B-C4B-NB	-2.83	107.89	110.52
39	P	311	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
50	7	304	A1EB1	C40-C32-C31	-2.83	107.94	110.47
43	7	310	DD6	C15-C14-C13	-2.83	120.01	125.99
50	E	301	A1EB1	C28-C27-C26	-2.83	121.23	124.93
43	U	204	DD6	C10-C9-C8	-2.83	114.39	123.22
39	z	309	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
49	M	313	KC2	CBD-CHA-C1A	2.83	134.15	128.88
50	0	302	A1EB1	O6-C42-C44	2.83	120.78	111.91
47	M	301	SQD	O47-C7-O49	-2.83	116.87	123.70
39	Y	304	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
51	M	316	A1ECV	O2-CMC-O1	-2.83	117.92	123.45
43	G	306	DD6	C37-C36-C35	2.83	119.59	114.36
39	R	307	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
43	A	301	DD6	C3-C4-C5	-2.83	117.69	123.47
39	8	312	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
39	I	315	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
49	G	311	KC2	C2D-C1D-ND	-2.83	108.34	110.23
39	L	319	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
50	S	302	A1EB1	O4-C38-O5	-2.82	117.35	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Z	313	CLA	CHB-C4A-NA	2.82	128.42	124.51
49	H	311	KC2	C2D-C1D-ND	-2.82	108.34	110.23
48	3	307	A86	C9-C8-C6	-2.82	118.48	126.42
49	V	314	KC2	O1D-CGD-CBD	-2.82	118.71	124.48
39	a	811	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
48	4	306	A86	C40-C32-C31	-2.82	107.95	110.47
49	F	311	KC2	O1D-CGD-CBD	-2.82	118.71	124.48
49	5	305	KC2	C4D-C3D-CAD	2.82	109.32	107.42
39	T	310	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	x	306	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	b	842	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	U	201	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	0	310	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	1	316	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	S	319	CLA	CHB-C4A-NA	2.82	128.41	124.51
43	P	304	DD6	C14-C13-C11	-2.82	121.15	125.53
49	9	311	KC2	CBD-CHA-C1A	2.82	134.14	128.88
49	V	314	KC2	CHC-C4B-C3B	-2.82	120.43	125.26
48	P	302	A86	C9-C8-C6	-2.82	118.49	126.42
39	8	313	CLA	CAA-C2A-C3A	-2.82	109.52	116.10
49	6	319	KC2	CHB-C1B-C2B	-2.82	119.56	125.48
39	B	206	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
39	F	315	CLA	CHB-C4A-NA	2.82	128.41	124.51
42	a	844	BCR	C38-C26-C25	-2.82	121.36	124.53
49	B	208	KC2	O1D-CGD-CBD	-2.82	118.72	124.48
39	E	317	CLA	CHB-C4A-NA	2.82	128.41	124.51
45	b	849	DGD	CDB-CCB-CBB	-2.82	100.11	114.42
51	Z	314	A1ECV	O2-CMC-C2C	2.82	119.03	112.27
39	1	311	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
49	6	316	KC2	CHC-C4B-C3B	-2.82	120.44	125.26
51	X	313	A1ECV	C4B-CHC-C1C	2.82	125.06	115.73
39	Y	314	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
48	J	301	A86	C3-C2-C1	-2.82	123.29	127.31
49	I	312	KC2	O1D-CGD-CBD	-2.82	118.72	124.48
39	Z	313	CLA	CMC-C2C-C1C	-2.82	120.75	125.04
50	h	203	A1EB1	C34-O4-C38	-2.82	112.65	117.90
39	6	321	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
49	2	313	KC2	C2D-C1D-ND	-2.81	108.34	110.23
51	x	310	A1ECV	C4B-CHC-C1C	2.81	125.06	115.73
39	F	312	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
39	X	308	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
39	0	322	CLA	CHB-C4A-NA	2.81	128.40	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	307	A86	C34-O4-C38	-2.81	112.65	117.90
51	R	313	A1ECV	CMB-C2B-C1B	2.81	130.04	124.73
39	Z	306	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
49	R	312	KC2	C1D-ND-C4D	2.81	108.33	106.33
39	7	325	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
43	O	305	DD6	C37-C36-C31	-2.81	120.53	124.35
49	W	315	KC2	C2D-C1D-ND	-2.81	108.35	110.23
48	V	301	A86	C33-C32-C31	2.81	111.94	109.21
39	b	819	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
51	O	315	A1ECV	CMA-C3A-C2A	2.81	129.94	124.68
43	Q	306	DD6	O1-C20-C19	-2.81	111.27	113.38
39	Y	307	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
48	1	306	A86	C25-C26-C27	-2.81	123.30	127.31
49	C	312	KC2	C1D-ND-C4D	2.81	108.33	106.33
39	5	306	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
48	S	304	A86	C-C1-C2	-2.81	118.99	122.92
39	y	310	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
48	Z	303	A86	C40-C32-C31	-2.81	107.96	110.47
50	R	303	A1EB1	C41-C32-C31	-2.81	107.96	110.47
39	Q	311	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
39	U	211	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
42	a	843	BCR	C38-C26-C27	2.81	119.01	113.62
39	a	829	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
39	P	314	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
50	L	303	A1EB1	O6-C42-C44	2.81	120.72	111.91
48	6	305	A86	O1-C20-C21	-2.81	111.69	115.06
50	3	309	A1EB1	O6-C42-C44	2.81	120.72	111.91
49	V	314	KC2	CBD-CHA-C1A	2.81	134.12	128.88
39	a	817	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
39	Z	316	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
52	M	322	A1EB4	O3-C39-C43	2.81	120.72	111.91
48	2	302	A86	C34-O4-C38	-2.81	112.66	117.90
39	D	311	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
39	a	816	CLA	CHB-C1B-NB	2.81	127.23	124.26
49	5	314	KC2	C2D-C1D-ND	-2.81	108.35	110.23
39	A	306	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
39	a	847	CLA	C3B-C4B-NB	-2.81	107.91	110.52
39	6	321	CLA	C3B-C4B-NB	-2.81	107.91	110.52
39	E	313	CLA	CHB-C4A-NA	2.81	128.39	124.51
39	Z	316	CLA	CHB-C4A-NA	2.81	128.39	124.51
50	4	302	A1EB1	C17-C16-C15	2.81	112.03	109.16
48	1	303	A86	O1-C20-C19	-2.81	111.27	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B	206	CLA	C3B-C4B-NB	-2.81	107.91	110.52
51	7	323	A1ECV	CMB-C2B-C1B	2.81	130.03	124.73
49	L	314	KC2	C1D-ND-C4D	2.81	108.33	106.33
39	T	309	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
49	Y	308	KC2	CHB-C1B-C2B	-2.80	119.60	125.48
49	4	317	KC2	CBD-CHA-C1A	2.80	134.11	128.88
39	b	812	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
39	x	314	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
50	5	302	A1EB1	C33-C32-C31	2.80	111.94	109.21
39	a	822	CLA	CHB-C4A-NA	2.80	128.39	124.51
39	b	813	CLA	CHB-C4A-NA	2.80	128.39	124.51
39	0	323	CLA	CHB-C4A-NA	2.80	128.39	124.51
39	b	813	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
39	L	310	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
39	1	308	CLA	C3B-C4B-NB	-2.80	107.92	110.52
39	a	824	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
39	b	840	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
39	J	308	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
39	M	318	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
50	J	302	A1EB1	O1-C15-C14	-2.80	107.59	113.21
39	C	308	CLA	CHB-C4A-NA	2.80	128.39	124.51
51	X	310	A1ECV	O2-CMC-C2C	2.80	118.99	112.27
39	b	811	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
50	E	301	A1EB1	O6-C42-C44	2.80	120.70	111.91
39	R	307	CLA	CMB-C2B-C1B	-2.80	121.10	125.37
39	B	205	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
50	3	309	A1EB1	C4-C3-C2	-2.80	117.74	123.47
39	M	321	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
39	E	307	CLA	CHB-C1B-NB	2.80	127.22	124.26
48	4	328	A86	C33-C32-C31	2.80	111.93	109.21
51	T	317	A1ECV	CMA-C3A-C2A	2.80	129.92	124.68
51	G	316	A1ECV	C4B-CHC-C1C	2.80	125.00	115.73
48	0	308	A86	C21-C20-C19	2.80	117.43	114.28
39	b	802	CLA	CMB-C2B-C1B	-2.80	121.11	125.37
50	3	303	A1EB1	O1-C15-C14	-2.80	107.59	113.21
39	o	201	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
39	7	316	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
39	9	319	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
48	O	302	A86	C23-C16-C22	-2.80	103.24	107.37
49	G	317	KC2	O1D-CGD-CBD	-2.80	118.76	124.48
50	H	301	A1EB1	C12-C11-C13	2.80	120.72	116.02
39	O	318	CLA	O2D-CGD-O1D	-2.80	118.37	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	L	303	A1EB1	O4-C38-O5	-2.80	117.41	122.96
39	E	314	CLA	C3B-C4B-NB	-2.80	107.92	110.52
39	E	316	CLA	CHB-C4A-NA	2.80	128.38	124.51
52	P	319	A1EB4	O3-C39-C43	2.80	120.69	111.91
39	W	309	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
39	b	830	CLA	CHB-C1B-NB	2.80	127.22	124.26
48	M	303	A86	C35-C34-C33	2.80	114.75	109.88
48	8	309	A86	C25-C24-C1	-2.80	118.56	126.42
39	b	819	CLA	CHB-C4A-NA	2.80	128.38	124.51
39	b	820	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
39	K	311	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
39	I	311	CLA	CHB-C4A-NA	2.79	128.38	124.51
39	7	324	CLA	CAA-C2A-C3A	-2.79	109.58	116.10
39	z	318	CLA	CMB-C2B-C1B	-2.79	121.11	125.37
50	6	304	A1EB1	C40-C32-C31	-2.79	107.97	110.47
39	4	314	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
39	5	310	CLA	C3B-C4B-NB	-2.79	107.92	110.52
39	F	309	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
48	3	308	A86	C21-C20-C19	2.79	117.42	114.28
49	X	318	KC2	CBD-CHA-C1A	2.79	134.09	128.88
39	F	321	CLA	C3B-C4B-NB	-2.79	107.92	110.52
43	o	204	DD6	C37-C36-C31	-2.79	120.56	124.35
50	x	301	A1EB1	O4-C38-O5	-2.79	117.42	122.96
39	D	316	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
39	3	322	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
43	O	303	DD6	C10-C9-C8	-2.79	114.51	123.22
39	X	311	CLA	C3B-C4B-NB	-2.79	107.93	110.52
51	M	316	A1ECV	C4B-CHC-C1C	2.79	124.97	115.73
48	G	301	A86	C34-O4-C38	-2.79	112.70	117.90
39	b	842	CLA	C3B-C4B-NB	-2.79	107.93	110.52
39	I	309	CLA	C3B-C4B-NB	-2.79	107.93	110.52
51	W	317	A1ECV	O2-CMC-C2C	2.79	118.96	112.27
42	j	103	BCR	C10-C11-C12	-2.79	114.51	123.22
49	A	310	KC2	CHC-C4B-C3B	-2.79	120.49	125.26
39	W	309	CLA	C3B-C4B-NB	-2.79	107.93	110.52
39	o	202	CLA	CHB-C4A-NA	2.79	128.37	124.51
39	b	836	CLA	CHB-C1B-NB	2.79	127.21	124.26
43	J	306	DD6	C25-C24-C1	-2.79	118.58	126.42
39	Y	314	CLA	CHB-C4A-NA	2.79	128.37	124.51
39	H	312	CLA	C3B-C4B-NB	-2.79	107.93	110.52
39	K	308	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
39	Q	320	CLA	O2D-CGD-O1D	-2.79	118.39	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Q	321	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
39	b	815	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
49	M	311	KC2	C2D-C1D-ND	-2.79	108.36	110.23
39	F	321	CLA	CHB-C4A-NA	2.79	128.37	124.51
39	4	322	CLA	CHB-C4A-NA	2.79	128.37	124.51
39	U	208	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
39	R	311	CLA	C3B-C4B-NB	-2.79	107.93	110.52
39	0	320	CLA	C3B-C4B-NB	-2.79	107.93	110.52
50	R	303	A1EB1	C28-C27-C26	-2.79	121.29	124.93
39	C	304	CLA	C3B-C4B-NB	-2.78	107.93	110.52
39	D	315	CLA	CHB-C4A-NA	2.78	128.36	124.51
39	b	821	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
50	V	302	A1EB1	C28-C27-C26	-2.78	121.29	124.93
46	F	320	LMG	O8-C28-C29	2.78	120.64	111.91
43	M	304	DD6	C15-C14-C13	-2.78	120.11	125.99
43	X	304	DD6	C28-C27-C29	2.78	122.35	116.84
47	D	321	SQD	O8-S-C6	2.78	110.17	105.74
39	I	310	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
49	Q	313	KC2	O2D-CGD-O1D	-2.78	118.40	123.84
39	E	306	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
48	S	307	A86	C12-C11-C13	2.78	120.70	116.02
42	h	202	BCR	C7-C8-C9	-2.78	122.03	126.23
39	Z	312	CLA	CAA-C2A-C3A	-2.78	109.61	116.10
52	X	305	A1EB4	C3-C2-C1	-2.78	123.34	127.31
48	P	302	A86	O4-C38-O5	-2.78	117.44	122.96
47	M	301	SQD	O8-S-C6	2.78	110.17	105.74
48	M	306	A86	C12-C11-C13	2.78	120.69	116.02
49	S	314	KC2	C2D-C1D-ND	-2.78	108.37	110.23
49	5	311	KC2	C2D-C1D-ND	-2.78	108.37	110.23
39	K	307	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
51	O	315	A1ECV	C4B-CHC-C1C	2.78	124.94	115.73
39	E	318	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
39	b	803	CLA	CHB-C4A-NA	2.78	128.35	124.51
39	H	308	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
43	K	303	DD6	C37-C36-C31	-2.78	120.57	124.35
48	X	302	A86	C34-O4-C38	-2.78	112.72	117.90
39	x	308	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
46	W	302	LMG	C8-O7-C10	-2.78	110.95	117.79
43	W	305	DD6	C14-C13-C11	-2.78	121.22	125.53
39	J	313	CLA	CHB-C4A-NA	2.78	128.35	124.51
49	K	310	KC2	CBD-CHA-C1A	2.78	134.06	128.88
39	a	832	CLA	O2D-CGD-O1D	-2.78	118.41	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B	207	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
39	I	309	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
39	J	313	CLA	C3B-C4B-NB	-2.78	107.94	110.52
39	3	323	CLA	CHB-C4A-NA	2.78	128.35	124.51
48	y	306	A86	O1-C20-C21	-2.78	111.73	115.06
39	P	309	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
39	S	320	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
39	U	215	CLA	C3B-C4B-NB	-2.78	107.94	110.52
39	T	311	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
43	R	304	DD6	C34-C35-C36	-2.78	106.33	111.85
43	J	305	DD6	C37-C36-C35	2.77	119.50	114.36
39	F	321	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
50	U	205	A1EB1	O6-C42-C44	2.77	120.61	111.91
46	P	317	LMG	C8-O7-C10	-2.77	110.96	117.79
39	a	829	CLA	CHB-C4A-NA	2.77	128.35	124.51
51	X	313	A1ECV	CMB-C2B-C1B	2.77	129.97	124.73
49	9	318	KC2	CHB-C1B-C2B	-2.77	119.66	125.48
42	i	102	BCR	C2-C1-C6	2.77	114.75	110.48
39	E	319	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
49	X	312	KC2	O1D-CGD-CBD	-2.77	118.81	124.48
50	4	303	A1EB1	C4-C3-C2	-2.77	117.79	123.47
52	P	318	A1EB4	C21-C20-C15	-2.77	117.63	122.32
52	P	305	A1EB4	O3-C39-C43	2.77	120.61	111.91
48	6	309	A86	C4-C5-C6	-2.77	123.35	127.31
43	Q	306	DD6	C32-C31-C36	-2.77	118.72	122.63
49	T	314	KC2	C1A-NA-C4A	-2.77	105.46	106.71
39	2	318	CLA	CAA-C2A-C3A	-2.77	109.63	116.10
39	a	818	CLA	CHB-C4A-NA	2.77	128.34	124.51
39	b	818	CLA	C3B-C4B-NB	-2.77	107.94	110.52
39	J	309	CLA	C3B-C4B-NB	-2.77	107.94	110.52
48	O	307	A86	C4-C3-C2	-2.77	117.80	123.47
48	S	305	A86	C3-C4-C5	-2.77	117.80	123.47
39	D	310	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
50	G	307	A1EB1	C3-C2-C1	-2.77	123.36	127.31
39	a	836	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
39	b	822	CLA	CHB-C4A-NA	2.77	128.34	124.51
39	b	836	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
52	R	305	A1EB4	O3-C39-C43	2.77	120.59	111.91
39	Q	314	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
39	2	310	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
51	5	309	A1ECV	O2-CMC-C2C	2.77	118.91	112.27
39	1	311	CLA	CAA-C2A-C3A	-2.77	109.64	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	2	317	KC2	O1D-CGD-CBD	-2.77	118.82	124.48
50	6	308	A1EB1	O6-C42-C44	2.77	120.59	111.91
43	F	305	DD6	O1-C20-C19	-2.77	111.30	113.38
39	Q	314	CLA	CHB-C4A-NA	2.77	128.34	124.51
43	D	306	DD6	C9-C10-C11	-2.77	123.36	127.31
51	7	317	A1ECV	O2D-CGD-O1D	-2.77	118.43	123.84
39	A	305	CLA	C3B-C4B-NB	-2.76	107.95	110.52
39	k	201	CLA	O2A-CGA-O1A	-2.76	116.61	123.59
50	G	302	A1EB1	C33-C32-C31	2.76	111.90	109.21
39	J	316	CLA	CHB-C4A-NA	2.76	128.34	124.51
49	J	315	KC2	CBD-CHA-C1A	2.76	134.04	128.88
39	O	311	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
48	C	303	A86	C40-C32-C31	-2.76	108.00	110.47
49	F	307	KC2	O2D-CGD-CBD	2.76	116.18	111.27
48	B	201	A86	C4-C5-C6	-2.76	123.36	127.31
50	D	308	A1EB1	O6-C42-C44	2.76	120.58	111.91
42	b	846	BCR	C39-C30-C25	-2.76	105.82	110.30
39	b	819	CLA	C3B-C4B-NB	-2.76	107.95	110.52
39	f	802	CLA	C3B-C4B-NB	-2.76	107.95	110.52
39	I	313	CLA	C3B-C4B-NB	-2.76	107.95	110.52
51	S	318	A1ECV	C4B-CHC-C1C	2.76	124.89	115.73
46	7	326	LMG	O6-C1-O1	-2.76	103.43	109.97
39	L	313	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
39	a	817	CLA	CHB-C4A-NA	2.76	128.33	124.51
39	2	310	CLA	CHB-C4A-NA	2.76	128.33	124.51
51	y	311	A1ECV	C4B-CHC-C1C	2.76	124.88	115.73
47	F	319	SQD	C4-C3-C2	2.76	115.64	110.82
39	U	214	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
39	1	320	CLA	C3B-C4B-NB	-2.76	107.95	110.52
43	A	304	DD6	O1-C20-C21	-2.76	111.75	115.06
39	a	816	CLA	CMB-C2B-C1B	-2.76	121.16	125.37
50	x	301	A1EB1	O6-C42-C44	2.76	120.57	111.91
43	S	306	DD6	C19-C18-C17	2.76	116.11	110.77
39	T	318	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
39	W	319	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
52	W	306	A1EB4	O3-C39-C43	2.76	120.57	111.91
42	l	202	BCR	C34-C9-C10	-2.76	119.06	122.92
39	T	309	CLA	CMB-C2B-C1B	-2.76	121.17	125.37
50	7	303	A1EB1	C3-C4-C5	-2.76	117.82	123.47
39	x	307	CLA	CAA-C2A-C3A	-2.76	109.66	116.10
49	V	312	KC2	C2D-C1D-ND	-2.76	108.38	110.23
39	b	840	CLA	CHB-C4A-NA	2.76	128.33	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	5	311	KC2	O1D-CGD-CBD	-2.76	118.84	124.48
50	V	306	A1EB1	O6-C42-C44	2.76	120.57	111.91
43	z	305	DD6	C9-C10-C11	-2.76	123.37	127.31
49	G	315	KC2	CBD-CHA-C1A	2.76	134.03	128.88
50	1	305	A1EB1	O4-C38-O5	-2.76	117.48	122.96
52	X	305	A1EB4	C12-C11-C13	2.76	119.93	115.30
48	Z	301	A86	C25-C24-C1	-2.76	118.67	126.42
43	Q	303	DD6	C37-C36-C31	-2.76	120.60	124.35
46	D	322	LMG	O6-C1-O1	-2.76	103.44	109.97
43	5	303	DD6	C37-C36-C31	-2.76	120.60	124.35
39	J	318	CLA	CHB-C4A-NA	2.76	128.32	124.51
47	E	320	SQD	O8-S-C6	2.76	110.13	105.74
39	y	312	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
39	y	318	CLA	C3B-C4B-NB	-2.76	107.96	110.52
48	4	305	A86	C25-C26-C27	-2.76	123.38	127.31
48	U	202	A86	C34-O4-C38	-2.76	112.76	117.90
48	O	307	A86	C40-C32-C31	-2.76	108.00	110.47
39	D	312	CLA	C3B-C4B-NB	-2.76	107.96	110.52
39	M	309	CLA	CHB-C4A-NA	2.76	128.32	124.51
48	Q	305	A86	C4-C3-C2	-2.76	117.83	123.47
43	3	304	DD6	C37-C36-C35	2.76	119.46	114.36
39	b	808	CLA	CHB-C4A-NA	2.76	128.32	124.51
39	X	316	CLA	CHB-C4A-NA	2.76	128.32	124.51
49	M	313	KC2	CHD-C4C-NC	2.76	128.38	124.20
39	b	803	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
39	U	215	CLA	CHB-C4A-NA	2.75	128.32	124.51
39	7	314	CLA	CHB-C4A-NA	2.75	128.32	124.51
50	8	308	A1EB1	C33-C32-C31	2.75	111.89	109.21
50	R	303	A1EB1	O1-C20-C21	-2.75	111.76	115.06
39	S	309	CLA	C3B-C4B-NB	-2.75	107.96	110.52
49	Q	313	KC2	CHD-C4C-NC	2.75	128.38	124.20
48	3	308	A86	C12-C11-C13	2.75	120.65	116.02
39	O	318	CLA	CMB-C2B-C1B	-2.75	121.18	125.37
50	D	308	A1EB1	O4-C38-O5	-2.75	117.49	122.96
39	8	311	CLA	CHB-C4A-NA	2.75	128.32	124.51
39	D	313	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
39	Z	316	CLA	C3B-C4B-NB	-2.75	107.96	110.52
43	x	304	DD6	C10-C9-C8	-2.75	114.63	123.22
39	X	311	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
45	C	314	DGD	O6D-C1D-O3G	-2.75	103.46	109.97
39	R	315	CLA	CHB-C4A-NA	2.75	128.32	124.51
39	0	318	CLA	O2D-CGD-O1D	-2.75	118.46	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	6	310	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
49	0	317	KC2	C2D-C1D-ND	-2.75	108.39	110.23
48	U	206	A86	C9-C10-C11	-2.75	118.52	126.61
39	9	310	CLA	CMA-C3A-C2A	-2.75	109.68	116.10
48	W	303	A86	O1-C20-C21	-2.75	111.76	115.06
39	l	204	CLA	CHB-C4A-NA	2.75	128.31	124.51
39	a	837	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
39	6	315	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
48	8	305	A86	C7-C6-C5	-2.75	119.07	122.92
51	7	317	A1ECV	CMA-C3A-C2A	2.75	129.82	124.68
51	z	310	A1ECV	C4B-CHC-C1C	2.75	124.83	115.73
39	6	313	CLA	C3B-C4B-NB	-2.75	107.97	110.52
50	H	304	A1EB1	O6-C42-C44	2.75	120.53	111.91
51	5	309	A1ECV	C4B-CHC-C1C	2.75	124.83	115.73
50	U	203	A1EB1	O6-C42-C44	2.75	120.53	111.91
48	9	303	A86	C25-C26-C27	-2.75	123.39	127.31
39	Q	311	CLA	C3B-C4B-NB	-2.75	107.97	110.52
49	7	319	KC2	C2D-C1D-ND	-2.75	108.39	110.23
39	E	312	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
52	R	305	A1EB4	C4-C3-C2	-2.75	117.85	123.47
50	7	304	A1EB1	C34-O4-C38	-2.75	112.78	117.90
51	X	313	A1ECV	O2-CMC-O1	-2.75	118.08	123.45
39	K	311	CLA	CMB-C2B-C1B	-2.74	121.19	125.37
43	a	846	DD6	C33-C34-C35	-2.74	106.55	110.30
39	a	838	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
49	T	315	KC2	CBD-CHA-C1A	2.74	134.00	128.88
39	E	307	CLA	C3B-C4B-NB	-2.74	107.97	110.52
50	E	301	A1EB1	C25-C26-C27	-2.74	123.36	127.26
52	R	305	A1EB4	C3-C2-C1	-2.74	123.40	127.31
48	3	308	A86	C25-C24-C1	-2.74	118.71	126.42
48	Z	301	A86	C9-C8-C6	-2.74	118.71	126.42
50	8	304	A1EB1	C36-C31-C32	2.74	122.42	119.70
50	8	306	A1EB1	C33-C32-C31	2.74	111.88	109.21
39	D	319	CLA	CHB-C4A-NA	2.74	128.30	124.51
49	M	313	KC2	C1D-ND-C4D	2.74	108.28	106.33
49	6	314	KC2	CHB-C4A-C3A	-2.74	120.70	124.98
51	M	316	A1ECV	C2A-CAA-CBA	-2.74	122.45	128.63
49	5	313	KC2	C2D-C1D-ND	-2.74	108.39	110.23
39	1	316	CLA	C3B-C4B-NB	-2.74	107.97	110.52
39	F	313	CLA	CHB-C4A-NA	2.74	128.30	124.51
39	7	324	CLA	CHB-C4A-NA	2.74	128.30	124.51
39	Q	310	CLA	O2D-CGD-O1D	-2.74	118.48	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	4	316	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
48	B	201	A86	C40-C32-C31	-2.74	108.02	110.47
50	G	302	A1EB1	C17-C16-C15	2.74	111.96	109.16
39	M	321	CLA	CHB-C4A-NA	2.74	128.30	124.51
42	k	204	BCR	C3-C4-C5	-2.74	109.19	114.08
49	L	312	KC2	CHC-C4B-C3B	-2.74	120.57	125.26
39	K	309	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
39	E	315	CLA	CHB-C4A-NA	2.74	128.30	124.51
39	Z	313	CLA	CAA-C2A-C3A	-2.74	109.71	116.10
48	3	308	A86	O1-C20-C19	-2.74	111.33	113.38
49	6	317	KC2	C1D-ND-C4D	2.74	108.28	106.33
39	S	310	CLA	CHB-C4A-NA	2.74	128.30	124.51
49	G	315	KC2	O1D-CGD-CBD	-2.74	118.88	124.48
49	4	318	KC2	CBD-CHA-C1A	2.74	133.99	128.88
39	a	815	CLA	CHB-C4A-NA	2.74	128.30	124.51
39	a	809	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
39	1	317	CLA	C3B-C4B-NB	-2.74	107.98	110.52
39	x	306	CLA	C3B-C4B-NB	-2.74	107.98	110.52
43	I	306	DD6	C37-C36-C31	-2.74	120.63	124.35
48	y	305	A86	C36-C31-C32	2.74	122.41	119.70
49	P	312	KC2	O1D-CGD-CBD	-2.74	118.89	124.48
39	o	205	CLA	C3B-C4B-NB	-2.74	107.98	110.52
39	y	310	CLA	C3B-C4B-NB	-2.74	107.98	110.52
49	J	315	KC2	C2D-C1D-ND	-2.74	108.40	110.23
49	4	318	KC2	C2D-C1D-ND	-2.74	108.40	110.23
39	a	808	CLA	CHB-C4A-NA	2.74	128.29	124.51
39	6	322	CLA	CHB-C4A-NA	2.74	128.29	124.51
50	T	302	A1EB1	O6-C42-C44	2.74	120.49	111.91
39	Z	309	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
51	W	317	A1ECV	C4B-CHC-C1C	2.74	124.79	115.73
39	L	319	CLA	CHB-C4A-NA	2.73	128.29	124.51
39	O	316	CLA	CHB-C4A-NA	2.73	128.29	124.51
49	0	319	KC2	O1D-CGD-CBD	-2.73	118.89	124.48
43	V	303	DD6	C37-C36-C31	-2.73	120.63	124.35
39	O	313	CLA	CHB-C4A-NA	2.73	128.29	124.51
49	X	314	KC2	C2D-C1D-ND	-2.73	108.40	110.23
50	5	302	A1EB1	O6-C42-C44	2.73	120.49	111.91
51	7	317	A1ECV	O1D-CGD-CBD	-2.73	120.19	124.74
48	8	302	A86	C36-C31-C32	2.73	122.41	119.70
49	C	312	KC2	CBD-CHA-C1A	2.73	133.98	128.88
47	9	322	SQD	O8-S-C6	2.73	110.09	105.74
39	Y	310	CLA	C3B-C4B-NB	-2.73	107.98	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	M	315	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
39	a	828	CLA	CHB-C4A-NA	2.73	128.29	124.51
39	a	836	CLA	CHB-C4A-NA	2.73	128.29	124.51
39	b	818	CLA	CHB-C4A-NA	2.73	128.29	124.51
50	9	302	A1EB1	O6-C42-C44	2.73	120.48	111.91
39	b	837	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
39	J	313	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
39	3	316	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
39	4	322	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
39	1	313	CLA	C3B-C4B-NB	-2.73	107.98	110.52
39	8	315	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
51	T	317	A1ECV	O2-CMC-O1	-2.73	118.11	123.45
39	2	319	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
51	2	311	A1ECV	O2D-CGD-O1D	-2.73	118.50	123.84
51	R	310	A1ECV	C4B-CHC-C1C	2.73	124.78	115.73
39	a	828	CLA	C3B-C4B-NB	-2.73	107.98	110.52
39	b	806	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
43	j	102	DD6	C37-C36-C31	-2.73	120.64	124.35
51	y	317	A1ECV	C2A-CAA-CBA	-2.73	122.47	128.63
48	Q	302	A86	C41-C32-C31	-2.73	108.03	110.47
39	R	308	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
51	Z	314	A1ECV	CMA-C3A-C2A	2.73	129.78	124.68
50	V	305	A1EB1	C3-C4-C5	-2.73	117.88	123.47
39	L	316	CLA	C3B-C4B-NB	-2.73	107.98	110.52
49	K	310	KC2	C1A-NA-C4A	-2.73	105.48	106.71
49	6	319	KC2	CHC-C4B-C3B	-2.73	120.59	125.26
51	T	317	A1ECV	CMB-C2B-C1B	2.73	129.88	124.73
51	V	317	A1ECV	C4B-CHC-C1C	2.73	124.77	115.73
46	W	320	LMG	O6-C1-O1	-2.73	103.51	109.97
39	M	318	CLA	CHB-C4A-NA	2.73	128.28	124.51
43	I	306	DD6	C15-C14-C13	-2.73	120.23	125.99
49	G	317	KC2	CHB-C4A-C3A	-2.73	120.72	124.98
39	O	310	CLA	CHB-C1B-NB	2.73	127.14	124.26
39	b	809	CLA	CHB-C4A-NA	2.73	128.28	124.51
49	9	313	KC2	C2D-C1D-ND	-2.73	108.40	110.23
50	4	301	A1EB1	C4-C5-C6	-2.73	123.42	127.31
39	b	814	CLA	CHB-C4A-NA	2.73	128.28	124.51
39	F	312	CLA	CHB-C4A-NA	2.73	128.28	124.51
49	8	317	KC2	O1D-CGD-CBD	-2.73	118.91	124.48
39	a	810	CLA	C3B-C4B-NB	-2.73	107.99	110.52
50	z	301	A1EB1	O1-C20-C21	-2.73	111.79	115.06
48	Q	304	A86	C-C1-C2	-2.73	119.11	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	1	313	CLA	CHB-C4A-NA	2.73	128.28	124.51
43	j	102	DD6	C33-C34-C35	-2.73	106.57	110.30
49	T	314	KC2	C1D-ND-C4D	2.73	108.27	106.33
39	z	308	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
48	k	206	A86	C34-O4-C38	-2.72	112.82	117.90
39	a	834	CLA	CHB-C4A-NA	2.72	128.28	124.51
39	b	817	CLA	CHB-C4A-NA	2.72	128.28	124.51
39	O	309	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
48	L	305	A86	C40-C32-C31	-2.72	108.03	110.47
49	G	315	KC2	C2D-C1D-ND	-2.72	108.41	110.23
49	P	310	KC2	C2D-C1D-ND	-2.72	108.41	110.23
49	P	320	KC2	C2D-C1D-ND	-2.72	108.41	110.23
39	5	315	CLA	CHB-C4A-NA	2.72	128.28	124.51
50	7	303	A1EB1	O4-C38-O5	-2.72	117.55	122.96
50	O	301	A1EB1	C12-C11-C13	2.72	120.60	116.02
49	G	313	KC2	C2D-C1D-ND	-2.72	108.41	110.23
39	8	310	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
50	6	301	A1EB1	C12-C11-C10	-2.72	116.84	123.42
43	A	303	DD6	C13-C11-C10	2.72	123.12	118.94
39	J	307	CLA	CHB-C4A-NA	2.72	128.28	124.51
50	x	301	A1EB1	O1-C15-C14	-2.72	107.75	113.21
39	T	320	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
48	9	305	A86	C25-C26-C27	-2.72	123.43	127.31
39	a	806	CLA	CHB-C4A-NA	2.72	128.27	124.51
39	Z	307	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
39	2	315	CLA	CAA-C2A-C3A	-2.72	109.75	116.10
43	X	304	DD6	C3-C2-C1	-2.72	123.43	127.31
43	z	304	DD6	C32-C31-C36	-2.72	118.79	122.63
39	b	832	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
39	b	833	CLA	CHB-C4A-NA	2.72	128.27	124.51
48	4	305	A86	C34-O4-C38	-2.72	112.83	117.90
51	R	313	A1ECV	O1D-CGD-CBD	-2.72	120.21	124.74
39	U	213	CLA	CHB-C4A-NA	2.72	128.27	124.51
43	j	102	DD6	C21-C20-C15	-2.72	117.70	122.26
39	S	316	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
39	a	833	CLA	CHB-C4A-NA	2.72	128.27	124.51
39	R	309	CLA	CHB-C4A-NA	2.72	128.27	124.51
42	b	845	BCR	C30-C25-C26	-2.72	118.78	122.61
39	S	308	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
40	b	843	PQN	C2M-C2-C1	2.72	120.78	116.27
49	x	313	KC2	C2D-C1D-ND	-2.72	108.41	110.23
39	o	206	CLA	O2D-CGD-O1D	-2.72	118.53	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	F	318	SQD	O8-S-C6	2.72	110.07	105.74
51	9	317	A1ECV	CMA-C3A-C2A	2.72	129.76	124.68
39	F	306	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
39	X	307	CLA	C3B-C4B-NB	-2.72	108.00	110.52
49	T	314	KC2	CHD-C4C-NC	2.72	128.32	124.20
39	9	310	CLA	CHB-C4A-NA	2.72	128.27	124.51
51	R	313	A1ECV	C3-O2-CMC	2.72	121.07	115.83
49	R	314	KC2	C2D-C1D-ND	-2.71	108.41	110.23
49	3	315	KC2	CHB-C4A-C3A	-2.71	120.74	124.98
48	T	305	A86	C34-O4-C38	-2.71	112.84	117.90
43	y	303	DD6	C9-C10-C11	-2.71	123.44	127.31
48	G	305	A86	C33-C32-C31	2.71	111.85	109.21
48	B	201	A86	C12-C11-C13	2.71	120.58	116.02
39	a	847	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
39	8	322	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
48	3	307	A86	C21-C20-C19	2.71	117.33	114.28
46	0	324	LMG	O8-C28-C29	2.71	120.42	111.91
49	V	312	KC2	C1A-NA-C4A	-2.71	105.49	106.71
49	6	314	KC2	C1A-NA-C4A	-2.71	105.49	106.71
49	Q	315	KC2	C2D-C1D-ND	-2.71	108.41	110.23
42	b	845	BCR	C38-C26-C27	2.71	118.83	113.62
49	z	312	KC2	CBD-CHA-C1A	2.71	133.94	128.88
48	8	307	A86	C21-C20-C19	2.71	117.33	114.28
39	9	310	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
50	6	308	A1EB1	O4-C38-O5	-2.71	117.57	122.96
39	W	318	CLA	CHB-C4A-NA	2.71	128.26	124.51
39	1	319	CLA	CHB-C4A-NA	2.71	128.26	124.51
48	L	305	A86	C34-O4-C38	-2.71	112.84	117.90
39	E	309	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
49	M	307	KC2	CHB-C4A-C3A	-2.71	120.74	124.98
51	9	314	A1ECV	CMB-C2B-C1B	2.71	129.85	124.73
39	b	822	CLA	C3B-C4B-NB	-2.71	108.00	110.52
39	T	308	CLA	C3B-C4B-NB	-2.71	108.00	110.52
49	5	305	KC2	CHD-C4C-NC	2.71	128.32	124.20
39	z	306	CLA	C3B-C4B-NB	-2.71	108.00	110.52
39	b	835	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
39	5	310	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
43	3	304	DD6	C4-C3-C2	-2.71	117.92	123.47
51	y	311	A1ECV	O2D-CGD-O1D	-2.71	118.54	123.84
43	D	306	DD6	C10-C9-C8	-2.71	114.76	123.22
50	6	308	A1EB1	C17-C16-C15	2.71	111.93	109.16
39	7	313	CLA	O2D-CGD-O1D	-2.71	118.54	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	X	306	KC2	CHC-C4B-C3B	-2.71	120.62	125.26
43	W	305	DD6	C15-C14-C13	-2.71	120.27	125.99
39	J	312	CLA	CHB-C4A-NA	2.71	128.26	124.51
39	M	315	CLA	CHB-C4A-NA	2.71	128.26	124.51
50	9	302	A1EB1	C4-C3-C2	-2.71	117.92	123.47
51	5	312	A1ECV	O2-CMC-O1	-2.71	118.16	123.45
39	b	816	CLA	C3B-C4B-NB	-2.71	108.00	110.52
39	G	314	CLA	C3B-C4B-NB	-2.71	108.00	110.52
39	7	324	CLA	C3B-C4B-NB	-2.71	108.00	110.52
48	L	304	A86	C17-C16-C15	2.71	111.92	109.16
42	f	804	BCR	C38-C26-C25	-2.71	121.49	124.53
43	H	305	DD6	C21-C20-C15	-2.71	117.72	122.26
39	H	310	CLA	CHB-C4A-NA	2.71	128.25	124.51
39	M	317	CLA	CHB-C4A-NA	2.71	128.25	124.51
39	O	310	CLA	C3B-C4B-NB	-2.71	108.00	110.52
49	8	316	KC2	C2D-C1D-ND	-2.71	108.42	110.23
39	5	307	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
39	P	307	CLA	C3B-C4B-NB	-2.71	108.00	110.52
51	S	312	A1ECV	CMA-C3A-C2A	2.71	129.74	124.68
39	X	309	CLA	CHB-C4A-NA	2.71	128.25	124.51
39	W	310	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
39	4	313	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
39	V	313	CLA	CHB-C4A-NA	2.70	128.25	124.51
39	x	309	CLA	CHB-C4A-NA	2.70	128.25	124.51
50	G	308	A1EB1	O6-C42-C44	2.70	120.39	111.91
39	b	806	CLA	C3B-C4B-NB	-2.70	108.01	110.52
51	5	309	A1ECV	CMA-C3A-C2A	2.70	129.74	124.68
49	T	315	KC2	C2D-C1D-ND	-2.70	108.42	110.23
43	X	304	DD6	C14-C13-C11	-2.70	121.33	125.53
39	S	313	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
50	Q	307	A1EB1	C41-C32-C31	-2.70	108.05	110.47
47	7	302	SQD	C44-O6-C1	2.70	119.02	113.74
39	a	834	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
51	4	315	A1ECV	O2D-CGD-O1D	-2.70	118.55	123.84
46	W	302	LMG	O8-C28-C29	2.70	120.39	111.91
50	K	304	A1EB1	O6-C42-C44	2.70	120.39	111.91
43	x	303	DD6	C25-C24-C1	-2.70	118.82	126.42
39	Z	313	CLA	CMC-C2C-C3C	2.70	133.46	126.12
51	L	318	A1ECV	CHC-C4B-C3B	-2.70	122.34	126.66
39	5	316	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
43	S	306	DD6	C25-C26-C27	-2.70	118.73	126.58
43	O	304	DD6	C14-C13-C11	-2.70	121.34	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	V	303	DD6	C33-C34-C35	-2.70	106.61	110.30
43	J	304	DD6	C7-C6-C5	-2.70	119.14	122.92
46	P	317	LMG	O8-C28-C29	2.70	120.38	111.91
39	3	312	CLA	CHB-C4A-NA	2.70	128.25	124.51
39	C	306	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
50	z	301	A1EB1	C4-C3-C2	-2.70	117.94	123.47
51	R	310	A1ECV	CMB-C2B-C1B	2.70	129.83	124.73
39	I	310	CLA	CHB-C4A-NA	2.70	128.25	124.51
45	C	314	DGD	C3G-C2G-C1G	-2.70	105.40	111.79
50	S	303	A1EB1	O6-C42-C44	2.70	120.38	111.91
43	J	306	DD6	C9-C8-C6	-2.70	118.83	126.42
42	b	845	BCR	C15-C16-C17	-2.70	117.94	123.47
39	Q	311	CLA	CHB-C4A-NA	2.70	128.25	124.51
39	6	315	CLA	CHB-C4A-NA	2.70	128.25	124.51
49	W	315	KC2	CHC-C4B-C3B	-2.70	120.64	125.26
39	6	312	CLA	C3B-C4B-NB	-2.70	108.01	110.52
39	E	306	CLA	CHB-C4A-NA	2.70	128.24	124.51
47	F	319	SQD	O6-C1-C2	2.70	112.52	108.30
48	H	302	A86	O1-C20-C21	-2.70	111.82	115.06
39	B	207	CLA	CHB-C4A-NA	2.70	128.24	124.51
50	h	203	A1EB1	C33-C32-C31	2.70	111.83	109.21
39	x	317	CLA	CAA-C2A-C3A	-2.70	109.80	116.10
48	K	301	A86	C3-C4-C5	-2.70	117.95	123.47
50	Q	307	A1EB1	O6-C42-C44	2.70	120.37	111.91
50	4	303	A1EB1	O6-C42-C44	2.70	120.37	111.91
52	W	321	A1EB4	O3-C39-C43	2.70	120.37	111.91
43	2	303	DD6	C9-C8-C6	-2.70	118.84	126.42
49	0	314	KC2	C2D-C1D-ND	-2.70	108.42	110.23
39	H	306	CLA	CHB-C4A-NA	2.70	128.24	124.51
39	b	831	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
39	4	311	CLA	O2A-CGA-O1A	-2.70	116.79	123.59
50	9	302	A1EB1	C3-C2-C1	-2.70	123.46	127.31
48	9	303	A86	C26-C25-C24	-2.70	114.80	123.22
43	J	306	DD6	C37-C36-C35	2.70	119.35	114.36
39	9	319	CLA	CHB-C4A-NA	2.70	128.24	124.51
39	5	306	CLA	C3B-C4B-NB	-2.70	108.01	110.52
49	X	312	KC2	C1A-NA-C4A	-2.70	105.49	106.71
39	H	307	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
39	b	827	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
43	X	304	DD6	O1-C20-C21	-2.69	111.83	115.06
39	a	817	CLA	C3B-C4B-NB	-2.69	108.02	110.52
39	a	823	CLA	C3B-C4B-NB	-2.69	108.02	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	z	305	DD6	C37-C36-C31	-2.69	120.69	124.35
49	8	320	KC2	O1D-CGD-CBD	-2.69	118.97	124.48
42	f	801	BCR	C33-C5-C6	-2.69	121.50	124.53
39	1	319	CLA	C3B-C4B-NB	-2.69	108.02	110.52
39	Z	304	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
39	D	317	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
39	K	314	CLA	CAA-C2A-C3A	-2.69	109.81	116.10
39	8	315	CLA	CHB-C4A-NA	2.69	128.24	124.51
39	I	309	CLA	CHB-C4A-NA	2.69	128.23	124.51
39	U	212	CLA	C3B-C4B-NB	-2.69	108.02	110.52
39	b	807	CLA	CMB-C2B-C1B	-2.69	121.27	125.37
39	F	310	CLA	CHB-C4A-NA	2.69	128.23	124.51
39	x	309	CLA	C3B-C4B-NB	-2.69	108.02	110.52
39	y	312	CLA	C3B-C4B-NB	-2.69	108.02	110.52
48	J	301	A86	C33-C32-C31	2.69	111.83	109.21
49	T	312	KC2	O1D-CGD-CBD	-2.69	118.98	124.48
39	a	821	CLA	CHB-C4A-NA	2.69	128.23	124.51
39	Y	304	CLA	CHB-C4A-NA	2.69	128.23	124.51
51	S	312	A1ECV	O2D-CGD-O1D	-2.69	118.58	123.84
39	b	807	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
39	4	323	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
39	o	206	CLA	CHB-C4A-NA	2.69	128.23	124.51
39	L	316	CLA	CHB-C4A-NA	2.69	128.23	124.51
47	W	301	SQD	C44-O6-C1	2.69	118.99	113.74
43	E	302	DD6	C33-C34-C35	-2.69	106.62	110.30
49	Y	309	KC2	C2D-C1D-ND	-2.69	108.43	110.23
39	J	307	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
39	x	311	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
39	z	314	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
49	T	312	KC2	O2D-CGD-O1D	-2.69	118.58	123.84
49	3	317	KC2	CHC-C4B-C3B	-2.69	120.66	125.26
42	b	848	BCR	C16-C15-C14	-2.69	117.97	123.47
39	o	201	CLA	CHB-C4A-NA	2.69	128.23	124.51
39	y	318	CLA	CHB-C4A-NA	2.69	128.23	124.51
39	J	308	CLA	C3B-C4B-NB	-2.69	108.02	110.52
39	a	831	CLA	CHB-C4A-NA	2.69	128.23	124.51
39	A	309	CLA	CHB-C4A-NA	2.69	128.23	124.51
39	y	315	CLA	CHB-C4A-NA	2.69	128.23	124.51
42	f	801	BCR	C11-C10-C9	-2.69	123.48	127.31
39	O	312	CLA	CHB-C4A-NA	2.69	128.22	124.51
39	U	211	CLA	CHB-C4A-NA	2.69	128.22	124.51
39	Z	306	CLA	CHB-C4A-NA	2.69	128.22	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	2	314	KC2	C1A-NA-C4A	-2.68	105.50	106.71
43	S	306	DD6	C25-C24-C1	-2.68	118.87	126.42
39	E	310	CLA	CHB-C4A-NA	2.68	128.22	124.51
43	I	305	DD6	C14-C13-C11	-2.68	121.36	125.53
39	A	312	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
39	b	815	CLA	C3B-C4B-NB	-2.68	108.03	110.52
39	b	807	CLA	C3B-C4B-NB	-2.68	108.03	110.52
39	A	311	CLA	CHB-C4A-NA	2.68	128.22	124.51
43	4	307	DD6	C37-C36-C35	2.68	119.33	114.36
49	G	315	KC2	C2A-C3A-C4A	2.68	108.48	106.49
39	B	203	CLA	CHB-C4A-NA	2.68	128.22	124.51
39	7	318	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
39	l	205	CLA	C3B-C4B-NB	-2.68	108.03	110.52
39	E	306	CLA	C3B-C4B-NB	-2.68	108.03	110.52
39	L	309	CLA	CHB-C4A-NA	2.68	128.22	124.51
39	P	316	CLA	CHB-C4A-NA	2.68	128.22	124.51
39	T	318	CLA	CHB-C4A-NA	2.68	128.22	124.51
39	z	317	CLA	CHB-C4A-NA	2.68	128.22	124.51
50	J	302	A1EB1	O6-C42-C44	2.68	120.32	111.91
48	2	305	A86	C9-C8-C6	-2.68	118.88	126.42
43	A	301	DD6	C33-C34-C35	-2.68	106.63	110.30
49	L	317	KC2	C2D-C1D-ND	-2.68	108.44	110.23
49	G	311	KC2	C1A-NA-C4A	-2.68	105.50	106.71
48	9	305	A86	C12-C11-C13	2.68	120.52	116.02
50	L	303	A1EB1	C17-C16-C15	2.68	111.90	109.16
48	3	307	A86	C35-C34-C33	2.68	114.55	109.88
43	I	305	DD6	C37-C36-C31	-2.68	120.71	124.35
39	b	816	CLA	CHB-C4A-NA	2.68	128.22	124.51
39	b	835	CLA	CHB-C4A-NA	2.68	128.22	124.51
39	b	838	CLA	CHB-C4A-NA	2.68	128.22	124.51
49	y	313	KC2	C2D-C1D-ND	-2.68	108.44	110.23
39	Y	305	CLA	C3B-C4B-NB	-2.68	108.03	110.52
39	X	307	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
43	K	303	DD6	C14-C13-C11	-2.68	121.37	125.53
48	O	306	A86	C34-O4-C38	-2.68	112.91	117.90
49	W	312	KC2	C2D-C1D-ND	-2.68	108.44	110.23
48	M	306	A86	C40-C32-C31	-2.68	108.08	110.47
48	M	306	A86	O1-C15-C14	-2.68	107.84	113.21
39	Y	311	CLA	CAA-C2A-C3A	-2.68	109.85	116.10
50	4	302	A1EB1	C28-C27-C26	-2.68	121.43	124.93
48	4	309	A86	C36-C31-C32	2.68	122.35	119.70
50	U	205	A1EB1	C12-C11-C13	2.68	120.52	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	6	313	CLA	CHB-C4A-NA	2.68	128.21	124.51
52	M	322	A1EB4	C-C1-C2	-2.68	119.17	122.92
50	6	306	A1EB1	C12-C11-C13	2.68	120.52	116.02
46	M	319	LMG	O8-C28-C29	2.67	120.30	111.91
51	Y	312	A1ECV	C4B-CHC-C1C	2.67	124.59	115.73
50	G	304	A1EB1	O6-C42-C44	2.67	120.30	111.91
49	S	315	KC2	CHB-C4A-C3A	-2.67	120.80	124.98
39	D	311	CLA	CHB-C4A-NA	2.67	128.21	124.51
43	3	301	DD6	C37-C36-C35	2.67	119.31	114.36
50	S	302	A1EB1	O6-C42-C44	2.67	120.30	111.91
39	l	204	CLA	CHD-C1D-ND	-2.67	122.00	124.45
39	7	321	CLA	CHB-C4A-NA	2.67	128.21	124.51
48	R	301	A86	C35-C34-C33	2.67	114.54	109.88
49	L	321	KC2	O1D-CGD-CBD	-2.67	119.01	124.48
49	8	320	KC2	C2D-C1D-ND	-2.67	108.44	110.23
39	D	318	CLA	CHB-C4A-NA	2.67	128.21	124.51
39	y	307	CLA	C3B-C4B-NB	-2.67	108.04	110.52
39	Q	320	CLA	CHB-C4A-NA	2.67	128.21	124.51
39	U	208	CLA	CHB-C4A-NA	2.67	128.21	124.51
50	7	306	A1EB1	C28-C27-C26	-2.67	121.44	124.93
48	R	302	A86	C9-C10-C11	-2.67	118.75	126.61
43	4	307	DD6	C9-C10-C11	-2.67	123.50	127.31
49	C	312	KC2	C1A-NA-C4A	-2.67	105.50	106.71
39	L	313	CLA	CHB-C4A-NA	2.67	128.21	124.51
49	V	312	KC2	CHB-C4A-C3A	-2.67	120.81	124.98
39	Z	305	CLA	C3B-C4B-NB	-2.67	108.04	110.52
39	V	309	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
43	D	307	DD6	C4-C3-C2	-2.67	118.00	123.47
39	R	308	CLA	C3B-C4B-NB	-2.67	108.04	110.52
43	4	307	DD6	C3-C4-C5	-2.67	118.00	123.47
43	Z	302	DD6	C9-C8-C6	-2.67	118.92	126.42
50	S	303	A1EB1	O4-C38-O5	-2.67	117.66	122.96
50	0	302	A1EB1	C33-C32-C31	2.67	111.81	109.21
39	0	310	CLA	C3B-C4B-NB	-2.67	108.04	110.52
49	7	320	KC2	C2D-C1D-ND	-2.67	108.44	110.23
49	6	314	KC2	C2D-C1D-ND	-2.67	108.44	110.23
39	b	824	CLA	CHB-C4A-NA	2.67	128.20	124.51
39	P	308	CLA	CHB-C4A-NA	2.67	128.20	124.51
39	i	103	CLA	C3B-C4B-NB	-2.67	108.04	110.52
43	G	306	DD6	C4-C3-C2	-2.67	118.01	123.47
39	a	819	CLA	CHB-C4A-NA	2.67	128.20	124.51
49	V	320	KC2	O1D-CGD-CBD	-2.67	119.03	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	X	318	KC2	C1A-NA-C4A	-2.67	105.51	106.71
39	U	207	CLA	C3B-C4B-NB	-2.67	108.04	110.52
46	F	317	LMG	O8-C28-C29	2.67	120.28	111.91
48	R	301	A86	C12-C11-C13	2.67	120.50	116.02
48	D	305	A86	C4-C5-C6	-2.67	123.50	127.31
39	a	807	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
39	b	810	CLA	C3B-C4B-NB	-2.67	108.04	110.52
50	O	301	A1EB1	C3-C4-C5	-2.67	118.01	123.47
48	W	307	A86	C35-C34-C33	2.67	114.53	109.88
50	x	301	A1EB1	O1-C20-C19	-2.67	111.38	113.38
48	O	302	A86	C40-C32-C31	-2.66	108.09	110.47
48	7	307	A86	O4-C38-O5	-2.66	117.67	122.96
39	a	803	CLA	CHB-C4A-NA	2.66	128.20	124.51
39	b	814	CLA	C3B-C4B-NB	-2.66	108.04	110.52
50	7	304	A1EB1	C17-C16-C15	2.66	111.88	109.16
50	6	301	A1EB1	C-C1-C2	-2.66	119.19	122.92
39	a	832	CLA	CHB-C4A-NA	2.66	128.20	124.51
50	V	306	A1EB1	C33-C32-C31	-2.66	106.62	109.21
49	G	313	KC2	C1A-C2A-C3A	-2.66	105.00	107.11
39	E	318	CLA	C3B-C4B-NB	-2.66	108.04	110.52
39	Y	310	CLA	CHB-C4A-NA	2.66	128.19	124.51
39	b	802	CLA	CHD-C1D-ND	-2.66	122.01	124.45
39	a	814	CLA	CHB-C4A-NA	2.66	128.19	124.51
43	O	305	DD6	C33-C34-C35	-2.66	106.66	110.30
39	a	810	CLA	CHB-C4A-NA	2.66	128.19	124.51
39	3	320	CLA	CHB-C4A-NA	2.66	128.19	124.51
39	3	322	CLA	CHB-C4A-NA	2.66	128.19	124.51
43	F	305	DD6	C-C1-C2	-2.66	119.20	122.92
43	Q	303	DD6	C20-C19-C18	-2.66	107.49	112.75
51	x	316	A1ECV	C2A-CAA-CBA	-2.66	122.63	128.63
42	a	845	BCR	C38-C26-C25	-2.66	121.54	124.53
52	M	322	A1EB4	O4-C38-O43	-2.66	117.68	122.96
39	X	307	CLA	CHB-C4A-NA	2.66	128.19	124.51
39	x	306	CLA	CHB-C4A-NA	2.66	128.19	124.51
49	W	308	KC2	CHD-C4C-NC	2.66	128.24	124.20
47	S	301	SQD	O9-S-C6	2.66	110.10	106.94
39	7	314	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
48	P	303	A86	C17-C16-C15	2.66	111.88	109.16
39	0	312	CLA	CHB-C4A-NA	2.66	128.19	124.51
49	Q	318	KC2	C2D-C1D-ND	-2.66	108.45	110.23
49	X	315	KC2	C2D-C1D-ND	-2.66	108.45	110.23
50	4	302	A1EB1	O6-C42-C44	2.66	120.25	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	P	315	A1ECV	C4B-CHC-C1C	2.66	124.53	115.73
51	Q	319	A1ECV	O2D-CGD-O1D	-2.66	118.64	123.84
39	o	203	CLA	CHB-C4A-NA	2.66	128.19	124.51
47	S	301	SQD	O8-S-C6	2.66	109.97	105.74
52	X	305	A1EB4	O1-C15-C14	-2.66	113.02	115.71
50	3	302	A1EB1	O6-C42-C44	2.66	120.25	111.91
50	V	302	A1EB1	C36-C31-C32	2.66	122.33	119.70
50	V	307	A1EB1	C40-C32-C31	-2.66	108.09	110.47
39	l	201	CLA	C3B-C4B-NB	-2.66	108.05	110.52
39	C	306	CLA	C3B-C4B-NB	-2.66	108.05	110.52
39	8	322	CLA	C3B-C4B-NB	-2.66	108.05	110.52
39	9	319	CLA	C3B-C4B-NB	-2.66	108.05	110.52
39	b	802	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
50	4	301	A1EB1	O6-C42-C44	2.66	120.25	111.91
39	b	821	CLA	CHB-C1B-NB	2.66	127.07	124.26
49	V	315	KC2	CBD-CHA-C1A	2.66	133.83	128.88
39	a	809	CLA	CHB-C4A-NA	2.66	128.19	124.51
39	3	314	CLA	CHB-C4A-NA	2.66	128.19	124.51
39	P	309	CLA	C3B-C4B-NB	-2.66	108.05	110.52
49	T	312	KC2	C1A-NA-C4A	-2.66	105.51	106.71
50	V	307	A1EB1	O6-C42-C44	2.66	120.24	111.91
52	P	319	A1EB4	C-C1-C2	-2.66	119.20	122.92
39	H	307	CLA	CHB-C4A-NA	2.66	128.18	124.51
49	M	314	KC2	C2D-C1D-ND	-2.66	108.45	110.23
47	M	301	SQD	O6-C1-C2	2.65	112.45	108.30
42	k	204	BCR	C33-C5-C4	2.65	118.72	113.62
39	J	311	CLA	CHB-C4A-NA	2.65	128.18	124.51
49	0	319	KC2	C1B-CHB-C4A	-2.65	120.33	126.06
49	Z	310	KC2	O1D-CGD-CBD	-2.65	119.05	124.48
49	1	312	KC2	CHC-C4B-C3B	-2.65	120.72	125.26
39	6	318	CLA	CHB-C4A-NA	2.65	128.18	124.51
47	4	327	SQD	O8-S-C6	2.65	109.97	105.74
49	x	312	KC2	C2D-C1D-ND	-2.65	108.45	110.23
49	Y	308	KC2	CHC-C4B-C3B	-2.65	120.72	125.26
49	V	308	KC2	C1A-NA-C4A	-2.65	105.51	106.71
50	4	301	A1EB1	C35-C34-C33	-2.65	105.25	109.88
39	a	804	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
39	I	308	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
50	8	304	A1EB1	C28-O6-C42	2.65	121.58	115.68
39	L	311	CLA	CHB-C4A-NA	2.65	128.18	124.51
48	Q	308	A86	C34-O4-C38	-2.65	112.95	117.90
48	U	202	A86	C9-C8-C6	-2.65	118.97	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	l	202	BCR	C20-C21-C22	-2.65	123.53	127.31
39	a	837	CLA	C3B-C4B-NB	-2.65	108.06	110.52
50	3	324	A1EB1	C7-C6-C8	2.65	122.25	118.08
50	0	303	A1EB1	C41-C32-C31	-2.65	108.10	110.47
39	V	311	CLA	CHB-C4A-NA	2.65	128.18	124.51
42	a	842	BCR	C33-C5-C6	-2.65	121.55	124.53
39	a	802	CLA	C3B-C4B-NB	-2.65	108.06	110.52
50	5	302	A1EB1	C17-C16-C15	2.65	111.87	109.16
50	1	305	A1EB1	O6-C42-C44	2.65	120.22	111.91
48	3	307	A86	O1-C15-C14	-2.65	107.89	113.21
39	3	319	CLA	CHB-C4A-NA	2.65	128.18	124.51
39	Y	305	CLA	CHB-C4A-NA	2.65	128.18	124.51
39	Z	304	CLA	CHB-C4A-NA	2.65	128.18	124.51
50	G	304	A1EB1	C17-C16-C15	2.65	111.86	109.16
49	1	312	KC2	CHB-C1B-C2B	-2.65	119.92	125.48
39	0	313	CLA	CHB-C4A-NA	2.65	128.17	124.51
51	T	317	A1ECV	C4B-CHC-C1C	2.65	124.50	115.73
43	y	303	DD6	C37-C36-C31	-2.65	120.75	124.35
48	W	304	A86	C17-C16-C15	2.65	111.86	109.16
39	D	316	CLA	CHB-C4A-NA	2.65	128.17	124.51
39	6	318	CLA	C3B-C4B-NB	-2.65	108.06	110.52
51	9	314	A1ECV	CMA-C3A-C2A	2.65	129.63	124.68
52	P	319	A1EB4	O4-C38-O43	-2.65	117.70	122.96
52	W	306	A1EB4	C40-C32-C31	-2.65	108.10	110.47
39	R	316	CLA	CHB-C4A-NA	2.65	128.17	124.51
42	j	103	BCR	C38-C26-C25	-2.65	121.56	124.53
48	y	305	A86	C33-C32-C31	2.65	111.78	109.21
39	H	309	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
49	S	317	KC2	C2D-C1D-ND	-2.65	108.46	110.23
39	B	206	CLA	CHB-C4A-NA	2.65	128.17	124.51
39	D	309	CLA	CHB-C4A-NA	2.65	128.17	124.51
48	W	303	A86	C40-C32-C31	-2.65	108.10	110.47
39	V	319	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
39	6	321	CLA	CHB-C4A-NA	2.65	128.17	124.51
39	a	804	CLA	C3B-C4B-NB	-2.65	108.06	110.52
42	b	847	BCR	C4-C5-C6	-2.64	118.89	122.73
49	Z	310	KC2	C2D-C1D-ND	-2.64	108.46	110.23
39	U	209	CLA	CHB-C4A-NA	2.64	128.17	124.51
49	2	317	KC2	CBD-CHA-C1A	2.64	133.81	128.88
49	x	315	KC2	O1D-CGD-CBD	-2.64	119.07	124.48
39	E	319	CLA	C3B-C4B-NB	-2.64	108.06	110.52
39	H	307	CLA	C3B-C4B-NB	-2.64	108.06	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	H	303	DD6	C33-C34-C35	-2.64	106.69	110.30
50	9	302	A1EB1	C9-C10-C11	-2.64	118.84	126.61
39	B	205	CLA	CAA-C2A-C3A	-2.64	107.66	114.26
41	a	840	LHG	C11-C10-C9	-2.64	101.01	114.42
49	V	314	KC2	C1A-NA-C4A	-2.64	105.52	106.71
48	H	302	A86	C12-C11-C13	2.64	120.46	116.02
39	2	307	CLA	CHB-C4A-NA	2.64	128.17	124.51
43	F	305	DD6	C15-C14-C13	-2.64	120.41	125.99
39	a	818	CLA	C3B-C4B-NB	-2.64	108.06	110.52
39	b	824	CLA	C3B-C4B-NB	-2.64	108.06	110.52
48	3	308	A86	C3-C4-C5	-2.64	118.06	123.47
48	8	305	A86	C35-C34-C33	2.64	114.49	109.88
39	4	319	CLA	CHB-C4A-NA	2.64	128.16	124.51
50	C	302	A1EB1	O1-C20-C21	-2.64	111.89	115.06
43	4	308	DD6	C37-C36-C31	-2.64	120.76	124.35
39	b	831	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	F	316	CLA	C3B-C4B-NB	-2.64	108.06	110.52
49	2	314	KC2	C2D-C1D-ND	-2.64	108.46	110.23
39	1	310	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	V	313	CLA	C3B-C4B-NB	-2.64	108.07	110.52
39	3	319	CLA	C3B-C4B-NB	-2.64	108.07	110.52
48	8	305	A86	C17-C16-C15	2.64	111.86	109.16
51	2	311	A1ECV	C4B-CHC-C1C	2.64	124.47	115.73
39	U	201	CLA	CHB-C4A-NA	2.64	128.16	124.51
48	3	308	A86	C19-C18-C17	2.64	115.87	110.77
51	Z	308	A1ECV	C4B-CHC-C1C	2.64	124.47	115.73
43	T	303	DD6	C21-C20-C15	-2.64	117.84	122.26
39	y	310	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	z	308	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	8	318	CLA	C3B-C4B-NB	-2.64	108.07	110.52
48	V	304	A86	C12-C11-C13	2.64	120.45	116.02
39	k	203	CLA	C3B-C4B-NB	-2.64	108.07	110.52
43	y	303	DD6	C15-C14-C13	-2.64	120.42	125.99
48	9	301	A86	C12-C11-C13	2.64	120.45	116.02
49	O	317	KC2	CHB-C1B-C2B	-2.64	119.95	125.48
39	J	308	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	K	309	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	Q	312	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	5	308	CLA	CHB-C4A-NA	2.64	128.16	124.51
48	8	302	A86	C34-O4-C38	-2.64	112.98	117.90
49	P	320	KC2	C4D-C3D-CAD	2.64	109.20	107.42
39	E	312	CLA	CHB-C4A-NA	2.64	128.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	U	210	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	x	314	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	F	312	CLA	C3B-C4B-NB	-2.64	108.07	110.52
46	S	321	LMG	O6-C1-O1	-2.64	103.73	109.97
50	U	205	A1EB1	O1-C20-C21	-2.64	111.90	115.06
39	U	212	CLA	CHB-C4A-NA	2.64	128.16	124.51
47	D	321	SQD	C44-O6-C1	2.64	118.89	113.74
49	Y	309	KC2	CBD-CHA-C1A	2.64	133.79	128.88
43	F	305	DD6	C37-C36-C35	2.64	119.24	114.36
48	3	307	A86	C9-C10-C11	-2.63	118.86	126.61
39	a	811	CLA	C3B-C4B-NB	-2.63	108.07	110.52
39	H	313	CLA	C3B-C4B-NB	-2.63	108.07	110.52
42	a	845	BCR	C34-C9-C10	-2.63	119.23	122.92
48	6	309	A86	C34-O4-C38	-2.63	112.99	117.90
48	0	304	A86	C26-C25-C24	-2.63	115.00	123.22
39	J	310	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
49	T	316	KC2	C1A-NA-C4A	-2.63	105.52	106.71
50	8	304	A1EB1	O6-C42-C44	2.63	120.17	111.91
42	b	844	BCR	C10-C11-C12	-2.63	115.00	123.22
39	b	833	CLA	CHD-C1D-ND	-2.63	122.03	124.45
39	o	205	CLA	CHB-C4A-NA	2.63	128.15	124.51
39	Y	302	CLA	CHB-C4A-NA	2.63	128.15	124.51
52	P	305	A1EB4	C40-C32-C31	-2.63	108.12	110.47
48	8	309	A86	C12-C11-C13	2.63	120.44	116.02
50	8	301	A1EB1	O6-C42-C44	2.63	120.17	111.91
43	5	303	DD6	C33-C34-C35	-2.63	106.70	110.30
49	O	317	KC2	C1B-CHB-C4A	-2.63	120.38	126.06
43	y	303	DD6	O1-C20-C19	-2.63	111.41	113.38
43	J	305	DD6	C9-C8-C6	-2.63	119.02	126.42
39	i	103	CLA	CHB-C4A-NA	2.63	128.15	124.51
39	0	315	CLA	CHB-C4A-NA	2.63	128.15	124.51
48	7	308	A86	C40-C32-C31	-2.63	108.12	110.47
39	3	322	CLA	C3B-C4B-NB	-2.63	108.07	110.52
39	9	312	CLA	C3B-C4B-NB	-2.63	108.07	110.52
48	8	323	A86	C33-C32-C31	2.63	111.77	109.21
39	E	313	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
39	2	319	CLA	CAA-C2A-C1A	2.63	120.60	111.97
42	h	202	BCR	C38-C26-C25	-2.63	121.57	124.53
49	F	307	KC2	O2D-CGD-O1D	-2.63	118.69	123.84
48	Y	301	A86	C40-C32-C31	-2.63	108.12	110.47
39	a	816	CLA	C3B-C4B-NB	-2.63	108.08	110.52
39	W	311	CLA	C3B-C4B-NB	-2.63	108.08	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	b	801	CLA	CHB-C4A-NA	2.63	128.15	124.51
39	2	312	CLA	CHB-C4A-NA	2.63	128.15	124.51
43	V	303	DD6	C14-C13-C11	-2.63	121.45	125.53
39	D	312	CLA	CHB-C4A-NA	2.63	128.15	124.51
39	1	316	CLA	CHB-C4A-NA	2.63	128.15	124.51
42	a	843	BCR	C30-C25-C26	-2.63	118.91	122.61
43	4	307	DD6	C25-C26-C27	-2.63	118.95	126.58
43	3	301	DD6	C21-C20-C15	-2.63	117.85	122.26
39	H	313	CLA	CHB-C4A-NA	2.63	128.15	124.51
39	x	308	CLA	CHB-C4A-NA	2.63	128.15	124.51
51	S	318	A1ECV	O2-CMC-O1	-2.63	118.31	123.45
50	3	303	A1EB1	C35-C34-C33	2.63	114.46	109.88
50	O	301	A1EB1	C41-C32-C31	-2.63	108.12	110.47
39	X	309	CLA	C3B-C4B-NB	-2.63	108.08	110.52
52	W	321	A1EB4	C20-C19-C18	-2.63	107.55	112.75
48	F	301	A86	O-C13-C11	-2.63	115.34	121.15
50	J	302	A1EB1	C9-C8-C6	-2.63	119.04	126.42
39	0	315	CLA	CMB-C2B-C1B	-2.63	121.37	125.37
39	b	803	CLA	C3B-C4B-NB	-2.63	108.08	110.52
39	A	315	CLA	C3B-C4B-NB	-2.63	108.08	110.52
39	E	310	CLA	C3B-C4B-NB	-2.63	108.08	110.52
48	7	312	A86	O4-C34-C35	2.63	114.13	107.59
39	a	805	CLA	CHB-C4A-NA	2.63	128.14	124.51
39	x	311	CLA	CHB-C4A-NA	2.63	128.14	124.51
48	6	305	A86	C12-C11-C13	2.63	120.43	116.02
39	Q	320	CLA	C3B-C4B-NB	-2.63	108.08	110.52
39	S	319	CLA	C3B-C4B-NB	-2.63	108.08	110.52
50	0	303	A1EB1	O6-C42-C44	2.63	120.15	111.91
39	Z	313	CLA	CHC-C1C-NC	2.63	128.19	124.20
42	b	848	BCR	C8-C7-C6	-2.63	119.83	127.20
39	W	319	CLA	CHB-C4A-NA	2.63	128.14	124.51
39	2	308	CLA	CHB-C4A-NA	2.63	128.14	124.51
50	x	302	A1EB1	C28-O6-C42	2.62	121.52	115.68
39	b	808	CLA	C3B-C4B-NB	-2.62	108.08	110.52
39	D	316	CLA	C3B-C4B-NB	-2.62	108.08	110.52
52	X	305	A1EB4	C10-C9-C8	-2.62	115.03	123.22
39	a	804	CLA	CHB-C4A-NA	2.62	128.14	124.51
39	a	811	CLA	CHB-C4A-NA	2.62	128.14	124.51
43	W	305	DD6	C37-C36-C31	-2.62	120.78	124.35
50	7	303	A1EB1	C4-C5-C6	-2.62	123.56	127.31
48	G	305	A86	O4-C34-C33	2.62	114.13	107.59
39	9	320	CLA	CHB-C4A-NA	2.62	128.14	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	3	303	A1EB1	O6-C42-C44	2.62	120.14	111.91
43	F	305	DD6	C10-C9-C8	-2.62	115.03	123.22
50	F	304	A1EB1	O6-C42-C44	2.62	120.14	111.91
39	X	308	CLA	CHB-C4A-NA	2.62	128.14	124.51
39	a	812	CLA	C3B-C4B-NB	-2.62	108.08	110.52
39	Y	314	CLA	C3B-C4B-NB	-2.62	108.08	110.52
39	a	824	CLA	CHB-C4A-NA	2.62	128.14	124.51
39	a	826	CLA	CMB-C2B-C1B	-2.62	121.38	125.37
39	o	203	CLA	C3B-C4B-NB	-2.62	108.08	110.52
39	L	308	CLA	CHB-C4A-NA	2.62	128.14	124.51
39	O	314	CLA	CHB-C4A-NA	2.62	128.14	124.51
46	S	322	LMG	O8-C28-C29	2.62	120.13	111.91
49	V	314	KC2	C2D-C1D-ND	-2.62	108.47	110.23
39	0	322	CLA	C3B-C4B-NB	-2.62	108.08	110.52
39	1	310	CLA	C3B-C4B-NB	-2.62	108.08	110.52
48	U	202	A86	C40-C32-C31	-2.62	108.13	110.47
48	V	304	A86	O4-C38-O5	-2.62	117.76	122.96
49	9	318	KC2	CHC-C4B-C3B	-2.62	120.78	125.26
48	W	303	A86	C9-C8-C6	-2.62	119.06	126.42
50	6	308	A1EB1	C9-C8-C6	-2.62	119.06	126.42
39	L	319	CLA	C3B-C4B-NB	-2.62	108.08	110.52
43	2	303	DD6	C20-C19-C18	-2.62	107.57	112.75
48	4	310	A86	O4-C34-C33	2.62	114.11	107.59
43	3	304	DD6	C8-C6-C5	2.62	122.96	118.94
39	Y	311	CLA	CHB-C4A-NA	2.62	128.13	124.51
39	3	311	CLA	C3B-C4B-NB	-2.62	108.09	110.52
39	4	322	CLA	C3B-C4B-NB	-2.62	108.09	110.52
39	6	322	CLA	C3B-C4B-NB	-2.62	108.09	110.52
43	z	304	DD6	C21-C20-C15	-2.62	117.87	122.26
49	K	313	KC2	C4D-C3D-CAD	2.62	109.19	107.42
43	j	102	DD6	C14-C13-C11	-2.62	121.47	125.53
47	F	318	SQD	C4-C3-C2	2.62	115.39	110.82
39	k	202	CLA	CHB-C4A-NA	2.62	128.13	124.51
39	H	312	CLA	CHB-C4A-NA	2.62	128.13	124.51
39	a	831	CLA	O2D-CGD-CBD	2.62	115.92	111.27
39	5	308	CLA	C3B-C4B-NB	-2.62	108.09	110.52
43	1	304	DD6	C9-C8-C6	-2.62	119.07	126.42
48	L	306	A86	C9-C10-C11	-2.62	118.92	126.61
43	7	309	DD6	O1-C20-C19	-2.62	111.42	113.38
52	T	304	A1EB4	C41-C32-C31	-2.62	108.13	110.47
49	4	324	KC2	O1D-CGD-CBD	-2.62	119.13	124.48
42	l	202	BCR	C15-C16-C17	-2.62	118.12	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	b	827	CLA	C3B-C4B-NB	-2.62	108.09	110.52
49	y	316	KC2	C2D-C1D-ND	-2.61	108.48	110.23
51	9	317	A1ECV	O2D-CGD-O1D	-2.61	118.73	123.84
39	Z	304	CLA	C3B-C4B-NB	-2.61	108.09	110.52
49	8	317	KC2	CBD-CHA-C1A	2.61	133.75	128.88
50	y	301	A1EB1	C3-C4-C5	-2.61	118.12	123.47
49	3	318	KC2	CHB-C4A-C3A	-2.61	120.90	124.98
48	9	304	A86	C28-C27-C26	-2.61	119.26	122.92
39	I	301	CLA	CHB-C4A-NA	2.61	128.13	124.51
49	H	314	KC2	C2D-C1D-ND	-2.61	108.48	110.23
48	U	206	A86	C9-C8-C6	-2.61	119.08	126.42
39	F	315	CLA	O2D-CGD-CBD	2.61	115.91	111.27
50	K	304	A1EB1	C35-C34-C33	2.61	114.44	109.88
42	b	844	BCR	C4-C5-C6	-2.61	118.94	122.73
50	x	302	A1EB1	O6-C42-C44	2.61	120.11	111.91
39	0	311	CLA	CMB-C2B-C1B	-2.61	121.39	125.37
39	3	316	CLA	C3B-C4B-NB	-2.61	108.09	110.52
39	J	310	CLA	CHB-C4A-NA	2.61	128.12	124.51
39	z	314	CLA	CHB-C4A-NA	2.61	128.12	124.51
51	O	315	A1ECV	O1D-CGD-CBD	-2.61	120.39	124.74
48	S	307	A86	C34-O4-C38	-2.61	113.03	117.90
39	P	309	CLA	CHB-C4A-NA	2.61	128.12	124.51
39	8	322	CLA	CHB-C4A-NA	2.61	128.12	124.51
39	h	201	CLA	CHB-C4A-NA	2.61	128.12	124.51
39	F	310	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
48	8	309	A86	C40-C32-C31	-2.61	108.14	110.47
50	0	307	A1EB1	C36-C31-C32	2.61	122.29	119.70
50	6	308	A1EB1	O1-C20-C21	-2.61	111.93	115.06
43	7	309	DD6	C37-C36-C31	-2.61	120.80	124.35
51	6	320	A1ECV	O1D-CGD-CBD	-2.61	120.39	124.74
39	z	306	CLA	CHB-C4A-NA	2.61	128.12	124.51
49	W	314	KC2	C1A-NA-C4A	-2.61	105.53	106.71
49	Z	310	KC2	CHD-C4C-NC	2.61	128.16	124.20
46	Q	322	LMG	O8-C28-C29	2.61	120.09	111.91
39	A	305	CLA	CHB-C4A-NA	2.61	128.12	124.51
39	E	319	CLA	CHB-C4A-NA	2.61	128.12	124.51
39	8	321	CLA	CHB-C4A-NA	2.61	128.12	124.51
39	Z	307	CLA	CHB-C4A-NA	2.61	128.12	124.51
50	7	304	A1EB1	O6-C42-C44	2.61	120.09	111.91
39	G	312	CLA	CHB-C4A-NA	2.61	128.12	124.51
51	X	310	A1ECV	C4B-CHC-C1C	2.61	124.37	115.73
49	z	315	KC2	CHD-C4C-NC	2.61	128.16	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	z	317	CLA	C3B-C4B-NB	-2.61	108.10	110.52
49	Q	318	KC2	O1D-CGD-CBD	-2.61	119.15	124.48
47	E	320	SQD	O5-C1-C2	2.61	115.87	110.35
50	O	301	A1EB1	C35-C34-C33	2.61	114.42	109.88
48	L	307	A86	C33-C32-C31	2.61	111.74	109.21
39	W	316	CLA	CMB-C2B-C1B	-2.61	121.40	125.37
50	H	304	A1EB1	C9-C8-C6	-2.61	119.10	126.42
39	0	323	CLA	C3B-C4B-NB	-2.61	108.10	110.52
39	8	312	CLA	C3B-C4B-NB	-2.61	108.10	110.52
50	E	301	A1EB1	C4-C3-C2	-2.60	118.14	123.47
39	B	205	CLA	CHB-C4A-NA	2.60	128.11	124.51
39	C	307	CLA	CHB-C4A-NA	2.60	128.11	124.51
39	O	308	CLA	CHB-C4A-NA	2.60	128.11	124.51
39	S	308	CLA	CHB-C4A-NA	2.60	128.11	124.51
49	V	308	KC2	CHB-C4A-C3A	-2.60	120.91	124.98
43	F	305	DD6	C25-C26-C27	-2.60	119.02	126.58
39	I	315	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
49	9	318	KC2	C1B-CHB-C4A	-2.60	120.44	126.06
39	C	307	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
39	a	835	CLA	CHB-C4A-NA	2.60	128.11	124.51
42	m	101	BCR	C11-C10-C9	-2.60	123.60	127.31
49	L	315	KC2	C2D-C1D-ND	-2.60	108.49	110.23
49	V	320	KC2	C2D-C1D-ND	-2.60	108.49	110.23
43	H	303	DD6	C21-C20-C15	-2.60	117.90	122.26
49	T	314	KC2	O2D-CGD-O1D	-2.60	118.75	123.84
39	a	816	CLA	CHB-C4A-NA	2.60	128.11	124.51
39	7	315	CLA	CHB-C4A-NA	2.60	128.11	124.51
39	y	309	CLA	CHB-C4A-NA	2.60	128.11	124.51
39	z	309	CLA	CHB-C4A-NA	2.60	128.11	124.51
49	R	312	KC2	O1D-CGD-CBD	-2.60	119.16	124.48
39	1	309	CLA	C3B-C4B-NB	-2.60	108.10	110.52
39	9	312	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
39	J	309	CLA	CHB-C4A-NA	2.60	128.11	124.51
39	x	317	CLA	CHB-C4A-NA	2.60	128.11	124.51
39	z	318	CLA	CHB-C4A-NA	2.60	128.11	124.51
50	4	304	A1EB1	O6-C42-C44	2.60	120.07	111.91
39	6	311	CLA	O2D-CGD-O1D	-2.60	118.19	124.09
49	8	317	KC2	CHD-C4C-NC	2.60	128.15	124.20
48	6	307	A86	C4-C3-C2	-2.60	118.15	123.47
48	L	306	A86	O4-C38-O5	-2.60	117.80	122.96
50	G	307	A1EB1	O6-C42-C44	2.60	120.06	111.91
39	D	313	CLA	CHB-C4A-NA	2.60	128.11	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	8	312	CLA	CHB-C4A-NA	2.60	128.11	124.51
48	1	307	A86	C12-C11-C13	2.60	120.39	116.02
42	b	847	BCR	C21-C20-C19	-2.60	115.11	123.22
50	K	305	A1EB1	O6-C42-C44	2.60	120.06	111.91
39	S	310	CLA	CAA-C2A-C1A	2.60	117.89	112.14
39	T	310	CLA	CHB-C4A-NA	2.60	128.10	124.51
52	W	306	A1EB4	C21-C20-C15	-2.60	117.93	122.32
49	3	321	KC2	O1D-CGD-CBD	-2.60	119.17	124.48
43	Z	302	DD6	C20-C19-C18	-2.60	107.61	112.75
39	F	313	CLA	C3B-C4B-NB	-2.60	108.11	110.52
39	H	309	CLA	CHB-C4A-NA	2.60	128.10	124.51
49	2	313	KC2	CHB-C4A-C3A	-2.60	120.92	124.98
52	P	305	A1EB4	C21-C20-C15	-2.60	117.93	122.32
48	8	323	A86	C36-C31-C32	2.60	122.27	119.70
39	E	314	CLA	CHB-C4A-NA	2.60	128.10	124.51
39	M	310	CLA	CHB-C4A-NA	2.60	128.10	124.51
39	y	307	CLA	CHB-C4A-NA	2.60	128.10	124.51
51	9	314	A1ECV	O1D-CGD-CBD	-2.60	120.41	124.74
39	y	315	CLA	C3B-C4B-NB	-2.60	108.11	110.52
39	Y	303	CLA	C3B-C4B-NB	-2.60	108.11	110.52
39	6	310	CLA	C3B-C4B-NB	-2.60	108.11	110.52
47	D	304	SQD	O8-S-C6	2.60	109.88	105.74
49	4	320	KC2	CHD-C4C-NC	2.60	128.14	124.20
39	5	306	CLA	CHB-C4A-NA	2.60	128.10	124.51
49	M	314	KC2	CBD-CHA-C1A	2.60	133.72	128.88
51	4	321	A1ECV	CMA-C3A-C2A	2.60	129.53	124.68
43	z	305	DD6	C25-C26-C27	-2.60	119.04	126.58
39	0	311	CLA	CHB-C1B-NB	2.60	127.00	124.26
51	R	313	A1ECV	O2D-CGD-O1D	-2.60	118.76	123.84
39	F	306	CLA	CHB-C4A-NA	2.60	128.10	124.51
50	V	307	A1EB1	C33-C32-C31	2.59	111.73	109.21
39	H	309	CLA	C3B-C4B-NB	-2.59	108.11	110.52
39	5	316	CLA	C3B-C4B-NB	-2.59	108.11	110.52
49	B	208	KC2	C2D-C1D-ND	-2.59	108.49	110.23
39	E	318	CLA	CHB-C4A-NA	2.59	128.10	124.51
39	F	316	CLA	CHB-C4A-NA	2.59	128.10	124.51
43	Q	303	DD6	C12-C11-C10	-2.59	119.29	122.92
39	8	310	CLA	CHB-C4A-NA	2.59	128.10	124.51
48	M	306	A86	C35-C34-C33	2.59	114.40	109.88
49	G	313	KC2	CMA-C3A-C4A	-2.59	121.09	125.04
41	a	841	LHG	C11-C10-C9	-2.59	101.26	114.42
52	X	305	A1EB4	C21-C20-C15	-2.59	117.94	122.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	J	310	CLA	C3B-C4B-NB	-2.59	108.11	110.52
39	3	314	CLA	C3B-C4B-NB	-2.59	108.11	110.52
43	R	304	DD6	C21-C20-C15	-2.59	117.92	122.26
49	5	311	KC2	C3C-C2C-C1C	2.59	108.41	106.49
49	0	317	KC2	CHB-C4A-C3A	-2.59	120.93	124.98
39	a	825	CLA	CHB-C4A-NA	2.59	128.10	124.51
39	y	312	CLA	CHB-C4A-NA	2.59	128.10	124.51
51	Q	319	A1ECV	CMA-C3A-C2A	2.59	129.53	124.68
39	k	201	CLA	C3B-C4B-NB	-2.59	108.11	110.52
39	k	203	CLA	CHB-C4A-NA	2.59	128.09	124.51
39	U	214	CLA	CHB-C4A-NA	2.59	128.09	124.51
39	y	308	CLA	CHB-C4A-NA	2.59	128.09	124.51
39	9	320	CLA	CAA-C2A-C3A	-2.59	110.05	116.10
43	P	304	DD6	C7-C6-C5	-2.59	119.29	122.92
49	M	313	KC2	CHC-C4B-C3B	-2.59	120.83	125.26
39	b	809	CLA	C3B-C4B-NB	-2.59	108.11	110.52
39	L	309	CLA	C3B-C4B-NB	-2.59	108.11	110.52
50	8	308	A1EB1	O6-C42-C44	2.59	120.04	111.91
48	R	301	A86	C40-C32-C31	-2.59	108.15	110.47
48	0	306	A86	C40-C32-C31	-2.59	108.15	110.47
49	5	311	KC2	C1A-NA-C4A	-2.59	105.54	106.71
43	O	305	DD6	O1-C20-C21	-2.59	111.95	115.06
39	F	309	CLA	CHB-C4A-NA	2.59	128.09	124.51
39	Z	315	CLA	CHB-C4A-NA	2.59	128.09	124.51
39	O	312	CLA	C3B-C4B-NB	-2.59	108.11	110.52
49	0	316	KC2	C2D-C1D-ND	-2.59	108.50	110.23
39	I	308	CLA	CMB-C2B-C1B	-2.59	121.43	125.37
52	P	305	A1EB4	O1-C15-C14	-2.59	113.09	115.71
39	8	313	CLA	C3B-C4B-NB	-2.59	108.11	110.52
43	x	303	DD6	C21-C20-C15	-2.59	117.92	122.26
49	9	313	KC2	C1A-NA-C4A	-2.59	105.54	106.71
39	i	103	CLA	CMB-C2B-C1B	-2.59	121.43	125.37
39	B	203	CLA	C3B-C4B-NB	-2.59	108.12	110.52
48	R	317	A86	C12-C11-C13	2.59	120.37	116.02
49	P	320	KC2	CHD-C4C-NC	2.59	128.13	124.20
49	X	312	KC2	CHD-C4C-NC	2.59	128.13	124.20
41	j	104	LHG	O8-C23-C24	2.59	120.02	111.91
39	M	308	CLA	CHB-C4A-NA	2.59	128.09	124.51
39	b	837	CLA	CMB-C2B-C3B	2.58	132.85	126.59
39	R	315	CLA	C3B-C4B-NB	-2.58	108.12	110.52
43	z	305	DD6	C4-C5-C6	-2.58	123.62	127.31
39	b	827	CLA	CHB-C4A-NA	2.58	128.09	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	V	309	CLA	CHB-C4A-NA	2.58	128.09	124.51
50	z	302	A1EB1	O1-C20-C19	-2.58	111.44	113.38
39	F	310	CLA	C3B-C4B-NB	-2.58	108.12	110.52
39	W	310	CLA	C3B-C4B-NB	-2.58	108.12	110.52
52	R	305	A1EB4	C33-C32-C31	2.58	111.72	109.21
49	R	318	KC2	C2D-C1D-ND	-2.58	108.50	110.23
48	B	201	A86	O1-C20-C21	-2.58	111.96	115.06
43	1	304	DD6	C19-C18-C17	-2.58	105.78	110.77
49	W	308	KC2	CHB-C4A-C3A	-2.58	120.94	124.98
49	Z	310	KC2	C1A-NA-C4A	-2.58	105.55	106.71
39	B	204	CLA	CHB-C4A-NA	2.58	128.08	124.51
50	6	301	A1EB1	C10-C9-C8	-2.58	115.16	123.22
48	Q	308	A86	C25-C26-C27	-2.58	123.62	127.31
49	L	314	KC2	CHD-C4C-NC	2.58	128.12	124.20
49	S	317	KC2	CHD-C4C-NC	2.58	128.12	124.20
39	i	101	CLA	CHB-C4A-NA	2.58	128.08	124.51
39	W	309	CLA	CHB-C4A-NA	2.58	128.08	124.51
39	W	311	CLA	CHB-C4A-NA	2.58	128.08	124.51
39	a	814	CLA	C3B-C4B-NB	-2.58	108.12	110.52
39	A	308	CLA	C3B-C4B-NB	-2.58	108.12	110.52
48	B	201	A86	C34-O4-C38	-2.58	113.08	117.90
42	a	843	BCR	C16-C15-C14	-2.58	118.19	123.47
42	b	845	BCR	C33-C5-C4	2.58	118.58	113.62
49	T	315	KC2	CHD-C4C-NC	2.58	128.12	124.20
39	a	807	CLA	C3B-C4B-NB	-2.58	108.12	110.52
50	0	303	A1EB1	C34-O4-C38	-2.58	113.09	117.90
39	E	307	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
39	L	310	CLA	CHB-C4A-NA	2.58	128.08	124.51
49	5	314	KC2	C1A-NA-C4A	-2.58	105.55	106.71
50	G	307	A1EB1	C17-C16-C15	2.58	111.80	109.16
39	V	309	CLA	C3B-C4B-NB	-2.58	108.12	110.52
49	V	315	KC2	C2D-C1D-ND	-2.58	108.50	110.23
50	7	306	A1EB1	C34-O4-C38	-2.58	113.09	117.90
39	5	307	CLA	CHB-C1B-NB	2.58	126.99	124.26
49	Y	308	KC2	C1B-CHB-C4A	-2.58	120.50	126.06
51	Y	306	A1ECV	O2-CMC-O1	-2.58	118.41	123.45
42	a	842	BCR	C28-C27-C26	-2.58	109.47	114.08
48	F	301	A86	C34-O4-C38	-2.58	113.09	117.90
39	b	830	CLA	C2D-C1D-ND	-2.58	108.20	110.10
39	P	314	CLA	CHB-C4A-NA	2.58	128.08	124.51
50	4	304	A1EB1	C28-C27-C26	-2.58	121.56	124.93
48	I	304	A86	C34-O4-C38	-2.58	113.09	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	3	323	CLA	C3B-C4B-NB	-2.58	108.12	110.52
50	E	301	A1EB1	O1-C20-C19	-2.58	111.45	113.38
48	O	302	A86	C3-C2-C1	-2.58	123.63	127.31
50	K	302	A1EB1	C35-C34-C33	-2.58	105.38	109.88
48	P	302	A86	C34-O4-C38	-2.58	113.09	117.90
48	0	304	A86	O4-C38-O5	-2.58	117.84	122.96
39	b	828	CLA	CHB-C4A-NA	2.58	128.07	124.51
39	C	306	CLA	CHB-C4A-NA	2.58	128.07	124.51
39	E	309	CLA	CHB-C4A-NA	2.58	128.07	124.51
39	1	317	CLA	CHB-C4A-NA	2.58	128.07	124.51
50	h	203	A1EB1	C35-C34-C33	-2.58	105.38	109.88
39	Q	309	CLA	C3B-C4B-NB	-2.58	108.12	110.52
48	4	328	A86	C34-O4-C38	-2.58	113.09	117.90
49	X	312	KC2	C2D-C1D-ND	-2.58	108.50	110.23
49	Z	311	KC2	C2D-C1D-ND	-2.58	108.50	110.23
39	V	310	CLA	CHB-C4A-NA	2.58	128.07	124.51
49	2	317	KC2	C4D-C3D-CAD	2.58	109.16	107.42
49	2	317	KC2	CHB-C4A-C3A	-2.58	120.95	124.98
48	7	312	A86	O1-C20-C21	-2.58	111.97	115.06
39	L	313	CLA	C3B-C4B-NB	-2.58	108.13	110.52
48	4	328	A86	C4-C5-C6	-2.58	123.64	127.31
39	O	310	CLA	CHD-C1D-ND	-2.57	122.09	124.45
42	m	101	BCR	C15-C14-C13	-2.57	123.64	127.31
39	O	310	CLA	CBC-CAC-C3C	-2.57	105.33	112.43
50	3	324	A1EB1	C9-C8-C6	-2.57	119.19	126.42
46	4	325	LMG	O6-C1-O1	-2.57	103.88	109.97
49	F	307	KC2	C1A-NA-C4A	-2.57	105.55	106.71
39	b	802	CLA	CMB-C2B-C3B	2.57	132.82	126.59
49	X	318	KC2	C2D-C1D-ND	-2.57	108.51	110.23
49	4	320	KC2	C2D-C1D-ND	-2.57	108.51	110.23
39	o	206	CLA	C3B-C4B-NB	-2.57	108.13	110.52
39	M	317	CLA	C3B-C4B-NB	-2.57	108.13	110.52
50	C	302	A1EB1	C9-C8-C6	-2.57	119.19	126.42
49	P	306	KC2	C4D-C3D-CAD	2.57	109.16	107.42
39	a	827	CLA	O2D-CGD-CBD	2.57	115.84	111.27
39	G	314	CLA	O2D-CGD-CBD	2.57	115.84	111.27
51	4	321	A1ECV	C4B-CHC-C1C	2.57	124.25	115.73
49	0	314	KC2	CHB-C4A-C3A	-2.57	120.96	124.98
47	W	301	SQD	O6-C1-C2	2.57	112.32	108.30
39	b	810	CLA	CHB-C4A-NA	2.57	128.07	124.51
39	b	842	CLA	CHB-C4A-NA	2.57	128.07	124.51
49	C	313	KC2	O1D-CGD-CBD	-2.57	119.23	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	T	316	KC2	CHD-C4C-NC	2.57	128.10	124.20
43	5	303	DD6	C21-C20-C15	-2.57	117.95	122.26
50	F	304	A1EB1	C40-C32-C31	-2.57	108.17	110.47
50	U	205	A1EB1	C4-C3-C2	-2.57	118.21	123.47
39	z	314	CLA	C3B-C4B-NB	-2.57	108.13	110.52
50	6	301	A1EB1	C35-C34-C33	2.57	114.36	109.88
39	0	320	CLA	CHB-C4A-NA	2.57	128.06	124.51
39	z	307	CLA	CHB-C4A-NA	2.57	128.06	124.51
43	7	309	DD6	C3-C4-C5	-2.57	118.21	123.47
39	a	835	CLA	C3B-C4B-NB	-2.57	108.13	110.52
39	P	316	CLA	C3B-C4B-NB	-2.57	108.13	110.52
50	z	302	A1EB1	C9-C8-C6	-2.57	119.20	126.42
39	K	314	CLA	CMA-C3A-C2A	-2.57	110.11	116.10
48	2	305	A86	C12-C11-C13	2.57	120.33	116.02
48	J	303	A86	C33-C32-C31	2.57	111.71	109.21
49	T	316	KC2	CBD-CHA-C1A	2.57	133.67	128.88
50	7	306	A1EB1	C28-O6-C42	2.57	121.39	115.68
49	L	317	KC2	C1A-NA-C4A	-2.57	105.55	106.71
39	R	307	CLA	C3B-C4B-NB	-2.57	108.13	110.52
39	b	851	CLA	CHB-C4A-NA	2.57	128.06	124.51
43	C	301	DD6	C14-C13-C11	-2.57	121.55	125.53
48	D	305	A86	C40-C32-C31	-2.57	108.18	110.47
48	8	307	A86	O1-C15-C14	-2.57	108.06	113.21
49	z	313	KC2	O1D-CGD-CBD	-2.57	119.73	124.51
39	a	823	CLA	O2D-CGD-CBD	2.57	115.83	111.27
49	Z	311	KC2	CHD-C4C-NC	2.56	128.09	124.20
48	6	309	A86	C12-C11-C13	2.56	120.33	116.02
50	O	301	A1EB1	O6-C42-C44	2.56	119.95	111.91
39	9	309	CLA	CHB-C4A-NA	2.56	128.06	124.51
48	1	303	A86	C25-C24-C1	-2.56	119.21	126.42
39	G	309	CLA	CHB-C4A-NA	2.56	128.06	124.51
39	J	307	CLA	C3B-C4B-NB	-2.56	108.14	110.52
50	U	203	A1EB1	C41-C32-C31	-2.56	108.18	110.47
43	5	303	DD6	C3-C2-C1	-2.56	123.65	127.31
39	L	309	CLA	O2D-CGD-O1D	-2.56	118.27	124.09
39	4	311	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
39	C	304	CLA	CHB-C4A-NA	2.56	128.06	124.51
39	F	308	CLA	CHB-C4A-NA	2.56	128.06	124.51
39	0	318	CLA	CHB-C4A-NA	2.56	128.06	124.51
43	E	305	DD6	C37-C36-C31	-2.56	120.87	124.35
42	a	843	BCR	C3-C4-C5	-2.56	109.50	114.08
50	8	306	A1EB1	C28-O6-C42	2.56	121.38	115.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	2	314	KC2	CHD-C4C-NC	2.56	128.09	124.20
43	7	309	DD6	C21-C20-C15	-2.56	117.97	122.26
50	y	301	A1EB1	O6-C42-C44	2.56	119.94	111.91
39	f	803	CLA	CHB-C4A-NA	2.56	128.05	124.51
52	M	305	A1EB4	O3-C39-C43	2.56	119.94	111.91
49	W	314	KC2	C2D-C1D-ND	-2.56	108.52	110.23
39	R	307	CLA	CHB-C4A-NA	2.56	128.05	124.51
39	W	310	CLA	CHB-C4A-NA	2.56	128.05	124.51
39	I	314	CLA	CHB-C4A-NA	2.56	128.05	124.51
39	G	310	CLA	C3B-C4B-NB	-2.56	108.14	110.52
42	i	102	BCR	C15-C16-C17	-2.56	118.23	123.47
49	T	315	KC2	O1D-CGD-CBD	-2.56	119.25	124.48
43	4	307	DD6	C21-C20-C15	-2.56	117.97	122.26
49	x	313	KC2	CHD-C4C-NC	2.56	128.08	124.20
43	U	204	DD6	O1-C20-C21	-2.56	111.99	115.06
48	S	305	A86	C33-C32-C31	2.56	111.70	109.21
39	a	809	CLA	C3B-C4B-NB	-2.56	108.14	110.52
43	E	305	DD6	C4-C3-C2	-2.56	118.24	123.47
48	5	301	A86	C25-C24-C1	-2.56	119.23	126.42
39	D	319	CLA	C3B-C4B-NB	-2.56	108.14	110.52
39	6	311	CLA	CMA-C3A-C2A	-2.56	110.13	116.10
48	8	307	A86	C40-C32-C31	-2.56	108.18	110.47
51	V	317	A1ECV	CMB-C2B-C1B	2.56	129.56	124.73
46	7	301	LMG	O8-C28-C29	2.56	119.93	111.91
49	X	306	KC2	CBD-CHA-C1A	2.56	133.65	128.88
39	4	314	CLA	C3B-C4B-NB	-2.56	108.14	110.52
48	D	305	A86	C28-C27-C26	-2.56	119.34	122.92
39	E	308	CLA	CHB-C4A-NA	2.56	128.05	124.51
49	L	317	KC2	CHD-C4C-NC	2.56	128.08	124.20
49	z	315	KC2	C2D-C1D-ND	-2.56	108.52	110.23
50	V	302	A1EB1	O6-C42-C44	2.56	119.93	111.91
39	T	311	CLA	CHB-C4A-NA	2.55	128.04	124.51
39	I	316	CLA	CHB-C4A-NA	2.55	128.04	124.51
51	x	310	A1ECV	O1D-CGD-CBD	-2.55	120.48	124.74
39	3	320	CLA	C3B-C4B-NB	-2.55	108.14	110.52
48	7	312	A86	C3-C4-C5	-2.55	118.24	123.47
51	6	320	A1ECV	C4B-CHC-C1C	2.55	124.19	115.73
49	0	319	KC2	O2D-CGD-O1D	-2.55	118.84	123.84
50	K	304	A1EB1	C12-C11-C13	2.55	120.31	116.02
50	0	305	A1EB1	C35-C34-C33	2.55	114.33	109.88
39	C	309	CLA	CHB-C4A-NA	2.55	128.04	124.51
49	y	316	KC2	CHB-C4A-C3A	-2.55	120.99	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	y	301	A1EB1	C40-C32-C31	-2.55	108.19	110.47
42	b	847	BCR	C33-C5-C6	-2.55	121.66	124.53
48	U	206	A86	O4-C38-O5	-2.55	117.89	122.96
51	4	321	A1ECV	O2-CMC-O1	-2.55	118.46	123.45
51	X	313	A1ECV	O1D-CGD-CBD	-2.55	120.49	124.74
46	A	316	LMG	O1-C7-C8	-2.55	104.74	110.90
39	1	308	CLA	CHB-C4A-NA	2.55	128.04	124.51
39	b	851	CLA	C3B-C4B-NB	-2.55	108.15	110.52
48	9	303	A86	C12-C11-C13	2.55	120.31	116.02
39	F	308	CLA	C3B-C4B-NB	-2.55	108.15	110.52
39	H	315	CLA	C3B-C4B-NB	-2.55	108.15	110.52
39	L	308	CLA	C3B-C4B-NB	-2.55	108.15	110.52
39	2	318	CLA	CHB-C4A-NA	2.55	128.04	124.51
49	L	314	KC2	O1D-CGD-CBD	-2.55	119.26	124.48
41	D	302	LHG	C11-C10-C9	-2.55	101.47	114.42
52	W	306	A1EB4	O1-C15-C14	-2.55	113.13	115.71
49	3	321	KC2	C2D-C1D-ND	-2.55	108.52	110.23
39	b	815	CLA	CHB-C4A-NA	2.55	128.04	124.51
39	K	307	CLA	CHB-C4A-NA	2.55	128.04	124.51
49	y	314	KC2	CBD-CHA-C1A	2.55	133.64	128.88
39	a	806	CLA	C3B-C4B-NB	-2.55	108.15	110.52
39	b	837	CLA	C3B-C4B-NB	-2.55	108.15	110.52
39	6	311	CLA	C3B-C4B-NB	-2.55	108.15	110.52
42	b	845	BCR	C38-C26-C25	-2.55	121.67	124.53
39	V	310	CLA	CAA-CBA-CGA	-2.55	105.80	113.25
39	4	311	CLA	CHB-C4A-NA	2.55	128.04	124.51
51	W	317	A1ECV	O2-CMC-O1	-2.55	118.47	123.45
39	x	314	CLA	C3B-C4B-NB	-2.55	108.15	110.52
52	5	304	A1EB4	O3-C39-C43	2.55	119.90	111.91
39	G	318	CLA	CAC-C3C-C4C	2.55	128.12	124.81
39	S	313	CLA	CHB-C4A-NA	2.55	128.03	124.51
42	b	850	BCR	C38-C26-C25	-2.55	121.67	124.53
50	G	302	A1EB1	O6-C42-C44	2.55	119.90	111.91
49	K	313	KC2	C2A-C3A-C4A	2.55	108.38	106.49
46	4	326	LMG	O8-C28-C29	2.55	119.90	111.91
39	A	308	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
39	A	311	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
49	9	318	KC2	O2D-CGD-O1D	-2.55	118.86	123.84
39	R	311	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
50	J	302	A1EB1	C25-C24-C1	-2.55	119.27	126.42
43	A	303	DD6	C20-C19-C18	-2.55	107.71	112.75
48	7	312	A86	C12-C11-C13	2.55	120.30	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	G	316	A1ECV	O2D-CGD-O1D	-2.55	118.86	123.84
39	C	309	CLA	C3B-C4B-NB	-2.54	108.15	110.52
39	T	311	CLA	C3B-C4B-NB	-2.54	108.15	110.52
50	F	304	A1EB1	C7-C6-C5	-2.54	119.36	122.92
39	b	821	CLA	CHB-C4A-NA	2.54	128.03	124.51
48	G	305	A86	O1-C20-C21	-2.54	112.01	115.06
47	E	320	SQD	C3-C4-C5	2.54	114.78	110.24
49	0	316	KC2	CHD-C4C-NC	2.54	128.06	124.20
39	O	308	CLA	CMA-C3A-C2A	-2.54	110.16	116.10
43	x	303	DD6	C9-C10-C11	-2.54	123.68	127.31
39	S	308	CLA	C3B-C4B-NB	-2.54	108.16	110.52
46	I	302	LMG	C1-C2-C3	-2.54	104.70	110.00
49	Q	318	KC2	CHB-C4A-C3A	-2.54	121.00	124.98
49	W	314	KC2	O1D-CGD-CBD	-2.54	119.28	124.48
39	M	310	CLA	C3B-C4B-NB	-2.54	108.16	110.52
39	b	823	CLA	CHB-C4A-NA	2.54	128.03	124.51
49	7	319	KC2	C1A-NA-C4A	-2.54	105.56	106.71
49	3	321	KC2	C2A-C3A-C4A	2.54	108.37	106.49
43	K	303	DD6	O1-C20-C21	-2.54	112.01	115.06
43	z	305	DD6	O1-C20-C21	-2.54	112.01	115.06
39	F	309	CLA	C3B-C4B-NB	-2.54	108.16	110.52
39	G	312	CLA	C3B-C4B-NB	-2.54	108.16	110.52
39	Z	305	CLA	CHB-C4A-NA	2.54	128.03	124.51
48	J	303	A86	C36-C31-C32	2.54	122.22	119.70
39	O	311	CLA	CHB-C4A-NA	2.54	128.03	124.51
39	4	312	CLA	CHB-C4A-NA	2.54	128.02	124.51
52	5	304	A1EB4	C4-C5-C6	-2.54	123.69	127.31
52	P	318	A1EB4	C35-C34-C33	-2.54	105.44	109.88
50	0	305	A1EB1	O6-C42-C44	2.54	119.88	111.91
49	C	313	KC2	C2D-C1D-ND	-2.54	108.53	110.23
50	K	302	A1EB1	O6-C42-C44	2.54	119.87	111.91
48	9	304	A86	C3-C4-C5	-2.54	118.27	123.47
50	G	308	A1EB1	C19-C18-C17	-2.54	105.87	110.77
48	6	303	A86	C3-C4-C5	-2.54	118.28	123.47
39	2	309	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
39	7	316	CLA	CHB-C4A-NA	2.54	128.02	124.51
43	y	303	DD6	C25-C24-C1	-2.54	119.29	126.42
39	6	312	CLA	CHB-C4A-NA	2.54	128.02	124.51
48	4	309	A86	C17-C16-C15	2.54	111.75	109.16
39	a	826	CLA	C3B-C4B-NB	-2.54	108.16	110.52
39	J	312	CLA	C3B-C4B-NB	-2.54	108.16	110.52
39	4	319	CLA	C3B-C4B-NB	-2.54	108.16	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	a	846	DD6	C25-C24-C1	-2.54	119.29	126.42
39	6	310	CLA	CHB-C4A-NA	2.54	128.02	124.51
50	x	302	A1EB1	O1-C20-C19	-2.54	111.48	113.38
39	b	829	CLA	CMB-C2B-C1B	-2.54	121.51	125.37
49	3	318	KC2	C1A-NA-C4A	-2.54	105.57	106.71
50	z	302	A1EB1	C3-C4-C5	-2.54	118.28	123.47
39	b	832	CLA	CHB-C4A-NA	2.54	128.02	124.51
39	C	311	CLA	CHB-C4A-NA	2.53	128.02	124.51
39	Q	309	CLA	CHB-C4A-NA	2.53	128.02	124.51
39	Z	315	CLA	C3B-C4B-NB	-2.53	108.16	110.52
39	P	307	CLA	CHB-C4A-NA	2.53	128.02	124.51
48	4	310	A86	C41-C32-C31	-2.53	108.20	110.47
50	L	303	A1EB1	C40-C32-C31	-2.53	108.20	110.47
43	5	303	DD6	C14-C13-C11	-2.53	121.60	125.53
39	b	837	CLA	CHB-C4A-NA	2.53	128.01	124.51
49	V	315	KC2	CHB-C4A-C3A	-2.53	121.02	124.98
50	8	306	A1EB1	C12-C11-C13	2.53	120.28	116.02
48	0	304	A86	O1-C20-C21	-2.53	112.02	115.06
39	a	833	CLA	C3B-C4B-NB	-2.53	108.17	110.52
39	b	817	CLA	C3B-C4B-NB	-2.53	108.17	110.52
48	4	310	A86	C12-C11-C13	2.53	120.28	116.02
50	8	308	A1EB1	O4-C38-O5	-2.53	117.93	122.96
50	4	303	A1EB1	C33-C32-C31	2.53	111.67	109.21
39	Q	321	CLA	CHB-C1B-NB	2.53	126.94	124.26
39	K	314	CLA	CHB-C4A-NA	2.53	128.01	124.51
39	O	309	CLA	CHB-C4A-NA	2.53	128.01	124.51
39	V	316	CLA	CHB-C4A-NA	2.53	128.01	124.51
51	R	310	A1ECV	O1D-CGD-CBD	-2.53	120.53	124.74
39	J	318	CLA	C3B-C4B-NB	-2.53	108.17	110.52
48	L	304	A86	C41-C32-C31	-2.53	108.21	110.47
48	0	309	A86	C34-O4-C38	-2.53	113.18	117.90
39	D	310	CLA	CHB-C1B-NB	2.53	126.93	124.26
49	M	307	KC2	C4D-C3D-CAD	2.53	109.13	107.42
43	R	304	DD6	C33-C34-C35	-2.53	106.84	110.30
49	7	322	KC2	O1D-CGD-CBD	-2.53	119.31	124.48
39	a	807	CLA	CHB-C4A-NA	2.53	128.01	124.51
49	6	319	KC2	C1B-CHB-C4A	-2.53	120.60	126.06
39	7	325	CLA	CHB-C4A-NA	2.53	128.01	124.51
51	T	317	A1ECV	O2D-CGD-O1D	-2.53	118.90	123.84
43	S	306	DD6	C37-C36-C35	2.53	119.04	114.36
49	X	306	KC2	C1B-CHB-C4A	-2.53	120.61	126.06
39	E	309	CLA	C3B-C4B-NB	-2.53	108.17	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	a	840	LHG	C20-C19-C18	-2.53	101.60	114.42
48	U	206	A86	C41-C32-C31	-2.53	108.21	110.47
43	C	301	DD6	C25-C24-C1	-2.53	119.32	126.42
48	P	302	A86	C12-C11-C13	2.53	120.27	116.02
43	T	303	DD6	C37-C36-C31	-2.53	120.92	124.35
50	9	302	A1EB1	C9-C8-C6	-2.53	119.32	126.42
42	a	842	BCR	C38-C26-C25	-2.53	121.69	124.53
43	K	303	DD6	C15-C14-C13	-2.52	120.66	125.99
49	X	314	KC2	CHD-C4C-NC	2.52	128.03	124.20
47	k	205	SQD	C44-O6-C1	2.52	118.67	113.74
46	Q	322	LMG	C8-O7-C10	-2.52	111.58	117.79
52	M	305	A1EB4	O4-C38-O43	-2.52	117.95	122.96
48	F	302	A86	C4-C3-C2	-2.52	118.30	123.47
39	b	811	CLA	C3B-C4B-NB	-2.52	108.17	110.52
50	2	304	A1EB1	C12-C11-C13	2.52	120.26	116.02
41	D	301	LHG	O8-C23-C24	2.52	119.83	111.91
43	V	303	DD6	O1-C20-C19	-2.52	111.49	113.38
49	6	316	KC2	C2D-C1D-ND	-2.52	108.54	110.23
48	S	304	A86	C-C1-C24	2.52	122.05	118.08
48	3	305	A86	O1-C20-C21	-2.52	112.03	115.06
49	F	307	KC2	CHB-C4A-C3A	-2.52	121.04	124.98
50	R	303	A1EB1	C3-C4-C5	-2.52	118.31	123.47
39	b	801	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
48	y	305	A86	C34-O4-C38	-2.52	113.20	117.90
39	I	311	CLA	C3B-C4B-NB	-2.52	108.18	110.52
39	Y	302	CLA	C3B-C4B-NB	-2.52	108.18	110.52
51	X	313	A1ECV	O2D-CGD-O1D	-2.52	118.91	123.84
39	a	830	CLA	CHB-C4A-NA	2.52	128.00	124.51
39	X	317	CLA	CHB-C4A-NA	2.52	128.00	124.51
50	h	203	A1EB1	O6-C42-C44	2.52	119.82	111.91
48	1	303	A86	C12-C11-C13	2.52	120.26	116.02
39	8	313	CLA	CHB-C4A-NA	2.52	128.00	124.51
49	V	308	KC2	O2D-CGD-O1D	-2.52	118.91	123.84
50	8	306	A1EB1	C25-C24-C1	-2.52	119.34	126.42
49	5	313	KC2	CHD-C4C-NC	2.52	128.03	124.20
51	X	313	A1ECV	C3-O2-CMC	2.52	120.69	115.83
48	7	307	A86	C12-C11-C13	2.52	120.25	116.02
41	j	104	LHG	C11-C10-C9	-2.52	101.63	114.42
39	8	318	CLA	CHB-C4A-NA	2.52	128.00	124.51
39	x	307	CLA	C3B-C4B-NB	-2.52	108.18	110.52
39	W	316	CLA	CHB-C4A-NA	2.52	128.00	124.51
39	5	316	CLA	CHB-C4A-NA	2.52	128.00	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	T	302	A1EB1	C3-C4-C5	-2.52	118.31	123.47
49	M	307	KC2	C2D-C1D-ND	-2.52	108.54	110.23
49	I	303	KC2	C2D-C1D-ND	-2.52	108.54	110.23
43	y	303	DD6	C21-C20-C15	-2.52	118.04	122.26
39	a	837	CLA	CHB-C4A-NA	2.52	127.99	124.51
39	T	309	CLA	CHB-C4A-NA	2.52	127.99	124.51
52	X	305	A1EB4	O3-C39-C43	2.52	119.81	111.91
39	T	313	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
49	Q	318	KC2	CHD-C4C-NC	2.52	128.02	124.20
49	A	313	KC2	C1B-CHB-C4A	-2.52	120.63	126.06
39	4	313	CLA	CHB-C4A-NA	2.52	127.99	124.51
48	G	301	A86	C25-C24-C1	-2.52	119.35	126.42
39	7	324	CLA	CHB-C1B-NB	2.52	126.92	124.26
51	Y	306	A1ECV	C4B-CHC-C1C	2.52	124.06	115.73
49	S	314	KC2	CHD-C4C-NC	2.52	128.02	124.20
39	z	311	CLA	CHB-C4A-NA	2.52	127.99	124.51
39	o	201	CLA	C3B-C4B-NB	-2.51	108.18	110.52
39	x	308	CLA	CMB-C2B-C1B	-2.51	121.54	125.37
50	T	307	A1EB1	C17-C16-C15	2.51	111.73	109.16
49	I	303	KC2	C1A-C2A-C3A	-2.51	105.12	107.11
48	9	305	A86	O1-C15-C14	-2.51	108.17	113.21
43	A	302	DD6	C33-C34-C35	-2.51	106.86	110.30
50	G	304	A1EB1	C33-C32-C31	2.51	111.65	109.21
49	P	310	KC2	C1A-NA-C4A	-2.51	105.58	106.71
43	M	304	DD6	O1-C20-C19	-2.51	111.49	113.38
48	0	308	A86	C7-C6-C8	2.51	122.04	118.08
49	0	316	KC2	O1D-CGD-CBD	-2.51	119.34	124.48
39	z	311	CLA	CAA-C2A-C3A	-2.51	110.23	116.10
48	X	302	A86	C17-C16-C15	2.51	111.73	109.16
39	B	205	CLA	C3B-C4B-NB	-2.51	108.19	110.52
39	C	305	CLA	CHB-C4A-NA	2.51	127.98	124.51
42	l	202	BCR	C21-C20-C19	-2.51	115.38	123.22
49	6	317	KC2	C1A-NA-C4A	-2.51	105.58	106.71
51	P	315	A1ECV	CMA-C3A-C2A	2.51	129.38	124.68
48	Z	303	A86	C12-C11-C13	2.51	120.24	116.02
48	2	302	A86	C40-C32-C31	-2.51	108.22	110.47
39	R	309	CLA	C3B-C4B-NB	-2.51	108.19	110.52
39	W	318	CLA	C3B-C4B-NB	-2.51	108.19	110.52
39	7	316	CLA	CMB-C2B-C1B	-2.51	121.55	125.37
48	M	302	A86	C25-C24-C1	-2.51	119.36	126.42
50	z	301	A1EB1	C34-O4-C38	-2.51	113.22	117.90
39	H	308	CLA	C3B-C4B-NB	-2.51	108.19	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	W	313	CLA	C3B-C4B-NB	-2.51	108.19	110.52
48	4	306	A86	C34-O4-C38	-2.51	113.22	117.90
39	4	314	CLA	CHB-C4A-NA	2.51	127.98	124.51
49	L	317	KC2	CHB-C4A-C3A	-2.51	121.06	124.98
49	y	316	KC2	CHD-C4C-NC	2.51	128.01	124.20
39	A	306	CLA	CHB-C1B-NB	2.51	126.91	124.26
39	I	313	CLA	CHB-C4A-NA	2.51	127.98	124.51
49	C	312	KC2	C2D-C1D-ND	-2.51	108.55	110.23
49	6	317	KC2	C2D-C1D-ND	-2.51	108.55	110.23
48	3	307	A86	C41-C32-C31	-2.51	108.23	110.47
49	R	314	KC2	CHD-C4C-NC	2.51	128.01	124.20
39	J	311	CLA	C3B-C4B-NB	-2.51	108.19	110.52
48	G	305	A86	O4-C38-O5	-2.51	117.98	122.96
50	7	303	A1EB1	O6-C42-C44	2.51	119.77	111.91
39	R	316	CLA	C3B-C4B-NB	-2.51	108.19	110.52
39	T	309	CLA	C3B-C4B-NB	-2.51	108.19	110.52
51	L	318	A1ECV	C4B-CHC-C1C	2.51	124.03	115.73
42	h	202	BCR	C11-C10-C9	-2.51	123.73	127.31
52	M	322	A1EB4	C20-C19-C18	-2.51	107.79	112.75
49	W	314	KC2	CHD-C4C-NC	2.51	128.00	124.20
39	b	836	CLA	CHB-C4A-NA	2.50	127.97	124.51
49	6	317	KC2	CHD-C4C-NC	2.50	128.00	124.20
39	8	315	CLA	C3B-C4B-NB	-2.50	108.19	110.52
39	J	318	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
50	y	302	A1EB1	C35-C34-C33	-2.50	105.51	109.88
39	M	308	CLA	C3B-C4B-NB	-2.50	108.19	110.52
48	7	307	A86	C4-C5-C6	-2.50	123.74	127.31
43	D	307	DD6	C37-C36-C31	-2.50	120.95	124.35
39	Y	313	CLA	CHB-C4A-NA	2.50	127.97	124.51
43	J	304	DD6	C12-C11-C10	-2.50	119.42	122.92
39	R	315	CLA	O2D-CGD-CBD	2.50	115.71	111.27
50	3	302	A1EB1	C12-C11-C13	2.50	120.22	116.02
39	Z	312	CLA	CHB-C4A-NA	2.50	127.97	124.51
39	9	312	CLA	CHD-C1D-ND	-2.50	122.16	124.45
51	L	318	A1ECV	O1D-CGD-CBD	-2.50	120.58	124.74
50	C	302	A1EB1	C34-O4-C38	-2.50	113.24	117.90
49	3	317	KC2	C2D-C1D-ND	-2.50	108.56	110.23
50	8	306	A1EB1	O1-C20-C19	-2.50	111.50	113.38
39	a	822	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
48	7	311	A86	C41-C32-C31	-2.50	108.23	110.47
47	W	301	SQD	C4-C3-C2	2.50	115.19	110.82
51	z	310	A1ECV	O1D-CGD-CBD	-2.50	120.58	124.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	V	319	CLA	C3B-C4B-NB	-2.50	108.20	110.52
39	0	313	CLA	C3B-C4B-NB	-2.50	108.20	110.52
48	y	305	A86	C9-C8-C6	-2.50	119.40	126.42
50	V	302	A1EB1	O4-C34-C33	2.50	113.81	107.59
43	y	304	DD6	C25-C26-C27	-2.50	119.33	126.58
39	7	313	CLA	CHB-C4A-NA	2.50	127.97	124.51
39	Y	303	CLA	CHB-C4A-NA	2.50	127.97	124.51
39	b	829	CLA	C3B-C4B-NB	-2.50	108.20	110.52
39	z	318	CLA	C3B-C4B-NB	-2.50	108.20	110.52
50	V	305	A1EB1	C41-C32-C31	-2.50	108.24	110.47
48	J	303	A86	C25-C26-C27	-2.50	123.75	127.31
46	M	320	LMG	O6-C1-O1	-2.50	104.06	109.97
50	T	307	A1EB1	O6-C42-C44	2.50	119.74	111.91
49	4	324	KC2	C2D-C1D-ND	-2.50	108.56	110.23
39	O	310	CLA	CMB-C2B-C1B	-2.50	121.57	125.37
51	Q	316	A1ECV	C3-O2-CMC	2.50	120.65	115.83
39	H	308	CLA	CHB-C4A-NA	2.50	127.96	124.51
43	y	304	DD6	C10-C9-C8	-2.50	115.43	123.22
48	0	309	A86	O4-C38-O5	-2.50	118.00	122.96
48	0	309	A86	C25-C24-C1	-2.50	119.40	126.42
39	G	310	CLA	CHB-C4A-NA	2.50	127.96	124.51
39	2	315	CLA	CHB-C4A-NA	2.50	127.96	124.51
49	W	312	KC2	CHD-C4C-NC	2.50	127.99	124.20
39	D	313	CLA	C3B-C4B-NB	-2.50	108.20	110.52
39	b	813	CLA	CMB-C2B-C3B	2.50	130.06	123.59
39	Q	310	CLA	CMB-C2B-C1B	-2.50	121.57	125.37
43	y	303	DD6	C3-C4-C5	-2.50	118.36	123.47
49	V	314	KC2	CHD-C4C-NC	2.49	127.99	124.20
49	4	318	KC2	CHB-C4A-C3A	-2.49	121.08	124.98
43	H	303	DD6	C9-C10-C11	-2.49	123.75	127.31
39	0	312	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
39	a	808	CLA	C3B-C4B-NB	-2.49	108.20	110.52
48	3	305	A86	C7-C6-C5	-2.49	119.43	122.92
49	J	315	KC2	O1D-CGD-CBD	-2.49	119.38	124.48
39	a	825	CLA	CMB-C2B-C3B	2.49	132.63	126.59
48	L	306	A86	O1-C15-C14	-2.49	108.21	113.21
49	X	315	KC2	CHD-C4C-NC	2.49	127.99	124.20
39	0	310	CLA	CHB-C4A-NA	2.49	127.96	124.51
46	9	321	LMG	O6-C1-O1	-2.49	104.07	109.97
49	5	314	KC2	CHD-C4C-NC	2.49	127.98	124.20
39	b	830	CLA	CHB-C4A-NA	2.49	127.96	124.51
52	P	318	A1EB4	O3-C39-C43	2.49	119.73	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	W	307	A86	C12-C11-C13	2.49	120.21	116.02
48	X	302	A86	O1-C20-C21	-2.49	112.07	115.06
49	7	319	KC2	O1D-CGD-CBD	-2.49	119.39	124.48
51	x	310	A1ECV	O2D-CGD-O1D	-2.49	118.97	123.84
49	Q	313	KC2	C1B-CHB-C4A	-2.49	120.68	126.06
50	J	302	A1EB1	C4-C3-C2	-2.49	118.37	123.47
48	4	309	A86	C34-O4-C38	-2.49	113.25	117.90
48	1	302	A86	C33-C32-C31	2.49	111.63	109.21
42	f	801	BCR	C7-C8-C9	-2.49	122.47	126.23
39	O	309	CLA	CHC-C4B-NB	2.49	126.89	124.26
48	6	302	A86	C4-C3-C2	-2.49	118.37	123.47
48	4	310	A86	O1-C20-C21	-2.49	112.07	115.06
43	z	305	DD6	C21-C20-C15	-2.49	118.09	122.26
50	V	306	A1EB1	C36-C31-C32	2.49	122.17	119.70
39	b	812	CLA	C3B-C4B-NB	-2.49	108.20	110.52
42	m	101	BCR	C27-C26-C25	2.49	126.35	122.73
49	8	314	KC2	O2D-CGD-O1D	-2.49	118.97	123.84
48	R	301	A86	C4-C3-C2	-2.49	118.37	123.47
43	B	202	DD6	C15-C14-C13	-2.49	120.73	125.99
49	F	307	KC2	CHD-C4C-NC	2.49	127.98	124.20
39	S	316	CLA	CHB-C4A-NA	2.49	127.95	124.51
49	3	317	KC2	CHD-C4C-NC	2.49	127.98	124.20
39	F	321	CLA	C1-C2-C3	-2.49	121.74	126.04
39	b	813	CLA	CAB-C3B-C2B	2.49	130.04	123.59
41	X	301	LHG	O8-C23-C24	2.49	119.72	111.91
39	4	323	CLA	C3B-C4B-NB	-2.49	108.21	110.52
49	x	312	KC2	CHD-C4C-NC	2.49	127.98	124.20
50	h	203	A1EB1	C40-C32-C31	-2.49	108.25	110.47
50	z	302	A1EB1	C40-C32-C31	-2.49	108.25	110.47
50	0	305	A1EB1	C25-C24-C1	-2.49	119.43	126.42
49	V	315	KC2	C1A-NA-C4A	-2.49	105.59	106.71
48	K	301	A86	C10-C9-C8	-2.49	115.46	123.22
52	P	319	A1EB4	C20-C19-C18	-2.49	107.83	112.75
49	8	317	KC2	C2D-C1D-ND	-2.49	108.57	110.23
39	4	312	CLA	O2D-CGD-CBD	2.49	115.68	111.27
39	A	306	CLA	CMB-C2B-C3B	2.48	132.61	126.59
39	H	316	CLA	C3B-C4B-NB	-2.48	108.21	110.52
39	V	311	CLA	C3B-C4B-NB	-2.48	108.21	110.52
48	V	301	A86	C12-C11-C13	2.48	120.20	116.02
43	P	304	DD6	C24-C1-C2	2.48	122.75	118.94
48	C	303	A86	C12-C11-C13	2.48	120.19	116.02
39	7	324	CLA	O2D-CGD-CBD	2.48	115.68	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	0	307	A1EB1	O6-C42-C44	2.48	119.70	111.91
39	M	309	CLA	C3B-C4B-NB	-2.48	108.21	110.52
48	L	301	A86	C34-O4-C38	-2.48	113.27	117.90
50	8	306	A1EB1	O6-C42-C44	2.48	119.70	111.91
50	V	305	A1EB1	C28-C27-C26	-2.48	121.69	124.93
39	4	312	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
48	D	305	A86	O4-C38-O5	-2.48	118.03	122.96
39	A	307	CLA	C3B-C4B-NB	-2.48	108.21	110.52
49	z	313	KC2	CHC-C4B-C3B	-2.48	121.01	125.26
49	L	317	KC2	O1D-CGD-CBD	-2.48	119.41	124.48
48	J	301	A86	O4-C38-O5	-2.48	118.03	122.96
48	T	305	A86	O4-C38-O5	-2.48	118.03	122.96
43	D	306	DD6	C15-C14-C13	-2.48	120.75	125.99
50	R	303	A1EB1	C10-C9-C8	-2.48	115.47	123.22
39	A	312	CLA	CHB-C4A-NA	2.48	127.94	124.51
48	8	323	A86	C25-C24-C1	-2.48	119.45	126.42
49	P	306	KC2	CHB-C4A-C3A	-2.48	121.10	124.98
49	T	316	KC2	C2D-C1D-ND	-2.48	108.57	110.23
50	7	305	A1EB1	C40-C32-C31	-2.48	108.25	110.47
39	6	311	CLA	CHB-C4A-NA	2.48	127.94	124.51
51	x	316	A1ECV	O1D-CGD-CBD	-2.48	120.61	124.74
48	T	306	A86	C26-C25-C24	-2.48	115.48	123.22
39	H	310	CLA	C3B-C4B-NB	-2.48	108.22	110.52
49	P	320	KC2	CHB-C4A-C3A	-2.48	121.11	124.98
51	9	314	A1ECV	O2D-CGD-O1D	-2.48	118.99	123.84
42	j	103	BCR	C28-C27-C26	-2.48	109.65	114.08
50	3	324	A1EB1	C33-C32-C31	2.48	111.62	109.21
39	S	320	CLA	C3B-C4B-NB	-2.48	108.22	110.52
39	Z	312	CLA	C3B-C4B-NB	-2.48	108.22	110.52
49	Y	309	KC2	CHD-C4C-NC	2.48	127.96	124.20
49	L	314	KC2	C2D-C1D-ND	-2.48	108.57	110.23
47	M	301	SQD	O5-C5-C4	2.48	114.19	109.69
51	0	321	A1ECV	C1B-CHB-C4A	2.48	123.94	115.73
49	C	313	KC2	CHD-C4C-NC	2.48	127.96	124.20
52	R	305	A1EB4	C12-C11-C13	2.48	119.46	115.30
43	7	310	DD6	C32-C31-C36	-2.48	119.14	122.63
49	M	307	KC2	CHD-C4C-NC	2.48	127.96	124.20
39	V	319	CLA	CHB-C4A-NA	2.48	127.94	124.51
48	2	302	A86	O4-C38-O5	-2.48	118.04	122.96
39	7	321	CLA	C3B-C4B-NB	-2.48	108.22	110.52
39	I	316	CLA	C3B-C4B-NB	-2.48	108.22	110.52
49	L	315	KC2	C1A-NA-C4A	-2.48	105.59	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	a	801	CLA	CHB-C4A-NA	2.48	127.94	124.51
51	y	317	A1ECV	O1D-CGD-CBD	-2.47	120.62	124.74
43	x	303	DD6	C25-C26-C27	-2.47	119.39	126.58
39	R	308	CLA	CHB-C4A-NA	2.47	127.93	124.51
39	T	320	CLA	CHB-C4A-NA	2.47	127.93	124.51
39	9	315	CLA	CHB-C4A-NA	2.47	127.93	124.51
47	9	322	SQD	C4-C3-C2	2.47	115.14	110.82
50	9	302	A1EB1	C35-C34-C33	-2.47	105.56	109.88
43	P	304	DD6	C8-C6-C5	2.47	122.74	118.94
49	x	315	KC2	CHD-C4C-NC	2.47	127.96	124.20
43	X	304	DD6	C37-C36-C35	2.47	118.94	114.36
42	b	848	BCR	C34-C9-C8	2.47	121.97	118.08
39	O	311	CLA	CHB-C1B-NB	2.47	126.88	124.26
42	f	804	BCR	C15-C16-C17	-2.47	118.41	123.47
49	C	312	KC2	CHD-C4C-NC	2.47	127.95	124.20
49	K	310	KC2	CHD-C4C-NC	2.47	127.95	124.20
39	a	847	CLA	CHB-C4A-NA	2.47	127.93	124.51
39	a	832	CLA	C3B-C4B-NB	-2.47	108.22	110.52
39	8	310	CLA	C3B-C4B-NB	-2.47	108.22	110.52
50	G	302	A1EB1	C3-C4-C5	-2.47	118.41	123.47
39	O	313	CLA	C1-C2-C3	-2.47	122.75	126.75
49	6	316	KC2	CHD-C4C-NC	2.47	127.95	124.20
49	3	315	KC2	C4D-C3D-CAD	2.47	109.09	107.42
49	2	317	KC2	CHD-C4C-NC	2.47	127.95	124.20
42	a	843	BCR	C27-C26-C25	-2.47	119.14	122.73
49	K	313	KC2	O1D-CGD-CBD	-2.47	119.43	124.48
48	8	302	A86	O4-C38-O5	-2.47	118.06	122.96
48	k	206	A86	C35-C34-C33	-2.47	105.57	109.88
49	G	317	KC2	C2D-C1D-ND	-2.47	108.58	110.23
49	C	312	KC2	O1D-CGD-CBD	-2.47	119.43	124.48
43	j	102	DD6	C15-C14-C13	-2.47	120.78	125.99
43	3	304	DD6	C12-C11-C10	-2.47	119.47	122.92
49	P	313	KC2	O2D-CGD-O1D	-2.47	119.01	123.84
50	y	302	A1EB1	O6-C42-C44	2.47	119.65	111.91
48	J	301	A86	C4-C3-C2	-2.47	118.42	123.47
42	f	801	BCR	C15-C14-C13	-2.47	123.79	127.31
50	R	303	A1EB1	C33-C32-C31	2.47	111.61	109.21
50	y	301	A1EB1	C33-C32-C31	2.47	111.61	109.21
39	U	213	CLA	C3B-C4B-NB	-2.47	108.23	110.52
50	4	303	A1EB1	O1-C20-C21	-2.47	112.10	115.06
48	H	302	A86	C25-C26-C27	-2.47	123.79	127.31
39	D	317	CLA	C3B-C4B-NB	-2.47	108.23	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	K	312	CLA	C3B-C4B-NB	-2.47	108.23	110.52
50	L	303	A1EB1	C35-C34-C33	-2.46	105.58	109.88
39	K	308	CLA	CHB-C4A-NA	2.46	127.92	124.51
39	S	311	CLA	CHB-C4A-NA	2.46	127.92	124.51
52	T	304	A1EB4	O4-C38-O43	-2.46	118.07	122.96
48	Q	301	A86	C35-C34-C33	2.46	114.18	109.88
39	K	309	CLA	C3B-C4B-NB	-2.46	108.23	110.52
39	J	314	CLA	CHB-C4A-NA	2.46	127.92	124.51
39	J	318	CLA	CMB-C2B-C1B	-2.46	121.62	125.37
48	X	302	A86	C9-C10-C11	-2.46	119.36	126.61
39	R	316	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
39	a	812	CLA	CHB-C4A-NA	2.46	127.92	124.51
39	O	310	CLA	CHB-C4A-NA	2.46	127.92	124.51
49	L	314	KC2	C4D-C3D-CAD	2.46	109.08	107.42
49	V	318	KC2	C1B-CHB-C4A	-2.46	120.75	126.06
49	P	310	KC2	CHD-C4C-NC	2.46	127.94	124.20
52	M	305	A1EB4	C21-C20-C15	-2.46	118.16	122.32
39	J	317	CLA	CHB-C4A-NA	2.46	127.92	124.51
39	7	318	CLA	CHB-C4A-NA	2.46	127.92	124.51
43	O	304	DD6	C-C1-C2	-2.46	119.47	122.92
50	V	307	A1EB1	C28-O6-C42	2.46	121.16	115.68
49	P	312	KC2	CHD-C4C-NC	2.46	127.94	124.20
39	T	313	CLA	C3B-C4B-NB	-2.46	108.23	110.52
39	2	319	CLA	C3B-C4B-NB	-2.46	108.23	110.52
49	M	311	KC2	CHD-C4C-NC	2.46	127.94	124.20
48	O	302	A86	C19-C18-C17	2.46	115.52	110.77
42	b	847	BCR	C8-C7-C6	-2.46	120.29	127.20
49	R	312	KC2	CHD-C4C-NC	2.46	127.94	124.20
49	M	313	KC2	C2D-C1D-ND	-2.46	108.58	110.23
42	b	845	BCR	C28-C27-C26	-2.46	109.69	114.08
42	b	850	BCR	C16-C15-C14	-2.46	118.44	123.47
47	M	301	SQD	O48-C23-C24	2.46	119.62	111.91
51	G	316	A1ECV	O1D-CGD-CBD	-2.46	120.64	124.74
48	O	307	A86	C9-C10-C11	-2.46	119.38	126.61
49	y	313	KC2	CHD-C4C-NC	2.46	127.93	124.20
39	S	319	CLA	O2D-CGD-CBD	2.46	115.64	111.27
39	b	829	CLA	CHB-C4A-NA	2.46	127.91	124.51
48	L	302	A86	C12-C11-C13	2.46	120.15	116.02
49	3	318	KC2	CBD-CHA-C1A	2.46	133.46	128.88
51	5	309	A1ECV	C3-O2-CMC	2.46	120.57	115.83
50	G	304	A1EB1	C26-C25-C24	-2.46	115.55	123.22
39	Z	306	CLA	C3B-C4B-NB	-2.46	108.24	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	H	315	CLA	CHB-C4A-NA	2.46	127.91	124.51
47	F	318	SQD	C44-O6-C1	2.46	118.54	113.74
48	C	303	A86	C35-C34-C33	2.46	114.16	109.88
43	A	304	DD6	C4-C3-C2	-2.46	118.44	123.47
39	b	806	CLA	C1-C2-C3	-2.46	121.80	126.04
48	M	302	A86	C9-C8-C6	-2.46	119.52	126.42
39	U	207	CLA	CHB-C4A-NA	2.46	127.91	124.51
50	D	308	A1EB1	C35-C34-C33	-2.46	105.59	109.88
43	z	305	DD6	C10-C9-C8	-2.45	115.56	123.22
51	y	311	A1ECV	O1D-CGD-CBD	-2.45	120.65	124.74
39	a	823	CLA	CHB-C4A-NA	2.45	127.91	124.51
39	B	203	CLA	CHD-C1D-ND	-2.45	122.20	124.45
48	L	304	A86	C26-C25-C24	-2.45	115.56	123.22
48	4	310	A86	C4-C3-C2	-2.45	118.45	123.47
43	R	304	DD6	C37-C36-C31	-2.45	121.02	124.35
47	W	301	SQD	O5-C5-C4	2.45	114.15	109.69
39	a	824	CLA	CHB-C1B-NB	2.45	126.85	124.26
48	Q	305	A86	C12-C11-C13	2.45	120.14	116.02
49	5	305	KC2	CHB-C4A-C3A	-2.45	121.15	124.98
41	D	301	LHG	C11-C10-C9	-2.45	101.97	114.42
42	i	102	BCR	C10-C11-C12	-2.45	115.56	123.22
39	a	819	CLA	C3B-C4B-NB	-2.45	108.24	110.52
39	D	318	CLA	C3B-C4B-NB	-2.45	108.24	110.52
39	l	203	CLA	CHB-C4A-NA	2.45	127.90	124.51
39	D	309	CLA	O2D-CGD-CBD	2.45	115.62	111.27
50	3	310	A1EB1	C34-O4-C38	-2.45	113.33	117.90
39	C	305	CLA	C3B-C4B-NB	-2.45	108.24	110.52
49	P	306	KC2	C1A-NA-C4A	-2.45	105.60	106.71
49	W	312	KC2	C1A-NA-C4A	-2.45	105.60	106.71
49	Z	311	KC2	C1A-NA-C4A	-2.45	105.60	106.71
50	7	306	A1EB1	C9-C10-C11	-2.45	119.40	126.61
48	G	301	A86	O4-C38-O5	-2.45	118.09	122.96
50	O	301	A1EB1	C25-C24-C1	-2.45	119.53	126.42
48	L	304	A86	C40-C32-C31	-2.45	108.28	110.47
39	E	312	CLA	CHB-C1B-NB	2.45	126.85	124.26
51	6	320	A1ECV	O2D-CGD-O1D	-2.45	119.05	123.84
42	b	844	BCR	C20-C19-C18	-2.45	119.53	126.42
49	O	317	KC2	CHC-C4B-C3B	-2.45	121.07	125.26
49	H	314	KC2	CHD-C4C-NC	2.45	127.92	124.20
42	i	102	BCR	C20-C19-C18	-2.45	119.54	126.42
49	2	317	KC2	C1A-C2A-C3A	-2.45	105.17	107.11
42	h	202	BCR	C10-C11-C12	-2.45	115.58	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	4	327	SQD	O5-C5-C4	2.45	114.14	109.69
49	V	318	KC2	CHD-C4C-NC	2.45	127.92	124.20
50	4	301	A1EB1	C3-C4-C5	-2.45	118.46	123.47
51	0	321	A1ECV	O2D-CGD-O1D	-2.45	119.05	123.84
49	H	314	KC2	O1D-CGD-CBD	-2.45	119.48	124.48
49	6	316	KC2	O1D-CGD-CBD	-2.45	119.48	124.48
43	O	304	DD6	C3-C4-C5	-2.45	118.46	123.47
48	S	307	A86	C4-C3-C2	-2.45	118.46	123.47
39	C	308	CLA	C3B-C4B-NB	-2.45	108.25	110.52
39	b	835	CLA	C3B-C4B-NB	-2.44	108.25	110.52
39	4	313	CLA	C3B-C4B-NB	-2.44	108.25	110.52
39	2	315	CLA	C3B-C4B-NB	-2.44	108.25	110.52
52	X	305	A1EB4	C12-O3-C39	2.44	121.12	115.68
49	A	313	KC2	O1D-CGD-CBD	-2.44	119.48	124.48
39	V	316	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
42	l	207	BCR	C33-C5-C6	-2.44	121.78	124.53
39	1	311	CLA	CHB-C4A-NA	2.44	127.89	124.51
50	0	303	A1EB1	C4-C3-C2	-2.44	118.47	123.47
50	7	303	A1EB1	C41-C32-C31	-2.44	108.29	110.47
39	O	308	CLA	C3B-C4B-NB	-2.44	108.25	110.52
39	Y	311	CLA	C3B-C4B-NB	-2.44	108.25	110.52
49	0	316	KC2	C2A-C3A-C4A	2.44	108.30	106.49
39	V	310	CLA	CHB-C1B-NB	2.44	126.84	124.26
50	7	306	A1EB1	O6-C42-C44	2.44	119.57	111.91
48	L	307	A86	C7-C6-C8	2.44	121.92	118.08
48	1	306	A86	C34-O4-C38	-2.44	113.35	117.90
39	O	318	CLA	C3B-C4B-NB	-2.44	108.25	110.52
39	I	314	CLA	C3B-C4B-NB	-2.44	108.25	110.52
48	X	303	A86	C41-C32-C31	-2.44	108.29	110.47
42	a	843	BCR	C38-C26-C25	-2.44	121.79	124.53
42	l	202	BCR	C38-C26-C27	2.44	118.31	113.62
48	4	310	A86	O4-C38-O5	-2.44	118.11	122.96
49	0	314	KC2	CHD-C4C-NC	2.44	127.91	124.20
39	T	308	CLA	CHB-C4A-NA	2.44	127.89	124.51
39	b	818	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
49	I	303	KC2	CHD-C4C-NC	2.44	127.90	124.20
42	b	844	BCR	C2-C1-C6	2.44	114.23	110.48
51	x	316	A1ECV	C4B-CHC-C1C	2.44	123.81	115.73
39	9	310	CLA	C3B-C4B-NB	-2.44	108.25	110.52
39	b	801	CLA	C1-C2-C3	-2.44	121.83	126.04
49	z	315	KC2	C4D-C3D-CAD	2.44	109.06	107.42
48	6	307	A86	C25-C24-C1	-2.44	119.57	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	b	847	BCR	C38-C26-C25	-2.44	121.79	124.53
43	B	202	DD6	C9-C8-C6	-2.44	119.57	126.42
39	C	307	CLA	C3B-C4B-NB	-2.44	108.25	110.52
39	y	308	CLA	C3B-C4B-NB	-2.44	108.25	110.52
39	3	311	CLA	CHB-C4A-NA	2.44	127.88	124.51
39	G	310	CLA	CAC-C3C-C4C	2.44	127.97	124.81
50	z	301	A1EB1	C33-C32-C31	2.44	111.58	109.21
49	T	312	KC2	CHB-C4A-C3A	-2.44	121.17	124.98
48	S	305	A86	C25-C24-C1	-2.44	119.57	126.42
39	Q	314	CLA	C3B-C4B-NB	-2.44	108.25	110.52
51	y	317	A1ECV	C4B-CHC-C1C	2.44	123.80	115.73
39	b	839	CLA	CHB-C4A-NA	2.44	127.88	124.51
50	T	307	A1EB1	C28-O6-C42	2.44	121.10	115.68
39	K	306	CLA	CHB-C4A-NA	2.43	127.88	124.51
49	8	316	KC2	CHD-C4C-NC	2.43	127.90	124.20
43	Q	306	DD6	C21-C20-C15	-2.43	118.18	122.26
51	7	323	A1ECV	CMA-C3A-C2A	2.43	129.23	124.68
39	z	311	CLA	C3B-C4B-NB	-2.43	108.26	110.52
39	b	836	CLA	CMB-C2B-C3B	2.43	132.48	126.59
50	5	302	A1EB1	O4-C38-O5	-2.43	118.13	122.96
49	7	320	KC2	CHD-C4C-NC	2.43	127.89	124.20
49	7	322	KC2	CHD-C4C-NC	2.43	127.89	124.20
49	3	321	KC2	CHB-C1B-C2B	-2.43	120.38	125.48
39	U	209	CLA	C3B-C4B-NB	-2.43	108.26	110.52
49	3	321	KC2	O2D-CGD-O1D	-2.43	119.08	123.84
48	V	304	A86	C10-C9-C8	-2.43	115.63	123.22
48	9	301	A86	C4-C3-C2	-2.43	118.49	123.47
48	Z	301	A86	C9-C10-C11	-2.43	119.46	126.61
48	6	307	A86	C34-O4-C38	-2.43	113.37	117.90
39	z	307	CLA	CMB-C2B-C3B	2.43	132.47	126.59
43	D	303	DD6	C9-C8-C6	-2.43	119.59	126.42
50	x	302	A1EB1	C9-C8-C6	-2.43	119.59	126.42
49	M	314	KC2	C2A-C3A-C4A	2.43	108.29	106.49
49	0	314	KC2	C4D-C3D-CAD	2.43	109.06	107.42
49	M	314	KC2	CHD-C4C-NC	2.43	127.89	124.20
49	X	318	KC2	CHD-C4C-NC	2.43	127.89	124.20
48	1	306	A86	C25-C24-C1	-2.43	119.59	126.42
48	1	307	A86	C4-C3-C2	-2.43	118.50	123.47
48	M	306	A86	O1-C20-C19	-2.43	111.56	113.38
39	T	319	CLA	C3B-C4B-NB	-2.43	108.26	110.52
50	F	304	A1EB1	C26-C25-C24	-2.43	115.64	123.22
49	G	311	KC2	CHD-C4C-NC	2.43	127.89	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	Q	319	A1ECV	C4B-CHC-C1C	2.43	123.78	115.73
43	X	304	DD6	C40-C32-C31	-2.43	106.61	110.47
48	X	303	A86	C3-C4-C5	-2.43	118.50	123.47
49	J	315	KC2	CHD-C4C-NC	2.43	127.89	124.20
43	Q	306	DD6	C9-C10-C11	-2.43	123.85	127.31
48	W	303	A86	C4-C3-C2	-2.43	118.50	123.47
49	1	315	KC2	CHD-C4C-NC	2.43	127.89	124.20
48	2	301	A86	C36-C31-C32	2.43	122.10	119.70
48	Q	305	A86	O4-C38-O5	-2.43	118.14	122.96
50	K	305	A1EB1	C25-C26-C27	-2.43	123.81	127.26
39	E	307	CLA	CMB-C2B-C3B	2.43	132.46	126.59
49	M	311	KC2	CHB-C4A-C3A	-2.43	121.19	124.98
48	L	302	A86	C34-O4-C38	-2.42	113.38	117.90
52	M	305	A1EB4	O1-C15-C14	-2.42	113.25	115.71
50	0	307	A1EB1	C20-C19-C18	-2.42	107.95	112.75
49	P	320	KC2	C1A-NA-C4A	-2.42	105.62	106.71
39	1	311	CLA	C3B-C4B-NB	-2.42	108.27	110.52
48	3	307	A86	O4-C38-O5	-2.42	118.15	122.96
50	K	302	A1EB1	O4-C38-O5	-2.42	118.15	122.96
49	1	314	KC2	O1D-CGD-CBD	-2.42	119.52	124.48
49	9	316	KC2	O2D-CGD-O1D	-2.42	119.10	123.84
39	O	314	CLA	CHB-C1B-NB	2.42	126.82	124.26
48	6	305	A86	C41-C32-C31	-2.42	108.30	110.47
49	C	313	KC2	CHB-C4A-C3A	-2.42	121.19	124.98
49	M	313	KC2	O1D-CGD-CBD	-2.42	119.53	124.48
50	H	301	A1EB1	O6-C42-C44	2.42	119.51	111.91
48	6	307	A86	C9-C10-C11	-2.42	119.49	126.61
49	X	315	KC2	C1A-NA-C4A	-2.42	105.62	106.71
39	a	809	CLA	CHD-C1D-ND	-2.42	122.23	124.45
39	7	318	CLA	C3B-C4B-NB	-2.42	108.27	110.52
51	1	318	A1ECV	O1D-CGD-CBD	-2.42	120.70	124.74
42	b	847	BCR	C11-C12-C13	-2.42	119.61	126.42
39	L	309	CLA	CMB-C2B-C3B	2.42	132.45	126.59
47	F	318	SQD	O48-C23-C24	2.42	119.51	111.91
42	l	206	BCR	C15-C16-C17	-2.42	118.51	123.47
48	8	323	A86	O4-C38-O5	-2.42	118.15	122.96
49	I	303	KC2	C4D-C3D-CAD	2.42	109.05	107.42
49	Z	311	KC2	C4D-C3D-CAD	2.42	109.05	107.42
49	G	317	KC2	CHD-C4C-NC	2.42	127.88	124.20
50	6	304	A1EB1	C28-O6-C42	2.42	121.07	115.68
48	9	306	A86	C3-C4-C5	-2.42	118.52	123.47
39	a	827	CLA	CHB-C4A-NA	2.42	127.86	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	H	318	SQD	O48-C23-C24	2.42	119.50	111.91
39	9	310	CLA	CMB-C2B-C3B	2.42	132.45	126.59
49	1	315	KC2	CBD-CHA-C4D	-2.42	103.35	109.14
39	8	322	CLA	CHD-C1D-ND	-2.42	122.23	124.45
49	A	313	KC2	C1A-NA-C4A	-2.42	105.62	106.71
47	E	320	SQD	O48-C23-C24	2.42	119.50	111.91
39	j	101	CLA	CMB-C2B-C3B	2.42	132.45	126.59
48	4	328	A86	O4-C38-O5	-2.42	118.16	122.96
50	H	301	A1EB1	C4-C3-C2	-2.42	118.52	123.47
48	S	304	A86	O4-C38-O5	-2.42	118.16	122.96
48	3	308	A86	O4-C38-O5	-2.42	118.16	122.96
39	b	807	CLA	CAC-C3C-C4C	2.42	127.95	124.81
42	k	204	BCR	C16-C15-C14	-2.42	118.52	123.47
48	7	311	A86	C36-C31-C32	2.42	122.09	119.70
50	H	301	A1EB1	O1-C20-C21	-2.42	112.16	115.06
39	E	307	CLA	CHB-C4A-NA	2.42	127.85	124.51
49	Y	308	KC2	O1D-CGD-CBD	-2.42	119.54	124.48
39	i	101	CLA	C3B-C4B-NB	-2.42	108.27	110.52
39	x	317	CLA	C3B-C4B-NB	-2.42	108.27	110.52
50	y	302	A1EB1	O4-C38-O5	-2.42	118.16	122.96
39	a	829	CLA	CMB-C2B-C1B	-2.42	121.69	125.37
49	x	313	KC2	C1A-NA-C4A	-2.42	105.62	106.71
49	4	320	KC2	C4D-C3D-CAD	2.42	109.05	107.42
49	L	312	KC2	C1B-CHB-C4A	-2.42	120.85	126.06
39	K	311	CLA	CHB-C4A-NA	2.42	127.85	124.51
48	5	301	A86	C34-O4-C38	-2.42	113.39	117.90
39	b	830	CLA	CMB-C2B-C3B	2.41	132.44	126.59
50	F	304	A1EB1	C41-C32-C31	-2.41	108.31	110.47
39	K	307	CLA	C3B-C4B-NB	-2.41	108.28	110.52
47	S	301	SQD	O5-C1-C2	2.41	115.46	110.35
39	D	310	CLA	CHB-C4A-NA	2.41	127.85	124.51
39	y	319	CLA	CHB-C4A-NA	2.41	127.85	124.51
48	B	201	A86	O4-C38-O5	-2.41	118.17	122.96
39	Q	317	CLA	C3B-C4B-NB	-2.41	108.28	110.52
49	0	314	KC2	C1A-NA-C4A	-2.41	105.62	106.71
49	7	320	KC2	C1A-NA-C4A	-2.41	105.62	106.71
51	X	310	A1ECV	O1D-CGD-CBD	-2.41	120.72	124.74
43	H	305	DD6	C28-C27-C29	2.41	121.62	116.84
39	a	820	CLA	CHB-C4A-NA	2.41	127.85	124.51
49	S	315	KC2	CHD-C4C-NC	2.41	127.86	124.20
50	V	302	A1EB1	C40-C32-C31	-2.41	108.31	110.47
48	6	309	A86	C28-C27-C26	-2.41	119.54	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	y	317	A1ECV	O2D-CGD-O1D	-2.41	119.12	123.84
47	7	302	SQD	O47-C7-O49	-2.41	117.87	123.70
39	b	841	CLA	CHB-C4A-NA	2.41	127.85	124.51
50	U	205	A1EB1	C9-C8-C6	-2.41	119.64	126.42
39	i	103	CLA	CHB-C1B-NB	2.41	126.81	124.26
49	0	319	KC2	CHB-C1B-C2B	-2.41	120.42	125.48
48	3	307	A86	C-C1-C2	-2.41	119.55	122.92
50	z	302	A1EB1	C28-O6-C42	2.41	121.04	115.68
49	R	312	KC2	C2A-C3A-C4A	2.41	108.27	106.49
51	R	310	A1ECV	O2-CMC-O1	-2.41	118.74	123.45
43	B	202	DD6	C32-C31-C36	-2.41	119.23	122.63
48	F	302	A86	C3-C2-C1	-2.41	123.87	127.31
47	k	205	SQD	C4-C3-C2	2.41	115.03	110.82
50	1	301	A1EB1	C28-O6-C42	2.41	121.04	115.68
39	h	201	CLA	C3B-C4B-NB	-2.41	108.28	110.52
49	M	311	KC2	C1A-NA-C4A	-2.41	105.62	106.71
39	1	309	CLA	CHB-C4A-NA	2.41	127.84	124.51
39	Y	304	CLA	C3B-C4B-NB	-2.41	108.28	110.52
48	6	303	A86	C40-C32-C31	-2.41	108.32	110.47
39	A	306	CLA	CHB-C4A-NA	2.41	127.84	124.51
43	I	305	DD6	C41-C32-C31	-2.41	106.64	110.47
50	H	301	A1EB1	C9-C8-C6	-2.41	119.65	126.42
48	1	303	A86	C33-C32-C31	2.41	111.55	109.21
48	S	304	A86	C34-O4-C38	-2.41	113.41	117.90
39	A	308	CLA	CHB-C4A-NA	2.41	127.84	124.51
43	x	303	DD6	C32-C31-C36	-2.40	119.24	122.63
39	H	306	CLA	C3B-C4B-NB	-2.40	108.28	110.52
50	3	302	A1EB1	C28-O6-C42	2.40	121.03	115.68
39	b	811	CLA	O2D-CGD-CBD	2.40	115.54	111.27
49	5	305	KC2	C2D-C1D-ND	-2.40	108.62	110.23
50	S	302	A1EB1	O1-C20-C21	-2.40	112.17	115.06
49	4	320	KC2	CHB-C4A-C3A	-2.40	121.22	124.98
48	0	304	A86	O1-C20-C19	-2.40	111.58	113.38
52	X	305	A1EB4	C25-C26-C27	-2.40	123.88	127.31
48	0	308	A86	C34-O4-C38	2.40	122.38	117.90
50	6	308	A1EB1	C4-C3-C2	-2.40	118.55	123.47
51	y	317	A1ECV	C3-O2-CMC	2.40	120.47	115.83
42	a	843	BCR	C33-C5-C4	2.40	118.23	113.62
48	D	305	A86	C19-C18-C17	2.40	115.41	110.77
48	I	304	A86	O4-C38-O5	-2.40	118.19	122.96
49	W	312	KC2	CHB-C4A-C3A	-2.40	121.22	124.98
39	O	316	CLA	C3B-C4B-NB	-2.40	108.29	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	K	313	KC2	CHD-C4C-NC	2.40	127.85	124.20
39	b	811	CLA	C1-C2-C3	-2.40	121.89	126.04
48	G	305	A86	C4-C3-C2	-2.40	118.55	123.47
49	y	313	KC2	C1A-NA-C4A	-2.40	105.63	106.71
50	0	302	A1EB1	O4-C38-O5	-2.40	118.19	122.96
51	Y	306	A1ECV	C3-O2-CMC	2.40	120.46	115.83
50	7	305	A1EB1	O6-C42-C44	2.40	119.44	111.91
49	R	306	KC2	CBD-CHA-C1A	2.40	133.36	128.88
39	D	309	CLA	C3B-C4B-NB	-2.40	108.29	110.52
50	8	301	A1EB1	C33-C32-C31	2.40	111.55	109.21
49	M	311	KC2	C4D-C3D-CAD	2.40	109.04	107.42
48	y	306	A86	C9-C8-C6	-2.40	119.67	126.42
49	G	313	KC2	O1D-CGD-CBD	-2.40	119.57	124.48
49	Q	315	KC2	O1D-CGD-CBD	-2.40	119.57	124.48
49	V	312	KC2	O1D-CGD-CBD	-2.40	119.57	124.48
48	1	303	A86	O4-C38-O5	-2.40	118.19	122.96
39	D	317	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
47	k	205	SQD	O48-C23-C24	2.40	119.44	111.91
39	T	308	CLA	O2D-CGD-CBD	2.40	115.53	111.27
48	Q	301	A86	C25-C24-C1	-2.40	119.67	126.42
48	Q	304	A86	O4-C38-O5	-2.40	118.19	122.96
39	9	308	CLA	C3B-C4B-NB	-2.40	108.29	110.52
39	3	313	CLA	CHB-C4A-NA	2.40	127.83	124.51
39	5	307	CLA	CHB-C4A-NA	2.40	127.83	124.51
42	b	846	BCR	C20-C21-C22	-2.40	123.89	127.31
39	a	801	CLA	C2D-C1D-ND	-2.40	108.34	110.10
39	4	323	CLA	CHB-C4A-NA	2.40	127.83	124.51
48	9	305	A86	O4-C38-O5	-2.40	118.20	122.96
48	6	307	A86	O4-C38-O5	-2.40	118.20	122.96
39	Q	317	CLA	CHB-C4A-NA	2.40	127.83	124.51
48	y	306	A86	C4-C3-C2	-2.40	118.56	123.47
52	5	304	A1EB4	C25-C26-C27	-2.40	123.89	127.31
48	8	323	A86	C12-C11-C13	2.40	120.05	116.02
50	0	302	A1EB1	C34-O4-C38	-2.40	113.43	117.90
39	4	312	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
48	y	306	A86	C25-C24-C1	-2.40	119.68	126.42
39	0	318	CLA	C3B-C4B-NB	-2.40	108.29	110.52
49	9	313	KC2	CHB-C4A-C3A	-2.40	121.24	124.98
39	k	201	CLA	CHB-C4A-NA	2.40	127.83	124.51
39	x	318	CLA	CHB-C4A-NA	2.40	127.83	124.51
50	6	304	A1EB1	C35-C34-C33	-2.40	105.70	109.88
50	Q	323	A1EB1	C25-C24-C1	-2.40	119.69	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	G	311	KC2	O1D-CGD-CBD	-2.40	119.58	124.48
50	y	302	A1EB1	C28-O6-C42	2.40	121.01	115.68
39	L	320	CLA	C3B-C4B-NB	-2.40	108.29	110.52
42	b	844	BCR	C11-C10-C9	-2.39	123.89	127.31
49	P	310	KC2	CHB-C4A-C3A	-2.39	121.24	124.98
43	3	304	DD6	C25-C24-C1	-2.39	119.69	126.42
50	6	301	A1EB1	O4-C38-O5	-2.39	118.20	122.96
43	C	301	DD6	C37-C36-C35	2.39	118.79	114.36
43	U	204	DD6	C12-C11-C13	2.39	121.85	118.08
39	D	313	CLA	CMB-C2B-C1B	-2.39	121.72	125.37
48	W	303	A86	C41-C32-C31	-2.39	108.33	110.47
49	C	313	KC2	C1A-NA-C4A	-2.39	105.63	106.71
49	P	312	KC2	C1A-NA-C4A	-2.39	105.63	106.71
39	D	317	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
50	K	304	A1EB1	C17-C16-C15	2.39	111.60	109.16
48	3	307	A86	C20-C19-C18	2.39	117.48	112.75
47	S	301	SQD	O48-C23-C24	2.39	119.42	111.91
43	A	302	DD6	C37-C36-C35	2.39	118.79	114.36
48	8	307	A86	O4-C38-O5	-2.39	118.21	122.96
51	Z	308	A1ECV	C3-O2-CMC	2.39	120.44	115.83
43	x	304	DD6	C21-C20-C15	-2.39	118.25	122.26
39	I	310	CLA	C3B-C4B-NB	-2.39	108.30	110.52
49	7	319	KC2	CHB-C4A-C3A	-2.39	121.24	124.98
42	b	845	BCR	C3-C4-C5	-2.39	109.81	114.08
39	b	806	CLA	CHB-C4A-NA	2.39	127.82	124.51
39	l	201	CLA	CHB-C4A-NA	2.39	127.82	124.51
50	4	302	A1EB1	C12-C11-C13	2.39	120.04	116.02
48	J	303	A86	O4-C38-O5	-2.39	118.21	122.96
49	M	314	KC2	O1D-CGD-CBD	-2.39	119.59	124.48
49	V	315	KC2	O1D-CGD-CBD	-2.39	119.59	124.48
48	M	303	A86	C34-O4-C38	-2.39	113.44	117.90
49	V	312	KC2	CHD-C4C-NC	2.39	127.83	124.20
39	a	821	CLA	C3B-C4B-NB	-2.39	108.30	110.52
39	A	309	CLA	C3B-C4B-NB	-2.39	108.30	110.52
48	0	306	A86	O1-C20-C21	-2.39	112.19	115.06
49	W	312	KC2	O1D-CGD-CBD	-2.39	119.59	124.48
43	o	204	DD6	C15-C14-C13	-2.39	120.94	125.99
39	S	309	CLA	CMB-C2B-C3B	2.39	132.38	126.59
43	3	304	DD6	C9-C8-C6	-2.39	119.70	126.42
50	7	306	A1EB1	C9-C8-C6	-2.39	119.70	126.42
49	0	316	KC2	C4D-C3D-CAD	2.39	109.03	107.42
39	a	830	CLA	C3B-C4B-NB	-2.39	108.30	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	E	317	CLA	C3B-C4B-NB	-2.39	108.30	110.52
50	V	307	A1EB1	C36-C31-C32	2.39	122.07	119.70
50	G	307	A1EB1	C25-C26-C27	-2.39	123.86	127.26
48	0	301	A86	C12-C11-C13	2.39	120.03	116.02
48	Q	302	A86	O4-C38-O5	-2.39	118.22	122.96
49	y	313	KC2	O1D-CGD-CBD	-2.39	119.60	124.48
39	D	312	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
49	P	310	KC2	O1D-CGD-CBD	-2.39	119.60	124.48
51	G	316	A1ECV	O2-CMC-O1	-2.39	118.78	123.45
49	9	311	KC2	CHD-C4C-NC	2.39	127.83	124.20
49	9	316	KC2	CHD-C4C-NC	2.39	127.83	124.20
45	b	849	DGD	CFB-CEB-CDB	-2.39	102.31	114.42
50	T	307	A1EB1	C9-C10-C11	-2.39	119.59	126.61
49	V	318	KC2	CHB-C4A-C3A	-2.39	121.25	124.98
49	8	319	KC2	CBD-CHA-C1A	2.39	133.33	128.88
39	U	210	CLA	CHB-C1B-NB	2.39	126.78	124.26
39	K	314	CLA	C3B-C4B-NB	-2.39	108.30	110.52
50	y	301	A1EB1	C9-C8-C6	-2.38	119.72	126.42
39	1	320	CLA	CHB-C4A-NA	2.38	127.81	124.51
39	b	838	CLA	O2A-CGA-O1A	-2.38	117.57	123.59
48	L	305	A86	C41-C32-C31	-2.38	108.34	110.47
49	8	317	KC2	C1A-NA-C4A	-2.38	105.63	106.71
49	S	317	KC2	CHB-C4A-C3A	-2.38	121.25	124.98
39	S	309	CLA	CHB-C4A-NA	2.38	127.81	124.51
39	x	307	CLA	CHB-C4A-NA	2.38	127.81	124.51
50	2	304	A1EB1	O4-C38-O5	-2.38	118.23	122.96
49	8	314	KC2	CBD-CHA-C1A	2.38	133.33	128.88
49	4	324	KC2	CHD-C4C-NC	2.38	127.82	124.20
50	0	302	A1EB1	C36-C31-C32	2.38	122.06	119.70
47	M	301	SQD	C45-O47-C7	2.38	123.66	117.79
50	J	302	A1EB1	O4-C38-O5	-2.38	118.23	122.96
48	K	301	A86	O4-C38-O5	-2.38	118.23	122.96
48	0	309	A86	C28-C27-C26	-2.38	119.59	122.92
49	V	308	KC2	CHD-C4C-NC	2.38	127.81	124.20
49	3	317	KC2	O1D-CGD-CBD	-2.38	119.62	124.48
49	z	315	KC2	CHB-C4A-C3A	-2.38	121.26	124.98
47	7	302	SQD	O5-C5-C4	2.38	114.01	109.69
48	L	301	A86	C9-C8-C6	-2.38	119.74	126.42
49	X	315	KC2	CHB-C4A-C3A	-2.38	121.27	124.98
50	V	306	A1EB1	C28-O6-C42	2.38	120.97	115.68
51	6	320	A1ECV	C3-O2-CMC	2.38	120.42	115.83
50	G	302	A1EB1	C28-C27-C26	-2.38	121.82	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	y	314	KC2	C1B-CHB-C4A	-2.38	120.93	126.06
39	b	836	CLA	C3B-C4B-NB	-2.38	108.31	110.52
39	b	812	CLA	CHB-C4A-NA	2.38	127.80	124.51
50	3	310	A1EB1	O6-C28-C27	2.38	114.97	109.07
39	b	815	CLA	CBC-CAC-C3C	2.38	118.98	112.43
48	0	306	A86	C12-C11-C13	2.38	120.01	116.02
41	X	301	LHG	C20-C19-C18	-2.37	102.37	114.42
43	O	303	DD6	C7-C6-C8	2.37	121.82	118.08
47	P	301	SQD	O48-C23-C24	2.37	119.36	111.91
48	7	311	A86	C28-C27-C26	-2.37	119.60	122.92
50	O	301	A1EB1	C17-C16-C15	2.37	111.58	109.16
43	z	305	DD6	C37-C36-C35	2.37	118.75	114.36
43	D	306	DD6	C26-C25-C24	-2.37	115.81	123.22
43	R	304	DD6	C14-C13-C11	-2.37	121.85	125.53
51	2	311	A1ECV	O1D-CGD-CBD	-2.37	120.79	124.74
50	R	303	A1EB1	O4-C34-C35	2.37	113.50	107.59
52	5	304	A1EB4	C26-C25-C24	-2.37	115.81	123.22
43	J	305	DD6	C12-C11-C10	-2.37	119.60	122.92
51	W	317	A1ECV	CMB-C2B-C1B	2.37	129.21	124.73
48	Y	301	A86	C12-C11-C13	2.37	120.01	116.02
50	2	304	A1EB1	C3-C4-C5	-2.37	118.61	123.47
48	z	303	A86	O4-C38-O5	-2.37	118.25	122.96
51	O	315	A1ECV	O2D-CGD-O1D	-2.37	119.20	123.84
48	O	307	A86	C12-C11-C13	2.37	120.01	116.02
50	G	304	A1EB1	C12-C11-C13	2.37	120.01	116.02
50	y	302	A1EB1	C9-C10-C11	-2.37	119.64	126.61
43	J	304	DD6	C33-C34-C35	-2.37	107.06	110.30
39	a	826	CLA	CHB-C4A-NA	2.37	127.79	124.51
50	y	302	A1EB1	C41-C32-C31	-2.37	108.35	110.47
48	W	303	A86	C28-C27-C26	-2.37	119.60	122.92
41	X	301	LHG	C11-C10-C9	-2.37	102.39	114.42
49	R	318	KC2	O1D-CGD-CBD	-2.37	119.63	124.48
51	x	316	A1ECV	O2D-CGD-O1D	-2.37	119.20	123.84
51	z	310	A1ECV	O2D-CGD-O1D	-2.37	119.20	123.84
39	J	314	CLA	CHD-C1D-ND	-2.37	122.28	124.45
49	X	306	KC2	O2D-CGD-O1D	-2.37	119.20	123.84
49	S	314	KC2	O1D-CGD-CBD	-2.37	119.64	124.48
39	T	309	CLA	CHB-C1B-NB	2.37	126.77	124.26
39	I	308	CLA	CHB-C4A-NA	2.37	127.79	124.51
39	a	834	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
48	W	303	A86	C25-C24-C1	-2.37	119.76	126.42
49	3	318	KC2	CHD-C4C-NC	2.37	127.80	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	R	312	KC2	C2D-C1D-ND	-2.37	108.64	110.23
48	X	303	A86	C33-C32-C31	2.37	111.51	109.21
48	9	306	A86	O1-C20-C21	-2.37	112.22	115.06
51	P	315	A1ECV	C3-O2-CMC	2.37	120.40	115.83
50	2	306	A1EB1	C4-C3-C2	-2.37	118.62	123.47
48	z	303	A86	C12-C11-C13	2.37	120.00	116.02
49	5	314	KC2	CHB-C4A-C3A	-2.37	121.28	124.98
50	T	302	A1EB1	O1-C20-C21	-2.37	112.22	115.06
51	Z	308	A1ECV	C1D-CHD-C4C	-2.37	107.90	115.73
49	4	317	KC2	O1D-CGD-CBD	-2.37	119.64	124.48
39	U	208	CLA	CHB-C1B-NB	2.37	126.76	124.26
39	f	802	CLA	CHD-C1D-ND	-2.37	122.28	124.45
49	V	320	KC2	CHD-C4C-NC	2.37	127.79	124.20
39	Z	313	CLA	CHC-C1C-C2C	-2.37	120.16	126.73
39	f	802	CLA	CHB-C4A-NA	2.37	127.78	124.51
40	a	839	PQN	C2M-C2-C3	-2.37	120.54	124.40
39	K	306	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
52	M	305	A1EB4	C3-C4-C5	-2.37	118.63	123.47
39	U	214	CLA	C3B-C4B-NB	-2.36	108.32	110.52
48	M	302	A86	C12-C11-C13	2.36	120.00	116.02
39	A	307	CLA	CHB-C4A-NA	2.36	127.78	124.51
48	Q	305	A86	C26-C25-C24	-2.36	115.84	123.22
49	H	314	KC2	C1A-NA-C4A	-2.36	105.64	106.71
39	A	314	CLA	O2D-CGD-CBD	2.36	115.47	111.27
48	Z	301	A86	C36-C31-C32	2.36	122.04	119.70
46	M	319	LMG	C1-C2-C3	-2.36	105.07	110.00
48	M	306	A86	O4-C38-O5	-2.36	118.27	122.96
50	y	301	A1EB1	C25-C24-C1	-2.36	119.78	126.42
39	R	307	CLA	CMB-C2B-C3B	2.36	132.31	126.59
50	4	304	A1EB1	C40-C32-C31	-2.36	108.36	110.47
43	I	305	DD6	C21-C20-C15	-2.36	118.30	122.26
48	Q	302	A86	C34-O4-C38	-2.36	113.49	117.90
50	G	304	A1EB1	O1-C20-C21	-2.36	112.22	115.06
39	6	315	CLA	CMB-C2B-C3B	2.36	132.31	126.59
49	G	315	KC2	C1A-NA-C4A	-2.36	105.64	106.71
39	z	318	CLA	CMB-C2B-C3B	2.36	132.31	126.59
48	T	306	A86	C12-C11-C13	2.36	119.99	116.02
46	F	320	LMG	C1-O6-C5	2.36	118.32	113.69
48	M	303	A86	C9-C10-C11	-2.36	119.66	126.61
39	b	839	CLA	C3B-C4B-NB	-2.36	108.32	110.52
48	4	306	A86	C28-C27-C26	-2.36	119.61	122.92
49	Q	318	KC2	O2D-CGD-O1D	-2.36	119.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	R	316	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
42	a	843	BCR	C8-C7-C6	-2.36	120.57	127.20
50	0	305	A1EB1	C3-C4-C5	-2.36	118.64	123.47
50	x	302	A1EB1	O1-C20-C21	-2.36	112.23	115.06
49	L	315	KC2	CHB-C4A-C3A	-2.36	121.29	124.98
49	R	318	KC2	C1A-NA-C4A	-2.36	105.64	106.71
48	7	307	A86	O4-C34-C35	2.36	113.47	107.59
48	R	301	A86	O4-C38-O5	-2.36	118.28	122.96
52	T	304	A1EB4	C4-C5-C6	-2.36	123.94	127.31
49	Z	311	KC2	O1D-CGD-CBD	-2.36	119.66	124.48
50	0	305	A1EB1	O4-C38-O5	-2.36	118.28	122.96
39	b	834	CLA	CHB-C4A-NA	2.36	127.77	124.51
50	3	310	A1EB1	C9-C8-C6	-2.36	119.79	126.42
42	j	103	BCR	C15-C16-C17	-2.36	118.65	123.47
39	E	310	CLA	C1-C2-C3	-2.36	121.97	126.04
48	M	302	A86	C41-C32-C31	-2.36	108.36	110.47
49	M	313	KC2	C1B-CHB-C4A	-2.36	120.97	126.06
39	a	822	CLA	O2D-CGD-CBD	2.36	115.45	111.27
48	4	306	A86	C25-C24-C1	-2.36	119.80	126.42
43	y	304	DD6	C21-C20-C15	-2.36	118.31	122.26
42	m	101	BCR	C7-C8-C9	-2.36	122.67	126.23
39	3	316	CLA	C1-C2-C3	-2.36	122.94	126.75
52	W	306	A1EB4	C10-C9-C8	-2.36	115.87	123.22
50	F	304	A1EB1	C3-C2-C1	-2.36	123.95	127.31
43	W	305	DD6	O1-C20-C19	-2.35	111.61	113.38
39	R	311	CLA	C1-C2-C3	-2.35	122.94	126.75
41	a	840	LHG	O8-C23-C24	2.35	119.30	111.91
49	X	315	KC2	C4D-C3D-CAD	2.35	109.01	107.42
39	M	321	CLA	C3B-C4B-NB	-2.35	108.33	110.52
39	x	318	CLA	CMB-C2B-C1B	-2.35	121.78	125.37
43	E	302	DD6	C9-C10-C11	-2.35	123.95	127.31
49	0	317	KC2	CHD-C4C-NC	2.35	127.77	124.20
43	D	303	DD6	C3-C4-C5	-2.35	118.65	123.47
43	E	305	DD6	C37-C36-C35	2.35	118.71	114.36
48	y	305	A86	C4-C3-C2	-2.35	118.66	123.47
46	Q	322	LMG	C1-O6-C5	2.35	118.30	113.69
42	b	848	BCR	C15-C16-C17	-2.35	118.66	123.47
39	2	308	CLA	CHD-C1D-ND	-2.35	122.29	124.45
50	G	302	A1EB1	C28-O6-C42	2.35	120.91	115.68
39	y	319	CLA	CHB-C1B-NB	2.35	126.75	124.26
50	0	305	A1EB1	C40-C32-C31	-2.35	108.37	110.47
49	L	321	KC2	C1B-CHB-C4A	-2.35	120.99	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	J	305	DD6	C-C1-C2	-2.35	119.63	122.92
39	b	820	CLA	CHB-C4A-NA	2.35	127.76	124.51
39	x	317	CLA	O2D-CGD-CBD	2.35	115.44	111.27
49	8	314	KC2	C1B-CHB-C4A	-2.35	120.99	126.06
48	1	306	A86	C33-C32-C31	2.35	111.49	109.21
50	G	302	A1EB1	O1-C20-C21	-2.35	112.24	115.06
43	1	304	DD6	C12-C11-C10	-2.35	119.63	122.92
39	b	823	CLA	C3B-C4B-NB	-2.35	108.34	110.52
39	Y	313	CLA	C3B-C4B-NB	-2.35	108.34	110.52
39	M	315	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
49	R	314	KC2	CHB-C4A-C3A	-2.35	121.31	124.98
43	R	304	DD6	C9-C8-C6	-2.35	119.82	126.42
52	5	304	A1EB4	C21-C20-C15	-2.35	118.35	122.32
49	1	314	KC2	C1A-NA-C4A	-2.35	105.65	106.71
52	P	305	A1EB4	C10-C9-C8	-2.35	115.89	123.22
48	S	307	A86	C20-C19-C18	-2.35	108.11	112.75
39	V	310	CLA	CMB-C2B-C1B	-2.35	121.80	125.37
39	a	834	CLA	C3B-C4B-NB	-2.35	108.34	110.52
46	l	208	LMG	C1-O6-C5	2.35	118.29	113.69
52	X	305	A1EB4	C34-O4-C38	-2.35	113.53	117.90
50	G	307	A1EB1	C4-C3-C2	-2.35	118.67	123.47
40	b	843	PQN	C14-C13-C15	2.35	119.22	115.27
48	L	306	A86	C28-C27-C26	-2.35	119.64	122.92
48	U	202	A86	O4-C38-O5	-2.34	118.30	122.96
50	7	303	A1EB1	O4-C34-C33	2.34	113.43	107.59
49	X	318	KC2	O1D-CGD-CBD	-2.34	119.69	124.48
48	O	306	A86	C33-C32-C31	2.34	111.49	109.21
42	j	103	BCR	C11-C10-C9	-2.34	123.97	127.31
39	7	316	CLA	C3B-C4B-NB	-2.34	108.34	110.52
51	P	315	A1ECV	O2D-CGD-O1D	-2.34	119.26	123.84
48	L	304	A86	C28-C27-C26	-2.34	119.64	122.92
39	a	814	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
49	L	314	KC2	C2A-C3A-C4A	2.34	108.22	106.49
48	3	306	A86	O4-C38-O5	-2.34	118.31	122.96
48	E	304	A86	O4-C34-C35	2.34	113.43	107.59
39	a	801	CLA	C3B-C4B-NB	-2.34	108.34	110.52
48	U	202	A86	C9-C10-C11	-2.34	119.72	126.61
39	x	318	CLA	C3B-C4B-NB	-2.34	108.34	110.52
39	8	310	CLA	CBA-CAA-C2A	2.34	120.77	113.86
48	S	305	A86	C7-C6-C8	2.34	121.77	118.08
39	a	823	CLA	CHD-C1D-ND	-2.34	122.30	124.45
49	1	314	KC2	CHD-C4C-NC	2.34	127.75	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	9	305	A86	C35-C34-C33	2.34	113.96	109.88
43	I	306	DD6	C4-C3-C2	-2.34	118.68	123.47
43	A	303	DD6	C15-C14-C13	-2.34	121.05	125.99
52	W	321	A1EB4	C-C1-C2	-2.34	119.64	122.92
49	Q	318	KC2	C4D-C3D-CAD	2.34	109.00	107.42
39	a	814	CLA	O2D-CGD-CBD	2.34	115.42	111.27
49	V	314	KC2	CHB-C4A-C3A	-2.34	121.33	124.98
50	8	301	A1EB1	C35-C34-C33	-2.34	105.80	109.88
48	G	301	A86	O1-C20-C21	-2.34	112.25	115.06
39	I	301	CLA	CHD-C1D-ND	-2.34	122.31	124.45
49	x	315	KC2	CBD-CHA-C1A	2.34	133.24	128.88
49	X	314	KC2	CHB-C4A-C3A	-2.34	121.33	124.98
49	0	319	KC2	CBD-CHA-C4D	-2.34	103.55	109.14
52	R	305	A1EB4	C40-C32-C31	-2.34	108.38	110.47
49	x	315	KC2	C1B-CHB-C4A	-2.34	121.02	126.06
49	C	313	KC2	O2D-CGD-O1D	-2.34	119.27	123.84
49	8	319	KC2	CHD-C4C-NC	2.34	127.75	124.20
39	A	309	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
39	l	205	CLA	CAC-C3C-C4C	2.34	127.84	124.81
48	6	303	A86	O4-C38-O5	-2.34	118.32	122.96
49	T	314	KC2	C2D-C1D-ND	-2.34	108.67	110.23
49	8	320	KC2	CHB-C4A-C3A	-2.34	121.33	124.98
49	J	315	KC2	C1A-NA-C4A	-2.34	105.66	106.71
49	C	312	KC2	O2D-CGD-O1D	-2.34	119.27	123.84
39	H	313	CLA	CHD-C1D-ND	-2.34	122.31	124.45
48	G	301	A86	C28-C27-C26	-2.34	119.65	122.92
48	6	305	A86	O4-C38-O5	-2.34	118.32	122.96
43	C	301	DD6	C32-C33-C34	-2.33	108.37	113.64
49	P	312	KC2	C1B-CHB-C4A	-2.33	121.02	126.06
49	K	310	KC2	CHB-C4A-C3A	-2.33	121.33	124.98
48	1	306	A86	C20-C19-C18	2.33	117.37	112.75
39	M	312	CLA	C3B-C4B-NB	-2.33	108.35	110.52
39	x	311	CLA	C3B-C4B-NB	-2.33	108.35	110.52
52	R	305	A1EB4	C34-O4-C38	-2.33	113.55	117.90
51	Y	306	A1ECV	C1D-CHD-C4C	-2.33	108.01	115.73
49	9	316	KC2	CHB-C4A-C3A	-2.33	121.33	124.98
50	9	302	A1EB1	C41-C32-C31	-2.33	108.38	110.47
39	H	308	CLA	CHD-C1D-ND	-2.33	122.31	124.45
46	F	317	LMG	C1-O6-C5	2.33	118.27	113.69
43	4	307	DD6	C32-C31-C36	-2.33	119.34	122.63
49	3	321	KC2	CHD-C4C-NC	2.33	127.74	124.20
43	D	307	DD6	C9-C10-C11	-2.33	123.98	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	0	303	A1EB1	C20-C19-C18	-2.33	108.14	112.75
48	E	304	A86	O4-C38-O5	-2.33	118.33	122.96
49	R	318	KC2	CHD-C4C-NC	2.33	127.74	124.20
49	T	315	KC2	C2A-C3A-C4A	2.33	108.22	106.49
39	S	310	CLA	C2A-C1A-CHA	2.33	127.94	123.86
39	a	838	CLA	C3B-C4B-NB	-2.33	108.35	110.52
39	F	315	CLA	C3B-C4B-NB	-2.33	108.35	110.52
50	Q	323	A1EB1	O4-C38-O5	-2.33	118.33	122.96
49	5	313	KC2	CHB-C4A-C3A	-2.33	121.34	124.98
49	1	312	KC2	C1B-CHB-C4A	-2.33	121.03	126.06
49	x	312	KC2	O1D-CGD-CBD	-2.33	119.72	124.48
48	1	307	A86	C35-C34-C33	-2.33	105.81	109.88
48	L	307	A86	O4-C38-O5	-2.33	118.33	122.96
39	7	325	CLA	C3B-C4B-NB	-2.33	108.35	110.52
47	7	302	SQD	O5-C1-C2	2.33	115.28	110.35
51	V	317	A1ECV	O2D-CGD-O1D	-2.33	119.28	123.84
50	4	304	A1EB1	C9-C10-C11	-2.33	119.76	126.61
48	6	307	A86	C28-C27-C26	-2.33	119.66	122.92
49	8	317	KC2	CHB-C4A-C3A	-2.33	121.34	124.98
50	V	302	A1EB1	O1-C20-C19	-2.33	111.63	113.38
39	z	309	CLA	C3B-C4B-NB	-2.33	108.35	110.52
39	D	314	CLA	CHB-C4A-NA	2.33	127.73	124.51
49	W	308	KC2	C2D-C1D-ND	-2.33	108.67	110.23
49	R	306	KC2	CHB-C4A-C3A	-2.33	121.34	124.98
48	9	301	A86	O4-C38-O5	-2.33	118.34	122.96
42	b	844	BCR	C38-C26-C25	-2.33	121.91	124.53
43	O	303	DD6	C32-C31-C36	-2.33	119.35	122.63
39	F	314	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
49	A	310	KC2	C1B-CHB-C4A	-2.33	121.04	126.06
42	a	844	BCR	C16-C15-C14	-2.33	118.71	123.47
48	1	303	A86	O1-C15-C14	-2.33	108.54	113.21
52	T	304	A1EB4	C25-C26-C27	-2.33	123.99	127.31
49	G	311	KC2	C1B-CHB-C4A	-2.33	121.04	126.06
50	y	301	A1EB1	O1-C15-C20	-2.33	57.13	59.40
49	9	311	KC2	C1B-CHB-C4A	-2.33	121.04	126.06
50	G	304	A1EB1	C28-C27-C26	-2.33	121.89	124.93
50	6	304	A1EB1	C4-C3-C2	-2.33	118.71	123.47
48	Q	304	A86	C3-C4-C5	-2.33	118.71	123.47
48	D	305	A86	C-C1-C2	-2.33	119.67	122.92
49	G	315	KC2	C4D-C3D-CAD	2.32	108.99	107.42
50	3	303	A1EB1	O1-C15-C20	-2.32	57.13	59.40
43	R	304	DD6	C41-C32-C31	-2.32	106.77	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	9	303	A86	O4-C34-C35	2.32	113.38	107.59
50	1	305	A1EB1	C12-C11-C13	2.32	119.93	116.02
39	a	829	CLA	C3B-C4B-NB	-2.32	108.36	110.52
39	2	312	CLA	O2D-CGD-CBD	2.32	115.40	111.27
45	C	314	DGD	C1D-C2D-C3D	-2.32	105.16	110.00
43	x	304	DD6	O1-C20-C21	-2.32	112.27	115.06
48	L	301	A86	O4-C38-O5	-2.32	118.35	122.96
48	9	304	A86	O4-C38-O5	-2.32	118.35	122.96
48	8	307	A86	C-C1-C2	-2.32	119.67	122.92
49	P	306	KC2	CHD-C4C-NC	2.32	127.73	124.20
49	7	319	KC2	CHD-C4C-NC	2.32	127.73	124.20
46	0	324	LMG	O7-C10-O9	-2.32	118.35	122.96
39	b	808	CLA	O2D-CGD-CBD	2.32	115.39	111.27
39	E	313	CLA	C3B-C4B-NB	-2.32	108.36	110.52
49	1	314	KC2	C1B-CHB-C4A	-2.32	121.05	126.06
49	y	316	KC2	O1D-CGD-CBD	-2.32	119.73	124.48
48	7	308	A86	C33-C32-C31	2.32	111.47	109.21
51	Y	312	A1ECV	O2-CMC-O1	-2.32	118.91	123.45
39	o	202	CLA	CAA-C2A-C3A	-2.32	108.46	114.26
49	R	318	KC2	CHB-C4A-C3A	-2.32	121.35	124.98
48	T	301	A86	C12-C11-C13	2.32	119.92	116.02
48	k	206	A86	O4-C38-O5	-2.32	118.35	122.96
48	7	308	A86	O4-C38-O5	-2.32	118.36	122.96
48	W	304	A86	C9-C10-C11	-2.32	119.79	126.61
48	R	301	A86	O1-C15-C14	-2.32	108.56	113.21
50	G	308	A1EB1	C34-O4-C38	-2.32	113.58	117.90
50	8	306	A1EB1	O1-C20-C21	-2.32	112.28	115.06
49	5	314	KC2	C4D-C3D-CAD	2.32	108.98	107.42
52	P	318	A1EB4	O4-C38-O43	-2.32	118.36	122.96
39	7	324	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
49	H	314	KC2	C1B-CHB-C4A	-2.32	121.06	126.06
48	2	301	A86	O1-C15-C20	-2.32	57.14	59.40
51	Y	312	A1ECV	O2-CMC-C2C	2.32	117.83	112.27
39	2	318	CLA	C3B-C4B-NB	-2.32	108.37	110.52
48	M	302	A86	C40-C32-C31	-2.32	108.40	110.47
50	G	302	A1EB1	C40-C32-C31	-2.32	108.40	110.47
49	T	315	KC2	O2D-CGD-O1D	-2.32	119.31	123.84
48	S	307	A86	O4-C38-O5	-2.32	118.36	122.96
39	E	308	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
50	R	303	A1EB1	O6-C42-C44	2.32	119.17	111.91
39	J	308	CLA	C1-C2-C3	-2.32	123.00	126.75
49	R	306	KC2	C1B-CHB-C4A	-2.32	121.06	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	Q	313	KC2	C1A-NA-C4A	-2.32	105.67	106.71
49	Q	315	KC2	C1A-NA-C4A	-2.32	105.67	106.71
49	z	315	KC2	C1A-NA-C4A	-2.32	105.67	106.71
49	1	315	KC2	O2D-CGD-O1D	-2.32	119.31	123.84
39	J	317	CLA	C3B-C4B-NB	-2.32	108.37	110.52
49	2	314	KC2	CHB-C4A-C3A	-2.32	121.36	124.98
48	T	305	A86	C10-C9-C8	-2.31	115.99	123.22
50	V	307	A1EB1	O4-C38-O5	-2.31	118.36	122.96
48	Z	303	A86	C-C1-C2	-2.31	119.68	122.92
39	a	805	CLA	CMB-C2B-C3B	2.31	132.19	126.59
49	9	311	KC2	O1D-CGD-CBD	-2.31	119.75	124.48
43	F	303	DD6	C33-C34-C35	-2.31	107.14	110.30
43	I	305	DD6	C3-C4-C5	-2.31	118.73	123.47
39	9	307	CLA	CHB-C4A-NA	2.31	127.71	124.51
50	J	302	A1EB1	C12-C11-C13	2.31	119.91	116.02
48	0	308	A86	O4-C34-C35	2.31	113.35	107.59
49	2	313	KC2	O1D-CGD-CBD	-2.31	119.75	124.48
48	4	309	A86	C12-C11-C13	2.31	119.91	116.02
48	0	304	A86	C9-C8-C6	-2.31	119.92	126.42
49	C	313	KC2	C4D-C3D-CAD	2.31	108.98	107.42
39	2	308	CLA	CHB-C1B-NB	2.31	126.70	124.26
50	y	301	A1EB1	O4-C38-O5	-2.31	118.37	122.96
39	8	321	CLA	C3B-C4B-NB	-2.31	108.37	110.52
48	F	301	A86	C33-C32-C31	2.31	111.46	109.21
48	M	302	A86	C35-C34-C33	-2.31	105.84	109.88
51	5	312	A1ECV	C3-O2-CMC	2.31	120.29	115.83
49	W	315	KC2	C1B-CHB-C4A	-2.31	121.07	126.06
51	R	313	A1ECV	CMA-C3A-C2A	2.31	129.00	124.68
50	h	203	A1EB1	C3-C4-C5	-2.31	118.74	123.47
47	D	321	SQD	O48-C23-C24	2.31	119.16	111.91
49	K	313	KC2	C1B-CHB-C4A	-2.31	121.08	126.06
49	4	320	KC2	C1A-NA-C4A	-2.31	105.67	106.71
50	V	307	A1EB1	O1-C15-C20	-2.31	57.14	59.40
49	V	308	KC2	C4D-C3D-CAD	2.31	108.98	107.42
39	b	831	CLA	CHB-C1B-NB	2.31	126.70	124.26
48	M	306	A86	C19-C18-C17	2.31	115.23	110.77
43	y	304	DD6	C4-C5-C6	-2.31	124.02	127.31
48	9	301	A86	C28-C27-C26	-2.31	119.69	122.92
50	6	301	A1EB1	C7-C6-C5	-2.31	119.69	122.92
49	J	315	KC2	O2D-CGD-O1D	-2.31	119.33	123.84
50	7	304	A1EB1	C3-C4-C5	-2.31	118.75	123.47
39	S	320	CLA	CHB-C4A-NA	2.31	127.70	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	z	312	KC2	O1D-CGD-CBD	-2.31	119.76	124.48
49	V	318	KC2	C1A-NA-C4A	-2.31	105.67	106.71
48	F	301	A86	C3-C4-C5	-2.31	118.75	123.47
48	8	303	A86	O4-C38-O5	-2.31	118.38	122.96
49	y	314	KC2	CHD-C4C-NC	2.31	127.70	124.20
48	0	301	A86	O4-C34-C35	2.31	113.33	107.59
48	8	305	A86	C12-C11-C13	2.31	119.89	116.02
39	F	314	CLA	C3B-C4B-NB	-2.30	108.38	110.52
49	J	315	KC2	CHB-C4A-C3A	-2.30	121.38	124.98
48	9	306	A86	O4-C38-O5	-2.30	118.38	122.96
48	4	306	A86	C3-C4-C5	-2.30	118.75	123.47
49	S	317	KC2	C4D-C3D-CAD	2.30	108.97	107.42
49	8	319	KC2	C4D-C3D-CAD	2.30	108.97	107.42
49	R	314	KC2	C1B-CHB-C4A	-2.30	121.09	126.06
39	Z	313	CLA	C3C-C4C-NC	-2.30	107.99	110.57
50	4	304	A1EB1	C9-C8-C6	-2.30	119.94	126.42
48	Z	303	A86	O4-C38-O5	-2.30	118.39	122.96
52	R	305	A1EB4	C21-C20-C15	-2.30	118.43	122.32
49	K	313	KC2	CHB-C4A-C3A	-2.30	121.38	124.98
43	I	306	DD6	C4-C5-C6	-2.30	124.02	127.31
48	D	305	A86	C10-C9-C8	-2.30	116.03	123.22
49	1	315	KC2	C1B-CHB-C4A	-2.30	121.09	126.06
50	3	309	A1EB1	C41-C32-C31	-2.30	108.41	110.47
43	K	303	DD6	O1-C20-C19	-2.30	111.65	113.38
49	6	317	KC2	C4D-C3D-CAD	2.30	108.97	107.42
46	W	302	LMG	C4-C3-C2	-2.30	106.81	110.82
49	X	312	KC2	C2A-C3A-C4A	2.30	108.19	106.49
49	6	314	KC2	O1D-CGD-CBD	-2.30	119.78	124.48
50	V	302	A1EB1	C3-C4-C5	-2.30	118.76	123.47
50	V	302	A1EB1	C17-C16-C15	2.30	111.51	109.16
46	P	317	LMG	C4-C3-C2	-2.30	106.81	110.82
39	P	311	CLA	C3B-C4B-NB	-2.30	108.38	110.52
46	D	322	LMG	O3-C3-C2	-2.30	105.03	110.35
48	1	307	A86	C9-C8-C6	-2.30	119.95	126.42
49	L	314	KC2	C1A-NA-C4A	-2.30	105.67	106.71
43	I	307	DD6	C9-C8-C6	-2.30	119.95	126.42
50	7	304	A1EB1	C33-C32-C31	2.30	111.45	109.21
48	7	311	A86	O1-C15-C20	-2.30	57.15	59.40
49	M	314	KC2	CHB-C4A-C3A	-2.30	121.39	124.98
39	b	828	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
48	2	301	A86	O4-C38-O5	-2.30	118.39	122.96
50	V	307	A1EB1	C7-C6-C8	2.30	121.70	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	G	306	DD6	C21-C20-C15	-2.30	118.41	122.26
39	0	312	CLA	CAA-CBA-CGA	-2.30	106.54	113.25
39	L	320	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
49	M	307	KC2	O2D-CGD-O1D	-2.30	119.34	123.84
49	B	208	KC2	C4D-C3D-CAD	2.30	108.97	107.42
49	6	316	KC2	C1A-NA-C4A	-2.30	105.67	106.71
49	H	314	KC2	CBD-CHA-C1A	2.30	133.17	128.88
49	B	208	KC2	O2A-CGA-O1A	-2.30	117.90	122.67
42	b	845	BCR	C11-C12-C13	-2.30	119.96	126.42
39	X	317	CLA	C3B-C4B-NB	-2.30	108.38	110.52
39	Z	307	CLA	C3B-C4B-NB	-2.30	108.38	110.52
50	2	304	A1EB1	O1-C15-C20	-2.30	57.15	59.40
39	Q	310	CLA	CHB-C4A-NA	2.30	127.69	124.51
49	C	312	KC2	C1B-CHB-C4A	-2.30	121.10	126.06
39	S	316	CLA	C3B-C4B-NB	-2.30	108.39	110.52
39	W	316	CLA	C3B-C4B-NB	-2.30	108.39	110.52
51	T	317	A1ECV	C2A-CAA-CBA	-2.30	123.45	128.63
42	j	103	BCR	C38-C26-C27	2.30	118.03	113.62
39	2	319	CLA	CAA-CBA-CGA	-2.29	106.55	113.25
39	K	311	CLA	CMB-C2B-C3B	2.29	132.15	126.59
50	5	302	A1EB1	C12-C11-C13	2.29	119.88	116.02
43	O	305	DD6	C21-C20-C15	-2.29	118.42	122.26
48	B	201	A86	C35-C34-C33	-2.29	105.87	109.88
48	Q	308	A86	C3-C4-C5	-2.29	118.77	123.47
48	4	310	A86	C20-C19-C18	-2.29	108.21	112.75
48	6	302	A86	C25-C24-C1	-2.29	119.97	126.42
49	G	311	KC2	CHB-C4A-C3A	-2.29	121.40	124.98
39	O	318	CLA	CMB-C2B-C3B	2.29	132.14	126.59
49	I	312	KC2	O2D-CGD-O1D	-2.29	119.36	123.84
49	5	313	KC2	C1B-CHB-C4A	-2.29	121.11	126.06
48	7	307	A86	C3-C4-C5	-2.29	118.78	123.47
48	O	302	A86	O4-C38-O5	-2.29	118.41	122.96
48	W	307	A86	O4-C38-O5	-2.29	118.41	122.96
39	b	834	CLA	C3B-C4B-NB	-2.29	108.39	110.52
39	0	315	CLA	C3B-C4B-NB	-2.29	108.39	110.52
39	b	831	CLA	C1-C2-C3	-2.29	123.04	126.75
49	X	312	KC2	CHB-C4A-C3A	-2.29	121.40	124.98
49	T	314	KC2	C2A-C3A-C4A	2.29	108.19	106.49
50	h	203	A1EB1	C10-C9-C8	-2.29	116.07	123.22
50	0	307	A1EB1	C25-C24-C1	-2.29	119.98	126.42
50	3	302	A1EB1	O1-C15-C20	-2.29	57.16	59.40
49	Z	311	KC2	CHB-C4A-C3A	-2.29	121.40	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	P	306	KC2	C1B-CHB-C4A	-2.29	121.12	126.06
39	M	315	CLA	C3B-C4B-NB	-2.29	108.39	110.52
39	L	311	CLA	CHD-C1D-ND	-2.29	122.35	124.45
43	E	303	DD6	C14-C13-C11	-2.29	121.98	125.53
39	X	308	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
39	4	311	CLA	CHB-C1B-NB	2.29	126.68	124.26
49	X	314	KC2	C1B-CHB-C4A	-2.29	121.12	126.06
43	O	305	DD6	C25-C24-C1	-2.29	119.98	126.42
48	7	308	A86	C7-C6-C8	2.29	121.68	118.08
52	M	322	A1EB4	C24-C1-C2	2.29	122.45	118.94
50	G	304	A1EB1	O1-C15-C20	-2.29	57.16	59.40
49	F	311	KC2	O2D-CGD-O1D	-2.29	119.36	123.84
39	z	308	CLA	C3B-C4B-NB	-2.29	108.39	110.52
49	5	311	KC2	CHB-C4A-C3A	-2.29	121.41	124.98
48	0	301	A86	C3-C4-C5	-2.29	118.79	123.47
48	Q	304	A86	C17-C16-C15	2.29	111.50	109.16
42	m	101	BCR	C15-C16-C17	-2.29	118.79	123.47
43	E	305	DD6	C25-C24-C1	-2.29	119.99	126.42
49	2	314	KC2	C4D-C3D-CAD	2.29	108.96	107.42
39	4	316	CLA	C3B-C4B-NB	-2.29	108.39	110.52
49	W	315	KC2	O1D-CGD-CBD	-2.29	119.81	124.48
43	y	304	DD6	C32-C31-C36	-2.29	119.41	122.63
39	T	313	CLA	CHB-C1B-NB	2.29	126.68	124.26
50	0	302	A1EB1	C9-C10-C11	-2.29	119.89	126.61
39	D	311	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
49	6	314	KC2	CHD-C4C-NC	2.29	127.67	124.20
47	4	327	SQD	O5-C1-C2	2.29	115.19	110.35
49	8	319	KC2	C1B-CHB-C4A	-2.29	121.13	126.06
39	a	801	CLA	C4D-C3D-CAD	-2.28	105.40	108.10
49	H	311	KC2	C1B-CHB-C4A	-2.28	121.13	126.06
48	U	202	A86	C28-C27-C26	-2.28	119.72	122.92
43	z	304	DD6	O1-C20-C19	-2.28	111.67	113.38
39	a	802	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
48	8	307	A86	C3-C4-C5	-2.28	118.80	123.47
49	P	313	KC2	CHB-C4A-C3A	-2.28	121.41	124.98
49	8	320	KC2	CHD-C4C-NC	2.28	127.67	124.20
50	U	205	A1EB1	O1-C15-C20	-2.28	57.17	59.40
49	9	313	KC2	C1B-CHB-C4A	-2.28	121.13	126.06
48	L	307	A86	C35-C34-C33	-2.28	105.89	109.88
43	7	309	DD6	C9-C10-C11	-2.28	124.05	127.31
49	8	320	KC2	C1B-CHB-C4A	-2.28	121.13	126.06
51	Q	316	A1ECV	O2D-CGD-O1D	-2.28	119.37	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	F	320	LMG	C8-O7-C10	-2.28	112.17	117.79
39	Q	310	CLA	C3B-C4B-NB	-2.28	108.40	110.52
39	C	310	CLA	O2D-CGD-CBD	2.28	115.32	111.27
49	8	314	KC2	C2D-C1D-ND	-2.28	108.70	110.23
39	2	307	CLA	C3B-C4B-NB	-2.28	108.40	110.52
39	Z	313	CLA	O2D-CGD-CBD	2.28	115.32	111.27
52	X	305	A1EB4	O4-C38-O43	-2.28	118.43	122.96
48	Y	301	A86	C33-C32-C31	2.28	111.43	109.21
48	8	307	A86	C20-C19-C18	2.28	117.26	112.75
50	H	301	A1EB1	C20-C19-C18	2.28	117.26	112.75
39	9	315	CLA	C3B-C4B-NB	-2.28	108.40	110.52
48	X	302	A86	C7-C6-C5	-2.28	119.73	122.92
50	7	304	A1EB1	O1-C15-C14	2.28	117.79	113.21
48	H	302	A86	C36-C31-C32	2.28	121.96	119.70
42	a	845	BCR	C20-C19-C18	-2.28	120.01	126.42
39	I	308	CLA	CMB-C2B-C3B	2.28	132.11	126.59
42	f	804	BCR	C33-C5-C4	2.28	118.00	113.62
49	L	317	KC2	C1B-CHB-C4A	-2.28	121.14	126.06
48	L	305	A86	C12-C11-C13	2.28	119.85	116.02
50	G	307	A1EB1	C12-C11-C13	2.28	119.85	116.02
49	T	314	KC2	C1A-C2A-C3A	-2.28	105.31	107.11
49	G	317	KC2	O2D-CGD-O1D	-2.28	119.38	123.84
50	G	302	A1EB1	C12-C11-C13	2.28	119.85	116.02
39	S	319	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
43	3	304	DD6	C32-C31-C36	-2.28	119.42	122.63
48	T	305	A86	C33-C32-C31	2.28	111.42	109.21
48	3	306	A86	C33-C32-C31	2.28	111.42	109.21
39	Q	321	CLA	CHB-C4A-NA	2.28	127.66	124.51
39	X	317	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
49	8	314	KC2	CHD-C4C-NC	2.28	127.66	124.20
52	5	304	A1EB4	C40-C32-C31	-2.28	108.43	110.47
43	O	304	DD6	C33-C34-C35	-2.28	107.19	110.30
39	X	316	CLA	C2D-C1D-ND	-2.28	108.43	110.10
42	j	103	BCR	C2-C1-C6	2.28	113.99	110.48
39	R	307	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
48	H	302	A86	C20-C19-C18	-2.28	108.25	112.75
39	2	310	CLA	C3B-C4B-NB	-2.28	108.40	110.52
39	U	201	CLA	CHC-C4B-NB	2.28	126.67	124.26
42	h	202	BCR	C15-C16-C17	-2.28	118.81	123.47
49	Y	309	KC2	C1B-CHB-C4A	-2.28	121.15	126.06
49	G	313	KC2	C4D-C3D-CAD	2.28	108.96	107.42
47	D	304	SQD	O5-C1-C2	2.28	115.17	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	7	309	DD6	C10-C9-C8	-2.28	116.12	123.22
48	Q	302	A86	C26-C25-C24	-2.28	116.12	123.22
39	D	313	CLA	CHD-C1D-ND	-2.28	122.36	124.45
48	9	304	A86	C33-C32-C31	2.27	111.42	109.21
52	T	304	A1EB4	C3-C4-C5	-2.27	118.81	123.47
39	X	307	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
43	U	204	DD6	C25-C26-C27	-2.27	119.98	126.58
39	Y	303	CLA	CMA-C3A-C2A	-2.27	110.79	116.10
39	a	805	CLA	C3B-C4B-NB	-2.27	108.41	110.52
43	T	303	DD6	C14-C13-C11	-2.27	122.00	125.53
48	O	307	A86	O4-C38-O5	-2.27	118.44	122.96
49	0	314	KC2	C1B-CHB-C4A	-2.27	121.15	126.06
49	7	319	KC2	C1B-CHB-C4A	-2.27	121.15	126.06
49	6	316	KC2	C1B-CHB-C4A	-2.27	121.15	126.06
48	Q	304	A86	C33-C32-C31	2.27	111.42	109.21
50	U	205	A1EB1	O4-C38-O5	-2.27	118.44	122.96
49	H	311	KC2	CHD-C4C-NC	2.27	127.65	124.20
49	4	317	KC2	C1A-NA-C4A	-2.27	105.68	106.71
49	R	318	KC2	C4D-C3D-CAD	2.27	108.95	107.42
39	Z	309	CLA	CHB-C4A-NA	2.27	127.66	124.51
48	z	303	A86	C25-C24-C1	-2.27	120.03	126.42
39	l	204	CLA	CHB-C1B-NB	2.27	126.66	124.26
39	L	311	CLA	CHB-C1B-NB	2.27	126.66	124.26
47	D	304	SQD	O48-C23-C24	2.27	119.04	111.91
43	I	305	DD6	C28-C27-C29	2.27	121.34	116.84
43	A	304	DD6	C25-C24-C1	-2.27	120.03	126.42
39	2	309	CLA	CHB-C4A-NA	2.27	127.65	124.51
49	3	317	KC2	CHB-C4A-C3A	-2.27	121.43	124.98
48	0	306	A86	O4-C38-O5	-2.27	118.45	122.96
43	z	304	DD6	C25-C24-C1	-2.27	120.03	126.42
49	P	312	KC2	O2D-CGD-O1D	-2.27	119.40	123.84
49	5	311	KC2	O2D-CGD-O1D	-2.27	119.40	123.84
39	a	831	CLA	C3B-C4B-NB	-2.27	108.41	110.52
42	a	842	BCR	C16-C15-C14	-2.27	118.82	123.47
48	S	305	A86	C34-O4-C38	-2.27	113.66	117.90
49	G	315	KC2	C1B-CHB-C4A	-2.27	121.16	126.06
49	K	310	KC2	C1B-CHB-C4A	-2.27	121.16	126.06
39	7	325	CLA	C1-C2-C3	-2.27	123.08	126.75
50	4	304	A1EB1	O4-C38-O5	-2.27	118.45	122.96
48	x	305	A86	O1-C15-C20	-2.27	57.18	59.40
49	M	313	KC2	CHB-C4A-C3A	-2.27	121.43	124.98
43	o	204	DD6	C37-C36-C35	2.27	118.56	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	W	319	CLA	C3B-C4B-NB	-2.27	108.41	110.52
50	S	303	A1EB1	C9-C10-C11	-2.27	119.94	126.61
39	a	811	CLA	CHD-C1D-ND	-2.27	122.37	124.45
50	1	305	A1EB1	C35-C34-C33	-2.27	105.92	109.88
50	4	302	A1EB1	C25-C24-C1	-2.27	120.04	126.42
39	k	203	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
39	0	315	CLA	CMB-C2B-C3B	2.27	132.08	126.59
49	R	306	KC2	CHD-C4C-NC	2.27	127.64	124.20
42	b	848	BCR	C33-C5-C4	2.27	117.97	113.62
39	b	807	CLA	CMB-C2B-C3B	2.27	132.08	126.59
48	Q	301	A86	C9-C8-C6	-2.27	120.05	126.42
46	M	319	LMG	C8-O7-C10	-2.27	112.21	117.79
51	Z	314	A1ECV	O1D-CGD-CBD	-2.27	120.96	124.74
48	1	307	A86	C25-C24-C1	-2.27	120.05	126.42
49	V	314	KC2	O2D-CGD-O1D	-2.27	119.41	123.84
50	U	203	A1EB1	C4-C3-C2	-2.27	118.83	123.47
52	5	304	A1EB4	C3-C2-C1	-2.27	124.08	127.31
49	W	308	KC2	O2D-CGD-O1D	-2.27	119.41	123.84
39	3	312	CLA	C3B-C4B-NB	-2.27	108.41	110.52
48	8	309	A86	O4-C38-O5	-2.27	118.46	122.96
48	Y	301	A86	O4-C38-O5	-2.27	118.46	122.96
50	K	305	A1EB1	C12-C11-C13	2.27	119.83	116.02
52	R	305	A1EB4	C4-C5-C6	-2.27	124.08	127.31
49	2	317	KC2	O2D-CGD-O1D	-2.27	119.41	123.84
48	B	201	A86	C-C1-C2	-2.27	119.75	122.92
50	V	306	A1EB1	O1-C20-C21	-2.27	112.34	115.06
49	4	318	KC2	C1B-CHB-C4A	-2.26	121.17	126.06
47	M	301	SQD	C1-O5-C5	2.26	118.13	113.69
43	F	305	DD6	C25-C24-C1	-2.26	120.06	126.42
49	Y	308	KC2	O2D-CGD-O1D	-2.26	119.41	123.84
39	F	316	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
48	1	302	A86	C9-C8-C6	-2.26	120.06	126.42
52	P	319	A1EB4	C24-C1-C2	2.26	122.42	118.94
52	W	321	A1EB4	C40-C32-C31	-2.26	108.45	110.47
48	W	304	A86	O1-C15-C20	-2.26	57.19	59.40
48	Q	301	A86	C34-O4-C38	-2.26	113.68	117.90
52	R	305	A1EB4	C10-C9-C8	-2.26	116.15	123.22
48	z	303	A86	O1-C20-C19	-2.26	111.68	113.38
48	Q	305	A86	C9-C8-C6	-2.26	120.06	126.42
49	G	315	KC2	CHD-C4C-NC	2.26	127.64	124.20
49	z	312	KC2	CHD-C4C-NC	2.26	127.64	124.20
39	B	204	CLA	CHB-C1B-NB	2.26	126.65	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	7	307	A86	O1-C15-C20	-2.26	57.19	59.40
49	S	315	KC2	C1B-CHB-C4A	-2.26	121.18	126.06
39	Y	307	CLA	C3B-C4B-NB	-2.26	108.42	110.52
48	Y	301	A86	C25-C24-C1	-2.26	120.06	126.42
50	1	301	A1EB1	C34-O4-C38	-2.26	113.68	117.90
46	W	320	LMG	O1-C7-C8	-2.26	105.44	110.90
39	b	806	CLA	O2D-CGD-CBD	2.26	115.28	111.27
39	b	840	CLA	CHB-C1B-NB	2.26	126.65	124.26
50	z	302	A1EB1	C17-C16-C15	2.26	111.47	109.16
43	Q	306	DD6	C25-C24-C1	-2.26	120.07	126.42
51	5	312	A1ECV	O1D-CGD-CBD	-2.26	120.97	124.74
51	O	315	A1ECV	C3-O2-CMC	2.26	120.19	115.83
50	3	309	A1EB1	C12-C11-C13	2.26	119.82	116.02
48	U	206	A86	C-C1-C2	-2.26	119.76	122.92
50	K	305	A1EB1	C20-C19-C18	-2.26	108.28	112.75
48	9	304	A86	C25-C24-C1	-2.26	120.07	126.42
39	L	310	CLA	C3B-C4B-NB	-2.26	108.42	110.52
50	E	301	A1EB1	C40-C32-C31	-2.26	108.45	110.47
49	1	312	KC2	CBD-CHA-C4D	-2.26	103.74	109.14
48	1	302	A86	C36-C31-C32	2.26	121.94	119.70
49	P	313	KC2	C2A-C3A-C4A	2.26	108.16	106.49
50	G	302	A1EB1	C9-C8-C6	-2.26	120.07	126.42
43	O	305	DD6	C37-C36-C35	2.26	118.54	114.36
48	3	308	A86	O4-C34-C35	2.26	113.22	107.59
39	4	322	CLA	CHB-C1B-NB	2.26	126.65	124.26
48	R	301	A86	C33-C32-C31	2.26	111.41	109.21
39	b	832	CLA	C3B-C4B-NB	-2.26	108.42	110.52
48	1	303	A86	C40-C32-C31	-2.26	108.45	110.47
50	7	305	A1EB1	C41-C32-C31	-2.26	108.45	110.47
50	9	302	A1EB1	C19-C18-C17	-2.26	106.41	110.77
43	1	304	DD6	C7-C6-C5	-2.26	119.76	122.92
39	7	314	CLA	CHD-C1D-ND	-2.26	122.38	124.45
51	E	311	A1ECV	CHC-C4B-C3B	-2.26	123.06	126.66
43	A	303	DD6	C7-C6-C5	-2.26	119.76	122.92
48	9	303	A86	O1-C15-C20	-2.26	57.19	59.40
48	M	303	A86	C9-C8-C6	-2.26	120.08	126.42
49	8	316	KC2	CHB-C4A-C3A	-2.26	121.45	124.98
43	1	304	DD6	C28-C27-C29	2.26	121.31	116.84
49	M	311	KC2	C1B-CHB-C4A	-2.26	121.19	126.06
48	8	307	A86	C35-C34-C33	-2.26	105.94	109.88
49	H	314	KC2	O2D-CGD-O1D	-2.26	119.43	123.84
48	R	317	A86	C34-O4-C38	-2.26	113.69	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	D	308	A1EB1	C28-O6-C42	2.26	120.70	115.68
49	9	316	KC2	C1B-CHB-C4A	-2.26	121.19	126.06
39	5	307	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
48	Z	303	A86	C3-C4-C5	-2.26	118.85	123.47
49	3	321	KC2	CBD-CHA-C1A	2.26	133.09	128.88
49	7	322	KC2	C4D-C3D-CAD	2.26	108.94	107.42
49	x	315	KC2	O2D-CGD-O1D	-2.26	119.43	123.84
50	3	303	A1EB1	O4-C38-O5	-2.26	118.48	122.96
39	x	318	CLA	CHB-C1B-NB	2.25	126.64	124.26
43	7	309	DD6	C34-C35-C36	-2.25	107.36	111.85
43	z	304	DD6	C14-C13-C11	-2.25	122.03	125.53
49	0	319	KC2	CHC-C4B-C3B	-2.25	121.40	125.26
50	2	304	A1EB1	C40-C32-C31	-2.25	108.45	110.47
46	Q	322	LMG	C4-C3-C2	-2.25	106.89	110.82
52	5	304	A1EB4	O1-C15-C14	-2.25	113.43	115.71
49	H	311	KC2	CHB-C4A-C3A	-2.25	121.46	124.98
49	8	316	KC2	C1B-CHB-C4A	-2.25	121.20	126.06
47	D	320	SQD	O48-C23-C24	2.25	118.98	111.91
47	M	301	SQD	O47-C7-C8	2.25	116.36	111.50
39	J	316	CLA	C3B-C4B-NB	-2.25	108.42	110.52
48	L	307	A86	C20-C19-C18	-2.25	108.29	112.75
50	4	301	A1EB1	O4-C38-O5	-2.25	118.49	122.96
49	2	313	KC2	C4D-C3D-CAD	2.25	108.94	107.42
49	V	314	KC2	C1B-CHB-C4A	-2.25	121.20	126.06
48	L	301	A86	O1-C15-C20	-2.25	57.20	59.40
51	X	310	A1ECV	O2-CMC-O1	-2.25	119.05	123.45
51	M	316	A1ECV	O2D-CGD-O1D	-2.25	119.44	123.84
48	T	301	A86	O1-C15-C20	-2.25	57.20	59.40
41	H	317	LHG	O8-C23-C24	2.25	118.97	111.91
49	Q	315	KC2	C1B-CHB-C4A	-2.25	121.20	126.06
47	9	322	SQD	O48-C23-C24	2.25	118.97	111.91
49	R	318	KC2	C1B-CHB-C4A	-2.25	121.20	126.06
49	Z	310	KC2	C1B-CHB-C4A	-2.25	121.20	126.06
50	x	302	A1EB1	O4-C38-O5	-2.25	118.49	122.96
42	h	202	BCR	C16-C15-C14	-2.25	118.86	123.47
39	7	325	CLA	O2D-CGD-CBD	2.25	115.27	111.27
50	2	304	A1EB1	C35-C34-C33	-2.25	105.95	109.88
49	3	318	KC2	C1B-CHB-C4A	-2.25	121.20	126.06
39	y	308	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
42	b	845	BCR	C27-C26-C25	-2.25	119.47	122.73
39	L	320	CLA	CHA-C1A-NA	-2.25	121.25	126.40
49	X	314	KC2	C1A-NA-C4A	-2.25	105.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S	317	KC2	O1D-CGD-CBD	-2.25	119.88	124.48
49	L	317	KC2	O2D-CGD-O1D	-2.25	119.44	123.84
50	H	301	A1EB1	C19-C18-C17	2.25	115.11	110.77
48	7	308	A86	C25-C24-C1	-2.25	120.10	126.42
49	V	315	KC2	CHD-C4C-NC	2.25	127.61	124.20
49	y	313	KC2	CHB-C4A-C3A	-2.25	121.47	124.98
49	X	312	KC2	C1B-CHB-C4A	-2.25	121.21	126.06
49	7	322	KC2	O2D-CGD-O1D	-2.25	119.44	123.84
48	L	307	A86	C4-C5-C6	-2.25	124.10	127.31
47	7	302	SQD	O48-C23-C24	2.25	118.96	111.91
48	4	305	A86	C12-C11-C13	2.25	119.80	116.02
39	7	314	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
49	9	316	KC2	O1D-CGD-CBD	-2.25	119.89	124.48
48	K	301	A86	O1-C15-C20	-2.25	57.20	59.40
39	U	211	CLA	CHD-C1D-ND	-2.25	122.39	124.45
48	J	301	A86	C9-C10-C11	-2.25	120.01	126.61
39	5	306	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
48	y	306	A86	C12-C11-C13	2.24	119.79	116.02
45	b	849	DGD	CBB-CAB-C9B	-2.24	103.03	114.42
51	M	316	A1ECV	C3-O2-CMC	2.24	120.16	115.83
39	F	306	CLA	C3B-C4B-NB	-2.24	108.43	110.52
50	V	302	A1EB1	C33-C32-C31	2.24	111.39	109.21
50	C	302	A1EB1	C9-C10-C11	-2.24	120.01	126.61
49	F	307	KC2	C1B-CHB-C4A	-2.24	121.22	126.06
50	J	302	A1EB1	C9-C10-C11	-2.24	120.01	126.61
48	J	301	A86	C9-C8-C6	-2.24	120.11	126.42
43	D	307	DD6	C21-C20-C15	-2.24	118.50	122.26
50	y	302	A1EB1	C19-C18-C17	-2.24	106.44	110.77
48	0	304	A86	C34-O4-C38	-2.24	113.72	117.90
48	x	305	A86	C28-C27-C26	-2.24	119.78	122.92
49	L	315	KC2	C1B-CHB-C4A	-2.24	121.22	126.06
39	7	321	CLA	CHD-C1D-ND	-2.24	122.39	124.45
42	b	846	BCR	C16-C15-C14	-2.24	118.88	123.47
43	3	304	DD6	C3-C2-C1	-2.24	124.11	127.31
46	F	317	LMG	C4-C3-C2	-2.24	106.91	110.82
48	Q	308	A86	C12-C11-C13	2.24	119.79	116.02
39	b	835	CLA	CHD-C1D-ND	-2.24	122.39	124.45
43	7	310	DD6	C-C1-C2	-2.24	119.78	122.92
50	4	302	A1EB1	O1-C15-C20	-2.24	57.21	59.40
41	X	301	LHG	C18-C17-C16	-2.24	103.05	114.42
39	b	841	CLA	CHB-C1B-NB	2.24	126.63	124.26
39	A	307	CLA	CHD-C1D-ND	-2.24	122.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	l	208	LMG	C4-C3-C2	-2.24	106.91	110.82
39	T	309	CLA	CMB-C2B-C3B	2.24	132.01	126.59
48	L	301	A86	C28-C27-C26	-2.24	119.78	122.92
48	2	305	A86	O4-C38-O5	-2.24	118.51	122.96
49	8	317	KC2	O2D-CGD-O1D	-2.24	119.46	123.84
49	B	208	KC2	C1B-CHB-C4A	-2.24	121.23	126.06
50	V	306	A1EB1	O4-C38-O5	-2.24	118.51	122.96
48	O	307	A86	C25-C24-C1	-2.24	120.13	126.42
48	0	306	A86	C9-C8-C6	-2.24	120.13	126.42
49	T	312	KC2	C1B-CHB-C4A	-2.24	121.23	126.06
50	S	303	A1EB1	O1-C20-C21	-2.24	112.37	115.06
50	0	305	A1EB1	O1-C20-C21	-2.24	112.37	115.06
51	W	317	A1ECV	O2D-CGD-O1D	-2.24	119.46	123.84
39	0	310	CLA	CHB-C1B-NB	2.24	126.63	124.26
39	F	314	CLA	C4-C3-C5	2.24	119.03	115.27
50	0	307	A1EB1	O4-C38-O5	-2.24	118.52	122.96
48	x	305	A86	C36-C31-C32	2.24	121.92	119.70
39	J	309	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
43	4	307	DD6	C10-C9-C8	-2.24	116.24	123.22
46	F	320	LMG	C4-C3-C2	-2.24	106.92	110.82
43	Q	306	DD6	C4-C3-C2	-2.24	118.89	123.47
50	E	301	A1EB1	O1-C15-C20	-2.24	57.21	59.40
39	a	825	CLA	C3B-C4B-NB	-2.24	108.44	110.52
42	b	846	BCR	C23-C22-C21	2.24	122.37	118.94
49	A	313	KC2	CHD-C4C-NC	2.24	127.60	124.20
49	L	321	KC2	CHD-C4C-NC	2.24	127.60	124.20
50	U	203	A1EB1	O4-C38-O5	-2.24	118.52	122.96
39	S	313	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
48	4	306	A86	C4-C3-C2	-2.24	118.89	123.47
50	0	307	A1EB1	C9-C8-C6	-2.24	120.13	126.42
39	W	316	CLA	CMB-C2B-C3B	2.24	132.00	126.59
49	7	322	KC2	C1B-CHB-C4A	-2.24	121.23	126.06
39	S	319	CLA	CHB-C1B-NB	2.24	126.62	124.26
46	7	326	LMG	O3-C3-C2	-2.24	105.18	110.35
43	E	305	DD6	C15-C14-C13	-2.24	121.27	125.99
49	K	310	KC2	O1D-CGD-CBD	-2.24	119.91	124.48
49	R	312	KC2	C1A-NA-C4A	-2.24	105.70	106.71
49	R	314	KC2	C1A-NA-C4A	-2.24	105.70	106.71
49	5	313	KC2	C1A-NA-C4A	-2.24	105.70	106.71
50	8	301	A1EB1	O4-C38-O5	-2.24	118.52	122.96
49	W	315	KC2	CHD-C4C-NC	2.24	127.59	124.20
49	W	312	KC2	C1B-CHB-C4A	-2.24	121.24	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	4	303	A1EB1	O4-C38-O5	-2.23	118.52	122.96
51	P	315	A1ECV	O2-CMC-O1	-2.23	119.08	123.45
49	A	310	KC2	CHD-C4C-NC	2.23	127.59	124.20
50	y	302	A1EB1	C9-C8-C6	-2.23	120.14	126.42
50	V	306	A1EB1	C41-C32-C31	2.23	112.47	110.47
49	3	315	KC2	C1B-CHB-C4A	-2.23	121.24	126.06
43	O	305	DD6	C25-C26-C27	-2.23	120.10	126.58
48	x	305	A86	C12-C11-C13	2.23	119.77	116.02
52	P	318	A1EB4	C36-C31-C32	2.23	121.91	119.70
39	0	322	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
39	l	203	CLA	CHB-C1B-NB	2.23	126.62	124.26
39	7	314	CLA	CHB-C1B-NB	2.23	126.62	124.26
43	x	304	DD6	C25-C26-C27	-2.23	120.10	126.58
48	T	301	A86	C9-C8-C6	-2.23	120.15	126.42
46	I	302	LMG	C38-C37-C36	-2.23	103.09	114.42
48	8	302	A86	O1-C15-C20	-2.23	57.22	59.40
42	j	103	BCR	C34-C9-C8	2.23	121.59	118.08
49	F	311	KC2	CHB-C4A-NA	2.23	127.72	124.20
48	0	309	A86	C12-C11-C13	2.23	119.77	116.02
39	A	314	CLA	C3B-C4B-NB	-2.23	108.44	110.52
49	4	317	KC2	CHD-C4C-NC	2.23	127.59	124.20
49	W	314	KC2	C1B-CHB-C4A	-2.23	121.25	126.06
43	A	304	DD6	C25-C26-C27	-2.23	120.10	126.58
49	V	308	KC2	O1D-CGD-CBD	-2.23	119.92	124.48
48	8	302	A86	C9-C8-C6	-2.23	120.15	126.42
49	z	312	KC2	C1B-CHB-C4A	-2.23	121.25	126.06
48	L	302	A86	O1-C15-C20	-2.23	57.22	59.40
39	y	319	CLA	CMB-C2B-C3B	2.23	131.99	126.59
52	5	304	A1EB4	O1-C20-C21	-2.23	112.39	115.06
49	L	321	KC2	CBD-CHA-C1A	2.23	133.04	128.88
49	S	317	KC2	C1A-NA-C4A	-2.23	105.70	106.71
50	F	304	A1EB1	C-C1-C24	2.23	121.59	118.08
48	E	304	A86	O1-C15-C20	-2.23	57.22	59.40
43	J	306	DD6	C-C1-C2	-2.23	119.80	122.92
43	M	304	DD6	C9-C8-C6	-2.23	120.16	126.42
43	Q	303	DD6	C13-C11-C10	2.23	122.36	118.94
49	I	312	KC2	CHB-C4A-NA	2.23	127.71	124.20
49	2	314	KC2	C1B-CHB-C4A	-2.23	121.25	126.06
39	S	310	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
39	B	207	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
50	Q	307	A1EB1	C3-C4-C5	-2.23	118.92	123.47
50	8	304	A1EB1	C12-C11-C13	2.23	119.76	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	8	308	A1EB1	C35-C34-C33	2.23	113.76	109.88
48	L	305	A86	C9-C8-C6	-2.23	120.17	126.42
51	Z	308	A1ECV	O1D-CGD-CBD	-2.23	121.03	124.74
49	G	315	KC2	O2D-CGD-O1D	-2.22	119.49	123.84
49	P	310	KC2	C1B-CHB-C4A	-2.22	121.26	126.06
48	C	303	A86	C33-C32-C31	2.22	111.37	109.21
39	L	309	CLA	CHB-C1B-NB	2.22	126.61	124.26
39	Q	311	CLA	CHD-C1D-ND	-2.22	122.41	124.45
49	6	316	KC2	C2A-C3A-C4A	2.22	108.14	106.49
39	9	308	CLA	C2A-C1A-CHA	2.22	127.75	123.86
51	5	309	A1ECV	O1D-CGD-CBD	-2.22	121.03	124.74
42	a	845	BCR	C38-C26-C27	2.22	117.89	113.62
50	8	308	A1EB1	C25-C24-C1	-2.22	120.17	126.42
50	x	301	A1EB1	C25-C24-C1	-2.22	120.17	126.42
39	S	319	CLA	C3A-C2A-C1A	2.22	104.67	101.34
39	b	809	CLA	CHD-C1D-ND	-2.22	122.41	124.45
48	9	304	A86	C36-C31-C32	2.22	121.90	119.70
50	O	301	A1EB1	O4-C38-O5	-2.22	118.55	122.96
46	S	321	LMG	C1-C2-C3	-2.22	105.37	110.00
49	y	316	KC2	C1B-CHB-C4A	-2.22	121.26	126.06
46	A	316	LMG	O3-C3-C2	-2.22	105.21	110.35
39	b	826	CLA	CHB-C4A-NA	2.22	127.58	124.51
39	a	802	CLA	CHD-C1D-ND	-2.22	122.41	124.45
39	F	310	CLA	CHD-C1D-ND	-2.22	122.41	124.45
39	9	320	CLA	CHD-C1D-ND	-2.22	122.41	124.45
49	8	314	KC2	O1D-CGD-CBD	-2.22	119.94	124.48
39	a	810	CLA	CHB-C1B-NB	2.22	126.61	124.26
39	I	315	CLA	C3B-C4B-NB	-2.22	108.45	110.52
39	F	321	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
48	P	303	A86	C9-C10-C11	-2.22	120.08	126.61
48	T	305	A86	C3-C4-C5	-2.22	118.92	123.47
50	8	301	A1EB1	C3-C4-C5	-2.22	118.92	123.47
49	z	315	KC2	C1B-CHB-C4A	-2.22	121.27	126.06
48	4	309	A86	O1-C15-C20	-2.22	57.23	59.40
49	4	317	KC2	CHB-C4A-C3A	-2.22	121.51	124.98
50	5	302	A1EB1	C25-C24-C1	-2.22	120.18	126.42
39	a	847	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
51	4	321	A1ECV	O2D-CGD-O1D	-2.22	119.50	123.84
46	4	325	LMG	C1-C2-C3	-2.22	105.37	110.00
50	7	305	A1EB1	C25-C24-C1	-2.22	120.18	126.42
50	3	303	A1EB1	C12-C11-C13	2.22	119.75	116.02
39	b	808	CLA	CMB-C2B-C1B	-2.22	121.99	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	J	309	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
39	T	318	CLA	C3B-C4B-NB	-2.22	108.46	110.52
39	z	307	CLA	C3B-C4B-NB	-2.22	108.46	110.52
49	4	320	KC2	O1D-CGD-CBD	-2.22	119.94	124.48
48	1	307	A86	O1-C20-C19	-2.22	111.72	113.38
50	3	303	A1EB1	C25-C24-C1	-2.22	120.18	126.42
39	a	801	CLA	CBA-CAA-C2A	-2.22	107.31	113.86
51	X	313	A1ECV	CMA-C3A-C2A	2.22	128.83	124.68
49	H	311	KC2	O1D-CGD-CBD	-2.22	119.94	124.48
43	7	309	DD6	C12-C11-C13	2.22	121.57	118.08
49	S	314	KC2	C4D-C3D-CAD	2.22	108.92	107.42
48	0	308	A86	C28-C27-C26	-2.22	119.82	122.92
43	O	303	DD6	C25-C26-C27	-2.22	120.14	126.58
49	x	313	KC2	C1B-CHB-C4A	-2.22	121.27	126.06
39	a	822	CLA	C2A-C1A-CHA	2.22	127.74	123.86
43	o	204	DD6	C26-C25-C24	-2.22	116.30	123.22
48	Z	301	A86	C3-C4-C5	-2.22	118.93	123.47
39	V	316	CLA	C3B-C4B-NB	-2.22	108.46	110.52
39	a	813	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
48	2	301	A86	C12-C11-C13	2.22	119.75	116.02
48	L	305	A86	C25-C24-C1	-2.22	120.19	126.42
48	I	304	A86	O1-C20-C21	-2.22	112.40	115.06
43	T	303	DD6	C3-C2-C1	-2.22	124.15	127.31
42	i	102	BCR	C28-C27-C26	-2.22	110.12	114.08
48	Q	301	A86	C12-C11-C13	2.22	119.74	116.02
50	J	302	A1EB1	O1-C15-C20	-2.22	57.23	59.40
43	O	304	DD6	C37-C36-C35	2.22	118.46	114.36
50	G	307	A1EB1	O1-C15-C20	-2.22	57.23	59.40
48	T	306	A86	O4-C38-O5	-2.21	118.56	122.96
42	l	206	BCR	C23-C24-C25	-2.21	120.98	127.20
48	M	303	A86	O1-C15-C20	-2.21	57.24	59.40
48	M	306	A86	C33-C32-C31	2.21	111.36	109.21
48	W	304	A86	C12-C11-C13	2.21	119.74	116.02
39	j	101	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
39	S	308	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
49	Q	315	KC2	CHD-C4C-NC	2.21	127.56	124.20
39	a	806	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
39	5	316	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
48	x	305	A86	C34-O4-C38	-2.21	113.77	117.90
39	7	313	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
49	2	313	KC2	C1B-CHB-C4A	-2.21	121.28	126.06
48	R	317	A86	O4-C38-O5	-2.21	118.57	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B	208	KC2	CHD-C4C-NC	2.21	127.56	124.20
52	5	304	A1EB4	C34-O4-C38	-2.21	113.77	117.90
49	V	312	KC2	C1B-CHB-C4A	-2.21	121.28	126.06
39	o	201	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
51	x	316	A1ECV	C3-O2-CMC	2.21	120.10	115.83
49	S	315	KC2	O1D-CGD-CBD	-2.21	119.96	124.48
43	X	304	DD6	C4-C3-C2	-2.21	118.94	123.47
49	5	314	KC2	C1A-C2A-C3A	-2.21	105.36	107.11
39	a	807	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
39	S	309	CLA	CHD-C1D-ND	-2.21	122.42	124.45
50	L	303	A1EB1	C28-O6-C42	2.21	120.60	115.68
49	L	314	KC2	CHB-C4A-C3A	-2.21	121.53	124.98
49	x	313	KC2	CHB-C4A-C3A	-2.21	121.53	124.98
48	J	303	A86	C12-C11-C13	2.21	119.74	116.02
39	Y	311	CLA	O2D-CGD-CBD	2.21	115.20	111.27
48	Y	301	A86	O1-C15-C20	-2.21	57.24	59.40
50	3	324	A1EB1	C-C1-C2	-2.21	119.83	122.92
39	H	308	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
50	x	301	A1EB1	O1-C15-C20	-2.21	57.24	59.40
48	7	311	A86	C10-C9-C8	-2.21	116.32	123.22
50	4	304	A1EB1	C19-C18-C17	-2.21	106.50	110.77
50	R	303	A1EB1	O1-C15-C20	-2.21	57.24	59.40
42	a	844	BCR	C33-C5-C4	2.21	117.86	113.62
50	G	302	A1EB1	O1-C15-C20	-2.21	57.24	59.40
49	X	314	KC2	O1D-CGD-CBD	-2.21	119.96	124.48
43	C	301	DD6	C12-C11-C13	2.21	121.56	118.08
48	8	305	A86	O4-C38-O5	-2.21	118.57	122.96
48	6	307	A86	O1-C15-C20	-2.21	57.24	59.40
51	Y	306	A1ECV	O1D-CGD-CBD	-2.21	121.06	124.74
48	S	307	A86	C10-C9-C8	-2.21	116.32	123.22
50	0	302	A1EB1	C35-C34-C33	-2.21	106.02	109.88
48	4	309	A86	C4-C3-C2	-2.21	118.95	123.47
48	G	301	A86	C-C1-C2	-2.21	119.83	122.92
49	L	321	KC2	O2D-CGD-O1D	-2.21	119.52	123.84
39	I	315	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
48	Z	301	A86	O4-C38-O5	-2.21	118.58	122.96
48	O	306	A86	C-C1-C2	-2.21	119.83	122.92
39	b	838	CLA	O2D-CGD-CBD	2.21	115.19	111.27
50	U	203	A1EB1	C12-C11-C13	2.21	119.73	116.02
48	V	304	A86	O1-C15-C20	-2.21	57.24	59.40
49	Q	313	KC2	CHB-C4A-C3A	-2.21	121.53	124.98
49	4	320	KC2	C1B-CHB-C4A	-2.21	121.30	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	302	A86	O4-C38-O5	-2.21	118.58	122.96
43	A	301	DD6	C14-C13-C11	-2.21	122.11	125.53
50	K	302	A1EB1	O1-C15-C20	-2.21	57.24	59.40
39	x	307	CLA	CMA-C3A-C2A	-2.21	110.95	116.10
48	P	303	A86	C12-C11-C13	2.21	119.73	116.02
39	O	314	CLA	CHD-C1D-ND	-2.21	122.43	124.45
39	P	314	CLA	CHD-C1D-ND	-2.21	122.43	124.45
50	H	304	A1EB1	O4-C38-O5	-2.21	118.58	122.96
39	b	837	CLA	CHB-C1B-NB	2.21	126.59	124.26
48	0	308	A86	O4-C34-C33	2.21	113.08	107.59
49	4	317	KC2	C1B-CHB-C4A	-2.21	121.30	126.06
39	0	312	CLA	C1-C2-C3	-2.21	122.23	126.04
51	y	317	A1ECV	C1D-CHD-C4C	-2.20	108.44	115.73
50	3	310	A1EB1	O1-C15-C20	-2.20	57.25	59.40
48	M	302	A86	C28-C27-C26	-2.20	119.83	122.92
49	T	314	KC2	C1B-CHB-C4A	-2.20	121.30	126.06
39	9	320	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
49	0	317	KC2	C1A-C2A-C3A	-2.20	105.36	107.11
43	y	304	DD6	C-C1-C2	-2.20	119.84	122.92
49	9	316	KC2	CBD-CHA-C1A	2.20	132.99	128.88
48	8	305	A86	C7-C6-C8	-2.20	114.61	118.08
49	V	312	KC2	C4D-C3D-CAD	2.20	108.91	107.42
39	3	320	CLA	O2D-CGD-CBD	2.20	115.18	111.27
48	W	307	A86	C33-C32-C31	2.20	111.35	109.21
48	0	301	A86	C19-C18-C17	2.20	115.03	110.77
48	9	305	A86	C34-O4-C38	-2.20	113.79	117.90
43	Z	302	DD6	C25-C24-C1	-2.20	120.23	126.42
48	9	305	A86	O1-C15-C20	-2.20	57.25	59.40
50	E	301	A1EB1	C26-C25-C24	-2.20	116.34	123.22
39	5	315	CLA	C2D-C1D-ND	-2.20	108.48	110.10
49	5	313	KC2	O1D-CGD-CBD	-2.20	119.98	124.48
49	T	316	KC2	C1B-CHB-C4A	-2.20	121.31	126.06
48	L	302	A86	O3-C36-C37	-2.20	105.47	109.39
46	4	325	LMG	O1-C7-C8	-2.20	105.59	110.90
49	F	311	KC2	C4D-C3D-CAD	2.20	108.91	107.42
43	F	305	DD6	C7-C6-C8	2.20	121.55	118.08
39	b	841	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
39	T	309	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
43	y	303	DD6	C25-C26-C27	-2.20	120.19	126.58
48	G	305	A86	C12-C11-C13	2.20	119.72	116.02
48	y	306	A86	O4-C34-C33	2.20	113.07	107.59
39	4	314	CLA	CMB-C2B-C1B	-2.20	122.02	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	7	304	A1EB1	C10-C9-C8	-2.20	116.35	123.22
51	9	314	A1ECV	C3-O2-CMC	2.20	120.08	115.83
48	J	301	A86	O1-C15-C20	-2.20	57.25	59.40
50	6	304	A1EB1	O1-C20-C21	-2.20	112.42	115.06
41	a	840	LHG	C27-C26-C25	-2.20	103.26	114.42
49	x	312	KC2	C1A-NA-C4A	-2.20	105.72	106.71
49	4	324	KC2	C1B-CHB-C4A	-2.20	121.31	126.06
48	P	303	A86	O1-C15-C20	-2.20	57.25	59.40
49	6	314	KC2	C1A-C2A-C3A	-2.20	105.37	107.11
43	G	303	DD6	C14-C13-C11	-2.20	122.12	125.53
49	R	314	KC2	O1D-CGD-CBD	-2.20	119.98	124.48
49	7	319	KC2	C4D-C3D-CAD	2.20	108.90	107.42
49	3	315	KC2	CHD-C4C-NC	2.20	127.54	124.20
43	a	846	DD6	C9-C8-C6	-2.20	120.24	126.42
48	U	202	A86	O1-C15-C20	-2.20	57.25	59.40
48	0	309	A86	C40-C32-C31	-2.20	108.50	110.47
39	M	315	CLA	CMA-C3A-C2A	-2.20	110.97	116.10
50	3	303	A1EB1	C3-C4-C5	-2.20	118.97	123.47
48	2	301	A86	C17-C16-C15	2.20	111.41	109.16
39	W	311	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
50	4	304	A1EB1	C28-O6-C42	2.20	120.57	115.68
43	X	304	DD6	C21-C20-C15	-2.20	118.58	122.26
39	A	311	CLA	CHD-C1D-ND	-2.20	122.44	124.45
39	b	841	CLA	C3B-C4B-NB	-2.20	108.48	110.52
39	K	306	CLA	C2A-C1A-CHA	2.20	127.70	123.86
49	G	317	KC2	C1B-CHB-C4A	-2.20	121.32	126.06
39	k	202	CLA	CHD-C1D-ND	-2.20	122.44	124.45
39	5	310	CLA	C1-C2-C3	-2.20	123.20	126.75
48	C	303	A86	O1-C20-C21	-2.20	112.42	115.06
49	6	317	KC2	CHB-C4A-C3A	-2.20	121.55	124.98
51	L	318	A1ECV	C3-O2-CMC	2.20	120.07	115.83
39	K	312	CLA	CHD-C1D-ND	-2.19	122.44	124.45
42	l	206	BCR	C21-C20-C19	-2.19	116.37	123.22
49	Z	311	KC2	C1B-CHB-C4A	-2.19	121.32	126.06
43	H	305	DD6	C33-C34-C35	-2.19	107.30	110.30
49	X	315	KC2	O1D-CGD-CBD	-2.19	119.99	124.48
49	F	311	KC2	C1B-CHB-C4A	-2.19	121.32	126.06
50	8	304	A1EB1	C9-C8-C6	-2.19	120.25	126.42
48	6	303	A86	O1-C15-C20	-2.19	57.26	59.40
50	5	302	A1EB1	C3-C4-C5	-2.19	118.98	123.47
50	z	301	A1EB1	O4-C38-O5	-2.19	118.60	122.96
39	A	305	CLA	CHB-C1B-NB	2.19	126.58	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	8	302	A86	C35-C34-C33	-2.19	106.05	109.88
39	X	316	CLA	O2D-CGD-CBD	2.19	115.17	111.27
39	b	805	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
49	J	315	KC2	C1B-CHB-C4A	-2.19	121.33	126.06
49	y	313	KC2	C1B-CHB-C4A	-2.19	121.33	126.06
48	8	305	A86	C-C1-C2	-2.19	119.85	122.92
48	J	301	A86	C26-C25-C24	-2.19	116.38	123.22
50	S	303	A1EB1	C26-C25-C24	-2.19	116.38	123.22
50	D	308	A1EB1	C33-C32-C31	2.19	111.34	109.21
50	6	308	A1EB1	C9-C10-C11	-2.19	120.16	126.61
42	a	843	BCR	C28-C27-C26	-2.19	110.16	114.08
39	O	310	CLA	C3C-C4C-NC	-2.19	108.11	110.57
43	F	305	DD6	C33-C34-C35	-2.19	107.31	110.30
39	E	313	CLA	CHD-C1D-ND	-2.19	122.44	124.45
39	G	312	CLA	CHD-C1D-ND	-2.19	122.44	124.45
39	a	805	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
48	L	307	A86	C25-C24-C1	-2.19	120.26	126.42
50	T	307	A1EB1	C-C1-C24	2.19	121.53	118.08
49	V	312	KC2	C1A-C2A-C3A	-2.19	105.38	107.11
49	8	317	KC2	C1B-CHB-C4A	-2.19	121.33	126.06
50	V	306	A1EB1	C9-C8-C6	-2.19	120.26	126.42
39	Z	316	CLA	C2A-C1A-CHA	2.19	127.68	123.85
39	3	312	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
49	I	312	KC2	CHC-C1C-C2C	-2.19	121.56	124.98
49	3	317	KC2	C1B-CHB-C4A	-2.19	121.33	126.06
52	R	305	A1EB4	O1-C20-C21	-2.19	112.43	115.06
48	2	302	A86	O1-C15-C20	-2.19	57.26	59.40
39	b	815	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
49	5	311	KC2	C1B-CHB-C4A	-2.19	121.34	126.06
49	I	312	KC2	C1B-CHB-C4A	-2.19	121.34	126.06
48	M	303	A86	C12-C11-C13	2.19	119.70	116.02
48	O	302	A86	C9-C10-C11	-2.19	120.17	126.61
49	X	312	KC2	C4D-C3D-CAD	2.19	108.90	107.42
48	6	309	A86	O1-C15-C20	-2.19	57.26	59.40
39	0	311	CLA	CHB-C4A-NA	2.19	127.54	124.51
48	T	305	A86	O1-C15-C20	-2.19	57.26	59.40
46	9	321	LMG	O3-C3-C2	-2.19	105.29	110.35
39	V	310	CLA	CAA-C2A-C1A	-2.19	104.81	111.97
43	a	846	DD6	C25-C26-C27	-2.19	120.23	126.58
39	a	836	CLA	C3B-C4B-NB	-2.19	108.49	110.52
42	b	844	BCR	C16-C15-C14	-2.19	118.99	123.47
49	Y	309	KC2	CHB-C4A-C3A	-2.19	121.56	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	G	313	KC2	CHD-C4C-NC	2.19	127.52	124.20
39	E	313	CLA	CMB-C2B-C3B	2.19	131.88	126.59
49	I	312	KC2	C4D-C3D-CAD	2.19	108.89	107.42
49	I	303	KC2	CMA-C3A-C4A	-2.19	121.71	125.04
48	O	306	A86	C28-C27-C26	-2.19	119.86	122.92
48	3	307	A86	C7-C6-C5	-2.19	119.86	122.92
39	0	310	CLA	CHD-C1D-ND	-2.19	122.45	124.45
39	5	308	CLA	CHD-C1D-ND	-2.19	122.45	124.45
39	B	209	CLA	C3B-C4B-NB	-2.18	108.49	110.52
50	O	301	A1EB1	O1-C20-C21	-2.18	112.44	115.06
48	8	302	A86	C17-C16-C15	2.18	111.39	109.16
52	P	319	A1EB4	C10-C9-C8	-2.18	116.40	123.22
50	C	302	A1EB1	O4-C38-O5	-2.18	118.62	122.96
50	K	304	A1EB1	O1-C15-C20	-2.18	57.26	59.40
49	0	316	KC2	CMB-C2B-C1B	2.18	128.56	124.71
39	C	311	CLA	C3B-C4B-NB	-2.18	108.49	110.52
50	8	308	A1EB1	C9-C8-C6	-2.18	120.28	126.42
43	J	305	DD6	C3-C4-C5	-2.18	119.00	123.47
51	Q	319	A1ECV	O2-CMC-O1	-2.18	119.18	123.45
48	F	302	A86	O4-C38-O5	-2.18	118.62	122.96
48	L	302	A86	C4-C5-C6	-2.18	124.19	127.31
39	b	801	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
49	3	321	KC2	CMB-C2B-C1B	2.18	128.56	124.71
39	I	315	CLA	CMB-C2B-C3B	2.18	131.87	126.59
48	9	306	A86	C33-C32-C31	2.18	111.33	109.21
50	2	306	A1EB1	C41-C32-C31	-2.18	108.52	110.47
39	8	311	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
49	S	317	KC2	C1B-CHB-C4A	-2.18	121.35	126.06
50	G	302	A1EB1	C25-C24-C1	-2.18	120.29	126.42
50	6	308	A1EB1	C28-O6-C42	2.18	120.53	115.68
48	Z	303	A86	C25-C26-C27	-2.18	124.20	127.31
51	V	317	A1ECV	CMA-C3A-C2A	2.18	128.76	124.68
48	4	305	A86	O4-C38-O5	-2.18	118.63	122.96
49	X	315	KC2	C1B-CHB-C4A	-2.18	121.35	126.06
50	z	301	A1EB1	C-C1-C24	2.18	121.51	118.08
39	y	308	CLA	O2A-CGA-O1A	-2.18	117.86	123.30
48	y	305	A86	O1-C15-C20	-2.18	57.27	59.40
50	T	307	A1EB1	O1-C15-C20	-2.18	57.27	59.40
48	3	307	A86	C28-C27-C26	-2.18	119.87	122.92
50	H	301	A1EB1	C40-C32-C31	-2.18	108.52	110.47
48	L	304	A86	C10-C9-C8	-2.18	116.41	123.22
49	7	320	KC2	C1B-CHB-C4A	-2.18	121.36	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	b	850	BCR	C3-C4-C5	-2.18	110.19	114.08
48	W	304	A86	C9-C8-C6	-2.18	120.29	126.42
46	7	326	LMG	C1-C2-C3	-2.18	105.46	110.00
48	8	303	A86	O1-C15-C20	-2.18	57.27	59.40
43	2	303	DD6	C34-C35-C36	-2.18	107.51	111.85
39	A	309	CLA	CHD-C1D-ND	-2.18	122.45	124.45
50	6	306	A1EB1	O4-C38-O5	-2.18	118.64	122.96
39	3	313	CLA	CHB-C1B-NB	2.18	126.56	124.26
49	y	314	KC2	O1D-CGD-CBD	-2.18	120.03	124.48
39	a	826	CLA	CMB-C2B-C3B	2.18	131.86	126.59
49	O	317	KC2	O1A-CGA-CBA	-2.18	118.24	125.67
48	8	307	A86	C9-C8-C6	-2.18	120.30	126.42
42	h	202	BCR	C36-C18-C19	2.18	121.51	118.08
50	3	302	A1EB1	O4-C34-C33	2.18	113.01	107.59
49	7	320	KC2	O1D-CGD-CBD	-2.18	120.03	124.48
39	a	816	CLA	C1-C2-C3	-2.18	122.28	126.04
42	k	204	BCR	C11-C12-C13	-2.18	120.31	126.42
39	M	318	CLA	C3B-C4B-NB	-2.18	108.50	110.52
48	Z	303	A86	C28-C27-C26	-2.18	119.88	122.92
47	4	327	SQD	O48-C23-C24	2.17	118.73	111.91
39	D	314	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
50	U	205	A1EB1	C40-C32-C31	-2.17	108.53	110.47
49	V	308	KC2	C1B-CHB-C4A	-2.17	121.37	126.06
46	4	325	LMG	O3-C3-C2	-2.17	105.32	110.35
43	2	303	DD6	C25-C24-C1	-2.17	120.31	126.42
39	Y	314	CLA	C2A-C1A-CHA	2.17	127.65	123.85
52	M	322	A1EB4	C10-C9-C8	-2.17	116.44	123.22
39	P	314	CLA	C3B-C4B-NB	-2.17	108.50	110.52
39	Q	310	CLA	CHD-C1D-ND	-2.17	122.46	124.45
48	C	303	A86	O4-C38-O5	-2.17	118.64	122.96
39	2	310	CLA	CAA-C2A-C3A	-2.17	108.83	114.26
48	Q	304	A86	O1-C15-C20	-2.17	57.28	59.40
49	F	311	KC2	CHC-C1C-C2C	-2.17	121.58	124.98
48	H	302	A86	O4-C38-O5	-2.17	118.65	122.96
43	R	304	DD6	C33-C32-C31	2.17	114.02	109.62
39	b	826	CLA	CHB-C1B-NB	2.17	126.56	124.26
48	0	306	A86	C20-C19-C18	-2.17	108.45	112.75
43	D	303	DD6	C24-C1-C2	2.17	122.27	118.94
46	S	321	LMG	O7-C10-O9	-2.17	118.46	123.70
49	y	316	KC2	C4D-C3D-CAD	2.17	108.89	107.42
43	x	304	DD6	C4-C5-C6	-2.17	124.21	127.31
48	Z	301	A86	O1-C15-C20	-2.17	57.28	59.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	K	306	CLA	C3B-C4B-NB	-2.17	108.50	110.52
39	b	816	CLA	CHD-C1D-ND	-2.17	122.46	124.45
39	D	309	CLA	CHB-C1B-NB	2.17	126.55	124.26
43	T	303	DD6	C4-C5-C6	-2.17	124.21	127.31
46	M	320	LMG	O3-C3-C2	-2.17	105.33	110.35
50	1	305	A1EB1	C34-O4-C38	-2.17	113.85	117.90
39	a	802	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
39	8	313	CLA	CMA-C3A-C2A	-2.17	111.04	116.10
39	a	825	CLA	CHD-C1D-ND	-2.17	122.46	124.45
39	X	308	CLA	CHD-C1D-ND	-2.17	122.46	124.45
49	y	316	KC2	C1A-NA-C4A	-2.17	105.73	106.71
39	V	316	CLA	C1-C2-C3	-2.17	123.24	126.75
39	7	315	CLA	C1-C2-C3	-2.17	123.24	126.75
49	W	315	KC2	O2D-CGD-O1D	-2.17	119.60	123.84
48	1	302	A86	O1-C15-C20	-2.17	57.28	59.40
39	8	322	CLA	O2D-CGD-CBD	2.17	115.12	111.27
39	X	311	CLA	C1-C2-C3	-2.17	123.24	126.75
48	Q	304	A86	C12-C11-C13	2.17	119.66	116.02
48	8	307	A86	C12-C11-C13	2.17	119.66	116.02
52	P	319	A1EB4	C7-C6-C5	-2.17	119.89	122.92
48	V	301	A86	O1-C15-C20	-2.17	57.28	59.40
52	W	306	A1EB4	C25-C24-C1	-2.17	120.33	126.42
39	U	211	CLA	C1-C2-C3	-2.17	122.30	126.04
42	a	842	BCR	C2-C1-C6	2.17	113.82	110.48
39	Q	311	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
39	0	312	CLA	C3B-C4B-NB	-2.17	108.50	110.52
39	l	203	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
52	P	305	A1EB4	C4-C3-C2	-2.17	119.04	123.47
39	b	851	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
48	0	308	A86	O1-C15-C20	-2.17	57.28	59.40
43	o	204	DD6	C28-C27-C29	2.17	121.13	116.84
39	b	818	CLA	CMB-C2B-C3B	2.17	131.83	126.59
39	D	312	CLA	CHB-C1B-NB	2.17	126.55	124.26
48	J	303	A86	O1-C15-C20	-2.17	57.28	59.40
39	O	308	CLA	CHD-C4C-C3C	2.17	128.02	124.84
50	0	307	A1EB1	C12-C11-C13	2.17	119.66	116.02
48	J	303	A86	C9-C8-C6	-2.17	120.33	126.42
49	6	317	KC2	C1B-CHB-C4A	-2.17	121.39	126.06
39	l	204	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
43	Q	306	DD6	O1-C20-C21	-2.16	112.46	115.06
48	9	301	A86	O1-C15-C20	-2.16	57.28	59.40
52	P	305	A1EB4	O4-C38-O43	-2.16	118.66	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	A	313	KC2	C2A-C3A-C4A	2.16	108.09	106.49
43	3	304	DD6	C25-C26-C27	-2.16	120.30	126.58
43	X	304	DD6	C33-C32-C31	2.16	114.01	109.62
39	b	817	CLA	C1-C2-C3	-2.16	122.30	126.04
48	0	308	A86	C36-C31-C32	2.16	121.84	119.70
39	b	825	CLA	C3B-C4B-NB	-2.16	108.51	110.52
39	l	201	CLA	CHD-C1D-ND	-2.16	122.47	124.45
49	S	314	KC2	C1B-CHB-C4A	-2.16	121.39	126.06
39	a	835	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
39	h	201	CLA	O2D-CGD-CBD	2.16	115.11	111.27
48	3	306	A86	C4-C3-C2	-2.16	119.04	123.47
50	S	302	A1EB1	C7-C6-C5	-2.16	119.89	122.92
50	V	306	A1EB1	O6-C42-O43	-2.16	118.13	123.59
50	6	304	A1EB1	C19-C18-C17	-2.16	106.60	110.77
47	P	301	SQD	C3-C4-C5	2.16	114.10	110.24
39	a	822	CLA	CMB-C2B-C3B	2.16	131.83	126.59
49	6	319	KC2	CHD-C4C-NC	2.16	127.48	124.20
51	S	318	A1ECV	O2D-CGD-O1D	-2.16	119.61	123.84
52	P	318	A1EB4	C-C1-C2	-2.16	119.89	122.92
39	T	313	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
39	b	821	CLA	CHD-C1D-ND	-2.16	122.47	124.45
49	M	311	KC2	O1D-CGD-CBD	-2.16	120.06	124.48
52	P	305	A1EB4	C25-C24-C1	-2.16	120.34	126.42
43	x	304	DD6	C12-C11-C13	2.16	121.48	118.08
49	I	303	KC2	CHB-C4A-NA	2.16	127.61	124.20
39	b	825	CLA	C2D-C1D-ND	-2.16	108.51	110.10
49	x	312	KC2	C4D-C3D-CAD	2.16	108.88	107.42
39	L	310	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
49	Q	318	KC2	C1B-CHB-C4A	-2.16	121.39	126.06
49	0	317	KC2	C1B-CHB-C4A	-2.16	121.39	126.06
47	T	321	SQD	O48-C23-C24	2.16	118.69	111.91
39	V	310	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
39	a	816	CLA	CHD-C1D-ND	-2.16	122.47	124.45
39	D	318	CLA	CHD-C1D-ND	-2.16	122.47	124.45
39	F	306	CLA	CHD-C1D-ND	-2.16	122.47	124.45
43	W	305	DD6	C25-C26-C27	-2.16	120.31	126.58
39	b	820	CLA	CAA-CBA-CGA	-2.16	106.94	113.25
43	4	308	DD6	C9-C10-C11	-2.16	124.23	127.31
48	6	302	A86	O1-C15-C20	-2.16	57.29	59.40
39	a	815	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
39	F	313	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
39	A	308	CLA	CHB-C1B-NB	2.16	126.54	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	2	313	KC2	CHD-C4C-NC	2.16	127.48	124.20
49	3	318	KC2	O1D-CGD-CBD	-2.16	120.07	124.48
43	M	304	DD6	C28-C27-C29	2.16	121.11	116.84
49	Z	310	KC2	CHB-C4A-C3A	-2.16	121.61	124.98
39	b	812	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
46	W	320	LMG	O3-C3-C2	-2.16	105.36	110.35
42	f	801	BCR	C10-C11-C12	-2.16	116.48	123.22
49	x	313	KC2	O1D-CGD-CBD	-2.16	120.07	124.48
48	0	306	A86	C3-C4-C5	-2.16	119.05	123.47
52	W	306	A1EB4	C4-C3-C2	-2.16	119.05	123.47
50	K	305	A1EB1	C9-C8-C6	-2.16	120.36	126.42
49	W	308	KC2	C4D-C3D-CAD	2.16	108.88	107.42
49	W	312	KC2	C4D-C3D-CAD	2.16	108.88	107.42
49	T	316	KC2	CHB-C4A-C3A	-2.16	121.61	124.98
39	O	310	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
39	U	209	CLA	O2D-CGD-CBD	2.16	115.10	111.27
39	W	311	CLA	CHD-C1D-ND	-2.16	122.47	124.45
45	b	849	DGD	C3G-C2G-C1G	-2.16	106.69	111.79
49	x	312	KC2	C1B-CHB-C4A	-2.16	121.41	126.06
50	D	308	A1EB1	C-C1-C2	-2.16	119.90	122.92
48	U	202	A86	C25-C24-C1	-2.16	120.36	126.42
50	K	305	A1EB1	C34-O4-C38	-2.16	113.88	117.90
43	x	304	DD6	C7-C6-C8	2.16	121.47	118.08
48	7	312	A86	C26-C25-C24	-2.16	116.49	123.22
48	k	206	A86	C7-C6-C5	-2.16	119.90	122.92
48	0	304	A86	C28-C27-C26	-2.16	119.90	122.92
39	T	320	CLA	C3B-C4B-NB	-2.16	108.52	110.52
51	L	318	A1ECV	O2D-CGD-O1D	-2.16	119.62	123.84
48	0	301	A86	C20-C19-C18	2.16	117.01	112.75
49	L	317	KC2	C4D-C3D-CAD	2.16	108.88	107.42
39	M	310	CLA	CHD-C1D-ND	-2.16	122.47	124.45
50	4	301	A1EB1	C36-C31-C32	2.16	121.83	119.70
50	0	302	A1EB1	C20-C19-C18	-2.16	108.48	112.75
39	G	318	CLA	CHB-C4A-NA	2.16	127.49	124.51
50	G	304	A1EB1	C-C1-C24	2.15	121.47	118.08
48	D	305	A86	C7-C6-C8	2.15	121.47	118.08
50	V	305	A1EB1	C7-C6-C8	2.15	121.47	118.08
48	6	302	A86	O4-C38-O5	-2.15	118.68	122.96
39	j	101	CLA	O2D-CGD-CBD	2.15	115.09	111.27
50	V	302	A1EB1	C35-C34-C33	-2.15	106.12	109.88
50	3	324	A1EB1	O4-C38-O5	-2.15	118.68	122.96
46	7	301	LMG	C8-O7-C10	-2.15	112.49	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	b	837	CLA	CBA-CAA-C2A	-2.15	107.51	113.86
50	1	301	A1EB1	C3-C4-C5	-2.15	119.06	123.47
49	V	320	KC2	C4D-C3D-CAD	2.15	108.87	107.42
39	9	312	CLA	CAC-C3C-C4C	2.15	127.60	124.81
50	C	302	A1EB1	O1-C20-C19	-2.15	111.77	113.38
48	8	309	A86	O1-C15-C20	-2.15	57.30	59.40
48	2	301	A86	C35-C34-C33	-2.15	106.12	109.88
43	A	301	DD6	C21-C20-C15	-2.15	118.65	122.26
39	b	828	CLA	C3B-C4B-NB	-2.15	108.52	110.52
49	H	314	KC2	CHB-C4A-C3A	-2.15	121.62	124.98
39	7	314	CLA	O2D-CGD-CBD	2.15	115.09	111.27
48	0	309	A86	C3-C4-C5	-2.15	119.07	123.47
49	L	314	KC2	O2D-CGD-O1D	-2.15	119.63	123.84
43	A	303	DD6	C9-C8-C6	-2.15	120.37	126.42
39	a	820	CLA	C2D-C1D-ND	-2.15	108.52	110.10
48	3	308	A86	C20-C19-C18	2.15	117.00	112.75
48	O	306	A86	O1-C15-C20	-2.15	57.30	59.40
39	b	823	CLA	CHD-C1D-ND	-2.15	122.48	124.45
39	S	316	CLA	CHD-C1D-ND	-2.15	122.48	124.45
49	7	322	KC2	CHB-C4A-C3A	-2.15	121.62	124.98
49	3	317	KC2	C2A-C3A-C4A	2.15	108.08	106.49
39	x	308	CLA	CMB-C2B-C3B	2.15	131.79	126.59
50	3	324	A1EB1	C8-C6-C5	-2.15	115.64	118.94
39	0	320	CLA	O2D-CGD-CBD	2.15	115.09	111.27
39	A	315	CLA	CHD-C1D-ND	-2.15	122.48	124.45
48	X	303	A86	O4-C38-O5	-2.15	118.69	122.96
49	R	312	KC2	O2D-CGD-O1D	-2.15	119.64	123.84
43	Z	302	DD6	C-C1-C2	-2.15	119.91	122.92
39	b	818	CLA	CHD-C1D-ND	-2.15	122.48	124.45
39	a	834	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
48	4	310	A86	C25-C24-C1	-2.15	120.38	126.42
50	1	301	A1EB1	O4-C38-O5	-2.15	118.69	122.96
50	V	302	A1EB1	C28-O6-C42	2.15	120.46	115.68
50	7	305	A1EB1	C35-C34-C33	-2.15	106.13	109.88
49	B	208	KC2	CHB-C4A-NA	2.15	127.59	124.20
48	F	302	A86	O1-C15-C20	-2.15	57.30	59.40
48	Z	303	A86	C34-O4-C38	-2.15	113.89	117.90
39	S	308	CLA	CHD-C1D-ND	-2.15	122.48	124.45
49	C	313	KC2	C1B-CHB-C4A	-2.15	121.43	126.06
50	6	306	A1EB1	C25-C24-C1	-2.15	120.39	126.42
49	P	310	KC2	C4D-C3D-CAD	2.15	108.87	107.42
39	Q	310	CLA	CMB-C2B-C3B	2.15	131.79	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	U	203	A1EB1	C33-C32-C31	2.15	111.30	109.21
39	A	311	CLA	CHB-C1B-NB	2.15	126.53	124.26
49	F	311	KC2	CHD-C4C-NC	2.15	127.46	124.20
43	B	202	DD6	C21-C20-C15	-2.15	118.66	122.26
50	4	302	A1EB1	O4-C38-O5	-2.15	118.70	122.96
49	0	316	KC2	CHB-C4A-C3A	-2.15	121.63	124.98
41	H	317	LHG	O8-C23-O10	-2.15	118.18	123.59
43	Q	306	DD6	C10-C9-C8	-2.15	116.52	123.22
52	W	306	A1EB4	O4-C38-O43	-2.15	118.70	122.96
50	3	324	A1EB1	C-C1-C24	2.15	121.46	118.08
39	8	311	CLA	O2D-CGD-CBD	2.15	115.08	111.27
39	G	312	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
49	G	315	KC2	C1A-C2A-C3A	-2.14	105.41	107.11
43	A	303	DD6	C3-C4-C5	-2.14	119.08	123.47
50	G	304	A1EB1	C28-O6-C42	2.14	120.45	115.68
50	Q	323	A1EB1	C28-O6-C42	2.14	120.45	115.68
43	R	304	DD6	C40-C32-C31	-2.14	107.06	110.47
47	D	320	SQD	C4-C3-C2	2.14	114.57	110.82
43	x	303	DD6	C-C1-C2	-2.14	119.92	122.92
48	L	301	A86	C25-C24-C1	-2.14	120.39	126.42
48	y	305	A86	C9-C10-C11	-2.14	120.31	126.61
48	J	301	A86	C34-O4-C38	-2.14	113.90	117.90
42	i	102	BCR	C16-C15-C14	-2.14	119.08	123.47
49	Z	310	KC2	O2D-CGD-O1D	-2.14	119.65	123.84
49	z	313	KC2	CAA-CBA-CGA	-2.14	119.93	123.66
51	y	317	A1ECV	O2-CMC-O1	-2.14	119.26	123.45
39	x	307	CLA	CHD-C1D-ND	-2.14	122.48	124.45
48	U	202	A86	C4-C3-C2	-2.14	119.08	123.47
39	b	825	CLA	O2D-CGD-CBD	2.14	115.08	111.27
49	V	315	KC2	C1B-CHB-C4A	-2.14	121.44	126.06
50	Q	307	A1EB1	C33-C32-C31	2.14	111.29	109.21
48	Q	305	A86	C34-O4-C38	-2.14	113.90	117.90
39	V	319	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
39	0	311	CLA	CHD-C1D-ND	-2.14	122.49	124.45
51	7	323	A1ECV	C1B-CHB-C4A	2.14	122.83	115.73
39	b	803	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
43	7	309	DD6	C25-C24-C1	-2.14	120.40	126.42
39	9	308	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
49	A	313	KC2	O2A-CGA-O1A	-2.14	118.22	122.67
49	Y	309	KC2	O1D-CGD-CBD	-2.14	120.11	124.48
49	6	316	KC2	CHB-C4A-C3A	-2.14	121.64	124.98
49	3	321	KC2	C1A-C2A-C3A	-2.14	105.42	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	P	313	KC2	C1A-NA-C4A	-2.14	105.74	106.71
49	4	324	KC2	CHB-C4A-NA	2.14	127.58	124.20
49	1	312	KC2	O1D-CGD-CBD	-2.14	120.11	124.48
50	L	303	A1EB1	O1-C20-C21	-2.14	112.49	115.06
48	R	301	A86	O1-C15-C20	-2.14	57.31	59.40
50	Q	307	A1EB1	O1-C15-C20	-2.14	57.31	59.40
48	L	304	A86	O4-C38-O5	-2.14	118.71	122.96
43	3	301	DD6	C-C1-C2	-2.14	119.93	122.92
48	8	303	A86	C28-C27-C26	-2.14	119.93	122.92
49	4	317	KC2	C4D-C3D-CAD	2.14	108.86	107.42
48	J	301	A86	C41-C32-C31	-2.14	108.56	110.47
49	W	314	KC2	O2D-CGD-O1D	-2.14	119.66	123.84
48	O	306	A86	C7-C6-C5	-2.14	119.93	122.92
46	4	326	LMG	C8-O7-C10	-2.14	112.53	117.79
48	8	302	A86	C4-C3-C2	-2.14	119.10	123.47
39	b	825	CLA	C2A-C1A-CHA	2.14	127.59	123.86
48	L	306	A86	O1-C15-C20	-2.14	57.31	59.40
50	8	306	A1EB1	C35-C34-C33	2.14	113.60	109.88
42	a	844	BCR	C8-C7-C6	-2.14	121.20	127.20
41	a	840	LHG	C18-C17-C16	-2.14	103.58	114.42
48	Q	301	A86	O1-C15-C20	-2.14	57.31	59.40
39	P	309	CLA	CHD-C1D-ND	-2.14	122.49	124.45
42	b	846	BCR	C38-C26-C25	-2.14	122.13	124.53
49	M	313	KC2	O2D-CGD-O1D	-2.14	119.66	123.84
50	E	301	A1EB1	C41-C32-C31	-2.14	108.56	110.47
39	T	309	CLA	CHD-C1D-ND	-2.13	122.49	124.45
50	7	306	A1EB1	C26-C25-C24	-2.13	116.56	123.22
39	R	315	CLA	C2A-C1A-CHA	2.13	127.59	123.86
39	F	310	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
51	P	315	A1ECV	O1D-CGD-CBD	-2.13	121.19	124.74
39	I	314	CLA	CHD-C1D-ND	-2.13	122.49	124.45
39	J	310	CLA	CHB-C1B-NB	2.13	126.52	124.26
48	E	304	A86	C3-C4-C5	-2.13	119.10	123.47
49	9	313	KC2	O1D-CGD-CBD	-2.13	120.12	124.48
48	8	309	A86	C9-C8-C6	-2.13	120.42	126.42
43	z	304	DD6	C25-C26-C27	-2.13	120.39	126.58
50	4	302	A1EB1	C33-C32-C31	2.13	111.28	109.21
50	4	304	A1EB1	C35-C34-C33	-2.13	106.15	109.88
48	8	303	A86	C4-C3-C2	-2.13	119.11	123.47
39	3	322	CLA	CHD-C1D-ND	-2.13	122.49	124.45
49	M	307	KC2	C1B-CHB-C4A	-2.13	121.46	126.06
39	T	310	CLA	C3B-C4B-NB	-2.13	108.54	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B	204	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
39	B	209	CLA	CHB-C1B-NB	2.13	126.51	124.26
39	K	308	CLA	CHB-C1B-NB	2.13	126.51	124.26
49	1	314	KC2	CBD-CHA-C1A	2.13	132.86	128.88
43	Z	302	DD6	C34-C35-C36	-2.13	107.61	111.85
48	J	301	A86	C25-C26-C27	-2.13	124.27	127.31
39	b	809	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
39	P	309	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
39	D	310	CLA	C3B-C4B-NB	-2.13	108.54	110.52
49	X	306	KC2	CHD-C4C-NC	2.13	127.44	124.20
49	T	315	KC2	CHB-C4A-C3A	-2.13	121.65	124.98
49	T	316	KC2	O2D-CGD-O1D	-2.13	119.67	123.84
48	1	303	A86	O1-C15-C20	-2.13	57.32	59.40
49	L	314	KC2	C1B-CHB-C4A	-2.13	121.46	126.06
48	L	302	A86	O4-C38-O5	-2.13	118.73	122.96
39	K	312	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
39	9	308	CLA	CBA-CAA-C2A	2.13	120.15	113.86
49	X	312	KC2	O2D-CGD-O1D	-2.13	119.67	123.84
39	f	802	CLA	CHB-C1B-NB	2.13	126.51	124.26
39	U	215	CLA	CHB-C1B-NB	2.13	126.51	124.26
50	K	304	A1EB1	C4-C3-C2	-2.13	119.11	123.47
49	V	320	KC2	C1B-CHB-C4A	-2.13	121.46	126.06
48	7	307	A86	C40-C32-C31	-2.13	108.57	110.47
49	O	317	KC2	CBD-CHA-C1A	2.13	132.85	128.88
50	3	324	A1EB1	C35-C34-C33	2.13	113.59	109.88
43	2	303	DD6	C-C1-C2	-2.13	119.94	122.92
39	l	203	CLA	O2D-CGD-CBD	2.13	115.05	111.27
49	I	312	KC2	CHD-C4C-NC	2.13	127.43	124.20
39	D	314	CLA	C3B-C4B-NB	-2.13	108.54	110.52
49	P	320	KC2	C1B-CHB-C4A	-2.13	121.47	126.06
48	B	201	A86	C28-C27-C26	-2.13	119.94	122.92
39	U	201	CLA	C2A-C1A-CHA	2.13	127.58	123.86
39	7	313	CLA	CHD-C1D-ND	-2.13	122.50	124.45
39	B	209	CLA	CHB-C4A-NA	2.13	127.45	124.51
50	3	309	A1EB1	O4-C38-O5	-2.13	118.73	122.96
51	Y	312	A1ECV	O1D-CGD-CBD	-2.13	121.19	124.74
50	4	302	A1EB1	C28-O6-C42	2.13	120.41	115.68
39	j	101	CLA	C3B-C4B-NB	-2.13	108.54	110.52
49	C	312	KC2	CHB-C4A-C3A	-2.13	121.66	124.98
46	S	321	LMG	C3-C4-C5	-2.13	106.44	110.24
49	V	320	KC2	CHB-C4A-NA	2.13	127.56	124.20
48	Q	308	A86	O4-C38-O5	-2.13	118.74	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	304	DD6	C26-C25-C24	-2.13	116.58	123.22
48	8	309	A86	C28-C27-C26	-2.13	119.94	122.92
49	4	318	KC2	CHD-C4C-NC	2.13	127.43	124.20
39	V	309	CLA	CHB-C1B-NB	2.13	126.51	124.26
39	a	806	CLA	O2D-CGD-CBD	2.13	115.05	111.27
48	0	304	A86	C12-C11-C13	2.13	119.59	116.02
50	8	308	A1EB1	C34-O4-C38	-2.13	113.93	117.90
39	L	320	CLA	O2A-CGA-O1A	-2.13	116.48	123.14
39	a	819	CLA	CAA-C2A-C3A	-2.13	106.96	112.78
43	z	305	DD6	C-C1-C2	-2.13	119.94	122.92
39	l	205	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
49	0	319	KC2	C2A-C3A-C4A	2.13	108.06	106.49
48	M	306	A86	C4-C3-C2	-2.13	119.12	123.47
49	P	313	KC2	O2A-CGA-O1A	-2.13	118.25	122.67
39	a	824	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
39	U	209	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
39	W	316	CLA	CHD-C1D-ND	-2.13	122.50	124.45
39	4	312	CLA	CHD-C1D-ND	-2.13	122.50	124.45
39	3	322	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
42	l	207	BCR	C38-C26-C27	2.12	117.70	113.62
43	y	304	DD6	O1-C20-C21	-2.12	112.51	115.06
50	U	203	A1EB1	C28-O6-C42	2.12	120.41	115.68
43	K	303	DD6	C4-C3-C2	-2.12	119.12	123.47
43	J	304	DD6	C-C1-C2	-2.12	119.95	122.92
48	C	303	A86	C25-C24-C1	-2.12	120.45	126.42
49	S	314	KC2	C1A-NA-C4A	-2.12	105.75	106.71
43	X	304	DD6	C37-C36-C31	-2.12	121.46	124.35
48	R	302	A86	C-C1-C2	-2.12	119.95	122.92
49	G	313	KC2	C1B-CHB-C4A	-2.12	121.48	126.06
43	O	304	DD6	C28-C27-C29	2.12	121.05	116.84
39	b	812	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
49	Y	308	KC2	CHD-C4C-NC	2.12	127.42	124.20
49	I	303	KC2	C2A-C3A-C4A	2.12	108.06	106.49
49	2	317	KC2	C1B-CHB-C4A	-2.12	121.48	126.06
48	1	303	A86	C9-C8-C6	-2.12	120.45	126.42
50	T	307	A1EB1	C26-C25-C24	-2.12	116.59	123.22
43	z	304	DD6	C34-C35-C36	-2.12	107.63	111.85
50	L	303	A1EB1	C9-C8-C6	-2.12	120.45	126.42
49	T	315	KC2	C1A-C2A-C3A	-2.12	105.43	107.11
43	O	304	DD6	C41-C32-C31	-2.12	107.09	110.47
48	7	312	A86	O4-C38-O5	-2.12	118.75	122.96
49	K	310	KC2	O2D-CGD-O1D	-2.12	119.69	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	I	308	CLA	C3B-C4B-NB	-2.12	108.55	110.52
50	V	302	A1EB1	C12-C11-C13	2.12	119.59	116.02
51	x	310	A1ECV	CMB-C2B-C1B	2.12	128.74	124.73
50	y	301	A1EB1	C9-C10-C11	-2.12	120.37	126.61
49	1	315	KC2	CHB-C4A-C3A	-2.12	121.67	124.98
50	O	301	A1EB1	C28-O6-C42	2.12	120.40	115.68
43	H	303	DD6	C26-C25-C24	-2.12	116.60	123.22
39	7	315	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
49	0	317	KC2	C4C-C3C-C2C	-2.12	105.43	107.11
39	a	803	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
43	W	305	DD6	C4-C3-C2	-2.12	119.13	123.47
39	l	205	CLA	CHB-C4A-NA	2.12	127.44	124.51
50	7	305	A1EB1	O4-C38-O5	-2.12	118.75	122.96
50	U	205	A1EB1	C34-O4-C38	-2.12	113.95	117.90
47	M	301	SQD	C4-C3-C2	2.12	114.52	110.82
51	4	321	A1ECV	C3-O2-CMC	2.12	119.92	115.83
50	z	302	A1EB1	O4-C34-C35	2.12	112.87	107.59
50	S	303	A1EB1	C28-O6-C42	2.12	120.39	115.68
51	9	317	A1ECV	C1B-CHB-C4A	2.12	122.75	115.73
48	9	305	A86	C7-C6-C8	2.12	121.41	118.08
50	V	306	A1EB1	C9-C10-C11	-2.12	120.38	126.61
51	M	316	A1ECV	CED-O2D-CGD	2.12	120.73	115.94
39	l	204	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
43	D	303	DD6	C37-C36-C35	2.12	118.28	114.36
49	A	313	KC2	C4D-C3D-CAD	2.12	108.85	107.42
39	2	309	CLA	C3B-C4B-NB	-2.12	108.55	110.52
39	C	304	CLA	CHB-C1B-NB	2.12	126.50	124.26
39	b	825	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
39	I	313	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
39	z	309	CLA	CMB-C2B-C1B	-2.12	122.15	125.37
51	Q	316	A1ECV	O1D-CGD-CBD	-2.12	121.22	124.74
43	F	303	DD6	C14-C13-C11	-2.12	122.25	125.53
49	6	316	KC2	C4D-C3D-CAD	2.12	108.85	107.42
39	F	314	CLA	CMB-C2B-C1B	-2.12	122.15	125.37
50	K	302	A1EB1	C28-C27-C26	-2.12	122.17	124.93
50	C	302	A1EB1	C3-C4-C5	-2.12	119.14	123.47
50	K	305	A1EB1	C4-C3-C2	-2.12	119.14	123.47
52	M	322	A1EB4	C7-C6-C5	-2.12	119.96	122.92
39	y	319	CLA	C3B-C4B-NB	-2.11	108.55	110.52
39	6	312	CLA	CAA-C2A-C3A	-2.11	108.98	114.26
43	O	304	DD6	C21-C20-C15	-2.11	118.72	122.26
49	V	320	KC2	O2D-CGD-O1D	-2.11	119.70	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	8	310	CLA	CAA-C2A-C1A	2.11	118.90	111.97
43	A	304	DD6	C15-C14-C13	-2.11	121.52	125.99
39	4	312	CLA	CHB-C1B-NB	2.11	126.50	124.26
39	2	309	CLA	CHB-C1B-NB	2.11	126.50	124.26
50	E	301	A1EB1	C33-C32-C31	2.11	111.27	109.21
49	S	315	KC2	C1A-C2A-C3A	-2.11	105.44	107.11
48	0	304	A86	C9-C10-C11	-2.11	120.39	126.61
43	E	303	DD6	C3-C4-C5	-2.11	119.14	123.47
43	A	304	DD6	C37-C36-C35	2.11	118.27	114.36
39	0	315	CLA	C1-C2-C3	-2.11	123.33	126.75
39	a	838	CLA	C2D-C1D-ND	-2.11	108.55	110.10
39	0	311	CLA	CMB-C2B-C3B	2.11	131.71	126.59
39	C	307	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
43	4	307	DD6	C12-C11-C13	2.11	121.41	118.08
39	3	312	CLA	O2D-CGD-CBD	2.11	115.02	111.27
42	f	801	BCR	C33-C5-C4	2.11	117.67	113.62
49	9	318	KC2	CHD-C4C-NC	2.11	127.41	124.20
48	Q	308	A86	C20-C19-C18	-2.11	108.57	112.75
50	S	302	A1EB1	C17-C16-C15	2.11	111.32	109.16
43	A	302	DD6	C26-C25-C24	-2.11	116.63	123.22
50	3	310	A1EB1	C9-C10-C11	-2.11	120.40	126.61
49	3	317	KC2	C4D-C3D-CAD	2.11	108.84	107.42
42	i	102	BCR	C8-C7-C6	-2.11	121.27	127.20
39	S	313	CLA	C3B-C4B-NB	-2.11	108.56	110.52
46	W	320	LMG	O2-C2-C1	-2.11	104.92	110.05
39	8	311	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
39	B	207	CLA	CHB-C1B-NB	2.11	126.49	124.26
39	E	318	CLA	CHD-C1D-ND	-2.11	122.52	124.45
39	I	314	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
43	2	303	DD6	C7-C6-C5	-2.11	119.97	122.92
52	P	319	A1EB4	C25-C24-C1	-2.11	120.49	126.42
43	z	305	DD6	C7-C6-C8	2.11	121.40	118.08
48	z	303	A86	C28-C27-C26	-2.11	119.97	122.92
49	2	313	KC2	C1A-NA-C4A	-2.11	105.76	106.71
48	2	302	A86	C9-C8-C6	-2.11	120.49	126.42
39	J	318	CLA	CHB-C1B-NB	2.11	126.49	124.26
51	G	316	A1ECV	C3-O2-CMC	2.11	119.90	115.83
49	y	313	KC2	C4D-C3D-CAD	2.11	108.84	107.42
50	9	302	A1EB1	C28-O6-C42	2.11	120.37	115.68
48	O	306	A86	O4-C38-O5	-2.11	118.78	122.96
39	Q	310	CLA	CHB-C1B-NB	2.11	126.49	124.26
39	7	316	CLA	CMB-C2B-C3B	2.11	131.69	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	P	304	DD6	C9-C8-C6	-2.11	120.50	126.42
39	4	322	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
49	G	317	KC2	C4D-C3D-CAD	2.11	108.84	107.42
42	a	844	BCR	C38-C26-C27	2.11	117.66	113.62
48	8	323	A86	C35-C34-C33	-2.11	106.20	109.88
39	a	832	CLA	CHC-C4B-NB	2.11	126.49	124.26
39	b	814	CLA	CHB-C1B-NB	2.11	126.49	124.26
39	b	818	CLA	CHB-C1B-NB	2.11	126.49	124.26
49	5	314	KC2	O1D-CGD-CBD	-2.11	120.17	124.48
39	i	103	CLA	C2A-C1A-CHA	2.11	127.54	123.86
49	3	318	KC2	O2A-CGA-O1A	-2.11	118.29	122.67
39	8	322	CLA	C3C-C4C-NC	-2.11	108.21	110.57
49	8	319	KC2	CHB-C4A-C3A	-2.11	121.69	124.98
48	3	305	A86	C28-C27-C26	-2.11	119.97	122.92
39	D	312	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
39	6	315	CLA	C3B-C4B-NB	-2.11	108.56	110.52
39	3	316	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
49	5	314	KC2	C1B-CHB-C4A	-2.10	121.52	126.06
39	b	831	CLA	C2D-C1D-ND	-2.10	108.55	110.10
49	2	314	KC2	O1D-CGD-CBD	-2.10	120.18	124.48
51	x	316	A1ECV	C1D-CHD-C4C	-2.10	108.77	115.73
50	h	203	A1EB1	O4-C38-O5	-2.10	118.78	122.96
39	x	318	CLA	C2A-C1A-CHA	2.10	127.53	123.85
52	W	321	A1EB4	C25-C24-C1	-2.10	120.51	126.42
49	V	318	KC2	C4D-C3D-CAD	2.10	108.84	107.42
39	J	311	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
50	Q	307	A1EB1	O4-C34-C35	2.10	112.83	107.59
43	C	301	DD6	C10-C9-C8	-2.10	116.65	123.22
52	W	321	A1EB4	O4-C38-O43	-2.10	118.78	122.96
50	2	306	A1EB1	C40-C32-C31	-2.10	108.59	110.47
48	1	307	A86	O1-C15-C20	-2.10	57.34	59.40
39	W	313	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
48	9	305	A86	C10-C9-C8	-2.10	116.66	123.22
48	T	305	A86	C25-C24-C1	-2.10	120.51	126.42
43	J	305	DD6	C7-C6-C5	-2.10	119.98	122.92
48	C	303	A86	C9-C8-C6	-2.10	120.51	126.42
52	R	305	A1EB4	C25-C26-C27	-2.10	124.31	127.31
48	8	323	A86	C9-C8-C6	-2.10	120.51	126.42
46	D	322	LMG	O2-C2-C1	-2.10	104.94	110.05
39	L	316	CLA	O2D-CGD-CBD	2.10	115.00	111.27
49	6	314	KC2	O2D-CGD-O1D	-2.10	119.73	123.84
39	b	842	CLA	O2A-CGA-O1A	-2.10	118.29	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	l	206	BCR	C33-C5-C4	2.10	117.65	113.62
43	F	305	DD6	C12-C11-C13	2.10	121.39	118.08
51	5	312	A1ECV	O2D-CGD-O1D	-2.10	119.73	123.84
48	2	305	A86	C9-C10-C11	-2.10	120.43	126.61
43	O	304	DD6	C34-C35-C36	-2.10	107.67	111.85
49	P	320	KC2	C1A-C2A-C3A	-2.10	105.45	107.11
50	7	303	A1EB1	C7-C6-C8	2.10	121.39	118.08
48	1	306	A86	C9-C10-C11	-2.10	120.43	126.61
43	T	303	DD6	C3-C4-C5	-2.10	119.17	123.47
48	9	301	A86	C25-C24-C1	-2.10	120.52	126.42
49	5	305	KC2	C1A-NA-C4A	-2.10	105.76	106.71
49	Y	309	KC2	C4D-C3D-CAD	2.10	108.84	107.42
50	7	303	A1EB1	C28-O6-C42	2.10	120.35	115.68
49	6	316	KC2	O2D-CGD-O1D	-2.10	119.73	123.84
39	b	839	CLA	CHD-C1D-ND	-2.10	122.53	124.45
39	O	308	CLA	CHD-C1D-ND	-2.10	122.53	124.45
39	Q	317	CLA	CHD-C1D-ND	-2.10	122.53	124.45
48	M	302	A86	C-C1-C2	-2.10	119.98	122.92
50	6	306	A1EB1	C3-C4-C5	-2.10	119.17	123.47
39	Q	321	CLA	O2D-CGD-CBD	2.10	115.00	111.27
39	E	319	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
50	S	303	A1EB1	C35-C34-C33	-2.10	106.22	109.88
39	6	311	CLA	CHD-C1D-ND	-2.10	122.53	124.45
39	E	309	CLA	CHB-C1B-NB	2.10	126.48	124.26
43	x	304	DD6	O1-C20-C19	-2.10	111.81	113.38
51	S	318	A1ECV	CED-O2D-CGD	2.10	120.68	115.94
50	D	308	A1EB1	C25-C24-C1	-2.10	120.52	126.42
48	Z	301	A86	C12-C11-C13	2.10	119.55	116.02
39	F	308	CLA	O2D-CGD-CBD	2.10	115.00	111.27
39	1	320	CLA	O2D-CGD-CBD	2.10	115.00	111.27
48	3	306	A86	C40-C32-C31	-2.10	108.59	110.47
50	D	308	A1EB1	O6-C42-O43	-2.10	118.30	123.59
39	C	307	CLA	CHD-C1D-ND	-2.10	122.53	124.45
49	6	314	KC2	C1B-CHB-C4A	-2.10	121.53	126.06
52	M	322	A1EB4	C25-C24-C1	-2.10	120.53	126.42
39	S	319	CLA	C2A-C1A-CHA	2.10	127.53	123.86
49	M	314	KC2	C4D-C3D-CAD	2.10	108.83	107.42
48	I	304	A86	C41-C32-C31	-2.10	108.60	110.47
39	a	818	CLA	CHB-C1B-NB	2.10	126.48	124.26
43	F	305	DD6	C3-C4-C5	-2.10	119.18	123.47
39	E	310	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
43	3	301	DD6	C10-C9-C8	-2.10	116.68	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	0	314	KC2	O1D-CGD-CBD	-2.10	120.20	124.48
50	G	304	A1EB1	O4-C38-O5	-2.09	118.80	122.96
49	5	311	KC2	C2A-C3A-C4A	2.09	108.04	106.49
39	X	311	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	Y	307	CLA	CAA-C2A-C3A	-2.09	111.21	116.10
46	M	320	LMG	O2-C2-C1	-2.09	104.96	110.05
48	7	307	A86	C41-C32-C31	-2.09	108.60	110.47
39	b	834	CLA	CAA-CBA-CGA	-2.09	107.13	113.25
48	4	306	A86	C33-C32-C31	2.09	111.25	109.21
51	7	317	A1ECV	CBB-CAB-C3B	-2.09	117.33	127.49
48	0	301	A86	O1-C15-C20	-2.09	57.35	59.40
39	Z	309	CLA	C3B-C4B-NB	-2.09	108.57	110.52
49	R	312	KC2	C1B-CHB-C4A	-2.09	121.54	126.06
39	Y	307	CLA	CHB-C4A-NA	2.09	127.41	124.51
39	V	310	CLA	CMB-C2B-C3B	2.09	131.66	126.59
39	V	316	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
49	7	320	KC2	CHB-C4A-C3A	-2.09	121.71	124.98
48	I	304	A86	C26-C25-C24	-2.09	116.69	123.22
48	9	303	A86	C9-C8-C6	-2.09	120.54	126.42
48	0	308	A86	C12-C11-C13	2.09	119.54	116.02
39	X	309	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	1	309	CLA	CHB-C1B-NB	2.09	126.47	124.26
48	5	301	A86	C4-C3-C2	-2.09	119.19	123.47
49	x	312	KC2	CHB-C4A-C3A	-2.09	121.71	124.98
50	0	307	A1EB1	C9-C10-C11	-2.09	120.46	126.61
50	0	303	A1EB1	C33-C32-C31	2.09	111.24	109.21
50	4	301	A1EB1	C40-C32-C31	-2.09	108.60	110.47
39	L	308	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
39	a	804	CLA	CHC-C4B-NB	2.09	126.47	124.26
39	W	313	CLA	CHB-C1B-NB	2.09	126.47	124.26
39	J	311	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	3	312	CLA	CHD-C1D-ND	-2.09	122.53	124.45
48	L	304	A86	C4-C3-C2	-2.09	119.19	123.47
43	F	305	DD6	C34-C35-C36	-2.09	107.69	111.85
43	M	304	DD6	C14-C13-C11	-2.09	122.29	125.53
48	V	304	A86	C26-C25-C24	-2.09	116.69	123.22
39	a	835	CLA	CHB-C1B-NB	2.09	126.47	124.26
49	3	318	KC2	C2A-C3A-C4A	2.09	108.04	106.49
43	A	303	DD6	C34-C35-C36	-2.09	107.69	111.85
39	a	819	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
49	G	317	KC2	CHB-C4A-NA	2.09	127.50	124.20
39	b	838	CLA	CHD-C1D-ND	-2.09	122.53	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	D	312	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	X	307	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	5	310	CLA	CHD-C1D-ND	-2.09	122.53	124.45
46	9	321	LMG	O2-C2-C1	-2.09	104.97	110.05
43	G	303	DD6	C40-C32-C31	-2.09	107.15	110.47
39	a	825	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
50	3	309	A1EB1	O1-C15-C20	-2.09	57.36	59.40
43	E	305	DD6	C25-C26-C27	-2.09	120.52	126.58
39	a	834	CLA	CMB-C2B-C3B	2.09	131.65	126.59
39	U	201	CLA	C2D-C1D-ND	-2.09	108.56	110.10
50	G	307	A1EB1	C28-O6-C42	2.09	120.33	115.68
39	a	819	CLA	CHD-C1D-ND	-2.09	122.53	124.45
50	7	306	A1EB1	O1-C20-C21	-2.09	112.55	115.06
48	W	303	A86	C12-C11-C13	2.09	119.53	116.02
48	1	302	A86	C12-C11-C13	2.09	119.53	116.02
39	l	201	CLA	O2D-CGD-CBD	2.09	114.98	111.27
51	E	311	A1ECV	C1B-CHB-C4A	2.09	122.65	115.73
39	b	819	CLA	CHB-C1B-NB	2.09	126.47	124.26
39	U	212	CLA	CHB-C1B-NB	2.09	126.47	124.26
50	7	306	A1EB1	O4-C38-O5	-2.09	118.81	122.96
39	a	823	CLA	CAA-C2A-C1A	-2.09	105.14	111.97
50	Q	307	A1EB1	C9-C10-C11	-2.09	120.47	126.61
50	K	302	A1EB1	C36-C31-C32	2.09	121.77	119.70
50	7	303	A1EB1	C4-C3-C2	-2.09	119.20	123.47
39	P	308	CLA	C3B-C4B-NB	-2.09	108.58	110.52
42	a	845	BCR	C35-C13-C12	2.09	121.36	118.08
49	P	310	KC2	O2D-CGD-O1D	-2.09	119.76	123.84
50	T	307	A1EB1	C3-C2-C1	-2.09	124.33	127.31
51	Q	319	A1ECV	C3-O2-CMC	2.09	119.86	115.83
49	W	308	KC2	O1D-CGD-CBD	-2.09	120.22	124.48
48	y	305	A86	O4-C38-O5	-2.09	118.82	122.96
48	V	301	A86	C9-C8-C6	-2.09	120.56	126.42
49	9	311	KC2	C4D-C3D-CAD	2.09	108.83	107.42
48	7	312	A86	C10-C9-C8	-2.09	116.71	123.22
39	F	314	CLA	C2A-C1A-CHA	2.09	127.51	123.86
51	0	321	A1ECV	CED-O2D-CGD	2.09	120.65	115.94
51	7	317	A1ECV	C3-O2-CMC	2.09	119.85	115.83
42	a	842	BCR	C38-C26-C27	2.09	117.62	113.62
47	T	321	SQD	O5-C1-C2	2.09	114.76	110.35
50	0	302	A1EB1	C9-C8-C6	-2.08	120.56	126.42
50	G	304	A1EB1	C35-C34-C33	2.08	113.51	109.88
49	T	315	KC2	C1B-CHB-C4A	-2.08	121.56	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	6	314	KC2	C4D-C3D-CAD	2.08	108.83	107.42
48	W	304	A86	O4-C38-O5	-2.08	118.82	122.96
48	8	303	A86	C12-C11-C13	2.08	119.52	116.02
39	F	314	CLA	C4-C3-C2	-2.08	118.33	123.68
43	j	102	DD6	C7-C6-C5	-2.08	120.00	122.92
39	b	814	CLA	CHD-C1D-ND	-2.08	122.54	124.45
39	Q	314	CLA	CHD-C1D-ND	-2.08	122.54	124.45
49	B	208	KC2	O2D-CGD-O1D	-2.08	119.77	123.84
48	X	303	A86	C35-C34-C33	-2.08	106.24	109.88
49	X	306	KC2	O1D-CGD-CBD	-2.08	120.22	124.48
51	Q	319	A1ECV	O1D-CGD-CBD	-2.08	121.27	124.74
48	W	304	A86	C3-C4-C5	-2.08	119.21	123.47
39	a	803	CLA	CHB-C1B-NB	2.08	126.46	124.26
39	J	314	CLA	CHB-C1B-NB	2.08	126.46	124.26
39	i	103	CLA	CMB-C2B-C3B	2.08	131.63	126.59
50	S	303	A1EB1	C34-O4-C38	-2.08	114.02	117.90
39	A	307	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
48	Q	301	A86	C9-C10-C11	-2.08	120.49	126.61
50	7	304	A1EB1	C25-C24-C1	-2.08	120.57	126.42
42	k	204	BCR	C7-C8-C9	-2.08	123.09	126.23
48	W	307	A86	O1-C15-C20	-2.08	57.37	59.40
49	X	318	KC2	C1B-CHB-C4A	-2.08	121.57	126.06
46	D	322	LMG	O1-C1-C2	-2.08	105.05	108.30
46	A	316	LMG	O2-C2-C1	-2.08	104.99	110.05
39	y	308	CLA	CHD-C1D-ND	-2.08	122.54	124.45
43	E	305	DD6	C33-C34-C35	-2.08	107.46	110.30
42	h	202	BCR	C34-C9-C8	2.08	121.36	118.08
43	I	305	DD6	C4-C5-C6	-2.08	124.34	127.31
43	x	303	DD6	C34-C35-C36	-2.08	107.71	111.85
45	b	849	DGD	CAB-C9B-C8B	-2.08	103.86	114.42
42	l	206	BCR	C10-C11-C12	-2.08	116.73	123.22
42	j	103	BCR	C30-C25-C24	2.08	121.66	115.78
39	E	307	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
49	Q	315	KC2	CHB-C4A-C3A	-2.08	121.73	124.98
39	a	835	CLA	CHD-C1D-ND	-2.08	122.54	124.45
52	X	305	A1EB4	C-C1-C24	2.08	121.35	118.08
39	V	310	CLA	C1-C2-C3	-2.08	122.45	126.04
39	Q	310	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
39	0	313	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
50	0	305	A1EB1	C12-C11-C13	2.08	119.51	116.02
39	T	310	CLA	CHD-C1D-ND	-2.08	122.54	124.45
39	R	309	CLA	O2D-CGD-CBD	2.08	114.96	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	f	803	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
50	1	301	A1EB1	C4-C3-C2	-2.08	119.22	123.47
43	Z	302	DD6	C7-C6-C5	-2.08	120.01	122.92
39	3	319	CLA	O2D-CGD-CBD	2.08	114.96	111.27
39	D	310	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
42	b	848	BCR	C35-C13-C12	2.08	121.35	118.08
39	B	206	CLA	CHD-C1D-ND	-2.08	122.55	124.45
39	D	315	CLA	CHD-C1D-ND	-2.08	122.55	124.45
39	W	313	CLA	CHD-C1D-ND	-2.08	122.55	124.45
39	0	311	CLA	C4D-CHA-C1A	2.08	123.78	121.25
49	P	320	KC2	C2A-C3A-C4A	2.08	108.03	106.49
48	G	305	A86	C41-C32-C31	-2.08	108.61	110.47
39	R	315	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
49	W	308	KC2	C1B-CHB-C4A	-2.08	121.58	126.06
39	a	802	CLA	CMB-C2B-C3B	2.08	131.62	126.59
39	U	207	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
52	R	305	A1EB4	C26-C25-C24	-2.08	116.74	123.22
39	H	313	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
49	P	313	KC2	C1B-CHB-C4A	-2.08	121.58	126.06
48	8	307	A86	C28-C27-C26	-2.08	120.02	122.92
50	z	301	A1EB1	C9-C10-C11	-2.08	120.50	126.61
50	7	306	A1EB1	C35-C34-C33	-2.08	106.25	109.88
42	f	804	BCR	C38-C26-C27	2.08	117.60	113.62
52	R	305	A1EB4	C-C1-C24	2.08	121.35	118.08
48	O	307	A86	C28-C27-C26	-2.08	120.02	122.92
50	x	302	A1EB1	C4-C3-C2	-2.08	119.22	123.47
52	X	305	A1EB4	C9-C10-C11	-2.08	124.51	127.00
48	6	305	A86	C40-C32-C31	-2.07	108.61	110.47
52	W	321	A1EB4	O1-C20-C21	-2.07	112.57	115.06
39	U	210	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
48	4	309	A86	C41-C32-C31	2.07	112.33	110.47
49	y	316	KC2	O2D-CGD-O1D	-2.07	119.78	123.84
39	L	311	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
39	6	310	CLA	CAA-C2A-C3A	-2.07	109.08	114.26
50	3	310	A1EB1	C25-C24-C1	-2.07	120.59	126.42
39	J	318	CLA	CMB-C2B-C3B	2.07	131.61	126.59
39	T	313	CLA	CHD-C1D-ND	-2.07	122.55	124.45
50	0	303	A1EB1	C-C1-C24	2.07	121.34	118.08
50	0	302	A1EB1	C40-C32-C31	-2.07	108.62	110.47
43	D	303	DD6	C25-C26-C27	-2.07	120.56	126.58
52	W	321	A1EB4	C21-C20-C15	-2.07	118.82	122.32
39	i	103	CLA	O2A-CGA-O1A	-2.07	118.36	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	L	318	A1ECV	O2-CMC-O1	-2.07	119.40	123.45
50	D	308	A1EB1	C20-C19-C18	-2.07	108.65	112.75
48	3	305	A86	C36-C31-C32	2.07	121.75	119.70
39	C	308	CLA	CHD-C1D-ND	-2.07	122.55	124.45
49	M	314	KC2	C1B-CHB-C4A	-2.07	121.59	126.06
39	4	312	CLA	CMB-C2B-C1B	-2.07	122.21	125.37
39	b	833	CLA	CHB-C1B-NB	2.07	126.45	124.26
39	W	311	CLA	CHB-C1B-NB	2.07	126.45	124.26
39	a	829	CLA	CMB-C2B-C3B	2.07	131.60	126.59
49	A	313	KC2	CHB-C4A-C3A	-2.07	121.74	124.98
39	T	319	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
39	b	839	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
49	W	312	KC2	O2D-CGD-O1D	-2.07	119.79	123.84
49	G	317	KC2	C1A-NA-C4A	-2.07	105.78	106.71
42	a	844	BCR	C10-C11-C12	-2.07	116.75	123.22
46	I	302	LMG	O3-C3-C2	-2.07	105.56	110.35
48	y	306	A86	C9-C10-C11	-2.07	120.52	126.61
39	E	306	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
50	h	203	A1EB1	C28-O6-C42	2.07	120.28	115.68
39	7	314	CLA	C2A-C1A-CHA	2.07	127.48	123.86
39	3	314	CLA	CHD-C1D-ND	-2.07	122.55	124.45
49	2	313	KC2	O2D-CGD-O1D	-2.07	119.79	123.84
50	4	303	A1EB1	C17-C16-C15	2.07	111.27	109.16
41	a	840	LHG	O8-C6-C5	-2.07	102.41	108.43
49	L	312	KC2	CHB-C4A-C3A	-2.07	121.75	124.98
43	x	304	DD6	C-C1-C2	-2.07	120.03	122.92
48	P	302	A86	C9-C10-C11	-2.07	120.53	126.61
39	4	316	CLA	CHD-C1D-ND	-2.07	122.55	124.45
48	F	302	A86	C9-C8-C6	-2.07	120.61	126.42
42	b	846	BCR	C1-C6-C5	-2.07	119.70	122.61
48	M	306	A86	C20-C19-C18	2.07	116.84	112.75
39	l	205	CLA	CHB-C1B-NB	2.07	126.45	124.26
39	B	205	CLA	CHB-C1B-NB	2.07	126.45	124.26
48	P	303	A86	O4-C38-O5	-2.07	118.86	122.96
39	b	821	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
42	a	844	BCR	C20-C19-C18	-2.07	120.61	126.42
50	3	302	A1EB1	C9-C8-C6	-2.07	120.61	126.42
39	P	309	CLA	CHB-C1B-NB	2.07	126.44	124.26
39	W	309	CLA	CHB-C1B-NB	2.07	126.44	124.26
39	7	315	CLA	CHB-C1B-NB	2.07	126.44	124.26
48	T	301	A86	O4-C38-O5	-2.07	118.86	122.96
39	D	313	CLA	CMB-C2B-C3B	2.07	131.59	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	303	DD6	C25-C26-C27	-2.07	120.58	126.58
41	X	301	LHG	C27-C26-C25	-2.07	103.94	114.42
39	D	313	CLA	CHB-C1B-NB	2.07	126.44	124.26
39	x	307	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
43	S	306	DD6	C21-C20-C15	-2.07	118.80	122.26
49	L	315	KC2	O1D-CGD-CBD	-2.07	120.26	124.48
39	D	317	CLA	CMB-C2B-C3B	2.07	131.59	126.59
39	D	310	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
50	7	306	A1EB1	C41-C32-C31	-2.06	108.62	110.47
39	P	308	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
48	Q	301	A86	O4-C38-O5	-2.06	118.86	122.96
48	X	303	A86	C7-C6-C8	2.06	121.33	118.08
50	S	302	A1EB1	C26-C25-C24	-2.06	116.77	123.22
39	1	319	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
39	a	812	CLA	CHD-C1D-ND	-2.06	122.56	124.45
43	A	303	DD6	C37-C36-C35	2.06	118.18	114.36
48	W	303	A86	C9-C10-C11	-2.06	120.54	126.61
50	S	303	A1EB1	C19-C18-C17	-2.06	106.79	110.77
39	b	816	CLA	C2D-C1D-ND	-2.06	108.58	110.10
49	S	315	KC2	C2A-C3A-C4A	2.06	108.02	106.49
48	E	304	A86	C9-C10-C11	-2.06	120.54	126.61
50	z	301	A1EB1	C9-C8-C6	-2.06	120.62	126.42
46	F	317	LMG	O7-C10-O9	-2.06	118.72	123.70
39	a	818	CLA	CHD-C1D-ND	-2.06	122.56	124.45
39	a	828	CLA	CHD-C1D-ND	-2.06	122.56	124.45
39	Z	306	CLA	CHD-C1D-ND	-2.06	122.56	124.45
39	a	824	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
39	E	313	CLA	CHB-C1B-NB	2.06	126.44	124.26
39	D	309	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
50	y	302	A1EB1	C40-C32-C31	-2.06	108.63	110.47
39	U	209	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
39	0	311	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
48	L	306	A86	C8-C6-C5	2.06	122.11	118.94
43	O	305	DD6	C7-C6-C5	-2.06	120.03	122.92
48	M	303	A86	C3-C4-C5	-2.06	119.25	123.47
48	Q	302	A86	O1-C15-C20	-2.06	57.39	59.40
49	Q	315	KC2	C2A-C3A-C4A	2.06	108.02	106.49
39	a	801	CLA	C1-C2-C3	-2.06	122.48	126.04
49	J	315	KC2	C1A-C2A-C3A	-2.06	105.48	107.11
49	R	312	KC2	C1A-C2A-C3A	-2.06	105.48	107.11
48	7	308	A86	C28-C27-C26	-2.06	120.04	122.92
43	2	303	DD6	C28-C27-C29	2.06	120.92	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	U	206	A86	C33-C32-C31	2.06	111.21	109.21
39	b	801	CLA	C2D-C1D-ND	-2.06	108.59	110.10
39	B	209	CLA	O2D-CGD-CBD	2.06	114.93	111.27
50	2	306	A1EB1	O4-C38-O5	-2.06	118.87	122.96
39	b	834	CLA	C4-C3-C5	2.06	118.73	115.27
39	b	832	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
39	b	838	CLA	C1-C2-C3	-2.06	122.48	126.04
39	l	205	CLA	C3C-C4C-NC	-2.06	108.26	110.57
39	0	315	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
39	3	311	CLA	CHD-C1D-ND	-2.06	122.56	124.45
51	6	320	A1ECV	O2-CMC-O1	-2.06	119.43	123.45
50	K	305	A1EB1	O4-C38-O5	-2.06	118.87	122.96
43	a	846	DD6	C37-C36-C35	2.06	118.17	114.36
39	a	827	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
39	E	309	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
50	V	302	A1EB1	C25-C24-C1	-2.06	120.64	126.42
42	f	804	BCR	C35-C13-C14	-2.06	120.04	122.92
39	b	805	CLA	CMB-C2B-C3B	2.06	131.57	126.59
43	Q	303	DD6	C3-C4-C5	-2.06	119.26	123.47
50	h	203	A1EB1	O1-C15-C20	-2.06	57.39	59.40
49	x	313	KC2	C4D-C3D-CAD	2.06	108.81	107.42
42	i	102	BCR	C38-C26-C27	2.06	117.57	113.62
48	M	303	A86	C4-C3-C2	-2.06	119.26	123.47
48	U	206	A86	O1-C15-C20	-2.06	57.39	59.40
49	6	317	KC2	O1D-CGD-CBD	-2.06	120.28	124.48
39	a	810	CLA	CHD-C1D-ND	-2.06	122.56	124.45
39	h	201	CLA	CHD-C1D-ND	-2.06	122.56	124.45
50	0	303	A1EB1	C9-C10-C11	-2.06	120.56	126.61
39	a	834	CLA	C1-C2-C3	-2.06	122.49	126.04
43	5	303	DD6	C40-C32-C31	-2.06	107.20	110.47
49	S	314	KC2	CHB-C4A-C3A	-2.06	121.77	124.98
48	2	302	A86	C-C1-C2	-2.06	120.04	122.92
49	0	316	KC2	C1B-CHB-C4A	-2.06	121.62	126.06
48	L	305	A86	C35-C34-C33	-2.06	106.29	109.88
43	Z	302	DD6	C25-C26-C27	-2.05	120.61	126.58
48	8	309	A86	C33-C32-C31	2.05	111.21	109.21
50	z	302	A1EB1	O1-C20-C21	-2.05	112.59	115.06
52	T	304	A1EB4	O4-C34-C35	2.05	112.71	107.59
39	8	318	CLA	O2D-CGD-CBD	2.05	114.92	111.27
50	y	301	A1EB1	C-C1-C2	-2.05	120.05	122.92
48	8	303	A86	C25-C24-C1	-2.05	120.64	126.42
50	0	305	A1EB1	O1-C20-C19	-2.05	111.84	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	X	302	A86	C28-C27-C26	-2.05	120.05	122.92
39	T	308	CLA	CHB-C1B-NB	2.05	126.43	124.26
39	E	308	CLA	C3B-C4B-NB	-2.05	108.61	110.52
39	G	314	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
50	E	301	A1EB1	O6-C42-O43	-2.05	118.41	123.59
49	L	312	KC2	CHD-C4C-NC	2.05	127.32	124.20
48	4	309	A86	O4-C38-O5	-2.05	118.88	122.96
48	X	302	A86	C-C1-C2	-2.05	120.05	122.92
49	5	305	KC2	C2A-C3A-C4A	2.05	108.01	106.49
39	M	315	CLA	CMB-C2B-C3B	2.05	131.56	126.59
50	H	304	A1EB1	C12-C11-C13	2.05	119.47	116.02
50	U	203	A1EB1	C20-C19-C18	-2.05	108.69	112.75
50	x	302	A1EB1	C17-C16-C15	2.05	111.26	109.16
48	W	303	A86	C-C1-C2	-2.05	120.05	122.92
43	S	306	DD6	C23-C16-C17	2.05	112.55	108.98
39	A	312	CLA	C1-C2-C3	-2.05	122.49	126.04
49	Q	315	KC2	C4D-C3D-CAD	2.05	108.81	107.42
49	P	320	KC2	O1D-CGD-CBD	-2.05	120.29	124.48
48	3	308	A86	O1-C15-C20	-2.05	57.40	59.40
48	Q	301	A86	C3-C4-C5	-2.05	119.27	123.47
39	R	308	CLA	CHB-C1B-NB	2.05	126.43	124.26
39	V	309	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
48	T	305	A86	C35-C34-C33	-2.05	106.30	109.88
42	b	847	BCR	C2-C1-C6	2.05	113.64	110.48
39	a	805	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	K	314	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	T	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
46	l	208	LMG	C8-O7-C10	-2.05	112.74	117.79
43	7	309	DD6	O1-C20-C21	-2.05	112.60	115.06
39	a	810	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
43	x	303	DD6	C10-C9-C8	-2.05	116.82	123.22
51	W	317	A1ECV	O1D-CGD-CBD	-2.05	121.33	124.74
51	0	321	A1ECV	CHC-C4B-C3B	-2.05	123.39	126.66
49	R	312	KC2	C4D-C3D-CAD	2.05	108.80	107.42
48	0	304	A86	C35-C34-C33	2.05	113.45	109.88
48	Q	302	A86	C12-C11-C13	2.05	119.46	116.02
50	z	302	A1EB1	C12-C11-C13	2.05	119.46	116.02
39	A	312	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
39	I	301	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
50	7	304	A1EB1	C35-C34-C33	-2.05	106.30	109.88
39	T	320	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
52	P	318	A1EB4	C12-C11-C13	2.05	118.74	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	C	305	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	R	309	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	I	315	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	a	823	CLA	CHB-C1B-NB	2.05	126.42	124.26
50	S	303	A1EB1	C9-C8-C6	-2.05	120.66	126.42
43	S	306	DD6	C-C1-C2	-2.05	120.06	122.92
39	E	308	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
39	K	306	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
42	b	846	BCR	C21-C20-C19	-2.05	116.83	123.22
39	V	316	CLA	CHB-C1B-NB	2.05	126.42	124.26
39	I	314	CLA	CHB-C1B-NB	2.05	126.42	124.26
39	K	309	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	a	812	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
42	b	845	BCR	C21-C20-C19	-2.05	116.83	123.22
47	P	301	SQD	O47-C7-O49	-2.05	118.76	123.70
49	2	313	KC2	CHB-C4A-NA	2.05	127.43	124.20
39	U	210	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	b	807	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
50	6	308	A1EB1	C12-C11-C13	2.05	119.46	116.02
49	L	312	KC2	O1D-CGD-CBD	-2.04	120.30	124.48
50	U	205	A1EB1	C26-C25-C24	-2.04	116.84	123.22
50	J	302	A1EB1	C35-C34-C33	-2.04	106.31	109.88
48	1	307	A86	O1-C15-C14	-2.04	109.11	113.21
49	X	318	KC2	CHB-C4A-C3A	-2.04	121.78	124.98
50	H	304	A1EB1	C34-O4-C38	-2.04	114.09	117.90
49	M	307	KC2	C1A-NA-C4A	-2.04	105.79	106.71
50	1	301	A1EB1	C10-C9-C8	-2.04	116.84	123.22
39	o	205	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
49	V	314	KC2	C2A-C3A-C4A	2.04	108.00	106.49
39	G	309	CLA	CHB-C1B-NB	2.04	126.42	124.26
39	0	312	CLA	CHB-C1B-NB	2.04	126.42	124.26
52	R	305	A1EB4	O4-C38-O43	-2.04	118.90	122.96
39	C	308	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
39	7	325	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
39	O	311	CLA	CAA-C2A-C3A	-2.04	109.16	114.26
39	a	833	CLA	O2D-CGD-CBD	2.04	114.90	111.27
50	y	301	A1EB1	C12-C11-C13	2.04	119.45	116.02
42	k	204	BCR	C38-C26-C27	2.04	117.54	113.62
48	G	301	A86	C9-C10-C11	-2.04	120.60	126.61
43	Z	302	DD6	C28-C27-C29	2.04	120.88	116.84
48	U	206	A86	C25-C26-C27	-2.04	124.40	127.31
39	b	831	CLA	O2A-CGA-O1A	-2.04	118.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	4	321	A1ECV	CED-O2D-CGD	2.04	120.56	115.94
48	4	328	A86	C-C1-C2	-2.04	120.06	122.92
50	2	306	A1EB1	C7-C6-C5	-2.04	120.06	122.92
39	I	308	CLA	CHD-C1D-ND	-2.04	122.58	124.45
49	G	313	KC2	CHC-C1C-C2C	-2.04	121.79	124.98
39	U	211	CLA	CHB-C1B-NB	2.04	126.42	124.26
43	y	303	DD6	C-C1-C2	-2.04	120.06	122.92
48	Q	308	A86	C26-C25-C24	-2.04	116.85	123.22
39	V	309	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
49	3	317	KC2	CMB-C2B-C1B	2.04	128.31	124.71
51	2	311	A1ECV	C3-O2-CMC	2.04	119.77	115.83
43	T	303	DD6	C12-C11-C10	-2.04	120.06	122.92
39	E	312	CLA	C4-C3-C5	2.04	118.70	115.27
52	W	321	A1EB4	C12-O3-C39	2.04	120.22	115.68
48	6	307	A86	C7-C6-C5	-2.04	120.07	122.92
48	J	303	A86	C9-C10-C11	-2.04	120.61	126.61
48	S	307	A86	C25-C24-C1	-2.04	120.69	126.42
50	y	301	A1EB1	C28-O6-C42	2.04	120.22	115.68
48	K	301	A86	C40-C32-C31	-2.04	108.65	110.47
52	M	322	A1EB4	C41-C32-C31	-2.04	108.65	110.47
39	E	316	CLA	CHD-C1D-ND	-2.04	122.58	124.45
50	L	303	A1EB1	C19-C18-C17	-2.04	106.83	110.77
39	M	309	CLA	O2D-CGD-CBD	2.04	114.89	111.27
39	V	316	CLA	CMB-C2B-C3B	2.04	131.53	126.59
50	3	310	A1EB1	C4-C3-C2	-2.04	119.30	123.47
43	O	303	DD6	C12-C11-C13	2.04	121.29	118.08
49	V	314	KC2	C4D-C3D-CAD	2.04	108.80	107.42
49	X	314	KC2	C4D-C3D-CAD	2.04	108.80	107.42
39	b	836	CLA	CHD-C1D-ND	-2.04	122.58	124.45
47	D	321	SQD	O6-C1-C2	2.04	111.48	108.30
39	a	835	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
48	6	309	A86	O4-C38-O5	-2.04	118.92	122.96
39	E	317	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
39	a	827	CLA	CMB-C2B-C3B	2.04	131.52	126.59
48	Q	304	A86	C-C1-C24	2.04	121.29	118.08
39	P	311	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
39	H	309	CLA	CHB-C1B-NB	2.04	126.41	124.26
39	A	314	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
50	K	302	A1EB1	C28-O6-C42	2.04	120.21	115.68
39	Z	307	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
42	f	801	BCR	C27-C26-C25	-2.04	119.78	122.73
39	H	306	CLA	O2A-CGA-O1A	-2.04	118.45	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	I	304	A86	C10-C9-C8	-2.04	116.86	123.22
39	T	313	CLA	CHB-C4A-NA	2.04	127.33	124.51
49	W	314	KC2	CHB-C4A-C3A	-2.04	121.80	124.98
39	M	310	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
48	T	306	A86	C34-O4-C38	-2.04	114.10	117.90
43	D	306	DD6	C3-C4-C5	-2.04	119.31	123.47
48	U	206	A86	C25-C24-C1	-2.04	120.70	126.42
39	G	310	CLA	CHD-C1D-ND	-2.03	122.58	124.45
39	I	316	CLA	CHD-C1D-ND	-2.03	122.58	124.45
49	4	324	KC2	O2D-CGD-O1D	-2.03	119.86	123.84
50	7	303	A1EB1	C25-C24-C1	-2.03	120.70	126.42
47	H	318	SQD	C1-O5-C5	2.03	117.68	113.69
39	a	837	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
49	1	312	KC2	C2A-C3A-C4A	2.03	108.00	106.49
49	z	312	KC2	C4D-C3D-CAD	2.03	108.79	107.42
48	O	307	A86	O1-C20-C21	-2.03	112.62	115.06
39	F	312	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
42	b	850	BCR	C38-C26-C27	2.03	117.52	113.62
39	V	309	CLA	C4-C3-C5	2.03	118.69	115.27
39	A	314	CLA	C1-C2-C3	-2.03	122.53	126.04
39	J	307	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
39	b	828	CLA	C1-C2-C3	-2.03	122.53	126.04
39	H	315	CLA	CHC-C4B-NB	2.03	126.41	124.26
48	Q	302	A86	C3-C4-C5	-2.03	119.31	123.47
39	a	813	CLA	CHD-C1D-ND	-2.03	122.59	124.45
50	G	308	A1EB1	O4-C38-O5	-2.03	118.92	122.96
48	0	301	A86	C23-C16-C17	2.03	112.51	108.98
39	5	315	CLA	O2D-CGD-CBD	2.03	114.88	111.27
39	a	805	CLA	CHB-C1B-NB	2.03	126.41	124.26
39	I	313	CLA	CHB-C1B-NB	2.03	126.41	124.26
51	S	318	A1ECV	O1D-CGD-CBD	-2.03	121.36	124.74
39	b	805	CLA	CHD-C1D-ND	-2.03	122.59	124.45
39	M	315	CLA	CHD-C1D-ND	-2.03	122.59	124.45
50	3	310	A1EB1	O4-C38-O5	-2.03	118.93	122.96
42	k	204	BCR	C8-C9-C10	2.03	122.06	118.94
50	2	306	A1EB1	O-C13-C14	-2.03	117.53	121.66
39	f	802	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
39	a	816	CLA	CMB-C2B-C3B	2.03	131.51	126.59
39	E	308	CLA	CMB-C2B-C3B	2.03	131.51	126.59
49	8	320	KC2	C4D-C3D-CAD	2.03	108.79	107.42
50	2	306	A1EB1	O6-C42-O43	-2.03	118.47	123.59
39	Q	321	CLA	C1-C2-C3	-2.03	122.53	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	D	316	CLA	CHD-C1D-ND	-2.03	122.59	124.45
46	S	321	LMG	O3-C3-C2	-2.03	105.66	110.35
52	M	322	A1EB4	C12-O3-C39	2.03	120.20	115.68
48	F	302	A86	C-C1-C24	2.03	121.28	118.08
52	5	304	A1EB4	C-C1-C24	2.03	121.28	118.08
39	9	308	CLA	O2A-C1-C2	2.03	113.97	108.64
39	R	309	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
39	U	211	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
39	X	308	CLA	CMB-C2B-C3B	2.03	131.50	126.59
48	0	308	A86	C8-C6-C5	-2.03	115.83	118.94
39	a	816	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
49	M	314	KC2	O2A-CGA-O1A	-2.03	118.45	122.67
39	b	817	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
39	3	320	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
46	F	320	LMG	O7-C10-O9	-2.03	118.80	123.70
47	4	327	SQD	O47-C7-O49	-2.03	118.80	123.70
39	R	315	CLA	C3A-C2A-C1A	2.03	104.38	101.34
51	x	316	A1ECV	O2-CMC-O1	-2.03	119.48	123.45
42	a	842	BCR	C31-C1-C6	-2.03	107.01	110.30
48	V	304	A86	C3-C4-C5	-2.03	119.32	123.47
39	0	313	CLA	CHD-C1D-ND	-2.03	122.59	124.45
49	M	307	KC2	O1D-CGD-CBD	-2.03	120.33	124.48
49	V	318	KC2	O1D-CGD-CBD	-2.03	120.33	124.48
39	E	308	CLA	O2D-CGD-CBD	2.03	114.87	111.27
39	O	318	CLA	C2A-C1A-CHA	2.03	127.41	123.86
50	x	301	A1EB1	O6-C42-O43	-2.03	118.47	123.59
52	P	318	A1EB4	C23-C16-C22	2.03	110.36	107.37
39	I	311	CLA	O2D-CGD-CBD	2.03	114.87	111.27
48	S	307	A86	O1-C20-C21	-2.03	112.63	115.06
52	5	304	A1EB4	C33-C32-C31	2.03	111.18	109.21
50	K	304	A1EB1	O4-C38-O5	-2.03	118.94	122.96
52	P	318	A1EB4	C40-C32-C31	-2.03	108.66	110.47
48	H	302	A86	C3-C4-C5	-2.03	119.32	123.47
49	4	318	KC2	O1D-CGD-CBD	-2.03	120.34	124.48
39	X	311	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
50	K	304	A1EB1	C9-C8-C6	-2.03	120.72	126.42
39	Q	310	CLA	C1-C2-C3	-2.03	122.54	126.04
39	k	202	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
48	0	301	A86	C26-C25-C24	-2.03	116.89	123.22
51	0	321	A1ECV	CMB-C2B-C1B	2.03	128.55	124.73
49	0	316	KC2	O2D-CGD-O1D	-2.03	119.88	123.84
48	6	309	A86	C35-C34-C33	-2.03	106.34	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	i	101	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
49	5	311	KC2	C4D-C3D-CAD	2.03	108.79	107.42
48	7	311	A86	C3-C4-C5	-2.02	119.33	123.47
50	0	303	A1EB1	O4-C38-O5	-2.02	118.94	122.96
39	b	826	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
47	9	322	SQD	O6-C1-C2	2.02	111.46	108.30
39	b	829	CLA	CMB-C2B-C3B	2.02	131.49	126.59
43	o	204	DD6	C3-C4-C5	-2.02	119.33	123.47
39	P	307	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
43	G	306	DD6	C7-C6-C5	-2.02	120.09	122.92
48	G	301	A86	C7-C6-C5	-2.02	120.09	122.92
43	U	204	DD6	C21-C20-C15	-2.02	118.87	122.26
50	z	302	A1EB1	C25-C24-C1	-2.02	120.73	126.42
39	P	308	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
48	S	307	A86	C40-C32-C31	-2.02	108.66	110.47
48	T	305	A86	C40-C32-C31	-2.02	108.66	110.47
39	E	316	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
49	2	314	KC2	O2D-CGD-O1D	-2.02	119.88	123.84
39	f	803	CLA	CHB-C1B-NB	2.02	126.40	124.26
39	I	301	CLA	CHB-C1B-NB	2.02	126.40	124.26
39	B	206	CLA	C2D-C1D-ND	-2.02	108.61	110.10
39	J	310	CLA	CMB-C2B-C3B	2.02	131.49	126.59
48	X	303	A86	C25-C24-C1	-2.02	120.73	126.42
48	O	302	A86	C7-C6-C5	-2.02	120.09	122.92
39	a	812	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
49	Y	309	KC2	C1A-NA-C4A	-2.02	105.80	106.71
51	M	316	A1ECV	O1D-CGD-CBD	-2.02	121.37	124.74
46	M	320	LMG	O1-C7-C8	-2.02	106.02	110.90
48	S	307	A86	C41-C32-C31	-2.02	108.66	110.47
39	I	310	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
48	G	301	A86	O-C13-C11	-2.02	116.68	121.15
50	4	301	A1EB1	C26-C25-C24	-2.02	116.91	123.22
48	0	306	A86	C9-C10-C11	-2.02	120.67	126.61
39	a	823	CLA	CAA-CBA-CGA	-2.02	107.35	113.25
49	M	307	KC2	CHB-C4A-NA	2.02	127.39	124.20
49	Z	310	KC2	C4D-C3D-CAD	2.02	108.78	107.42
39	T	318	CLA	C2A-C1A-CHA	2.02	127.39	123.86
42	a	844	BCR	C23-C24-C25	-2.02	121.53	127.20
39	H	312	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
39	b	817	CLA	CHB-C1B-NB	2.02	126.39	124.26
48	9	306	A86	C20-C19-C18	-2.02	108.75	112.75
39	H	309	CLA	O2A-CGA-O1A	-2.02	118.50	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	S	309	CLA	C2D-C1D-ND	-2.02	108.62	110.10
48	J	303	A86	C35-C34-C33	-2.02	106.35	109.88
46	4	326	LMG	O7-C10-O9	-2.02	118.82	123.70
39	2	319	CLA	CHC-C4B-NB	2.02	126.39	124.26
50	0	302	A1EB1	C3-C4-C5	-2.02	119.34	123.47
39	H	312	CLA	C1-C2-C3	-2.02	122.55	126.04
39	F	308	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
48	9	305	A86	C26-C25-C24	-2.02	116.92	123.22
50	8	308	A1EB1	C12-C11-C13	2.02	119.41	116.02
39	D	319	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
39	F	321	CLA	CHD-C1D-ND	-2.02	122.60	124.45
39	9	319	CLA	CHD-C1D-ND	-2.02	122.60	124.45
42	j	103	BCR	C23-C24-C25	-2.02	121.54	127.20
48	U	202	A86	O4-C34-C35	2.02	112.61	107.59
39	A	309	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
39	b	815	CLA	C1-C2-C3	-2.02	122.56	126.04
50	K	302	A1EB1	C12-C11-C13	2.02	119.41	116.02
39	b	829	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
39	x	309	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
50	4	301	A1EB1	C7-C6-C8	2.02	121.25	118.08
50	K	302	A1EB1	C17-C16-C15	2.02	111.22	109.16
51	4	321	A1ECV	O1D-CGD-CBD	-2.02	121.38	124.74
46	7	301	LMG	O7-C10-O9	-2.02	118.83	123.70
39	A	312	CLA	CHB-C1B-NB	2.02	126.39	124.26
52	X	305	A1EB4	C26-C25-C24	-2.02	116.93	123.22
49	H	314	KC2	O2A-CGA-O1A	-2.02	118.48	122.67
39	M	309	CLA	O1D-CGD-CBD	2.02	128.61	124.48
46	D	322	LMG	O1-C7-C8	-2.01	106.04	110.90
39	F	313	CLA	O2D-CGD-CBD	2.01	114.85	111.27
52	P	319	A1EB4	C41-C32-C31	-2.01	108.67	110.47
48	6	305	A86	O4-C34-C35	2.01	112.61	107.59
39	a	832	CLA	CHD-C1D-ND	-2.01	122.60	124.45
50	F	304	A1EB1	C28-O6-C42	2.01	120.16	115.68
39	A	309	CLA	CMB-C2B-C3B	2.01	131.47	126.59
39	i	103	CLA	O1D-CGD-CBD	2.01	128.60	124.48
47	D	321	SQD	C4-C3-C2	2.01	114.34	110.82
49	3	321	KC2	C1B-CHB-C4A	-2.01	121.71	126.06
51	y	311	A1ECV	C3-O2-CMC	2.01	119.72	115.83
43	A	304	DD6	C12-C11-C10	-2.01	120.10	122.92
49	1	314	KC2	CHB-C4A-C3A	-2.01	121.83	124.98
50	2	306	A1EB1	C34-O4-C38	-2.01	114.14	117.90
39	b	810	CLA	O2A-CGA-O1A	-2.01	118.51	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	L	305	A86	C3-C4-C5	-2.01	119.35	123.47
42	b	848	BCR	C7-C8-C9	-2.01	123.19	126.23
48	8	305	A86	C28-C27-C26	-2.01	120.10	122.92
48	M	303	A86	O4-C38-O5	-2.01	118.96	122.96
50	9	302	A1EB1	C25-C24-C1	-2.01	120.76	126.42
49	1	312	KC2	O2D-CGD-O1D	-2.01	119.90	123.84
49	6	317	KC2	O2D-CGD-O1D	-2.01	119.90	123.84
48	G	305	A86	C35-C34-C33	-2.01	106.36	109.88
50	G	308	A1EB1	C33-C32-C31	2.01	111.17	109.21
39	E	317	CLA	CMB-C2B-C1B	-2.01	122.30	125.37
47	M	301	SQD	C44-O6-C1	2.01	117.67	113.74
50	V	307	A1EB1	C17-C16-C15	2.01	111.22	109.16
39	A	315	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
43	S	306	DD6	C20-C19-C18	2.01	116.73	112.75
49	K	313	KC2	CHB-C4A-NA	2.01	127.37	124.20
39	4	322	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
39	D	319	CLA	CHB-C1B-NB	2.01	126.39	124.26
39	3	319	CLA	CHB-C1B-NB	2.01	126.39	124.26
39	9	307	CLA	CHB-C1B-NB	2.01	126.39	124.26
48	8	307	A86	O1-C15-C20	-2.01	57.43	59.40
39	M	321	CLA	CHD-C1D-ND	-2.01	122.61	124.45
39	4	311	CLA	CHD-C1D-ND	-2.01	122.61	124.45
47	P	301	SQD	O48-C23-O10	-2.01	118.52	123.59
39	E	313	CLA	O2D-CGD-CBD	2.01	114.84	111.27
39	S	320	CLA	O2D-CGD-CBD	2.01	114.84	111.27
49	0	317	KC2	O1D-CGD-CBD	-2.01	120.37	124.48
39	a	823	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
48	M	302	A86	O1-C20-C21	-2.01	112.65	115.06
39	J	309	CLA	CMB-C2B-C3B	2.01	131.46	126.59
43	U	204	DD6	C3-C4-C5	-2.01	119.36	123.47
48	D	305	A86	O-C13-C11	-2.01	116.71	121.15
39	F	321	CLA	C1-O2A-CGA	2.01	121.72	116.44
49	P	306	KC2	O1D-CGD-CBD	-2.01	120.37	124.48
39	G	309	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
48	O	306	A86	C24-C1-C2	2.01	122.03	118.94
47	F	319	SQD	C3-C4-C5	2.01	113.82	110.24
48	x	305	A86	C-C1-C2	-2.01	120.11	122.92
42	a	845	BCR	C10-C11-C12	-2.01	116.95	123.22
39	2	309	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
39	D	317	CLA	C2A-C1A-CHA	2.01	127.37	123.86
49	T	312	KC2	C1A-C2A-C3A	-2.01	105.52	107.11
50	K	302	A1EB1	C3-C4-C5	-2.01	119.36	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	W	303	A86	O1-C20-C19	-2.01	111.87	113.38
39	E	310	CLA	CHD-C1D-ND	-2.01	122.61	124.45
48	O	302	A86	C9-C8-C6	-2.01	120.77	126.42
39	2	319	CLA	CHA-C1A-NA	-2.01	121.80	126.40
39	C	306	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
39	Z	305	CLA	CMA-C3A-C2A	-2.01	111.41	116.10
39	a	813	CLA	CHC-C1C-NC	2.01	127.25	124.20
50	V	302	A1EB1	O4-C38-O5	-2.01	118.97	122.96
39	y	309	CLA	C3B-C4B-NB	-2.01	108.65	110.52
39	D	314	CLA	C1-C2-C3	-2.01	122.57	126.04
39	4	311	CLA	C2A-C1A-CHA	2.01	127.37	123.86
47	S	301	SQD	O5-C5-C4	2.01	113.34	109.69
39	0	315	CLA	CHD-C1D-ND	-2.01	122.61	124.45
42	b	844	BCR	C30-C25-C26	-2.01	119.79	122.61
50	x	302	A1EB1	C3-C4-C5	-2.01	119.36	123.47
39	b	805	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
39	X	317	CLA	CHB-C1B-NB	2.01	126.38	124.26
39	G	318	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
51	5	309	A1ECV	O2-CMC-O1	-2.01	119.53	123.45
39	a	804	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
39	o	206	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
48	V	301	A86	C36-C31-C32	2.01	121.69	119.70
39	y	309	CLA	CHB-C1B-NB	2.01	126.38	124.26
50	1	301	A1EB1	O6-C42-O43	-2.01	118.53	123.59
39	9	309	CLA	C3B-C4B-NB	-2.01	108.65	110.52
42	a	844	BCR	C21-C20-C19	-2.01	116.96	123.22
39	b	809	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
49	J	315	KC2	C2A-C3A-C4A	2.01	107.97	106.49
39	S	320	CLA	C1-C2-C3	-2.01	122.57	126.04
39	P	316	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
48	P	302	A86	C17-C16-C15	2.01	111.21	109.16
39	b	801	CLA	CHB-C1B-NB	2.01	126.38	124.26
39	S	311	CLA	CHB-C1B-NB	2.01	126.38	124.26
39	b	806	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
50	8	306	A1EB1	C-C1-C2	-2.01	120.11	122.92
48	E	304	A86	C9-C8-C6	-2.01	120.78	126.42
49	I	303	KC2	C1B-CHB-C4A	-2.01	121.73	126.06
39	b	822	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
50	T	307	A1EB1	O4-C38-O5	-2.00	118.98	122.96
39	o	202	CLA	CHB-C1B-NB	2.00	126.38	124.26
49	6	319	KC2	C2A-C3A-C4A	2.00	107.97	106.49
42	a	843	BCR	C10-C11-C12	-2.00	116.96	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	8	302	A86	C25-C24-C1	-2.00	120.79	126.42
48	1	303	A86	C4-C3-C2	-2.00	119.37	123.47
50	2	304	A1EB1	C-C1-C2	-2.00	120.12	122.92
48	7	312	A86	O4-C34-C33	2.00	112.58	107.59
48	V	301	A86	C4-C3-C2	-2.00	119.37	123.47
39	o	203	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
48	V	304	A86	C34-O4-C38	-2.00	114.16	117.90
48	5	301	A86	C7-C6-C5	-2.00	120.12	122.92
39	a	812	CLA	O2D-CGD-CBD	2.00	114.83	111.27
49	J	315	KC2	C4D-C3D-CAD	2.00	108.77	107.42
39	W	310	CLA	CHB-C1B-NB	2.00	126.38	124.26
39	J	308	CLA	CHD-C1D-ND	-2.00	122.61	124.45
39	S	313	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
50	7	303	A1EB1	C26-C25-C24	-2.00	116.97	123.22
43	5	303	DD6	C-C1-C24	2.00	121.23	118.08
39	F	314	CLA	C1-O2A-CGA	2.00	121.70	116.44
39	Q	321	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
43	T	303	DD6	C28-C27-C29	2.00	120.80	116.84
42	l	207	BCR	C16-C15-C14	-2.00	119.37	123.47
39	b	826	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
43	4	307	DD6	O1-C20-C21	-2.00	112.66	115.06
50	G	307	A1EB1	O4-C34-C33	2.00	112.58	107.59
47	D	320	SQD	O5-C1-C2	2.00	114.58	110.35
48	9	304	A86	O1-C15-C20	-2.00	57.44	59.40
39	b	840	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
49	M	314	KC2	O2D-CGD-O1D	-2.00	119.93	123.84
50	8	308	A1EB1	O1-C20-C19	-2.00	111.88	113.38
39	D	319	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
50	3	303	A1EB1	C17-C16-C15	2.00	111.20	109.16
48	Q	302	A86	C35-C34-C33	2.00	113.37	109.88
48	F	301	A86	C7-C6-C8	2.00	121.23	118.08
39	a	821	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
39	M	308	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
39	D	314	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (115) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
51	E	311	A1ECV	ND
51	E	311	A1ECV	NA
51	E	311	A1ECV	NB
51	G	316	A1ECV	ND

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Mol	Chain	Res	Type	Atom
51	G	316	A1ECV	NA
51	G	316	A1ECV	NB
51	L	318	A1ECV	ND
51	L	318	A1ECV	NA
51	L	318	A1ECV	NB
51	M	316	A1ECV	ND
51	M	316	A1ECV	NA
51	M	316	A1ECV	NB
51	O	315	A1ECV	ND
51	O	315	A1ECV	NA
51	O	315	A1ECV	NB
51	P	315	A1ECV	ND
51	P	315	A1ECV	NA
51	P	315	A1ECV	NB
51	Q	316	A1ECV	ND
51	Q	316	A1ECV	NA
51	Q	316	A1ECV	NB
51	Q	319	A1ECV	ND
51	Q	319	A1ECV	NA
51	Q	319	A1ECV	NB
51	R	310	A1ECV	ND
51	R	310	A1ECV	NA
51	R	310	A1ECV	NB
51	R	313	A1ECV	ND
51	R	313	A1ECV	NA
51	R	313	A1ECV	NB
51	S	312	A1ECV	ND
51	S	312	A1ECV	NA
51	S	312	A1ECV	NB
51	S	318	A1ECV	ND
51	S	318	A1ECV	NA
51	S	318	A1ECV	NB
51	T	317	A1ECV	ND
51	T	317	A1ECV	NA
51	T	317	A1ECV	NB
51	V	317	A1ECV	ND
51	V	317	A1ECV	NA
51	V	317	A1ECV	NB
51	W	317	A1ECV	ND
51	W	317	A1ECV	NA
51	W	317	A1ECV	NB
51	X	310	A1ECV	ND

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Mol	Chain	Res	Type	Atom
51	X	310	A1ECV	NA
51	X	310	A1ECV	NB
51	X	313	A1ECV	ND
51	X	313	A1ECV	NA
51	X	313	A1ECV	NB
51	0	321	A1ECV	NA
51	0	321	A1ECV	NB
51	1	318	A1ECV	ND
51	1	318	A1ECV	NA
51	1	318	A1ECV	NB
51	4	315	A1ECV	ND
51	4	315	A1ECV	NA
51	4	315	A1ECV	NB
51	4	321	A1ECV	ND
51	4	321	A1ECV	NA
51	4	321	A1ECV	NB
51	5	309	A1ECV	ND
51	5	309	A1ECV	NA
51	5	309	A1ECV	NB
51	5	312	A1ECV	ND
51	5	312	A1ECV	NA
51	5	312	A1ECV	NB
51	7	317	A1ECV	ND
51	7	317	A1ECV	NA
51	7	317	A1ECV	NB
51	7	323	A1ECV	NA
51	7	323	A1ECV	NB
51	9	314	A1ECV	ND
51	9	314	A1ECV	NA
51	9	314	A1ECV	NB
51	9	317	A1ECV	ND
51	9	317	A1ECV	NA
51	9	317	A1ECV	NB
51	x	310	A1ECV	ND
51	x	310	A1ECV	NA
51	x	310	A1ECV	NB
51	x	316	A1ECV	ND
51	x	316	A1ECV	NA
51	x	316	A1ECV	NB
51	y	311	A1ECV	ND
51	y	311	A1ECV	NA
51	y	311	A1ECV	NB

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Mol	Chain	Res	Type	Atom
51	y	317	A1ECV	ND
51	y	317	A1ECV	NA
51	y	317	A1ECV	NB
51	z	310	A1ECV	ND
51	z	310	A1ECV	NA
51	z	310	A1ECV	NB
51	z	316	A1ECV	ND
51	z	316	A1ECV	NA
51	z	316	A1ECV	NB
51	Y	306	A1ECV	ND
51	Y	306	A1ECV	NA
51	Y	306	A1ECV	NB
51	Y	312	A1ECV	ND
51	Y	312	A1ECV	NA
51	Y	312	A1ECV	NB
51	Z	308	A1ECV	ND
51	Z	308	A1ECV	NA
51	Z	308	A1ECV	NB
51	Z	314	A1ECV	ND
51	Z	314	A1ECV	NA
51	Z	314	A1ECV	NB
51	2	311	A1ECV	ND
51	2	311	A1ECV	NA
51	2	311	A1ECV	NB
51	6	320	A1ECV	ND
51	6	320	A1ECV	NA
51	6	320	A1ECV	NB

All (7546) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	a	801	CLA	CBD-CGD-O2D-CED
39	a	802	CLA	C1A-C2A-CAA-CBA
39	a	803	CLA	CHA-CBD-CGD-O1D
39	a	803	CLA	CHA-CBD-CGD-O2D
39	a	803	CLA	CAD-CBD-CGD-O1D
39	a	806	CLA	C3A-C2A-CAA-CBA
39	a	807	CLA	C4B-C3B-CAB-CBB
39	a	808	CLA	CHA-CBD-CGD-O1D
39	a	808	CLA	CHA-CBD-CGD-O2D
39	a	809	CLA	C2-C3-C5-C6
39	a	809	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
39	a	812	CLA	CBD-CGD-O2D-CED
39	a	813	CLA	CHA-CBD-CGD-O1D
39	a	813	CLA	CHA-CBD-CGD-O2D
39	a	815	CLA	C1A-C2A-CAA-CBA
39	a	815	CLA	C3A-C2A-CAA-CBA
39	a	815	CLA	C4B-C3B-CAB-CBB
39	a	816	CLA	C1A-C2A-CAA-CBA
39	a	816	CLA	C3A-C2A-CAA-CBA
39	a	820	CLA	CHA-CBD-CGD-O1D
39	a	821	CLA	C1A-C2A-CAA-CBA
39	a	821	CLA	C3A-C2A-CAA-CBA
39	a	821	CLA	C2B-C3B-CAB-CBB
39	a	821	CLA	C4B-C3B-CAB-CBB
39	a	825	CLA	C1A-C2A-CAA-CBA
39	a	826	CLA	CHA-CBD-CGD-O1D
39	a	826	CLA	CHA-CBD-CGD-O2D
39	a	830	CLA	CBD-CGD-O2D-CED
39	a	832	CLA	C2B-C3B-CAB-CBB
39	a	832	CLA	C4B-C3B-CAB-CBB
39	a	833	CLA	C1A-C2A-CAA-CBA
39	a	833	CLA	CAD-CBD-CGD-O2D
39	a	836	CLA	CHA-CBD-CGD-O1D
39	a	847	CLA	C2B-C3B-CAB-CBB
39	a	847	CLA	C4B-C3B-CAB-CBB
39	a	847	CLA	CBD-CGD-O2D-CED
39	b	803	CLA	CHA-CBD-CGD-O1D
39	b	803	CLA	CHA-CBD-CGD-O2D
39	b	805	CLA	CBD-CGD-O2D-CED
39	b	806	CLA	CBD-CGD-O2D-CED
39	b	809	CLA	C3A-C2A-CAA-CBA
39	b	809	CLA	CHA-CBD-CGD-O1D
39	b	809	CLA	CHA-CBD-CGD-O2D
39	b	811	CLA	C2B-C3B-CAB-CBB
39	b	811	CLA	C4B-C3B-CAB-CBB
39	b	811	CLA	CHA-CBD-CGD-O2D
39	b	812	CLA	CHA-CBD-CGD-O1D
39	b	812	CLA	CHA-CBD-CGD-O2D
39	b	815	CLA	C1A-C2A-CAA-CBA
39	b	816	CLA	C1A-C2A-CAA-CBA
39	b	816	CLA	C3A-C2A-CAA-CBA
39	b	817	CLA	C1A-C2A-CAA-CBA
39	b	818	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	b	818	CLA	CHA-CBD-CGD-O2D
39	b	818	CLA	CAD-CBD-CGD-O1D
39	b	818	CLA	C2-C3-C5-C6
39	b	818	CLA	C4-C3-C5-C6
39	b	820	CLA	C1A-C2A-CAA-CBA
39	b	820	CLA	C3A-C2A-CAA-CBA
39	b	821	CLA	C2B-C3B-CAB-CBB
39	b	821	CLA	C4B-C3B-CAB-CBB
39	b	822	CLA	C4B-C3B-CAB-CBB
39	b	823	CLA	C1A-C2A-CAA-CBA
39	b	823	CLA	C3A-C2A-CAA-CBA
39	b	824	CLA	CHA-CBD-CGD-O1D
39	b	824	CLA	CHA-CBD-CGD-O2D
39	b	826	CLA	CBD-CGD-O2D-CED
39	b	828	CLA	C1A-C2A-CAA-CBA
39	b	828	CLA	C3A-C2A-CAA-CBA
39	b	828	CLA	CHA-CBD-CGD-O1D
39	b	829	CLA	C1A-C2A-CAA-CBA
39	b	829	CLA	C3A-C2A-CAA-CBA
39	b	830	CLA	C2-C3-C5-C6
39	b	830	CLA	C4-C3-C5-C6
39	b	831	CLA	C1A-C2A-CAA-CBA
39	b	831	CLA	C3A-C2A-CAA-CBA
39	b	834	CLA	C2B-C3B-CAB-CBB
39	b	834	CLA	C4B-C3B-CAB-CBB
39	b	835	CLA	C1A-C2A-CAA-CBA
39	b	835	CLA	C3A-C2A-CAA-CBA
39	b	837	CLA	C1A-C2A-CAA-CBA
39	b	838	CLA	CHA-CBD-CGD-O1D
39	b	838	CLA	CHA-CBD-CGD-O2D
39	b	840	CLA	C4B-C3B-CAB-CBB
39	f	803	CLA	CBD-CGD-O2D-CED
39	i	101	CLA	CHA-CBD-CGD-O1D
39	i	103	CLA	C1A-C2A-CAA-CBA
39	i	103	CLA	CHA-CBD-CGD-O1D
39	i	103	CLA	CHA-CBD-CGD-O2D
39	i	103	CLA	CAD-CBD-CGD-O1D
39	i	103	CLA	CBD-CGD-O2D-CED
39	l	201	CLA	CBD-CGD-O2D-CED
39	k	201	CLA	C2B-C3B-CAB-CBB
39	k	201	CLA	C4B-C3B-CAB-CBB
39	k	201	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
39	k	202	CLA	C1A-C2A-CAA-CBA
39	k	202	CLA	C3A-C2A-CAA-CBA
39	k	202	CLA	C2A-CAA-CBA-CGA
39	k	202	CLA	C4B-C3B-CAB-CBB
39	k	202	CLA	CHA-CBD-CGD-O1D
39	k	202	CLA	CHA-CBD-CGD-O2D
39	o	201	CLA	C1A-C2A-CAA-CBA
39	o	201	CLA	C3A-C2A-CAA-CBA
39	o	202	CLA	C4B-C3B-CAB-CBB
39	o	203	CLA	CHA-CBD-CGD-O1D
39	o	203	CLA	CHA-CBD-CGD-O2D
39	o	206	CLA	C2-C3-C5-C6
39	o	206	CLA	C4-C3-C5-C6
39	A	309	CLA	CHA-CBD-CGD-O1D
39	A	312	CLA	C1A-C2A-CAA-CBA
39	A	312	CLA	C3A-C2A-CAA-CBA
39	A	315	CLA	C1A-C2A-CAA-CBA
39	A	315	CLA	C3A-C2A-CAA-CBA
39	A	315	CLA	CBD-CGD-O2D-CED
39	A	315	CLA	O1D-CGD-O2D-CED
39	B	203	CLA	CHA-CBD-CGD-O1D
39	B	203	CLA	CHA-CBD-CGD-O2D
39	B	206	CLA	C1A-C2A-CAA-CBA
39	B	206	CLA	C3A-C2A-CAA-CBA
39	B	209	CLA	C11-C10-C8-C7
39	C	304	CLA	C1A-C2A-CAA-CBA
39	C	304	CLA	C3A-C2A-CAA-CBA
39	C	305	CLA	C2B-C3B-CAB-CBB
39	C	305	CLA	C4B-C3B-CAB-CBB
39	C	305	CLA	C2-C3-C5-C6
39	C	305	CLA	C4-C3-C5-C6
39	C	308	CLA	CBD-CGD-O2D-CED
39	C	309	CLA	C4B-C3B-CAB-CBB
39	C	309	CLA	CHA-CBD-CGD-O1D
39	C	309	CLA	CHA-CBD-CGD-O2D
39	C	309	CLA	CAD-CBD-CGD-O1D
39	C	309	CLA	CBD-CGD-O2D-CED
39	D	309	CLA	C4B-C3B-CAB-CBB
39	D	310	CLA	C2B-C3B-CAB-CBB
39	D	310	CLA	C4B-C3B-CAB-CBB
39	D	310	CLA	C11-C10-C8-C9
39	D	310	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
39	D	312	CLA	C1A-C2A-CAA-CBA
39	D	312	CLA	C3A-C2A-CAA-CBA
39	D	313	CLA	CHA-CBD-CGD-O1D
39	D	313	CLA	CHA-CBD-CGD-O2D
39	D	313	CLA	CAD-CBD-CGD-O1D
39	D	313	CLA	C14-C13-C15-C16
39	D	315	CLA	C1A-C2A-CAA-CBA
39	D	317	CLA	C1A-C2A-CAA-CBA
39	D	317	CLA	C2-C3-C5-C6
39	D	317	CLA	C4-C3-C5-C6
39	D	318	CLA	C1A-C2A-CAA-CBA
39	D	318	CLA	C3A-C2A-CAA-CBA
39	D	318	CLA	C2B-C3B-CAB-CBB
39	D	318	CLA	C4B-C3B-CAB-CBB
39	E	314	CLA	C2-C3-C5-C6
39	E	314	CLA	C4-C3-C5-C6
39	E	315	CLA	CHA-CBD-CGD-O1D
39	E	315	CLA	CAD-CBD-CGD-O1D
39	E	315	CLA	CAD-CBD-CGD-O2D
39	E	316	CLA	C2B-C3B-CAB-CBB
39	E	316	CLA	C4B-C3B-CAB-CBB
39	E	317	CLA	CBD-CGD-O2D-CED
39	E	318	CLA	C1A-C2A-CAA-CBA
39	E	319	CLA	C1A-C2A-CAA-CBA
39	E	319	CLA	C3A-C2A-CAA-CBA
39	E	319	CLA	C4B-C3B-CAB-CBB
39	E	319	CLA	CHA-CBD-CGD-O1D
39	E	319	CLA	CHA-CBD-CGD-O2D
39	F	313	CLA	C1A-C2A-CAA-CBA
39	F	313	CLA	C3A-C2A-CAA-CBA
39	F	314	CLA	C1A-C2A-CAA-CBA
39	F	314	CLA	C2-C3-C5-C6
39	F	314	CLA	C4-C3-C5-C6
39	F	321	CLA	CBA-CGA-O2A-C1
39	F	321	CLA	O1A-CGA-O2A-C1
39	F	321	CLA	C2-C3-C5-C6
39	F	321	CLA	C4-C3-C5-C6
39	G	309	CLA	CHA-CBD-CGD-O1D
39	G	309	CLA	CHA-CBD-CGD-O2D
39	G	309	CLA	CBD-CGD-O2D-CED
39	G	312	CLA	C1A-C2A-CAA-CBA
39	G	312	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
39	G	314	CLA	O1A-CGA-O2A-C1
39	G	314	CLA	C4B-C3B-CAB-CBB
39	H	306	CLA	C1A-C2A-CAA-CBA
39	H	306	CLA	C3A-C2A-CAA-CBA
39	H	306	CLA	CBD-CGD-O2D-CED
39	H	310	CLA	CHA-CBD-CGD-O1D
39	H	310	CLA	CHA-CBD-CGD-O2D
39	H	312	CLA	C1A-C2A-CAA-CBA
39	H	312	CLA	C3A-C2A-CAA-CBA
39	H	312	CLA	C2-C3-C5-C6
39	H	312	CLA	C4-C3-C5-C6
39	H	313	CLA	CBD-CGD-O2D-CED
39	H	315	CLA	CHA-CBD-CGD-O1D
39	H	315	CLA	CHA-CBD-CGD-O2D
39	H	315	CLA	CBD-CGD-O2D-CED
39	H	316	CLA	CBA-CGA-O2A-C1
39	H	316	CLA	CHA-CBD-CGD-O1D
39	H	316	CLA	CHA-CBD-CGD-O2D
39	H	316	CLA	CBD-CGD-O2D-CED
39	J	308	CLA	C4B-C3B-CAB-CBB
39	J	309	CLA	C2-C3-C5-C6
39	J	309	CLA	C4-C3-C5-C6
39	J	312	CLA	C4B-C3B-CAB-CBB
39	J	312	CLA	CBD-CGD-O2D-CED
39	J	313	CLA	C1A-C2A-CAA-CBA
39	J	313	CLA	C3A-C2A-CAA-CBA
39	J	313	CLA	C2B-C3B-CAB-CBB
39	J	313	CLA	C4B-C3B-CAB-CBB
39	J	317	CLA	CBD-CGD-O2D-CED
39	J	317	CLA	O1D-CGD-O2D-CED
39	K	306	CLA	C2-C3-C5-C6
39	K	306	CLA	C4-C3-C5-C6
39	K	307	CLA	C2-C3-C5-C6
39	K	307	CLA	C4-C3-C5-C6
39	K	308	CLA	C4B-C3B-CAB-CBB
39	K	314	CLA	CHA-CBD-CGD-O1D
39	K	314	CLA	CHA-CBD-CGD-O2D
39	K	314	CLA	CAD-CBD-CGD-O1D
39	L	308	CLA	C1A-C2A-CAA-CBA
39	L	309	CLA	C1A-C2A-CAA-CBA
39	L	316	CLA	CHA-CBD-CGD-O1D
39	L	316	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	L	316	CLA	CAD-CBD-CGD-O2D
39	L	320	CLA	C3A-C2A-CAA-CBA
39	L	320	CLA	CBD-CGD-O2D-CED
39	M	310	CLA	CHA-CBD-CGD-O1D
39	M	310	CLA	CHA-CBD-CGD-O2D
39	M	310	CLA	CBD-CGD-O2D-CED
39	M	312	CLA	C2B-C3B-CAB-CBB
39	M	312	CLA	C4B-C3B-CAB-CBB
39	M	315	CLA	CHA-CBD-CGD-O1D
39	M	315	CLA	CHA-CBD-CGD-O2D
39	M	315	CLA	CAD-CBD-CGD-O1D
39	M	317	CLA	C2B-C3B-CAB-CBB
39	M	317	CLA	C4B-C3B-CAB-CBB
39	M	317	CLA	CBD-CGD-O2D-CED
39	M	321	CLA	C4B-C3B-CAB-CBB
39	O	308	CLA	C4B-C3B-CAB-CBB
39	O	308	CLA	C2C-C3C-CAC-CBC
39	O	308	CLA	C4C-C3C-CAC-CBC
39	O	312	CLA	CBA-CGA-O2A-C1
39	O	312	CLA	CHA-CBD-CGD-O1D
39	O	312	CLA	CHA-CBD-CGD-O2D
39	O	313	CLA	C1A-C2A-CAA-CBA
39	O	313	CLA	C3A-C2A-CAA-CBA
39	O	313	CLA	C4B-C3B-CAB-CBB
39	O	316	CLA	CBD-CGD-O2D-CED
39	P	309	CLA	CHA-CBD-CGD-O1D
39	P	309	CLA	CHA-CBD-CGD-O2D
39	P	309	CLA	CBD-CGD-O2D-CED
39	P	314	CLA	CHA-CBD-CGD-O1D
39	P	314	CLA	CHA-CBD-CGD-O2D
39	P	314	CLA	CAD-CBD-CGD-O1D
39	P	314	CLA	CAD-CBD-CGD-O2D
39	P	316	CLA	C4B-C3B-CAB-CBB
39	P	316	CLA	CBD-CGD-O2D-CED
39	P	316	CLA	C4-C3-C5-C6
39	Q	309	CLA	CHA-CBD-CGD-O1D
39	Q	309	CLA	CHA-CBD-CGD-O2D
39	Q	310	CLA	CHA-CBD-CGD-O1D
39	Q	310	CLA	CHA-CBD-CGD-O2D
39	Q	310	CLA	CBD-CGD-O2D-CED
39	Q	317	CLA	CBD-CGD-O2D-CED
39	Q	320	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	Q	321	CLA	C1A-C2A-CAA-CBA
39	R	307	CLA	C2-C3-C5-C6
39	R	307	CLA	C4-C3-C5-C6
39	R	308	CLA	C2-C3-C5-C6
39	R	308	CLA	C4-C3-C5-C6
39	R	315	CLA	C4B-C3B-CAB-CBB
39	R	315	CLA	CBD-CGD-O2D-CED
39	S	308	CLA	C4B-C3B-CAB-CBB
39	S	308	CLA	CHA-CBD-CGD-O1D
39	S	308	CLA	CHA-CBD-CGD-O2D
39	S	308	CLA	C2-C3-C5-C6
39	S	308	CLA	C4-C3-C5-C6
39	S	309	CLA	CHA-CBD-CGD-O1D
39	S	309	CLA	C4-C3-C5-C6
39	S	310	CLA	C1A-C2A-CAA-CBA
39	S	316	CLA	CHA-CBD-CGD-O1D
39	S	316	CLA	CHA-CBD-CGD-O2D
39	S	316	CLA	CAD-CBD-CGD-O1D
39	S	319	CLA	C1A-C2A-CAA-CBA
39	S	319	CLA	C2B-C3B-CAB-CBB
39	S	319	CLA	C4B-C3B-CAB-CBB
39	S	320	CLA	C1A-C2A-CAA-CBA
39	T	308	CLA	CBA-CGA-O2A-C1
39	T	308	CLA	CHA-CBD-CGD-O1D
39	T	308	CLA	CHA-CBD-CGD-O2D
39	T	309	CLA	CHA-CBD-CGD-O1D
39	T	309	CLA	CHA-CBD-CGD-O2D
39	T	310	CLA	CBD-CGD-O2D-CED
39	T	318	CLA	C4B-C3B-CAB-CBB
39	T	319	CLA	C2A-CAA-CBA-CGA
39	T	320	CLA	CHA-CBD-CGD-O2D
39	T	320	CLA	CBD-CGD-O2D-CED
39	U	207	CLA	O1A-CGA-O2A-C1
39	U	207	CLA	CHA-CBD-CGD-O1D
39	U	207	CLA	CHA-CBD-CGD-O2D
39	U	208	CLA	CBD-CGD-O2D-CED
39	U	209	CLA	C1A-C2A-CAA-CBA
39	U	209	CLA	C3A-C2A-CAA-CBA
39	U	209	CLA	C2A-CAA-CBA-CGA
39	U	211	CLA	CBD-CGD-O2D-CED
39	U	212	CLA	CBA-CGA-O2A-C1
39	U	212	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	U	213	CLA	CBD-CGD-O2D-CED
39	U	215	CLA	C4B-C3B-CAB-CBB
39	V	309	CLA	C11-C12-C13-C14
39	V	311	CLA	CAD-CBD-CGD-O1D
39	V	311	CLA	CAD-CBD-CGD-O2D
39	W	311	CLA	CHA-CBD-CGD-O1D
39	W	311	CLA	CHA-CBD-CGD-O2D
39	W	311	CLA	CBD-CGD-O2D-CED
39	W	313	CLA	C1A-C2A-CAA-CBA
39	W	313	CLA	C4-C3-C5-C6
39	W	318	CLA	C4B-C3B-CAB-CBB
39	X	307	CLA	C4-C3-C5-C6
39	X	308	CLA	C2-C3-C5-C6
39	X	308	CLA	C4-C3-C5-C6
39	X	316	CLA	C4B-C3B-CAB-CBB
39	X	316	CLA	CBD-CGD-O2D-CED
39	X	317	CLA	CBD-CGD-O2D-CED
39	0	310	CLA	C1A-C2A-CAA-CBA
39	0	310	CLA	C2-C3-C5-C6
39	0	310	CLA	C4-C3-C5-C6
39	0	311	CLA	C1A-C2A-CAA-CBA
39	0	311	CLA	CHA-CBD-CGD-O1D
39	0	311	CLA	CHA-CBD-CGD-O2D
39	0	312	CLA	CBA-CGA-O2A-C1
39	0	312	CLA	O1A-CGA-O2A-C1
39	0	318	CLA	C4B-C3B-CAB-CBB
39	0	320	CLA	C4B-C3B-CAB-CBB
39	0	322	CLA	C2B-C3B-CAB-CBB
39	0	322	CLA	C4B-C3B-CAB-CBB
39	0	322	CLA	CAD-CBD-CGD-O1D
39	0	322	CLA	CAD-CBD-CGD-O2D
39	0	322	CLA	C2-C3-C5-C6
39	0	322	CLA	C4-C3-C5-C6
39	0	323	CLA	C1A-C2A-CAA-CBA
39	0	323	CLA	C4B-C3B-CAB-CBB
39	1	308	CLA	C2B-C3B-CAB-CBB
39	1	308	CLA	C4B-C3B-CAB-CBB
39	1	308	CLA	CHA-CBD-CGD-O1D
39	1	308	CLA	CHA-CBD-CGD-O2D
39	1	308	CLA	CBD-CGD-O2D-CED
39	1	309	CLA	CBD-CGD-O2D-CED
39	1	310	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	1	310	CLA	CBD-CGD-O2D-CED
39	1	311	CLA	CHA-CBD-CGD-O1D
39	1	311	CLA	CHA-CBD-CGD-O2D
39	1	313	CLA	C2B-C3B-CAB-CBB
39	1	313	CLA	C4B-C3B-CAB-CBB
39	1	316	CLA	C2B-C3B-CAB-CBB
39	1	316	CLA	C4B-C3B-CAB-CBB
39	1	317	CLA	C4B-C3B-CAB-CBB
39	1	317	CLA	CBD-CGD-O2D-CED
39	1	320	CLA	C2B-C3B-CAB-CBB
39	1	320	CLA	C4B-C3B-CAB-CBB
39	1	320	CLA	CHA-CBD-CGD-O1D
39	1	320	CLA	CHA-CBD-CGD-O2D
39	1	320	CLA	CBD-CGD-O2D-CED
39	3	312	CLA	CHA-CBD-CGD-O1D
39	3	312	CLA	CHA-CBD-CGD-O2D
39	3	312	CLA	C11-C12-C13-C14
39	3	314	CLA	CBD-CGD-O2D-CED
39	3	316	CLA	C4B-C3B-CAB-CBB
39	3	319	CLA	CAD-CBD-CGD-O1D
39	3	319	CLA	CAD-CBD-CGD-O2D
39	3	322	CLA	C1A-C2A-CAA-CBA
39	3	323	CLA	CBD-CGD-O2D-CED
39	4	311	CLA	C1A-C2A-CAA-CBA
39	4	311	CLA	CBA-CGA-O2A-C1
39	4	311	CLA	O1A-CGA-O2A-C1
39	4	311	CLA	C4B-C3B-CAB-CBB
39	4	311	CLA	CHA-CBD-CGD-O1D
39	4	311	CLA	CHA-CBD-CGD-O2D
39	4	312	CLA	C1A-C2A-CAA-CBA
39	4	323	CLA	CBD-CGD-O2D-CED
39	5	306	CLA	C2-C3-C5-C6
39	5	306	CLA	C4-C3-C5-C6
39	5	307	CLA	O1A-CGA-O2A-C1
39	5	310	CLA	C2B-C3B-CAB-CBB
39	5	310	CLA	C4B-C3B-CAB-CBB
39	5	315	CLA	CBD-CGD-O2D-CED
39	5	316	CLA	C2-C3-C5-C6
39	5	316	CLA	C4-C3-C5-C6
39	7	313	CLA	C1A-C2A-CAA-CBA
39	7	313	CLA	C2A-CAA-CBA-CGA
39	7	313	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	7	313	CLA	CHA-CBD-CGD-O1D
39	7	313	CLA	CHA-CBD-CGD-O2D
39	7	313	CLA	C2-C3-C5-C6
39	7	313	CLA	C4-C3-C5-C6
39	7	314	CLA	C1A-C2A-CAA-CBA
39	7	314	CLA	C3A-C2A-CAA-CBA
39	7	314	CLA	CBD-CGD-O2D-CED
39	7	321	CLA	CHA-CBD-CGD-O1D
39	7	321	CLA	CHA-CBD-CGD-O2D
39	7	321	CLA	CAD-CBD-CGD-O1D
39	7	321	CLA	CAD-CBD-CGD-O2D
39	7	324	CLA	C2B-C3B-CAB-CBB
39	7	324	CLA	C4B-C3B-CAB-CBB
39	7	325	CLA	C2A-CAA-CBA-CGA
39	8	310	CLA	C1A-C2A-CAA-CBA
39	8	311	CLA	CHA-CBD-CGD-O1D
39	8	311	CLA	CHA-CBD-CGD-O2D
39	8	311	CLA	C4-C3-C5-C6
39	8	312	CLA	CHA-CBD-CGD-O1D
39	8	312	CLA	CHA-CBD-CGD-O2D
39	8	318	CLA	C4B-C3B-CAB-CBB
39	8	322	CLA	C2B-C3B-CAB-CBB
39	8	322	CLA	C4B-C3B-CAB-CBB
39	8	322	CLA	CBD-CGD-O2D-CED
39	9	307	CLA	CBD-CGD-O2D-CED
39	9	310	CLA	CHA-CBD-CGD-O1D
39	9	312	CLA	C4B-C3B-CAB-CBB
39	9	315	CLA	C2B-C3B-CAB-CBB
39	9	315	CLA	C4B-C3B-CAB-CBB
39	9	319	CLA	CHA-CBD-CGD-O1D
39	9	320	CLA	C2B-C3B-CAB-CBB
39	9	320	CLA	C4B-C3B-CAB-CBB
39	9	320	CLA	CBD-CGD-O2D-CED
39	9	320	CLA	O1D-CGD-O2D-CED
39	I	310	CLA	C2-C3-C5-C6
39	I	310	CLA	C4-C3-C5-C6
39	I	313	CLA	C4B-C3B-CAB-CBB
39	I	316	CLA	CHA-CBD-CGD-O1D
39	x	306	CLA	C4B-C3B-CAB-CBB
39	x	307	CLA	CHA-CBD-CGD-O1D
39	x	307	CLA	CHA-CBD-CGD-O2D
39	x	309	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	x	317	CLA	CBD-CGD-O2D-CED
39	x	318	CLA	CHA-CBD-CGD-O1D
39	x	318	CLA	CHA-CBD-CGD-O2D
39	x	318	CLA	CAD-CBD-CGD-O1D
39	x	318	CLA	CAD-CBD-CGD-O2D
39	y	307	CLA	C4B-C3B-CAB-CBB
39	y	308	CLA	C1A-C2A-CAA-CBA
39	y	308	CLA	C3A-C2A-CAA-CBA
39	y	308	CLA	CHA-CBD-CGD-O1D
39	y	308	CLA	CHA-CBD-CGD-O2D
39	y	309	CLA	CBD-CGD-O2D-CED
39	y	312	CLA	CBD-CGD-O2D-CED
39	y	315	CLA	CHA-CBD-CGD-O1D
39	y	315	CLA	CHA-CBD-CGD-O2D
39	y	315	CLA	CAD-CBD-CGD-O1D
39	y	315	CLA	CAD-CBD-CGD-O2D
39	y	318	CLA	C4B-C3B-CAB-CBB
39	y	318	CLA	CHA-CBD-CGD-O1D
39	y	318	CLA	CHA-CBD-CGD-O2D
39	y	319	CLA	CHA-CBD-CGD-O1D
39	y	319	CLA	CHA-CBD-CGD-O2D
39	z	306	CLA	C4B-C3B-CAB-CBB
39	z	307	CLA	CBD-CGD-O2D-CED
39	z	309	CLA	CBD-CGD-O2D-CED
39	z	311	CLA	CBD-CGD-O2D-CED
39	z	314	CLA	CHA-CBD-CGD-O1D
39	z	314	CLA	CHA-CBD-CGD-O2D
39	z	317	CLA	CBD-CGD-O2D-CED
39	z	318	CLA	CHA-CBD-CGD-O1D
39	z	318	CLA	CHA-CBD-CGD-O2D
39	z	318	CLA	CAD-CBD-CGD-O1D
39	Y	303	CLA	CBD-CGD-O2D-CED
39	Y	304	CLA	CBA-CGA-O2A-C1
39	Y	304	CLA	O1A-CGA-O2A-C1
39	Y	310	CLA	C4B-C3B-CAB-CBB
39	Y	310	CLA	CBD-CGD-O2D-CED
39	Y	310	CLA	O1D-CGD-O2D-CED
39	Y	311	CLA	C4B-C3B-CAB-CBB
39	Y	311	CLA	CAD-CBD-CGD-O1D
39	Y	313	CLA	CBD-CGD-O2D-CED
39	Y	314	CLA	C4B-C3B-CAB-CBB
39	Y	314	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	Y	314	CLA	CAD-CBD-CGD-O2D
39	Z	306	CLA	CBA-CGA-O2A-C1
39	Z	312	CLA	CBD-CGD-O2D-CED
39	Z	313	CLA	C4B-C3B-CAB-CBB
39	Z	313	CLA	CBD-CGD-O2D-CED
39	Z	313	CLA	O1D-CGD-O2D-CED
39	Z	315	CLA	CBD-CGD-O2D-CED
39	Z	316	CLA	CHA-CBD-CGD-O1D
39	Z	316	CLA	CHA-CBD-CGD-O2D
39	Z	316	CLA	CAD-CBD-CGD-O1D
39	2	308	CLA	CBA-CGA-O2A-C1
39	2	308	CLA	CHA-CBD-CGD-O1D
39	2	308	CLA	CHA-CBD-CGD-O2D
39	2	308	CLA	CBD-CGD-O2D-CED
39	2	309	CLA	CBA-CGA-O2A-C1
39	2	309	CLA	O1A-CGA-O2A-C1
39	2	309	CLA	CBD-CGD-O2D-CED
39	2	312	CLA	C4B-C3B-CAB-CBB
39	2	312	CLA	CHA-CBD-CGD-O1D
39	2	312	CLA	CHA-CBD-CGD-O2D
39	2	315	CLA	CBD-CGD-O2D-CED
39	2	316	CLA	C2B-C3B-CAB-CBB
39	2	316	CLA	C4B-C3B-CAB-CBB
39	2	319	CLA	CBA-CGA-O2A-C1
39	2	319	CLA	CHA-CBD-CGD-O1D
39	2	319	CLA	CAD-CBD-CGD-O1D
39	2	319	CLA	CAD-CBD-CGD-O2D
39	6	310	CLA	C1A-C2A-CAA-CBA
39	6	310	CLA	C3A-C2A-CAA-CBA
39	6	310	CLA	C4B-C3B-CAB-CBB
39	6	313	CLA	CBD-CGD-O2D-CED
39	6	318	CLA	CHA-CBD-CGD-O1D
39	6	318	CLA	CAD-CBD-CGD-O1D
39	6	318	CLA	CAD-CBD-CGD-O2D
39	6	321	CLA	C2B-C3B-CAB-CBB
39	6	321	CLA	C4B-C3B-CAB-CBB
39	6	322	CLA	C1A-C2A-CAA-CBA
39	6	322	CLA	C2A-CAA-CBA-CGA
39	6	322	CLA	CBA-CGA-O2A-C1
39	6	322	CLA	O1A-CGA-O2A-C1
39	6	322	CLA	CBD-CGD-O2D-CED
41	a	840	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
41	a	840	LHG	C1-C2-C3-O3
41	a	841	LHG	O1-C1-C2-O2
41	a	841	LHG	O1-C1-C2-C3
41	j	104	LHG	O2-C2-C3-O3
41	j	104	LHG	C3-O3-P-O5
41	j	104	LHG	C4-O6-P-O3
41	j	104	LHG	O9-C7-O7-C5
41	j	104	LHG	C8-C7-O7-C5
41	D	301	LHG	C4-O6-P-O5
41	D	302	LHG	O1-C1-C2-C3
41	D	302	LHG	C3-O3-P-O4
41	D	302	LHG	C3-O3-P-O6
41	H	317	LHG	C3-O3-P-O5
41	H	317	LHG	C8-C7-O7-C5
41	X	301	LHG	C2-C3-O3-P
41	X	301	LHG	C3-O3-P-O5
41	X	301	LHG	C4-O6-P-O5
42	b	844	BCR	C7-C8-C9-C10
42	b	844	BCR	C7-C8-C9-C34
42	b	844	BCR	C11-C12-C13-C35
42	b	847	BCR	C7-C8-C9-C10
42	b	847	BCR	C7-C8-C9-C34
42	b	847	BCR	C21-C22-C23-C24
42	b	847	BCR	C37-C22-C23-C24
42	m	101	BCR	C7-C8-C9-C10
42	m	101	BCR	C7-C8-C9-C34
42	m	101	BCR	C20-C21-C22-C37
42	m	101	BCR	C23-C24-C25-C30
42	h	202	BCR	C7-C8-C9-C10
42	h	202	BCR	C7-C8-C9-C34
43	A	304	DD6	C10-C11-C13-C14
43	A	304	DD6	C12-C11-C13-C14
43	B	202	DD6	C10-C11-C13-C14
43	B	202	DD6	C12-C11-C13-C14
43	B	202	DD6	C27-C29-C30-C31
43	C	301	DD6	C10-C11-C13-C14
43	C	301	DD6	C12-C11-C13-C14
43	E	305	DD6	C10-C11-C13-C14
43	E	305	DD6	C12-C11-C13-C14
43	E	305	DD6	C13-C14-C15-O1
43	F	305	DD6	C27-C29-C30-C31
43	G	306	DD6	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
43	H	305	DD6	C13-C14-C15-O1
43	J	305	DD6	C10-C11-C13-C14
43	J	305	DD6	C12-C11-C13-C14
43	O	303	DD6	C-C1-C24-C25
43	O	303	DD6	C2-C1-C24-C25
43	O	305	DD6	C13-C14-C15-O1
43	P	304	DD6	C12-C11-C13-C14
43	Q	303	DD6	C13-C14-C15-O1
43	3	301	DD6	C27-C29-C30-C31
43	4	308	DD6	C27-C29-C30-C31
43	7	309	DD6	C-C1-C24-C25
43	7	309	DD6	C2-C1-C24-C25
43	x	303	DD6	C13-C14-C15-O1
43	y	303	DD6	C13-C14-C15-O1
43	z	304	DD6	C5-C6-C8-C9
43	z	304	DD6	C7-C6-C8-C9
43	Z	302	DD6	C-C1-C24-C25
43	2	303	DD6	C-C1-C24-C25
45	C	314	DGD	C2B-C1B-O2G-C2G
45	C	314	DGD	O1B-C1B-O2G-C2G
46	l	208	LMG	C2-C1-O1-C7
46	l	208	LMG	O6-C1-O1-C7
46	F	317	LMG	C2-C1-O1-C7
46	F	317	LMG	O6-C1-O1-C7
46	M	319	LMG	C11-C10-O7-C8
46	M	320	LMG	C2-C1-O1-C7
46	M	320	LMG	O6-C1-O1-C7
46	M	320	LMG	O9-C10-O7-C8
46	M	320	LMG	C11-C10-O7-C8
46	Q	322	LMG	C2-C1-O1-C7
46	Q	322	LMG	O6-C1-O1-C7
46	S	322	LMG	O1-C7-C8-O7
46	S	322	LMG	O9-C10-O7-C8
46	W	320	LMG	C2-C1-O1-C7
46	W	320	LMG	O6-C1-O1-C7
46	W	320	LMG	O9-C10-O7-C8
46	W	320	LMG	C11-C10-O7-C8
46	0	324	LMG	C2-C1-O1-C7
46	0	324	LMG	O6-C1-O1-C7
46	4	325	LMG	O6-C1-O1-C7
46	4	325	LMG	O7-C8-C9-O8
46	4	326	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
46	4	326	LMG	O9-C10-O7-C8
46	7	301	LMG	O1-C7-C8-O7
46	7	301	LMG	O9-C10-O7-C8
46	9	321	LMG	C11-C10-O7-C8
46	I	302	LMG	C2-C1-O1-C7
46	I	302	LMG	O6-C1-O1-C7
46	I	302	LMG	C11-C10-O7-C8
47	k	205	SQD	C2-C1-O6-C44
47	k	205	SQD	O5-C1-O6-C44
47	k	205	SQD	O5-C5-C6-S
47	D	304	SQD	C5-C6-S-O7
47	D	304	SQD	C5-C6-S-O8
47	D	304	SQD	C5-C6-S-O9
47	D	320	SQD	C2-C1-O6-C44
47	D	320	SQD	O5-C1-O6-C44
47	D	321	SQD	O49-C7-O47-C45
47	D	321	SQD	C8-C7-O47-C45
47	D	321	SQD	C5-C6-S-O7
47	D	321	SQD	C5-C6-S-O8
47	D	321	SQD	C5-C6-S-O9
47	E	320	SQD	O49-C7-O47-C45
47	E	320	SQD	C8-C7-O47-C45
47	F	318	SQD	C2-C1-O6-C44
47	F	318	SQD	O5-C1-O6-C44
47	F	318	SQD	C5-C6-S-O7
47	F	319	SQD	O5-C5-C6-S
47	H	318	SQD	O47-C45-C46-O48
47	H	318	SQD	O5-C5-C6-S
47	S	301	SQD	C2-C1-O6-C44
47	S	301	SQD	O5-C1-O6-C44
47	S	301	SQD	O49-C7-O47-C45
47	S	301	SQD	C8-C7-O47-C45
47	S	301	SQD	C5-C6-S-O7
47	S	301	SQD	C5-C6-S-O8
47	T	321	SQD	C2-C1-O6-C44
47	T	321	SQD	O5-C1-O6-C44
47	W	301	SQD	C5-C6-S-O7
47	W	301	SQD	C5-C6-S-O8
47	4	327	SQD	C2-C1-O6-C44
47	4	327	SQD	O5-C1-O6-C44
47	4	327	SQD	O49-C7-O47-C45
47	4	327	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
47	4	327	SQD	C5-C6-S-O7
47	4	327	SQD	C5-C6-S-O8
47	4	327	SQD	C5-C6-S-O9
47	7	302	SQD	C2-C1-O6-C44
47	7	302	SQD	O5-C1-O6-C44
47	7	302	SQD	O6-C44-C45-O47
47	7	302	SQD	O49-C7-O47-C45
47	7	302	SQD	C8-C7-O47-C45
47	7	302	SQD	C5-C6-S-O7
47	7	302	SQD	C5-C6-S-O8
47	7	302	SQD	C5-C6-S-O9
47	9	322	SQD	O6-C44-C45-O47
47	9	322	SQD	C8-C7-O47-C45
47	9	322	SQD	O5-C5-C6-S
48	k	206	A86	C13-C14-C15-O1
48	k	206	A86	C28-C27-C29-C30
48	k	206	A86	C39-C38-O4-C34
48	k	206	A86	O5-C38-O4-C34
48	B	201	A86	C13-C14-C15-O1
48	B	201	A86	C39-C38-O4-C34
48	B	201	A86	O5-C38-O4-C34
48	C	303	A86	C13-C14-C15-O1
48	C	303	A86	C26-C27-C29-C30
48	D	305	A86	C39-C38-O4-C34
48	F	301	A86	C10-C11-C13-O
48	F	301	A86	C12-C11-C13-O
48	F	301	A86	C13-C14-C15-O1
48	F	302	A86	C39-C38-O4-C34
48	G	301	A86	C39-C38-O4-C34
48	G	301	A86	O5-C38-O4-C34
48	G	301	A86	C7-C6-C8-C9
48	G	305	A86	C13-C14-C15-O1
48	G	305	A86	C33-C34-O4-C38
48	G	305	A86	C39-C38-O4-C34
48	G	305	A86	C5-C6-C8-C9
48	G	305	A86	C7-C6-C8-C9
48	H	302	A86	C12-C11-C13-C14
48	H	302	A86	C39-C38-O4-C34
48	J	301	A86	C39-C38-O4-C34
48	J	301	A86	O5-C38-O4-C34
48	J	303	A86	C12-C11-C13-C14
48	J	303	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
48	J	303	A86	O5-C38-O4-C34
48	K	301	A86	C10-C11-C13-O
48	K	301	A86	C12-C11-C13-O
48	K	301	A86	C39-C38-O4-C34
48	K	301	A86	O5-C38-O4-C34
48	L	301	A86	C39-C38-O4-C34
48	L	301	A86	O5-C38-O4-C34
48	L	302	A86	C-C1-C24-C25
48	L	302	A86	C2-C1-C24-C25
48	L	302	A86	C10-C11-C13-O
48	L	302	A86	C12-C11-C13-O
48	L	302	A86	C24-C25-C26-C27
48	L	304	A86	C-C1-C24-C25
48	L	304	A86	C2-C1-C24-C25
48	L	304	A86	C39-C38-O4-C34
48	L	306	A86	C10-C11-C13-O
48	L	306	A86	C12-C11-C13-O
48	L	306	A86	C39-C38-O4-C34
48	L	306	A86	O5-C38-O4-C34
48	M	302	A86	C13-C14-C15-O1
48	M	302	A86	C39-C38-O4-C34
48	M	306	A86	C39-C38-O4-C34
48	M	306	A86	O5-C38-O4-C34
48	O	302	A86	C39-C38-O4-C34
48	O	302	A86	O5-C38-O4-C34
48	O	306	A86	C-C1-C24-C25
48	O	306	A86	C2-C1-C24-C25
48	O	307	A86	C13-C14-C15-C16
48	O	307	A86	C39-C38-O4-C34
48	O	307	A86	O5-C38-O4-C34
48	O	307	A86	C5-C6-C8-C9
48	O	307	A86	C7-C6-C8-C9
48	P	302	A86	C-C1-C24-C25
48	P	302	A86	C26-C27-C29-C30
48	P	302	A86	C28-C27-C29-C30
48	Q	302	A86	C39-C38-O4-C34
48	Q	302	A86	O5-C38-O4-C34
48	Q	302	A86	C5-C6-C8-C9
48	Q	302	A86	C7-C6-C8-C9
48	Q	304	A86	C39-C38-O4-C34
48	Q	304	A86	O5-C38-O4-C34
48	Q	305	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
48	Q	305	A86	C12-C11-C13-O
48	Q	305	A86	C13-C14-C15-O1
48	Q	305	A86	C39-C38-O4-C34
48	Q	305	A86	O5-C38-O4-C34
48	Q	305	A86	C3-C4-C5-C6
48	R	301	A86	C39-C38-O4-C34
48	R	301	A86	O5-C38-O4-C34
48	R	302	A86	C-C1-C24-C25
48	R	302	A86	C2-C1-C24-C25
48	R	302	A86	C13-C14-C15-O1
48	S	304	A86	C5-C6-C8-C9
48	S	304	A86	C7-C6-C8-C9
48	S	305	A86	C13-C14-C15-O1
48	S	307	A86	C39-C38-O4-C34
48	T	301	A86	C39-C38-O4-C34
48	T	305	A86	C12-C11-C13-O
48	T	305	A86	C39-C38-O4-C34
48	T	306	A86	C39-C38-O4-C34
48	U	202	A86	C-C1-C24-C25
48	U	202	A86	C2-C1-C24-C25
48	U	202	A86	C39-C38-O4-C34
48	U	202	A86	O5-C38-O4-C34
48	U	206	A86	C39-C38-O4-C34
48	V	301	A86	O5-C38-O4-C34
48	V	304	A86	C39-C38-O4-C34
48	V	304	A86	O5-C38-O4-C34
48	W	303	A86	C13-C14-C15-O1
48	W	307	A86	C39-C38-O4-C34
48	W	307	A86	O5-C38-O4-C34
48	X	303	A86	C10-C11-C13-O
48	X	303	A86	C12-C11-C13-O
48	X	303	A86	C13-C14-C15-O1
48	0	301	A86	C35-C34-O4-C38
48	0	304	A86	C10-C11-C13-O
48	0	304	A86	C12-C11-C13-O
48	0	304	A86	C13-C14-C15-O1
48	0	306	A86	C39-C38-O4-C34
48	0	309	A86	C28-C27-C29-C30
48	0	309	A86	C39-C38-O4-C34
48	0	309	A86	O5-C38-O4-C34
48	1	306	A86	C-C1-C24-C25
48	1	306	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
48	1	306	A86	C5-C6-C8-C9
48	1	306	A86	C7-C6-C8-C9
48	3	305	A86	C-C1-C24-C25
48	3	305	A86	C12-C11-C13-C14
48	3	305	A86	C13-C14-C15-O1
48	3	305	A86	C26-C27-C29-C30
48	3	305	A86	C35-C34-O4-C38
48	3	305	A86	C39-C38-O4-C34
48	3	306	A86	C39-C38-O4-C34
48	3	306	A86	O5-C38-O4-C34
48	3	306	A86	C5-C6-C8-C9
48	3	306	A86	C7-C6-C8-C9
48	3	307	A86	C26-C27-C29-C30
48	3	307	A86	C33-C34-O4-C38
48	3	307	A86	C39-C38-O4-C34
48	3	308	A86	C35-C34-O4-C38
48	3	308	A86	C39-C38-O4-C34
48	4	306	A86	C13-C14-C15-O1
48	4	309	A86	C11-C10-C9-C8
48	4	310	A86	C13-C14-C15-O1
48	4	310	A86	C33-C34-O4-C38
48	4	310	A86	C39-C38-O4-C34
48	4	328	A86	C2-C1-C24-C25
48	4	328	A86	C12-C11-C13-C14
48	4	328	A86	C13-C14-C15-C16
48	4	328	A86	C39-C38-O4-C34
48	7	307	A86	C35-C34-O4-C38
48	7	307	A86	C39-C38-O4-C34
48	7	308	A86	C10-C11-C13-O
48	7	308	A86	C12-C11-C13-O
48	7	308	A86	C13-C14-C15-O1
48	7	312	A86	C35-C34-O4-C38
48	7	312	A86	C39-C38-O4-C34
48	8	302	A86	C12-C11-C13-O
48	8	302	A86	C39-C38-O4-C34
48	8	302	A86	O5-C38-O4-C34
48	8	303	A86	C-C1-C24-C25
48	8	303	A86	C39-C38-O4-C34
48	8	303	A86	O5-C38-O4-C34
48	8	305	A86	C10-C11-C13-O
48	8	305	A86	C12-C11-C13-O
48	8	305	A86	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
48	8	305	A86	C39-C38-O4-C34
48	8	305	A86	O5-C38-O4-C34
48	8	305	A86	C5-C6-C8-C9
48	8	305	A86	C7-C6-C8-C9
48	8	307	A86	C12-C11-C13-C14
48	8	309	A86	C39-C38-O4-C34
48	8	323	A86	C39-C38-O4-C34
48	8	323	A86	O5-C38-O4-C34
48	9	301	A86	C-C1-C24-C25
48	9	301	A86	C2-C1-C24-C25
48	9	301	A86	C12-C11-C13-C14
48	9	301	A86	C39-C38-O4-C34
48	9	301	A86	O5-C38-O4-C34
48	9	303	A86	C35-C34-O4-C38
48	9	304	A86	C12-C11-C13-O
48	9	304	A86	C39-C38-O4-C34
48	9	304	A86	O5-C38-O4-C34
48	9	305	A86	C39-C38-O4-C34
48	9	305	A86	O5-C38-O4-C34
48	9	306	A86	C39-C38-O4-C34
48	9	306	A86	O5-C38-O4-C34
48	I	304	A86	C-C1-C24-C25
48	I	304	A86	C2-C1-C24-C25
48	I	304	A86	C10-C11-C13-O
48	I	304	A86	C12-C11-C13-O
48	I	304	A86	C13-C14-C15-O1
48	I	304	A86	C39-C38-O4-C34
48	x	305	A86	C26-C27-C29-C30
48	y	306	A86	C13-C14-C15-O1
48	y	306	A86	C33-C34-O4-C38
48	y	306	A86	C39-C38-O4-C34
48	z	303	A86	C12-C11-C13-C14
48	z	303	A86	C39-C38-O4-C34
48	Y	301	A86	C11-C10-C9-C8
48	Z	301	A86	C26-C27-C29-C30
48	Z	301	A86	C28-C27-C29-C30
48	Z	303	A86	C39-C38-O4-C34
48	Z	303	A86	O5-C38-O4-C34
48	Z	303	A86	C5-C6-C8-C9
48	Z	303	A86	C7-C6-C8-C9
48	2	301	A86	C39-C38-O4-C34
48	2	301	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
48	2	302	A86	C26-C27-C29-C30
48	2	302	A86	C28-C27-C29-C30
48	2	305	A86	C12-C11-C13-O
48	2	305	A86	C39-C38-O4-C34
48	6	302	A86	C39-C38-O4-C34
48	6	302	A86	O5-C38-O4-C34
48	6	302	A86	C5-C6-C8-C9
48	6	302	A86	C7-C6-C8-C9
48	6	303	A86	C39-C38-O4-C34
48	6	303	A86	O5-C38-O4-C34
48	6	305	A86	C10-C11-C13-O
48	6	305	A86	C12-C11-C13-O
48	6	305	A86	C39-C38-O4-C34
48	6	305	A86	O5-C38-O4-C34
48	6	307	A86	C12-C11-C13-C14
48	6	307	A86	C39-C38-O4-C34
48	6	307	A86	O5-C38-O4-C34
48	6	309	A86	C11-C13-C14-C15
48	6	309	A86	C13-C14-C15-C20
48	6	309	A86	C13-C14-C15-O1
48	6	309	A86	C5-C6-C8-C9
48	6	309	A86	C7-C6-C8-C9
49	A	310	KC2	C1A-C2A-CAA-CBA
49	A	310	KC2	C2B-C3B-CAB-CBB
49	A	310	KC2	C4B-C3B-CAB-CBB
49	A	310	KC2	C2C-C3C-CAC-CBC
49	A	313	KC2	C1A-C2A-CAA-CBA
49	A	313	KC2	C3A-C2A-CAA-CBA
49	B	208	KC2	C1A-C2A-CAA-CBA
49	B	208	KC2	C3A-C2A-CAA-CBA
49	B	208	KC2	C2B-C3B-CAB-CBB
49	B	208	KC2	C4B-C3B-CAB-CBB
49	B	208	KC2	C4C-C3C-CAC-CBC
49	B	208	KC2	CAA-CBA-CGA-O2A
49	C	312	KC2	C1A-C2A-CAA-CBA
49	C	312	KC2	C3A-C2A-CAA-CBA
49	C	312	KC2	C2B-C3B-CAB-CBB
49	C	312	KC2	C4B-C3B-CAB-CBB
49	C	312	KC2	C2C-C3C-CAC-CBC
49	C	312	KC2	C4C-C3C-CAC-CBC
49	C	312	KC2	CBD-CGD-O2D-CED
49	C	312	KC2	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
49	C	313	KC2	C1A-C2A-CAA-CBA
49	C	313	KC2	C2B-C3B-CAB-CBB
49	C	313	KC2	C4B-C3B-CAB-CBB
49	C	313	KC2	C2C-C3C-CAC-CBC
49	C	313	KC2	C4C-C3C-CAC-CBC
49	C	313	KC2	CBD-CGD-O2D-CED
49	F	307	KC2	C1A-C2A-CAA-CBA
49	F	307	KC2	C3A-C2A-CAA-CBA
49	F	307	KC2	C2B-C3B-CAB-CBB
49	F	307	KC2	C4B-C3B-CAB-CBB
49	F	307	KC2	C2C-C3C-CAC-CBC
49	F	307	KC2	C4C-C3C-CAC-CBC
49	F	311	KC2	C1A-C2A-CAA-CBA
49	F	311	KC2	C3A-C2A-CAA-CBA
49	F	311	KC2	C2B-C3B-CAB-CBB
49	F	311	KC2	C4B-C3B-CAB-CBB
49	F	311	KC2	CAA-CBA-CGA-O1A
49	G	311	KC2	C1A-C2A-CAA-CBA
49	G	311	KC2	C2B-C3B-CAB-CBB
49	G	311	KC2	C4B-C3B-CAB-CBB
49	G	311	KC2	C2C-C3C-CAC-CBC
49	G	311	KC2	C4C-C3C-CAC-CBC
49	G	313	KC2	C2B-C3B-CAB-CBB
49	G	313	KC2	C4B-C3B-CAB-CBB
49	G	313	KC2	C2A-CAA-CBA-CGA
49	G	315	KC2	C1A-C2A-CAA-CBA
49	G	315	KC2	C3A-C2A-CAA-CBA
49	G	315	KC2	C2B-C3B-CAB-CBB
49	G	315	KC2	C4B-C3B-CAB-CBB
49	G	315	KC2	CAA-CBA-CGA-O1A
49	G	315	KC2	CHA-CBD-CGD-O2D
49	G	317	KC2	C1A-C2A-CAA-CBA
49	G	317	KC2	C3A-C2A-CAA-CBA
49	G	317	KC2	C2B-C3B-CAB-CBB
49	G	317	KC2	C4B-C3B-CAB-CBB
49	G	317	KC2	C2C-C3C-CAC-CBC
49	G	317	KC2	C4C-C3C-CAC-CBC
49	H	311	KC2	C1A-C2A-CAA-CBA
49	H	311	KC2	C2B-C3B-CAB-CBB
49	H	311	KC2	C4B-C3B-CAB-CBB
49	H	311	KC2	C2C-C3C-CAC-CBC
49	H	311	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
49	H	314	KC2	C1A-C2A-CAA-CBA
49	H	314	KC2	C3A-C2A-CAA-CBA
49	H	314	KC2	C2B-C3B-CAB-CBB
49	H	314	KC2	C4B-C3B-CAB-CBB
49	H	314	KC2	C2C-C3C-CAC-CBC
49	H	314	KC2	C4C-C3C-CAC-CBC
49	H	314	KC2	CBD-CGD-O2D-CED
49	J	315	KC2	C1A-C2A-CAA-CBA
49	J	315	KC2	C2B-C3B-CAB-CBB
49	J	315	KC2	C4B-C3B-CAB-CBB
49	J	315	KC2	C2C-C3C-CAC-CBC
49	J	315	KC2	C4C-C3C-CAC-CBC
49	J	315	KC2	C2A-CAA-CBA-CGA
49	J	315	KC2	CBD-CGD-O2D-CED
49	K	310	KC2	C1A-C2A-CAA-CBA
49	K	310	KC2	C2B-C3B-CAB-CBB
49	K	310	KC2	C4B-C3B-CAB-CBB
49	K	310	KC2	C2C-C3C-CAC-CBC
49	K	310	KC2	C4C-C3C-CAC-CBC
49	K	313	KC2	C1A-C2A-CAA-CBA
49	K	313	KC2	C3A-C2A-CAA-CBA
49	K	313	KC2	C2B-C3B-CAB-CBB
49	K	313	KC2	C4B-C3B-CAB-CBB
49	K	313	KC2	C2C-C3C-CAC-CBC
49	K	313	KC2	C4C-C3C-CAC-CBC
49	L	312	KC2	C1A-C2A-CAA-CBA
49	L	312	KC2	C2B-C3B-CAB-CBB
49	L	312	KC2	C4B-C3B-CAB-CBB
49	L	314	KC2	C1A-C2A-CAA-CBA
49	L	314	KC2	C3A-C2A-CAA-CBA
49	L	314	KC2	C2B-C3B-CAB-CBB
49	L	314	KC2	C4B-C3B-CAB-CBB
49	L	315	KC2	C1A-C2A-CAA-CBA
49	L	315	KC2	C3A-C2A-CAA-CBA
49	L	315	KC2	C2B-C3B-CAB-CBB
49	L	315	KC2	C4B-C3B-CAB-CBB
49	L	315	KC2	CBD-CGD-O2D-CED
49	L	317	KC2	C1A-C2A-CAA-CBA
49	L	317	KC2	C2B-C3B-CAB-CBB
49	L	317	KC2	C4B-C3B-CAB-CBB
49	L	317	KC2	C2C-C3C-CAC-CBC
49	L	317	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
49	L	317	KC2	CBD-CGD-O2D-CED
49	L	317	KC2	O1D-CGD-O2D-CED
49	L	321	KC2	C1A-C2A-CAA-CBA
49	L	321	KC2	C2B-C3B-CAB-CBB
49	L	321	KC2	C2C-C3C-CAC-CBC
49	L	321	KC2	C4C-C3C-CAC-CBC
49	M	307	KC2	C1A-C2A-CAA-CBA
49	M	307	KC2	C2B-C3B-CAB-CBB
49	M	307	KC2	C4B-C3B-CAB-CBB
49	M	307	KC2	C2C-C3C-CAC-CBC
49	M	307	KC2	C4C-C3C-CAC-CBC
49	M	311	KC2	C1A-C2A-CAA-CBA
49	M	311	KC2	C2B-C3B-CAB-CBB
49	M	311	KC2	C4B-C3B-CAB-CBB
49	M	311	KC2	C2C-C3C-CAC-CBC
49	M	311	KC2	CAA-CBA-CGA-O1A
49	M	313	KC2	C1A-C2A-CAA-CBA
49	M	313	KC2	C3A-C2A-CAA-CBA
49	M	313	KC2	C2B-C3B-CAB-CBB
49	M	313	KC2	C4B-C3B-CAB-CBB
49	M	313	KC2	C2C-C3C-CAC-CBC
49	M	314	KC2	C2B-C3B-CAB-CBB
49	M	314	KC2	C2C-C3C-CAC-CBC
49	O	317	KC2	C1A-C2A-CAA-CBA
49	O	317	KC2	C3A-C2A-CAA-CBA
49	O	317	KC2	C2B-C3B-CAB-CBB
49	O	317	KC2	C4B-C3B-CAB-CBB
49	O	317	KC2	C2A-CAA-CBA-CGA
49	O	317	KC2	CAA-CBA-CGA-O1A
49	P	306	KC2	C1A-C2A-CAA-CBA
49	P	306	KC2	C2B-C3B-CAB-CBB
49	P	306	KC2	C4B-C3B-CAB-CBB
49	P	306	KC2	C2C-C3C-CAC-CBC
49	P	306	KC2	C4C-C3C-CAC-CBC
49	P	310	KC2	C1A-C2A-CAA-CBA
49	P	310	KC2	C2B-C3B-CAB-CBB
49	P	310	KC2	C4B-C3B-CAB-CBB
49	P	310	KC2	C2C-C3C-CAC-CBC
49	P	310	KC2	C4C-C3C-CAC-CBC
49	P	310	KC2	CAA-CBA-CGA-O1A
49	P	312	KC2	C1A-C2A-CAA-CBA
49	P	312	KC2	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
49	P	312	KC2	C2B-C3B-CAB-CBB
49	P	312	KC2	C4B-C3B-CAB-CBB
49	P	312	KC2	C2C-C3C-CAC-CBC
49	P	313	KC2	C2B-C3B-CAB-CBB
49	P	320	KC2	C1A-C2A-CAA-CBA
49	P	320	KC2	C2B-C3B-CAB-CBB
49	P	320	KC2	C4B-C3B-CAB-CBB
49	P	320	KC2	C2C-C3C-CAC-CBC
49	P	320	KC2	C4C-C3C-CAC-CBC
49	Q	313	KC2	C2C-C3C-CAC-CBC
49	Q	313	KC2	C2A-CAA-CBA-CGA
49	Q	313	KC2	CAA-CBA-CGA-O1A
49	Q	315	KC2	C1A-C2A-CAA-CBA
49	Q	315	KC2	C2B-C3B-CAB-CBB
49	Q	315	KC2	C4B-C3B-CAB-CBB
49	Q	318	KC2	C1A-C2A-CAA-CBA
49	Q	318	KC2	C3A-C2A-CAA-CBA
49	Q	318	KC2	C2B-C3B-CAB-CBB
49	Q	318	KC2	C4B-C3B-CAB-CBB
49	Q	318	KC2	C2C-C3C-CAC-CBC
49	Q	318	KC2	C4C-C3C-CAC-CBC
49	R	306	KC2	C1A-C2A-CAA-CBA
49	R	306	KC2	C2B-C3B-CAB-CBB
49	R	306	KC2	C4B-C3B-CAB-CBB
49	R	306	KC2	C2C-C3C-CAC-CBC
49	R	306	KC2	C4C-C3C-CAC-CBC
49	R	312	KC2	C1A-C2A-CAA-CBA
49	R	312	KC2	C2B-C3B-CAB-CBB
49	R	312	KC2	C4B-C3B-CAB-CBB
49	R	312	KC2	C2C-C3C-CAC-CBC
49	R	314	KC2	C1A-C2A-CAA-CBA
49	R	314	KC2	C2B-C3B-CAB-CBB
49	R	314	KC2	C4B-C3B-CAB-CBB
49	R	314	KC2	C2C-C3C-CAC-CBC
49	R	314	KC2	C4C-C3C-CAC-CBC
49	R	318	KC2	C1A-C2A-CAA-CBA
49	R	318	KC2	C2B-C3B-CAB-CBB
49	R	318	KC2	C4B-C3B-CAB-CBB
49	S	314	KC2	C1A-C2A-CAA-CBA
49	S	314	KC2	C2B-C3B-CAB-CBB
49	S	314	KC2	C4B-C3B-CAB-CBB
49	S	315	KC2	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
49	S	315	KC2	C3A-C2A-CAA-CBA
49	S	317	KC2	C1A-C2A-CAA-CBA
49	S	317	KC2	C3A-C2A-CAA-CBA
49	S	317	KC2	C2B-C3B-CAB-CBB
49	S	317	KC2	C4B-C3B-CAB-CBB
49	S	317	KC2	C2C-C3C-CAC-CBC
49	S	317	KC2	C4C-C3C-CAC-CBC
49	T	312	KC2	C2B-C3B-CAB-CBB
49	T	312	KC2	C4B-C3B-CAB-CBB
49	T	312	KC2	C2A-CAA-CBA-CGA
49	T	312	KC2	CHA-CBD-CGD-O1D
49	T	314	KC2	C1A-C2A-CAA-CBA
49	T	314	KC2	C2B-C3B-CAB-CBB
49	T	314	KC2	C2C-C3C-CAC-CBC
49	T	314	KC2	C4C-C3C-CAC-CBC
49	T	315	KC2	C1A-C2A-CAA-CBA
49	T	315	KC2	C2C-C3C-CAC-CBC
49	T	315	KC2	C4C-C3C-CAC-CBC
49	T	316	KC2	C1A-C2A-CAA-CBA
49	T	316	KC2	C2B-C3B-CAB-CBB
49	T	316	KC2	C4B-C3B-CAB-CBB
49	T	316	KC2	C2C-C3C-CAC-CBC
49	T	316	KC2	C4C-C3C-CAC-CBC
49	V	308	KC2	C1A-C2A-CAA-CBA
49	V	308	KC2	C2B-C3B-CAB-CBB
49	V	308	KC2	C4B-C3B-CAB-CBB
49	V	308	KC2	C2C-C3C-CAC-CBC
49	V	308	KC2	C4C-C3C-CAC-CBC
49	V	312	KC2	C2B-C3B-CAB-CBB
49	V	312	KC2	C4B-C3B-CAB-CBB
49	V	312	KC2	C2C-C3C-CAC-CBC
49	V	312	KC2	C4C-C3C-CAC-CBC
49	V	312	KC2	C2A-CAA-CBA-CGA
49	V	314	KC2	C1A-C2A-CAA-CBA
49	V	314	KC2	C3A-C2A-CAA-CBA
49	V	314	KC2	C2B-C3B-CAB-CBB
49	V	314	KC2	C4B-C3B-CAB-CBB
49	V	315	KC2	C1A-C2A-CAA-CBA
49	V	315	KC2	C2A-CAA-CBA-CGA
49	V	315	KC2	CBD-CGD-O2D-CED
49	V	318	KC2	C1A-C2A-CAA-CBA
49	V	318	KC2	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
49	V	318	KC2	C4B-C3B-CAB-CBB
49	V	318	KC2	C2C-C3C-CAC-CBC
49	V	318	KC2	C4C-C3C-CAC-CBC
49	V	320	KC2	C1A-C2A-CAA-CBA
49	V	320	KC2	C2B-C3B-CAB-CBB
49	V	320	KC2	C4B-C3B-CAB-CBB
49	V	320	KC2	C2C-C3C-CAC-CBC
49	V	320	KC2	C4C-C3C-CAC-CBC
49	W	308	KC2	C1A-C2A-CAA-CBA
49	W	308	KC2	C2B-C3B-CAB-CBB
49	W	308	KC2	C4B-C3B-CAB-CBB
49	W	308	KC2	C2C-C3C-CAC-CBC
49	W	308	KC2	C4C-C3C-CAC-CBC
49	W	312	KC2	C1A-C2A-CAA-CBA
49	W	312	KC2	C2B-C3B-CAB-CBB
49	W	312	KC2	C4B-C3B-CAB-CBB
49	W	312	KC2	C2C-C3C-CAC-CBC
49	W	312	KC2	C4C-C3C-CAC-CBC
49	W	312	KC2	CAA-CBA-CGA-O1A
49	W	314	KC2	C1A-C2A-CAA-CBA
49	W	314	KC2	C3A-C2A-CAA-CBA
49	W	314	KC2	C2B-C3B-CAB-CBB
49	W	314	KC2	C4B-C3B-CAB-CBB
49	W	314	KC2	C2C-C3C-CAC-CBC
49	W	315	KC2	C1A-C2A-CAA-CBA
49	W	315	KC2	C2B-C3B-CAB-CBB
49	W	315	KC2	C4B-C3B-CAB-CBB
49	W	315	KC2	C2C-C3C-CAC-CBC
49	W	315	KC2	C4C-C3C-CAC-CBC
49	W	315	KC2	CBD-CGD-O2D-CED
49	X	306	KC2	C1A-C2A-CAA-CBA
49	X	306	KC2	C2B-C3B-CAB-CBB
49	X	306	KC2	C4B-C3B-CAB-CBB
49	X	306	KC2	C2C-C3C-CAC-CBC
49	X	306	KC2	CBD-CGD-O2D-CED
49	X	312	KC2	C1A-C2A-CAA-CBA
49	X	312	KC2	C3A-C2A-CAA-CBA
49	X	312	KC2	C2B-C3B-CAB-CBB
49	X	312	KC2	C4B-C3B-CAB-CBB
49	X	312	KC2	C2C-C3C-CAC-CBC
49	X	314	KC2	C1A-C2A-CAA-CBA
49	X	314	KC2	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
49	X	314	KC2	C4B-C3B-CAB-CBB
49	X	314	KC2	C2C-C3C-CAC-CBC
49	X	314	KC2	C4C-C3C-CAC-CBC
49	X	315	KC2	C1A-C2A-CAA-CBA
49	X	315	KC2	C2B-C3B-CAB-CBB
49	X	315	KC2	C4B-C3B-CAB-CBB
49	X	315	KC2	C2C-C3C-CAC-CBC
49	X	315	KC2	C4C-C3C-CAC-CBC
49	X	318	KC2	C1A-C2A-CAA-CBA
49	X	318	KC2	C2B-C3B-CAB-CBB
49	X	318	KC2	C4B-C3B-CAB-CBB
49	X	318	KC2	C2C-C3C-CAC-CBC
49	X	318	KC2	C4C-C3C-CAC-CBC
49	0	314	KC2	C1A-C2A-CAA-CBA
49	0	314	KC2	C3A-C2A-CAA-CBA
49	0	314	KC2	C2B-C3B-CAB-CBB
49	0	314	KC2	C4B-C3B-CAB-CBB
49	0	314	KC2	C2C-C3C-CAC-CBC
49	0	314	KC2	CAA-CBA-CGA-O1A
49	0	316	KC2	C1A-C2A-CAA-CBA
49	0	316	KC2	C3A-C2A-CAA-CBA
49	0	316	KC2	C2B-C3B-CAB-CBB
49	0	316	KC2	C4B-C3B-CAB-CBB
49	0	317	KC2	C1A-C2A-CAA-CBA
49	0	319	KC2	C1A-C2A-CAA-CBA
49	0	319	KC2	C3A-C2A-CAA-CBA
49	0	319	KC2	C2B-C3B-CAB-CBB
49	0	319	KC2	C4B-C3B-CAB-CBB
49	0	319	KC2	C2C-C3C-CAC-CBC
49	0	319	KC2	C4C-C3C-CAC-CBC
49	1	312	KC2	C1A-C2A-CAA-CBA
49	1	312	KC2	C2B-C3B-CAB-CBB
49	1	312	KC2	C4B-C3B-CAB-CBB
49	1	314	KC2	C1A-C2A-CAA-CBA
49	1	314	KC2	C2B-C3B-CAB-CBB
49	1	314	KC2	C4B-C3B-CAB-CBB
49	1	314	KC2	C2C-C3C-CAC-CBC
49	1	314	KC2	CBD-CGD-O2D-CED
49	1	315	KC2	C3A-C2A-CAA-CBA
49	1	315	KC2	C2B-C3B-CAB-CBB
49	1	315	KC2	C4B-C3B-CAB-CBB
49	1	315	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
49	1	315	KC2	C4C-C3C-CAC-CBC
49	1	315	KC2	C2A-CAA-CBA-CGA
49	1	315	KC2	CAD-CBD-CGD-O1D
49	1	315	KC2	CAD-CBD-CGD-O2D
49	1	315	KC2	CBD-CGD-O2D-CED
49	3	315	KC2	C2B-C3B-CAB-CBB
49	3	315	KC2	C4B-C3B-CAB-CBB
49	3	317	KC2	C1A-C2A-CAA-CBA
49	3	317	KC2	C3A-C2A-CAA-CBA
49	3	317	KC2	C2B-C3B-CAB-CBB
49	3	317	KC2	C4B-C3B-CAB-CBB
49	3	318	KC2	C3A-C2A-CAA-CBA
49	3	321	KC2	C1A-C2A-CAA-CBA
49	3	321	KC2	C2B-C3B-CAB-CBB
49	3	321	KC2	C4B-C3B-CAB-CBB
49	3	321	KC2	C2C-C3C-CAC-CBC
49	3	321	KC2	C4C-C3C-CAC-CBC
49	3	321	KC2	CBD-CGD-O2D-CED
49	4	317	KC2	C1A-C2A-CAA-CBA
49	4	317	KC2	C2B-C3B-CAB-CBB
49	4	317	KC2	C4B-C3B-CAB-CBB
49	4	318	KC2	C1A-C2A-CAA-CBA
49	4	318	KC2	C2C-C3C-CAC-CBC
49	4	320	KC2	C1A-C2A-CAA-CBA
49	4	320	KC2	C3A-C2A-CAA-CBA
49	4	320	KC2	C2B-C3B-CAB-CBB
49	4	320	KC2	C4B-C3B-CAB-CBB
49	4	320	KC2	C2C-C3C-CAC-CBC
49	4	320	KC2	C4C-C3C-CAC-CBC
49	4	324	KC2	C1A-C2A-CAA-CBA
49	4	324	KC2	C3A-C2A-CAA-CBA
49	4	324	KC2	C2B-C3B-CAB-CBB
49	4	324	KC2	C4B-C3B-CAB-CBB
49	4	324	KC2	C2C-C3C-CAC-CBC
49	4	324	KC2	C4C-C3C-CAC-CBC
49	5	305	KC2	C1A-C2A-CAA-CBA
49	5	305	KC2	C2B-C3B-CAB-CBB
49	5	305	KC2	C4B-C3B-CAB-CBB
49	5	305	KC2	C2C-C3C-CAC-CBC
49	5	305	KC2	C4C-C3C-CAC-CBC
49	5	311	KC2	C1A-C2A-CAA-CBA
49	5	311	KC2	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
49	5	311	KC2	C4B-C3B-CAB-CBB
49	5	313	KC2	C1A-C2A-CAA-CBA
49	5	313	KC2	C2B-C3B-CAB-CBB
49	5	313	KC2	C4B-C3B-CAB-CBB
49	5	313	KC2	C2C-C3C-CAC-CBC
49	5	313	KC2	C4C-C3C-CAC-CBC
49	5	314	KC2	C2B-C3B-CAB-CBB
49	5	314	KC2	C4B-C3B-CAB-CBB
49	5	314	KC2	C2C-C3C-CAC-CBC
49	5	314	KC2	C4C-C3C-CAC-CBC
49	7	319	KC2	C1A-C2A-CAA-CBA
49	7	319	KC2	C2B-C3B-CAB-CBB
49	7	319	KC2	C4B-C3B-CAB-CBB
49	7	320	KC2	C1A-C2A-CAA-CBA
49	7	322	KC2	C1A-C2A-CAA-CBA
49	7	322	KC2	C3A-C2A-CAA-CBA
49	7	322	KC2	C2B-C3B-CAB-CBB
49	7	322	KC2	C4B-C3B-CAB-CBB
49	7	322	KC2	C2C-C3C-CAC-CBC
49	7	322	KC2	C4C-C3C-CAC-CBC
49	7	322	KC2	CHA-CBD-CGD-O1D
49	8	314	KC2	C1A-C2A-CAA-CBA
49	8	314	KC2	C2B-C3B-CAB-CBB
49	8	314	KC2	C4B-C3B-CAB-CBB
49	8	314	KC2	CBD-CGD-O2D-CED
49	8	316	KC2	C1A-C2A-CAA-CBA
49	8	316	KC2	C3A-C2A-CAA-CBA
49	8	316	KC2	C2B-C3B-CAB-CBB
49	8	316	KC2	C4B-C3B-CAB-CBB
49	8	316	KC2	C2C-C3C-CAC-CBC
49	8	316	KC2	C2A-CAA-CBA-CGA
49	8	316	KC2	CHA-CBD-CGD-O1D
49	8	317	KC2	C1A-C2A-CAA-CBA
49	8	317	KC2	C2C-C3C-CAC-CBC
49	8	317	KC2	C4C-C3C-CAC-CBC
49	8	317	KC2	CHA-CBD-CGD-O1D
49	8	319	KC2	C1A-C2A-CAA-CBA
49	8	319	KC2	C3A-C2A-CAA-CBA
49	8	319	KC2	C2B-C3B-CAB-CBB
49	8	319	KC2	C4B-C3B-CAB-CBB
49	8	319	KC2	C2C-C3C-CAC-CBC
49	8	319	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
49	8	319	KC2	CAA-CBA-CGA-O2A
49	8	319	KC2	CHA-CBD-CGD-O1D
49	8	319	KC2	CBD-CGD-O2D-CED
49	8	319	KC2	O1D-CGD-O2D-CED
49	8	320	KC2	C1A-C2A-CAA-CBA
49	8	320	KC2	C3A-C2A-CAA-CBA
49	8	320	KC2	C2B-C3B-CAB-CBB
49	8	320	KC2	C4B-C3B-CAB-CBB
49	8	320	KC2	C4C-C3C-CAC-CBC
49	9	311	KC2	C1A-C2A-CAA-CBA
49	9	311	KC2	C3A-C2A-CAA-CBA
49	9	311	KC2	C2B-C3B-CAB-CBB
49	9	311	KC2	C4B-C3B-CAB-CBB
49	9	311	KC2	C2C-C3C-CAC-CBC
49	9	311	KC2	C4C-C3C-CAC-CBC
49	9	313	KC2	C1A-C2A-CAA-CBA
49	9	313	KC2	C2B-C3B-CAB-CBB
49	9	313	KC2	C4B-C3B-CAB-CBB
49	9	313	KC2	CBD-CGD-O2D-CED
49	9	316	KC2	C1A-C2A-CAA-CBA
49	9	316	KC2	C2B-C3B-CAB-CBB
49	9	316	KC2	C4B-C3B-CAB-CBB
49	9	316	KC2	C2C-C3C-CAC-CBC
49	9	316	KC2	C4C-C3C-CAC-CBC
49	9	316	KC2	CBD-CGD-O2D-CED
49	9	316	KC2	O1D-CGD-O2D-CED
49	9	318	KC2	C1A-C2A-CAA-CBA
49	9	318	KC2	C3A-C2A-CAA-CBA
49	9	318	KC2	C2B-C3B-CAB-CBB
49	9	318	KC2	C4B-C3B-CAB-CBB
49	9	318	KC2	C2C-C3C-CAC-CBC
49	9	318	KC2	C4C-C3C-CAC-CBC
49	9	318	KC2	CBD-CGD-O2D-CED
49	I	303	KC2	C2B-C3B-CAB-CBB
49	I	303	KC2	C4B-C3B-CAB-CBB
49	I	312	KC2	C1A-C2A-CAA-CBA
49	I	312	KC2	C3A-C2A-CAA-CBA
49	I	312	KC2	C2B-C3B-CAB-CBB
49	I	312	KC2	C4B-C3B-CAB-CBB
49	I	312	KC2	CAA-CBA-CGA-O1A
49	x	312	KC2	C1A-C2A-CAA-CBA
49	x	312	KC2	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
49	x	312	KC2	C2B-C3B-CAB-CBB
49	x	312	KC2	C4B-C3B-CAB-CBB
49	x	312	KC2	C2C-C3C-CAC-CBC
49	x	313	KC2	C1A-C2A-CAA-CBA
49	x	313	KC2	C2B-C3B-CAB-CBB
49	x	313	KC2	C4B-C3B-CAB-CBB
49	x	313	KC2	C2C-C3C-CAC-CBC
49	x	313	KC2	C4C-C3C-CAC-CBC
49	x	315	KC2	C1A-C2A-CAA-CBA
49	x	315	KC2	C3A-C2A-CAA-CBA
49	x	315	KC2	C2B-C3B-CAB-CBB
49	x	315	KC2	C4B-C3B-CAB-CBB
49	x	315	KC2	C2C-C3C-CAC-CBC
49	x	315	KC2	C4C-C3C-CAC-CBC
49	x	315	KC2	C2A-CAA-CBA-CGA
49	y	313	KC2	C1A-C2A-CAA-CBA
49	y	313	KC2	C2B-C3B-CAB-CBB
49	y	313	KC2	C4B-C3B-CAB-CBB
49	y	313	KC2	C2C-C3C-CAC-CBC
49	y	313	KC2	C4C-C3C-CAC-CBC
49	y	314	KC2	C1A-C2A-CAA-CBA
49	y	314	KC2	C2B-C3B-CAB-CBB
49	y	314	KC2	C4B-C3B-CAB-CBB
49	y	314	KC2	C2C-C3C-CAC-CBC
49	y	314	KC2	C4C-C3C-CAC-CBC
49	y	316	KC2	C1A-C2A-CAA-CBA
49	y	316	KC2	C3A-C2A-CAA-CBA
49	y	316	KC2	C2B-C3B-CAB-CBB
49	y	316	KC2	C4B-C3B-CAB-CBB
49	y	316	KC2	C2C-C3C-CAC-CBC
49	y	316	KC2	C4C-C3C-CAC-CBC
49	z	312	KC2	C1A-C2A-CAA-CBA
49	z	312	KC2	C3A-C2A-CAA-CBA
49	z	312	KC2	C2B-C3B-CAB-CBB
49	z	312	KC2	C4B-C3B-CAB-CBB
49	z	312	KC2	C2C-C3C-CAC-CBC
49	z	313	KC2	C2B-C3B-CAB-CBB
49	z	313	KC2	C4B-C3B-CAB-CBB
49	z	313	KC2	C2C-C3C-CAC-CBC
49	z	313	KC2	C4C-C3C-CAC-CBC
49	z	315	KC2	C1A-C2A-CAA-CBA
49	z	315	KC2	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
49	z	315	KC2	C2B-C3B-CAB-CBB
49	z	315	KC2	C4B-C3B-CAB-CBB
49	z	315	KC2	C2C-C3C-CAC-CBC
49	z	315	KC2	C4C-C3C-CAC-CBC
49	z	315	KC2	CBD-CGD-O2D-CED
49	Y	308	KC2	C1A-C2A-CAA-CBA
49	Y	308	KC2	C3A-C2A-CAA-CBA
49	Y	308	KC2	C2B-C3B-CAB-CBB
49	Y	308	KC2	C4B-C3B-CAB-CBB
49	Y	308	KC2	C2C-C3C-CAC-CBC
49	Y	308	KC2	C4C-C3C-CAC-CBC
49	Y	309	KC2	C1A-C2A-CAA-CBA
49	Y	309	KC2	C3A-C2A-CAA-CBA
49	Y	309	KC2	C2B-C3B-CAB-CBB
49	Y	309	KC2	C4B-C3B-CAB-CBB
49	Y	309	KC2	C2C-C3C-CAC-CBC
49	Y	309	KC2	C4C-C3C-CAC-CBC
49	Z	310	KC2	C1A-C2A-CAA-CBA
49	Z	310	KC2	C3A-C2A-CAA-CBA
49	Z	310	KC2	C2B-C3B-CAB-CBB
49	Z	310	KC2	C4B-C3B-CAB-CBB
49	Z	310	KC2	C2C-C3C-CAC-CBC
49	Z	310	KC2	C4C-C3C-CAC-CBC
49	Z	311	KC2	C1A-C2A-CAA-CBA
49	Z	311	KC2	C3A-C2A-CAA-CBA
49	Z	311	KC2	C2B-C3B-CAB-CBB
49	Z	311	KC2	C4B-C3B-CAB-CBB
49	Z	311	KC2	C2C-C3C-CAC-CBC
49	Z	311	KC2	C4C-C3C-CAC-CBC
49	2	313	KC2	C1A-C2A-CAA-CBA
49	2	313	KC2	C3A-C2A-CAA-CBA
49	2	313	KC2	C2C-C3C-CAC-CBC
49	2	313	KC2	CBD-CGD-O2D-CED
49	2	314	KC2	C1A-C2A-CAA-CBA
49	2	314	KC2	C2B-C3B-CAB-CBB
49	2	314	KC2	C4B-C3B-CAB-CBB
49	2	314	KC2	C2C-C3C-CAC-CBC
49	2	314	KC2	C4C-C3C-CAC-CBC
49	2	314	KC2	C2A-CAA-CBA-CGA
49	2	314	KC2	CBD-CGD-O2D-CED
49	2	317	KC2	C2C-C3C-CAC-CBC
49	2	317	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
49	6	314	KC2	C2B-C3B-CAB-CBB
49	6	314	KC2	C4B-C3B-CAB-CBB
49	6	314	KC2	C2C-C3C-CAC-CBC
49	6	314	KC2	C2A-CAA-CBA-CGA
49	6	316	KC2	C1A-C2A-CAA-CBA
49	6	316	KC2	C3A-C2A-CAA-CBA
49	6	316	KC2	C2B-C3B-CAB-CBB
49	6	316	KC2	C4B-C3B-CAB-CBB
49	6	317	KC2	C1A-C2A-CAA-CBA
49	6	317	KC2	C3A-C2A-CAA-CBA
49	6	317	KC2	C2B-C3B-CAB-CBB
49	6	317	KC2	C2C-C3C-CAC-CBC
49	6	317	KC2	C4C-C3C-CAC-CBC
49	6	317	KC2	CBD-CGD-O2D-CED
49	6	319	KC2	C1A-C2A-CAA-CBA
49	6	319	KC2	C3A-C2A-CAA-CBA
49	6	319	KC2	C2B-C3B-CAB-CBB
49	6	319	KC2	C4B-C3B-CAB-CBB
49	6	319	KC2	C2C-C3C-CAC-CBC
49	6	319	KC2	C4C-C3C-CAC-CBC
49	6	319	KC2	C2A-CAA-CBA-CGA
50	C	302	A1EB1	C13-C14-C15-O1
50	D	308	A1EB1	C13-C14-C15-O1
50	D	308	A1EB1	O5-C38-O4-C34
50	D	308	A1EB1	C44-C42-O6-C28
50	D	308	A1EB1	O43-C42-O6-C28
50	E	301	A1EB1	C10-C11-C13-O
50	E	301	A1EB1	C12-C11-C13-O
50	E	301	A1EB1	C35-C34-O4-C38
50	F	304	A1EB1	C13-C14-C15-O1
50	F	304	A1EB1	C26-C27-C28-O6
50	G	302	A1EB1	C33-C34-O4-C38
50	G	304	A1EB1	C39-C38-O4-C34
50	G	307	A1EB1	C-C1-C24-C25
50	G	307	A1EB1	C2-C1-C24-C25
50	G	307	A1EB1	C33-C34-O4-C38
50	G	307	A1EB1	C5-C6-C8-C9
50	G	307	A1EB1	C7-C6-C8-C9
50	G	308	A1EB1	C44-C42-O6-C28
50	G	308	A1EB1	O43-C42-O6-C28
50	G	308	A1EB1	C5-C6-C8-C9
50	H	301	A1EB1	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
50	H	301	A1EB1	C12-C11-C13-O
50	H	304	A1EB1	C13-C14-C15-O1
50	H	304	A1EB1	C39-C38-O4-C34
50	J	302	A1EB1	C39-C38-O4-C34
50	K	304	A1EB1	C10-C11-C13-O
50	K	304	A1EB1	C12-C11-C13-O
50	K	304	A1EB1	C39-C38-O4-C34
50	K	305	A1EB1	C26-C27-C28-O6
50	L	303	A1EB1	O5-C38-O4-C34
50	L	303	A1EB1	C5-C6-C8-C9
50	L	303	A1EB1	C7-C6-C8-C9
50	O	301	A1EB1	C13-C14-C15-O1
50	O	301	A1EB1	C27-C28-O6-C42
50	O	301	A1EB1	C5-C6-C8-C9
50	O	301	A1EB1	C7-C6-C8-C9
50	Q	307	A1EB1	C35-C34-O4-C38
50	Q	323	A1EB1	C10-C11-C13-O
50	Q	323	A1EB1	C12-C11-C13-O
50	Q	323	A1EB1	C13-C14-C15-O1
50	Q	323	A1EB1	C44-C42-O6-C28
50	Q	323	A1EB1	O43-C42-O6-C28
50	R	303	A1EB1	C10-C11-C13-O
50	R	303	A1EB1	C12-C11-C13-O
50	R	303	A1EB1	C35-C34-O4-C38
50	R	303	A1EB1	C39-C38-O4-C34
50	S	302	A1EB1	C10-C11-C13-O
50	S	302	A1EB1	C10-C11-C13-C14
50	S	302	A1EB1	C12-C11-C13-O
50	S	302	A1EB1	C13-C14-C15-O1
50	S	302	A1EB1	C39-C38-O4-C34
50	S	302	A1EB1	O5-C38-O4-C34
50	S	302	A1EB1	C44-C42-O6-C28
50	S	302	A1EB1	O43-C42-O6-C28
50	S	302	A1EB1	C5-C6-C8-C9
50	S	302	A1EB1	C7-C6-C8-C9
50	S	303	A1EB1	C13-C14-C15-O1
50	S	303	A1EB1	C39-C38-O4-C34
50	T	302	A1EB1	C26-C27-C28-O6
50	T	302	A1EB1	C35-C34-O4-C38
50	U	203	A1EB1	C44-C42-O6-C28
50	U	203	A1EB1	O43-C42-O6-C28
50	U	205	A1EB1	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
50	V	302	A1EB1	C33-C34-O4-C38
50	V	302	A1EB1	C39-C38-O4-C34
50	V	305	A1EB1	C10-C11-C13-O
50	V	305	A1EB1	C12-C11-C13-O
50	V	305	A1EB1	C13-C14-C15-O1
50	V	306	A1EB1	C39-C38-O4-C34
50	V	307	A1EB1	C27-C28-O6-C42
50	V	307	A1EB1	C39-C38-O4-C34
50	V	307	A1EB1	O5-C38-O4-C34
50	V	307	A1EB1	C5-C6-C8-C9
50	V	307	A1EB1	C7-C6-C8-C9
50	0	302	A1EB1	C39-C38-O4-C34
50	0	303	A1EB1	C13-C14-C15-O1
50	0	305	A1EB1	C-C1-C24-C25
50	0	305	A1EB1	C2-C1-C24-C25
50	0	305	A1EB1	C13-C14-C15-O1
50	0	305	A1EB1	C39-C38-O4-C34
50	0	305	A1EB1	C5-C6-C8-C9
50	0	305	A1EB1	C7-C6-C8-C9
50	0	307	A1EB1	C10-C11-C13-O
50	0	307	A1EB1	C12-C11-C13-O
50	0	307	A1EB1	C27-C28-O6-C42
50	0	307	A1EB1	C33-C34-O4-C38
50	0	307	A1EB1	C39-C38-O4-C34
50	1	301	A1EB1	C39-C38-O4-C34
50	1	301	A1EB1	C44-C42-O6-C28
50	1	301	A1EB1	O43-C42-O6-C28
50	1	305	A1EB1	C10-C11-C13-O
50	1	305	A1EB1	C10-C11-C13-C14
50	1	305	A1EB1	C12-C11-C13-O
50	1	305	A1EB1	O5-C38-O4-C34
50	3	302	A1EB1	C10-C11-C13-O
50	3	302	A1EB1	C12-C11-C13-O
50	3	302	A1EB1	C33-C34-O4-C38
50	3	302	A1EB1	C44-C42-O6-C28
50	3	302	A1EB1	O43-C42-O6-C28
50	3	302	A1EB1	C5-C6-C8-C9
50	3	302	A1EB1	C7-C6-C8-C9
50	3	303	A1EB1	C44-C42-O6-C28
50	3	303	A1EB1	O43-C42-O6-C28
50	3	309	A1EB1	C35-C34-O4-C38
50	3	309	A1EB1	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
50	3	310	A1EB1	O-C13-C14-C15
50	3	310	A1EB1	C11-C13-C14-C15
50	3	310	A1EB1	C13-C14-C15-C20
50	3	310	A1EB1	C29-C27-C28-O6
50	3	310	A1EB1	C44-C42-O6-C28
50	3	310	A1EB1	O43-C42-O6-C28
50	3	324	A1EB1	C11-C10-C9-C8
50	3	324	A1EB1	C10-C11-C13-O
50	3	324	A1EB1	C12-C11-C13-O
50	3	324	A1EB1	C26-C27-C28-O6
50	3	324	A1EB1	C29-C27-C28-O6
50	3	324	A1EB1	C33-C34-O4-C38
50	3	324	A1EB1	C39-C38-O4-C34
50	3	324	A1EB1	C5-C6-C8-C9
50	3	324	A1EB1	C7-C6-C8-C9
50	4	301	A1EB1	C10-C11-C13-O
50	4	301	A1EB1	C12-C11-C13-O
50	4	301	A1EB1	C13-C14-C15-O1
50	4	301	A1EB1	C39-C38-O4-C34
50	4	302	A1EB1	C39-C38-O4-C34
50	4	302	A1EB1	C44-C42-O6-C28
50	4	302	A1EB1	O43-C42-O6-C28
50	4	302	A1EB1	C5-C6-C8-C9
50	4	302	A1EB1	C7-C6-C8-C9
50	4	303	A1EB1	C10-C11-C13-O
50	4	303	A1EB1	C12-C11-C13-O
50	4	303	A1EB1	C39-C38-O4-C34
50	4	303	A1EB1	O5-C38-O4-C34
50	4	303	A1EB1	C44-C42-O6-C28
50	4	303	A1EB1	O43-C42-O6-C28
50	4	303	A1EB1	C5-C6-C8-C9
50	4	303	A1EB1	C7-C6-C8-C9
50	4	304	A1EB1	C13-C14-C15-O1
50	4	304	A1EB1	C39-C38-O4-C34
50	5	302	A1EB1	C39-C38-O4-C34
50	5	302	A1EB1	C44-C42-O6-C28
50	5	302	A1EB1	O43-C42-O6-C28
50	7	303	A1EB1	C10-C11-C13-O
50	7	303	A1EB1	C10-C11-C13-C14
50	7	303	A1EB1	C12-C11-C13-O
50	7	303	A1EB1	C13-C14-C15-O1
50	7	303	A1EB1	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
50	7	303	A1EB1	C39-C38-O4-C34
50	7	303	A1EB1	C7-C6-C8-C9
50	7	304	A1EB1	C10-C11-C13-O
50	7	304	A1EB1	C12-C11-C13-O
50	7	304	A1EB1	C39-C38-O4-C34
50	7	304	A1EB1	O5-C38-O4-C34
50	7	305	A1EB1	C10-C11-C13-O
50	7	305	A1EB1	C12-C11-C13-O
50	7	305	A1EB1	C35-C34-O4-C38
50	7	305	A1EB1	C39-C38-O4-C34
50	7	305	A1EB1	C44-C42-O6-C28
50	7	305	A1EB1	O43-C42-O6-C28
50	7	305	A1EB1	C5-C6-C8-C9
50	7	305	A1EB1	C7-C6-C8-C9
50	7	306	A1EB1	C13-C14-C15-O1
50	7	306	A1EB1	C39-C38-O4-C34
50	8	301	A1EB1	C10-C11-C13-O
50	8	301	A1EB1	C12-C11-C13-O
50	8	301	A1EB1	C44-C42-O6-C28
50	8	301	A1EB1	O43-C42-O6-C28
50	8	304	A1EB1	C5-C6-C8-C9
50	8	304	A1EB1	C7-C6-C8-C9
50	8	308	A1EB1	C12-C11-C13-C14
50	8	308	A1EB1	C13-C14-C15-O1
50	8	308	A1EB1	C39-C38-O4-C34
50	8	308	A1EB1	O5-C38-O4-C34
50	9	302	A1EB1	C10-C11-C13-O
50	9	302	A1EB1	C12-C11-C13-O
50	9	302	A1EB1	C13-C14-C15-O1
50	9	302	A1EB1	C39-C38-O4-C34
50	9	302	A1EB1	C44-C42-O6-C28
50	9	302	A1EB1	O43-C42-O6-C28
50	h	203	A1EB1	C39-C38-O4-C34
50	x	301	A1EB1	C12-C11-C13-C14
50	x	301	A1EB1	O5-C38-O4-C34
50	x	301	A1EB1	C5-C6-C8-C9
50	x	301	A1EB1	C7-C6-C8-C9
50	x	302	A1EB1	C-C1-C24-C25
50	x	302	A1EB1	C2-C1-C24-C25
50	x	302	A1EB1	C27-C28-O6-C42
50	x	302	A1EB1	C39-C38-O4-C34
50	y	302	A1EB1	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
50	y	302	A1EB1	C39-C38-O4-C34
50	y	302	A1EB1	O5-C38-O4-C34
50	z	301	A1EB1	C13-C14-C15-O1
50	z	301	A1EB1	C39-C38-O4-C34
50	z	302	A1EB1	C35-C34-O4-C38
50	z	302	A1EB1	C44-C42-O6-C28
50	z	302	A1EB1	O43-C42-O6-C28
50	2	304	A1EB1	C-C1-C24-C25
50	2	304	A1EB1	C2-C1-C24-C25
50	2	304	A1EB1	C10-C11-C13-O
50	2	304	A1EB1	C12-C11-C13-O
50	2	306	A1EB1	C10-C11-C13-O
50	2	306	A1EB1	C12-C11-C13-O
50	2	306	A1EB1	C39-C38-O4-C34
50	2	306	A1EB1	O5-C38-O4-C34
50	2	306	A1EB1	C5-C6-C8-C9
50	2	306	A1EB1	C7-C6-C8-C9
50	6	301	A1EB1	C5-C6-C8-C9
50	6	301	A1EB1	C7-C6-C8-C9
50	6	304	A1EB1	C5-C6-C8-C9
50	6	304	A1EB1	C7-C6-C8-C9
50	6	306	A1EB1	C13-C14-C15-O1
50	6	306	A1EB1	C39-C38-O4-C34
50	6	308	A1EB1	C12-C11-C13-O
50	6	308	A1EB1	C13-C14-C15-O1
50	6	308	A1EB1	C24-C25-C26-C27
50	6	308	A1EB1	O5-C38-O4-C34
51	E	311	A1ECV	C1A-C2A-CAA-CBA
51	E	311	A1ECV	C3A-C2A-CAA-CBA
51	E	311	A1ECV	C2B-C3B-CAB-CBB
51	E	311	A1ECV	C4B-C3B-CAB-CBB
51	E	311	A1ECV	CHA-CBD-CGD-O2D
51	G	316	A1ECV	C1A-C2A-CAA-CBA
51	G	316	A1ECV	C3A-C2A-CAA-CBA
51	G	316	A1ECV	C2B-C3B-CAB-CBB
51	G	316	A1ECV	C4B-C3B-CAB-CBB
51	G	316	A1ECV	CBD-CGD-O2D-CED
51	L	318	A1ECV	C1A-C2A-CAA-CBA
51	L	318	A1ECV	C3A-C2A-CAA-CBA
51	L	318	A1ECV	C1C-C2C-CMC-O1
51	L	318	A1ECV	C1C-C2C-CMC-O2
51	L	318	A1ECV	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
51	L	318	A1ECV	C4B-C3B-CAB-CBB
51	L	318	A1ECV	CBD-CGD-O2D-CED
51	L	318	A1ECV	C2C-CMC-O2-C3
51	M	316	A1ECV	C1A-C2A-CAA-CBA
51	M	316	A1ECV	C3A-C2A-CAA-CBA
51	M	316	A1ECV	C2B-C3B-CAB-CBB
51	M	316	A1ECV	C4B-C3B-CAB-CBB
51	O	315	A1ECV	C1A-C2A-CAA-CBA
51	O	315	A1ECV	C3A-C2A-CAA-CBA
51	O	315	A1ECV	C2B-C3B-CAB-CBB
51	O	315	A1ECV	C4B-C3B-CAB-CBB
51	P	315	A1ECV	C1A-C2A-CAA-CBA
51	P	315	A1ECV	C3A-C2A-CAA-CBA
51	P	315	A1ECV	C2B-C3B-CAB-CBB
51	P	315	A1ECV	C4B-C3B-CAB-CBB
51	P	315	A1ECV	CBD-CGD-O2D-CED
51	P	315	A1ECV	C2C-CMC-O2-C3
51	Q	316	A1ECV	C1A-C2A-CAA-CBA
51	Q	316	A1ECV	C3A-C2A-CAA-CBA
51	Q	316	A1ECV	C2B-C3B-CAB-CBB
51	Q	316	A1ECV	C4B-C3B-CAB-CBB
51	Q	319	A1ECV	C1A-C2A-CAA-CBA
51	Q	319	A1ECV	C3A-C2A-CAA-CBA
51	Q	319	A1ECV	C1C-C2C-CMC-O1
51	Q	319	A1ECV	C1C-C2C-CMC-O2
51	Q	319	A1ECV	C2B-C3B-CAB-CBB
51	Q	319	A1ECV	C4B-C3B-CAB-CBB
51	R	310	A1ECV	C1A-C2A-CAA-CBA
51	R	310	A1ECV	C3A-C2A-CAA-CBA
51	R	310	A1ECV	C2B-C3B-CAB-CBB
51	R	310	A1ECV	C4B-C3B-CAB-CBB
51	R	310	A1ECV	C2C-CMC-O2-C3
51	R	313	A1ECV	C1A-C2A-CAA-CBA
51	R	313	A1ECV	C3A-C2A-CAA-CBA
51	R	313	A1ECV	C2B-C3B-CAB-CBB
51	R	313	A1ECV	C4B-C3B-CAB-CBB
51	S	312	A1ECV	C1A-C2A-CAA-CBA
51	S	312	A1ECV	C3A-C2A-CAA-CBA
51	S	312	A1ECV	C2B-C3B-CAB-CBB
51	S	312	A1ECV	C4B-C3B-CAB-CBB
51	S	318	A1ECV	C1A-C2A-CAA-CBA
51	S	318	A1ECV	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
51	S	318	A1ECV	C4B-C3B-CAB-CBB
51	T	317	A1ECV	C1A-C2A-CAA-CBA
51	T	317	A1ECV	C3A-C2A-CAA-CBA
51	T	317	A1ECV	C2B-C3B-CAB-CBB
51	T	317	A1ECV	C4B-C3B-CAB-CBB
51	V	317	A1ECV	C1A-C2A-CAA-CBA
51	V	317	A1ECV	C3A-C2A-CAA-CBA
51	V	317	A1ECV	C2B-C3B-CAB-CBB
51	V	317	A1ECV	C4B-C3B-CAB-CBB
51	V	317	A1ECV	CBD-CGD-O2D-CED
51	V	317	A1ECV	C2C-CMC-O2-C3
51	W	317	A1ECV	C1A-C2A-CAA-CBA
51	W	317	A1ECV	C3A-C2A-CAA-CBA
51	W	317	A1ECV	C2B-C3B-CAB-CBB
51	W	317	A1ECV	C4B-C3B-CAB-CBB
51	W	317	A1ECV	CBD-CGD-O2D-CED
51	W	317	A1ECV	C2C-CMC-O2-C3
51	X	310	A1ECV	C1A-C2A-CAA-CBA
51	X	310	A1ECV	C3A-C2A-CAA-CBA
51	X	310	A1ECV	C2B-C3B-CAB-CBB
51	X	310	A1ECV	C4B-C3B-CAB-CBB
51	X	310	A1ECV	C2C-CMC-O2-C3
51	X	313	A1ECV	C1A-C2A-CAA-CBA
51	X	313	A1ECV	C3A-C2A-CAA-CBA
51	X	313	A1ECV	C2B-C3B-CAB-CBB
51	X	313	A1ECV	C4B-C3B-CAB-CBB
51	0	321	A1ECV	C1A-C2A-CAA-CBA
51	0	321	A1ECV	C3A-C2A-CAA-CBA
51	0	321	A1ECV	C2B-C3B-CAB-CBB
51	0	321	A1ECV	C4B-C3B-CAB-CBB
51	0	321	A1ECV	CBD-CGD-O2D-CED
51	1	318	A1ECV	C1A-C2A-CAA-CBA
51	1	318	A1ECV	C3A-C2A-CAA-CBA
51	1	318	A1ECV	C2B-C3B-CAB-CBB
51	1	318	A1ECV	C4B-C3B-CAB-CBB
51	1	318	A1ECV	C2C-CMC-O2-C3
51	4	315	A1ECV	C1A-C2A-CAA-CBA
51	4	315	A1ECV	C3A-C2A-CAA-CBA
51	4	315	A1ECV	C2B-C3B-CAB-CBB
51	4	315	A1ECV	C4B-C3B-CAB-CBB
51	4	321	A1ECV	C1A-C2A-CAA-CBA
51	4	321	A1ECV	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
51	4	321	A1ECV	C1C-C2C-CMC-O1
51	4	321	A1ECV	C2B-C3B-CAB-CBB
51	4	321	A1ECV	C4B-C3B-CAB-CBB
51	4	321	A1ECV	C2C-CMC-O2-C3
51	5	309	A1ECV	C1A-C2A-CAA-CBA
51	5	309	A1ECV	C3A-C2A-CAA-CBA
51	5	309	A1ECV	C2B-C3B-CAB-CBB
51	5	309	A1ECV	C4B-C3B-CAB-CBB
51	5	309	A1ECV	C2C-CMC-O2-C3
51	5	312	A1ECV	C1A-C2A-CAA-CBA
51	5	312	A1ECV	C3A-C2A-CAA-CBA
51	5	312	A1ECV	C2B-C3B-CAB-CBB
51	5	312	A1ECV	C4B-C3B-CAB-CBB
51	7	317	A1ECV	C1A-C2A-CAA-CBA
51	7	317	A1ECV	C3A-C2A-CAA-CBA
51	7	317	A1ECV	C2B-C3B-CAB-CBB
51	7	317	A1ECV	C4B-C3B-CAB-CBB
51	7	323	A1ECV	C1A-C2A-CAA-CBA
51	7	323	A1ECV	C3A-C2A-CAA-CBA
51	7	323	A1ECV	C2B-C3B-CAB-CBB
51	7	323	A1ECV	C4B-C3B-CAB-CBB
51	7	323	A1ECV	C2C-CMC-O2-C3
51	9	314	A1ECV	C1A-C2A-CAA-CBA
51	9	314	A1ECV	C3A-C2A-CAA-CBA
51	9	314	A1ECV	C2B-C3B-CAB-CBB
51	9	317	A1ECV	C1A-C2A-CAA-CBA
51	9	317	A1ECV	C3A-C2A-CAA-CBA
51	9	317	A1ECV	C2B-C3B-CAB-CBB
51	9	317	A1ECV	C4B-C3B-CAB-CBB
51	9	317	A1ECV	C2C-CMC-O2-C3
51	x	310	A1ECV	C1A-C2A-CAA-CBA
51	x	310	A1ECV	C3A-C2A-CAA-CBA
51	x	316	A1ECV	C1A-C2A-CAA-CBA
51	x	316	A1ECV	C3A-C2A-CAA-CBA
51	x	316	A1ECV	C1C-C2C-CMC-O1
51	x	316	A1ECV	C1C-C2C-CMC-O2
51	x	316	A1ECV	C2B-C3B-CAB-CBB
51	x	316	A1ECV	C4B-C3B-CAB-CBB
51	x	316	A1ECV	C2C-CMC-O2-C3
51	y	311	A1ECV	C1A-C2A-CAA-CBA
51	y	311	A1ECV	C3A-C2A-CAA-CBA
51	y	311	A1ECV	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
51	y	311	A1ECV	C4B-C3B-CAB-CBB
51	y	317	A1ECV	C1A-C2A-CAA-CBA
51	y	317	A1ECV	C3A-C2A-CAA-CBA
51	y	317	A1ECV	C1C-C2C-CMC-O1
51	y	317	A1ECV	C1C-C2C-CMC-O2
51	y	317	A1ECV	C2B-C3B-CAB-CBB
51	y	317	A1ECV	C4B-C3B-CAB-CBB
51	z	310	A1ECV	C1A-C2A-CAA-CBA
51	z	310	A1ECV	C3A-C2A-CAA-CBA
51	z	310	A1ECV	C2B-C3B-CAB-CBB
51	z	310	A1ECV	C4B-C3B-CAB-CBB
51	z	316	A1ECV	C1A-C2A-CAA-CBA
51	z	316	A1ECV	C3A-C2A-CAA-CBA
51	z	316	A1ECV	C2B-C3B-CAB-CBB
51	z	316	A1ECV	C4B-C3B-CAB-CBB
51	z	316	A1ECV	C2C-CMC-O2-C3
51	Y	306	A1ECV	C1A-C2A-CAA-CBA
51	Y	306	A1ECV	C3A-C2A-CAA-CBA
51	Y	306	A1ECV	C2B-C3B-CAB-CBB
51	Y	306	A1ECV	C4B-C3B-CAB-CBB
51	Y	312	A1ECV	C1A-C2A-CAA-CBA
51	Y	312	A1ECV	C3A-C2A-CAA-CBA
51	Y	312	A1ECV	C2B-C3B-CAB-CBB
51	Y	312	A1ECV	C4B-C3B-CAB-CBB
51	Y	312	A1ECV	C2C-CMC-O2-C3
51	Y	312	A1ECV	O1-CMC-O2-C3
51	Z	308	A1ECV	C1A-C2A-CAA-CBA
51	Z	308	A1ECV	C3A-C2A-CAA-CBA
51	Z	308	A1ECV	C2B-C3B-CAB-CBB
51	Z	308	A1ECV	C4B-C3B-CAB-CBB
51	Z	314	A1ECV	C1A-C2A-CAA-CBA
51	Z	314	A1ECV	C3A-C2A-CAA-CBA
51	Z	314	A1ECV	C2B-C3B-CAB-CBB
51	Z	314	A1ECV	C4B-C3B-CAB-CBB
51	Z	314	A1ECV	C2C-CMC-O2-C3
51	2	311	A1ECV	C1A-C2A-CAA-CBA
51	2	311	A1ECV	C3A-C2A-CAA-CBA
51	2	311	A1ECV	C2B-C3B-CAB-CBB
51	2	311	A1ECV	C4B-C3B-CAB-CBB
51	6	320	A1ECV	C1A-C2A-CAA-CBA
51	6	320	A1ECV	C3A-C2A-CAA-CBA
51	6	320	A1ECV	C1C-C2C-CMC-O1

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Mol	Chain	Res	Type	Atoms
51	6	320	A1ECV	C1C-C2C-CMC-O2
51	6	320	A1ECV	C2B-C3B-CAB-CBB
51	6	320	A1ECV	C4B-C3B-CAB-CBB
51	6	320	A1ECV	CBD-CGD-O2D-CED
51	6	320	A1ECV	C2C-CMC-O2-C3
52	M	305	A1EB4	C10-C11-C12-O3
52	M	305	A1EB4	C42-C38-O4-C34
52	M	305	A1EB4	O43-C38-O4-C34
52	P	305	A1EB4	C-C1-C24-C25
52	P	305	A1EB4	C2-C1-C24-C25
52	P	305	A1EB4	C42-C38-O4-C34
52	P	318	A1EB4	C11-C12-O3-C39
52	P	318	A1EB4	O43-C38-O4-C34
52	P	318	A1EB4	C5-C6-C8-C9
52	P	318	A1EB4	C7-C6-C8-C9
52	R	305	A1EB4	C10-C11-C12-O3
52	T	304	A1EB4	C42-C38-O4-C34
52	T	304	A1EB4	O43-C38-O4-C34
52	W	306	A1EB4	C-C1-C24-C25
52	W	306	A1EB4	C2-C1-C24-C25
52	W	306	A1EB4	C42-C38-O4-C34
52	5	304	A1EB4	C10-C11-C12-O3
48	L	302	A86	C39-C38-O4-C34
48	P	302	A86	C39-C38-O4-C34
48	S	304	A86	C39-C38-O4-C34
48	S	304	A86	O5-C38-O4-C34
48	T	306	A86	O5-C38-O4-C34
48	U	206	A86	O5-C38-O4-C34
48	0	301	A86	C39-C38-O4-C34
48	0	304	A86	C39-C38-O4-C34
48	3	307	A86	O5-C38-O4-C34
48	7	308	A86	C39-C38-O4-C34
48	8	307	A86	C39-C38-O4-C34
48	8	309	A86	O5-C38-O4-C34
48	9	303	A86	C39-C38-O4-C34
48	I	304	A86	O5-C38-O4-C34
48	2	302	A86	C39-C38-O4-C34
50	D	308	A1EB1	C39-C38-O4-C34
50	E	301	A1EB1	C39-C38-O4-C34
50	F	304	A1EB1	O5-C38-O4-C34
50	G	302	A1EB1	C39-C38-O4-C34
50	G	307	A1EB1	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
50	G	308	A1EB1	C39-C38-O4-C34
50	L	303	A1EB1	C39-C38-O4-C34
50	Q	307	A1EB1	C39-C38-O4-C34
50	Q	323	A1EB1	C39-C38-O4-C34
50	T	302	A1EB1	C39-C38-O4-C34
50	U	203	A1EB1	C39-C38-O4-C34
50	V	305	A1EB1	O5-C38-O4-C34
50	V	306	A1EB1	O5-C38-O4-C34
50	0	302	A1EB1	O5-C38-O4-C34
50	3	302	A1EB1	C39-C38-O4-C34
50	3	303	A1EB1	C39-C38-O4-C34
50	3	324	A1EB1	O5-C38-O4-C34
50	7	306	A1EB1	O5-C38-O4-C34
50	8	301	A1EB1	C39-C38-O4-C34
50	9	302	A1EB1	O5-C38-O4-C34
50	x	301	A1EB1	C39-C38-O4-C34
50	y	301	A1EB1	C39-C38-O4-C34
50	z	301	A1EB1	O5-C38-O4-C34
50	z	302	A1EB1	C39-C38-O4-C34
50	6	301	A1EB1	C39-C38-O4-C34
50	6	306	A1EB1	O5-C38-O4-C34
52	P	318	A1EB4	C42-C38-O4-C34
52	R	305	A1EB4	C42-C38-O4-C34
52	X	305	A1EB4	C42-C38-O4-C34
39	f	803	CLA	O1D-CGD-O2D-CED
39	A	305	CLA	O1D-CGD-O2D-CED
39	H	315	CLA	O1D-CGD-O2D-CED
39	J	318	CLA	O1D-CGD-O2D-CED
39	M	310	CLA	O1D-CGD-O2D-CED
39	M	317	CLA	O1D-CGD-O2D-CED
39	P	309	CLA	O1D-CGD-O2D-CED
39	P	316	CLA	O1D-CGD-O2D-CED
39	T	320	CLA	O1D-CGD-O2D-CED
39	U	215	CLA	O1D-CGD-O2D-CED
39	W	311	CLA	O1D-CGD-O2D-CED
39	W	318	CLA	O1D-CGD-O2D-CED
39	0	313	CLA	O1D-CGD-O2D-CED
39	1	308	CLA	O1D-CGD-O2D-CED
39	1	311	CLA	O1D-CGD-O2D-CED
39	1	317	CLA	O1D-CGD-O2D-CED
39	1	320	CLA	O1D-CGD-O2D-CED
39	7	324	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	Y	311	CLA	O1D-CGD-O2D-CED
39	Z	316	CLA	O1D-CGD-O2D-CED
39	2	315	CLA	O1D-CGD-O2D-CED
39	6	322	CLA	O1D-CGD-O2D-CED
49	C	313	KC2	O1D-CGD-O2D-CED
49	H	314	KC2	O1D-CGD-O2D-CED
49	J	315	KC2	O1D-CGD-O2D-CED
49	z	315	KC2	O1D-CGD-O2D-CED
49	2	314	KC2	O1D-CGD-O2D-CED
51	P	315	A1ECV	O1D-CGD-O2D-CED
51	V	317	A1ECV	O1D-CGD-O2D-CED
51	6	320	A1ECV	O1D-CGD-O2D-CED
51	W	317	A1ECV	O1-CMC-O2-C3
51	X	310	A1ECV	O1-CMC-O2-C3
51	G	316	A1ECV	C2C-CMC-O2-C3
51	Q	316	A1ECV	C2C-CMC-O2-C3
51	Q	319	A1ECV	C2C-CMC-O2-C3
51	R	313	A1ECV	C2C-CMC-O2-C3
51	S	312	A1ECV	C2C-CMC-O2-C3
51	S	318	A1ECV	C2C-CMC-O2-C3
51	T	317	A1ECV	C2C-CMC-O2-C3
51	X	313	A1ECV	C2C-CMC-O2-C3
51	4	315	A1ECV	C2C-CMC-O2-C3
51	5	312	A1ECV	C2C-CMC-O2-C3
51	7	317	A1ECV	C2C-CMC-O2-C3
51	9	314	A1ECV	C2C-CMC-O2-C3
51	x	310	A1ECV	C2C-CMC-O2-C3
51	y	311	A1ECV	C2C-CMC-O2-C3
51	y	317	A1ECV	C2C-CMC-O2-C3
51	z	310	A1ECV	C2C-CMC-O2-C3
51	Y	306	A1ECV	C2C-CMC-O2-C3
51	Z	308	A1ECV	C2C-CMC-O2-C3
51	2	311	A1ECV	C2C-CMC-O2-C3
48	C	303	A86	C39-C38-O4-C34
48	D	305	A86	O5-C38-O4-C34
48	F	302	A86	O5-C38-O4-C34
48	G	305	A86	O5-C38-O4-C34
48	H	302	A86	O5-C38-O4-C34
48	L	304	A86	O5-C38-O4-C34
48	P	302	A86	O5-C38-O4-C34
48	Q	308	A86	C39-C38-O4-C34
48	T	305	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
48	V	301	A86	C39-C38-O4-C34
48	W	303	A86	C39-C38-O4-C34
48	X	302	A86	C39-C38-O4-C34
48	0	304	A86	O5-C38-O4-C34
48	0	306	A86	O5-C38-O4-C34
48	1	303	A86	C39-C38-O4-C34
48	3	308	A86	O5-C38-O4-C34
48	4	310	A86	O5-C38-O4-C34
48	4	328	A86	O5-C38-O4-C34
48	7	307	A86	O5-C38-O4-C34
48	7	312	A86	O5-C38-O4-C34
48	y	306	A86	O5-C38-O4-C34
48	Z	301	A86	C39-C38-O4-C34
48	2	302	A86	O5-C38-O4-C34
48	2	305	A86	O5-C38-O4-C34
50	F	304	A1EB1	C39-C38-O4-C34
50	G	304	A1EB1	O5-C38-O4-C34
50	H	301	A1EB1	C39-C38-O4-C34
50	H	301	A1EB1	O5-C38-O4-C34
50	J	302	A1EB1	O5-C38-O4-C34
50	K	302	A1EB1	C39-C38-O4-C34
50	O	301	A1EB1	C39-C38-O4-C34
50	S	303	A1EB1	O5-C38-O4-C34
50	U	203	A1EB1	O5-C38-O4-C34
50	V	302	A1EB1	O5-C38-O4-C34
50	V	305	A1EB1	C39-C38-O4-C34
50	0	303	A1EB1	C39-C38-O4-C34
50	0	307	A1EB1	O5-C38-O4-C34
50	1	301	A1EB1	O5-C38-O4-C34
50	1	305	A1EB1	C39-C38-O4-C34
50	4	301	A1EB1	O5-C38-O4-C34
50	4	302	A1EB1	O5-C38-O4-C34
50	4	304	A1EB1	O5-C38-O4-C34
50	7	303	A1EB1	O5-C38-O4-C34
50	7	305	A1EB1	O5-C38-O4-C34
50	8	301	A1EB1	O5-C38-O4-C34
50	h	203	A1EB1	O5-C38-O4-C34
50	x	302	A1EB1	O5-C38-O4-C34
50	y	301	A1EB1	O5-C38-O4-C34
50	2	304	A1EB1	C39-C38-O4-C34
50	6	308	A1EB1	C39-C38-O4-C34
52	P	305	A1EB4	O43-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
52	W	306	A1EB4	O43-C38-O4-C34
39	b	807	CLA	O1D-CGD-O2D-CED
39	b	826	CLA	O1D-CGD-O2D-CED
39	i	103	CLA	O1D-CGD-O2D-CED
39	E	317	CLA	O1D-CGD-O2D-CED
39	H	316	CLA	O1D-CGD-O2D-CED
39	J	312	CLA	O1D-CGD-O2D-CED
39	J	314	CLA	O1D-CGD-O2D-CED
39	K	309	CLA	O1D-CGD-O2D-CED
39	Q	317	CLA	O1D-CGD-O2D-CED
39	U	201	CLA	O1D-CGD-O2D-CED
39	U	211	CLA	O1D-CGD-O2D-CED
39	U	213	CLA	O1D-CGD-O2D-CED
39	X	316	CLA	O1D-CGD-O2D-CED
39	1	309	CLA	O1D-CGD-O2D-CED
39	5	315	CLA	O1D-CGD-O2D-CED
39	I	314	CLA	O1D-CGD-O2D-CED
39	x	317	CLA	O1D-CGD-O2D-CED
39	z	317	CLA	O1D-CGD-O2D-CED
39	Y	314	CLA	O1D-CGD-O2D-CED
39	2	308	CLA	O1D-CGD-O2D-CED
39	2	309	CLA	O1D-CGD-O2D-CED
39	2	319	CLA	O1D-CGD-O2D-CED
49	L	315	KC2	O1D-CGD-O2D-CED
49	V	315	KC2	O1D-CGD-O2D-CED
49	W	315	KC2	O1D-CGD-O2D-CED
49	0	319	KC2	O1D-CGD-O2D-CED
49	3	321	KC2	O1D-CGD-O2D-CED
49	8	314	KC2	O1D-CGD-O2D-CED
49	9	318	KC2	O1D-CGD-O2D-CED
49	2	313	KC2	O1D-CGD-O2D-CED
49	6	317	KC2	O1D-CGD-O2D-CED
51	G	316	A1ECV	O1D-CGD-O2D-CED
51	L	318	A1ECV	O1D-CGD-O2D-CED
51	W	317	A1ECV	O1D-CGD-O2D-CED
39	a	833	CLA	CBD-CGD-O2D-CED
39	b	807	CLA	CBD-CGD-O2D-CED
39	b	810	CLA	CBD-CGD-O2D-CED
39	b	828	CLA	CBD-CGD-O2D-CED
39	b	836	CLA	CBD-CGD-O2D-CED
39	A	305	CLA	CBD-CGD-O2D-CED
39	A	309	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	B	206	CLA	CBD-CGD-O2D-CED
39	C	311	CLA	CBD-CGD-O2D-CED
39	D	314	CLA	CBD-CGD-O2D-CED
39	D	317	CLA	CBD-CGD-O2D-CED
39	E	312	CLA	CBD-CGD-O2D-CED
39	F	312	CLA	CBD-CGD-O2D-CED
39	F	315	CLA	CBD-CGD-O2D-CED
39	J	310	CLA	CBD-CGD-O2D-CED
39	J	311	CLA	CBD-CGD-O2D-CED
39	J	314	CLA	CBD-CGD-O2D-CED
39	J	318	CLA	CBD-CGD-O2D-CED
39	K	309	CLA	CBD-CGD-O2D-CED
39	L	311	CLA	CBD-CGD-O2D-CED
39	L	316	CLA	CBD-CGD-O2D-CED
39	L	319	CLA	CBD-CGD-O2D-CED
39	O	311	CLA	CBD-CGD-O2D-CED
39	O	318	CLA	CBD-CGD-O2D-CED
39	S	319	CLA	CBD-CGD-O2D-CED
39	S	320	CLA	CBD-CGD-O2D-CED
39	T	318	CLA	CBD-CGD-O2D-CED
39	U	201	CLA	CBD-CGD-O2D-CED
39	U	212	CLA	CBD-CGD-O2D-CED
39	U	215	CLA	CBD-CGD-O2D-CED
39	V	319	CLA	CBD-CGD-O2D-CED
39	W	318	CLA	CBD-CGD-O2D-CED
39	0	313	CLA	CBD-CGD-O2D-CED
39	0	322	CLA	CBD-CGD-O2D-CED
39	0	323	CLA	CBD-CGD-O2D-CED
39	1	311	CLA	CBD-CGD-O2D-CED
39	1	319	CLA	CBD-CGD-O2D-CED
39	3	320	CLA	CBD-CGD-O2D-CED
39	4	312	CLA	CBD-CGD-O2D-CED
39	7	324	CLA	CBD-CGD-O2D-CED
39	7	325	CLA	CBD-CGD-O2D-CED
39	8	310	CLA	CBD-CGD-O2D-CED
39	8	318	CLA	CBD-CGD-O2D-CED
39	I	314	CLA	CBD-CGD-O2D-CED
39	I	315	CLA	CBD-CGD-O2D-CED
39	x	306	CLA	CBD-CGD-O2D-CED
39	x	307	CLA	CBD-CGD-O2D-CED
39	x	308	CLA	CBD-CGD-O2D-CED
39	x	318	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	y	307	CLA	CBD-CGD-O2D-CED
39	y	310	CLA	CBD-CGD-O2D-CED
39	z	306	CLA	CBD-CGD-O2D-CED
39	Y	311	CLA	CBD-CGD-O2D-CED
39	Y	314	CLA	CBD-CGD-O2D-CED
39	Z	305	CLA	CBD-CGD-O2D-CED
39	Z	316	CLA	CBD-CGD-O2D-CED
39	2	307	CLA	CBD-CGD-O2D-CED
39	2	318	CLA	CBD-CGD-O2D-CED
39	2	319	CLA	CBD-CGD-O2D-CED
49	L	314	KC2	CBD-CGD-O2D-CED
49	P	313	KC2	CBD-CGD-O2D-CED
49	T	312	KC2	CBD-CGD-O2D-CED
49	0	319	KC2	CBD-CGD-O2D-CED
49	8	316	KC2	CBD-CGD-O2D-CED
49	8	317	KC2	CBD-CGD-O2D-CED
49	6	319	KC2	CBD-CGD-O2D-CED
39	f	802	CLA	O1A-CGA-O2A-C1
39	D	312	CLA	O1A-CGA-O2A-C1
39	E	307	CLA	O1A-CGA-O2A-C1
39	E	312	CLA	O1A-CGA-O2A-C1
39	K	306	CLA	O1A-CGA-O2A-C1
39	S	308	CLA	O1A-CGA-O2A-C1
46	W	320	LMG	O10-C28-O8-C9
50	K	302	A1EB1	O43-C42-O6-C28
50	Q	307	A1EB1	O43-C42-O6-C28
39	O	312	CLA	O1A-CGA-O2A-C1
39	T	308	CLA	O1A-CGA-O2A-C1
39	Z	306	CLA	O1A-CGA-O2A-C1
39	2	319	CLA	O1A-CGA-O2A-C1
50	6	301	A1EB1	O5-C38-O4-C34
51	L	318	A1ECV	O1-CMC-O2-C3
51	Q	319	A1ECV	O1-CMC-O2-C3
51	R	313	A1ECV	O1-CMC-O2-C3
51	X	313	A1ECV	O1-CMC-O2-C3
51	1	318	A1ECV	O1-CMC-O2-C3
51	5	309	A1ECV	O1-CMC-O2-C3
51	7	323	A1ECV	O1-CMC-O2-C3
51	x	316	A1ECV	O1-CMC-O2-C3
51	z	316	A1ECV	O1-CMC-O2-C3
51	6	320	A1ECV	O1-CMC-O2-C3
39	B	206	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	J	310	CLA	O1D-CGD-O2D-CED
39	O	316	CLA	O1D-CGD-O2D-CED
39	O	318	CLA	O1D-CGD-O2D-CED
39	R	315	CLA	O1D-CGD-O2D-CED
39	U	212	CLA	O1D-CGD-O2D-CED
39	0	322	CLA	O1D-CGD-O2D-CED
39	3	320	CLA	O1D-CGD-O2D-CED
39	7	314	CLA	O1D-CGD-O2D-CED
39	8	310	CLA	O1D-CGD-O2D-CED
39	z	307	CLA	O1D-CGD-O2D-CED
39	Z	315	CLA	O1D-CGD-O2D-CED
51	0	321	A1ECV	O1D-CGD-O2D-CED
39	C	309	CLA	CBA-CGA-O2A-C1
39	J	318	CLA	CBA-CGA-O2A-C1
39	L	320	CLA	CBA-CGA-O2A-C1
39	3	323	CLA	CBA-CGA-O2A-C1
48	1	302	A86	C39-C38-O4-C34
50	U	205	A1EB1	C33-C34-O4-C38
39	a	801	CLA	O1D-CGD-O2D-CED
39	a	812	CLA	O1D-CGD-O2D-CED
39	C	308	CLA	O1D-CGD-O2D-CED
39	D	317	CLA	O1D-CGD-O2D-CED
39	L	311	CLA	O1D-CGD-O2D-CED
39	T	310	CLA	O1D-CGD-O2D-CED
39	1	310	CLA	O1D-CGD-O2D-CED
39	9	307	CLA	O1D-CGD-O2D-CED
39	x	309	CLA	O1D-CGD-O2D-CED
39	y	309	CLA	O1D-CGD-O2D-CED
39	Y	303	CLA	O1D-CGD-O2D-CED
39	Z	312	CLA	O1D-CGD-O2D-CED
39	6	313	CLA	O1D-CGD-O2D-CED
49	9	313	KC2	O1D-CGD-O2D-CED
39	l	201	CLA	CBA-CGA-O2A-C1
39	D	312	CLA	CBA-CGA-O2A-C1
39	E	307	CLA	CBA-CGA-O2A-C1
39	3	322	CLA	CBA-CGA-O2A-C1
46	0	324	LMG	C29-C28-O8-C9
50	K	302	A1EB1	C44-C42-O6-C28
50	Q	307	A1EB1	C44-C42-O6-C28
51	Z	314	A1ECV	O1-CMC-O2-C3
39	a	808	CLA	CBD-CGD-O2D-CED
39	a	818	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	a	820	CLA	CBD-CGD-O2D-CED
39	a	825	CLA	CBD-CGD-O2D-CED
39	b	809	CLA	CBD-CGD-O2D-CED
39	b	833	CLA	CBD-CGD-O2D-CED
39	E	315	CLA	CBD-CGD-O2D-CED
39	F	306	CLA	CBD-CGD-O2D-CED
39	F	316	CLA	CBD-CGD-O2D-CED
39	H	310	CLA	CBD-CGD-O2D-CED
39	J	313	CLA	CBD-CGD-O2D-CED
39	K	306	CLA	CBD-CGD-O2D-CED
39	L	308	CLA	CBD-CGD-O2D-CED
39	P	308	CLA	CBD-CGD-O2D-CED
39	Q	311	CLA	CBD-CGD-O2D-CED
39	Q	314	CLA	CBD-CGD-O2D-CED
39	Q	320	CLA	CBD-CGD-O2D-CED
39	S	310	CLA	CBD-CGD-O2D-CED
39	T	308	CLA	CBD-CGD-O2D-CED
39	U	207	CLA	CBD-CGD-O2D-CED
39	V	316	CLA	CBD-CGD-O2D-CED
39	0	311	CLA	CBD-CGD-O2D-CED
39	3	312	CLA	CBD-CGD-O2D-CED
39	3	313	CLA	CBD-CGD-O2D-CED
39	3	316	CLA	CBD-CGD-O2D-CED
39	8	312	CLA	CBD-CGD-O2D-CED
39	8	313	CLA	CBD-CGD-O2D-CED
39	9	319	CLA	CBD-CGD-O2D-CED
39	I	313	CLA	CBD-CGD-O2D-CED
39	y	308	CLA	CBD-CGD-O2D-CED
39	y	315	CLA	CBD-CGD-O2D-CED
39	z	318	CLA	CBD-CGD-O2D-CED
39	Y	302	CLA	CBD-CGD-O2D-CED
39	Y	304	CLA	CBD-CGD-O2D-CED
39	Y	305	CLA	CBD-CGD-O2D-CED
39	6	318	CLA	CBD-CGD-O2D-CED
39	6	321	CLA	CBD-CGD-O2D-CED
49	7	322	KC2	CBD-CGD-O2D-CED
49	I	303	KC2	CBD-CGD-O2D-CED
49	x	315	KC2	CBD-CGD-O2D-CED
49	y	316	KC2	CBD-CGD-O2D-CED
49	6	316	KC2	CBD-CGD-O2D-CED
51	Q	316	A1ECV	CBD-CGD-O2D-CED
51	5	312	A1ECV	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
48	9	303	A86	O5-C38-O4-C34
50	3	302	A1EB1	O5-C38-O4-C34
39	a	802	CLA	O1A-CGA-O2A-C1
39	a	803	CLA	O1A-CGA-O2A-C1
39	a	816	CLA	O1A-CGA-O2A-C1
39	a	838	CLA	O1A-CGA-O2A-C1
39	l	201	CLA	O1A-CGA-O2A-C1
39	k	202	CLA	O1A-CGA-O2A-C1
39	o	205	CLA	O1A-CGA-O2A-C1
39	D	311	CLA	O1A-CGA-O2A-C1
39	E	306	CLA	O1A-CGA-O2A-C1
39	G	312	CLA	O1A-CGA-O2A-C1
39	G	318	CLA	O1A-CGA-O2A-C1
39	H	306	CLA	O1A-CGA-O2A-C1
39	J	309	CLA	O1A-CGA-O2A-C1
39	L	308	CLA	O1A-CGA-O2A-C1
39	R	311	CLA	O1A-CGA-O2A-C1
39	S	309	CLA	O1A-CGA-O2A-C1
39	S	319	CLA	O1A-CGA-O2A-C1
39	V	309	CLA	O1A-CGA-O2A-C1
39	W	310	CLA	O1A-CGA-O2A-C1
39	X	311	CLA	O1A-CGA-O2A-C1
39	3	322	CLA	O1A-CGA-O2A-C1
39	5	310	CLA	O1A-CGA-O2A-C1
39	I	310	CLA	O1A-CGA-O2A-C1
46	A	316	LMG	O10-C28-O8-C9
46	M	320	LMG	O10-C28-O8-C9
46	0	324	LMG	O10-C28-O8-C9
46	9	321	LMG	O10-C28-O8-C9
46	I	302	LMG	O10-C28-O8-C9
47	k	205	SQD	O10-C23-O48-C46
50	R	303	A1EB1	O43-C42-O6-C28
50	0	305	A1EB1	O43-C42-O6-C28
50	7	304	A1EB1	O43-C42-O6-C28
39	2	308	CLA	O1A-CGA-O2A-C1
39	a	830	CLA	O1D-CGD-O2D-CED
39	a	847	CLA	O1D-CGD-O2D-CED
39	b	806	CLA	O1D-CGD-O2D-CED
39	G	309	CLA	O1D-CGD-O2D-CED
39	H	313	CLA	O1D-CGD-O2D-CED
39	L	320	CLA	O1D-CGD-O2D-CED
39	3	323	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	4	323	CLA	O1D-CGD-O2D-CED
39	y	312	CLA	O1D-CGD-O2D-CED
39	Y	313	CLA	O1D-CGD-O2D-CED
49	F	307	KC2	O1D-CGD-O2D-CED
49	G	315	KC2	CAA-CBA-CGA-O2A
49	T	312	KC2	CAA-CBA-CGA-O2A
48	0	301	A86	O5-C38-O4-C34
48	3	305	A86	O5-C38-O4-C34
50	E	301	A1EB1	O5-C38-O4-C34
50	G	302	A1EB1	O5-C38-O4-C34
50	G	307	A1EB1	O5-C38-O4-C34
50	G	308	A1EB1	O5-C38-O4-C34
50	Q	307	A1EB1	O5-C38-O4-C34
50	T	302	A1EB1	O5-C38-O4-C34
50	z	302	A1EB1	O5-C38-O4-C34
51	Q	316	A1ECV	O1-CMC-O2-C3
51	S	318	A1ECV	O1-CMC-O2-C3
51	T	317	A1ECV	O1-CMC-O2-C3
51	5	312	A1ECV	O1-CMC-O2-C3
51	7	317	A1ECV	O1-CMC-O2-C3
51	9	314	A1ECV	O1-CMC-O2-C3
51	x	310	A1ECV	O1-CMC-O2-C3
51	y	311	A1ECV	O1-CMC-O2-C3
51	y	317	A1ECV	O1-CMC-O2-C3
51	Y	306	A1ECV	O1-CMC-O2-C3
39	b	805	CLA	O1D-CGD-O2D-CED
39	l	201	CLA	O1D-CGD-O2D-CED
39	H	306	CLA	O1D-CGD-O2D-CED
39	Q	310	CLA	O1D-CGD-O2D-CED
39	U	208	CLA	O1D-CGD-O2D-CED
39	3	314	CLA	O1D-CGD-O2D-CED
39	8	322	CLA	O1D-CGD-O2D-CED
39	z	309	CLA	O1D-CGD-O2D-CED
49	1	315	KC2	O1D-CGD-O2D-CED
49	8	316	KC2	O1D-CGD-O2D-CED
50	T	307	A1EB1	C39-C38-O4-C34
50	8	306	A1EB1	C39-C38-O4-C34
39	b	801	CLA	CBD-CGD-O2D-CED
39	b	823	CLA	CBD-CGD-O2D-CED
39	b	830	CLA	CBD-CGD-O2D-CED
39	K	311	CLA	CBD-CGD-O2D-CED
39	R	307	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	T	311	CLA	CBD-CGD-O2D-CED
39	T	319	CLA	CBD-CGD-O2D-CED
39	0	310	CLA	CBD-CGD-O2D-CED
39	8	311	CLA	CBD-CGD-O2D-CED
39	x	314	CLA	CBD-CGD-O2D-CED
39	y	319	CLA	CBD-CGD-O2D-CED
39	2	316	CLA	CBD-CGD-O2D-CED
39	6	312	CLA	CBD-CGD-O2D-CED
49	6	314	KC2	CBD-CGD-O2D-CED
39	b	832	CLA	C5-C6-C7-C8
39	C	309	CLA	O1D-CGD-O2D-CED
39	L	319	CLA	O1D-CGD-O2D-CED
39	X	317	CLA	O1D-CGD-O2D-CED
39	0	323	CLA	O1D-CGD-O2D-CED
39	z	311	CLA	O1D-CGD-O2D-CED
41	D	302	LHG	O9-C7-O7-C5
41	H	317	LHG	O9-C7-O7-C5
46	M	319	LMG	O9-C10-O7-C8
46	4	325	LMG	O9-C10-O7-C8
46	I	302	LMG	O9-C10-O7-C8
47	D	320	SQD	O49-C7-O47-C45
47	F	318	SQD	O49-C7-O47-C45
47	M	301	SQD	O49-C7-O47-C45
47	T	321	SQD	O49-C7-O47-C45
39	B	204	CLA	CBA-CGA-O2A-C1
39	7	318	CLA	CBA-CGA-O2A-C1
39	y	309	CLA	CBA-CGA-O2A-C1
51	G	316	A1ECV	O1-CMC-O2-C3
51	S	312	A1ECV	O1-CMC-O2-C3
51	4	315	A1ECV	O1-CMC-O2-C3
51	z	310	A1ECV	O1-CMC-O2-C3
51	Z	308	A1ECV	O1-CMC-O2-C3
46	0	324	LMG	C11-C10-O7-C8
48	L	307	A86	C39-C38-O4-C34
48	R	302	A86	C39-C38-O4-C34
50	H	304	A1EB1	O5-C38-O4-C34
39	J	312	CLA	O1A-CGA-O2A-C1
39	O	318	CLA	O1A-CGA-O2A-C1
39	0	323	CLA	O1A-CGA-O2A-C1
39	7	318	CLA	O1A-CGA-O2A-C1
39	y	309	CLA	O1A-CGA-O2A-C1
39	z	308	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
52	X	305	A1EB4	C35-C34-O4-C38
51	E	311	A1ECV	C2C-CMC-O2-C3
39	a	823	CLA	C3-C5-C6-C7
39	b	812	CLA	C3-C5-C6-C7
39	b	814	CLA	C3-C5-C6-C7
39	b	816	CLA	C3-C5-C6-C7
39	b	820	CLA	C3-C5-C6-C7
39	b	821	CLA	C3-C5-C6-C7
39	j	101	CLA	C3-C5-C6-C7
39	o	206	CLA	C3-C5-C6-C7
39	A	314	CLA	C3-C5-C6-C7
39	C	307	CLA	C3-C5-C6-C7
39	C	310	CLA	C3-C5-C6-C7
39	D	310	CLA	C3-C5-C6-C7
39	D	316	CLA	C3-C5-C6-C7
39	E	309	CLA	C3-C5-C6-C7
39	F	308	CLA	C3-C5-C6-C7
39	H	312	CLA	C3-C5-C6-C7
39	J	310	CLA	C3-C5-C6-C7
39	J	311	CLA	C3-C5-C6-C7
39	J	314	CLA	C3-C5-C6-C7
39	K	308	CLA	C3-C5-C6-C7
39	K	311	CLA	C3-C5-C6-C7
39	O	314	CLA	C3-C5-C6-C7
39	P	309	CLA	C3-C5-C6-C7
39	Q	309	CLA	C3-C5-C6-C7
39	Q	312	CLA	C3-C5-C6-C7
39	R	307	CLA	C3-C5-C6-C7
39	S	309	CLA	C3-C5-C6-C7
39	T	309	CLA	C3-C5-C6-C7
39	W	310	CLA	C3-C5-C6-C7
39	X	307	CLA	C3-C5-C6-C7
39	0	310	CLA	C3-C5-C6-C7
39	0	311	CLA	C3-C5-C6-C7
39	4	311	CLA	C3-C5-C6-C7
39	4	312	CLA	C3-C5-C6-C7
39	4	314	CLA	C3-C5-C6-C7
39	5	306	CLA	C3-C5-C6-C7
39	7	313	CLA	C3-C5-C6-C7
39	7	314	CLA	C3-C5-C6-C7
39	I	314	CLA	C3-C5-C6-C7
39	a	802	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	a	838	CLA	CBA-CGA-O2A-C1
39	f	802	CLA	CBA-CGA-O2A-C1
39	k	202	CLA	CBA-CGA-O2A-C1
39	D	311	CLA	CBA-CGA-O2A-C1
39	E	312	CLA	CBA-CGA-O2A-C1
39	G	312	CLA	CBA-CGA-O2A-C1
39	G	314	CLA	CBA-CGA-O2A-C1
39	G	318	CLA	CBA-CGA-O2A-C1
39	K	306	CLA	CBA-CGA-O2A-C1
39	K	312	CLA	CBA-CGA-O2A-C1
39	R	311	CLA	CBA-CGA-O2A-C1
39	S	308	CLA	CBA-CGA-O2A-C1
39	S	309	CLA	CBA-CGA-O2A-C1
39	S	319	CLA	CBA-CGA-O2A-C1
39	U	207	CLA	CBA-CGA-O2A-C1
39	V	309	CLA	CBA-CGA-O2A-C1
39	X	311	CLA	CBA-CGA-O2A-C1
39	5	307	CLA	CBA-CGA-O2A-C1
39	5	310	CLA	CBA-CGA-O2A-C1
46	A	316	LMG	C29-C28-O8-C9
46	9	321	LMG	C29-C28-O8-C9
47	k	205	SQD	C24-C23-O48-C46
50	S	303	A1EB1	C44-C42-O6-C28
50	4	304	A1EB1	C44-C42-O6-C28
50	7	304	A1EB1	C44-C42-O6-C28
50	x	302	A1EB1	C44-C42-O6-C28
52	P	318	A1EB4	C43-C39-O3-C12
50	8	306	A1EB1	O5-C38-O4-C34
46	S	322	LMG	C11-C10-O7-C8
46	4	326	LMG	C11-C10-O7-C8
46	7	301	LMG	C11-C10-O7-C8
47	D	320	SQD	C8-C7-O47-C45
47	M	301	SQD	C8-C7-O47-C45
39	S	320	CLA	O1D-CGD-O2D-CED
39	z	306	CLA	O1D-CGD-O2D-CED
39	a	816	CLA	CBD-CGD-O2D-CED
39	a	831	CLA	CBD-CGD-O2D-CED
39	o	203	CLA	CBD-CGD-O2D-CED
39	A	312	CLA	CBD-CGD-O2D-CED
39	B	209	CLA	CBD-CGD-O2D-CED
39	E	318	CLA	CBD-CGD-O2D-CED
49	L	321	KC2	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
49	M	314	KC2	CBD-CGD-O2D-CED
48	M	302	A86	O5-C38-O4-C34
50	K	304	A1EB1	O5-C38-O4-C34
50	R	303	A1EB1	O5-C38-O4-C34
50	U	205	A1EB1	O5-C38-O4-C34
39	F	313	CLA	O1A-CGA-O2A-C1
50	V	302	A1EB1	O43-C42-O6-C28
50	V	307	A1EB1	O43-C42-O6-C28
39	H	316	CLA	O1A-CGA-O2A-C1
39	J	318	CLA	O1A-CGA-O2A-C1
39	L	320	CLA	O1A-CGA-O2A-C1
39	3	323	CLA	O1A-CGA-O2A-C1
48	S	307	A86	O5-C38-O4-C34
48	z	303	A86	O5-C38-O4-C34
50	0	305	A1EB1	O5-C38-O4-C34
50	3	309	A1EB1	O5-C38-O4-C34
50	5	302	A1EB1	O5-C38-O4-C34
51	2	311	A1ECV	O1-CMC-O2-C3
49	C	313	KC2	CAA-CBA-CGA-O1A
49	G	311	KC2	CAA-CBA-CGA-O1A
49	G	311	KC2	CAA-CBA-CGA-O2A
49	H	311	KC2	CAA-CBA-CGA-O2A
49	L	317	KC2	CAA-CBA-CGA-O2A
49	P	320	KC2	CAA-CBA-CGA-O2A
49	0	319	KC2	CAA-CBA-CGA-O2A
49	1	314	KC2	CAA-CBA-CGA-O2A
49	8	319	KC2	CAA-CBA-CGA-O1A
49	Y	309	KC2	CAA-CBA-CGA-O1A
49	Y	309	KC2	CAA-CBA-CGA-O2A
49	Z	311	KC2	CAA-CBA-CGA-O2A
49	6	319	KC2	CAA-CBA-CGA-O1A
49	6	319	KC2	CAA-CBA-CGA-O2A
51	R	310	A1ECV	CAA-CBA-CGA-O1A
51	R	310	A1ECV	CAA-CBA-CGA-O2A
51	X	310	A1ECV	CAA-CBA-CGA-O1A
51	X	310	A1ECV	CAA-CBA-CGA-O2A
51	y	311	A1ECV	CAA-CBA-CGA-O1A
51	y	311	A1ECV	CAA-CBA-CGA-O2A
51	Z	308	A1ECV	CAA-CBA-CGA-O1A
51	Z	308	A1ECV	CAA-CBA-CGA-O2A
39	E	315	CLA	CBA-CGA-O2A-C1
39	J	312	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	O	318	CLA	CBA-CGA-O2A-C1
39	0	323	CLA	CBA-CGA-O2A-C1
39	z	308	CLA	CBA-CGA-O2A-C1
48	L	302	A86	O5-C38-O4-C34
48	R	317	A86	C39-C38-O4-C34
48	T	301	A86	O5-C38-O4-C34
48	4	306	A86	C39-C38-O4-C34
48	8	307	A86	O5-C38-O4-C34
50	3	303	A1EB1	O5-C38-O4-C34
52	R	305	A1EB4	O43-C38-O4-C34
52	X	305	A1EB4	O43-C38-O4-C34
39	b	805	CLA	C4-C3-C5-C6
39	b	834	CLA	C4-C3-C5-C6
39	D	311	CLA	C4-C3-C5-C6
39	K	312	CLA	C4-C3-C5-C6
39	O	310	CLA	C4-C3-C5-C6
39	4	312	CLA	C4-C3-C5-C6
39	7	314	CLA	C4-C3-C5-C6
39	K	312	CLA	C2-C3-C5-C6
39	X	307	CLA	C2-C3-C5-C6
39	4	312	CLA	C2-C3-C5-C6
39	b	824	CLA	CBD-CGD-O2D-CED
39	D	316	CLA	CBD-CGD-O2D-CED
39	F	313	CLA	CBD-CGD-O2D-CED
39	3	322	CLA	CBD-CGD-O2D-CED
39	Z	306	CLA	CBD-CGD-O2D-CED
49	F	307	KC2	CBD-CGD-O2D-CED
39	a	818	CLA	C2A-CAA-CBA-CGA
39	a	838	CLA	C2A-CAA-CBA-CGA
39	b	840	CLA	C2A-CAA-CBA-CGA
39	o	201	CLA	C2A-CAA-CBA-CGA
39	D	317	CLA	C2A-CAA-CBA-CGA
39	J	316	CLA	C2A-CAA-CBA-CGA
39	R	307	CLA	C2A-CAA-CBA-CGA
39	U	201	CLA	C2A-CAA-CBA-CGA
39	U	214	CLA	C2A-CAA-CBA-CGA
39	V	309	CLA	C2A-CAA-CBA-CGA
39	X	307	CLA	C2A-CAA-CBA-CGA
39	0	323	CLA	C2A-CAA-CBA-CGA
39	5	306	CLA	C2A-CAA-CBA-CGA
39	Z	306	CLA	C2A-CAA-CBA-CGA
51	P	315	A1ECV	O1-CMC-O2-C3

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Mol	Chain	Res	Type	Atoms
39	7	314	CLA	O1A-CGA-O2A-C1
50	4	301	A1EB1	O43-C42-O6-C28
48	7	308	A86	O5-C38-O4-C34
39	B	204	CLA	O1A-CGA-O2A-C1
39	a	805	CLA	C3-C5-C6-C7
39	b	834	CLA	C3-C5-C6-C7
39	A	306	CLA	C3-C5-C6-C7
39	B	207	CLA	C3-C5-C6-C7
39	D	312	CLA	C3-C5-C6-C7
39	D	317	CLA	C3-C5-C6-C7
39	E	312	CLA	C3-C5-C6-C7
39	E	313	CLA	C3-C5-C6-C7
39	M	309	CLA	C3-C5-C6-C7
39	Q	310	CLA	C3-C5-C6-C7
39	W	311	CLA	C3-C5-C6-C7
39	W	313	CLA	C3-C5-C6-C7
39	I	313	CLA	C3-C5-C6-C7
39	a	803	CLA	CBA-CGA-O2A-C1
39	a	816	CLA	CBA-CGA-O2A-C1
39	b	824	CLA	CBA-CGA-O2A-C1
39	o	205	CLA	CBA-CGA-O2A-C1
39	A	311	CLA	CBA-CGA-O2A-C1
39	E	306	CLA	CBA-CGA-O2A-C1
39	H	306	CLA	CBA-CGA-O2A-C1
39	J	309	CLA	CBA-CGA-O2A-C1
39	K	307	CLA	CBA-CGA-O2A-C1
39	L	308	CLA	CBA-CGA-O2A-C1
39	T	318	CLA	CBA-CGA-O2A-C1
39	W	310	CLA	CBA-CGA-O2A-C1
39	X	307	CLA	CBA-CGA-O2A-C1
39	4	312	CLA	CBA-CGA-O2A-C1
39	5	306	CLA	CBA-CGA-O2A-C1
39	7	314	CLA	CBA-CGA-O2A-C1
39	I	310	CLA	CBA-CGA-O2A-C1
45	C	314	DGD	C2A-C1A-O1G-C1G
46	M	320	LMG	C29-C28-O8-C9
50	R	303	A1EB1	C44-C42-O6-C28
50	V	302	A1EB1	C44-C42-O6-C28
50	V	307	A1EB1	C44-C42-O6-C28
50	0	305	A1EB1	C44-C42-O6-C28
50	4	301	A1EB1	C44-C42-O6-C28
50	y	302	A1EB1	C44-C42-O6-C28

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Mol	Chain	Res	Type	Atoms
50	6	308	A1EB1	C44-C42-O6-C28
45	b	849	DGD	O6E-C5E-C6E-O5E
48	Q	301	A86	C39-C38-O4-C34
50	K	302	A1EB1	O5-C38-O4-C34
50	O	301	A1EB1	O5-C38-O4-C34
50	Q	323	A1EB1	O5-C38-O4-C34
50	0	303	A1EB1	O5-C38-O4-C34
39	a	814	CLA	CBD-CGD-O2D-CED
39	G	318	CLA	CBD-CGD-O2D-CED
39	K	307	CLA	CBD-CGD-O2D-CED
39	O	309	CLA	CBD-CGD-O2D-CED
39	9	309	CLA	CBD-CGD-O2D-CED
39	y	318	CLA	CBD-CGD-O2D-CED
49	A	313	KC2	CBD-CGD-O2D-CED
48	C	303	A86	O5-C38-O4-C34
48	Q	308	A86	O5-C38-O4-C34
48	x	305	A86	C39-C38-O4-C34
39	a	833	CLA	O1D-CGD-O2D-CED
39	C	311	CLA	O1D-CGD-O2D-CED
39	F	315	CLA	O1D-CGD-O2D-CED
39	J	311	CLA	O1D-CGD-O2D-CED
39	O	311	CLA	O1D-CGD-O2D-CED
39	V	319	CLA	O1D-CGD-O2D-CED
39	1	319	CLA	O1D-CGD-O2D-CED
39	x	318	CLA	O1D-CGD-O2D-CED
39	y	307	CLA	O1D-CGD-O2D-CED
39	2	307	CLA	O1D-CGD-O2D-CED
46	9	321	LMG	O9-C10-O7-C8
47	P	301	SQD	O49-C7-O47-C45
47	9	322	SQD	O49-C7-O47-C45
39	a	835	CLA	O1A-CGA-O2A-C1
39	b	820	CLA	O1A-CGA-O2A-C1
39	A	311	CLA	O1A-CGA-O2A-C1
39	A	315	CLA	O1A-CGA-O2A-C1
39	K	307	CLA	O1A-CGA-O2A-C1
39	K	311	CLA	O1A-CGA-O2A-C1
39	K	312	CLA	O1A-CGA-O2A-C1
39	L	319	CLA	O1A-CGA-O2A-C1
39	Q	314	CLA	O1A-CGA-O2A-C1
39	T	318	CLA	O1A-CGA-O2A-C1
45	C	314	DGD	O1A-C1A-O1G-C1G
50	4	304	A1EB1	O43-C42-O6-C28

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Mol	Chain	Res	Type	Atoms
50	x	302	A1EB1	O43-C42-O6-C28
52	P	318	A1EB4	O54-C39-O3-C12
51	4	321	A1ECV	O1-CMC-O2-C3
48	Z	301	A86	O5-C38-O4-C34
52	W	321	A1EB4	C45-C46-C47-C51
39	C	309	CLA	O1A-CGA-O2A-C1
39	E	315	CLA	O1A-CGA-O2A-C1
39	E	312	CLA	O1D-CGD-O2D-CED
39	4	312	CLA	O1D-CGD-O2D-CED
39	x	306	CLA	O1D-CGD-O2D-CED
43	1	304	DD6	C1-C2-C3-C4
43	1	304	DD6	C3-C4-C5-C6
43	3	304	DD6	C11-C10-C9-C8
48	O	307	A86	C3-C4-C5-C6
48	1	306	A86	C1-C2-C3-C4
48	Y	301	A86	C24-C25-C26-C27
48	6	309	A86	C11-C10-C9-C8
49	z	313	KC2	C3A-C2A-CAA-CBA
50	F	304	A1EB1	C24-C25-C26-C27
50	S	302	A1EB1	C11-C10-C9-C8
50	4	303	A1EB1	C11-C10-C9-C8
50	7	305	A1EB1	C11-C10-C9-C8
50	z	301	A1EB1	C24-C25-C26-C27
48	W	303	A86	O5-C38-O4-C34
48	X	302	A86	O5-C38-O4-C34
49	P	320	KC2	CAA-CBA-CGA-O1A
49	1	314	KC2	CAA-CBA-CGA-O1A
49	5	314	KC2	CAA-CBA-CGA-O2A
39	b	815	CLA	CBD-CGD-O2D-CED
39	b	817	CLA	CBD-CGD-O2D-CED
39	b	834	CLA	CBD-CGD-O2D-CED
39	o	205	CLA	CBD-CGD-O2D-CED
39	A	306	CLA	CBD-CGD-O2D-CED
39	B	203	CLA	CBD-CGD-O2D-CED
39	B	207	CLA	CBD-CGD-O2D-CED
39	D	311	CLA	CBD-CGD-O2D-CED
39	F	314	CLA	CBD-CGD-O2D-CED
39	J	316	CLA	CBD-CGD-O2D-CED
39	L	310	CLA	CBD-CGD-O2D-CED
39	V	311	CLA	CBD-CGD-O2D-CED
39	3	311	CLA	CBD-CGD-O2D-CED
49	K	310	KC2	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
49	P	306	KC2	CBD-CGD-O2D-CED
51	R	310	A1ECV	O1-CMC-O2-C3
39	F	312	CLA	O1D-CGD-O2D-CED
39	S	319	CLA	O1D-CGD-O2D-CED
39	T	318	CLA	O1D-CGD-O2D-CED
41	a	840	LHG	O2-C2-C3-O3
39	a	821	CLA	C3-C5-C6-C7
39	b	810	CLA	C3-C5-C6-C7
39	A	311	CLA	C3-C5-C6-C7
39	E	307	CLA	C3-C5-C6-C7
39	L	308	CLA	C3-C5-C6-C7
39	L	309	CLA	C3-C5-C6-C7
39	U	207	CLA	C3-C5-C6-C7
39	7	316	CLA	C3-C5-C6-C7
39	a	808	CLA	CBA-CGA-O2A-C1
39	a	835	CLA	CBA-CGA-O2A-C1
39	b	820	CLA	CBA-CGA-O2A-C1
39	l	204	CLA	CBA-CGA-O2A-C1
39	F	313	CLA	CBA-CGA-O2A-C1
39	H	308	CLA	CBA-CGA-O2A-C1
39	K	311	CLA	CBA-CGA-O2A-C1
39	L	319	CLA	CBA-CGA-O2A-C1
39	O	310	CLA	CBA-CGA-O2A-C1
39	P	308	CLA	CBA-CGA-O2A-C1
39	Q	314	CLA	CBA-CGA-O2A-C1
39	R	307	CLA	CBA-CGA-O2A-C1
39	4	322	CLA	CBA-CGA-O2A-C1
39	I	308	CLA	CBA-CGA-O2A-C1
46	W	320	LMG	C29-C28-O8-C9
50	C	302	A1EB1	C44-C42-O6-C28
50	H	304	A1EB1	C44-C42-O6-C28
50	J	302	A1EB1	C44-C42-O6-C28
50	2	304	A1EB1	C44-C42-O6-C28
48	E	304	A86	C39-C38-O4-C34
50	8	304	A1EB1	C39-C38-O4-C34
50	6	304	A1EB1	C39-C38-O4-C34
39	4	322	CLA	O1A-CGA-O2A-C1
39	5	306	CLA	O1A-CGA-O2A-C1
47	M	301	SQD	O10-C23-O48-C46
50	S	303	A1EB1	O43-C42-O6-C28
50	0	303	A1EB1	O43-C42-O6-C28
49	6	319	KC2	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
51	V	317	A1ECV	O1-CMC-O2-C3
46	4	325	LMG	C11-C10-O7-C8
47	F	318	SQD	C8-C7-O47-C45
47	F	319	SQD	C8-C7-O47-C45
47	P	301	SQD	C8-C7-O47-C45
48	E	304	A86	O5-C38-O4-C34
48	1	303	A86	O5-C38-O4-C34
50	8	304	A1EB1	O5-C38-O4-C34
50	6	304	A1EB1	O5-C38-O4-C34
39	Q	311	CLA	CBA-CGA-O2A-C1
39	a	811	CLA	CBD-CGD-O2D-CED
39	a	819	CLA	CBD-CGD-O2D-CED
39	b	808	CLA	CBD-CGD-O2D-CED
39	A	308	CLA	CBD-CGD-O2D-CED
39	B	205	CLA	CBD-CGD-O2D-CED
39	G	314	CLA	CBD-CGD-O2D-CED
39	J	308	CLA	CBD-CGD-O2D-CED
39	S	308	CLA	CBD-CGD-O2D-CED
49	G	311	KC2	CBD-CGD-O2D-CED
49	M	307	KC2	CBD-CGD-O2D-CED
49	R	306	KC2	CBD-CGD-O2D-CED
46	9	321	LMG	O6-C5-C6-O5
51	9	317	A1ECV	O1-CMC-O2-C3
52	R	305	A1EB4	C35-C34-O4-C38
50	C	302	A1EB1	O43-C42-O6-C28
46	P	317	LMG	C13-C14-C15-C16
46	W	302	LMG	C13-C14-C15-C16
46	M	320	LMG	O6-C5-C6-O5
46	I	302	LMG	O6-C5-C6-O5
39	b	810	CLA	O1D-CGD-O2D-CED
39	I	315	CLA	O1D-CGD-O2D-CED
46	S	322	LMG	C32-C33-C34-C35
50	2	304	A1EB1	O5-C38-O4-C34
52	M	322	A1EB4	C43-C44-C45-C46
52	P	319	A1EB4	C43-C44-C45-C46
39	k	201	CLA	CBD-CGD-O2D-CED
39	4	311	CLA	CBD-CGD-O2D-CED
51	y	311	A1ECV	CBD-CGD-O2D-CED
39	a	829	CLA	C3-C5-C6-C7
39	a	838	CLA	C3-C5-C6-C7
39	b	806	CLA	C3-C5-C6-C7
39	b	811	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
39	b	832	CLA	C3-C5-C6-C7
39	V	313	CLA	C3-C5-C6-C7
39	A	315	CLA	CBA-CGA-O2A-C1
46	I	302	LMG	C29-C28-O8-C9
50	0	303	A1EB1	C44-C42-O6-C28
39	2	318	CLA	O1D-CGD-O2D-CED
49	A	313	KC2	CAA-CBA-CGA-O2A
49	L	315	KC2	CAA-CBA-CGA-O2A
49	3	321	KC2	CAA-CBA-CGA-O1A
49	4	320	KC2	CAA-CBA-CGA-O2A
49	z	315	KC2	CAA-CBA-CGA-O1A
51	G	316	A1ECV	CAA-CBA-CGA-O1A
51	V	317	A1ECV	CAA-CBA-CGA-O2A
51	4	321	A1ECV	CAA-CBA-CGA-O2A
51	5	312	A1ECV	CAA-CBA-CGA-O1A
51	Y	306	A1ECV	CAA-CBA-CGA-O1A
51	Y	306	A1ECV	CAA-CBA-CGA-O2A
51	2	311	A1ECV	CAA-CBA-CGA-O2A
45	b	849	DGD	C4E-C5E-C6E-O5E
39	b	824	CLA	O1A-CGA-O2A-C1
39	O	310	CLA	O1A-CGA-O2A-C1
39	P	308	CLA	O1A-CGA-O2A-C1
39	R	307	CLA	O1A-CGA-O2A-C1
39	X	307	CLA	O1A-CGA-O2A-C1
39	I	308	CLA	O1A-CGA-O2A-C1
50	6	308	A1EB1	O43-C42-O6-C28
39	a	821	CLA	C4-C3-C5-C6
39	a	829	CLA	C4-C3-C5-C6
39	E	312	CLA	C4-C3-C5-C6
39	E	313	CLA	C4-C3-C5-C6
39	R	316	CLA	C4-C3-C5-C6
39	U	207	CLA	C4-C3-C5-C6
39	U	210	CLA	C4-C3-C5-C6
39	V	309	CLA	C4-C3-C5-C6
39	a	821	CLA	C2-C3-C5-C6
39	a	829	CLA	C2-C3-C5-C6
39	b	834	CLA	C2-C3-C5-C6
39	E	312	CLA	C2-C3-C5-C6
39	E	313	CLA	C2-C3-C5-C6
39	R	316	CLA	C2-C3-C5-C6
39	S	309	CLA	C2-C3-C5-C6
39	U	207	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
39	U	210	CLA	C2-C3-C5-C6
39	V	309	CLA	C2-C3-C5-C6
39	W	313	CLA	C2-C3-C5-C6
39	7	314	CLA	C2-C3-C5-C6
39	8	311	CLA	C2-C3-C5-C6
39	T	309	CLA	CBD-CGD-O2D-CED
39	a	820	CLA	C2A-CAA-CBA-CGA
39	b	828	CLA	C2A-CAA-CBA-CGA
39	b	832	CLA	C2A-CAA-CBA-CGA
39	C	309	CLA	C2A-CAA-CBA-CGA
39	H	316	CLA	C2A-CAA-CBA-CGA
39	J	309	CLA	C2A-CAA-CBA-CGA
39	2	319	CLA	C2A-CAA-CBA-CGA
39	b	828	CLA	O1D-CGD-O2D-CED
39	b	836	CLA	O1D-CGD-O2D-CED
39	D	314	CLA	O1D-CGD-O2D-CED
39	7	325	CLA	O1D-CGD-O2D-CED
39	x	307	CLA	O1D-CGD-O2D-CED
39	x	308	CLA	O1D-CGD-O2D-CED
39	y	310	CLA	O1D-CGD-O2D-CED
46	S	322	LMG	C17-C18-C19-C20
46	4	326	LMG	C30-C31-C32-C33
46	7	301	LMG	C30-C31-C32-C33
39	a	808	CLA	O1A-CGA-O2A-C1
39	l	204	CLA	O1A-CGA-O2A-C1
39	H	308	CLA	O1A-CGA-O2A-C1
39	4	312	CLA	O1A-CGA-O2A-C1
50	H	304	A1EB1	O43-C42-O6-C28
50	J	302	A1EB1	O43-C42-O6-C28
50	y	302	A1EB1	O43-C42-O6-C28
50	2	304	A1EB1	O43-C42-O6-C28
46	S	322	LMG	O6-C1-O1-C7
46	4	326	LMG	O6-C1-O1-C7
46	7	301	LMG	O6-C1-O1-C7
39	f	803	CLA	CBA-CGA-O2A-C1
39	E	319	CLA	CBA-CGA-O2A-C1
46	P	317	LMG	C29-C28-O8-C9
46	W	302	LMG	C29-C28-O8-C9
47	M	301	SQD	C24-C23-O48-C46
50	F	304	A1EB1	C44-C42-O6-C28
50	L	303	A1EB1	C44-C42-O6-C28
50	O	301	A1EB1	C44-C42-O6-C28

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Mol	Chain	Res	Type	Atoms
50	7	306	A1EB1	C44-C42-O6-C28
52	M	305	A1EB4	C43-C39-O3-C12
52	R	305	A1EB4	C43-C39-O3-C12
48	Y	301	A86	C39-C38-O4-C34
39	8	321	CLA	CBD-CGD-O2D-CED
39	2	312	CLA	CBD-CGD-O2D-CED
39	L	316	CLA	O1D-CGD-O2D-CED
39	8	318	CLA	O1D-CGD-O2D-CED
39	Z	305	CLA	O1D-CGD-O2D-CED
39	A	309	CLA	O1D-CGD-O2D-CED
49	1	314	KC2	O1D-CGD-O2D-CED
39	f	803	CLA	O1A-CGA-O2A-C1
47	T	321	SQD	C8-C7-O47-C45
49	Y	308	KC2	CAA-CBA-CGA-O2A
51	L	318	A1ECV	CAA-CBA-CGA-O1A
51	4	321	A1ECV	CAA-CBA-CGA-O1A
51	6	320	A1ECV	CAA-CBA-CGA-O2A
48	8	303	A86	C33-C34-O4-C38
39	L	308	CLA	O1D-CGD-O2D-CED
39	P	308	CLA	O1D-CGD-O2D-CED
39	3	312	CLA	O1D-CGD-O2D-CED
39	9	319	CLA	O1D-CGD-O2D-CED
39	y	315	CLA	O1D-CGD-O2D-CED
39	a	826	CLA	CBD-CGD-O2D-CED
39	o	206	CLA	CBD-CGD-O2D-CED
39	S	309	CLA	CBD-CGD-O2D-CED
52	W	321	A1EB4	C42-C38-O4-C34
39	b	809	CLA	O1D-CGD-O2D-CED
39	F	306	CLA	O1D-CGD-O2D-CED
39	3	313	CLA	O1D-CGD-O2D-CED
39	8	313	CLA	O1D-CGD-O2D-CED
51	Q	316	A1ECV	O1D-CGD-O2D-CED
41	D	302	LHG	C1-C2-C3-O3
39	E	319	CLA	O1A-CGA-O2A-C1
46	P	317	LMG	O10-C28-O8-C9
46	W	302	LMG	O10-C28-O8-C9
50	L	303	A1EB1	O43-C42-O6-C28
50	7	306	A1EB1	O43-C42-O6-C28
48	1	302	A86	O5-C38-O4-C34
39	b	809	CLA	C3-C5-C6-C7
39	E	314	CLA	C3-C5-C6-C7
39	F	313	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
39	G	314	CLA	C3-C5-C6-C7
39	S	311	CLA	C3-C5-C6-C7
39	0	312	CLA	C3-C5-C6-C7
39	8	311	CLA	C3-C5-C6-C7
39	J	316	CLA	CBA-CGA-O2A-C1
39	J	313	CLA	O1D-CGD-O2D-CED
39	Q	314	CLA	O1D-CGD-O2D-CED
39	6	318	CLA	O1D-CGD-O2D-CED
39	6	321	CLA	O1D-CGD-O2D-CED
39	a	804	CLA	CBA-CGA-O2A-C1
39	a	819	CLA	CBA-CGA-O2A-C1
39	b	816	CLA	CBA-CGA-O2A-C1
39	b	819	CLA	CBA-CGA-O2A-C1
39	i	103	CLA	CBA-CGA-O2A-C1
39	k	203	CLA	CBA-CGA-O2A-C1
39	o	206	CLA	CBA-CGA-O2A-C1
39	C	305	CLA	CBA-CGA-O2A-C1
39	D	309	CLA	CBA-CGA-O2A-C1
39	D	310	CLA	CBA-CGA-O2A-C1
39	E	313	CLA	CBA-CGA-O2A-C1
39	F	316	CLA	CBA-CGA-O2A-C1
39	H	312	CLA	CBA-CGA-O2A-C1
39	M	317	CLA	CBA-CGA-O2A-C1
39	S	313	CLA	CBA-CGA-O2A-C1
39	U	209	CLA	CBA-CGA-O2A-C1
39	V	316	CLA	CBA-CGA-O2A-C1
39	X	317	CLA	CBA-CGA-O2A-C1
39	0	310	CLA	CBA-CGA-O2A-C1
39	5	316	CLA	CBA-CGA-O2A-C1
39	9	308	CLA	CBA-CGA-O2A-C1
39	I	313	CLA	CBA-CGA-O2A-C1
46	4	326	LMG	C29-C28-O8-C9
46	7	301	LMG	C29-C28-O8-C9
50	G	302	A1EB1	C44-C42-O6-C28
50	T	302	A1EB1	C44-C42-O6-C28
50	V	306	A1EB1	C44-C42-O6-C28
50	0	302	A1EB1	C44-C42-O6-C28
50	3	309	A1EB1	C44-C42-O6-C28
50	3	324	A1EB1	C44-C42-O6-C28
50	8	304	A1EB1	C44-C42-O6-C28
50	h	203	A1EB1	C44-C42-O6-C28
50	y	301	A1EB1	C44-C42-O6-C28

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Mol	Chain	Res	Type	Atoms
50	6	304	A1EB1	C44-C42-O6-C28
52	X	305	A1EB4	C43-C39-O3-C12
52	5	304	A1EB4	C43-C39-O3-C12
39	S	320	CLA	C8-C10-C11-C12
39	a	821	CLA	CBD-CGD-O2D-CED
39	b	837	CLA	CBD-CGD-O2D-CED
39	b	841	CLA	CBD-CGD-O2D-CED
39	4	319	CLA	CBD-CGD-O2D-CED
49	V	308	KC2	CBD-CGD-O2D-CED
46	9	321	LMG	C4-C5-C6-O5
39	a	818	CLA	O1D-CGD-O2D-CED
39	Y	302	CLA	O1D-CGD-O2D-CED
43	z	304	DD6	C11-C10-C9-C8
43	z	304	DD6	C1-C2-C3-C4
48	L	304	A86	C24-C25-C26-C27
48	0	304	A86	C24-C25-C26-C27
48	4	328	A86	C1-C2-C3-C4
48	4	328	A86	C3-C4-C5-C6
48	9	304	A86	C11-C10-C9-C8
50	Q	307	A1EB1	C11-C10-C9-C8
50	V	307	A1EB1	C11-C10-C9-C8
50	9	302	A1EB1	C11-C10-C9-C8
48	Q	308	A86	C33-C34-O4-C38
46	0	324	LMG	C28-C29-C30-C31
39	b	801	CLA	C10-C11-C12-C13
39	0	310	CLA	C8-C10-C11-C12
39	4	314	CLA	C5-C6-C7-C8
39	a	819	CLA	O1A-CGA-O2A-C1
46	I	302	LMG	C4-C5-C6-O5
49	L	317	KC2	CAA-CBA-CGA-O1A
49	P	313	KC2	CAA-CBA-CGA-O2A
49	3	321	KC2	CAA-CBA-CGA-O2A
49	7	322	KC2	CAA-CBA-CGA-O2A
49	z	313	KC2	CAA-CBA-CGA-O2A
49	z	315	KC2	CAA-CBA-CGA-O2A
51	L	318	A1ECV	CAA-CBA-CGA-O2A
51	M	316	A1ECV	CAA-CBA-CGA-O2A
51	P	315	A1ECV	CAA-CBA-CGA-O1A
51	P	315	A1ECV	CAA-CBA-CGA-O2A
51	S	312	A1ECV	CAA-CBA-CGA-O2A
51	V	317	A1ECV	CAA-CBA-CGA-O1A
51	5	312	A1ECV	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
51	2	311	A1ECV	CAA-CBA-CGA-O1A
51	6	320	A1ECV	CAA-CBA-CGA-O1A
39	8	312	CLA	O1D-CGD-O2D-CED
39	b	803	CLA	C15-C16-C17-C18
39	A	306	CLA	C8-C10-C11-C12
39	C	311	CLA	C8-C10-C11-C12
39	D	311	CLA	C10-C11-C12-C13
39	E	308	CLA	C8-C10-C11-C12
39	E	312	CLA	C5-C6-C7-C8
39	P	308	CLA	C10-C11-C12-C13
39	4	314	CLA	C10-C11-C12-C13
39	5	308	CLA	C10-C11-C12-C13
41	D	302	LHG	O2-C2-C3-O3
50	3	303	A1EB1	C42-C44-C45-C46
52	W	321	A1EB4	C39-C43-C44-C45
39	E	316	CLA	C3-C5-C6-C7
47	D	321	SQD	C2-C1-O6-C44
46	M	319	LMG	O7-C8-C9-O8
47	S	301	SQD	O6-C44-C45-O47
39	K	308	CLA	CBA-CGA-O2A-C1
39	Z	313	CLA	C2C-C3C-CAC-CBC
39	b	819	CLA	O1A-CGA-O2A-C1
39	C	305	CLA	O1A-CGA-O2A-C1
39	E	313	CLA	O1A-CGA-O2A-C1
39	F	316	CLA	O1A-CGA-O2A-C1
39	9	308	CLA	O1A-CGA-O2A-C1
39	I	313	CLA	O1A-CGA-O2A-C1
46	4	326	LMG	O10-C28-O8-C9
46	7	301	LMG	O10-C28-O8-C9
50	G	302	A1EB1	O43-C42-O6-C28
50	3	309	A1EB1	O43-C42-O6-C28
51	E	311	A1ECV	O1-CMC-O2-C3
39	I	313	CLA	C4-C3-C5-C6
39	b	805	CLA	C2-C3-C5-C6
39	a	811	CLA	C11-C12-C13-C14
39	a	815	CLA	C11-C10-C8-C9
39	a	830	CLA	C11-C10-C8-C9
39	b	809	CLA	C6-C7-C8-C9
39	b	810	CLA	C6-C7-C8-C9
39	b	840	CLA	C6-C7-C8-C9
39	j	101	CLA	C6-C7-C8-C9
39	l	201	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
39	A	314	CLA	C11-C10-C8-C9
39	C	305	CLA	C6-C7-C8-C9
39	C	307	CLA	C11-C10-C8-C9
39	C	310	CLA	C14-C13-C15-C16
39	D	314	CLA	C14-C13-C15-C16
39	D	318	CLA	C14-C13-C15-C16
39	D	319	CLA	C14-C13-C15-C16
39	E	312	CLA	C6-C7-C8-C9
39	E	312	CLA	C11-C10-C8-C9
39	E	312	CLA	C14-C13-C15-C16
39	E	313	CLA	C6-C7-C8-C9
39	F	308	CLA	C14-C13-C15-C16
39	J	314	CLA	C11-C12-C13-C14
39	K	306	CLA	C6-C7-C8-C9
39	K	307	CLA	C6-C7-C8-C9
39	K	311	CLA	C11-C12-C13-C14
39	K	312	CLA	C6-C7-C8-C9
39	L	310	CLA	C6-C7-C8-C9
39	M	309	CLA	C11-C12-C13-C14
39	P	308	CLA	C11-C12-C13-C14
39	Q	312	CLA	C14-C13-C15-C16
39	R	307	CLA	C11-C12-C13-C14
39	S	308	CLA	C6-C7-C8-C9
39	S	311	CLA	C11-C12-C13-C14
39	V	311	CLA	C14-C13-C15-C16
39	X	307	CLA	C11-C12-C13-C14
39	0	310	CLA	C6-C7-C8-C9
39	3	314	CLA	C11-C12-C13-C14
39	4	314	CLA	C11-C12-C13-C14
39	5	306	CLA	C11-C12-C13-C14
39	7	313	CLA	C6-C7-C8-C9
39	6	312	CLA	C14-C13-C15-C16
39	E	315	CLA	O1D-CGD-O2D-CED
39	T	308	CLA	O1D-CGD-O2D-CED
39	U	207	CLA	O1D-CGD-O2D-CED
39	I	313	CLA	O1D-CGD-O2D-CED
39	Y	304	CLA	O1D-CGD-O2D-CED
39	Y	305	CLA	O1D-CGD-O2D-CED
51	5	312	A1ECV	O1D-CGD-O2D-CED
51	Z	308	A1ECV	CBD-CGD-O2D-CED
48	L	301	A86	C33-C34-O4-C38
50	0	302	A1EB1	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
39	C	306	CLA	C5-C6-C7-C8
39	a	815	CLA	C2A-CAA-CBA-CGA
39	a	821	CLA	C2A-CAA-CBA-CGA
39	b	833	CLA	C2A-CAA-CBA-CGA
39	D	311	CLA	C2A-CAA-CBA-CGA
39	Y	304	CLA	C2A-CAA-CBA-CGA
42	a	845	BCR	C37-C22-C23-C24
42	f	801	BCR	C37-C22-C23-C24
42	i	102	BCR	C37-C22-C23-C24
42	j	103	BCR	C7-C8-C9-C34
42	l	206	BCR	C37-C22-C23-C24
42	k	204	BCR	C7-C8-C9-C34
43	j	102	DD6	C12-C11-C13-C14
43	o	204	DD6	C12-C11-C13-C14
43	A	303	DD6	C12-C11-C13-C14
43	O	305	DD6	C7-C6-C8-C9
43	Q	303	DD6	C12-C11-C13-C14
43	3	304	DD6	C12-C11-C13-C14
43	7	310	DD6	C12-C11-C13-C14
48	D	305	A86	C-C1-C24-C25
48	R	302	A86	C7-C6-C8-C9
48	0	304	A86	C-C1-C24-C25
48	1	302	A86	C7-C6-C8-C9
48	4	305	A86	C7-C6-C8-C9
48	8	307	A86	C7-C6-C8-C9
48	9	304	A86	C7-C6-C8-C9
50	G	308	A1EB1	C7-C6-C8-C9
50	Q	307	A1EB1	C7-C6-C8-C9
50	U	203	A1EB1	C-C1-C24-C25
50	9	302	A1EB1	C7-C6-C8-C9
50	z	301	A1EB1	C-C1-C24-C25
50	z	302	A1EB1	C7-C6-C8-C9
42	a	845	BCR	C21-C22-C23-C24
42	f	801	BCR	C21-C22-C23-C24
42	i	102	BCR	C21-C22-C23-C24
42	l	206	BCR	C21-C22-C23-C24
42	k	204	BCR	C7-C8-C9-C10
43	j	102	DD6	C10-C11-C13-C14
43	A	303	DD6	C10-C11-C13-C14
43	Q	303	DD6	C10-C11-C13-C14
43	3	304	DD6	C10-C11-C13-C14
43	7	310	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
48	L	306	A86	C5-C6-C8-C9
48	Q	305	A86	C2-C1-C24-C25
48	0	304	A86	C2-C1-C24-C25
48	1	302	A86	C5-C6-C8-C9
48	8	307	A86	C5-C6-C8-C9
48	9	304	A86	C5-C6-C8-C9
50	1	305	A1EB1	C5-C6-C8-C9
50	z	301	A1EB1	C2-C1-C24-C25
46	D	322	LMG	O6-C5-C6-O5
46	Q	322	LMG	C10-C11-C12-C13
47	7	302	SQD	C7-C8-C9-C10
50	3	302	A1EB1	C42-C44-C45-C46
39	a	804	CLA	O1A-CGA-O2A-C1
39	b	816	CLA	O1A-CGA-O2A-C1
39	V	316	CLA	O1A-CGA-O2A-C1
39	X	317	CLA	O1A-CGA-O2A-C1
50	V	306	A1EB1	O43-C42-O6-C28
50	0	302	A1EB1	O43-C42-O6-C28
50	8	304	A1EB1	O43-C42-O6-C28
50	y	301	A1EB1	O43-C42-O6-C28
50	6	304	A1EB1	O43-C42-O6-C28
39	a	826	CLA	C13-C15-C16-C17
39	b	838	CLA	C8-C10-C11-C12
39	l	204	CLA	C8-C10-C11-C12
39	C	306	CLA	C8-C10-C11-C12
39	D	313	CLA	C5-C6-C7-C8
39	J	309	CLA	C8-C10-C11-C12
39	J	314	CLA	C13-C15-C16-C17
39	K	312	CLA	C13-C15-C16-C17
39	R	309	CLA	C13-C15-C16-C17
39	S	311	CLA	C5-C6-C7-C8
39	W	310	CLA	C15-C16-C17-C18
39	4	316	CLA	C10-C11-C12-C13
39	5	308	CLA	C5-C6-C7-C8
39	3	316	CLA	O1D-CGD-O2D-CED
50	T	307	A1EB1	O5-C38-O4-C34
39	W	319	CLA	CBA-CGA-O2A-C1
46	S	322	LMG	O6-C5-C6-O5
46	7	301	LMG	O6-C5-C6-O5
45	C	314	DGD	C4E-C5E-C6E-O5E
49	T	312	KC2	CAA-CBA-CGA-O1A
49	3	315	KC2	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
51	G	316	A1ECV	CAA-CBA-CGA-O2A
51	S	312	A1ECV	CAA-CBA-CGA-O1A
51	4	315	A1ECV	CAA-CBA-CGA-O1A
51	4	315	A1ECV	CAA-CBA-CGA-O2A
51	z	310	A1ECV	CAA-CBA-CGA-O2A
39	z	318	CLA	O1D-CGD-O2D-CED
39	a	814	CLA	CBA-CGA-O2A-C1
39	b	817	CLA	CBA-CGA-O2A-C1
39	J	314	CLA	CBA-CGA-O2A-C1
39	0	322	CLA	CBA-CGA-O2A-C1
39	1	319	CLA	CBA-CGA-O2A-C1
46	F	317	LMG	C29-C28-O8-C9
47	D	304	SQD	C24-C23-O48-C46
50	H	301	A1EB1	C44-C42-O6-C28
50	K	305	A1EB1	C44-C42-O6-C28
39	a	814	CLA	C10-C11-C12-C13
39	a	825	CLA	C10-C11-C12-C13
39	a	847	CLA	C13-C15-C16-C17
39	b	809	CLA	C15-C16-C17-C18
39	b	842	CLA	C10-C11-C12-C13
39	j	101	CLA	C8-C10-C11-C12
39	C	307	CLA	C8-C10-C11-C12
39	D	314	CLA	C5-C6-C7-C8
39	E	308	CLA	C15-C16-C17-C18
39	E	310	CLA	C5-C6-C7-C8
39	F	312	CLA	C15-C16-C17-C18
39	F	321	CLA	C13-C15-C16-C17
39	H	308	CLA	C8-C10-C11-C12
39	H	310	CLA	C5-C6-C7-C8
39	L	309	CLA	C5-C6-C7-C8
39	P	309	CLA	C10-C11-C12-C13
39	W	309	CLA	C10-C11-C12-C13
39	3	312	CLA	C8-C10-C11-C12
39	4	323	CLA	C13-C15-C16-C17
39	7	313	CLA	C5-C6-C7-C8
46	4	326	LMG	O6-C5-C6-O5
48	G	301	A86	C33-C34-O4-C38
50	V	307	A1EB1	C35-C34-O4-C38
46	P	317	LMG	C10-C11-C12-C13
46	W	302	LMG	C10-C11-C12-C13
50	J	302	A1EB1	C42-C44-C45-C46
52	M	305	A1EB4	C39-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
39	a	808	CLA	O1D-CGD-O2D-CED
39	b	833	CLA	O1D-CGD-O2D-CED
39	F	316	CLA	O1D-CGD-O2D-CED
39	0	311	CLA	O1D-CGD-O2D-CED
39	y	308	CLA	O1D-CGD-O2D-CED
39	D	309	CLA	CBD-CGD-O2D-CED
39	a	804	CLA	C15-C16-C17-C18
39	a	806	CLA	C5-C6-C7-C8
39	a	830	CLA	C8-C10-C11-C12
39	a	847	CLA	C8-C10-C11-C12
39	b	815	CLA	C13-C15-C16-C17
39	b	824	CLA	C5-C6-C7-C8
39	b	840	CLA	C8-C10-C11-C12
39	b	851	CLA	C5-C6-C7-C8
39	b	851	CLA	C13-C15-C16-C17
39	l	201	CLA	C5-C6-C7-C8
39	A	306	CLA	C5-C6-C7-C8
39	F	321	CLA	C15-C16-C17-C18
39	G	309	CLA	C5-C6-C7-C8
39	L	310	CLA	C15-C16-C17-C18
39	M	309	CLA	C10-C11-C12-C13
39	M	309	CLA	C15-C16-C17-C18
39	P	311	CLA	C15-C16-C17-C18
39	Q	312	CLA	C13-C15-C16-C17
39	R	308	CLA	C10-C11-C12-C13
39	R	309	CLA	C10-C11-C12-C13
39	S	313	CLA	C8-C10-C11-C12
39	S	320	CLA	C13-C15-C16-C17
39	3	312	CLA	C10-C11-C12-C13
39	4	316	CLA	C5-C6-C7-C8
39	5	308	CLA	C13-C15-C16-C17
39	7	316	CLA	C10-C11-C12-C13
39	h	201	CLA	C5-C6-C7-C8
41	D	301	LHG	O1-C1-C2-O2
39	D	310	CLA	O1A-CGA-O2A-C1
39	0	310	CLA	O1A-CGA-O2A-C1
41	a	841	LHG	C7-C8-C9-C10
41	H	317	LHG	C23-C24-C25-C26
46	D	322	LMG	C28-C29-C30-C31
46	S	321	LMG	C10-C11-C12-C13
46	9	321	LMG	C28-C29-C30-C31
46	I	302	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
47	k	205	SQD	C7-C8-C9-C10
47	D	321	SQD	C23-C24-C25-C26
47	P	301	SQD	C23-C24-C25-C26
50	G	308	A1EB1	C42-C44-C45-C46
50	S	303	A1EB1	C42-C44-C45-C46
50	2	306	A1EB1	C42-C44-C45-C46
52	P	318	A1EB4	C39-C43-C44-C45
39	K	312	CLA	CBD-CGD-O2D-CED
39	6	310	CLA	CBD-CGD-O2D-CED
39	a	804	CLA	C8-C10-C11-C12
39	b	801	CLA	C15-C16-C17-C18
39	b	810	CLA	C5-C6-C7-C8
39	o	206	CLA	C5-C6-C7-C8
39	D	319	CLA	C10-C11-C12-C13
39	E	308	CLA	C5-C6-C7-C8
39	G	310	CLA	C15-C16-C17-C18
39	H	313	CLA	C5-C6-C7-C8
39	M	312	CLA	C10-C11-C12-C13
39	U	210	CLA	C10-C11-C12-C13
39	V	311	CLA	C10-C11-C12-C13
39	X	309	CLA	C13-C15-C16-C17
39	4	323	CLA	C8-C10-C11-C12
39	a	810	CLA	CBA-CGA-O2A-C1
39	D	314	CLA	CBA-CGA-O2A-C1
39	D	316	CLA	CBA-CGA-O2A-C1
39	F	312	CLA	CBA-CGA-O2A-C1
39	Q	321	CLA	CBA-CGA-O2A-C1
39	3	311	CLA	CBA-CGA-O2A-C1
46	F	320	LMG	C29-C28-O8-C9
47	T	321	SQD	C24-C23-O48-C46
50	8	308	A1EB1	C44-C42-O6-C28
48	L	302	A86	C35-C34-O4-C38
48	L	306	A86	C35-C34-O4-C38
48	0	308	A86	C33-C34-O4-C38
48	6	302	A86	C33-C34-O4-C38
39	a	825	CLA	O1D-CGD-O2D-CED
39	V	316	CLA	O1D-CGD-O2D-CED
46	A	316	LMG	O9-C10-O7-C8
49	B	208	KC2	CAA-CBA-CGA-O1A
49	C	313	KC2	CAA-CBA-CGA-O2A
49	H	314	KC2	CAA-CBA-CGA-O2A
49	Z	311	KC2	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
39	a	803	CLA	C2-C1-O2A-CGA
46	0	324	LMG	O9-C10-O7-C8
39	a	835	CLA	C13-C15-C16-C17
39	a	838	CLA	C8-C10-C11-C12
39	b	820	CLA	C5-C6-C7-C8
39	B	207	CLA	C5-C6-C7-C8
39	D	315	CLA	C8-C10-C11-C12
39	D	318	CLA	C13-C15-C16-C17
39	K	307	CLA	C15-C16-C17-C18
39	O	310	CLA	C10-C11-C12-C13
39	V	309	CLA	C8-C10-C11-C12
41	D	302	LHG	C23-C24-C25-C26
41	X	301	LHG	C23-C24-C25-C26
46	7	326	LMG	C10-C11-C12-C13
50	0	302	A1EB1	C42-C44-C45-C46
51	M	316	A1ECV	C2C-CMC-O2-C3
39	C	305	CLA	CBD-CGD-O2D-CED
39	E	318	CLA	CBA-CGA-O2A-C1
41	a	840	LHG	C28-C29-C30-C31
39	H	306	CLA	O2A-C1-C2-C3
46	S	322	LMG	C13-C14-C15-C16
39	a	823	CLA	C10-C11-C12-C13
39	b	801	CLA	C13-C15-C16-C17
39	b	830	CLA	C10-C11-C12-C13
39	k	202	CLA	C5-C6-C7-C8
39	F	308	CLA	C13-C15-C16-C17
39	7	316	CLA	C5-C6-C7-C8
46	P	317	LMG	O6-C5-C6-O5
39	2	316	CLA	O1D-CGD-O2D-CED
39	a	804	CLA	C11-C10-C8-C7
39	a	808	CLA	C6-C7-C8-C10
39	b	820	CLA	C11-C10-C8-C7
39	A	314	CLA	C11-C10-C8-C7
39	A	314	CLA	C12-C13-C15-C16
39	D	310	CLA	C11-C12-C13-C15
39	D	311	CLA	C11-C12-C13-C15
39	E	307	CLA	C11-C12-C13-C15
39	E	308	CLA	C6-C7-C8-C10
39	E	312	CLA	C6-C7-C8-C10
39	J	311	CLA	C6-C7-C8-C10
39	M	310	CLA	C11-C12-C13-C15
39	P	309	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
39	S	308	CLA	C6-C7-C8-C10
39	0	310	CLA	C6-C7-C8-C10
39	4	311	CLA	C11-C12-C13-C15
39	k	203	CLA	O1A-CGA-O2A-C1
39	D	309	CLA	O1A-CGA-O2A-C1
39	H	312	CLA	O1A-CGA-O2A-C1
39	S	313	CLA	O1A-CGA-O2A-C1
39	U	209	CLA	O1A-CGA-O2A-C1
39	5	316	CLA	O1A-CGA-O2A-C1
52	X	305	A1EB4	O54-C39-O3-C12
43	O	303	DD6	C24-C25-C26-C27
48	G	301	A86	C11-C10-C9-C8
48	1	306	A86	C24-C25-C26-C27
48	8	307	A86	C11-C10-C9-C8
48	9	303	A86	C11-C10-C9-C8
48	9	306	A86	C11-C10-C9-C8
48	z	303	A86	C11-C10-C9-C8
48	Z	301	A86	C24-C25-C26-C27
48	2	302	A86	C24-C25-C26-C27
48	6	305	A86	C24-C25-C26-C27
48	6	309	A86	C1-C2-C3-C4
48	6	309	A86	C3-C4-C5-C6
50	G	302	A1EB1	C24-C25-C26-C27
50	G	307	A1EB1	C24-C25-C26-C27
50	G	308	A1EB1	C11-C10-C9-C8
50	V	307	A1EB1	C1-C2-C3-C4
50	3	302	A1EB1	C11-C10-C9-C8
50	3	324	A1EB1	C1-C2-C3-C4
50	x	301	A1EB1	C24-C25-C26-C27
50	x	302	A1EB1	C11-C10-C9-C8
50	y	301	A1EB1	C24-C25-C26-C27
50	z	302	A1EB1	C11-C10-C9-C8
39	5	310	CLA	CBD-CGD-O2D-CED
48	L	301	A86	C35-C34-O4-C38
39	a	813	CLA	C2A-CAA-CBA-CGA
39	a	826	CLA	C2A-CAA-CBA-CGA
39	a	833	CLA	C2A-CAA-CBA-CGA
39	b	819	CLA	C2A-CAA-CBA-CGA
39	f	803	CLA	C2A-CAA-CBA-CGA
39	S	320	CLA	C2A-CAA-CBA-CGA
39	a	820	CLA	O1D-CGD-O2D-CED
39	b	801	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	H	310	CLA	O1D-CGD-O2D-CED
39	K	306	CLA	O1D-CGD-O2D-CED
39	Q	311	CLA	O1D-CGD-O2D-CED
39	Q	320	CLA	O1D-CGD-O2D-CED
39	R	307	CLA	O1D-CGD-O2D-CED
39	S	310	CLA	O1D-CGD-O2D-CED
39	0	310	CLA	O1D-CGD-O2D-CED
39	8	311	CLA	O1D-CGD-O2D-CED
39	y	319	CLA	O1D-CGD-O2D-CED
49	Q	313	KC2	O1D-CGD-O2D-CED
39	a	814	CLA	C5-C6-C7-C8
39	b	812	CLA	C13-C15-C16-C17
39	D	317	CLA	C5-C6-C7-C8
39	E	307	CLA	C15-C16-C17-C18
39	M	309	CLA	C13-C15-C16-C17
39	P	308	CLA	C5-C6-C7-C8
39	W	311	CLA	C10-C11-C12-C13
39	0	310	CLA	C10-C11-C12-C13
46	W	302	LMG	O6-C5-C6-O5
46	M	319	LMG	C13-C14-C15-C16
49	X	315	KC2	CAA-CBA-CGA-O2A
51	M	316	A1ECV	CAA-CBA-CGA-O1A
51	z	310	A1ECV	CAA-CBA-CGA-O1A
50	T	302	A1EB1	O43-C42-O6-C28
50	3	324	A1EB1	O43-C42-O6-C28
46	D	322	LMG	O6-C1-O1-C7
39	a	806	CLA	C8-C10-C11-C12
39	A	314	CLA	C13-C15-C16-C17
39	0	310	CLA	C5-C6-C7-C8
39	b	823	CLA	O1D-CGD-O2D-CED
39	b	830	CLA	O1D-CGD-O2D-CED
39	K	311	CLA	O1D-CGD-O2D-CED
39	T	319	CLA	O1D-CGD-O2D-CED
48	R	302	A86	O5-C38-O4-C34
42	m	101	BCR	C18-C19-C20-C21
39	a	831	CLA	O1D-CGD-O2D-CED
50	z	301	A1EB1	C35-C34-O4-C38
39	Q	311	CLA	O1A-CGA-O2A-C1
39	a	835	CLA	C15-C16-C17-C18
39	b	806	CLA	C10-C11-C12-C13
39	b	838	CLA	C13-C15-C16-C17
39	b	842	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
39	i	103	CLA	C13-C15-C16-C17
39	C	311	CLA	C15-C16-C17-C18
39	D	315	CLA	C13-C15-C16-C17
39	D	316	CLA	C13-C15-C16-C17
39	E	307	CLA	C5-C6-C7-C8
39	F	314	CLA	C5-C6-C7-C8
39	K	308	CLA	C5-C6-C7-C8
39	M	312	CLA	C8-C10-C11-C12
39	Q	312	CLA	C5-C6-C7-C8
39	S	311	CLA	C10-C11-C12-C13
39	S	313	CLA	C10-C11-C12-C13
39	4	316	CLA	CBA-CGA-O2A-C1
48	L	307	A86	O5-C38-O4-C34
49	X	306	KC2	O1D-CGD-O2D-CED
39	b	817	CLA	O1A-CGA-O2A-C1
39	i	103	CLA	O1A-CGA-O2A-C1
39	o	206	CLA	O1A-CGA-O2A-C1
39	D	316	CLA	O1A-CGA-O2A-C1
39	J	314	CLA	O1A-CGA-O2A-C1
39	K	308	CLA	O1A-CGA-O2A-C1
39	M	317	CLA	O1A-CGA-O2A-C1
50	F	304	A1EB1	O43-C42-O6-C28
50	H	301	A1EB1	O43-C42-O6-C28
50	O	301	A1EB1	O43-C42-O6-C28
50	h	203	A1EB1	O43-C42-O6-C28
52	R	305	A1EB4	O54-C39-O3-C12
52	5	304	A1EB4	O54-C39-O3-C12
39	T	319	CLA	CBA-CGA-O2A-C1
50	L	303	A1EB1	C42-C44-C45-C46
46	M	319	LMG	C4-C5-C6-O5
39	b	841	CLA	C13-C15-C16-C17
39	D	319	CLA	C15-C16-C17-C18
39	E	312	CLA	C13-C15-C16-C17
39	F	321	CLA	C10-C11-C12-C13
39	P	308	CLA	C15-C16-C17-C18
39	3	314	CLA	C5-C6-C7-C8
39	I	314	CLA	C5-C6-C7-C8
39	B	209	CLA	O1D-CGD-O2D-CED
39	E	318	CLA	O1D-CGD-O2D-CED
39	T	311	CLA	O1D-CGD-O2D-CED
39	x	314	CLA	O1D-CGD-O2D-CED
39	6	312	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
49	L	314	KC2	O1D-CGD-O2D-CED
39	l	203	CLA	CBD-CGD-O2D-CED
39	D	314	CLA	O1A-CGA-O2A-C1
46	F	320	LMG	O10-C28-O8-C9
50	8	308	A1EB1	O43-C42-O6-C28
52	M	305	A1EB4	O54-C39-O3-C12
49	x	315	KC2	CAA-CBA-CGA-O2A
52	M	322	A1EB4	C11-C13-C14-C15
52	P	305	A1EB4	C11-C13-C14-C15
52	P	318	A1EB4	C11-C13-C14-C15
52	P	319	A1EB4	C11-C13-C14-C15
52	R	305	A1EB4	C11-C13-C14-C15
52	W	306	A1EB4	C11-C13-C14-C15
52	W	321	A1EB4	C11-C13-C14-C15
52	5	304	A1EB4	C11-C13-C14-C15
39	a	836	CLA	C13-C15-C16-C17
39	b	825	CLA	C5-C6-C7-C8
39	j	101	CLA	C13-C15-C16-C17
39	l	201	CLA	C8-C10-C11-C12
39	C	306	CLA	C10-C11-C12-C13
39	C	310	CLA	C5-C6-C7-C8
39	D	311	CLA	C8-C10-C11-C12
39	D	313	CLA	C13-C15-C16-C17
39	E	307	CLA	C10-C11-C12-C13
39	J	314	CLA	C15-C16-C17-C18
39	K	312	CLA	C5-C6-C7-C8
39	M	310	CLA	C10-C11-C12-C13
39	S	311	CLA	C15-C16-C17-C18
39	V	311	CLA	C13-C15-C16-C17
39	X	308	CLA	C8-C10-C11-C12
48	L	302	A86	C33-C34-O4-C38
50	S	303	A1EB1	C35-C34-O4-C38
41	a	840	LHG	C3-O3-P-O6
41	a	841	LHG	C3-O3-P-O6
41	j	104	LHG	C3-O3-P-O6
41	D	302	LHG	C4-O6-P-O3
41	H	317	LHG	C4-O6-P-O3
41	X	301	LHG	C3-O3-P-O6
39	b	805	CLA	C3-C5-C6-C7
46	S	322	LMG	C34-C35-C36-C37
39	b	831	CLA	CBA-CGA-O2A-C1
39	l	203	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	C	307	CLA	CBA-CGA-O2A-C1
39	P	316	CLA	CBA-CGA-O2A-C1
47	9	322	SQD	C24-C23-O48-C46
50	8	306	A1EB1	C44-C42-O6-C28
39	b	835	CLA	CBD-CGD-O2D-CED
46	l	208	LMG	O6-C5-C6-O5
46	F	317	LMG	O6-C5-C6-O5
46	F	320	LMG	O6-C5-C6-O5
46	Q	322	LMG	O6-C5-C6-O5
39	b	803	CLA	C8-C10-C11-C12
39	b	826	CLA	C13-C15-C16-C17
39	b	851	CLA	C15-C16-C17-C18
39	D	316	CLA	C5-C6-C7-C8
39	P	311	CLA	C13-C15-C16-C17
39	V	310	CLA	C5-C6-C7-C8
50	K	305	A1EB1	O43-C42-O6-C28
39	V	319	CLA	C3-C5-C6-C7
39	a	816	CLA	O1D-CGD-O2D-CED
39	o	203	CLA	O1D-CGD-O2D-CED
39	A	312	CLA	O1D-CGD-O2D-CED
48	R	317	A86	O5-C38-O4-C34
39	a	825	CLA	C13-C15-C16-C17
46	P	317	LMG	C28-C29-C30-C31
46	W	302	LMG	C28-C29-C30-C31
46	4	325	LMG	C28-C29-C30-C31
50	6	301	A1EB1	C42-C44-C45-C46
39	Z	306	CLA	O1D-CGD-O2D-CED
41	j	104	LHG	C1-C2-C3-O3
39	D	310	CLA	C4-C3-C5-C6
39	X	317	CLA	C4-C3-C5-C6
39	D	314	CLA	C8-C10-C11-C12
39	J	309	CLA	C10-C11-C12-C13
39	Q	310	CLA	C5-C6-C7-C8
39	W	313	CLA	C5-C6-C7-C8
39	I	313	CLA	C5-C6-C7-C8
39	a	814	CLA	O1D-CGD-O2D-CED
39	b	824	CLA	O1D-CGD-O2D-CED
39	o	205	CLA	C2A-CAA-CBA-CGA
39	E	318	CLA	C2A-CAA-CBA-CGA
39	E	319	CLA	C2A-CAA-CBA-CGA
39	2	309	CLA	C2A-CAA-CBA-CGA
39	E	310	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
39	I	311	CLA	C16-C17-C18-C20
49	H	311	KC2	CAA-CBA-CGA-O1A
49	3	318	KC2	CAA-CBA-CGA-O2A
49	6	316	KC2	CAA-CBA-CGA-O2A
39	a	806	CLA	CBA-CGA-O2A-C1
39	b	809	CLA	CBA-CGA-O2A-C1
39	o	201	CLA	CBA-CGA-O2A-C1
39	I	301	CLA	CBA-CGA-O2A-C1
47	F	319	SQD	C24-C23-O48-C46
39	a	829	CLA	C5-C6-C7-C8
48	4	306	A86	O5-C38-O4-C34
39	0	322	CLA	O1A-CGA-O2A-C1
43	j	102	DD6	C11-C10-C9-C8
48	G	305	A86	C11-C10-C9-C8
48	L	301	A86	C11-C10-C9-C8
48	L	306	A86	C11-C10-C9-C8
48	Q	302	A86	C11-C10-C9-C8
48	Q	305	A86	C24-C25-C26-C27
48	R	302	A86	C24-C25-C26-C27
48	1	302	A86	C11-C10-C9-C8
48	1	306	A86	C11-C10-C9-C8
48	3	306	A86	C11-C10-C9-C8
48	3	308	A86	C24-C25-C26-C27
48	8	302	A86	C11-C10-C9-C8
48	I	304	A86	C24-C25-C26-C27
48	6	302	A86	C11-C10-C9-C8
50	K	305	A1EB1	C11-C10-C9-C8
50	L	303	A1EB1	C11-C10-C9-C8
50	U	205	A1EB1	C24-C25-C26-C27
50	0	305	A1EB1	C11-C10-C9-C8
50	0	305	A1EB1	C24-C25-C26-C27
50	1	305	A1EB1	C11-C10-C9-C8
50	3	310	A1EB1	C11-C10-C9-C8
50	4	302	A1EB1	C11-C10-C9-C8
50	8	304	A1EB1	C11-C10-C9-C8
50	x	301	A1EB1	C11-C10-C9-C8
50	z	301	A1EB1	C11-C10-C9-C8
50	2	304	A1EB1	C24-C25-C26-C27
50	6	304	A1EB1	C11-C10-C9-C8
50	z	301	A1EB1	C33-C34-O4-C38
46	4	325	LMG	C10-C11-C12-C13
50	4	304	A1EB1	C42-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
41	D	302	LHG	C12-C13-C14-C15
48	X	303	A86	C39-C38-O4-C34
39	k	202	CLA	CBD-CGD-O2D-CED
46	P	317	LMG	C11-C10-O7-C8
46	W	302	LMG	C11-C10-O7-C8
39	j	101	CLA	C10-C11-C12-C13
39	P	308	CLA	C3-C5-C6-C7
41	D	301	LHG	C11-C10-C9-C8
41	D	302	LHG	C11-C12-C13-C14
45	b	849	DGD	C2A-C3A-C4A-C5A
45	b	849	DGD	C8A-C9A-CAA-CBA
47	D	304	SQD	C10-C11-C12-C13
47	F	318	SQD	C12-C13-C14-C15
39	D	316	CLA	O1D-CGD-O2D-CED
39	3	322	CLA	O1D-CGD-O2D-CED
49	C	313	KC2	C2A-CAA-CBA-CGA
49	G	315	KC2	C2A-CAA-CBA-CGA
49	L	312	KC2	C2A-CAA-CBA-CGA
49	R	312	KC2	C2A-CAA-CBA-CGA
49	V	314	KC2	C2A-CAA-CBA-CGA
49	X	306	KC2	C2A-CAA-CBA-CGA
49	3	315	KC2	C2A-CAA-CBA-CGA
49	3	318	KC2	C2A-CAA-CBA-CGA
49	4	318	KC2	C2A-CAA-CBA-CGA
49	5	311	KC2	C2A-CAA-CBA-CGA
49	7	322	KC2	C2A-CAA-CBA-CGA
49	2	317	KC2	C2A-CAA-CBA-CGA
39	b	837	CLA	C11-C12-C13-C15
39	C	308	CLA	C11-C12-C13-C14
39	M	308	CLA	C16-C17-C18-C19
39	Q	312	CLA	C16-C17-C18-C20
39	R	315	CLA	CBA-CGA-O2A-C1
39	X	316	CLA	CBA-CGA-O2A-C1
50	T	307	A1EB1	C44-C42-O6-C28
41	j	104	LHG	C4-C5-O7-C7
47	M	301	SQD	C46-C45-O47-C7
39	G	318	CLA	O1D-CGD-O2D-CED
39	O	309	CLA	O1D-CGD-O2D-CED
39	y	318	CLA	O1D-CGD-O2D-CED
46	P	317	LMG	O9-C10-O7-C8
46	W	302	LMG	O9-C10-O7-C8
39	b	827	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
39	f	802	CLA	C13-C15-C16-C17
50	D	308	A1EB1	C42-C44-C45-C46
41	X	301	LHG	C16-C17-C18-C19
46	I	302	LMG	C31-C32-C33-C34
52	P	305	A1EB4	C43-C44-C45-C46
52	W	306	A1EB4	C43-C44-C45-C46
39	F	313	CLA	O1D-CGD-O2D-CED
39	K	307	CLA	O1D-CGD-O2D-CED
39	a	810	CLA	O1A-CGA-O2A-C1
41	X	301	LHG	O6-C4-C5-O7
41	j	104	LHG	C10-C11-C12-C13
46	4	326	LMG	C12-C13-C14-C15
46	7	301	LMG	C12-C13-C14-C15
39	V	311	CLA	O1D-CGD-O2D-CED
39	9	309	CLA	O1D-CGD-O2D-CED
39	D	317	CLA	C13-C15-C16-C17
39	E	308	CLA	C10-C11-C12-C13
39	J	311	CLA	C13-C15-C16-C17
39	X	309	CLA	C10-C11-C12-C13
45	b	849	DGD	C3A-C4A-C5A-C6A
46	D	322	LMG	C30-C31-C32-C33
47	F	318	SQD	C25-C26-C27-C28
48	Q	301	A86	O5-C38-O4-C34
48	x	305	A86	O5-C38-O4-C34
52	M	322	A1EB4	C45-C46-C47-C51
52	P	319	A1EB4	C45-C46-C47-C51
39	K	306	CLA	C3-C5-C6-C7
39	0	313	CLA	C3-C5-C6-C7
47	E	320	SQD	C7-C8-C9-C10
50	7	304	A1EB1	C42-C44-C45-C46
39	L	310	CLA	O1D-CGD-O2D-CED
45	C	314	DGD	C2D-C1D-O3G-C3G
45	C	314	DGD	C2E-C1E-O5D-C6D
46	D	322	LMG	C2-C1-O1-C7
46	4	325	LMG	C2-C1-O1-C7
47	F	319	SQD	O47-C45-C46-O48
39	b	830	CLA	CBA-CGA-O2A-C1
39	b	841	CLA	CBA-CGA-O2A-C1
39	R	316	CLA	CBA-CGA-O2A-C1
52	P	305	A1EB4	C43-C39-O3-C12
52	W	306	A1EB4	C43-C39-O3-C12
39	b	819	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
41	X	301	LHG	C11-C10-C9-C8
45	b	849	DGD	CEB-CFB-CGB-CHB
46	I	302	LMG	C12-C13-C14-C15
46	I	302	LMG	C33-C34-C35-C36
47	k	205	SQD	C11-C10-C9-C8
39	a	838	CLA	C5-C6-C7-C8
39	A	314	CLA	C8-C10-C11-C12
39	B	209	CLA	C5-C6-C7-C8
39	C	311	CLA	C5-C6-C7-C8
39	a	814	CLA	O1A-CGA-O2A-C1
39	b	809	CLA	O1A-CGA-O2A-C1
39	b	831	CLA	O1A-CGA-O2A-C1
39	P	316	CLA	O1A-CGA-O2A-C1
39	1	319	CLA	O1A-CGA-O2A-C1
39	3	311	CLA	O1A-CGA-O2A-C1
39	b	832	CLA	C16-C17-C18-C19
39	b	842	CLA	C16-C17-C18-C20
39	D	318	CLA	C16-C17-C18-C20
39	E	308	CLA	C16-C17-C18-C19
39	M	309	CLA	C16-C17-C18-C20
39	P	308	CLA	C16-C17-C18-C20
39	Q	310	CLA	C16-C17-C18-C20
39	W	309	CLA	C16-C17-C18-C19
39	b	834	CLA	O1D-CGD-O2D-CED
39	B	203	CLA	O1D-CGD-O2D-CED
39	B	207	CLA	O1D-CGD-O2D-CED
39	F	314	CLA	O1D-CGD-O2D-CED
45	C	314	DGD	O6E-C5E-C6E-O5E
41	a	840	LHG	C27-C28-C29-C30
46	I	302	LMG	C29-C30-C31-C32
39	D	311	CLA	C2-C3-C5-C6
39	h	201	CLA	C2-C3-C5-C6
39	a	801	CLA	C11-C12-C13-C14
39	a	816	CLA	C11-C10-C8-C9
39	b	828	CLA	C6-C7-C8-C9
39	f	802	CLA	C6-C7-C8-C9
39	i	103	CLA	C11-C10-C8-C9
39	K	307	CLA	C11-C10-C8-C9
39	Q	309	CLA	C11-C10-C8-C9
39	S	308	CLA	C11-C10-C8-C9
39	S	309	CLA	C11-C10-C8-C9
39	7	316	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
48	T	306	A86	C35-C34-O4-C38
48	3	307	A86	C35-C34-O4-C38
41	a	840	LHG	C23-C24-C25-C26
45	b	849	DGD	C4B-C5B-C6B-C7B
46	S	322	LMG	C14-C15-C16-C17
46	9	321	LMG	C32-C33-C34-C35
47	D	321	SQD	C9-C10-C11-C12
52	R	305	A1EB4	C43-C44-C45-C46
39	a	805	CLA	C15-C16-C17-C18
39	b	825	CLA	C10-C11-C12-C13
39	X	308	CLA	C5-C6-C7-C8
39	0	311	CLA	C5-C6-C7-C8
39	I	313	CLA	C10-C11-C12-C13
49	H	314	KC2	CAA-CBA-CGA-O1A
49	3	317	KC2	CAA-CBA-CGA-O2A
49	7	322	KC2	CAA-CBA-CGA-O1A
39	b	805	CLA	C2A-CAA-CBA-CGA
39	E	316	CLA	C2A-CAA-CBA-CGA
39	J	318	CLA	C2A-CAA-CBA-CGA
39	M	308	CLA	C2A-CAA-CBA-CGA
39	O	318	CLA	C2A-CAA-CBA-CGA
39	P	307	CLA	C2A-CAA-CBA-CGA
39	4	323	CLA	C2A-CAA-CBA-CGA
39	F	312	CLA	O1A-CGA-O2A-C1
39	Q	321	CLA	O1A-CGA-O2A-C1
39	4	316	CLA	O1A-CGA-O2A-C1
46	F	317	LMG	O10-C28-O8-C9
43	a	846	DD6	C12-C11-C13-C14
43	j	102	DD6	C7-C6-C8-C9
43	J	304	DD6	C12-C11-C13-C14
43	S	306	DD6	C12-C11-C13-C14
48	L	301	A86	C7-C6-C8-C9
48	L	306	A86	C7-C6-C8-C9
48	Q	305	A86	C-C1-C24-C25
48	4	328	A86	C-C1-C24-C25
48	6	305	A86	C-C1-C24-C25
50	1	305	A1EB1	C7-C6-C8-C9
46	7	326	LMG	C11-C12-C13-C14
41	j	104	LHG	O1-C1-C2-C3
41	D	301	LHG	O1-C1-C2-C3
41	H	317	LHG	O1-C1-C2-C3
41	X	301	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
43	j	102	DD6	C5-C6-C8-C9
43	J	304	DD6	C10-C11-C13-C14
43	P	304	DD6	C10-C11-C13-C14
43	S	306	DD6	C10-C11-C13-C14
48	L	301	A86	C5-C6-C8-C9
48	8	303	A86	C2-C1-C24-C25
48	6	305	A86	C2-C1-C24-C25
50	9	302	A1EB1	C5-C6-C8-C9
50	z	302	A1EB1	C5-C6-C8-C9
39	D	311	CLA	C3-C5-C6-C7
39	V	309	CLA	C3-C5-C6-C7
39	V	310	CLA	C3-C5-C6-C7
46	M	319	LMG	O6-C5-C6-O5
39	D	317	CLA	C8-C10-C11-C12
39	F	321	CLA	C8-C10-C11-C12
39	K	311	CLA	C10-C11-C12-C13
39	4	323	CLA	C10-C11-C12-C13
39	7	316	CLA	C13-C15-C16-C17
41	D	302	LHG	C8-C7-O7-C5
46	P	317	LMG	C33-C34-C35-C36
46	S	322	LMG	C18-C19-C20-C21
46	W	302	LMG	C33-C34-C35-C36
46	4	326	LMG	C16-C17-C18-C19
46	7	301	LMG	C16-C17-C18-C19
50	0	305	A1EB1	C44-C45-C46-C47
49	L	312	KC2	CBD-CGD-O2D-CED
41	D	301	LHG	C7-C8-C9-C10
47	T	321	SQD	C7-C8-C9-C10
50	V	302	A1EB1	C42-C44-C45-C46
50	3	309	A1EB1	C42-C44-C45-C46
39	J	316	CLA	O1D-CGD-O2D-CED
46	D	322	LMG	C32-C33-C34-C35
46	4	326	LMG	C29-C30-C31-C32
46	7	301	LMG	C29-C30-C31-C32
50	T	302	A1EB1	C44-C45-C46-C47
39	a	817	CLA	C4B-C3B-CAB-CBB
39	a	831	CLA	C4B-C3B-CAB-CBB
39	a	833	CLA	C4B-C3B-CAB-CBB
39	b	806	CLA	C4B-C3B-CAB-CBB
39	b	814	CLA	C4B-C3B-CAB-CBB
39	b	823	CLA	C4B-C3B-CAB-CBB
39	b	839	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	b	842	CLA	C4B-C3B-CAB-CBB
39	b	851	CLA	C4B-C3B-CAB-CBB
39	f	802	CLA	C4B-C3B-CAB-CBB
39	f	803	CLA	C4B-C3B-CAB-CBB
39	l	201	CLA	C4B-C3B-CAB-CBB
39	k	203	CLA	C4B-C3B-CAB-CBB
39	A	311	CLA	C4B-C3B-CAB-CBB
39	A	315	CLA	C4B-C3B-CAB-CBB
39	B	207	CLA	C4B-C3B-CAB-CBB
39	C	304	CLA	C4B-C3B-CAB-CBB
39	C	308	CLA	C4B-C3B-CAB-CBB
39	D	315	CLA	C4B-C3B-CAB-CBB
39	E	306	CLA	C4B-C3B-CAB-CBB
39	E	312	CLA	C4B-C3B-CAB-CBB
39	E	315	CLA	C4B-C3B-CAB-CBB
39	F	312	CLA	C4B-C3B-CAB-CBB
39	F	321	CLA	C4B-C3B-CAB-CBB
39	G	309	CLA	C4B-C3B-CAB-CBB
39	G	318	CLA	C4B-C3B-CAB-CBB
39	H	306	CLA	C4B-C3B-CAB-CBB
39	H	312	CLA	C4B-C3B-CAB-CBB
39	H	315	CLA	C4B-C3B-CAB-CBB
39	J	307	CLA	C4B-C3B-CAB-CBB
39	K	306	CLA	C4B-C3B-CAB-CBB
39	L	308	CLA	C4B-C3B-CAB-CBB
39	L	311	CLA	C4B-C3B-CAB-CBB
39	L	316	CLA	C4B-C3B-CAB-CBB
39	M	318	CLA	C4B-C3B-CAB-CBB
39	O	309	CLA	C4B-C3B-CAB-CBB
39	O	310	CLA	C4B-C3B-CAB-CBB
39	O	314	CLA	C4B-C3B-CAB-CBB
39	Q	317	CLA	C4B-C3B-CAB-CBB
39	R	311	CLA	C4B-C3B-CAB-CBB
39	T	319	CLA	C4B-C3B-CAB-CBB
39	U	201	CLA	C4B-C3B-CAB-CBB
39	U	210	CLA	C4B-C3B-CAB-CBB
39	U	213	CLA	C4B-C3B-CAB-CBB
39	W	313	CLA	C4B-C3B-CAB-CBB
39	W	319	CLA	C4B-C3B-CAB-CBB
39	X	311	CLA	C4B-C3B-CAB-CBB
39	0	310	CLA	C4B-C3B-CAB-CBB
39	1	311	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	1	319	CLA	C4B-C3B-CAB-CBB
39	3	311	CLA	C4B-C3B-CAB-CBB
39	3	320	CLA	C4B-C3B-CAB-CBB
39	3	323	CLA	C4B-C3B-CAB-CBB
39	4	313	CLA	C4B-C3B-CAB-CBB
39	7	315	CLA	C4B-C3B-CAB-CBB
39	7	325	CLA	C4B-C3B-CAB-CBB
39	8	321	CLA	C4B-C3B-CAB-CBB
39	9	307	CLA	C4B-C3B-CAB-CBB
39	9	319	CLA	C4B-C3B-CAB-CBB
39	x	317	CLA	C4B-C3B-CAB-CBB
39	y	310	CLA	C4B-C3B-CAB-CBB
39	z	308	CLA	C4B-C3B-CAB-CBB
39	Y	313	CLA	C4B-C3B-CAB-CBB
39	Z	306	CLA	C4B-C3B-CAB-CBB
39	Z	316	CLA	C4B-C3B-CAB-CBB
39	2	315	CLA	C4B-C3B-CAB-CBB
39	2	319	CLA	C4B-C3B-CAB-CBB
39	6	318	CLA	C4B-C3B-CAB-CBB
39	6	322	CLA	C4B-C3B-CAB-CBB
39	b	825	CLA	C16-C17-C18-C20
39	b	837	CLA	C11-C12-C13-C14
39	E	308	CLA	C16-C17-C18-C20
39	K	312	CLA	C16-C17-C18-C20
39	Q	312	CLA	C16-C17-C18-C19
39	V	313	CLA	C16-C17-C18-C19
39	9	308	CLA	C6-C7-C8-C9
39	9	308	CLA	C6-C7-C8-C10
45	C	314	DGD	O6D-C1D-O3G-C3G
45	C	314	DGD	O6E-C1E-O5D-C6D
39	b	811	CLA	C13-C15-C16-C17
48	8	303	A86	C35-C34-O4-C38
41	j	104	LHG	C9-C10-C11-C12
46	9	321	LMG	C30-C31-C32-C33
39	A	307	CLA	CBD-CGD-O2D-CED
39	O	310	CLA	CBD-CGD-O2D-CED
39	1	316	CLA	CBD-CGD-O2D-CED
39	D	311	CLA	O1D-CGD-O2D-CED
46	D	322	LMG	C12-C13-C14-C15
47	T	321	SQD	C24-C25-C26-C27
41	X	301	LHG	C7-C8-C9-C10
45	C	314	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
39	a	807	CLA	C5-C6-C7-C8
39	M	309	CLA	C5-C6-C7-C8
39	W	309	CLA	C15-C16-C17-C18
39	I	309	CLA	C13-C15-C16-C17
49	L	315	KC2	CAA-CBA-CGA-O1A
49	M	314	KC2	CAA-CBA-CGA-O2A
50	8	306	A1EB1	O43-C42-O6-C28
46	S	322	LMG	C19-C20-C21-C22
39	b	815	CLA	O1D-CGD-O2D-CED
39	o	205	CLA	O1D-CGD-O2D-CED
39	3	312	CLA	C3-C5-C6-C7
39	L	310	CLA	CBA-CGA-O2A-C1
39	T	309	CLA	CBA-CGA-O2A-C1
39	W	318	CLA	CBA-CGA-O2A-C1
39	7	313	CLA	CBA-CGA-O2A-C1
46	S	322	LMG	C29-C28-O8-C9
52	T	304	A1EB4	C43-C39-O3-C12
41	D	302	LHG	C11-C10-C9-C8
47	4	327	SQD	C10-C11-C12-C13
39	b	817	CLA	O1D-CGD-O2D-CED
39	a	804	CLA	C3A-C2A-CAA-CBA
39	a	830	CLA	C3A-C2A-CAA-CBA
39	a	834	CLA	C3A-C2A-CAA-CBA
39	b	815	CLA	C3A-C2A-CAA-CBA
39	b	827	CLA	C3A-C2A-CAA-CBA
39	b	837	CLA	C3A-C2A-CAA-CBA
39	f	803	CLA	C3A-C2A-CAA-CBA
39	l	201	CLA	C3A-C2A-CAA-CBA
39	D	317	CLA	C3A-C2A-CAA-CBA
39	E	318	CLA	C3A-C2A-CAA-CBA
39	F	314	CLA	C3A-C2A-CAA-CBA
39	G	312	CLA	C3A-C2A-CAA-CBA
39	M	318	CLA	C3A-C2A-CAA-CBA
39	M	321	CLA	C3A-C2A-CAA-CBA
39	Q	317	CLA	C3A-C2A-CAA-CBA
39	S	319	CLA	C3A-C2A-CAA-CBA
39	T	319	CLA	C3A-C2A-CAA-CBA
39	U	201	CLA	C3A-C2A-CAA-CBA
39	W	319	CLA	C3A-C2A-CAA-CBA
39	0	310	CLA	C3A-C2A-CAA-CBA
39	3	311	CLA	C3A-C2A-CAA-CBA
39	3	322	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	3	323	CLA	C3A-C2A-CAA-CBA
39	4	311	CLA	C3A-C2A-CAA-CBA
39	4	312	CLA	C3A-C2A-CAA-CBA
39	8	310	CLA	C3A-C2A-CAA-CBA
39	6	322	CLA	C3A-C2A-CAA-CBA
39	S	320	CLA	C10-C11-C12-C13
48	9	304	A86	C24-C25-C26-C27
46	F	317	LMG	C33-C34-C35-C36
46	S	322	LMG	C4-C5-C6-O5
46	4	326	LMG	C4-C5-C6-O5
46	7	301	LMG	C4-C5-C6-O5
39	C	307	CLA	O1A-CGA-O2A-C1
50	T	307	A1EB1	O43-C42-O6-C28
39	b	825	CLA	C16-C17-C18-C19
39	C	308	CLA	C11-C12-C13-C15
39	D	318	CLA	C16-C17-C18-C19
39	M	308	CLA	C16-C17-C18-C20
39	V	313	CLA	C16-C17-C18-C20
39	W	309	CLA	C16-C17-C18-C20
46	4	325	LMG	C11-C12-C13-C14
47	D	320	SQD	C26-C27-C28-C29
47	4	327	SQD	C9-C10-C11-C12
39	A	306	CLA	O1D-CGD-O2D-CED
41	X	301	LHG	O9-C7-O7-C5
39	b	842	CLA	CBD-CGD-O2D-CED
39	o	202	CLA	CBD-CGD-O2D-CED
39	H	312	CLA	CBD-CGD-O2D-CED
39	X	308	CLA	CBD-CGD-O2D-CED
49	5	305	KC2	CBD-CGD-O2D-CED
46	I	302	LMG	C36-C37-C38-C39
47	7	302	SQD	C11-C10-C9-C8
39	a	836	CLA	C3-C5-C6-C7
39	i	101	CLA	C3-C5-C6-C7
39	o	203	CLA	C3-C5-C6-C7
51	0	321	A1ECV	C2C-CMC-O2-C3
46	F	320	LMG	C10-C11-C12-C13
39	l	203	CLA	O1A-CGA-O2A-C1
39	b	815	CLA	C4-C3-C5-C6
39	K	308	CLA	C4-C3-C5-C6
39	A	312	CLA	CBA-CGA-O2A-C1
39	H	309	CLA	CBA-CGA-O2A-C1
39	j	101	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
39	K	308	CLA	C2-C3-C5-C6
39	O	310	CLA	C2-C3-C5-C6
46	A	316	LMG	C11-C10-O7-C8
46	F	320	LMG	C11-C10-O7-C8
49	9	316	KC2	CAA-CBA-CGA-O2A
39	S	308	CLA	O1D-CGD-O2D-CED
45	b	849	DGD	C4A-C5A-C6A-C7A
45	b	849	DGD	CDB-CEB-CFB-CGB
39	A	308	CLA	O1D-CGD-O2D-CED
39	b	825	CLA	C2A-CAA-CBA-CGA
39	b	835	CLA	C2A-CAA-CBA-CGA
41	j	104	LHG	O1-C1-C2-O2
41	D	302	LHG	O1-C1-C2-O2
46	4	326	LMG	C34-C35-C36-C37
39	o	201	CLA	O1A-CGA-O2A-C1
50	U	205	A1EB1	C42-C44-C45-C46
50	8	306	A1EB1	C42-C44-C45-C46
39	a	805	CLA	C16-C17-C18-C20
39	K	312	CLA	C16-C17-C18-C19
45	b	849	DGD	C7A-C8A-C9A-CAA
46	7	301	LMG	C34-C35-C36-C37
51	M	316	A1ECV	O1-CMC-O2-C3
39	J	316	CLA	O1A-CGA-O2A-C1
46	S	321	LMG	C4-C5-C6-O5
39	a	801	CLA	C2B-C3B-CAB-CBB
39	a	807	CLA	C2B-C3B-CAB-CBB
39	a	815	CLA	C2B-C3B-CAB-CBB
39	a	817	CLA	C2B-C3B-CAB-CBB
39	a	831	CLA	C2B-C3B-CAB-CBB
39	a	833	CLA	C2B-C3B-CAB-CBB
39	b	806	CLA	C2B-C3B-CAB-CBB
39	b	822	CLA	C2B-C3B-CAB-CBB
39	b	823	CLA	C2B-C3B-CAB-CBB
39	b	839	CLA	C2B-C3B-CAB-CBB
39	b	840	CLA	C2B-C3B-CAB-CBB
39	b	842	CLA	C2B-C3B-CAB-CBB
39	b	851	CLA	C2B-C3B-CAB-CBB
39	f	802	CLA	C2B-C3B-CAB-CBB
39	f	803	CLA	C2B-C3B-CAB-CBB
39	l	201	CLA	C2B-C3B-CAB-CBB
39	k	202	CLA	C2B-C3B-CAB-CBB
39	k	203	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	o	202	CLA	C2B-C3B-CAB-CBB
39	A	311	CLA	C2B-C3B-CAB-CBB
39	A	315	CLA	C2B-C3B-CAB-CBB
39	B	207	CLA	C2B-C3B-CAB-CBB
39	C	304	CLA	C2B-C3B-CAB-CBB
39	C	308	CLA	C2B-C3B-CAB-CBB
39	C	309	CLA	C2B-C3B-CAB-CBB
39	D	309	CLA	C2B-C3B-CAB-CBB
39	D	315	CLA	C2B-C3B-CAB-CBB
39	E	306	CLA	C2B-C3B-CAB-CBB
39	E	312	CLA	C2B-C3B-CAB-CBB
39	E	315	CLA	C2B-C3B-CAB-CBB
39	E	319	CLA	C2B-C3B-CAB-CBB
39	F	312	CLA	C2B-C3B-CAB-CBB
39	F	321	CLA	C2B-C3B-CAB-CBB
39	G	309	CLA	C2B-C3B-CAB-CBB
39	G	314	CLA	C2B-C3B-CAB-CBB
39	G	318	CLA	C2B-C3B-CAB-CBB
39	H	306	CLA	C2B-C3B-CAB-CBB
39	H	307	CLA	C2B-C3B-CAB-CBB
39	H	312	CLA	C2B-C3B-CAB-CBB
39	H	315	CLA	C2B-C3B-CAB-CBB
39	J	307	CLA	C2B-C3B-CAB-CBB
39	J	308	CLA	C2B-C3B-CAB-CBB
39	J	312	CLA	C2B-C3B-CAB-CBB
39	K	306	CLA	C2B-C3B-CAB-CBB
39	K	308	CLA	C2B-C3B-CAB-CBB
39	L	308	CLA	C2B-C3B-CAB-CBB
39	L	311	CLA	C2B-C3B-CAB-CBB
39	M	318	CLA	C2B-C3B-CAB-CBB
39	M	321	CLA	C2B-C3B-CAB-CBB
39	O	308	CLA	C2B-C3B-CAB-CBB
39	O	309	CLA	C2B-C3B-CAB-CBB
39	O	310	CLA	C2B-C3B-CAB-CBB
39	O	313	CLA	C2B-C3B-CAB-CBB
39	O	314	CLA	C2B-C3B-CAB-CBB
39	P	316	CLA	C2B-C3B-CAB-CBB
39	Q	317	CLA	C2B-C3B-CAB-CBB
39	R	311	CLA	C2B-C3B-CAB-CBB
39	R	315	CLA	C2B-C3B-CAB-CBB
39	S	308	CLA	C2B-C3B-CAB-CBB
39	T	318	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	T	319	CLA	C2B-C3B-CAB-CBB
39	U	201	CLA	C2B-C3B-CAB-CBB
39	U	210	CLA	C2B-C3B-CAB-CBB
39	U	213	CLA	C2B-C3B-CAB-CBB
39	U	215	CLA	C2B-C3B-CAB-CBB
39	W	313	CLA	C2B-C3B-CAB-CBB
39	W	318	CLA	C2B-C3B-CAB-CBB
39	W	319	CLA	C2B-C3B-CAB-CBB
39	X	311	CLA	C2B-C3B-CAB-CBB
39	X	316	CLA	C2B-C3B-CAB-CBB
39	0	310	CLA	C2B-C3B-CAB-CBB
39	0	318	CLA	C2B-C3B-CAB-CBB
39	0	320	CLA	C2B-C3B-CAB-CBB
39	0	323	CLA	C2B-C3B-CAB-CBB
39	1	310	CLA	C2B-C3B-CAB-CBB
39	1	311	CLA	C2B-C3B-CAB-CBB
39	1	317	CLA	C2B-C3B-CAB-CBB
39	1	319	CLA	C2B-C3B-CAB-CBB
39	3	311	CLA	C2B-C3B-CAB-CBB
39	3	316	CLA	C2B-C3B-CAB-CBB
39	3	320	CLA	C2B-C3B-CAB-CBB
39	3	323	CLA	C2B-C3B-CAB-CBB
39	4	311	CLA	C2B-C3B-CAB-CBB
39	7	313	CLA	C2B-C3B-CAB-CBB
39	7	315	CLA	C2B-C3B-CAB-CBB
39	7	325	CLA	C2B-C3B-CAB-CBB
39	8	318	CLA	C2B-C3B-CAB-CBB
39	8	321	CLA	C2B-C3B-CAB-CBB
39	9	307	CLA	C2B-C3B-CAB-CBB
39	9	312	CLA	C2B-C3B-CAB-CBB
39	9	319	CLA	C2B-C3B-CAB-CBB
39	I	313	CLA	C2B-C3B-CAB-CBB
39	x	306	CLA	C2B-C3B-CAB-CBB
39	x	317	CLA	C2B-C3B-CAB-CBB
39	y	307	CLA	C2B-C3B-CAB-CBB
39	y	310	CLA	C2B-C3B-CAB-CBB
39	y	318	CLA	C2B-C3B-CAB-CBB
39	z	306	CLA	C2B-C3B-CAB-CBB
39	z	308	CLA	C2B-C3B-CAB-CBB
39	Y	310	CLA	C2B-C3B-CAB-CBB
39	Y	311	CLA	C2B-C3B-CAB-CBB
39	Y	313	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	Y	314	CLA	C2B-C3B-CAB-CBB
39	Z	306	CLA	C2B-C3B-CAB-CBB
39	Z	313	CLA	C2B-C3B-CAB-CBB
39	Z	316	CLA	C2B-C3B-CAB-CBB
39	2	312	CLA	C2B-C3B-CAB-CBB
39	2	315	CLA	C2B-C3B-CAB-CBB
39	2	319	CLA	C2B-C3B-CAB-CBB
39	6	310	CLA	C2B-C3B-CAB-CBB
39	6	313	CLA	C2B-C3B-CAB-CBB
39	6	318	CLA	C2B-C3B-CAB-CBB
39	6	322	CLA	C2B-C3B-CAB-CBB
39	3	311	CLA	O1D-CGD-O2D-CED
39	a	822	CLA	C15-C16-C17-C18
47	H	318	SQD	C26-C27-C28-C29
39	J	309	CLA	C3-C5-C6-C7
39	R	308	CLA	C3-C5-C6-C7
39	X	308	CLA	C3-C5-C6-C7
46	M	320	LMG	C4-C5-C6-O5
39	a	806	CLA	O1A-CGA-O2A-C1
39	I	301	CLA	O1A-CGA-O2A-C1
48	Q	302	A86	C33-C34-O4-C38
48	7	308	A86	C35-C34-O4-C38
48	6	307	A86	C35-C34-O4-C38
39	C	307	CLA	C5-C6-C7-C8
39	0	313	CLA	C5-C6-C7-C8
41	a	840	LHG	O9-C7-O7-C5
46	F	320	LMG	O9-C10-O7-C8
49	K	313	KC2	CAA-CBA-CGA-O2A
39	1	319	CLA	C2-C1-O2A-CGA
45	b	849	DGD	C5A-C6A-C7A-C8A
47	S	301	SQD	C9-C10-C11-C12
47	7	302	SQD	C9-C10-C11-C12
48	Y	301	A86	O5-C38-O4-C34
50	D	308	A1EB1	C44-C45-C46-C47
50	0	303	A1EB1	C44-C45-C46-C47
39	b	820	CLA	C8-C10-C11-C12
39	b	825	CLA	C15-C16-C17-C18
39	C	307	CLA	C10-C11-C12-C13
39	J	310	CLA	C5-C6-C7-C8
39	K	311	CLA	C13-C15-C16-C17
40	b	843	PQN	C23-C25-C26-C27
39	b	830	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	b	841	CLA	O1A-CGA-O2A-C1
39	R	315	CLA	O1A-CGA-O2A-C1
39	W	318	CLA	O1A-CGA-O2A-C1
39	X	316	CLA	O1A-CGA-O2A-C1
39	7	313	CLA	O1A-CGA-O2A-C1
50	E	301	A1EB1	C44-C45-C46-C47
47	E	320	SQD	C23-C24-C25-C26
50	K	304	A1EB1	C42-C44-C45-C46
39	1	313	CLA	CBD-CGD-O2D-CED
39	W	319	CLA	O1A-CGA-O2A-C1
42	a	842	BCR	C23-C24-C25-C26
42	a	842	BCR	C23-C24-C25-C30
42	a	845	BCR	C23-C24-C25-C26
42	a	845	BCR	C23-C24-C25-C30
42	b	850	BCR	C23-C24-C25-C26
42	b	850	BCR	C23-C24-C25-C30
42	i	102	BCR	C23-C24-C25-C26
42	i	102	BCR	C23-C24-C25-C30
42	j	103	BCR	C23-C24-C25-C26
42	j	103	BCR	C23-C24-C25-C30
42	l	206	BCR	C23-C24-C25-C26
42	l	206	BCR	C23-C24-C25-C30
42	m	101	BCR	C23-C24-C25-C26
42	h	202	BCR	C1-C6-C7-C8
42	h	202	BCR	C5-C6-C7-C8
39	b	822	CLA	CBA-CGA-O2A-C1
39	b	835	CLA	CBA-CGA-O2A-C1
39	b	851	CLA	CBA-CGA-O2A-C1
39	M	308	CLA	CBA-CGA-O2A-C1
39	T	320	CLA	CBA-CGA-O2A-C1
39	3	316	CLA	CBA-CGA-O2A-C1
50	G	307	A1EB1	C44-C42-O6-C28
50	1	305	A1EB1	C44-C42-O6-C28
39	a	801	CLA	C8-C10-C11-C12
39	b	830	CLA	C5-C6-C7-C8
39	C	311	CLA	C10-C11-C12-C13
39	3	312	CLA	C15-C16-C17-C18
41	a	841	LHG	C8-C7-O7-C5
41	X	301	LHG	C11-C12-C13-C14
46	F	317	LMG	C12-C13-C14-C15
39	R	316	CLA	O1A-CGA-O2A-C1
52	P	305	A1EB4	O54-C39-O3-C12

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Mol	Chain	Res	Type	Atoms
52	T	304	A1EB4	O54-C39-O3-C12
52	W	306	A1EB4	O54-C39-O3-C12
39	C	310	CLA	CBD-CGD-O2D-CED
39	D	310	CLA	C14-C13-C15-C16
47	M	301	SQD	C23-C24-C25-C26
47	F	318	SQD	C9-C10-C11-C12
39	I	313	CLA	C8-C10-C11-C12
39	I	313	CLA	C15-C16-C17-C18
49	0	319	KC2	CAA-CBA-CGA-O1A
51	5	309	A1ECV	CAA-CBA-CGA-O2A
39	0	312	CLA	C5-C6-C7-C8
46	4	326	LMG	C22-C23-C24-C25
46	7	301	LMG	C22-C23-C24-C25
50	C	302	A1EB1	C39-C38-O4-C34
39	b	811	CLA	C4-C3-C5-C6
39	h	201	CLA	C4-C3-C5-C6
39	a	801	CLA	C11-C12-C13-C15
39	a	801	CLA	C12-C13-C15-C16
39	a	808	CLA	C2-C3-C5-C6
39	a	816	CLA	C11-C10-C8-C7
39	a	827	CLA	C11-C10-C8-C7
39	b	806	CLA	C12-C13-C15-C16
39	b	809	CLA	C6-C7-C8-C10
39	b	811	CLA	C2-C3-C5-C6
39	b	815	CLA	C2-C3-C5-C6
39	b	828	CLA	C6-C7-C8-C10
39	b	833	CLA	C6-C7-C8-C10
39	b	840	CLA	C6-C7-C8-C10
39	f	802	CLA	C6-C7-C8-C10
39	j	101	CLA	C6-C7-C8-C10
39	l	201	CLA	C6-C7-C8-C10
39	C	305	CLA	C6-C7-C8-C10
39	C	310	CLA	C12-C13-C15-C16
39	D	314	CLA	C12-C13-C15-C16
39	D	319	CLA	C12-C13-C15-C16
39	E	312	CLA	C11-C12-C13-C15
39	G	310	CLA	C11-C12-C13-C15
39	H	312	CLA	C11-C12-C13-C15
39	H	313	CLA	C11-C12-C13-C15
39	J	314	CLA	C11-C12-C13-C15
39	K	307	CLA	C11-C10-C8-C7
39	P	308	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
39	Q	309	CLA	C11-C10-C8-C7
39	S	309	CLA	C11-C10-C8-C7
39	U	207	CLA	C11-C10-C8-C7
39	W	311	CLA	C11-C12-C13-C15
39	3	311	CLA	C11-C12-C13-C15
39	4	311	CLA	C11-C10-C8-C7
39	4	316	CLA	C11-C12-C13-C15
39	I	313	CLA	C2-C3-C5-C6
39	I	313	CLA	C11-C12-C13-C15
39	a	824	CLA	C3-C5-C6-C7
39	A	312	CLA	O1A-CGA-O2A-C1
39	H	309	CLA	O1A-CGA-O2A-C1
39	L	310	CLA	O1A-CGA-O2A-C1
39	T	309	CLA	O1A-CGA-O2A-C1
46	S	322	LMG	O10-C28-O8-C9
46	4	325	LMG	O10-C28-O8-C9
50	G	307	A1EB1	O43-C42-O6-C28
47	M	301	SQD	C11-C10-C9-C8
50	6	304	A1EB1	O6-C42-C44-C45
39	b	810	CLA	C10-C11-C12-C13
39	b	829	CLA	C8-C10-C11-C12
39	f	802	CLA	C5-C6-C7-C8
39	K	311	CLA	C8-C10-C11-C12
39	V	310	CLA	C10-C11-C12-C13
50	Q	323	A1EB1	C24-C25-C26-C27
50	S	303	A1EB1	C3-C4-C5-C6
39	b	832	CLA	C16-C17-C18-C20
39	M	309	CLA	C16-C17-C18-C19
39	P	308	CLA	C16-C17-C18-C19
39	Q	310	CLA	C16-C17-C18-C19
48	S	307	A86	C35-C34-O4-C38
39	b	808	CLA	O1D-CGD-O2D-CED
49	T	312	KC2	O1D-CGD-O2D-CED
46	F	317	LMG	O9-C10-O7-C8
39	a	832	CLA	CBA-CGA-O2A-C1
39	b	805	CLA	CBA-CGA-O2A-C1
39	E	316	CLA	CBA-CGA-O2A-C1
39	L	309	CLA	CBA-CGA-O2A-C1
39	P	307	CLA	CBA-CGA-O2A-C1
39	0	315	CLA	CBA-CGA-O2A-C1
39	7	315	CLA	CBA-CGA-O2A-C1
50	U	205	A1EB1	C44-C42-O6-C28

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Mol	Chain	Res	Type	Atoms
50	7	303	A1EB1	C44-C42-O6-C28
39	a	810	CLA	C2A-CAA-CBA-CGA
39	a	811	CLA	C2A-CAA-CBA-CGA
39	a	814	CLA	C2A-CAA-CBA-CGA
39	b	820	CLA	C2A-CAA-CBA-CGA
39	b	829	CLA	C2A-CAA-CBA-CGA
39	L	319	CLA	C2A-CAA-CBA-CGA
39	7	314	CLA	C2A-CAA-CBA-CGA
39	9	308	CLA	C2A-CAA-CBA-CGA
39	2	308	CLA	C2A-CAA-CBA-CGA
39	a	811	CLA	O1D-CGD-O2D-CED
39	A	311	CLA	C8-C10-C11-C12
39	P	307	CLA	C15-C16-C17-C18
39	8	311	CLA	C5-C6-C7-C8
41	D	301	LHG	C9-C10-C11-C12
39	B	205	CLA	O1D-CGD-O2D-CED
39	J	308	CLA	O1D-CGD-O2D-CED
39	8	321	CLA	O1D-CGD-O2D-CED
39	D	310	CLA	C12-C13-C15-C16
50	x	301	A1EB1	C42-C44-C45-C46
39	a	819	CLA	O1D-CGD-O2D-CED
39	D	313	CLA	C10-C11-C12-C13
39	3	314	CLA	C10-C11-C12-C13
39	Z	313	CLA	C4C-C3C-CAC-CBC
41	j	104	LHG	C11-C10-C9-C8
49	A	313	KC2	C2B-C3B-CAB-CBB
49	B	208	KC2	C2C-C3C-CAC-CBC
49	G	315	KC2	C2C-C3C-CAC-CBC
49	Q	313	KC2	C2B-C3B-CAB-CBB
49	R	318	KC2	C2C-C3C-CAC-CBC
49	T	315	KC2	C2B-C3B-CAB-CBB
49	V	315	KC2	C2C-C3C-CAC-CBC
49	1	312	KC2	C2C-C3C-CAC-CBC
49	3	315	KC2	C2C-C3C-CAC-CBC
49	3	317	KC2	C2C-C3C-CAC-CBC
49	4	318	KC2	C2B-C3B-CAB-CBB
49	8	314	KC2	C2C-C3C-CAC-CBC
49	8	320	KC2	C2C-C3C-CAC-CBC
49	I	303	KC2	C2C-C3C-CAC-CBC
51	S	318	A1ECV	C2B-C3B-CAB-CBB
39	b	841	CLA	C3-C5-C6-C7
39	G	314	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	2	310	CLA	CBD-CGD-O2D-CED
39	a	823	CLA	C16-C17-C18-C20
39	U	210	CLA	C11-C12-C13-C14
46	D	322	LMG	C4-C5-C6-O5
47	D	321	SQD	O5-C1-O6-C44
39	b	803	CLA	C13-C15-C16-C17
39	l	204	CLA	C15-C16-C17-C18
46	0	324	LMG	C29-C30-C31-C32
47	D	321	SQD	C24-C25-C26-C27
39	E	318	CLA	O1A-CGA-O2A-C1
41	j	104	LHG	C7-C8-C9-C10
41	j	104	LHG	C23-C24-C25-C26
46	M	320	LMG	C28-C29-C30-C31
50	7	303	A1EB1	C42-C44-C45-C46
46	D	322	LMG	C11-C10-O7-C8
46	F	317	LMG	C11-C10-O7-C8
45	b	849	DGD	C3B-C4B-C5B-C6B
50	T	307	A1EB1	C44-C45-C46-C47
52	W	321	A1EB4	O43-C38-O4-C34
49	A	310	KC2	C4C-C3C-CAC-CBC
49	G	315	KC2	C4C-C3C-CAC-CBC
49	L	321	KC2	C4B-C3B-CAB-CBB
49	M	311	KC2	C4C-C3C-CAC-CBC
49	M	313	KC2	C4C-C3C-CAC-CBC
49	M	314	KC2	C4B-C3B-CAB-CBB
49	M	314	KC2	C4C-C3C-CAC-CBC
49	P	312	KC2	C4C-C3C-CAC-CBC
49	P	313	KC2	C4B-C3B-CAB-CBB
49	Q	313	KC2	C4B-C3B-CAB-CBB
49	Q	313	KC2	C4C-C3C-CAC-CBC
49	R	312	KC2	C4C-C3C-CAC-CBC
49	R	318	KC2	C4C-C3C-CAC-CBC
49	T	314	KC2	C4B-C3B-CAB-CBB
49	V	315	KC2	C4C-C3C-CAC-CBC
49	W	314	KC2	C4C-C3C-CAC-CBC
49	X	306	KC2	C4C-C3C-CAC-CBC
49	X	312	KC2	C4C-C3C-CAC-CBC
49	0	314	KC2	C4C-C3C-CAC-CBC
49	1	314	KC2	C4C-C3C-CAC-CBC
49	4	318	KC2	C4C-C3C-CAC-CBC
49	8	314	KC2	C4C-C3C-CAC-CBC
49	8	316	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
49	I	303	KC2	C4C-C3C-CAC-CBC
49	x	312	KC2	C4C-C3C-CAC-CBC
49	z	312	KC2	C4C-C3C-CAC-CBC
49	2	313	KC2	C4C-C3C-CAC-CBC
49	6	314	KC2	C4C-C3C-CAC-CBC
49	6	317	KC2	C4B-C3B-CAB-CBB
51	9	314	A1ECV	C4B-C3B-CAB-CBB
39	D	316	CLA	C8-C10-C11-C12
39	R	309	CLA	C5-C6-C7-C8
39	E	313	CLA	CBD-CGD-O2D-CED
39	M	308	CLA	CBD-CGD-O2D-CED
51	X	310	A1ECV	CBD-CGD-O2D-CED
50	1	305	A1EB1	O43-C42-O6-C28
39	b	825	CLA	C3-C5-C6-C7
46	S	322	LMG	C29-C30-C31-C32
41	j	104	LHG	O7-C5-C6-O8
45	b	849	DGD	O2G-C2G-C3G-O3G
45	C	314	DGD	O1G-C1G-C2G-O2G
46	S	321	LMG	O7-C8-C9-O8
47	4	327	SQD	O6-C44-C45-O47
49	A	313	KC2	CAA-CBA-CGA-O1A
49	x	315	KC2	CAA-CBA-CGA-O1A
39	b	851	CLA	O1A-CGA-O2A-C1
39	E	310	CLA	C16-C17-C18-C19
39	I	311	CLA	C16-C17-C18-C19
39	a	808	CLA	C4-C3-C5-C6
39	b	851	CLA	C4-C3-C5-C6
39	j	101	CLA	C4-C3-C5-C6
41	D	302	LHG	C7-C8-C9-C10
39	a	805	CLA	C2-C3-C5-C6
39	a	816	CLA	C2-C3-C5-C6
39	D	310	CLA	C2-C3-C5-C6
39	X	317	CLA	C2-C3-C5-C6
43	a	846	DD6	C27-C29-C30-C31
43	H	303	DD6	C27-C29-C30-C31
43	H	305	DD6	C27-C29-C30-C31
43	J	305	DD6	C27-C29-C30-C31
43	T	303	DD6	C27-C29-C30-C31
43	4	307	DD6	C27-C29-C30-C31
43	5	303	DD6	C27-C29-C30-C31
43	I	306	DD6	C27-C29-C30-C31
47	7	302	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
39	a	804	CLA	C11-C10-C8-C9
39	a	808	CLA	C6-C7-C8-C9
39	a	822	CLA	C11-C10-C8-C9
39	a	823	CLA	C11-C10-C8-C9
39	a	825	CLA	C11-C10-C8-C9
39	a	827	CLA	C11-C10-C8-C9
39	a	836	CLA	C14-C13-C15-C16
39	a	837	CLA	C14-C13-C15-C16
39	a	847	CLA	C14-C13-C15-C16
39	b	833	CLA	C6-C7-C8-C9
39	l	204	CLA	C14-C13-C15-C16
39	A	314	CLA	C14-C13-C15-C16
39	C	305	CLA	C11-C10-C8-C9
39	D	311	CLA	C11-C12-C13-C14
39	G	310	CLA	C11-C12-C13-C14
39	H	313	CLA	C11-C12-C13-C14
39	J	311	CLA	C6-C7-C8-C9
39	M	310	CLA	C11-C12-C13-C14
39	P	309	CLA	C11-C12-C13-C14
39	U	207	CLA	C11-C10-C8-C9
39	U	211	CLA	C11-C10-C8-C9
39	3	311	CLA	C11-C12-C13-C14
39	3	314	CLA	C6-C7-C8-C9
39	4	311	CLA	C11-C10-C8-C9
39	4	311	CLA	C11-C12-C13-C14
39	I	313	CLA	C11-C12-C13-C14
39	T	309	CLA	O1D-CGD-O2D-CED
39	4	311	CLA	O1D-CGD-O2D-CED
49	P	313	KC2	O1D-CGD-O2D-CED
50	0	307	A1EB1	C35-C34-O4-C38
41	X	301	LHG	C12-C13-C14-C15
39	a	804	CLA	C3-C5-C6-C7
39	b	802	CLA	C2A-CAA-CBA-CGA
39	b	807	CLA	C2A-CAA-CBA-CGA
39	b	816	CLA	C2A-CAA-CBA-CGA
39	B	207	CLA	C2A-CAA-CBA-CGA
39	C	307	CLA	C2A-CAA-CBA-CGA
39	C	311	CLA	C2A-CAA-CBA-CGA
39	F	316	CLA	C2A-CAA-CBA-CGA
39	H	312	CLA	C2A-CAA-CBA-CGA
39	K	307	CLA	C2A-CAA-CBA-CGA
39	Q	321	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
39	T	309	CLA	C2A-CAA-CBA-CGA
39	U	207	CLA	C2A-CAA-CBA-CGA
39	9	319	CLA	C2A-CAA-CBA-CGA
39	I	311	CLA	C2A-CAA-CBA-CGA
46	4	326	LMG	C18-C19-C20-C21
46	7	301	LMG	C18-C19-C20-C21
47	H	318	SQD	C27-C28-C29-C30
43	J	306	DD6	C12-C11-C13-C14
48	Z	301	A86	C-C1-C24-C25
39	a	826	CLA	O1D-CGD-O2D-CED
46	I	302	LMG	C35-C36-C37-C38
43	J	306	DD6	C10-C11-C13-C14
48	G	301	A86	C5-C6-C8-C9
39	b	822	CLA	O1A-CGA-O2A-C1
39	b	835	CLA	O1A-CGA-O2A-C1
39	M	308	CLA	O1A-CGA-O2A-C1
39	T	320	CLA	O1A-CGA-O2A-C1
39	7	315	CLA	O1A-CGA-O2A-C1
47	E	320	SQD	O10-C23-O48-C46
50	7	303	A1EB1	O43-C42-O6-C28
39	a	804	CLA	C1A-C2A-CAA-CBA
39	a	806	CLA	C1A-C2A-CAA-CBA
39	a	809	CLA	C1A-C2A-CAA-CBA
39	a	817	CLA	C1A-C2A-CAA-CBA
39	a	830	CLA	C1A-C2A-CAA-CBA
39	a	834	CLA	C1A-C2A-CAA-CBA
39	b	809	CLA	C1A-C2A-CAA-CBA
39	b	818	CLA	C1A-C2A-CAA-CBA
39	b	824	CLA	C1A-C2A-CAA-CBA
39	b	827	CLA	C1A-C2A-CAA-CBA
39	f	803	CLA	C1A-C2A-CAA-CBA
39	l	201	CLA	C1A-C2A-CAA-CBA
39	l	204	CLA	C1A-C2A-CAA-CBA
39	o	205	CLA	C1A-C2A-CAA-CBA
39	A	307	CLA	C1A-C2A-CAA-CBA
39	B	203	CLA	C1A-C2A-CAA-CBA
39	C	310	CLA	C1A-C2A-CAA-CBA
39	C	311	CLA	C1A-C2A-CAA-CBA
39	D	316	CLA	C1A-C2A-CAA-CBA
39	E	313	CLA	C1A-C2A-CAA-CBA
39	G	309	CLA	C1A-C2A-CAA-CBA
39	G	318	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	H	313	CLA	C1A-C2A-CAA-CBA
39	J	314	CLA	C1A-C2A-CAA-CBA
39	L	320	CLA	C1A-C2A-CAA-CBA
39	M	318	CLA	C1A-C2A-CAA-CBA
39	M	321	CLA	C1A-C2A-CAA-CBA
39	O	310	CLA	C1A-C2A-CAA-CBA
39	O	314	CLA	C1A-C2A-CAA-CBA
39	P	311	CLA	C1A-C2A-CAA-CBA
39	Q	310	CLA	C1A-C2A-CAA-CBA
39	Q	317	CLA	C1A-C2A-CAA-CBA
39	S	308	CLA	C1A-C2A-CAA-CBA
39	S	309	CLA	C1A-C2A-CAA-CBA
39	S	313	CLA	C1A-C2A-CAA-CBA
39	T	313	CLA	C1A-C2A-CAA-CBA
39	T	319	CLA	C1A-C2A-CAA-CBA
39	U	201	CLA	C1A-C2A-CAA-CBA
39	W	319	CLA	C1A-C2A-CAA-CBA
39	0	322	CLA	C1A-C2A-CAA-CBA
39	1	319	CLA	C1A-C2A-CAA-CBA
39	3	311	CLA	C1A-C2A-CAA-CBA
39	3	312	CLA	C1A-C2A-CAA-CBA
39	3	323	CLA	C1A-C2A-CAA-CBA
39	4	322	CLA	C1A-C2A-CAA-CBA
39	8	311	CLA	C1A-C2A-CAA-CBA
39	9	308	CLA	C1A-C2A-CAA-CBA
39	9	319	CLA	C1A-C2A-CAA-CBA
39	2	308	CLA	C1A-C2A-CAA-CBA
39	2	319	CLA	C1A-C2A-CAA-CBA
39	a	805	CLA	C16-C17-C18-C19
39	a	823	CLA	C16-C17-C18-C19
39	a	847	CLA	C16-C17-C18-C20
47	F	319	SQD	O49-C7-O47-C45
47	W	301	SQD	C8-C7-O47-C45
49	y	313	KC2	CAA-CBA-CGA-O2A
51	5	309	A1ECV	CAA-CBA-CGA-O1A
46	l	208	LMG	C33-C34-C35-C36
50	C	302	A1EB1	C24-C25-C26-C27
50	V	302	A1EB1	C24-C25-C26-C27
50	8	306	A1EB1	C24-C25-C26-C27
39	b	842	CLA	C13-C15-C16-C17
39	D	319	CLA	C13-C15-C16-C17
39	O	314	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
39	P	308	CLA	C13-C15-C16-C17
39	V	311	CLA	C8-C10-C11-C12
41	H	317	LHG	C3-O3-P-O6
50	K	305	A1EB1	C42-C44-C45-C46
39	F	309	CLA	CBD-CGD-O2D-CED
49	4	320	KC2	CBD-CGD-O2D-CED
39	L	309	CLA	O1A-CGA-O2A-C1
39	a	836	CLA	C10-C11-C12-C13
39	a	815	CLA	CBA-CGA-O2A-C1
39	Q	309	CLA	CBA-CGA-O2A-C1
50	K	304	A1EB1	C44-C42-O6-C28
41	j	104	LHG	O6-C4-C5-C6
41	X	301	LHG	O6-C4-C5-C6
39	T	319	CLA	O1A-CGA-O2A-C1
47	T	321	SQD	C23-C24-C25-C26
50	V	305	A1EB1	C42-C44-C45-C46
50	6	308	A1EB1	C42-C44-C45-C46
39	o	206	CLA	O1D-CGD-O2D-CED
41	a	840	LHG	C32-C33-C34-C35
48	6	302	A86	C35-C34-O4-C38
46	S	322	LMG	C22-C23-C24-C25
39	b	841	CLA	O1D-CGD-O2D-CED
49	C	312	KC2	CAA-CBA-CGA-O2A
49	T	316	KC2	CAA-CBA-CGA-O2A
41	D	302	LHG	C10-C11-C12-C13
39	a	830	CLA	C5-C6-C7-C8
39	Q	310	CLA	C8-C10-C11-C12
52	P	305	A1EB4	C10-C11-C12-O3
52	T	304	A1EB4	C10-C11-C12-O3
52	W	306	A1EB4	C10-C11-C12-O3
52	X	305	A1EB4	C10-C11-C12-O3
46	S	322	LMG	C28-C29-C30-C31
39	a	824	CLA	CBA-CGA-O2A-C1
39	b	812	CLA	CBA-CGA-O2A-C1
39	B	207	CLA	CBA-CGA-O2A-C1
39	a	816	CLA	C4-C3-C5-C6
45	b	849	DGD	C6A-C7A-C8A-C9A
39	a	821	CLA	O1D-CGD-O2D-CED
45	b	849	DGD	CAB-CBB-CCB-CDB
39	a	832	CLA	O1A-CGA-O2A-C1
39	b	805	CLA	O1A-CGA-O2A-C1
39	P	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	0	315	CLA	O1A-CGA-O2A-C1
39	3	316	CLA	O1A-CGA-O2A-C1
41	D	302	LHG	C14-C15-C16-C17
45	b	849	DGD	C2B-C3B-C4B-C5B
46	F	320	LMG	C15-C16-C17-C18
47	D	320	SQD	C28-C29-C30-C31
39	a	828	CLA	C2A-CAA-CBA-CGA
39	S	309	CLA	C2A-CAA-CBA-CGA
39	D	319	CLA	C16-C17-C18-C20
39	2	312	CLA	O1D-CGD-O2D-CED
39	b	833	CLA	C3-C5-C6-C7
41	j	104	LHG	C4-C5-C6-O8
41	X	301	LHG	C4-C5-C6-O8
46	l	208	LMG	O1-C7-C8-C9
46	A	316	LMG	O1-C7-C8-C9
46	F	317	LMG	O1-C7-C8-C9
46	F	317	LMG	C7-C8-C9-O8
46	F	320	LMG	C7-C8-C9-O8
46	M	319	LMG	C7-C8-C9-O8
46	S	322	LMG	C7-C8-C9-O8
46	0	324	LMG	O1-C7-C8-C9
46	0	324	LMG	C7-C8-C9-O8
46	7	326	LMG	C7-C8-C9-O8
47	D	320	SQD	O6-C44-C45-C46
47	D	321	SQD	C44-C45-C46-O48
47	F	319	SQD	C44-C45-C46-O48
47	S	301	SQD	O6-C44-C45-C46
47	4	327	SQD	O6-C44-C45-C46
47	9	322	SQD	O6-C44-C45-C46
51	Q	319	A1ECV	CAA-CBA-CGA-O1A
46	A	316	LMG	O6-C5-C6-O5
39	K	309	CLA	C10-C11-C12-C13
39	E	316	CLA	O1A-CGA-O2A-C1
46	A	316	LMG	C8-C7-O1-C1
46	0	324	LMG	C8-C7-O1-C1
39	4	319	CLA	O1D-CGD-O2D-CED
39	R	309	CLA	C8-C10-C11-C12
39	U	207	CLA	C5-C6-C7-C8
39	B	207	CLA	CAA-CBA-CGA-O2A
39	b	837	CLA	O1D-CGD-O2D-CED
50	C	302	A1EB1	C42-C44-C45-C46
39	J	313	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	W	309	CLA	C8-C10-C11-C12
39	D	310	CLA	CBD-CGD-O2D-CED
39	E	310	CLA	CBD-CGD-O2D-CED
49	S	315	KC2	CBD-CGD-O2D-CED
49	V	314	KC2	CBD-CGD-O2D-CED
41	a	840	LHG	O1-C1-C2-O2
41	X	301	LHG	O1-C1-C2-O2
50	D	308	A1EB1	C45-C46-C47-C48
49	R	318	KC2	CAA-CBA-CGA-O2A
49	9	318	KC2	CAA-CBA-CGA-O2A
51	Q	319	A1ECV	CAA-CBA-CGA-O2A
48	8	302	A86	C33-C34-O4-C38
50	3	324	A1EB1	C35-C34-O4-C38
50	6	306	A1EB1	C33-C34-O4-C38
39	L	310	CLA	C5-C6-C7-C8
50	U	205	A1EB1	O43-C42-O6-C28
46	W	320	LMG	C10-C11-C12-C13
39	k	201	CLA	O1D-CGD-O2D-CED
46	W	320	LMG	O6-C5-C6-O5
39	a	805	CLA	C4-C3-C5-C6
46	7	326	LMG	C12-C13-C14-C15
49	B	208	KC2	C2A-CAA-CBA-CGA
49	P	313	KC2	C2A-CAA-CBA-CGA
49	T	314	KC2	C2A-CAA-CBA-CGA
49	8	319	KC2	C2A-CAA-CBA-CGA
39	j	101	CLA	C16-C17-C18-C20
39	k	203	CLA	C6-C7-C8-C9
39	b	818	CLA	CBA-CGA-O2A-C1
39	D	319	CLA	CBA-CGA-O2A-C1
39	8	311	CLA	CBA-CGA-O2A-C1
47	4	327	SQD	C24-C23-O48-C46
52	M	322	A1EB4	C43-C39-O3-C12
52	P	319	A1EB4	C43-C39-O3-C12
39	H	307	CLA	CBD-CGD-O2D-CED
39	3	319	CLA	CBD-CGD-O2D-CED
39	a	809	CLA	C10-C11-C12-C13
39	a	847	CLA	C10-C11-C12-C13
39	i	103	CLA	C8-C10-C11-C12
39	D	319	CLA	C8-C10-C11-C12
39	M	312	CLA	C13-C15-C16-C17
39	S	309	CLA	O1D-CGD-O2D-CED
39	F	310	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
41	D	302	LHG	C6-C5-O7-C7
47	F	318	SQD	C44-C45-O47-C7
47	P	301	SQD	C46-C45-O47-C7
51	y	311	A1ECV	O1D-CGD-O2D-CED
39	a	806	CLA	C2A-CAA-CBA-CGA
39	L	308	CLA	C2A-CAA-CBA-CGA
49	G	317	KC2	CAA-CBA-CGA-O2A
49	5	314	KC2	CAA-CBA-CGA-O1A
39	b	832	CLA	C15-C16-C17-C18
39	P	307	CLA	C10-C11-C12-C13
39	I	308	CLA	C5-C6-C7-C8
39	b	807	CLA	C2-C1-O2A-CGA
39	C	305	CLA	O1D-CGD-O2D-CED
47	M	301	SQD	C11-C12-C13-C14
47	7	302	SQD	C12-C13-C14-C15
39	M	308	CLA	C8-C10-C11-C12
41	X	301	LHG	C15-C16-C17-C18
52	W	321	A1EB4	C46-C47-C51-C55
39	b	838	CLA	CBA-CGA-O2A-C1
39	T	313	CLA	CBA-CGA-O2A-C1
41	X	301	LHG	C24-C23-O8-C6
50	G	304	A1EB1	C44-C42-O6-C28
39	6	310	CLA	O1D-CGD-O2D-CED
39	j	101	CLA	C16-C17-C18-C19
39	E	314	CLA	C5-C6-C7-C8
39	O	310	CLA	C8-C10-C11-C12
49	8	317	KC2	O1D-CGD-O2D-CED
39	a	815	CLA	O1A-CGA-O2A-C1
39	b	812	CLA	O1A-CGA-O2A-C1
50	L	303	A1EB1	C44-C45-C46-C47
39	b	819	CLA	CBD-CGD-O2D-CED
49	S	315	KC2	CAA-CBA-CGA-O1A
49	8	320	KC2	CAA-CBA-CGA-O2A
39	j	101	CLA	C15-C16-C17-C18
39	F	312	CLA	C10-C11-C12-C13
39	F	313	CLA	C5-C6-C7-C8
39	Q	310	CLA	C10-C11-C12-C13
41	X	301	LHG	O7-C5-C6-O8
46	F	317	LMG	O7-C8-C9-O8
46	F	320	LMG	O7-C8-C9-O8
46	M	319	LMG	O1-C7-C8-O7
46	7	326	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
48	0	309	A86	C33-C34-O4-C38
46	I	302	LMG	C30-C31-C32-C33
45	b	849	DGD	O1B-C1B-O2G-C2G
39	b	806	CLA	C8-C10-C11-C12
39	P	308	CLA	C8-C10-C11-C12
39	a	824	CLA	O1A-CGA-O2A-C1
39	B	207	CLA	O1A-CGA-O2A-C1
39	S	320	CLA	C16-C17-C18-C19
39	U	210	CLA	C11-C12-C13-C15
51	E	311	A1ECV	CHA-CBD-CGD-O1D
51	0	321	A1ECV	CHA-CBD-CGD-O1D
51	0	321	A1ECV	CHA-CBD-CGD-O2D
46	S	321	LMG	C11-C12-C13-C14
50	y	302	A1EB1	C42-C44-C45-C46
39	A	309	CLA	C4-C3-C5-C6
39	I	314	CLA	C4-C3-C5-C6
47	H	318	SQD	C29-C30-C31-C32
39	K	312	CLA	O1D-CGD-O2D-CED
39	a	804	CLA	C12-C13-C15-C16
39	a	811	CLA	C11-C12-C13-C15
39	a	816	CLA	C11-C12-C13-C15
39	a	822	CLA	C11-C10-C8-C7
39	a	823	CLA	C11-C10-C8-C7
39	a	825	CLA	C11-C10-C8-C7
39	a	826	CLA	C12-C13-C15-C16
39	a	830	CLA	C6-C7-C8-C10
39	a	830	CLA	C11-C12-C13-C15
39	a	836	CLA	C12-C13-C15-C16
39	a	837	CLA	C12-C13-C15-C16
39	a	847	CLA	C12-C13-C15-C16
39	b	801	CLA	C11-C12-C13-C15
39	b	803	CLA	C11-C10-C8-C7
39	b	816	CLA	C11-C10-C8-C7
39	b	832	CLA	C11-C12-C13-C15
39	b	835	CLA	C11-C10-C8-C7
39	b	840	CLA	C11-C10-C8-C7
39	b	841	CLA	C11-C10-C8-C7
39	b	841	CLA	C11-C12-C13-C15
39	l	204	CLA	C12-C13-C15-C16
39	A	306	CLA	C11-C12-C13-C15
39	A	311	CLA	C11-C12-C13-C15
39	C	305	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
39	C	311	CLA	C12-C13-C15-C16
39	D	310	CLA	C6-C7-C8-C10
39	D	311	CLA	C12-C13-C15-C16
39	D	315	CLA	C11-C12-C13-C15
39	D	317	CLA	C6-C7-C8-C10
39	D	318	CLA	C12-C13-C15-C16
39	E	307	CLA	C12-C13-C15-C16
39	F	321	CLA	C11-C10-C8-C7
39	F	321	CLA	C11-C12-C13-C15
39	G	309	CLA	C6-C7-C8-C10
39	K	311	CLA	C12-C13-C15-C16
39	M	309	CLA	C11-C12-C13-C15
39	R	309	CLA	C12-C13-C15-C16
39	U	211	CLA	C11-C10-C8-C7
39	V	311	CLA	C11-C10-C8-C7
39	W	311	CLA	C12-C13-C15-C16
39	X	309	CLA	C11-C12-C13-C15
39	0	310	CLA	C11-C10-C8-C7
39	3	314	CLA	C6-C7-C8-C10
39	3	314	CLA	C11-C12-C13-C15
39	4	312	CLA	C11-C10-C8-C7
39	4	314	CLA	C11-C12-C13-C15
39	4	316	CLA	C11-C10-C8-C7
39	7	313	CLA	C6-C7-C8-C10
39	7	316	CLA	C6-C7-C8-C10
39	I	313	CLA	C12-C13-C15-C16
39	a	801	CLA	CAA-CBA-CGA-O2A
39	i	103	CLA	C3-C5-C6-C7
39	H	310	CLA	C3-C5-C6-C7
39	Q	309	CLA	O1A-CGA-O2A-C1
39	K	308	CLA	C11-C12-C13-C14
48	X	303	A86	O5-C38-O4-C34
39	a	804	CLA	C14-C13-C15-C16
39	a	805	CLA	C14-C13-C15-C16
39	a	806	CLA	C14-C13-C15-C16
39	a	809	CLA	C11-C10-C8-C9
39	a	816	CLA	C11-C12-C13-C14
39	a	826	CLA	C14-C13-C15-C16
39	a	830	CLA	C6-C7-C8-C9
39	a	830	CLA	C11-C12-C13-C14
39	a	838	CLA	C11-C12-C13-C14
39	a	847	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
39	b	803	CLA	C11-C10-C8-C9
39	b	810	CLA	C14-C13-C15-C16
39	b	816	CLA	C11-C10-C8-C9
39	b	827	CLA	C14-C13-C15-C16
39	b	832	CLA	C11-C12-C13-C14
39	b	833	CLA	C14-C13-C15-C16
39	b	835	CLA	C11-C10-C8-C9
39	b	835	CLA	C14-C13-C15-C16
39	b	840	CLA	C11-C10-C8-C9
39	b	841	CLA	C11-C10-C8-C9
39	b	841	CLA	C11-C12-C13-C14
39	i	103	CLA	C11-C12-C13-C14
39	A	306	CLA	C11-C12-C13-C14
39	A	311	CLA	C14-C13-C15-C16
39	C	310	CLA	C11-C12-C13-C14
39	C	311	CLA	C14-C13-C15-C16
39	D	310	CLA	C6-C7-C8-C9
39	D	315	CLA	C11-C12-C13-C14
39	D	317	CLA	C6-C7-C8-C9
39	D	319	CLA	C11-C10-C8-C9
39	E	307	CLA	C6-C7-C8-C9
39	E	307	CLA	C11-C12-C13-C14
39	E	307	CLA	C14-C13-C15-C16
39	E	312	CLA	C11-C12-C13-C14
39	F	321	CLA	C11-C10-C8-C9
39	H	308	CLA	C11-C10-C8-C9
39	H	312	CLA	C11-C12-C13-C14
39	K	308	CLA	C6-C7-C8-C9
39	K	309	CLA	C6-C7-C8-C9
39	P	308	CLA	C6-C7-C8-C9
39	P	308	CLA	C11-C10-C8-C9
39	R	309	CLA	C14-C13-C15-C16
39	V	311	CLA	C11-C10-C8-C9
39	X	308	CLA	C11-C10-C8-C9
39	X	309	CLA	C11-C10-C8-C9
39	0	310	CLA	C11-C10-C8-C9
39	3	312	CLA	C11-C10-C8-C9
39	3	312	CLA	C14-C13-C15-C16
39	4	312	CLA	C11-C10-C8-C9
39	4	316	CLA	C11-C10-C8-C9
39	7	316	CLA	C11-C12-C13-C14
39	I	308	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
39	I	313	CLA	C14-C13-C15-C16
40	a	839	PQN	C24-C23-C25-C26
39	b	835	CLA	O1D-CGD-O2D-CED
50	9	302	A1EB1	C1-C2-C3-C4
39	7	313	CLA	CBD-CGD-O2D-CED
49	Y	308	KC2	CBD-CGD-O2D-CED
48	G	301	A86	C35-C34-O4-C38
50	0	305	A1EB1	C33-C34-O4-C38
46	F	317	LMG	C31-C32-C33-C34
39	a	811	CLA	CBA-CGA-O2A-C1
39	E	309	CLA	CBA-CGA-O2A-C1
39	a	815	CLA	C8-C10-C11-C12
39	M	318	CLA	CBA-CGA-O2A-C1
39	b	808	CLA	C2A-CAA-CBA-CGA
39	A	314	CLA	C2A-CAA-CBA-CGA
47	M	301	SQD	C12-C13-C14-C15
50	K	304	A1EB1	O43-C42-O6-C28
43	G	306	DD6	C12-C11-C13-C14
43	O	305	DD6	C12-C11-C13-C14
48	4	328	A86	C7-C6-C8-C9
48	Z	303	A86	C-C1-C24-C25
50	H	301	A1EB1	C7-C6-C8-C9
50	H	304	A1EB1	C7-C6-C8-C9
52	T	304	A1EB4	C-C1-C24-C25
39	b	842	CLA	C16-C17-C18-C19
39	k	203	CLA	C6-C7-C8-C10
39	D	319	CLA	C16-C17-C18-C19
43	G	306	DD6	C10-C11-C13-C14
48	P	302	A86	C2-C1-C24-C25
48	4	328	A86	C5-C6-C8-C9
48	Z	303	A86	C2-C1-C24-C25
50	7	303	A1EB1	C5-C6-C8-C9
46	W	320	LMG	C30-C31-C32-C33
47	D	321	SQD	C25-C26-C27-C28
39	O	310	CLA	C3-C5-C6-C7
39	D	309	CLA	O1D-CGD-O2D-CED
39	a	826	CLA	C15-C16-C17-C18
39	5	306	CLA	C13-C15-C16-C17
50	G	304	A1EB1	O43-C42-O6-C28
39	b	842	CLA	CBA-CGA-O2A-C1
39	j	101	CLA	CBA-CGA-O2A-C1
39	J	307	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
39	L	311	CLA	CBA-CGA-O2A-C1
39	M	312	CLA	CBA-CGA-O2A-C1
39	Q	310	CLA	CBA-CGA-O2A-C1
39	I	314	CLA	CBA-CGA-O2A-C1
39	b	810	CLA	C15-C16-C17-C18
39	b	815	CLA	C10-C11-C12-C13
39	b	841	CLA	C10-C11-C12-C13
39	C	311	CLA	C13-C15-C16-C17
39	5	310	CLA	O1D-CGD-O2D-CED
49	F	307	KC2	CAA-CBA-CGA-O2A
49	X	318	KC2	CAA-CBA-CGA-O2A
39	D	312	CLA	CBD-CGD-O2D-CED
39	a	801	CLA	C4B-C3B-CAB-CBB
39	a	810	CLA	C4B-C3B-CAB-CBB
39	a	814	CLA	C4B-C3B-CAB-CBB
39	a	818	CLA	C4B-C3B-CAB-CBB
39	a	830	CLA	C4B-C3B-CAB-CBB
39	a	838	CLA	C4B-C3B-CAB-CBB
39	b	810	CLA	C4B-C3B-CAB-CBB
39	b	819	CLA	C4B-C3B-CAB-CBB
39	b	825	CLA	C4B-C3B-CAB-CBB
39	b	831	CLA	C4B-C3B-CAB-CBB
39	b	838	CLA	C4B-C3B-CAB-CBB
39	i	101	CLA	C4B-C3B-CAB-CBB
39	l	203	CLA	C4B-C3B-CAB-CBB
39	l	204	CLA	C4B-C3B-CAB-CBB
39	A	305	CLA	C4B-C3B-CAB-CBB
39	A	312	CLA	C4B-C3B-CAB-CBB
39	C	310	CLA	C4B-C3B-CAB-CBB
39	D	311	CLA	C4B-C3B-CAB-CBB
39	E	314	CLA	C4B-C3B-CAB-CBB
39	F	313	CLA	C4B-C3B-CAB-CBB
39	F	315	CLA	C4B-C3B-CAB-CBB
39	F	316	CLA	C4B-C3B-CAB-CBB
39	G	312	CLA	C4B-C3B-CAB-CBB
39	H	307	CLA	C4B-C3B-CAB-CBB
39	H	316	CLA	C4B-C3B-CAB-CBB
39	J	314	CLA	C4B-C3B-CAB-CBB
39	K	314	CLA	C4B-C3B-CAB-CBB
39	L	319	CLA	C4B-C3B-CAB-CBB
39	L	320	CLA	C4B-C3B-CAB-CBB
39	O	312	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	O	316	CLA	C4B-C3B-CAB-CBB
39	P	307	CLA	C4B-C3B-CAB-CBB
39	S	311	CLA	C4B-C3B-CAB-CBB
39	S	316	CLA	C4B-C3B-CAB-CBB
39	S	320	CLA	C4B-C3B-CAB-CBB
39	T	320	CLA	C4B-C3B-CAB-CBB
39	V	319	CLA	C4B-C3B-CAB-CBB
39	X	307	CLA	C4B-C3B-CAB-CBB
39	X	308	CLA	C4B-C3B-CAB-CBB
39	1	309	CLA	C4B-C3B-CAB-CBB
39	3	312	CLA	C4B-C3B-CAB-CBB
39	3	322	CLA	C4B-C3B-CAB-CBB
39	4	322	CLA	C4B-C3B-CAB-CBB
39	4	323	CLA	C4B-C3B-CAB-CBB
39	5	315	CLA	C4B-C3B-CAB-CBB
39	5	316	CLA	C4B-C3B-CAB-CBB
39	7	318	CLA	C4B-C3B-CAB-CBB
39	7	321	CLA	C4B-C3B-CAB-CBB
39	8	310	CLA	C4B-C3B-CAB-CBB
39	8	315	CLA	C4B-C3B-CAB-CBB
39	I	301	CLA	C4B-C3B-CAB-CBB
39	x	314	CLA	C4B-C3B-CAB-CBB
39	y	312	CLA	C4B-C3B-CAB-CBB
39	y	315	CLA	C4B-C3B-CAB-CBB
39	z	311	CLA	C4B-C3B-CAB-CBB
39	z	314	CLA	C4B-C3B-CAB-CBB
39	z	317	CLA	C4B-C3B-CAB-CBB
39	Y	303	CLA	C4B-C3B-CAB-CBB
39	Y	304	CLA	C4B-C3B-CAB-CBB
39	Z	305	CLA	C4B-C3B-CAB-CBB
39	Z	312	CLA	C4B-C3B-CAB-CBB
39	Z	315	CLA	C4B-C3B-CAB-CBB
39	2	307	CLA	C4B-C3B-CAB-CBB
39	2	318	CLA	C4B-C3B-CAB-CBB
39	6	313	CLA	C4B-C3B-CAB-CBB
39	4	323	CLA	C16-C17-C18-C19
39	b	819	CLA	C8-C10-C11-C12
39	i	103	CLA	C5-C6-C7-C8
39	S	313	CLA	C5-C6-C7-C8
41	a	840	LHG	O6-C4-C5-C6
39	C	305	CLA	C3-C5-C6-C7
48	L	306	A86	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
41	a	840	LHG	C12-C13-C14-C15
46	S	322	LMG	C21-C22-C23-C24
47	P	301	SQD	C24-C23-O48-C46
50	2	306	A1EB1	C44-C42-O6-C28
39	D	314	CLA	C13-C15-C16-C17
39	V	313	CLA	C13-C15-C16-C17
51	Z	308	A1ECV	O1D-CGD-O2D-CED
47	D	304	SQD	C9-C10-C11-C12
39	a	826	CLA	C4-C3-C5-C6
39	A	306	CLA	C4-C3-C5-C6
39	B	207	CLA	C4-C3-C5-C6
39	3	311	CLA	C4-C3-C5-C6
39	I	308	CLA	C4-C3-C5-C6
39	b	851	CLA	C2-C3-C5-C6
39	A	309	CLA	C2-C3-C5-C6
39	I	314	CLA	C2-C3-C5-C6
49	P	313	KC2	CAA-CBA-CGA-O1A
39	B	209	CLA	C11-C10-C8-C9
48	Z	301	A86	C33-C34-O4-C38
47	P	301	SQD	C9-C10-C11-C12
46	P	317	LMG	C29-C30-C31-C32
46	W	302	LMG	C29-C30-C31-C32
47	4	327	SQD	C12-C13-C14-C15
47	9	322	SQD	C10-C11-C12-C13
39	A	311	CLA	C13-C15-C16-C17
39	D	319	CLA	C2A-CAA-CBA-CGA
39	b	828	CLA	CBA-CGA-O2A-C1
39	b	829	CLA	CBA-CGA-O2A-C1
39	0	311	CLA	CBA-CGA-O2A-C1
41	D	301	LHG	C24-C23-O8-C6
47	k	205	SQD	C23-C24-C25-C26
47	M	301	SQD	C7-C8-C9-C10
41	H	317	LHG	C24-C25-C26-C27
47	M	301	SQD	C25-C26-C27-C28
39	O	310	CLA	O1D-CGD-O2D-CED
47	D	304	SQD	O10-C23-O48-C46
39	a	802	CLA	C3A-C2A-CAA-CBA
39	a	817	CLA	C3A-C2A-CAA-CBA
39	a	825	CLA	C3A-C2A-CAA-CBA
39	a	833	CLA	C3A-C2A-CAA-CBA
39	b	817	CLA	C3A-C2A-CAA-CBA
39	i	103	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	A	314	CLA	C3A-C2A-CAA-CBA
39	C	310	CLA	C3A-C2A-CAA-CBA
39	D	315	CLA	C3A-C2A-CAA-CBA
39	P	311	CLA	C3A-C2A-CAA-CBA
39	Q	321	CLA	C3A-C2A-CAA-CBA
39	S	320	CLA	C3A-C2A-CAA-CBA
39	U	210	CLA	C3A-C2A-CAA-CBA
39	W	313	CLA	C3A-C2A-CAA-CBA
39	9	308	CLA	C3A-C2A-CAA-CBA
39	a	830	CLA	C13-C15-C16-C17
43	U	204	DD6	C24-C25-C26-C27
48	O	306	A86	C24-C25-C26-C27
48	G	301	A86	O-C13-C14-C15
48	L	304	A86	O-C13-C14-C15
48	Q	301	A86	O-C13-C14-C15
48	Q	305	A86	O-C13-C14-C15
48	S	307	A86	O-C13-C14-C15
48	V	304	A86	O-C13-C14-C15
48	0	301	A86	O-C13-C14-C15
48	4	305	A86	O-C13-C14-C15
48	4	306	A86	O-C13-C14-C15
48	4	310	A86	O-C13-C14-C15
48	z	303	A86	O-C13-C14-C15
48	2	305	A86	O-C13-C14-C15
50	G	304	A1EB1	O-C13-C14-C15
50	H	301	A1EB1	O-C13-C14-C15
50	O	301	A1EB1	O-C13-C14-C15
50	3	324	A1EB1	O-C13-C14-C15
50	7	304	A1EB1	O-C13-C14-C15
50	8	306	A1EB1	O-C13-C14-C15
50	y	301	A1EB1	O-C13-C14-C15
50	z	302	A1EB1	O-C13-C14-C15
50	2	304	A1EB1	O-C13-C14-C15
50	0	302	A1EB1	C35-C34-O4-C38
49	1	312	KC2	CAA-CBA-CGA-O2A
39	P	311	CLA	C16-C17-C18-C20
39	b	833	CLA	CBA-CGA-O2A-C1
39	X	317	CLA	C3-C5-C6-C7
39	a	801	CLA	C13-C15-C16-C17
39	a	823	CLA	C15-C16-C17-C18
39	W	310	CLA	C13-C15-C16-C17
41	a	841	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
41	H	317	LHG	C4-C5-C6-O8
45	b	849	DGD	C1G-C2G-C3G-O3G
45	C	314	DGD	O1G-C1G-C2G-C3G
46	A	316	LMG	C7-C8-C9-O8
46	M	319	LMG	O1-C7-C8-C9
46	Q	322	LMG	C7-C8-C9-O8
46	S	321	LMG	C7-C8-C9-O8
46	4	326	LMG	O1-C7-C8-C9
46	7	301	LMG	O1-C7-C8-C9
46	9	321	LMG	C7-C8-C9-O8
47	F	319	SQD	O6-C44-C45-C46
47	M	301	SQD	C44-C45-C46-O48
47	P	301	SQD	O6-C44-C45-C46
47	P	301	SQD	C44-C45-C46-O48
47	T	321	SQD	C44-C45-C46-O48
47	7	302	SQD	O6-C44-C45-C46
49	Z	310	KC2	CBD-CGD-O2D-CED
46	P	317	LMG	C15-C16-C17-C18
46	W	302	LMG	C15-C16-C17-C18
47	F	318	SQD	C10-C11-C12-C13
50	G	304	A1EB1	C42-C44-C45-C46
52	P	319	A1EB4	O54-C39-O3-C12
46	A	316	LMG	C29-C30-C31-C32
39	a	803	CLA	O2A-C1-C2-C3
48	Q	302	A86	C35-C34-O4-C38
41	a	840	LHG	C10-C11-C12-C13
50	C	302	A1EB1	O5-C38-O4-C34
39	a	803	CLA	C3-C5-C6-C7
39	a	811	CLA	C3-C5-C6-C7
39	b	801	CLA	C3-C5-C6-C7
39	1	316	CLA	O1D-CGD-O2D-CED
46	S	321	LMG	O10-C28-O8-C9
52	M	322	A1EB4	O54-C39-O3-C12
39	a	814	CLA	C4-C3-C5-C6
39	a	818	CLA	C4-C3-C5-C6
39	W	310	CLA	C4-C3-C5-C6
47	E	320	SQD	C24-C23-O48-C46
41	X	301	LHG	C25-C26-C27-C28
39	l	203	CLA	O1D-CGD-O2D-CED
39	D	310	CLA	C10-C11-C12-C13
39	4	323	CLA	C15-C16-C17-C18
50	6	308	A1EB1	O6-C42-C44-C45

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Mol	Chain	Res	Type	Atoms
39	8	311	CLA	O1A-CGA-O2A-C1
46	S	321	LMG	O6-C5-C6-O5
39	k	202	CLA	O1D-CGD-O2D-CED
39	o	202	CLA	O1D-CGD-O2D-CED
39	a	807	CLA	C2A-CAA-CBA-CGA
39	a	834	CLA	C2A-CAA-CBA-CGA
39	E	308	CLA	C2A-CAA-CBA-CGA
46	4	326	LMG	C31-C32-C33-C34
46	7	301	LMG	C31-C32-C33-C34
41	a	841	LHG	O6-C4-C5-O7
50	x	301	A1EB1	C44-C42-O6-C28
46	7	326	LMG	C30-C31-C32-C33
39	b	818	CLA	O1A-CGA-O2A-C1
39	D	319	CLA	O1A-CGA-O2A-C1
49	H	311	KC2	C3A-C2A-CAA-CBA
49	M	314	KC2	C3A-C2A-CAA-CBA
49	P	313	KC2	C3A-C2A-CAA-CBA
49	y	314	KC2	C3A-C2A-CAA-CBA
49	4	318	KC2	CAA-CBA-CGA-O2A
39	a	814	CLA	C2B-C3B-CAB-CBB
39	a	830	CLA	C2B-C3B-CAB-CBB
39	a	838	CLA	C2B-C3B-CAB-CBB
39	b	814	CLA	C2B-C3B-CAB-CBB
39	b	819	CLA	C2B-C3B-CAB-CBB
39	b	838	CLA	C2B-C3B-CAB-CBB
39	l	204	CLA	C2B-C3B-CAB-CBB
39	A	305	CLA	C2B-C3B-CAB-CBB
39	C	310	CLA	C2B-C3B-CAB-CBB
39	E	314	CLA	C2B-C3B-CAB-CBB
39	F	313	CLA	C2B-C3B-CAB-CBB
39	F	315	CLA	C2B-C3B-CAB-CBB
39	F	316	CLA	C2B-C3B-CAB-CBB
39	G	312	CLA	C2B-C3B-CAB-CBB
39	L	316	CLA	C2B-C3B-CAB-CBB
39	L	319	CLA	C2B-C3B-CAB-CBB
39	L	320	CLA	C2B-C3B-CAB-CBB
39	O	316	CLA	C2B-C3B-CAB-CBB
39	T	320	CLA	C2B-C3B-CAB-CBB
39	V	319	CLA	C2B-C3B-CAB-CBB
39	X	307	CLA	C2B-C3B-CAB-CBB
39	X	308	CLA	C2B-C3B-CAB-CBB
39	4	313	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	4	322	CLA	C2B-C3B-CAB-CBB
39	4	323	CLA	C2B-C3B-CAB-CBB
39	5	315	CLA	C2B-C3B-CAB-CBB
39	7	318	CLA	C2B-C3B-CAB-CBB
39	x	314	CLA	C2B-C3B-CAB-CBB
39	y	312	CLA	C2B-C3B-CAB-CBB
39	y	315	CLA	C2B-C3B-CAB-CBB
39	z	311	CLA	C2B-C3B-CAB-CBB
39	z	317	CLA	C2B-C3B-CAB-CBB
39	2	307	CLA	C2B-C3B-CAB-CBB
39	S	309	CLA	C5-C6-C7-C8
39	T	313	CLA	O1A-CGA-O2A-C1
45	b	849	DGD	C9B-CAB-CBB-CCB
47	S	301	SQD	C12-C13-C14-C15
39	a	831	CLA	C3-C5-C6-C7
39	G	312	CLA	C4C-C3C-CAC-CBC
47	k	205	SQD	C24-C25-C26-C27
46	Q	322	LMG	O7-C8-C9-O8
47	D	320	SQD	O6-C44-C45-O47
39	D	318	CLA	CBD-CGD-O2D-CED
39	E	307	CLA	CBD-CGD-O2D-CED
39	3	312	CLA	CBA-CGA-O2A-C1
46	S	321	LMG	C29-C28-O8-C9
46	W	320	LMG	C13-C14-C15-C16
48	Q	308	A86	C35-C34-O4-C38
48	T	306	A86	C33-C34-O4-C38
52	R	305	A1EB4	C33-C34-O4-C38
39	a	816	CLA	C16-C17-C18-C19
39	a	847	CLA	C16-C17-C18-C19
39	P	311	CLA	C16-C17-C18-C19
39	0	313	CLA	C6-C7-C8-C9
39	a	831	CLA	C13-C15-C16-C17
39	E	312	CLA	C8-C10-C11-C12
48	F	301	A86	C10-C11-C13-C14
48	J	303	A86	C10-C11-C13-C14
48	K	301	A86	C10-C11-C13-C14
48	L	304	A86	C10-C11-C13-C14
48	L	306	A86	C10-C11-C13-C14
48	Q	305	A86	C10-C11-C13-C14
48	T	305	A86	C10-C11-C13-C14
48	X	303	A86	C10-C11-C13-C14
48	0	304	A86	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
48	3	305	A86	C10-C11-C13-C14
48	4	306	A86	C10-C11-C13-C14
48	7	308	A86	C10-C11-C13-C14
48	8	305	A86	C10-C11-C13-C14
48	9	301	A86	C10-C11-C13-C14
48	I	304	A86	C10-C11-C13-C14
48	x	305	A86	C10-C11-C13-C14
48	6	305	A86	C10-C11-C13-C14
48	6	307	A86	C10-C11-C13-C14
48	6	309	A86	C10-C11-C13-C14
50	E	301	A1EB1	C10-C11-C13-C14
50	G	307	A1EB1	C10-C11-C13-C14
50	H	301	A1EB1	C10-C11-C13-C14
50	J	302	A1EB1	C10-C11-C13-C14
50	K	304	A1EB1	C10-C11-C13-C14
50	Q	323	A1EB1	C10-C11-C13-C14
50	R	303	A1EB1	C10-C11-C13-C14
50	V	305	A1EB1	C10-C11-C13-C14
50	0	307	A1EB1	C10-C11-C13-C14
50	3	324	A1EB1	C10-C11-C13-C14
50	4	301	A1EB1	C10-C11-C13-C14
50	4	303	A1EB1	C10-C11-C13-C14
50	7	304	A1EB1	C10-C11-C13-C14
50	7	305	A1EB1	C10-C11-C13-C14
50	8	301	A1EB1	C10-C11-C13-C14
50	8	308	A1EB1	C10-C11-C13-C14
50	x	301	A1EB1	C10-C11-C13-C14
50	x	302	A1EB1	C10-C11-C13-C14
50	2	304	A1EB1	C10-C11-C13-C14
50	2	306	A1EB1	C10-C11-C13-C14
41	a	840	LHG	C11-C10-C9-C8
39	C	311	CLA	C2-C1-O2A-CGA
39	S	308	CLA	C2-C1-O2A-CGA
39	9	308	CLA	C2-C1-O2A-CGA
39	I	314	CLA	C2-C1-O2A-CGA
39	A	307	CLA	O1D-CGD-O2D-CED
39	a	826	CLA	C2-C3-C5-C6
39	B	207	CLA	C2-C3-C5-C6
39	S	308	CLA	C5-C6-C7-C8
39	a	804	CLA	C11-C12-C13-C14
39	a	811	CLA	C14-C13-C15-C16
39	a	831	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
39	b	807	CLA	C11-C10-C8-C9
39	b	820	CLA	C6-C7-C8-C9
39	b	820	CLA	C11-C10-C8-C9
39	b	832	CLA	C6-C7-C8-C9
39	A	311	CLA	C11-C12-C13-C14
39	C	305	CLA	C11-C12-C13-C14
39	D	313	CLA	C11-C10-C8-C9
39	D	319	CLA	C11-C12-C13-C14
39	E	308	CLA	C6-C7-C8-C9
39	J	314	CLA	C11-C10-C8-C9
39	K	311	CLA	C6-C7-C8-C9
39	K	311	CLA	C14-C13-C15-C16
39	L	308	CLA	C6-C7-C8-C9
39	R	309	CLA	C11-C10-C8-C9
39	W	313	CLA	C6-C7-C8-C9
39	4	311	CLA	C6-C7-C8-C9
39	7	325	CLA	CBA-CGA-O2A-C1
46	I	302	LMG	C16-C17-C18-C19
49	P	312	KC2	CBD-CGD-O2D-CED
48	C	303	A86	C33-C34-O4-C38
50	U	205	A1EB1	C35-C34-O4-C38
39	a	831	CLA	C5-C6-C7-C8
39	K	309	CLA	C5-C6-C7-C8
39	4	311	CLA	C8-C10-C11-C12
41	j	104	LHG	C2-C3-O3-P
49	5	314	KC2	C1A-C2A-CAA-CBA
39	a	811	CLA	O1A-CGA-O2A-C1
39	Q	310	CLA	O1A-CGA-O2A-C1
39	G	312	CLA	C2C-C3C-CAC-CBC
39	i	101	CLA	C2A-CAA-CBA-CGA
39	l	205	CLA	C2A-CAA-CBA-CGA
39	K	312	CLA	C2A-CAA-CBA-CGA
39	W	309	CLA	C2A-CAA-CBA-CGA
39	4	312	CLA	C2A-CAA-CBA-CGA
39	I	314	CLA	C2A-CAA-CBA-CGA
39	F	308	CLA	C16-C17-C18-C19
39	R	308	CLA	C11-C12-C13-C15
42	b	844	BCR	C1-C6-C7-C8
42	b	844	BCR	C5-C6-C7-C8
42	l	202	BCR	C1-C6-C7-C8
42	l	202	BCR	C5-C6-C7-C8
42	m	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
39	b	838	CLA	C5-C6-C7-C8
39	3	312	CLA	C13-C15-C16-C17
39	9	308	CLA	CAA-CBA-CGA-O2A
48	6	307	A86	C7-C6-C8-C9
50	3	324	A1EB1	C-C1-C24-C25
51	O	315	A1ECV	CAA-CBA-CGA-O1A
39	E	309	CLA	O1A-CGA-O2A-C1
39	X	308	CLA	O1D-CGD-O2D-CED
39	2	310	CLA	O1D-CGD-O2D-CED
39	1	309	CLA	C1A-C2A-CAA-CBA
39	9	312	CLA	C1A-C2A-CAA-CBA
39	y	312	CLA	C1A-C2A-CAA-CBA
39	y	318	CLA	C1A-C2A-CAA-CBA
39	z	307	CLA	C1A-C2A-CAA-CBA
39	z	317	CLA	C1A-C2A-CAA-CBA
39	2	310	CLA	C1A-C2A-CAA-CBA
39	6	313	CLA	C1A-C2A-CAA-CBA
43	o	204	DD6	C10-C11-C13-C14
43	O	305	DD6	C10-C11-C13-C14
43	Z	302	DD6	C2-C1-C24-C25
43	2	303	DD6	C2-C1-C24-C25
48	R	302	A86	C5-C6-C8-C9
48	3	305	A86	C2-C1-C24-C25
50	H	304	A1EB1	C5-C6-C8-C9
50	Q	307	A1EB1	C5-C6-C8-C9
50	U	203	A1EB1	C2-C1-C24-C25
50	V	307	A1EB1	C33-C34-O4-C38
50	3	324	A1EB1	C2-C1-C24-C25
39	D	318	CLA	C10-C11-C12-C13
39	J	311	CLA	C8-C10-C11-C12
39	4	316	CLA	C8-C10-C11-C12
41	a	841	LHG	O9-C7-O7-C5
41	X	301	LHG	C8-C7-O7-C5
52	M	322	A1EB4	C46-C47-C51-C55
52	P	319	A1EB4	C46-C47-C51-C55
39	b	842	CLA	O1A-CGA-O2A-C1
39	a	811	CLA	C16-C17-C18-C20
39	S	320	CLA	C16-C17-C18-C20
39	6	312	CLA	C16-C17-C18-C19
40	a	839	PQN	C26-C27-C28-C29
45	b	849	DGD	C5B-C6B-C7B-C8B
41	X	301	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
39	b	842	CLA	O1D-CGD-O2D-CED
39	1	313	CLA	O1D-CGD-O2D-CED
51	O	315	A1ECV	CAA-CBA-CGA-O2A
39	b	821	CLA	C13-C15-C16-C17
41	H	317	LHG	O6-C4-C5-C6
46	F	317	LMG	C30-C31-C32-C33
39	a	806	CLA	C12-C13-C15-C16
39	a	809	CLA	C11-C10-C8-C7
39	a	809	CLA	C11-C12-C13-C15
39	a	811	CLA	C12-C13-C15-C16
39	a	815	CLA	C11-C10-C8-C7
39	a	830	CLA	C11-C10-C8-C7
39	a	831	CLA	C6-C7-C8-C10
39	a	838	CLA	C11-C12-C13-C15
39	a	847	CLA	C11-C10-C8-C7
39	a	847	CLA	C11-C12-C13-C15
39	b	807	CLA	C6-C7-C8-C10
39	b	807	CLA	C11-C10-C8-C7
39	b	809	CLA	C11-C10-C8-C7
39	b	810	CLA	C6-C7-C8-C10
39	b	810	CLA	C12-C13-C15-C16
39	b	812	CLA	C6-C7-C8-C10
39	b	820	CLA	C6-C7-C8-C10
39	b	821	CLA	C6-C7-C8-C10
39	b	833	CLA	C12-C13-C15-C16
39	b	838	CLA	C11-C12-C13-C15
39	i	101	CLA	C11-C10-C8-C7
39	i	103	CLA	C11-C12-C13-C15
39	l	201	CLA	C11-C10-C8-C7
39	A	311	CLA	C12-C13-C15-C16
39	A	312	CLA	C11-C10-C8-C7
39	C	305	CLA	C11-C12-C13-C15
39	C	310	CLA	C11-C12-C13-C15
39	D	310	CLA	C11-C10-C8-C7
39	D	313	CLA	C11-C10-C8-C7
39	D	313	CLA	C12-C13-C15-C16
39	D	319	CLA	C11-C10-C8-C7
39	D	319	CLA	C11-C12-C13-C15
39	E	307	CLA	C11-C10-C8-C7
39	F	308	CLA	C12-C13-C15-C16
39	F	321	CLA	C12-C13-C15-C16
39	G	310	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
39	H	308	CLA	C11-C10-C8-C7
39	J	314	CLA	C6-C7-C8-C10
39	J	314	CLA	C11-C10-C8-C7
39	K	308	CLA	C6-C7-C8-C10
39	K	311	CLA	C6-C7-C8-C10
39	L	308	CLA	C6-C7-C8-C10
39	L	310	CLA	C11-C10-C8-C7
39	O	310	CLA	C11-C10-C8-C7
39	P	307	CLA	C11-C10-C8-C7
39	P	308	CLA	C11-C10-C8-C7
39	P	309	CLA	C11-C10-C8-C7
39	Q	310	CLA	C11-C12-C13-C15
39	Q	310	CLA	C12-C13-C15-C16
39	R	309	CLA	C11-C10-C8-C7
39	S	308	CLA	C11-C10-C8-C7
39	S	311	CLA	C11-C12-C13-C15
39	U	207	CLA	C6-C7-C8-C10
39	V	309	CLA	C11-C12-C13-C15
39	V	311	CLA	C12-C13-C15-C16
39	W	310	CLA	C12-C13-C15-C16
39	W	311	CLA	C11-C10-C8-C7
39	X	308	CLA	C11-C10-C8-C7
39	X	309	CLA	C11-C10-C8-C7
39	3	312	CLA	C11-C10-C8-C7
39	3	312	CLA	C12-C13-C15-C16
39	4	316	CLA	C12-C13-C15-C16
39	5	308	CLA	C11-C10-C8-C7
39	7	313	CLA	C11-C10-C8-C7
39	I	314	CLA	C11-C12-C13-C15
39	H	312	CLA	O1D-CGD-O2D-CED
39	L	311	CLA	O1A-CGA-O2A-C1
51	R	310	A1ECV	C1C-C2C-CMC-O1
51	4	321	A1ECV	C1C-C2C-CMC-O2
51	5	309	A1ECV	C1C-C2C-CMC-O1
51	5	309	A1ECV	C1C-C2C-CMC-O2
39	K	312	CLA	C15-C16-C17-C18
47	E	320	SQD	C45-C46-O48-C23
39	C	311	CLA	C16-C17-C18-C20
39	X	309	CLA	C15-C16-C17-C18
39	I	314	CLA	C10-C11-C12-C13
40	b	843	PQN	C20-C21-C22-C23
39	b	838	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
46	W	320	LMG	C29-C30-C31-C32
47	k	205	SQD	C25-C26-C27-C28
39	a	847	CLA	C15-C16-C17-C18
39	D	316	CLA	C15-C16-C17-C18
49	A	310	KC2	C2A-CAA-CBA-CGA
49	A	313	KC2	C2A-CAA-CBA-CGA
49	X	315	KC2	C2A-CAA-CBA-CGA
49	4	320	KC2	C2A-CAA-CBA-CGA
49	Z	310	KC2	C2A-CAA-CBA-CGA
39	6	312	CLA	C16-C17-C18-C20
39	a	807	CLA	C15-C16-C17-C18
39	E	310	CLA	C10-C11-C12-C13
39	F	308	CLA	C15-C16-C17-C18
39	a	826	CLA	CBA-CGA-O2A-C1
39	E	314	CLA	CBA-CGA-O2A-C1
39	V	310	CLA	CBA-CGA-O2A-C1
46	D	322	LMG	C33-C34-C35-C36
50	2	304	A1EB1	C44-C45-C46-C47
39	b	830	CLA	C13-C15-C16-C17
39	A	312	CLA	C10-C11-C12-C13
39	J	314	CLA	C10-C11-C12-C13
39	K	306	CLA	C5-C6-C7-C8
39	b	832	CLA	CBD-CGD-O2D-CED
39	I	311	CLA	CBD-CGD-O2D-CED
39	a	801	CLA	CAD-CBD-CGD-O2D
39	a	805	CLA	CAD-CBD-CGD-O2D
39	a	817	CLA	CAD-CBD-CGD-O2D
39	a	822	CLA	CAD-CBD-CGD-O2D
39	a	823	CLA	CAD-CBD-CGD-O2D
39	a	828	CLA	CAD-CBD-CGD-O2D
39	a	837	CLA	CAD-CBD-CGD-O2D
39	b	813	CLA	CAD-CBD-CGD-O2D
39	b	814	CLA	CAD-CBD-CGD-O2D
39	b	818	CLA	CAD-CBD-CGD-O2D
39	b	826	CLA	CAD-CBD-CGD-O2D
39	b	833	CLA	CAD-CBD-CGD-O2D
39	i	103	CLA	CAD-CBD-CGD-O2D
39	A	312	CLA	CAD-CBD-CGD-O2D
39	C	309	CLA	CAD-CBD-CGD-O2D
39	C	310	CLA	CAD-CBD-CGD-O2D
39	E	312	CLA	CAD-CBD-CGD-O2D
39	E	318	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
39	F	314	CLA	CAD-CBD-CGD-O2D
39	H	312	CLA	CAD-CBD-CGD-O2D
39	J	308	CLA	CAD-CBD-CGD-O2D
39	J	314	CLA	CAD-CBD-CGD-O2D
39	K	314	CLA	CAD-CBD-CGD-O2D
39	L	310	CLA	CAD-CBD-CGD-O2D
39	M	312	CLA	CAD-CBD-CGD-O2D
39	M	315	CLA	CAD-CBD-CGD-O2D
39	O	314	CLA	CAD-CBD-CGD-O2D
39	P	311	CLA	CAD-CBD-CGD-O2D
39	R	307	CLA	CAD-CBD-CGD-O2D
39	R	311	CLA	CAD-CBD-CGD-O2D
39	S	310	CLA	CAD-CBD-CGD-O2D
39	S	313	CLA	CAD-CBD-CGD-O2D
39	S	319	CLA	CAD-CBD-CGD-O2D
39	T	313	CLA	CAD-CBD-CGD-O2D
39	T	319	CLA	CAD-CBD-CGD-O2D
39	X	311	CLA	CAD-CBD-CGD-O2D
39	0	312	CLA	CAD-CBD-CGD-O2D
39	0	315	CLA	CAD-CBD-CGD-O2D
39	0	318	CLA	CAD-CBD-CGD-O2D
39	3	316	CLA	CAD-CBD-CGD-O2D
39	4	316	CLA	CAD-CBD-CGD-O2D
39	5	316	CLA	CAD-CBD-CGD-O2D
39	7	324	CLA	CAD-CBD-CGD-O2D
39	8	315	CLA	CAD-CBD-CGD-O2D
39	9	309	CLA	CAD-CBD-CGD-O2D
39	I	310	CLA	CAD-CBD-CGD-O2D
39	I	315	CLA	CAD-CBD-CGD-O2D
39	z	311	CLA	CAD-CBD-CGD-O2D
39	z	318	CLA	CAD-CBD-CGD-O2D
39	Y	311	CLA	CAD-CBD-CGD-O2D
39	Z	316	CLA	CAD-CBD-CGD-O2D
39	2	315	CLA	CAD-CBD-CGD-O2D
47	D	320	SQD	C46-C45-O47-C7
47	T	321	SQD	C46-C45-O47-C7
48	B	201	A86	C28-C27-C29-C30
48	C	303	A86	C28-C27-C29-C30
48	Q	305	A86	C28-C27-C29-C30
48	R	302	A86	C28-C27-C29-C30
48	X	302	A86	C28-C27-C29-C30
48	0	304	A86	C28-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
48	3	305	A86	C28-C27-C29-C30
48	3	307	A86	C28-C27-C29-C30
48	8	323	A86	C28-C27-C29-C30
48	I	304	A86	C28-C27-C29-C30
48	x	305	A86	C28-C27-C29-C30
48	2	305	A86	C28-C27-C29-C30
49	A	313	KC2	C2C-C3C-CAC-CBC
49	F	311	KC2	C2C-C3C-CAC-CBC
49	G	313	KC2	C2C-C3C-CAC-CBC
49	H	311	KC2	CAD-CBD-CGD-O2D
49	H	314	KC2	CAD-CBD-CGD-O2D
49	L	312	KC2	C2C-C3C-CAC-CBC
49	P	306	KC2	CAD-CBD-CGD-O2D
49	P	313	KC2	C2C-C3C-CAC-CBC
49	P	320	KC2	CAD-CBD-CGD-O2D
49	Q	313	KC2	CAD-CBD-CGD-O2D
49	Q	315	KC2	C2C-C3C-CAC-CBC
49	R	306	KC2	CAD-CBD-CGD-O2D
49	R	314	KC2	CAD-CBD-CGD-O2D
49	V	308	KC2	CAD-CBD-CGD-O2D
49	V	314	KC2	C2C-C3C-CAC-CBC
49	V	318	KC2	CAD-CBD-CGD-O2D
49	X	306	KC2	CAD-CBD-CGD-O2D
49	X	312	KC2	CAD-CBD-CGD-O2D
49	X	314	KC2	CAD-CBD-CGD-O2D
49	0	317	KC2	C2B-C3B-CAB-CBB
49	3	315	KC2	CAD-CBD-CGD-O2D
49	3	318	KC2	C2C-C3C-CAC-CBC
49	4	317	KC2	CAD-CBD-CGD-O2D
49	4	324	KC2	CAD-CBD-CGD-O2D
49	5	313	KC2	CAD-CBD-CGD-O2D
49	7	319	KC2	C2C-C3C-CAC-CBC
49	7	319	KC2	CAD-CBD-CGD-O2D
49	7	320	KC2	C2B-C3B-CAB-CBB
49	7	320	KC2	C2C-C3C-CAC-CBC
49	9	311	KC2	CAD-CBD-CGD-O2D
49	I	312	KC2	C2C-C3C-CAC-CBC
49	2	314	KC2	CAD-CBD-CGD-O2D
49	2	317	KC2	C2B-C3B-CAB-CBB
49	6	316	KC2	C2C-C3C-CAC-CBC
50	z	301	A1EB1	C28-C27-C29-C30
51	G	316	A1ECV	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
51	O	315	A1ECV	CAD-CBD-CGD-O2D
51	P	315	A1ECV	CAD-CBD-CGD-O2D
51	S	312	A1ECV	CAD-CBD-CGD-O2D
51	V	317	A1ECV	CAD-CBD-CGD-O2D
51	4	315	A1ECV	CAD-CBD-CGD-O2D
51	5	312	A1ECV	CAD-CBD-CGD-O2D
51	9	314	A1ECV	CAD-CBD-CGD-O2D
51	9	317	A1ECV	CAD-CBD-CGD-O2D
39	a	801	CLA	C3-C5-C6-C7
39	b	829	CLA	C10-C11-C12-C13
39	i	101	CLA	C5-C6-C7-C8
39	5	308	CLA	C8-C10-C11-C12
39	b	811	CLA	CBA-CGA-O2A-C1
41	a	840	LHG	C24-C23-O8-C6
39	b	828	CLA	C4-C3-C5-C6
39	L	309	CLA	C6-C7-C8-C10
39	4	323	CLA	C16-C17-C18-C20
47	D	304	SQD	O5-C1-O6-C44
39	C	306	CLA	C2-C3-C5-C6
41	a	840	LHG	C7-C8-C9-C10
46	D	322	LMG	C7-C8-C9-O8
46	S	322	LMG	O1-C7-C8-C9
46	4	325	LMG	O1-C7-C8-C9
46	4	325	LMG	C7-C8-C9-O8
47	H	318	SQD	C44-C45-C46-O48
48	H	302	A86	C12-C11-C13-O
48	J	303	A86	C12-C11-C13-O
48	L	304	A86	C12-C11-C13-O
48	S	305	A86	C12-C11-C13-O
48	3	305	A86	C12-C11-C13-O
48	4	305	A86	C12-C11-C13-O
48	4	306	A86	C12-C11-C13-O
48	4	328	A86	C12-C11-C13-O
48	8	307	A86	C12-C11-C13-O
48	9	301	A86	C12-C11-C13-O
48	9	303	A86	C12-C11-C13-O
48	9	305	A86	C12-C11-C13-O
48	x	305	A86	C12-C11-C13-O
48	z	303	A86	C12-C11-C13-O
48	6	307	A86	C12-C11-C13-O
50	G	307	A1EB1	C12-C11-C13-O
50	L	303	A1EB1	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
50	O	301	A1EB1	C12-C11-C13-O
50	S	303	A1EB1	C12-C11-C13-O
50	0	302	A1EB1	C12-C11-C13-O
50	1	301	A1EB1	C12-C11-C13-O
50	8	306	A1EB1	C12-C11-C13-O
50	8	308	A1EB1	C12-C11-C13-O
50	x	301	A1EB1	C12-C11-C13-O
50	x	302	A1EB1	C12-C11-C13-O
50	y	302	A1EB1	C12-C11-C13-O
50	z	302	A1EB1	C12-C11-C13-O
50	6	304	A1EB1	C12-C11-C13-O
39	3	312	CLA	O1A-CGA-O2A-C1
39	7	325	CLA	O1A-CGA-O2A-C1
39	I	314	CLA	O1A-CGA-O2A-C1
50	2	306	A1EB1	O43-C42-O6-C28
47	4	327	SQD	C26-C27-C28-C29
41	a	840	LHG	O6-C4-C5-O7
39	E	310	CLA	C8-C10-C11-C12
39	M	312	CLA	C15-C16-C17-C18
39	I	309	CLA	C15-C16-C17-C18
52	X	305	A1EB4	C33-C34-O4-C38
39	0	310	CLA	CAA-CBA-CGA-O2A
39	J	307	CLA	O2A-C1-C2-C3
49	1	312	KC2	C4C-C3C-CAC-CBC
49	3	315	KC2	C4C-C3C-CAC-CBC
49	3	317	KC2	C4C-C3C-CAC-CBC
49	4	318	KC2	C4B-C3B-CAB-CBB
49	7	320	KC2	CAA-CBA-CGA-O2A
39	R	308	CLA	CBA-CGA-O2A-C1
46	M	319	LMG	C29-C30-C31-C32
50	U	205	A1EB1	C44-C45-C46-C47
49	O	317	KC2	CBD-CGD-O2D-CED
39	M	312	CLA	O1A-CGA-O2A-C1
39	R	308	CLA	C11-C12-C13-C14
39	S	309	CLA	C16-C17-C18-C20
39	a	811	CLA	CHA-CBD-CGD-O1D
39	a	811	CLA	CHA-CBD-CGD-O2D
39	a	814	CLA	CHA-CBD-CGD-O1D
39	a	814	CLA	CHA-CBD-CGD-O2D
39	a	819	CLA	CHA-CBD-CGD-O1D
39	a	820	CLA	CHA-CBD-CGD-O2D
39	a	827	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	a	827	CLA	CHA-CBD-CGD-O2D
39	a	835	CLA	CHA-CBD-CGD-O1D
39	a	836	CLA	CHA-CBD-CGD-O2D
39	b	806	CLA	CHA-CBD-CGD-O1D
39	b	806	CLA	CHA-CBD-CGD-O2D
39	b	808	CLA	CHA-CBD-CGD-O1D
39	b	808	CLA	CHA-CBD-CGD-O2D
39	b	811	CLA	CHA-CBD-CGD-O1D
39	b	815	CLA	CHA-CBD-CGD-O1D
39	b	815	CLA	CHA-CBD-CGD-O2D
39	b	823	CLA	CHA-CBD-CGD-O1D
39	b	823	CLA	CHA-CBD-CGD-O2D
39	b	827	CLA	CHA-CBD-CGD-O1D
39	b	828	CLA	CHA-CBD-CGD-O2D
39	b	830	CLA	CHA-CBD-CGD-O1D
39	b	830	CLA	CHA-CBD-CGD-O2D
39	b	851	CLA	CHA-CBD-CGD-O1D
39	b	851	CLA	CHA-CBD-CGD-O2D
39	i	101	CLA	CHA-CBD-CGD-O2D
39	j	101	CLA	CHA-CBD-CGD-O1D
39	j	101	CLA	CHA-CBD-CGD-O2D
39	k	201	CLA	CHA-CBD-CGD-O1D
39	k	201	CLA	CHA-CBD-CGD-O2D
39	A	309	CLA	CHA-CBD-CGD-O2D
39	C	305	CLA	CHA-CBD-CGD-O1D
39	C	305	CLA	CHA-CBD-CGD-O2D
39	C	308	CLA	CHA-CBD-CGD-O1D
39	D	318	CLA	CHA-CBD-CGD-O1D
39	D	319	CLA	CHA-CBD-CGD-O1D
39	D	319	CLA	CHA-CBD-CGD-O2D
39	E	315	CLA	CHA-CBD-CGD-O2D
39	E	317	CLA	CHA-CBD-CGD-O1D
39	E	317	CLA	CHA-CBD-CGD-O2D
39	F	310	CLA	CHA-CBD-CGD-O1D
39	F	310	CLA	CHA-CBD-CGD-O2D
39	G	318	CLA	CHA-CBD-CGD-O1D
39	J	309	CLA	CHA-CBD-CGD-O1D
39	L	316	CLA	CHA-CBD-CGD-O2D
39	O	316	CLA	CHA-CBD-CGD-O1D
39	O	316	CLA	CHA-CBD-CGD-O2D
39	Q	320	CLA	CHA-CBD-CGD-O2D
39	R	309	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	R	309	CLA	CHA-CBD-CGD-O2D
39	S	309	CLA	CHA-CBD-CGD-O2D
39	T	320	CLA	CHA-CBD-CGD-O1D
39	U	201	CLA	CHA-CBD-CGD-O1D
39	U	209	CLA	CHA-CBD-CGD-O1D
39	U	213	CLA	CHA-CBD-CGD-O1D
39	U	213	CLA	CHA-CBD-CGD-O2D
39	U	215	CLA	CHA-CBD-CGD-O1D
39	U	215	CLA	CHA-CBD-CGD-O2D
39	V	316	CLA	CHA-CBD-CGD-O1D
39	V	316	CLA	CHA-CBD-CGD-O2D
39	W	316	CLA	CHA-CBD-CGD-O1D
39	W	316	CLA	CHA-CBD-CGD-O2D
39	0	320	CLA	CHA-CBD-CGD-O1D
39	0	320	CLA	CHA-CBD-CGD-O2D
39	0	323	CLA	CHA-CBD-CGD-O1D
39	0	323	CLA	CHA-CBD-CGD-O2D
39	4	312	CLA	CHA-CBD-CGD-O1D
39	5	308	CLA	CHA-CBD-CGD-O1D
39	5	308	CLA	CHA-CBD-CGD-O2D
39	9	308	CLA	CHA-CBD-CGD-O1D
39	9	308	CLA	CHA-CBD-CGD-O2D
39	9	310	CLA	CHA-CBD-CGD-O2D
39	9	319	CLA	CHA-CBD-CGD-O2D
39	I	316	CLA	CHA-CBD-CGD-O2D
39	x	314	CLA	CHA-CBD-CGD-O1D
39	x	314	CLA	CHA-CBD-CGD-O2D
39	y	310	CLA	CHA-CBD-CGD-O1D
39	y	310	CLA	CHA-CBD-CGD-O2D
39	z	309	CLA	CHA-CBD-CGD-O1D
39	z	309	CLA	CHA-CBD-CGD-O2D
39	z	317	CLA	CHA-CBD-CGD-O1D
39	z	317	CLA	CHA-CBD-CGD-O2D
39	Y	307	CLA	CHA-CBD-CGD-O1D
39	Y	314	CLA	CHA-CBD-CGD-O1D
39	2	310	CLA	CHA-CBD-CGD-O1D
39	2	310	CLA	CHA-CBD-CGD-O2D
39	2	319	CLA	CHA-CBD-CGD-O2D
39	6	318	CLA	CHA-CBD-CGD-O2D
49	K	313	KC2	CHA-CBD-CGD-O1D
49	K	313	KC2	CHA-CBD-CGD-O2D
49	R	312	KC2	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
49	S	314	KC2	CHA-CBD-CGD-O1D
49	V	315	KC2	CHA-CBD-CGD-O2D
49	V	320	KC2	CHA-CBD-CGD-O1D
49	V	320	KC2	CHA-CBD-CGD-O2D
49	8	316	KC2	CHA-CBD-CGD-O2D
49	8	317	KC2	CHA-CBD-CGD-O2D
49	8	320	KC2	CHA-CBD-CGD-O2D
49	I	303	KC2	CHA-CBD-CGD-O1D
39	b	821	CLA	C15-C16-C17-C18
39	b	828	CLA	O1A-CGA-O2A-C1
39	b	833	CLA	O1A-CGA-O2A-C1
39	j	101	CLA	O1A-CGA-O2A-C1
39	J	307	CLA	O1A-CGA-O2A-C1
39	K	307	CLA	C5-C6-C7-C8
41	a	841	LHG	O7-C5-C6-O8
46	A	316	LMG	O7-C8-C9-O8
46	0	324	LMG	O7-C8-C9-O8
46	9	321	LMG	O7-C8-C9-O8
47	k	205	SQD	O6-C44-C45-O47
47	E	320	SQD	O47-C45-C46-O48
47	F	318	SQD	O6-C44-C45-O47
47	F	319	SQD	O6-C44-C45-O47
47	P	301	SQD	O47-C45-C46-O48
39	C	308	CLA	CBA-CGA-O2A-C1
46	7	301	LMG	C32-C33-C34-C35
49	L	314	KC2	CAA-CBA-CGA-O2A
39	b	829	CLA	O1A-CGA-O2A-C1
47	T	321	SQD	O10-C23-O48-C46
50	x	301	A1EB1	O43-C42-O6-C28
46	4	326	LMG	C32-C33-C34-C35
39	D	311	CLA	C16-C17-C18-C20
39	S	309	CLA	C16-C17-C18-C19
48	H	302	A86	C10-C11-C13-O
48	J	303	A86	C10-C11-C13-O
48	L	304	A86	C10-C11-C13-O
48	L	305	A86	C10-C11-C13-O
48	O	307	A86	C13-C14-C15-O1
48	S	304	A86	C13-C14-C15-O1
48	S	305	A86	C10-C11-C13-O
48	S	307	A86	C13-C14-C15-O1
48	T	305	A86	C10-C11-C13-O
48	3	305	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
48	3	306	A86	C13-C14-C15-O1
48	4	305	A86	C13-C14-C15-O1
48	4	306	A86	C10-C11-C13-O
48	4	328	A86	C10-C11-C13-O
48	4	328	A86	C13-C14-C15-O1
48	8	302	A86	C10-C11-C13-O
48	8	307	A86	C10-C11-C13-O
48	9	301	A86	C10-C11-C13-O
48	9	304	A86	C10-C11-C13-O
48	9	305	A86	C10-C11-C13-O
48	x	305	A86	C10-C11-C13-O
48	z	303	A86	C10-C11-C13-O
48	z	303	A86	C13-C14-C15-O1
48	Z	303	A86	C10-C11-C13-O
48	2	305	A86	C10-C11-C13-O
48	6	307	A86	C10-C11-C13-O
48	6	309	A86	C10-C11-C13-O
50	G	307	A1EB1	C10-C11-C13-O
50	G	308	A1EB1	C13-C14-C15-O1
50	H	301	A1EB1	C13-C14-C15-O1
50	J	302	A1EB1	C10-C11-C13-O
50	K	305	A1EB1	C13-C14-C15-O1
50	L	303	A1EB1	C10-C11-C13-O
50	O	301	A1EB1	C10-C11-C13-O
50	S	303	A1EB1	C10-C11-C13-O
50	V	302	A1EB1	C10-C11-C13-O
50	V	306	A1EB1	C13-C14-C15-O1
50	0	302	A1EB1	C10-C11-C13-O
50	0	307	A1EB1	C13-C14-C15-O1
50	1	301	A1EB1	C10-C11-C13-O
50	3	310	A1EB1	C10-C11-C13-O
50	3	310	A1EB1	C13-C14-C15-O1
50	4	303	A1EB1	C13-C14-C15-O1
50	7	304	A1EB1	C13-C14-C15-O1
50	7	305	A1EB1	C13-C14-C15-O1
50	8	301	A1EB1	C13-C14-C15-O1
50	8	306	A1EB1	C10-C11-C13-O
50	8	306	A1EB1	C13-C14-C15-O1
50	8	308	A1EB1	C10-C11-C13-O
50	x	301	A1EB1	C10-C11-C13-O
50	x	302	A1EB1	C10-C11-C13-O
50	x	302	A1EB1	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
50	y	302	A1EB1	C10-C11-C13-O
50	z	302	A1EB1	C10-C11-C13-O
50	2	306	A1EB1	C13-C14-C15-O1
50	6	301	A1EB1	C13-C14-C15-O1
50	6	304	A1EB1	C10-C11-C13-O
50	6	304	A1EB1	C13-C14-C15-O1
50	6	308	A1EB1	C10-C11-C13-O
39	M	308	CLA	O1D-CGD-O2D-CED
39	C	306	CLA	C4-C3-C5-C6
39	0	311	CLA	O1A-CGA-O2A-C1
43	j	102	DD6	C27-C29-C30-C31
43	G	306	DD6	C27-C29-C30-C31
43	J	306	DD6	C27-C29-C30-C31
43	Q	306	DD6	C27-C29-C30-C31
43	S	306	DD6	C27-C29-C30-C31
43	W	305	DD6	C27-C29-C30-C31
43	I	307	DD6	C27-C29-C30-C31
43	z	305	DD6	C27-C29-C30-C31
39	a	809	CLA	C11-C12-C13-C14
39	b	807	CLA	C6-C7-C8-C9
39	b	821	CLA	C6-C7-C8-C9
39	j	101	CLA	C14-C13-C15-C16
39	A	312	CLA	C11-C12-C13-C14
39	J	314	CLA	C6-C7-C8-C9
39	L	310	CLA	C11-C10-C8-C9
39	P	309	CLA	C11-C10-C8-C9
39	U	207	CLA	C6-C7-C8-C9
39	V	313	CLA	C6-C7-C8-C9
39	3	311	CLA	C11-C10-C8-C9
39	7	313	CLA	C11-C10-C8-C9
39	I	314	CLA	C11-C12-C13-C14
39	F	309	CLA	O1D-CGD-O2D-CED
39	a	826	CLA	O1A-CGA-O2A-C1
47	9	322	SQD	O10-C23-O48-C46
46	W	320	LMG	C14-C15-C16-C17
47	D	320	SQD	C5-C6-S-O8
47	F	318	SQD	C5-C6-S-O8
47	F	319	SQD	C4-C5-C6-S
49	S	317	KC2	CAA-CBA-CGA-O2A
49	Z	310	KC2	CAA-CBA-CGA-O2A
50	E	301	A1EB1	C29-C27-C28-O6
50	G	304	A1EB1	C29-C27-C28-O6

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Mol	Chain	Res	Type	Atoms
50	H	304	A1EB1	C29-C27-C28-O6
50	K	302	A1EB1	C29-C27-C28-O6
50	U	205	A1EB1	C29-C27-C28-O6
50	4	301	A1EB1	C29-C27-C28-O6
50	7	305	A1EB1	C29-C27-C28-O6
50	8	306	A1EB1	C29-C27-C28-O6
50	2	304	A1EB1	C29-C27-C28-O6
39	7	313	CLA	O1D-CGD-O2D-CED
39	F	308	CLA	C2A-CAA-CBA-CGA
39	I	310	CLA	C2A-CAA-CBA-CGA
49	G	315	KC2	CBD-CGD-O2D-CED
51	z	310	A1ECV	CBD-CGD-O2D-CED
39	E	315	CLA	CAA-CBA-CGA-O2A
39	L	320	CLA	CAA-CBA-CGA-O2A
39	E	314	CLA	O1A-CGA-O2A-C1
42	b	850	BCR	C37-C22-C23-C24
43	A	303	DD6	C7-C6-C8-C9
43	1	304	DD6	C12-C11-C13-C14
48	2	301	A86	C35-C34-O4-C38
39	a	802	CLA	CBD-CGD-O2D-CED
52	W	321	A1EB4	C44-C45-C46-C47
42	b	850	BCR	C21-C22-C23-C24
42	j	103	BCR	C7-C8-C9-C10
43	a	846	DD6	C5-C6-C8-C9
43	O	305	DD6	C5-C6-C8-C9
48	D	305	A86	C2-C1-C24-C25
48	6	307	A86	C5-C6-C8-C9
39	E	313	CLA	O1D-CGD-O2D-CED
39	a	807	CLA	C1A-C2A-CAA-CBA
39	a	832	CLA	C1A-C2A-CAA-CBA
39	J	309	CLA	C1A-C2A-CAA-CBA
39	T	318	CLA	C1A-C2A-CAA-CBA
52	M	305	A1EB4	C13-C11-C12-O3
52	R	305	A1EB4	C13-C11-C12-O3
52	5	304	A1EB4	C13-C11-C12-O3
46	4	326	LMG	C28-C29-C30-C31
50	H	301	A1EB1	C42-C44-C45-C46
39	a	801	CLA	C16-C17-C18-C20
39	P	307	CLA	CBD-CGD-O2D-CED
52	T	304	A1EB4	C11-C13-C14-C15
48	3	306	A86	C3-C4-C5-C6
39	b	819	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	E	310	CLA	O1D-CGD-O2D-CED
46	A	316	LMG	C11-C12-C13-C14
39	a	847	CLA	C4-C3-C5-C6
39	H	307	CLA	O1D-CGD-O2D-CED
46	F	317	LMG	C32-C33-C34-C35
50	7	306	A1EB1	C44-C45-C46-C47
39	a	803	CLA	C4B-C3B-CAB-CBB
39	a	820	CLA	C4B-C3B-CAB-CBB
39	a	837	CLA	C4B-C3B-CAB-CBB
39	b	833	CLA	C4B-C3B-CAB-CBB
39	o	205	CLA	C4B-C3B-CAB-CBB
39	B	205	CLA	C4B-C3B-CAB-CBB
39	B	209	CLA	C4B-C3B-CAB-CBB
39	D	314	CLA	C4B-C3B-CAB-CBB
39	J	317	CLA	C4B-C3B-CAB-CBB
39	Q	309	CLA	C4B-C3B-CAB-CBB
39	Q	312	CLA	C4B-C3B-CAB-CBB
39	T	308	CLA	C4B-C3B-CAB-CBB
39	U	208	CLA	C4B-C3B-CAB-CBB
39	U	212	CLA	C4B-C3B-CAB-CBB
39	U	214	CLA	C4B-C3B-CAB-CBB
39	y	309	CLA	C4B-C3B-CAB-CBB
39	Y	307	CLA	C4B-C3B-CAB-CBB
41	a	840	LHG	C3-O3-P-O5
41	a	841	LHG	C3-O3-P-O5
41	j	104	LHG	C4-O6-P-O4
41	D	302	LHG	C3-O3-P-O5
41	D	302	LHG	C4-O6-P-O5
41	H	317	LHG	C4-O6-P-O5
39	b	813	CLA	C6-C7-C8-C9
39	3	312	CLA	C16-C17-C18-C20
46	7	301	LMG	C28-C29-C30-C31
50	8	304	A1EB1	C42-C44-C45-C46
39	E	313	CLA	C8-C10-C11-C12
39	b	832	CLA	CBA-CGA-O2A-C1
39	G	310	CLA	CBA-CGA-O2A-C1
41	a	841	LHG	O6-C4-C5-C6
49	T	315	KC2	CAA-CBA-CGA-O2A
39	C	310	CLA	O1D-CGD-O2D-CED
39	a	829	CLA	C2A-CAA-CBA-CGA
39	M	310	CLA	C2A-CAA-CBA-CGA
39	a	830	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
39	S	320	CLA	C15-C16-C17-C18
46	4	326	LMG	C14-C15-C16-C17
46	7	301	LMG	C14-C15-C16-C17
41	j	104	LHG	C24-C25-C26-C27
46	l	208	LMG	C12-C13-C14-C15
39	a	811	CLA	CAD-CBD-CGD-O1D
39	a	819	CLA	CAD-CBD-CGD-O1D
39	b	809	CLA	CAD-CBD-CGD-O1D
39	b	815	CLA	CAD-CBD-CGD-O1D
39	b	823	CLA	CAD-CBD-CGD-O1D
39	b	830	CLA	CAD-CBD-CGD-O1D
39	b	838	CLA	CAD-CBD-CGD-O1D
39	A	308	CLA	C2-C3-C5-C6
39	A	309	CLA	CAD-CBD-CGD-O1D
39	D	319	CLA	CAD-CBD-CGD-O1D
39	E	319	CLA	CAD-CBD-CGD-O1D
39	F	310	CLA	CAD-CBD-CGD-O1D
39	H	316	CLA	CAD-CBD-CGD-O1D
39	J	312	CLA	CAD-CBD-CGD-O1D
39	R	315	CLA	CAD-CBD-CGD-O1D
39	T	313	CLA	C2-C3-C5-C6
39	U	201	CLA	CAD-CBD-CGD-O1D
39	U	215	CLA	CAD-CBD-CGD-O1D
39	W	316	CLA	CAD-CBD-CGD-O1D
39	X	317	CLA	CAD-CBD-CGD-O1D
39	0	313	CLA	CAD-CBD-CGD-O1D
39	1	311	CLA	CAD-CBD-CGD-O1D
39	3	320	CLA	CAD-CBD-CGD-O1D
39	3	323	CLA	CAD-CBD-CGD-O1D
39	8	318	CLA	CAD-CBD-CGD-O1D
39	9	310	CLA	CAD-CBD-CGD-O1D
39	x	314	CLA	CAD-CBD-CGD-O1D
39	y	310	CLA	CAD-CBD-CGD-O1D
39	y	319	CLA	CAD-CBD-CGD-O1D
39	z	309	CLA	CAD-CBD-CGD-O1D
39	z	314	CLA	CAD-CBD-CGD-O1D
39	Y	313	CLA	CAD-CBD-CGD-O1D
39	2	310	CLA	CAD-CBD-CGD-O1D
39	2	312	CLA	CAD-CBD-CGD-O1D
39	2	318	CLA	CAD-CBD-CGD-O1D
47	E	320	SQD	O5-C5-C6-S
47	W	301	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
48	k	206	A86	C26-C27-C29-C30
48	B	201	A86	C26-C27-C29-C30
48	Q	305	A86	C26-C27-C29-C30
48	R	302	A86	C26-C27-C29-C30
48	X	302	A86	C26-C27-C29-C30
48	0	309	A86	C26-C27-C29-C30
48	8	323	A86	C26-C27-C29-C30
50	C	302	A1EB1	C26-C27-C28-O6
50	E	301	A1EB1	C26-C27-C28-O6
50	G	304	A1EB1	C26-C27-C28-O6
50	G	307	A1EB1	C26-C27-C28-O6
50	H	304	A1EB1	C26-C27-C28-O6
50	K	302	A1EB1	C26-C27-C28-O6
50	O	301	A1EB1	C26-C27-C28-O6
50	R	303	A1EB1	C26-C27-C28-O6
50	U	203	A1EB1	C26-C27-C28-O6
50	U	205	A1EB1	C26-C27-C28-O6
50	V	305	A1EB1	C26-C27-C28-O6
50	0	302	A1EB1	C26-C27-C28-O6
50	0	305	A1EB1	C26-C27-C28-O6
50	1	301	A1EB1	C26-C27-C28-O6
50	3	310	A1EB1	C26-C27-C28-O6
50	4	301	A1EB1	C26-C27-C28-O6
50	4	302	A1EB1	C26-C27-C28-O6
50	5	302	A1EB1	C26-C27-C28-O6
50	7	303	A1EB1	C26-C27-C28-O6
50	7	304	A1EB1	C26-C27-C28-O6
50	8	301	A1EB1	C26-C27-C28-O6
50	8	306	A1EB1	C26-C27-C28-O6
50	9	302	A1EB1	C26-C27-C28-O6
50	y	301	A1EB1	C26-C27-C28-O6
50	2	304	A1EB1	C26-C27-C28-O6
50	2	306	A1EB1	C26-C27-C28-O6
50	6	301	A1EB1	C26-C27-C28-O6
46	S	321	LMG	C28-C29-C30-C31
47	F	318	SQD	C7-C8-C9-C10
39	b	851	CLA	CAA-CBA-CGA-O2A
39	D	316	CLA	C10-C11-C12-C13
39	D	312	CLA	O1D-CGD-O2D-CED
39	R	308	CLA	O1A-CGA-O2A-C1
39	C	311	CLA	C3-C5-C6-C7
41	a	840	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
46	S	321	LMG	C30-C31-C32-C33
39	a	818	CLA	CBA-CGA-O2A-C1
39	T	311	CLA	CBA-CGA-O2A-C1
50	6	301	A1EB1	C44-C42-O6-C28
39	C	307	CLA	C13-C15-C16-C17
39	0	313	CLA	C6-C7-C8-C10
39	a	804	CLA	C11-C12-C13-C15
39	a	815	CLA	C11-C12-C13-C15
39	a	818	CLA	C2-C3-C5-C6
39	a	818	CLA	C6-C7-C8-C10
39	a	829	CLA	C6-C7-C8-C10
39	b	814	CLA	C3A-C2A-CAA-CBA
39	b	821	CLA	C11-C10-C8-C7
39	b	824	CLA	C11-C10-C8-C7
39	b	826	CLA	C6-C7-C8-C10
39	b	832	CLA	C6-C7-C8-C10
39	A	312	CLA	C11-C12-C13-C15
39	C	308	CLA	C6-C7-C8-C10
39	D	311	CLA	C11-C10-C8-C7
39	D	316	CLA	C11-C10-C8-C7
39	E	312	CLA	C12-C13-C15-C16
39	E	313	CLA	C6-C7-C8-C10
39	L	310	CLA	C6-C7-C8-C10
39	M	310	CLA	C11-C10-C8-C7
39	P	308	CLA	C12-C13-C15-C16
39	0	323	CLA	C3A-C2A-CAA-CBA
39	I	309	CLA	C6-C7-C8-C10
39	2	319	CLA	C3A-C2A-CAA-CBA
39	6	312	CLA	C12-C13-C15-C16
41	j	104	LHG	O6-C4-C5-O7
46	W	320	LMG	C28-C29-C30-C31
41	a	840	LHG	C25-C26-C27-C28
50	0	302	A1EB1	C24-C25-C26-C27
39	a	805	CLA	C13-C15-C16-C17
39	l	204	CLA	C13-C15-C16-C17
39	4	314	CLA	C13-C15-C16-C17
41	a	840	LHG	C8-C7-O7-C5
46	l	208	LMG	C34-C35-C36-C37
46	4	325	LMG	C30-C31-C32-C33
39	a	822	CLA	C8-C10-C11-C12
39	V	311	CLA	C5-C6-C7-C8
39	B	209	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
39	C	308	CLA	C2A-CAA-CBA-CGA
39	G	310	CLA	C2A-CAA-CBA-CGA
39	G	318	CLA	C2A-CAA-CBA-CGA
39	L	320	CLA	C2A-CAA-CBA-CGA
39	T	311	CLA	C2A-CAA-CBA-CGA
39	T	318	CLA	C2A-CAA-CBA-CGA
39	I	309	CLA	C2A-CAA-CBA-CGA
39	a	816	CLA	C16-C17-C18-C20
50	V	302	A1EB1	C27-C28-O6-C42
46	Q	322	LMG	O1-C7-C8-C9
46	I	302	LMG	O1-C7-C8-C9
47	k	205	SQD	O6-C44-C45-C46
39	C	308	CLA	O1A-CGA-O2A-C1
41	H	317	LHG	O7-C5-C6-O8
46	l	208	LMG	O1-C7-C8-O7
46	A	316	LMG	O1-C7-C8-O7
46	D	322	LMG	O7-C8-C9-O8
46	F	317	LMG	O1-C7-C8-O7
46	Q	322	LMG	O1-C7-C8-O7
46	S	322	LMG	O7-C8-C9-O8
46	0	324	LMG	O1-C7-C8-O7
46	4	325	LMG	O1-C7-C8-O7
46	I	302	LMG	O1-C7-C8-O7
47	D	321	SQD	O47-C45-C46-O48
47	P	301	SQD	O6-C44-C45-O47
47	k	205	SQD	C10-C11-C12-C13
39	b	825	CLA	C13-C15-C16-C17
39	V	310	CLA	O1A-CGA-O2A-C1
45	C	314	DGD	C5D-C6D-O5D-C1E
39	a	811	CLA	C16-C17-C18-C19
40	a	839	PQN	C26-C27-C28-C30
39	D	310	CLA	O1D-CGD-O2D-CED
39	G	310	CLA	O1A-CGA-O2A-C1
50	6	301	A1EB1	O43-C42-O6-C28
39	3	319	CLA	O1D-CGD-O2D-CED
39	b	802	CLA	C15-C16-C17-C18
39	b	807	CLA	C4-C3-C5-C6
46	4	325	LMG	C29-C28-O8-C9
41	H	317	LHG	C14-C15-C16-C17
48	L	304	A86	C13-C14-C15-C20
48	M	302	A86	C13-C14-C15-C20
48	Q	305	A86	C13-C14-C15-C20

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Mol	Chain	Res	Type	Atoms
48	R	302	A86	C13-C14-C15-C20
48	W	303	A86	C13-C14-C15-C20
48	X	302	A86	C13-C14-C15-C20
48	X	303	A86	C13-C14-C15-C20
48	0	304	A86	C13-C14-C15-C20
48	5	301	A86	C13-C14-C15-C20
48	8	305	A86	C13-C14-C15-C20
48	6	305	A86	C13-C14-C15-C20
49	4	320	KC2	CAA-CBA-CGA-O1A
50	C	302	A1EB1	C13-C14-C15-C20
50	H	304	A1EB1	C13-C14-C15-C20
50	S	303	A1EB1	C13-C14-C15-C20
50	V	305	A1EB1	C13-C14-C15-C20
50	1	301	A1EB1	C13-C14-C15-C20
50	4	304	A1EB1	C13-C14-C15-C20
50	7	306	A1EB1	C13-C14-C15-C20
50	8	308	A1EB1	C13-C14-C15-C20
50	9	302	A1EB1	C13-C14-C15-C20
50	2	306	A1EB1	C13-C14-C15-C20
50	6	308	A1EB1	C13-C14-C15-C20
39	a	847	CLA	C6-C7-C8-C9
39	a	847	CLA	C11-C12-C13-C14
39	b	812	CLA	C6-C7-C8-C9
39	b	838	CLA	C11-C12-C13-C14
39	i	101	CLA	C11-C10-C8-C9
39	l	201	CLA	C11-C10-C8-C9
39	o	206	CLA	C6-C7-C8-C9
39	A	309	CLA	C6-C7-C8-C9
39	A	312	CLA	C11-C10-C8-C9
39	E	307	CLA	C11-C10-C8-C9
39	E	314	CLA	C6-C7-C8-C9
39	F	308	CLA	C6-C7-C8-C9
39	F	321	CLA	C11-C12-C13-C14
39	G	310	CLA	C6-C7-C8-C9
39	O	310	CLA	C11-C10-C8-C9
39	P	307	CLA	C11-C10-C8-C9
39	P	308	CLA	C14-C13-C15-C16
39	Q	310	CLA	C11-C12-C13-C14
39	Q	310	CLA	C14-C13-C15-C16
39	W	311	CLA	C11-C10-C8-C9
39	4	316	CLA	C14-C13-C15-C16
39	5	308	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
39	7	313	CLA	C11-C12-C13-C14
46	S	322	LMG	C12-C13-C14-C15
39	C	311	CLA	C16-C17-C18-C19
39	D	311	CLA	C16-C17-C18-C19
39	F	308	CLA	C16-C17-C18-C20
39	I	311	CLA	O1D-CGD-O2D-CED
39	a	818	CLA	O1A-CGA-O2A-C1
39	T	311	CLA	O1A-CGA-O2A-C1
39	a	817	CLA	C2A-CAA-CBA-CGA
50	2	304	A1EB1	O6-C42-C44-C45
39	9	312	CLA	C2C-C3C-CAC-CBC
50	3	303	A1EB1	C35-C34-O4-C38
39	4	311	CLA	C5-C6-C7-C8
46	l	208	LMG	C15-C16-C17-C18
39	b	832	CLA	O1D-CGD-O2D-CED
42	b	844	BCR	C11-C12-C13-C14
48	4	305	A86	C5-C6-C8-C9
48	Z	301	A86	C2-C1-C24-C25
47	P	301	SQD	C11-C10-C9-C8
39	a	803	CLA	C2B-C3B-CAB-CBB
39	a	804	CLA	C2B-C3B-CAB-CBB
39	a	808	CLA	C2B-C3B-CAB-CBB
39	a	809	CLA	C2B-C3B-CAB-CBB
39	a	810	CLA	C2B-C3B-CAB-CBB
39	a	818	CLA	C2B-C3B-CAB-CBB
39	a	819	CLA	C2B-C3B-CAB-CBB
39	a	824	CLA	C2B-C3B-CAB-CBB
39	a	828	CLA	C2B-C3B-CAB-CBB
39	b	810	CLA	C2B-C3B-CAB-CBB
39	b	820	CLA	C2B-C3B-CAB-CBB
39	b	825	CLA	C2B-C3B-CAB-CBB
39	b	827	CLA	C2B-C3B-CAB-CBB
39	b	831	CLA	C2B-C3B-CAB-CBB
39	b	835	CLA	C2B-C3B-CAB-CBB
39	i	101	CLA	C2B-C3B-CAB-CBB
39	l	203	CLA	C2B-C3B-CAB-CBB
39	A	308	CLA	C2B-C3B-CAB-CBB
39	A	312	CLA	C2B-C3B-CAB-CBB
39	B	205	CLA	C2B-C3B-CAB-CBB
39	B	209	CLA	C2B-C3B-CAB-CBB
39	D	311	CLA	C2B-C3B-CAB-CBB
39	D	314	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	F	306	CLA	C2B-C3B-CAB-CBB
39	F	309	CLA	C2B-C3B-CAB-CBB
39	H	316	CLA	C2B-C3B-CAB-CBB
39	J	314	CLA	C2B-C3B-CAB-CBB
39	J	316	CLA	C2B-C3B-CAB-CBB
39	J	317	CLA	C2B-C3B-CAB-CBB
39	K	314	CLA	C2B-C3B-CAB-CBB
39	L	313	CLA	C2B-C3B-CAB-CBB
39	O	312	CLA	C2B-C3B-CAB-CBB
39	P	307	CLA	C2B-C3B-CAB-CBB
39	Q	320	CLA	C2B-C3B-CAB-CBB
39	R	308	CLA	C2B-C3B-CAB-CBB
39	R	316	CLA	C2B-C3B-CAB-CBB
39	S	311	CLA	C2B-C3B-CAB-CBB
39	S	316	CLA	C2B-C3B-CAB-CBB
39	S	320	CLA	C2B-C3B-CAB-CBB
39	U	207	CLA	C2B-C3B-CAB-CBB
39	U	212	CLA	C2B-C3B-CAB-CBB
39	U	214	CLA	C2B-C3B-CAB-CBB
39	V	309	CLA	C2B-C3B-CAB-CBB
39	V	311	CLA	C2B-C3B-CAB-CBB
39	W	309	CLA	C2B-C3B-CAB-CBB
39	W	310	CLA	C2B-C3B-CAB-CBB
39	X	317	CLA	C2B-C3B-CAB-CBB
39	1	309	CLA	C2B-C3B-CAB-CBB
39	3	312	CLA	C2B-C3B-CAB-CBB
39	3	319	CLA	C2B-C3B-CAB-CBB
39	3	322	CLA	C2B-C3B-CAB-CBB
39	4	319	CLA	C2B-C3B-CAB-CBB
39	5	306	CLA	C2B-C3B-CAB-CBB
39	5	307	CLA	C2B-C3B-CAB-CBB
39	5	308	CLA	C2B-C3B-CAB-CBB
39	5	316	CLA	C2B-C3B-CAB-CBB
39	7	321	CLA	C2B-C3B-CAB-CBB
39	8	310	CLA	C2B-C3B-CAB-CBB
39	8	312	CLA	C2B-C3B-CAB-CBB
39	8	315	CLA	C2B-C3B-CAB-CBB
39	I	301	CLA	C2B-C3B-CAB-CBB
39	I	309	CLA	C2B-C3B-CAB-CBB
39	x	311	CLA	C2B-C3B-CAB-CBB
39	x	318	CLA	C2B-C3B-CAB-CBB
39	z	314	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	Y	302	CLA	C2B-C3B-CAB-CBB
39	Y	303	CLA	C2B-C3B-CAB-CBB
39	Y	304	CLA	C2B-C3B-CAB-CBB
39	Z	304	CLA	C2B-C3B-CAB-CBB
39	Z	305	CLA	C2B-C3B-CAB-CBB
39	Z	309	CLA	C2B-C3B-CAB-CBB
39	Z	312	CLA	C2B-C3B-CAB-CBB
39	Z	315	CLA	C2B-C3B-CAB-CBB
39	2	318	CLA	C2B-C3B-CAB-CBB
39	6	312	CLA	C2B-C3B-CAB-CBB
39	b	832	CLA	O1A-CGA-O2A-C1
47	F	319	SQD	O10-C23-O48-C46
39	a	805	CLA	C5-C6-C7-C8
39	A	309	CLA	C5-C6-C7-C8
48	6	307	A86	C33-C34-O4-C38
50	3	309	A1EB1	C33-C34-O4-C38
49	S	315	KC2	CAA-CBA-CGA-O2A
50	2	306	A1EB1	C44-C45-C46-C47
46	I	302	LMG	C10-C11-C12-C13
39	a	819	CLA	C1-C2-C3-C4
39	l	203	CLA	C1-C2-C3-C4
39	D	309	CLA	C1-C2-C3-C4
39	E	306	CLA	C1-C2-C3-C4
39	G	318	CLA	C1-C2-C3-C5
39	J	307	CLA	C1-C2-C3-C4
50	8	306	A1EB1	O6-C42-C44-C45
46	P	317	LMG	C7-C8-O7-C10
46	W	302	LMG	C7-C8-O7-C10
46	4	326	LMG	C9-C8-O7-C10
46	7	301	LMG	C9-C8-O7-C10
47	E	320	SQD	C44-C45-O47-C7
39	a	835	CLA	C2A-CAA-CBA-CGA
39	b	815	CLA	C2A-CAA-CBA-CGA
39	A	307	CLA	C2A-CAA-CBA-CGA
39	C	306	CLA	C2A-CAA-CBA-CGA
39	H	308	CLA	C2A-CAA-CBA-CGA
39	S	311	CLA	C2A-CAA-CBA-CGA
39	W	311	CLA	C2A-CAA-CBA-CGA
39	1	319	CLA	C2A-CAA-CBA-CGA
39	A	311	CLA	C10-C11-C12-C13
39	a	806	CLA	C2-C1-O2A-CGA
39	b	803	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
39	b	851	CLA	C2-C1-O2A-CGA
39	A	312	CLA	C2-C1-O2A-CGA
39	H	306	CLA	C2-C1-O2A-CGA
39	H	309	CLA	C2-C1-O2A-CGA
39	L	309	CLA	C2-C1-O2A-CGA
39	R	316	CLA	C2-C1-O2A-CGA
39	S	320	CLA	C2-C1-O2A-CGA
39	0	315	CLA	C2-C1-O2A-CGA
39	0	322	CLA	C2-C1-O2A-CGA
39	4	323	CLA	C2-C1-O2A-CGA
39	J	313	CLA	O1A-CGA-O2A-C1
50	3	309	A1EB1	O6-C42-C44-C45
46	F	317	LMG	C11-C12-C13-C14
50	8	308	A1EB1	C42-C44-C45-C46
48	L	302	A86	C12-C11-C13-C14
48	L	304	A86	C12-C11-C13-C14
48	L	306	A86	C12-C11-C13-C14
48	Q	305	A86	C12-C11-C13-C14
48	S	305	A86	C12-C11-C13-C14
48	T	305	A86	C12-C11-C13-C14
48	X	303	A86	C12-C11-C13-C14
48	4	305	A86	C12-C11-C13-C14
48	4	306	A86	C12-C11-C13-C14
48	8	302	A86	C12-C11-C13-C14
48	8	305	A86	C12-C11-C13-C14
48	9	304	A86	C12-C11-C13-C14
48	9	305	A86	C12-C11-C13-C14
48	x	305	A86	C12-C11-C13-C14
48	2	305	A86	C12-C11-C13-C14
48	6	309	A86	C12-C11-C13-C14
50	G	307	A1EB1	C12-C11-C13-C14
50	J	302	A1EB1	C12-C11-C13-C14
50	O	301	A1EB1	C12-C11-C13-C14
50	V	305	A1EB1	C12-C11-C13-C14
50	0	307	A1EB1	C12-C11-C13-C14
50	3	302	A1EB1	C12-C11-C13-C14
50	7	305	A1EB1	C12-C11-C13-C14
50	9	302	A1EB1	C12-C11-C13-C14
50	x	302	A1EB1	C12-C11-C13-C14
50	2	304	A1EB1	C12-C11-C13-C14
50	6	308	A1EB1	C12-C11-C13-C14
46	S	322	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
39	E	307	CLA	O1D-CGD-O2D-CED
48	8	309	A86	C3-C4-C5-C6
41	H	317	LHG	O6-C4-C5-O7
39	a	815	CLA	CAA-CBA-CGA-O2A
39	E	319	CLA	O2A-C1-C2-C3
39	a	835	CLA	C4-C3-C5-C6
39	I	310	CLA	C4C-C3C-CAC-CBC
46	W	302	LMG	C34-C35-C36-C37
39	D	318	CLA	O1D-CGD-O2D-CED
39	b	819	CLA	C3-C5-C6-C7
42	l	207	BCR	C5-C6-C7-C8
42	m	101	BCR	C1-C6-C7-C8
42	h	202	BCR	C23-C24-C25-C26
42	h	202	BCR	C23-C24-C25-C30
39	a	814	CLA	C2-C3-C5-C6
39	a	847	CLA	C2-C3-C5-C6
39	b	828	CLA	C2-C3-C5-C6
39	3	311	CLA	C2-C3-C5-C6
39	M	309	CLA	O1A-CGA-O2A-C1
46	P	317	LMG	C34-C35-C36-C37
47	D	321	SQD	C24-C23-O48-C46
39	b	806	CLA	CAA-CBA-CGA-O2A
39	f	802	CLA	C8-C10-C11-C12
51	X	310	A1ECV	O1D-CGD-O2D-CED
39	a	826	CLA	C16-C17-C18-C19
39	X	308	CLA	C11-C12-C13-C14
49	V	320	KC2	CAA-CBA-CGA-O2A
45	b	849	DGD	O6E-C1E-O5D-C6D
52	M	305	A1EB4	C11-C13-C14-C15
47	M	301	SQD	O47-C45-C46-O48
47	T	321	SQD	O47-C45-C46-O48
41	X	301	LHG	C4-O6-P-O3
46	D	322	LMG	C14-C15-C16-C17
51	L	318	A1ECV	CHA-CBD-CGD-O1D
51	L	318	A1ECV	CHA-CBD-CGD-O2D
51	Q	319	A1ECV	CHA-CBD-CGD-O1D
51	Q	319	A1ECV	CHA-CBD-CGD-O2D
49	6	314	KC2	CAA-CBA-CGA-O1A
45	b	849	DGD	O1G-C1G-C2G-C3G
47	F	318	SQD	O6-C44-C45-C46
39	b	835	CLA	C12-C13-C15-C16
39	A	306	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
39	E	307	CLA	C6-C7-C8-C10
39	H	310	CLA	C6-C7-C8-C10
39	K	312	CLA	C6-C7-C8-C10
39	M	308	CLA	C11-C10-C8-C7
39	V	313	CLA	C6-C7-C8-C10
39	W	310	CLA	C2-C3-C5-C6
39	W	310	CLA	C11-C10-C8-C7
39	7	316	CLA	C11-C12-C13-C15
40	a	839	PQN	C22-C23-C25-C26
39	a	815	CLA	C11-C12-C13-C14
39	a	818	CLA	C6-C7-C8-C9
39	b	809	CLA	C11-C10-C8-C9
39	b	821	CLA	C11-C10-C8-C9
39	D	311	CLA	C14-C13-C15-C16
39	G	309	CLA	C6-C7-C8-C9
39	M	308	CLA	C11-C10-C8-C9
39	M	310	CLA	C11-C10-C8-C9
39	W	310	CLA	C14-C13-C15-C16
39	W	311	CLA	C14-C13-C15-C16
39	X	309	CLA	C11-C12-C13-C14
39	I	309	CLA	C6-C7-C8-C9
39	b	838	CLA	C15-C16-C17-C18
43	Q	303	DD6	C24-C25-C26-C27
50	0	303	A1EB1	C1-C2-C3-C4
50	x	302	A1EB1	C3-C4-C5-C6
39	b	813	CLA	C6-C7-C8-C10
39	A	314	CLA	C16-C17-C18-C20
39	M	309	CLA	CBA-CGA-O2A-C1
51	7	323	A1ECV	CAA-CBA-CGA-O2A
39	a	822	CLA	O1A-CGA-O2A-C1
39	o	205	CLA	C3-C5-C6-C7
39	W	310	CLA	C5-C6-C7-C8
50	H	304	A1EB1	C42-C44-C45-C46
48	3	306	A86	C33-C34-O4-C38
42	b	850	BCR	C7-C8-C9-C34
42	m	101	BCR	C37-C22-C23-C24
48	8	307	A86	C-C1-C24-C25
39	3	312	CLA	C16-C17-C18-C19
39	M	310	CLA	CBA-CGA-O2A-C1
46	P	317	LMG	C16-C17-C18-C19
46	W	302	LMG	C16-C17-C18-C19
39	U	201	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
39	b	802	CLA	C13-C15-C16-C17
39	M	308	CLA	C15-C16-C17-C18
39	5	308	CLA	C15-C16-C17-C18
41	H	317	LHG	O1-C1-C2-O2
39	I	308	CLA	C2-C3-C5-C6
39	a	827	CLA	CBA-CGA-O2A-C1
39	b	840	CLA	CBA-CGA-O2A-C1
39	G	309	CLA	CBA-CGA-O2A-C1
39	M	310	CLA	O1A-CGA-O2A-C1
49	Q	315	KC2	CBD-CGD-O2D-CED
39	a	825	CLA	C3-C5-C6-C7
50	7	303	A1EB1	C45-C46-C47-C48
51	0	321	A1ECV	O1-CMC-O2-C3
39	a	802	CLA	O1D-CGD-O2D-CED
46	4	326	LMG	C33-C34-C35-C36
46	7	301	LMG	C33-C34-C35-C36
39	b	840	CLA	O1A-CGA-O2A-C1
39	G	309	CLA	O1A-CGA-O2A-C1
39	M	318	CLA	O1A-CGA-O2A-C1
39	a	822	CLA	CBA-CGA-O2A-C1
39	a	808	CLA	C4B-C3B-CAB-CBB
39	a	809	CLA	C4B-C3B-CAB-CBB
39	a	812	CLA	C4B-C3B-CAB-CBB
39	a	819	CLA	C4B-C3B-CAB-CBB
39	a	828	CLA	C4B-C3B-CAB-CBB
39	a	835	CLA	C4B-C3B-CAB-CBB
39	b	816	CLA	C4B-C3B-CAB-CBB
39	b	820	CLA	C4B-C3B-CAB-CBB
39	b	827	CLA	C4B-C3B-CAB-CBB
39	b	835	CLA	C4B-C3B-CAB-CBB
39	A	308	CLA	C4B-C3B-CAB-CBB
39	E	307	CLA	C4B-C3B-CAB-CBB
39	F	306	CLA	C4B-C3B-CAB-CBB
39	F	309	CLA	C4B-C3B-CAB-CBB
39	H	309	CLA	C4B-C3B-CAB-CBB
39	J	316	CLA	C4B-C3B-CAB-CBB
39	L	313	CLA	C4B-C3B-CAB-CBB
39	M	309	CLA	C4B-C3B-CAB-CBB
39	P	311	CLA	C4B-C3B-CAB-CBB
39	Q	320	CLA	C4B-C3B-CAB-CBB
39	R	308	CLA	C4B-C3B-CAB-CBB
39	R	316	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	U	207	CLA	C4B-C3B-CAB-CBB
39	V	309	CLA	C4B-C3B-CAB-CBB
39	V	311	CLA	C4B-C3B-CAB-CBB
39	W	309	CLA	C4B-C3B-CAB-CBB
39	W	310	CLA	C4B-C3B-CAB-CBB
39	X	317	CLA	C4B-C3B-CAB-CBB
39	3	319	CLA	C4B-C3B-CAB-CBB
39	4	319	CLA	C4B-C3B-CAB-CBB
39	5	306	CLA	C4B-C3B-CAB-CBB
39	8	312	CLA	C4B-C3B-CAB-CBB
39	I	309	CLA	C4B-C3B-CAB-CBB
39	x	311	CLA	C4B-C3B-CAB-CBB
39	x	318	CLA	C4B-C3B-CAB-CBB
39	Y	302	CLA	C4B-C3B-CAB-CBB
39	Z	304	CLA	C4B-C3B-CAB-CBB
39	Z	309	CLA	C4B-C3B-CAB-CBB
39	2	308	CLA	C4B-C3B-CAB-CBB
39	6	312	CLA	C4B-C3B-CAB-CBB
39	L	311	CLA	C2A-CAA-CBA-CGA
39	O	314	CLA	C2A-CAA-CBA-CGA
39	U	211	CLA	C2A-CAA-CBA-CGA
39	0	313	CLA	C2A-CAA-CBA-CGA
39	a	826	CLA	C16-C17-C18-C20
43	C	301	DD6	C3-C4-C5-C6
48	L	307	A86	C24-C25-C26-C27
48	O	306	A86	C11-C10-C9-C8
48	S	305	A86	C1-C2-C3-C4
50	T	302	A1EB1	C24-C25-C26-C27
50	0	303	A1EB1	C24-C25-C26-C27
50	7	303	A1EB1	C11-C10-C9-C8
50	7	306	A1EB1	C24-C25-C26-C27
50	y	302	A1EB1	C11-C10-C9-C8
39	h	201	CLA	CBD-CGD-O2D-CED
39	a	803	CLA	C15-C16-C17-C18
39	H	312	CLA	C10-C11-C12-C13
39	M	308	CLA	C10-C11-C12-C13
41	H	317	LHG	C12-C13-C14-C15
45	b	849	DGD	C9A-CAA-CBA-CCA
49	9	316	KC2	CAA-CBA-CGA-O1A
41	D	302	LHG	O6-C4-C5-O7
39	C	310	CLA	C16-C17-C18-C20
39	M	312	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
49	A	313	KC2	C4B-C3B-CAB-CBB
49	F	311	KC2	C4C-C3C-CAC-CBC
49	G	313	KC2	C4C-C3C-CAC-CBC
49	L	312	KC2	C4C-C3C-CAC-CBC
49	T	315	KC2	C4B-C3B-CAB-CBB
49	3	318	KC2	C4C-C3C-CAC-CBC
49	I	312	KC2	C4C-C3C-CAC-CBC
49	6	316	KC2	C4C-C3C-CAC-CBC
50	6	306	A1EB1	C35-C34-O4-C38
39	9	308	CLA	C3-C5-C6-C7
47	4	327	SQD	C11-C12-C13-C14
39	a	803	CLA	C4-C3-C5-C6
39	B	209	CLA	C4-C3-C5-C6
39	D	312	CLA	C4-C3-C5-C6
39	E	307	CLA	C4-C3-C5-C6
39	T	309	CLA	C4-C3-C5-C6
39	b	833	CLA	C8-C10-C11-C12
39	5	306	CLA	C10-C11-C12-C13
39	a	803	CLA	C2-C3-C5-C6
39	b	835	CLA	C2-C3-C5-C6
46	l	208	LMG	C32-C33-C34-C35
50	4	304	A1EB1	C44-C45-C46-C47
51	7	323	A1ECV	CAA-CBA-CGA-O1A
39	a	820	CLA	C2-C1-O2A-CGA
39	a	821	CLA	C2-C1-O2A-CGA
39	a	825	CLA	C2-C1-O2A-CGA
39	k	202	CLA	C2-C1-O2A-CGA
39	P	308	CLA	C2-C1-O2A-CGA
40	a	839	PQN	C20-C21-C22-C23
39	A	309	CLA	C2A-CAA-CBA-CGA
39	D	313	CLA	C2A-CAA-CBA-CGA
39	F	310	CLA	C2A-CAA-CBA-CGA
39	H	313	CLA	C2A-CAA-CBA-CGA
39	P	309	CLA	C2A-CAA-CBA-CGA
39	Q	312	CLA	C2A-CAA-CBA-CGA
39	U	208	CLA	C2A-CAA-CBA-CGA
39	W	310	CLA	C2A-CAA-CBA-CGA
39	4	314	CLA	C2A-CAA-CBA-CGA
39	I	308	CLA	C2A-CAA-CBA-CGA
46	M	319	LMG	C14-C15-C16-C17
49	y	313	KC2	CBD-CGD-O2D-CED
39	B	207	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
49	V	312	KC2	CAA-CBA-CGA-O2A
49	6	316	KC2	CAA-CBA-CGA-O1A
39	F	316	CLA	C3A-C2A-CAA-CBA
39	7	313	CLA	C3A-C2A-CAA-CBA
39	0	320	CLA	O1D-CGD-O2D-CED
39	J	309	CLA	C16-C17-C18-C20
39	4	312	CLA	C16-C17-C18-C19
47	D	320	SQD	C24-C23-O48-C46
48	P	302	A86	O-C13-C14-C15
48	7	311	A86	O-C13-C14-C15
48	6	309	A86	O-C13-C14-C15
50	6	301	A1EB1	O-C13-C14-C15
50	6	308	A1EB1	O-C13-C14-C15
39	b	835	CLA	C4-C3-C5-C6
47	T	321	SQD	C11-C10-C9-C8
39	a	822	CLA	C11-C12-C13-C14
39	b	824	CLA	C11-C10-C8-C9
39	b	825	CLA	C14-C13-C15-C16
39	D	311	CLA	C11-C10-C8-C9
39	M	312	CLA	C11-C10-C8-C9
39	M	312	CLA	C14-C13-C15-C16
39	S	320	CLA	C11-C12-C13-C14
39	W	310	CLA	C11-C12-C13-C14
39	W	311	CLA	C11-C12-C13-C14
39	4	314	CLA	C6-C7-C8-C9
39	4	323	CLA	C11-C12-C13-C14
47	F	318	SQD	C11-C12-C13-C14
39	8	312	CLA	CAA-CBA-CGA-O1A
39	I	313	CLA	C13-C15-C16-C17
39	C	310	CLA	CBA-CGA-O2A-C1
45	C	314	DGD	C3B-C4B-C5B-C6B
42	b	846	BCR	C20-C21-C22-C37
42	f	804	BCR	C35-C13-C14-C15
42	l	202	BCR	C11-C10-C9-C34
46	9	321	LMG	O1-C7-C8-C9
48	L	302	A86	C25-C26-C27-C28
48	2	305	A86	C-C1-C2-C3
39	l	204	CLA	C2A-CAA-CBA-CGA
39	0	315	CLA	C2A-CAA-CBA-CGA
39	3	311	CLA	C2A-CAA-CBA-CGA
50	V	302	A1EB1	C44-C45-C46-C47
39	A	314	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
39	b	819	CLA	O2A-C1-C2-C3
50	O	301	A1EB1	C33-C34-O4-C38
39	P	307	CLA	O1D-CGD-O2D-CED
49	6	316	KC2	O1D-CGD-O2D-CED
43	a	846	DD6	C7-C6-C8-C9
43	7	310	DD6	C7-C6-C8-C9
48	Q	308	A86	C-C1-C24-C25
50	0	303	A1EB1	C7-C6-C8-C9
50	7	305	A1EB1	C-C1-C24-C25
39	a	827	CLA	O1A-CGA-O2A-C1
46	P	317	LMG	C9-C8-O7-C10
46	S	322	LMG	C7-C8-O7-C10
46	W	302	LMG	C9-C8-O7-C10
39	9	308	CLA	C4-C3-C5-C6
39	b	802	CLA	C1A-C2A-CAA-CBA
39	b	814	CLA	C1A-C2A-CAA-CBA
39	b	836	CLA	C1A-C2A-CAA-CBA
39	b	839	CLA	C1A-C2A-CAA-CBA
39	j	101	CLA	C1A-C2A-CAA-CBA
39	o	206	CLA	C1A-C2A-CAA-CBA
39	A	314	CLA	C1A-C2A-CAA-CBA
39	C	309	CLA	C1A-C2A-CAA-CBA
39	D	311	CLA	C1A-C2A-CAA-CBA
39	E	315	CLA	C1A-C2A-CAA-CBA
39	F	308	CLA	C1A-C2A-CAA-CBA
39	F	316	CLA	C1A-C2A-CAA-CBA
39	F	321	CLA	C1A-C2A-CAA-CBA
39	J	311	CLA	C1A-C2A-CAA-CBA
39	K	312	CLA	C1A-C2A-CAA-CBA
39	U	210	CLA	C1A-C2A-CAA-CBA
39	W	309	CLA	C1A-C2A-CAA-CBA
39	4	316	CLA	C1A-C2A-CAA-CBA
39	I	309	CLA	C1A-C2A-CAA-CBA
39	h	201	CLA	C1A-C2A-CAA-CBA
46	P	317	LMG	C4-C5-C6-O5
46	W	302	LMG	C4-C5-C6-O5
39	b	835	CLA	CAA-CBA-CGA-O2A
50	L	303	A1EB1	O6-C42-C44-C45
39	b	837	CLA	C11-C10-C8-C7
39	j	101	CLA	C12-C13-C15-C16
39	A	309	CLA	C11-C12-C13-C15
39	E	312	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
39	Q	310	CLA	C6-C7-C8-C10
39	Q	312	CLA	C12-C13-C15-C16
39	0	310	CLA	C11-C12-C13-C15
49	2	317	KC2	CAA-CBA-CGA-O2A
46	S	321	LMG	C12-C13-C14-C15
50	5	302	A1EB1	C44-C45-C46-C47
52	X	305	A1EB4	C11-C13-C14-C15
39	b	811	CLA	O1A-CGA-O2A-C1
39	C	310	CLA	O1A-CGA-O2A-C1
39	1	310	CLA	CAA-CBA-CGA-O2A
39	J	311	CLA	O1A-CGA-O2A-C1
39	1	310	CLA	CAA-CBA-CGA-O1A
47	4	327	SQD	C11-C10-C9-C8
39	Q	314	CLA	C6-C7-C8-C9
39	b	801	CLA	C2A-CAA-CBA-CGA
39	b	831	CLA	C2A-CAA-CBA-CGA
39	J	307	CLA	C2A-CAA-CBA-CGA
39	4	322	CLA	C2A-CAA-CBA-CGA
39	7	316	CLA	C2A-CAA-CBA-CGA
39	b	807	CLA	C13-C15-C16-C17
39	b	828	CLA	C10-C11-C12-C13
39	J	314	CLA	C5-C6-C7-C8
47	F	319	SQD	C7-C8-C9-C10
39	I	310	CLA	C2C-C3C-CAC-CBC
46	Q	322	LMG	C28-C29-C30-C31
39	A	305	CLA	O2A-C1-C2-C3
39	J	310	CLA	CBA-CGA-O2A-C1
46	I	302	LMG	C37-C38-C39-C40
49	A	310	KC2	C3A-C2A-CAA-CBA
49	G	311	KC2	C3A-C2A-CAA-CBA
49	G	313	KC2	C3A-C2A-CAA-CBA
49	J	315	KC2	C3A-C2A-CAA-CBA
49	K	310	KC2	C3A-C2A-CAA-CBA
49	L	312	KC2	C3A-C2A-CAA-CBA
49	L	317	KC2	C3A-C2A-CAA-CBA
49	L	321	KC2	C3A-C2A-CAA-CBA
49	M	307	KC2	C3A-C2A-CAA-CBA
49	M	311	KC2	C3A-C2A-CAA-CBA
49	P	310	KC2	C3A-C2A-CAA-CBA
49	Q	315	KC2	C3A-C2A-CAA-CBA
49	R	306	KC2	C3A-C2A-CAA-CBA
49	R	312	KC2	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
49	R	314	KC2	C3A-C2A-CAA-CBA
49	R	318	KC2	C3A-C2A-CAA-CBA
49	S	314	KC2	C3A-C2A-CAA-CBA
49	T	315	KC2	C3A-C2A-CAA-CBA
49	T	316	KC2	C3A-C2A-CAA-CBA
49	V	308	KC2	C3A-C2A-CAA-CBA
49	V	315	KC2	C3A-C2A-CAA-CBA
49	V	318	KC2	C3A-C2A-CAA-CBA
49	W	308	KC2	C3A-C2A-CAA-CBA
49	W	312	KC2	C3A-C2A-CAA-CBA
49	X	306	KC2	C3A-C2A-CAA-CBA
49	X	314	KC2	C3A-C2A-CAA-CBA
49	X	318	KC2	C3A-C2A-CAA-CBA
49	1	312	KC2	C3A-C2A-CAA-CBA
49	1	314	KC2	C3A-C2A-CAA-CBA
49	3	321	KC2	C3A-C2A-CAA-CBA
49	4	317	KC2	C3A-C2A-CAA-CBA
49	4	318	KC2	C3A-C2A-CAA-CBA
49	5	305	KC2	C3A-C2A-CAA-CBA
49	5	311	KC2	C3A-C2A-CAA-CBA
49	5	313	KC2	C3A-C2A-CAA-CBA
49	7	319	KC2	C3A-C2A-CAA-CBA
49	7	320	KC2	C3A-C2A-CAA-CBA
49	8	314	KC2	C3A-C2A-CAA-CBA
49	8	317	KC2	C3A-C2A-CAA-CBA
49	9	313	KC2	C3A-C2A-CAA-CBA
49	x	313	KC2	C3A-C2A-CAA-CBA
49	y	313	KC2	C3A-C2A-CAA-CBA
49	2	314	KC2	C3A-C2A-CAA-CBA
39	H	312	CLA	C16-C17-C18-C20
39	J	311	CLA	C16-C17-C18-C20
46	l	208	LMG	C11-C12-C13-C14
39	b	809	CLA	CAA-CBA-CGA-O2A
47	4	327	SQD	C24-C25-C26-C27
39	a	804	CLA	C5-C6-C7-C8
39	9	308	CLA	C5-C6-C7-C8
50	V	306	A1EB1	C42-C44-C45-C46
39	0	320	CLA	CBD-CGD-O2D-CED
39	a	835	CLA	C2B-C3B-CAB-CBB
39	a	837	CLA	C2B-C3B-CAB-CBB
39	b	826	CLA	C2B-C3B-CAB-CBB
39	b	833	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	o	205	CLA	C2B-C3B-CAB-CBB
39	o	206	CLA	C2B-C3B-CAB-CBB
39	B	204	CLA	C2B-C3B-CAB-CBB
39	B	206	CLA	C2B-C3B-CAB-CBB
39	D	316	CLA	C2B-C3B-CAB-CBB
39	D	319	CLA	C2B-C3B-CAB-CBB
39	F	308	CLA	C2B-C3B-CAB-CBB
39	G	310	CLA	C2B-C3B-CAB-CBB
39	H	309	CLA	C2B-C3B-CAB-CBB
39	H	313	CLA	C2B-C3B-CAB-CBB
39	M	309	CLA	C2B-C3B-CAB-CBB
39	Q	309	CLA	C2B-C3B-CAB-CBB
39	Q	312	CLA	C2B-C3B-CAB-CBB
39	T	308	CLA	C2B-C3B-CAB-CBB
39	U	208	CLA	C2B-C3B-CAB-CBB
39	U	211	CLA	C2B-C3B-CAB-CBB
39	0	313	CLA	C2B-C3B-CAB-CBB
39	3	313	CLA	C2B-C3B-CAB-CBB
39	7	314	CLA	C2B-C3B-CAB-CBB
39	8	313	CLA	C2B-C3B-CAB-CBB
39	h	201	CLA	C2B-C3B-CAB-CBB
39	y	309	CLA	C2B-C3B-CAB-CBB
39	Y	307	CLA	C2B-C3B-CAB-CBB
39	2	308	CLA	C2B-C3B-CAB-CBB
50	h	203	A1EB1	C44-C45-C46-C47
39	a	834	CLA	CBA-CGA-O2A-C1
39	8	310	CLA	CAA-CBA-CGA-O1A
39	R	308	CLA	C5-C6-C7-C8
50	8	304	A1EB1	C44-C45-C46-C47
46	F	317	LMG	C10-C11-C12-C13
46	Q	322	LMG	O9-C10-O7-C8
50	S	303	A1EB1	C33-C34-O4-C38
42	b	846	BCR	C20-C21-C22-C23
42	f	804	BCR	C12-C13-C14-C15
42	l	202	BCR	C11-C10-C9-C8
48	L	302	A86	C25-C26-C27-C29
48	8	307	A86	C13-C14-C15-C16
48	2	305	A86	C24-C1-C2-C3
48	2	305	A86	C13-C14-C15-C16
50	3	324	A1EB1	C13-C14-C15-C16
50	z	302	A1EB1	C13-C14-C15-C16
39	0	320	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
50	x	302	A1EB1	C45-C46-C47-C48
41	a	840	LHG	O7-C5-C6-O8
45	b	849	DGD	O1G-C1G-C2G-O2G
46	l	208	LMG	O7-C8-C9-O8
46	P	317	LMG	O7-C8-C9-O8
46	W	302	LMG	O7-C8-C9-O8
46	A	316	LMG	C8-C9-O8-C28
43	G	303	DD6	C11-C10-C9-C8
43	z	304	DD6	C3-C4-C5-C6
48	Q	308	A86	C24-C25-C26-C27
48	9	303	A86	C1-C2-C3-C4
50	H	304	A1EB1	C24-C25-C26-C27
50	V	307	A1EB1	C24-C25-C26-C27
50	7	303	A1EB1	C24-C25-C26-C27
39	0	320	CLA	CAA-CBA-CGA-O2A
48	S	307	A86	C33-C34-O4-C38
48	9	306	A86	C33-C34-O4-C38
50	1	301	A1EB1	C33-C34-O4-C38
39	h	201	CLA	O1D-CGD-O2D-CED
39	a	815	CLA	C16-C17-C18-C19
48	D	305	A86	C10-C11-C13-C14
48	H	302	A86	C10-C11-C13-C14
48	L	302	A86	C10-C11-C13-C14
48	M	302	A86	C10-C11-C13-C14
48	O	307	A86	C10-C11-C13-C14
48	P	302	A86	C10-C11-C13-C14
48	S	304	A86	C10-C11-C13-C14
48	S	305	A86	C10-C11-C13-C14
48	4	328	A86	C10-C11-C13-C14
48	8	307	A86	C10-C11-C13-C14
48	9	305	A86	C10-C11-C13-C14
48	z	303	A86	C10-C11-C13-C14
48	2	305	A86	C10-C11-C13-C14
50	L	303	A1EB1	C10-C11-C13-C14
50	O	301	A1EB1	C10-C11-C13-C14
50	S	303	A1EB1	C10-C11-C13-C14
50	3	302	A1EB1	C10-C11-C13-C14
50	9	302	A1EB1	C10-C11-C13-C14
50	h	203	A1EB1	C10-C11-C13-C14
50	y	302	A1EB1	C10-C11-C13-C14
50	6	308	A1EB1	C10-C11-C13-C14
39	K	309	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
39	0	312	CLA	C4-C3-C5-C6
40	b	843	PQN	C14-C13-C15-C16
39	a	828	CLA	C2-C1-O2A-CGA
39	E	309	CLA	C2-C1-O2A-CGA
39	F	316	CLA	C2-C1-O2A-CGA
39	J	309	CLA	C2-C1-O2A-CGA
39	V	310	CLA	C2-C1-O2A-CGA
39	V	319	CLA	C2-C1-O2A-CGA
39	0	311	CLA	C2-C1-O2A-CGA
39	4	311	CLA	C2-C1-O2A-CGA
39	b	829	CLA	CBD-CGD-O2D-CED
39	T	310	CLA	O1A-CGA-O2A-C1
39	J	309	CLA	C13-C15-C16-C17
39	8	312	CLA	CAA-CBA-CGA-O2A
45	b	849	DGD	C7B-C8B-C9B-CAB
46	W	320	LMG	C11-C12-C13-C14
39	X	308	CLA	C11-C12-C13-C15
39	a	814	CLA	C11-C10-C8-C9
39	a	826	CLA	C11-C12-C13-C14
39	b	801	CLA	C14-C13-C15-C16
39	b	842	CLA	C14-C13-C15-C16
39	P	311	CLA	C11-C12-C13-C14
39	W	309	CLA	C11-C10-C8-C9
39	J	310	CLA	O1A-CGA-O2A-C1
39	8	310	CLA	CAA-CBA-CGA-O2A
50	0	307	A1EB1	C45-C46-C47-C48
50	6	301	A1EB1	C44-C45-C46-C47
39	A	308	CLA	C4-C3-C5-C6
39	T	313	CLA	C4-C3-C5-C6
49	Q	313	KC2	C1A-C2A-CAA-CBA
49	T	312	KC2	C1A-C2A-CAA-CBA
49	1	315	KC2	C1A-C2A-CAA-CBA
49	3	315	KC2	C1A-C2A-CAA-CBA
49	3	318	KC2	C1A-C2A-CAA-CBA
39	k	203	CLA	CBD-CGD-O2D-CED
39	a	834	CLA	O1A-CGA-O2A-C1
39	J	314	CLA	C8-C10-C11-C12
39	V	313	CLA	C15-C16-C17-C18
39	E	317	CLA	C2A-CAA-CBA-CGA
39	K	309	CLA	C2A-CAA-CBA-CGA
39	V	311	CLA	C2A-CAA-CBA-CGA
39	3	314	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
39	I	309	CLA	C16-C17-C18-C20
39	T	310	CLA	CBA-CGA-O2A-C1
48	9	301	A86	C35-C34-O4-C38
39	a	801	CLA	CAA-CBA-CGA-O1A
42	a	842	BCR	C1-C6-C7-C8
42	a	842	BCR	C5-C6-C7-C8
42	b	848	BCR	C1-C6-C7-C8
42	l	206	BCR	C1-C6-C7-C8
42	l	207	BCR	C1-C6-C7-C8
39	a	830	CLA	C10-C11-C12-C13
51	z	310	A1ECV	O1D-CGD-O2D-CED
42	f	801	BCR	C36-C18-C19-C20
46	l	208	LMG	C7-C8-C9-O8
51	R	313	A1ECV	CAA-CBA-CGA-O2A
43	O	304	DD6	C1-C2-C3-C4
50	S	303	A1EB1	C1-C2-C3-C4
50	5	302	A1EB1	C24-C25-C26-C27
50	x	301	A1EB1	C1-C2-C3-C4
52	X	305	A1EB4	C1-C2-C3-C4
39	E	308	CLA	C4-C3-C5-C6
39	G	309	CLA	C4-C3-C5-C6
39	L	309	CLA	C4-C3-C5-C6
39	Q	310	CLA	C4-C3-C5-C6
43	A	303	DD6	C5-C6-C8-C9
50	7	305	A1EB1	C2-C1-C24-C25
52	T	304	A1EB4	C2-C1-C24-C25
39	C	310	CLA	C16-C17-C18-C19
39	A	307	CLA	C5-C6-C7-C8
39	I	308	CLA	C10-C11-C12-C13
39	b	806	CLA	C2-C3-C5-C6
39	b	807	CLA	C2-C3-C5-C6
39	C	308	CLA	C2-C3-C5-C6
39	9	308	CLA	C2-C3-C5-C6
46	I	302	LMG	C8-C7-O1-C1
47	H	318	SQD	C45-C44-O6-C1
39	X	316	CLA	C2-C1-O2A-CGA
46	M	319	LMG	C11-C12-C13-C14
39	A	311	CLA	C16-C17-C18-C20
47	W	301	SQD	C24-C23-O48-C46
39	4	312	CLA	C5-C6-C7-C8
39	a	831	CLA	C2A-CAA-CBA-CGA
39	5	316	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
45	b	849	DGD	C6B-C7B-C8B-C9B
46	M	320	LMG	C14-C15-C16-C17
39	3	311	CLA	CAA-CBA-CGA-O2A
39	J	311	CLA	CBA-CGA-O2A-C1
39	b	818	CLA	C3-C5-C6-C7
39	b	840	CLA	C3-C5-C6-C7
39	a	807	CLA	O1D-CGD-O2D-CED
39	a	804	CLA	C4B-C3B-CAB-CBB
39	a	824	CLA	C4B-C3B-CAB-CBB
39	b	826	CLA	C4B-C3B-CAB-CBB
39	b	828	CLA	C4B-C3B-CAB-CBB
39	o	206	CLA	C4B-C3B-CAB-CBB
39	B	204	CLA	C4B-C3B-CAB-CBB
39	D	316	CLA	C4B-C3B-CAB-CBB
39	D	319	CLA	C4B-C3B-CAB-CBB
39	E	309	CLA	C4B-C3B-CAB-CBB
39	E	310	CLA	C4B-C3B-CAB-CBB
39	E	318	CLA	C4B-C3B-CAB-CBB
39	F	308	CLA	C4B-C3B-CAB-CBB
39	G	310	CLA	C4B-C3B-CAB-CBB
39	H	313	CLA	C4B-C3B-CAB-CBB
39	U	211	CLA	C4B-C3B-CAB-CBB
39	0	313	CLA	C4B-C3B-CAB-CBB
39	3	313	CLA	C4B-C3B-CAB-CBB
39	3	314	CLA	C4B-C3B-CAB-CBB
39	5	307	CLA	C4B-C3B-CAB-CBB
39	5	308	CLA	C4B-C3B-CAB-CBB
39	7	314	CLA	C4B-C3B-CAB-CBB
39	8	313	CLA	C4B-C3B-CAB-CBB
39	I	310	CLA	C4B-C3B-CAB-CBB
39	h	201	CLA	C4B-C3B-CAB-CBB
39	P	309	CLA	C13-C15-C16-C17
39	a	804	CLA	C4-C3-C5-C6
39	3	313	CLA	C4-C3-C5-C6
46	Q	322	LMG	C11-C10-O7-C8
39	a	826	CLA	C11-C12-C13-C15
39	b	810	CLA	C11-C10-C8-C7
39	E	308	CLA	C2-C3-C5-C6
39	P	311	CLA	C11-C10-C8-C7
39	W	309	CLA	C11-C10-C8-C7
39	W	313	CLA	C11-C10-C8-C7
39	3	311	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
39	7	313	CLA	C11-C12-C13-C15
41	a	841	LHG	C24-C23-O8-C6
41	a	840	LHG	C17-C18-C19-C20
46	Q	322	LMG	C4-C5-C6-O5
51	P	315	A1ECV	C1C-C2C-CMC-O2
51	R	310	A1ECV	C1C-C2C-CMC-O2
51	9	314	A1ECV	C1C-C2C-CMC-O1
51	9	314	A1ECV	C1C-C2C-CMC-O2
43	A	303	DD6	C11-C10-C9-C8
43	E	303	DD6	C1-C2-C3-C4
45	b	849	DGD	C2E-C1E-O5D-C6D
48	7	308	A86	C33-C34-O4-C38
47	S	301	SQD	O47-C45-C46-O48
39	E	317	CLA	CBA-CGA-O2A-C1
39	a	803	CLA	CBD-CGD-O2D-CED
39	a	822	CLA	C13-C15-C16-C17
46	l	208	LMG	C4-C5-C6-O5
46	F	317	LMG	C4-C5-C6-O5
46	F	320	LMG	C4-C5-C6-O5
39	E	306	CLA	O2A-C1-C2-C3
39	b	807	CLA	CAA-CBA-CGA-O2A
39	E	319	CLA	CAA-CBA-CGA-O2A
39	4	312	CLA	C16-C17-C18-C20
49	8	314	KC2	CAA-CBA-CGA-O2A
39	a	803	CLA	O1D-CGD-O2D-CED
39	b	821	CLA	CBA-CGA-O2A-C1
39	I	311	CLA	CBA-CGA-O2A-C1
39	a	825	CLA	C4-C3-C5-C6
39	b	838	CLA	C4-C3-C5-C6
39	o	205	CLA	C4-C3-C5-C6
39	D	319	CLA	C4-C3-C5-C6
39	E	310	CLA	C4-C3-C5-C6
39	F	308	CLA	C4-C3-C5-C6
39	H	308	CLA	C4-C3-C5-C6
40	a	839	PQN	C14-C13-C15-C16
41	H	317	LHG	C11-C10-C9-C8
49	C	312	KC2	C2A-CAA-CBA-CGA
49	P	320	KC2	C2A-CAA-CBA-CGA
39	J	309	CLA	C16-C17-C18-C19
39	R	316	CLA	CAA-CBA-CGA-O2A
39	5	316	CLA	CAA-CBA-CGA-O2A
39	Z	306	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
50	F	304	A1EB1	O6-C42-C44-C45
47	7	302	SQD	C26-C27-C28-C29
39	a	801	CLA	C14-C13-C15-C16
39	a	829	CLA	C6-C7-C8-C9
39	b	826	CLA	C6-C7-C8-C9
39	C	308	CLA	C6-C7-C8-C9
39	D	316	CLA	C11-C10-C8-C9
39	F	313	CLA	C6-C7-C8-C9
39	H	312	CLA	C11-C10-C8-C9
39	M	310	CLA	C6-C7-C8-C9
39	S	309	CLA	C6-C7-C8-C9
39	S	311	CLA	C6-C7-C8-C9
39	W	310	CLA	C11-C10-C8-C9
39	4	316	CLA	C11-C12-C13-C14
47	M	301	SQD	C10-C11-C12-C13
50	6	308	A1EB1	O43-C42-C44-C45
39	a	820	CLA	C3A-C2A-CAA-CBA
39	b	802	CLA	C3A-C2A-CAA-CBA
39	j	101	CLA	C3A-C2A-CAA-CBA
39	E	312	CLA	C3A-C2A-CAA-CBA
39	E	316	CLA	C3A-C2A-CAA-CBA
39	G	309	CLA	C3A-C2A-CAA-CBA
39	J	307	CLA	C3A-C2A-CAA-CBA
39	0	311	CLA	C3A-C2A-CAA-CBA
39	3	314	CLA	C3A-C2A-CAA-CBA
39	I	301	CLA	C3A-C2A-CAA-CBA
39	b	816	CLA	C8-C10-C11-C12
39	b	825	CLA	O1A-CGA-O2A-C1
39	E	317	CLA	O1A-CGA-O2A-C1
39	3	323	CLA	CAA-CBA-CGA-O2A
47	D	321	SQD	O47-C7-C8-C9
39	a	807	CLA	CBD-CGD-O2D-CED
39	a	802	CLA	CAD-CBD-CGD-O2D
39	a	809	CLA	CAD-CBD-CGD-O2D
39	a	810	CLA	CAD-CBD-CGD-O2D
39	a	812	CLA	CAD-CBD-CGD-O2D
39	a	815	CLA	CAD-CBD-CGD-O2D
39	a	824	CLA	CAD-CBD-CGD-O2D
39	a	834	CLA	CAD-CBD-CGD-O2D
39	a	847	CLA	CAD-CBD-CGD-O2D
39	b	832	CLA	CAD-CBD-CGD-O2D
39	b	839	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
39	b	841	CLA	CAD-CBD-CGD-O2D
39	f	802	CLA	CAD-CBD-CGD-O2D
39	f	803	CLA	CAD-CBD-CGD-O2D
39	o	202	CLA	CAD-CBD-CGD-O2D
39	A	308	CLA	CAD-CBD-CGD-O2D
39	C	307	CLA	CAD-CBD-CGD-O2D
39	D	309	CLA	CAD-CBD-CGD-O2D
39	D	315	CLA	CAD-CBD-CGD-O2D
39	D	316	CLA	CAD-CBD-CGD-O2D
39	E	309	CLA	CAD-CBD-CGD-O2D
39	G	318	CLA	CAD-CBD-CGD-O2D
39	K	306	CLA	CAD-CBD-CGD-O2D
39	K	309	CLA	CAD-CBD-CGD-O2D
39	K	311	CLA	CAD-CBD-CGD-O2D
39	L	313	CLA	CAD-CBD-CGD-O2D
39	L	319	CLA	CAD-CBD-CGD-O2D
39	Q	314	CLA	CAD-CBD-CGD-O2D
39	Q	321	CLA	CAD-CBD-CGD-O2D
39	R	316	CLA	CAD-CBD-CGD-O2D
39	S	311	CLA	CAD-CBD-CGD-O2D
39	S	316	CLA	CAD-CBD-CGD-O2D
39	W	318	CLA	CAD-CBD-CGD-O2D
39	1	313	CLA	CAD-CBD-CGD-O2D
39	4	312	CLA	CAD-CBD-CGD-O2D
39	5	315	CLA	CAD-CBD-CGD-O2D
39	7	318	CLA	CAD-CBD-CGD-O2D
39	9	312	CLA	CAD-CBD-CGD-O2D
39	9	315	CLA	CAD-CBD-CGD-O2D
39	x	317	CLA	CAD-CBD-CGD-O2D
39	6	315	CLA	CAD-CBD-CGD-O2D
39	6	321	CLA	CAD-CBD-CGD-O2D
46	S	322	LMG	C9-C8-O7-C10
48	G	301	A86	C28-C27-C29-C30
48	L	306	A86	C28-C27-C29-C30
48	M	302	A86	C28-C27-C29-C30
48	O	306	A86	C28-C27-C29-C30
48	3	308	A86	C28-C27-C29-C30
48	5	301	A86	C28-C27-C29-C30
48	8	305	A86	C28-C27-C29-C30
48	y	306	A86	C28-C27-C29-C30
49	J	315	KC2	CAD-CBD-CGD-O2D
49	L	315	KC2	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
49	S	315	KC2	C2C-C3C-CAC-CBC
49	0	314	KC2	CAD-CBD-CGD-O2D
49	4	318	KC2	CAD-CBD-CGD-O2D
49	5	314	KC2	CAD-CBD-CGD-O2D
49	8	314	KC2	CAD-CBD-CGD-O2D
49	y	314	KC2	CAD-CBD-CGD-O2D
49	Z	311	KC2	CAD-CBD-CGD-O2D
49	6	317	KC2	CAD-CBD-CGD-O2D
51	Q	316	A1ECV	CAD-CBD-CGD-O2D
51	R	310	A1ECV	CAD-CBD-CGD-O2D
51	R	313	A1ECV	CAD-CBD-CGD-O2D
51	W	317	A1ECV	CAD-CBD-CGD-O2D
51	X	313	A1ECV	CAD-CBD-CGD-O2D
51	5	309	A1ECV	CAD-CBD-CGD-O2D
51	7	317	A1ECV	CAD-CBD-CGD-O2D
51	x	310	A1ECV	CAD-CBD-CGD-O2D
51	y	317	A1ECV	CAD-CBD-CGD-O2D
51	z	310	A1ECV	CAD-CBD-CGD-O2D
51	Y	306	A1ECV	CAD-CBD-CGD-O2D
51	Y	312	A1ECV	CAD-CBD-CGD-O2D
51	Z	308	A1ECV	CAD-CBD-CGD-O2D
51	Z	314	A1ECV	CAD-CBD-CGD-O2D
47	F	318	SQD	C23-C24-C25-C26
46	9	321	LMG	C33-C34-C35-C36
39	y	308	CLA	C2A-CAA-CBA-CGA
46	D	322	LMG	O9-C10-O7-C8
47	S	301	SQD	C26-C27-C28-C29
49	2	317	KC2	CBD-CGD-O2D-CED
39	a	807	CLA	C2-C1-O2A-CGA
39	a	830	CLA	C2-C1-O2A-CGA
39	I	313	CLA	C2-C1-O2A-CGA
39	I	315	CLA	C2-C1-O2A-CGA
39	G	318	CLA	CAA-CBA-CGA-O2A
39	K	308	CLA	CAA-CBA-CGA-O2A
39	Y	304	CLA	CAA-CBA-CGA-O2A
39	b	803	CLA	O1D-CGD-O2D-CED
39	a	836	CLA	C4-C3-C5-C6
39	b	802	CLA	C4-C3-C5-C6
39	b	803	CLA	C4-C3-C5-C6
39	b	806	CLA	C4-C3-C5-C6
39	b	820	CLA	C4-C3-C5-C6
39	b	825	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
39	F	313	CLA	C4-C3-C5-C6
39	4	314	CLA	C4-C3-C5-C6
39	b	803	CLA	C16-C17-C18-C19
39	a	833	CLA	CAA-CBA-CGA-O2A
39	b	808	CLA	CAA-CBA-CGA-O2A
48	K	301	A86	C35-C34-O4-C38
39	a	810	CLA	CAA-CBA-CGA-O2A
39	D	311	CLA	CAA-CBA-CGA-O2A
39	D	317	CLA	CAA-CBA-CGA-O2A
39	J	310	CLA	CAA-CBA-CGA-O2A
39	X	308	CLA	CAA-CBA-CGA-O2A
46	F	317	LMG	O8-C28-C29-C30
47	F	319	SQD	O47-C7-C8-C9
50	G	302	A1EB1	O6-C42-C44-C45
50	0	305	A1EB1	O6-C42-C44-C45
42	b	850	BCR	C7-C8-C9-C10
42	f	801	BCR	C17-C18-C19-C20
43	a	846	DD6	C10-C11-C13-C14
43	1	304	DD6	C10-C11-C13-C14
48	Q	308	A86	C2-C1-C24-C25
48	8	307	A86	C2-C1-C24-C25
48	Z	301	A86	C5-C6-C8-C9
50	H	301	A1EB1	C5-C6-C8-C9
50	0	303	A1EB1	C5-C6-C8-C9
39	E	314	CLA	C11-C10-C8-C9
39	L	311	CLA	C3-C5-C6-C7
49	W	315	KC2	CAA-CBA-CGA-O2A
49	X	315	KC2	CAA-CBA-CGA-O1A
43	A	304	DD6	C13-C14-C15-O1
43	3	301	DD6	C13-C14-C15-O1
43	z	304	DD6	C13-C14-C15-O1
48	L	305	A86	C12-C11-C13-O
48	P	302	A86	C12-C11-C13-O
48	Q	301	A86	C12-C11-C13-O
48	Z	301	A86	C12-C11-C13-O
48	Z	303	A86	C12-C11-C13-O
48	6	309	A86	C12-C11-C13-O
50	J	302	A1EB1	C12-C11-C13-O
50	T	302	A1EB1	C12-C11-C13-O
50	V	302	A1EB1	C12-C11-C13-O
50	3	303	A1EB1	C12-C11-C13-O
50	3	310	A1EB1	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
50	7	306	A1EB1	C12-C11-C13-O
50	h	203	A1EB1	C12-C11-C13-O
39	a	809	CLA	CBA-CGA-O2A-C1
39	b	825	CLA	CBA-CGA-O2A-C1
39	a	803	CLA	CAA-CBA-CGA-O2A
39	F	306	CLA	CBA-CGA-O2A-C1
39	I	310	CLA	C6-C7-C8-C9
41	X	301	LHG	C13-C14-C15-C16
46	7	301	LMG	C15-C16-C17-C18
39	a	828	CLA	O2A-C1-C2-C3
39	b	820	CLA	O2A-C1-C2-C3
39	F	314	CLA	O2A-C1-C2-C3
39	G	312	CLA	O2A-C1-C2-C3
39	L	310	CLA	O2A-C1-C2-C3
39	T	309	CLA	O2A-C1-C2-C3
39	X	307	CLA	O2A-C1-C2-C3
39	0	312	CLA	O2A-C1-C2-C3
39	9	308	CLA	O2A-C1-C2-C3
46	4	326	LMG	C15-C16-C17-C18
49	A	313	KC2	C4C-C3C-CAC-CBC
49	P	313	KC2	C4C-C3C-CAC-CBC
49	Q	315	KC2	C4C-C3C-CAC-CBC
49	S	315	KC2	C4C-C3C-CAC-CBC
49	V	314	KC2	C4C-C3C-CAC-CBC
49	0	317	KC2	C4B-C3B-CAB-CBB
49	7	319	KC2	C4C-C3C-CAC-CBC
49	7	320	KC2	C4B-C3B-CAB-CBB
49	7	320	KC2	C4C-C3C-CAC-CBC
49	2	317	KC2	C4B-C3B-CAB-CBB
39	a	819	CLA	C2A-CAA-CBA-CGA
39	J	313	CLA	C2A-CAA-CBA-CGA
39	0	310	CLA	C2A-CAA-CBA-CGA
39	C	304	CLA	C2A-CAA-CBA-CGA
39	A	307	CLA	C10-C11-C12-C13
39	G	310	CLA	C10-C11-C12-C13
50	3	309	A1EB1	C44-C45-C46-C47
39	F	309	CLA	CAA-CBA-CGA-O2A
39	Q	320	CLA	CAA-CBA-CGA-O2A
39	T	310	CLA	CAA-CBA-CGA-O2A
39	I	315	CLA	CAA-CBA-CGA-O2A
39	a	833	CLA	CAA-CBA-CGA-O1A
39	b	808	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
48	7	311	A86	O5-C38-O4-C34
39	b	827	CLA	C16-C17-C18-C19
39	f	803	CLA	C6-C7-C8-C10
39	H	312	CLA	C16-C17-C18-C19
39	L	309	CLA	C6-C7-C8-C9
39	a	806	CLA	CHA-CBD-CGD-O1D
39	a	806	CLA	CHA-CBD-CGD-O2D
39	a	819	CLA	CHA-CBD-CGD-O2D
39	a	821	CLA	CHA-CBD-CGD-O1D
39	a	821	CLA	CHA-CBD-CGD-O2D
39	a	831	CLA	CHA-CBD-CGD-O1D
39	a	831	CLA	CHA-CBD-CGD-O2D
39	a	835	CLA	CHA-CBD-CGD-O2D
39	b	817	CLA	CHA-CBD-CGD-O1D
39	b	827	CLA	CHA-CBD-CGD-O2D
39	b	837	CLA	CHA-CBD-CGD-O1D
39	A	314	CLA	CHA-CBD-CGD-O1D
39	A	314	CLA	CHA-CBD-CGD-O2D
39	B	209	CLA	CHA-CBD-CGD-O1D
39	B	209	CLA	CHA-CBD-CGD-O2D
39	C	306	CLA	CHA-CBD-CGD-O2D
39	C	308	CLA	CHA-CBD-CGD-O2D
39	D	317	CLA	CHA-CBD-CGD-O1D
39	D	318	CLA	CHA-CBD-CGD-O2D
39	E	307	CLA	CHA-CBD-CGD-O1D
39	E	307	CLA	CHA-CBD-CGD-O2D
39	E	318	CLA	CHA-CBD-CGD-O2D
39	F	308	CLA	CHA-CBD-CGD-O1D
39	F	308	CLA	CHA-CBD-CGD-O2D
39	F	321	CLA	CHA-CBD-CGD-O1D
39	G	312	CLA	CHA-CBD-CGD-O1D
39	G	312	CLA	CHA-CBD-CGD-O2D
39	J	309	CLA	CHA-CBD-CGD-O2D
39	J	318	CLA	CHA-CBD-CGD-O1D
39	J	318	CLA	CHA-CBD-CGD-O2D
39	L	308	CLA	CHA-CBD-CGD-O1D
39	L	308	CLA	CHA-CBD-CGD-O2D
39	U	201	CLA	CHA-CBD-CGD-O2D
39	U	209	CLA	CHA-CBD-CGD-O2D
39	U	211	CLA	CHA-CBD-CGD-O1D
39	U	211	CLA	CHA-CBD-CGD-O2D
39	U	214	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	X	309	CLA	CHA-CBD-CGD-O1D
39	X	309	CLA	CHA-CBD-CGD-O2D
39	0	310	CLA	CHA-CBD-CGD-O1D
39	0	310	CLA	CHA-CBD-CGD-O2D
39	1	316	CLA	CHA-CBD-CGD-O1D
39	1	317	CLA	CHA-CBD-CGD-O1D
39	1	317	CLA	CHA-CBD-CGD-O2D
39	3	322	CLA	CHA-CBD-CGD-O1D
39	3	322	CLA	CHA-CBD-CGD-O2D
39	4	312	CLA	CHA-CBD-CGD-O2D
39	4	322	CLA	CHA-CBD-CGD-O1D
39	8	313	CLA	CHA-CBD-CGD-O1D
39	I	308	CLA	CHA-CBD-CGD-O1D
39	I	308	CLA	CHA-CBD-CGD-O2D
39	I	311	CLA	CHA-CBD-CGD-O1D
39	I	311	CLA	CHA-CBD-CGD-O2D
39	Y	307	CLA	CHA-CBD-CGD-O2D
39	Y	314	CLA	CHA-CBD-CGD-O2D
39	Z	304	CLA	CHA-CBD-CGD-O1D
39	Z	304	CLA	CHA-CBD-CGD-O2D
39	2	316	CLA	CHA-CBD-CGD-O1D
39	2	316	CLA	CHA-CBD-CGD-O2D
39	6	322	CLA	CHA-CBD-CGD-O1D
39	6	322	CLA	CHA-CBD-CGD-O2D
48	U	206	A86	C11-C10-C9-C8
49	A	313	KC2	CHA-CBD-CGD-O2D
49	C	313	KC2	CHA-CBD-CGD-O1D
49	L	317	KC2	CHA-CBD-CGD-O1D
49	Q	315	KC2	CHA-CBD-CGD-O2D
49	S	314	KC2	CHA-CBD-CGD-O2D
49	T	312	KC2	CHA-CBD-CGD-O2D
49	V	314	KC2	CHA-CBD-CGD-O2D
49	V	315	KC2	CHA-CBD-CGD-O1D
49	1	314	KC2	CHA-CBD-CGD-O2D
49	5	311	KC2	CHA-CBD-CGD-O2D
49	9	318	KC2	CHA-CBD-CGD-O2D
49	x	312	KC2	CHA-CBD-CGD-O1D
49	x	312	KC2	CHA-CBD-CGD-O2D
49	z	312	KC2	CHA-CBD-CGD-O2D
39	O	309	CLA	CAA-CBA-CGA-O2A
39	C	308	CLA	C4-C3-C5-C6
39	L	311	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
39	a	836	CLA	C2-C3-C5-C6
49	W	314	KC2	CAA-CBA-CGA-O2A
41	a	840	LHG	C24-C25-C26-C27
39	a	816	CLA	C8-C10-C11-C12
39	C	307	CLA	CAA-CBA-CGA-O2A
39	J	309	CLA	CAA-CBA-CGA-O2A
39	L	308	CLA	CAA-CBA-CGA-O2A
39	S	309	CLA	CAA-CBA-CGA-O2A
39	S	311	CLA	CAA-CBA-CGA-O2A
39	3	314	CLA	CAA-CBA-CGA-O2A
39	7	315	CLA	CAA-CBA-CGA-O2A
50	3	302	A1EB1	O6-C42-C44-C45
46	9	321	LMG	O1-C7-C8-O7
39	D	310	CLA	C5-C6-C7-C8
39	I	311	CLA	C5-C6-C7-C8
39	x	306	CLA	CAA-CBA-CGA-O2A
39	T	320	CLA	CAA-CBA-CGA-O2A
39	V	310	CLA	CAA-CBA-CGA-O2A
50	7	304	A1EB1	O6-C42-C44-C45
46	P	317	LMG	C11-C12-C13-C14
46	W	302	LMG	C11-C12-C13-C14
39	X	316	CLA	C2A-CAA-CBA-CGA
48	D	305	A86	C10-C11-C13-O
48	D	305	A86	C13-C14-C15-O1
48	G	301	A86	C13-C14-C15-O1
48	L	304	A86	C13-C14-C15-O1
48	M	302	A86	C10-C11-C13-O
48	P	302	A86	C10-C11-C13-O
48	P	302	A86	C13-C14-C15-O1
48	Q	301	A86	C10-C11-C13-O
48	Q	308	A86	C13-C14-C15-O1
48	R	317	A86	C13-C14-C15-O1
48	S	304	A86	C10-C11-C13-O
48	T	306	A86	C13-C14-C15-O1
48	X	302	A86	C13-C14-C15-O1
48	0	309	A86	C13-C14-C15-O1
48	1	306	A86	C13-C14-C15-O1
48	5	301	A86	C13-C14-C15-O1
48	7	312	A86	C13-C14-C15-O1
48	9	303	A86	C10-C11-C13-O
48	9	306	A86	C13-C14-C15-O1
48	Z	301	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
48	2	305	A86	C13-C14-C15-O1
48	6	305	A86	C13-C14-C15-O1
50	L	303	A1EB1	C13-C14-C15-O1
50	T	302	A1EB1	C10-C11-C13-O
50	T	302	A1EB1	C13-C14-C15-O1
50	U	203	A1EB1	C13-C14-C15-O1
50	V	302	A1EB1	C13-C14-C15-O1
50	0	302	A1EB1	C13-C14-C15-O1
50	1	301	A1EB1	C13-C14-C15-O1
50	3	303	A1EB1	C10-C11-C13-O
50	3	324	A1EB1	C13-C14-C15-O1
50	4	304	A1EB1	C10-C11-C13-O
50	5	302	A1EB1	C13-C14-C15-O1
50	7	306	A1EB1	C10-C11-C13-O
50	8	304	A1EB1	C13-C14-C15-O1
50	h	203	A1EB1	C10-C11-C13-O
50	y	301	A1EB1	C10-C11-C13-O
50	z	301	A1EB1	C10-C11-C13-O
50	z	302	A1EB1	C13-C14-C15-O1
51	R	310	A1ECV	CHA-CBD-CGD-O1D
39	o	203	CLA	CBA-CGA-O2A-C1
39	A	314	CLA	CBA-CGA-O2A-C1
39	l	201	CLA	CAA-CBA-CGA-O2A
39	b	803	CLA	CBD-CGD-O2D-CED
49	6	314	KC2	CAA-CBA-CGA-O2A
39	a	806	CLA	C6-C7-C8-C10
39	a	835	CLA	C12-C13-C15-C16
39	b	803	CLA	C2-C3-C5-C6
39	b	812	CLA	C11-C12-C13-C15
39	b	842	CLA	C11-C12-C13-C15
39	o	206	CLA	C11-C10-C8-C7
39	D	319	CLA	C2-C3-C5-C6
39	F	308	CLA	C6-C7-C8-C10
39	5	306	CLA	C11-C12-C13-C15
39	5	308	CLA	C11-C12-C13-C15
39	I	311	CLA	C12-C13-C15-C16
43	I	305	DD6	C27-C29-C30-C31
50	7	303	A1EB1	C44-C45-C46-C47
39	L	310	CLA	CAA-CBA-CGA-O2A
39	W	319	CLA	CAA-CBA-CGA-O2A
39	3	322	CLA	CAA-CBA-CGA-O2A
46	F	320	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
47	W	301	SQD	O47-C7-C8-C9
39	b	812	CLA	C11-C12-C13-C14
39	b	837	CLA	C11-C10-C8-C9
39	F	321	CLA	C14-C13-C15-C16
39	M	312	CLA	C6-C7-C8-C9
39	Q	310	CLA	C6-C7-C8-C9
39	I	311	CLA	C14-C13-C15-C16
43	D	307	DD6	C24-C25-C26-C27
43	J	304	DD6	C11-C10-C9-C8
52	W	321	A1EB4	C3-C4-C5-C6
39	C	311	CLA	C2B-C3B-CAB-CBB
41	a	841	LHG	O2-C2-C3-O3
39	l	203	CLA	O2A-C1-C2-C3
39	b	821	CLA	O1A-CGA-O2A-C1
47	H	318	SQD	C24-C23-O48-C46
39	M	318	CLA	CAA-CBA-CGA-O2A
47	W	301	SQD	C4-C5-C6-S
47	9	322	SQD	C4-C5-C6-S
50	C	302	A1EB1	C29-C27-C28-O6
50	F	304	A1EB1	C29-C27-C28-O6
50	G	307	A1EB1	C29-C27-C28-O6
50	G	308	A1EB1	C29-C27-C28-O6
50	K	305	A1EB1	C29-C27-C28-O6
50	O	301	A1EB1	C29-C27-C28-O6
50	R	303	A1EB1	C29-C27-C28-O6
50	T	302	A1EB1	C29-C27-C28-O6
50	U	203	A1EB1	C29-C27-C28-O6
50	V	305	A1EB1	C29-C27-C28-O6
50	0	302	A1EB1	C29-C27-C28-O6
50	1	301	A1EB1	C29-C27-C28-O6
50	4	302	A1EB1	C29-C27-C28-O6
50	5	302	A1EB1	C29-C27-C28-O6
50	7	304	A1EB1	C29-C27-C28-O6
50	8	301	A1EB1	C29-C27-C28-O6
50	9	302	A1EB1	C29-C27-C28-O6
50	y	301	A1EB1	C29-C27-C28-O6
50	2	306	A1EB1	C29-C27-C28-O6
50	6	301	A1EB1	C29-C27-C28-O6
39	a	806	CLA	C16-C17-C18-C20
39	a	815	CLA	C16-C17-C18-C20
39	I	309	CLA	C16-C17-C18-C19
41	a	840	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
41	H	317	LHG	C15-C16-C17-C18
39	I	311	CLA	C13-C15-C16-C17
39	W	319	CLA	C2A-CAA-CBA-CGA
49	Z	311	KC2	CBD-CGD-O2D-CED
41	a	840	LHG	C30-C31-C32-C33
50	4	301	A1EB1	O6-C42-C44-C45
39	b	807	CLA	CAA-CBA-CGA-O1A
39	Y	304	CLA	CAA-CBA-CGA-O1A
47	W	301	SQD	O49-C7-C8-C9
39	b	803	CLA	C16-C17-C18-C20
39	X	309	CLA	C16-C17-C18-C20
47	P	301	SQD	C27-C28-C29-C30
39	o	203	CLA	O1A-CGA-O2A-C1
39	I	311	CLA	O1A-CGA-O2A-C1
39	D	312	CLA	C2-C3-C5-C6
50	L	303	A1EB1	C45-C46-C47-C48
50	8	301	A1EB1	C2-C1-C24-C25
52	M	305	A1EB4	C2-C1-C24-C25
39	W	311	CLA	CBA-CGA-O2A-C1
39	X	308	CLA	CBA-CGA-O2A-C1
49	7	322	KC2	O1D-CGD-O2D-CED
39	a	811	CLA	C1A-C2A-CAA-CBA
39	a	820	CLA	C1A-C2A-CAA-CBA
39	b	826	CLA	C1A-C2A-CAA-CBA
39	k	203	CLA	C1A-C2A-CAA-CBA
39	E	312	CLA	C1A-C2A-CAA-CBA
39	E	316	CLA	C1A-C2A-CAA-CBA
39	E	317	CLA	C1A-C2A-CAA-CBA
39	J	307	CLA	C1A-C2A-CAA-CBA
39	K	307	CLA	C1A-C2A-CAA-CBA
39	V	310	CLA	C1A-C2A-CAA-CBA
39	X	308	CLA	C1A-C2A-CAA-CBA
39	3	314	CLA	C1A-C2A-CAA-CBA
39	7	325	CLA	C1A-C2A-CAA-CBA
39	I	301	CLA	C1A-C2A-CAA-CBA
52	P	305	A1EB4	C13-C11-C12-O3
52	T	304	A1EB4	C13-C11-C12-O3
52	W	306	A1EB4	C13-C11-C12-O3
52	X	305	A1EB4	C13-C11-C12-O3
39	b	806	CLA	C16-C17-C18-C20
39	D	311	CLA	CAA-CBA-CGA-O1A
39	E	319	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
39	X	308	CLA	CAA-CBA-CGA-O1A
47	E	320	SQD	O49-C7-C8-C9
50	G	302	A1EB1	O43-C42-C44-C45
51	R	313	A1ECV	CAA-CBA-CGA-O1A
39	A	314	CLA	C2-C1-O2A-CGA
48	7	311	A86	C39-C38-O4-C34
39	a	810	CLA	CAA-CBA-CGA-O1A
39	K	308	CLA	CAA-CBA-CGA-O1A
39	Z	306	CLA	CAA-CBA-CGA-O1A
50	F	304	A1EB1	O43-C42-C44-C45
46	I	302	LMG	C15-C16-C17-C18
39	k	203	CLA	O1D-CGD-O2D-CED
39	b	810	CLA	CAA-CBA-CGA-O2A
39	E	314	CLA	CAA-CBA-CGA-O2A
39	a	806	CLA	C10-C11-C12-C13
39	E	313	CLA	C2A-CAA-CBA-CGA
39	R	309	CLA	C2A-CAA-CBA-CGA
39	U	212	CLA	C2A-CAA-CBA-CGA
39	X	309	CLA	C2A-CAA-CBA-CGA
39	0	312	CLA	C2A-CAA-CBA-CGA
39	J	311	CLA	C16-C17-C18-C19
39	L	311	CLA	CAA-CBA-CGA-O1A
39	5	316	CLA	CAA-CBA-CGA-O1A
46	4	325	LMG	C29-C30-C31-C32
39	l	205	CLA	CAA-CBA-CGA-O2A
39	o	205	CLA	CAA-CBA-CGA-O2A
39	P	309	CLA	CAA-CBA-CGA-O2A
39	T	308	CLA	CAA-CBA-CGA-O2A
50	y	301	A1EB1	O6-C42-C44-C45
39	b	833	CLA	C10-C11-C12-C13
46	l	208	LMG	O9-C10-O7-C8
41	D	301	LHG	C13-C14-C15-C16
39	G	318	CLA	CAA-CBA-CGA-O1A
39	L	310	CLA	CAA-CBA-CGA-O1A
39	R	316	CLA	CAA-CBA-CGA-O1A
39	9	308	CLA	CAA-CBA-CGA-O1A
41	X	301	LHG	O9-C7-C8-C9
47	M	301	SQD	O10-C23-C24-C25
47	9	322	SQD	O49-C7-C8-C9
39	a	835	CLA	C2-C3-C5-C6
39	B	209	CLA	C2-C3-C5-C6
39	E	307	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
50	4	303	A1EB1	C35-C34-O4-C38
46	F	320	LMG	C2-C1-O1-C7
39	a	801	CLA	C5-C6-C7-C8
39	a	823	CLA	C4B-C3B-CAB-CBB
39	B	206	CLA	C4B-C3B-CAB-CBB
39	C	311	CLA	C4B-C3B-CAB-CBB
39	V	310	CLA	C4B-C3B-CAB-CBB
39	I	314	CLA	C4B-C3B-CAB-CBB
39	x	309	CLA	C4B-C3B-CAB-CBB
39	a	803	CLA	CAA-CBA-CGA-O1A
39	C	307	CLA	CAA-CBA-CGA-O1A
39	J	309	CLA	CAA-CBA-CGA-O1A
39	J	310	CLA	CAA-CBA-CGA-O1A
39	L	308	CLA	CAA-CBA-CGA-O1A
39	S	309	CLA	CAA-CBA-CGA-O1A
39	T	310	CLA	CAA-CBA-CGA-O1A
39	T	320	CLA	CAA-CBA-CGA-O1A
39	3	323	CLA	CAA-CBA-CGA-O1A
39	I	315	CLA	CAA-CBA-CGA-O1A
39	a	807	CLA	CAA-CBA-CGA-O2A
49	T	314	KC2	CBD-CGD-O2D-CED
39	O	309	CLA	CAA-CBA-CGA-O1A
39	y	308	CLA	CAA-CBA-CGA-O2A
42	l	206	BCR	C5-C6-C7-C8
50	T	307	A1EB1	C33-C34-O4-C38
39	a	823	CLA	C8-C10-C11-C12
39	F	309	CLA	CAA-CBA-CGA-O1A
39	3	322	CLA	CAA-CBA-CGA-O1A
39	7	315	CLA	CAA-CBA-CGA-O1A
46	9	321	LMG	O9-C10-C11-C12
50	0	305	A1EB1	O43-C42-C44-C45
39	X	308	CLA	O1A-CGA-O2A-C1
49	P	310	KC2	C2A-CAA-CBA-CGA
49	W	312	KC2	C2A-CAA-CBA-CGA
39	a	813	CLA	CAA-CBA-CGA-O2A
39	D	313	CLA	CAA-CBA-CGA-O2A
39	K	309	CLA	CAA-CBA-CGA-O2A
39	M	309	CLA	CAA-CBA-CGA-O2A
39	4	314	CLA	CAA-CBA-CGA-O2A
50	4	302	A1EB1	O6-C42-C44-C45
39	x	306	CLA	CAA-CBA-CGA-O1A
39	K	307	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
39	O	310	CLA	C2A-CAA-CBA-CGA
39	5	308	CLA	C2A-CAA-CBA-CGA
39	l	201	CLA	CAA-CBA-CGA-O1A
39	D	317	CLA	CAA-CBA-CGA-O1A
39	0	310	CLA	CAA-CBA-CGA-O1A
39	A	314	CLA	O1A-CGA-O2A-C1
39	b	818	CLA	C5-C6-C7-C8
39	X	309	CLA	C5-C6-C7-C8
39	3	314	CLA	C8-C10-C11-C12
49	4	324	KC2	CAA-CBA-CGA-O2A
39	a	820	CLA	CAA-CBA-CGA-O2A
39	F	306	CLA	CAA-CBA-CGA-O2A
39	W	309	CLA	CAA-CBA-CGA-O2A
39	4	313	CLA	CAA-CBA-CGA-O2A
39	a	830	CLA	C15-C16-C17-C18
39	b	815	CLA	C4C-C3C-CAC-CBC
39	Q	320	CLA	CAA-CBA-CGA-O1A
39	3	314	CLA	CAA-CBA-CGA-O1A
39	a	807	CLA	C4-C3-C5-C6
39	M	309	CLA	C4-C3-C5-C6
48	P	302	A86	C24-C25-C26-C27
39	T	309	CLA	C2-C3-C5-C6
39	b	815	CLA	C5-C6-C7-C8
39	b	838	CLA	C10-C11-C12-C13
39	C	310	CLA	C10-C11-C12-C13
39	a	830	CLA	CAD-CBD-CGD-O1D
39	a	833	CLA	CAD-CBD-CGD-O1D
39	a	835	CLA	CAD-CBD-CGD-O1D
39	b	805	CLA	CAD-CBD-CGD-O1D
39	b	827	CLA	CAD-CBD-CGD-O1D
39	b	837	CLA	CAD-CBD-CGD-O1D
39	C	308	CLA	CAD-CBD-CGD-O1D
39	D	318	CLA	CAD-CBD-CGD-O1D
39	F	321	CLA	CAD-CBD-CGD-O1D
39	G	314	CLA	CAD-CBD-CGD-O1D
39	M	309	CLA	CAD-CBD-CGD-O1D
39	Q	317	CLA	CAD-CBD-CGD-O1D
39	S	319	CLA	CAD-CBD-CGD-O1D
39	U	209	CLA	CAD-CBD-CGD-O1D
39	X	316	CLA	CAD-CBD-CGD-O1D
39	1	309	CLA	CAD-CBD-CGD-O1D
39	1	319	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	3	314	CLA	CAD-CBD-CGD-O1D
39	x	306	CLA	CAD-CBD-CGD-O1D
39	x	309	CLA	CAD-CBD-CGD-O1D
39	Y	307	CLA	CAD-CBD-CGD-O1D
39	Z	304	CLA	CAD-CBD-CGD-O1D
47	F	318	SQD	O5-C5-C6-S
47	S	301	SQD	C5-C6-S-O9
48	D	305	A86	C26-C27-C29-C30
48	G	301	A86	C26-C27-C29-C30
48	O	306	A86	C26-C27-C29-C30
48	0	304	A86	C26-C27-C29-C30
48	3	308	A86	C26-C27-C29-C30
48	8	305	A86	C26-C27-C29-C30
48	I	304	A86	C26-C27-C29-C30
48	y	306	A86	C26-C27-C29-C30
48	Y	301	A86	C26-C27-C29-C30
49	I	303	KC2	CAD-CBD-CGD-O1D
50	z	301	A1EB1	C26-C27-C29-C30
51	Q	319	A1ECV	CAD-CBD-CGD-O1D
39	W	311	CLA	O1A-CGA-O2A-C1
39	S	311	CLA	CAA-CBA-CGA-O1A
46	F	320	LMG	O9-C10-C11-C12
50	7	304	A1EB1	O43-C42-C44-C45
39	M	321	CLA	CAA-CBA-CGA-O2A
39	0	313	CLA	CAA-CBA-CGA-O2A
50	8	301	A1EB1	O6-C42-C44-C45
39	a	806	CLA	C6-C7-C8-C9
39	b	801	CLA	C11-C12-C13-C14
39	b	806	CLA	C14-C13-C15-C16
39	b	842	CLA	C11-C12-C13-C14
39	A	309	CLA	C11-C12-C13-C14
39	G	310	CLA	C11-C10-C8-C9
39	V	313	CLA	C14-C13-C15-C16
39	0	310	CLA	C11-C12-C13-C14
39	3	314	CLA	C11-C10-C8-C9
39	5	306	CLA	C11-C10-C8-C9
39	b	807	CLA	C8-C10-C11-C12
39	7	314	CLA	C5-C6-C7-C8
40	a	839	PQN	C18-C20-C21-C22
50	T	302	A1EB1	C42-C44-C45-C46
39	A	308	CLA	CAA-CBA-CGA-O2A
39	F	314	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
39	Q	312	CLA	CAA-CBA-CGA-O2A
39	7	325	CLA	CAA-CBA-CGA-O2A
39	I	301	CLA	CAA-CBA-CGA-O2A
39	2	309	CLA	CAA-CBA-CGA-O2A
46	M	319	LMG	O7-C10-C11-C12
46	S	322	LMG	O8-C28-C29-C30
46	9	321	LMG	O7-C10-C11-C12
47	E	320	SQD	O47-C7-C8-C9
50	T	302	A1EB1	O6-C42-C44-C45
39	a	826	CLA	C8-C10-C11-C12
39	a	809	CLA	O1A-CGA-O2A-C1
39	A	305	CLA	O1A-CGA-O2A-C1
49	Y	308	KC2	CAA-CBA-CGA-O1A
39	b	814	CLA	CAA-CBA-CGA-O2A
39	i	101	CLA	CAA-CBA-CGA-O2A
39	A	309	CLA	CAA-CBA-CGA-O2A
39	E	313	CLA	CAA-CBA-CGA-O2A
39	J	307	CLA	CAA-CBA-CGA-O2A
39	0	322	CLA	CAA-CBA-CGA-O2A
39	5	307	CLA	CAA-CBA-CGA-O2A
39	7	316	CLA	CAA-CBA-CGA-O2A
39	I	309	CLA	CAA-CBA-CGA-O2A
39	h	201	CLA	CAA-CBA-CGA-O2A
47	D	321	SQD	O48-C23-C24-C25
50	G	307	A1EB1	O6-C42-C44-C45
50	V	306	A1EB1	O6-C42-C44-C45
50	h	203	A1EB1	O6-C42-C44-C45
39	a	805	CLA	C8-C10-C11-C12
39	a	838	CLA	CAA-CBA-CGA-O1A
39	R	309	CLA	CAA-CBA-CGA-O1A
50	3	302	A1EB1	O43-C42-C44-C45
41	D	302	LHG	C2-C3-O3-P
39	a	809	CLA	C8-C10-C11-C12
46	W	320	LMG	C12-C13-C14-C15
39	a	811	CLA	C3A-C2A-CAA-CBA
39	a	814	CLA	C11-C10-C8-C7
39	a	824	CLA	C6-C7-C8-C10
39	b	830	CLA	C11-C12-C13-C15
39	f	802	CLA	C11-C10-C8-C7
39	o	206	CLA	C6-C7-C8-C10
39	A	306	CLA	C11-C10-C8-C7
39	B	205	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	B	207	CLA	C3A-C2A-CAA-CBA
39	C	306	CLA	C11-C10-C8-C7
39	C	309	CLA	C3A-C2A-CAA-CBA
39	G	309	CLA	C2-C3-C5-C6
39	K	312	CLA	C12-C13-C15-C16
39	L	309	CLA	C3A-C2A-CAA-CBA
39	L	309	CLA	CHA-CBD-CGD-O1D
39	M	310	CLA	C6-C7-C8-C10
39	M	312	CLA	C6-C7-C8-C10
39	P	307	CLA	C11-C12-C13-C15
39	R	307	CLA	C11-C12-C13-C15
39	3	312	CLA	C11-C12-C13-C15
39	3	314	CLA	C11-C10-C8-C7
39	6	311	CLA	CAD-CBD-CGD-O2D
39	a	832	CLA	CAA-CBA-CGA-O1A
39	b	810	CLA	CAA-CBA-CGA-O1A
39	V	310	CLA	CAA-CBA-CGA-O1A
39	0	313	CLA	CAA-CBA-CGA-O1A
39	h	201	CLA	CAA-CBA-CGA-O1A
50	H	304	A1EB1	O43-C42-C44-C45
50	4	302	A1EB1	O43-C42-C44-C45
47	F	319	SQD	C10-C11-C12-C13
47	H	318	SQD	C11-C10-C9-C8
48	8	302	A86	C35-C34-O4-C38
39	a	806	CLA	CAA-CBA-CGA-O2A
39	a	838	CLA	CAA-CBA-CGA-O2A
39	A	307	CLA	CAA-CBA-CGA-O2A
39	D	318	CLA	CAA-CBA-CGA-O2A
39	F	310	CLA	CAA-CBA-CGA-O2A
39	K	306	CLA	CAA-CBA-CGA-O2A
39	P	308	CLA	CAA-CBA-CGA-O2A
39	R	309	CLA	CAA-CBA-CGA-O2A
39	V	311	CLA	CAA-CBA-CGA-O2A
39	X	309	CLA	CAA-CBA-CGA-O2A
39	1	319	CLA	CAA-CBA-CGA-O2A
39	I	311	CLA	CAA-CBA-CGA-O2A
39	2	308	CLA	CAA-CBA-CGA-O2A
50	H	304	A1EB1	O6-C42-C44-C45
50	V	305	A1EB1	O6-C42-C44-C45
50	9	302	A1EB1	O6-C42-C44-C45
50	F	304	A1EB1	C45-C46-C47-C48
42	b	845	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
42	b	846	BCR	C7-C8-C9-C10
43	D	307	DD6	C2-C1-C24-C25
43	7	310	DD6	C5-C6-C8-C9
48	M	302	A86	C5-C6-C8-C9
48	8	309	A86	C2-C1-C24-C25
48	9	306	A86	C5-C6-C8-C9
39	o	205	CLA	CAA-CBA-CGA-O1A
39	E	314	CLA	CAA-CBA-CGA-O1A
39	M	309	CLA	CAA-CBA-CGA-O1A
39	P	308	CLA	CAA-CBA-CGA-O1A
39	P	309	CLA	CAA-CBA-CGA-O1A
39	y	308	CLA	CAA-CBA-CGA-O1A
43	S	306	DD6	C11-C10-C9-C8
43	I	306	DD6	C3-C4-C5-C6
48	Q	305	A86	C1-C2-C3-C4
48	T	306	A86	C24-C25-C26-C27
50	2	306	A1EB1	C24-C25-C26-C27
48	O	307	A86	O-C13-C14-C15
48	S	304	A86	O-C13-C14-C15
48	X	302	A86	O-C13-C14-C15
48	0	309	A86	O-C13-C14-C15
48	1	306	A86	O-C13-C14-C15
48	4	328	A86	O-C13-C14-C15
48	6	305	A86	O-C13-C14-C15
39	E	309	CLA	CAA-CBA-CGA-O2A
39	O	318	CLA	CAA-CBA-CGA-O2A
39	S	308	CLA	CAA-CBA-CGA-O2A
39	T	318	CLA	CAA-CBA-CGA-O2A
46	4	325	LMG	O7-C10-C11-C12
46	F	320	LMG	O6-C1-O1-C7
39	K	312	CLA	C10-C11-C12-C13
39	a	807	CLA	CAA-CBA-CGA-O1A
39	A	307	CLA	CAA-CBA-CGA-O1A
39	A	308	CLA	CAA-CBA-CGA-O1A
39	T	308	CLA	CAA-CBA-CGA-O1A
39	V	311	CLA	CAA-CBA-CGA-O1A
39	I	309	CLA	CAA-CBA-CGA-O1A
50	4	301	A1EB1	O43-C42-C44-C45
50	8	301	A1EB1	O43-C42-C44-C45
50	y	301	A1EB1	O43-C42-C44-C45
39	a	832	CLA	CAA-CBA-CGA-O2A
39	Q	311	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
39	5	308	CLA	CAA-CBA-CGA-O2A
46	Q	322	LMG	O8-C28-C29-C30
39	0	322	CLA	CAA-CBA-CGA-O1A
39	A	306	CLA	C2A-CAA-CBA-CGA
39	J	308	CLA	C2A-CAA-CBA-CGA
48	0	308	A86	C35-C34-O4-C38
39	R	307	CLA	C13-C15-C16-C17
39	a	807	CLA	C3-C5-C6-C7
39	F	310	CLA	CAA-CBA-CGA-O1A
39	X	309	CLA	CAA-CBA-CGA-O1A
39	1	319	CLA	CAA-CBA-CGA-O1A
39	I	311	CLA	CAA-CBA-CGA-O1A
46	S	322	LMG	O10-C28-C29-C30
50	9	302	A1EB1	O43-C42-C44-C45
50	h	203	A1EB1	O43-C42-C44-C45
39	O	312	CLA	C4C-C3C-CAC-CBC
39	a	804	CLA	O1D-CGD-O2D-CED

There are no ring outliers.

444 monomers are involved in 929 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	I	308	CLA	3	0
39	R	309	CLA	1	0
39	a	837	CLA	1	0
39	I	309	CLA	2	0
39	6	313	CLA	1	0
46	Q	322	LMG	2	0
39	b	827	CLA	7	0
39	D	309	CLA	1	0
39	X	307	CLA	2	0
39	b	803	CLA	2	0
43	Q	303	DD6	5	0
39	f	802	CLA	1	0
39	6	310	CLA	1	0
39	F	313	CLA	3	0
39	a	818	CLA	3	0
41	H	317	LHG	3	0
46	M	319	LMG	10	0
39	X	317	CLA	3	0
39	9	319	CLA	2	0
39	a	835	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	H	309	CLA	2	0
39	3	320	CLA	1	0
39	E	312	CLA	3	0
39	i	101	CLA	4	0
39	Q	310	CLA	3	0
48	9	303	A86	1	0
39	y	310	CLA	1	0
39	A	312	CLA	1	0
51	1	318	A1ECV	1	0
39	1	308	CLA	2	0
48	F	302	A86	8	0
39	K	308	CLA	1	0
39	P	308	CLA	5	0
39	l	203	CLA	2	0
39	b	828	CLA	6	0
39	F	321	CLA	1	0
50	F	304	A1EB1	4	0
39	O	313	CLA	1	0
39	a	808	CLA	1	0
39	X	311	CLA	1	0
39	0	315	CLA	2	0
39	b	851	CLA	4	0
48	U	206	A86	1	0
47	4	327	SQD	1	0
47	T	321	SQD	1	0
39	k	203	CLA	1	0
49	Q	315	KC2	1	0
43	z	305	DD6	1	0
48	I	304	A86	1	0
39	b	841	CLA	4	0
50	x	302	A1EB1	2	0
39	o	201	CLA	2	0
39	b	838	CLA	4	0
39	8	321	CLA	1	0
39	L	313	CLA	1	0
39	a	825	CLA	7	0
39	b	842	CLA	2	0
39	a	831	CLA	4	0
43	O	305	DD6	1	0
52	P	319	A1EB4	2	0
39	b	801	CLA	7	0
39	A	315	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	C	305	CLA	1	0
39	a	804	CLA	2	0
39	H	306	CLA	3	0
47	P	301	SQD	1	0
39	l	201	CLA	3	0
39	a	824	CLA	5	0
39	R	316	CLA	2	0
39	B	204	CLA	1	0
49	P	312	KC2	2	0
39	1	309	CLA	1	0
39	a	803	CLA	3	0
39	T	311	CLA	1	0
39	J	311	CLA	4	0
49	X	314	KC2	19	0
39	a	847	CLA	2	0
39	3	314	CLA	3	0
39	4	316	CLA	1	0
39	E	314	CLA	5	0
39	T	319	CLA	1	0
39	Z	316	CLA	1	0
42	l	206	BCR	1	0
39	x	307	CLA	2	0
49	L	315	KC2	1	0
39	5	308	CLA	2	0
42	m	101	BCR	5	0
39	J	313	CLA	1	0
48	Q	304	A86	28	0
39	Z	306	CLA	1	0
39	D	310	CLA	2	0
46	4	325	LMG	2	0
39	L	310	CLA	2	0
39	D	312	CLA	2	0
39	1	310	CLA	1	0
39	Z	309	CLA	1	0
46	l	208	LMG	4	0
39	0	310	CLA	2	0
39	a	836	CLA	6	0
49	P	310	KC2	1	0
39	j	101	CLA	5	0
47	D	321	SQD	2	0
39	X	308	CLA	4	0
48	W	304	A86	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	U	207	CLA	3	0
39	x	311	CLA	1	0
49	0	314	KC2	2	0
49	V	315	KC2	1	0
39	S	319	CLA	2	0
51	7	317	A1ECV	2	0
43	4	308	DD6	1	0
39	F	310	CLA	1	0
48	1	307	A86	1	0
39	4	323	CLA	7	0
39	C	308	CLA	3	0
39	b	813	CLA	2	0
43	H	303	DD6	1	0
46	W	302	LMG	14	0
51	7	323	A1ECV	4	0
43	5	303	DD6	1	0
39	V	310	CLA	5	0
39	b	814	CLA	2	0
51	x	310	A1ECV	1	0
39	W	309	CLA	2	0
39	D	311	CLA	2	0
39	z	311	CLA	1	0
39	D	319	CLA	3	0
39	T	308	CLA	9	0
39	7	313	CLA	2	0
49	X	312	KC2	1	0
39	2	316	CLA	1	0
39	M	310	CLA	3	0
43	J	305	DD6	1	0
39	a	832	CLA	1	0
39	D	313	CLA	1	0
39	M	317	CLA	2	0
43	U	204	DD6	1	0
49	5	305	KC2	1	0
39	T	320	CLA	2	0
43	1	304	DD6	2	0
39	C	304	CLA	1	0
39	A	306	CLA	3	0
48	5	301	A86	2	0
39	U	209	CLA	1	0
46	7	301	LMG	20	0
39	D	317	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	9	307	CLA	1	0
48	Q	301	A86	1	0
39	T	313	CLA	2	0
39	a	826	CLA	3	0
39	9	308	CLA	3	0
39	I	301	CLA	3	0
39	I	315	CLA	1	0
47	k	205	SQD	2	0
39	K	314	CLA	1	0
39	H	313	CLA	2	0
39	M	309	CLA	2	0
39	J	318	CLA	2	0
39	J	314	CLA	3	0
49	W	315	KC2	1	0
52	W	321	A1EB4	1	0
39	V	319	CLA	1	0
39	I	313	CLA	2	0
39	8	311	CLA	2	0
39	X	309	CLA	2	0
46	S	322	LMG	20	0
39	S	308	CLA	2	0
39	b	832	CLA	5	0
39	3	322	CLA	2	0
48	W	307	A86	1	0
43	P	304	DD6	2	0
39	E	308	CLA	1	0
49	Y	308	KC2	1	0
49	O	317	KC2	1	0
39	a	807	CLA	3	0
39	L	308	CLA	3	0
50	H	304	A1EB1	1	0
39	K	312	CLA	2	0
51	T	317	A1ECV	1	0
39	J	310	CLA	1	0
39	U	208	CLA	2	0
43	O	304	DD6	1	0
39	G	318	CLA	1	0
46	0	324	LMG	4	0
50	7	306	A1EB1	1	0
39	Q	312	CLA	1	0
39	b	822	CLA	2	0
39	a	809	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	3	313	CLA	1	0
52	R	305	A1EB4	1	0
47	H	318	SQD	3	0
39	b	839	CLA	3	0
42	l	202	BCR	5	0
47	7	302	SQD	1	0
46	F	317	LMG	14	0
39	l	204	CLA	1	0
52	W	306	A1EB4	4	0
47	9	322	SQD	1	0
39	1	313	CLA	2	0
52	5	304	A1EB4	1	0
39	b	840	CLA	4	0
39	S	320	CLA	3	0
39	7	318	CLA	3	0
39	G	310	CLA	1	0
42	l	207	BCR	4	0
39	E	318	CLA	1	0
47	F	319	SQD	1	0
47	W	301	SQD	1	0
43	E	303	DD6	1	0
39	F	314	CLA	3	0
48	7	312	A86	1	0
48	E	304	A86	1	0
40	a	839	PQN	4	0
39	z	306	CLA	1	0
43	3	304	DD6	3	0
39	D	318	CLA	5	0
48	R	302	A86	2	0
39	Z	313	CLA	1	0
43	A	302	DD6	1	0
43	S	306	DD6	1	0
50	z	302	A1EB1	1	0
39	a	813	CLA	3	0
39	b	830	CLA	3	0
39	5	315	CLA	2	0
39	Q	321	CLA	3	0
39	8	313	CLA	1	0
39	a	814	CLA	2	0
39	b	818	CLA	3	0
42	f	801	BCR	3	0
41	a	840	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	X	301	LHG	2	0
43	F	305	DD6	1	0
47	D	304	SQD	2	0
39	H	310	CLA	3	0
39	H	312	CLA	2	0
39	V	316	CLA	10	0
39	I	311	CLA	1	0
46	A	316	LMG	1	0
39	C	310	CLA	3	0
39	b	817	CLA	3	0
39	K	309	CLA	1	0
39	b	820	CLA	3	0
42	a	845	BCR	5	0
49	F	307	KC2	1	0
49	x	312	KC2	1	0
39	b	809	CLA	5	0
39	J	309	CLA	3	0
39	b	810	CLA	3	0
39	b	811	CLA	2	0
39	2	308	CLA	1	0
39	i	103	CLA	6	0
39	b	815	CLA	4	0
39	W	318	CLA	1	0
50	2	304	A1EB1	1	0
39	M	308	CLA	1	0
39	f	803	CLA	1	0
52	P	318	A1EB4	3	0
42	a	844	BCR	3	0
39	7	316	CLA	4	0
39	A	314	CLA	3	0
39	K	311	CLA	1	0
39	b	807	CLA	3	0
39	b	825	CLA	2	0
39	a	823	CLA	3	0
39	F	308	CLA	3	0
39	A	311	CLA	2	0
39	a	829	CLA	2	0
49	5	313	KC2	26	0
39	Q	309	CLA	2	0
39	W	313	CLA	2	0
39	a	811	CLA	5	0
39	o	205	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	S	311	CLA	5	0
39	L	311	CLA	2	0
39	P	316	CLA	1	0
39	a	838	CLA	3	0
39	B	209	CLA	4	0
39	C	311	CLA	1	0
49	M	313	KC2	1	0
39	J	307	CLA	1	0
39	H	316	CLA	1	0
39	2	309	CLA	1	0
51	0	321	A1ECV	2	0
51	z	316	A1ECV	1	0
39	a	812	CLA	1	0
39	B	206	CLA	1	0
49	3	317	KC2	1	0
39	a	816	CLA	7	0
39	y	307	CLA	1	0
48	2	305	A86	1	0
47	M	301	SQD	3	0
39	a	801	CLA	6	0
39	7	321	CLA	1	0
39	a	817	CLA	2	0
39	Y	313	CLA	1	0
39	O	316	CLA	1	0
39	E	316	CLA	1	0
45	b	849	DGD	3	0
39	5	306	CLA	2	0
49	7	319	KC2	1	0
39	b	826	CLA	7	0
39	x	306	CLA	1	0
46	F	320	LMG	7	0
39	K	307	CLA	1	0
49	4	324	KC2	1	0
39	4	314	CLA	4	0
43	I	306	DD6	1	0
43	D	306	DD6	1	0
39	T	318	CLA	1	0
39	Q	311	CLA	3	0
43	F	303	DD6	6	0
39	x	308	CLA	1	0
40	b	843	PQN	3	0
39	b	819	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	b	833	CLA	3	0
39	V	311	CLA	1	0
39	0	311	CLA	3	0
39	2	310	CLA	1	0
39	U	215	CLA	1	0
39	b	829	CLA	2	0
49	T	315	KC2	2	0
42	b	846	BCR	4	0
39	Q	314	CLA	2	0
39	7	325	CLA	1	0
39	E	315	CLA	2	0
42	b	845	BCR	3	0
46	P	317	LMG	5	0
39	b	805	CLA	3	0
39	a	830	CLA	4	0
39	2	318	CLA	1	0
39	k	201	CLA	2	0
39	M	312	CLA	4	0
39	b	802	CLA	1	0
39	a	806	CLA	1	0
42	a	843	BCR	4	0
39	7	314	CLA	5	0
50	9	302	A1EB1	1	0
42	j	103	BCR	1	0
47	D	320	SQD	2	0
39	R	307	CLA	2	0
39	F	312	CLA	1	0
39	a	820	CLA	2	0
39	R	311	CLA	1	0
39	W	311	CLA	2	0
39	8	310	CLA	3	0
39	F	309	CLA	1	0
39	0	312	CLA	8	0
51	y	311	A1ECV	1	0
39	a	821	CLA	2	0
39	P	309	CLA	1	0
50	0	307	A1EB1	2	0
39	b	812	CLA	3	0
50	4	304	A1EB1	1	0
39	S	313	CLA	4	0
39	O	308	CLA	1	0
39	K	306	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	Y	305	CLA	1	0
39	U	201	CLA	1	0
39	E	313	CLA	2	0
39	A	305	CLA	1	0
49	R	314	KC2	15	0
39	O	309	CLA	1	0
39	D	314	CLA	2	0
39	D	315	CLA	1	0
49	F	311	KC2	7	0
39	B	207	CLA	2	0
49	W	314	KC2	2	0
39	b	837	CLA	1	0
39	A	309	CLA	1	0
39	E	310	CLA	4	0
39	b	823	CLA	1	0
42	i	102	BCR	6	0
43	2	303	DD6	1	0
42	b	844	BCR	2	0
49	6	316	KC2	1	0
39	7	324	CLA	4	0
41	j	104	LHG	1	0
39	S	309	CLA	2	0
48	0	304	A86	1	0
43	7	310	DD6	5	0
49	8	316	KC2	1	0
39	C	307	CLA	2	0
42	b	848	BCR	5	0
39	b	806	CLA	1	0
39	0	313	CLA	2	0
48	L	304	A86	4	0
46	I	302	LMG	1	0
49	2	313	KC2	1	0
47	S	301	SQD	4	0
39	x	317	CLA	1	0
39	6	321	CLA	1	0
39	a	827	CLA	2	0
39	R	308	CLA	1	0
39	D	316	CLA	2	0
43	M	304	DD6	2	0
39	P	307	CLA	3	0
51	9	317	A1ECV	2	0
46	7	326	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	O	310	CLA	4	0
48	Z	303	A86	1	0
42	h	202	BCR	4	0
39	b	824	CLA	4	0
50	0	303	A1EB1	2	0
39	5	316	CLA	2	0
39	Q	320	CLA	1	0
51	2	311	A1ECV	1	0
39	G	309	CLA	1	0
50	S	303	A1EB1	1	0
39	V	309	CLA	2	0
39	a	802	CLA	2	0
39	H	308	CLA	2	0
41	D	302	LHG	3	0
48	Q	302	A86	2	0
46	4	326	LMG	33	0
39	b	831	CLA	2	0
39	a	815	CLA	4	0
39	a	822	CLA	5	0
39	3	311	CLA	2	0
46	D	322	LMG	1	0
42	b	847	BCR	4	0
42	k	204	BCR	2	0
46	S	321	LMG	3	0
39	E	317	CLA	3	0
42	b	850	BCR	5	0
49	R	312	KC2	1	0
39	b	834	CLA	2	0
42	f	804	BCR	3	0
39	F	316	CLA	2	0
51	Y	306	A1ECV	1	0
48	D	305	A86	1	0
39	C	306	CLA	2	0
39	9	312	CLA	4	0
48	F	301	A86	1	0
39	0	323	CLA	2	0
39	b	821	CLA	2	0
39	V	313	CLA	5	0
39	W	310	CLA	7	0
39	b	808	CLA	1	0
39	b	835	CLA	1	0
39	l	205	CLA	7	0

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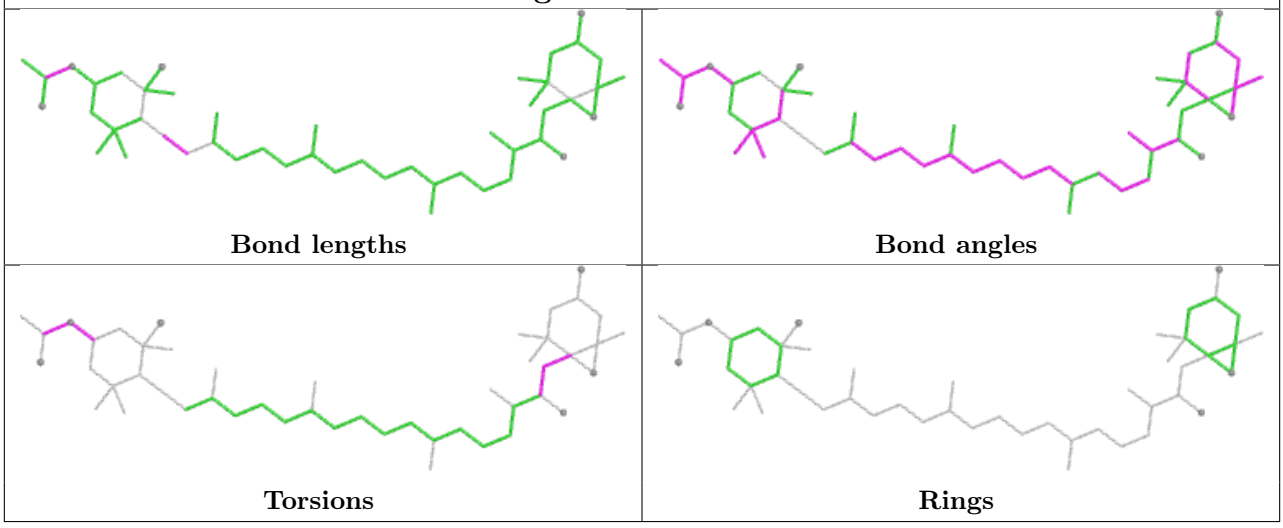
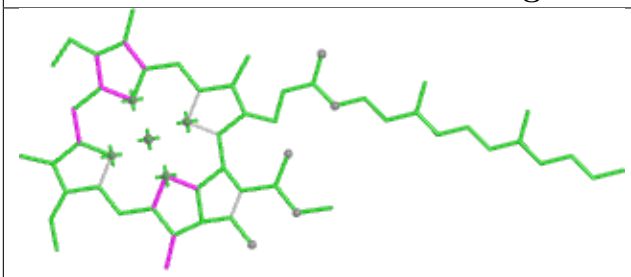
Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	o	206	CLA	2	0
39	4	312	CLA	2	0
39	3	312	CLA	4	0
42	a	842	BCR	5	0

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.

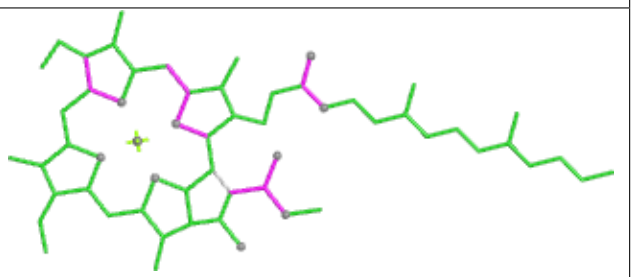
Ligand A86 S 307



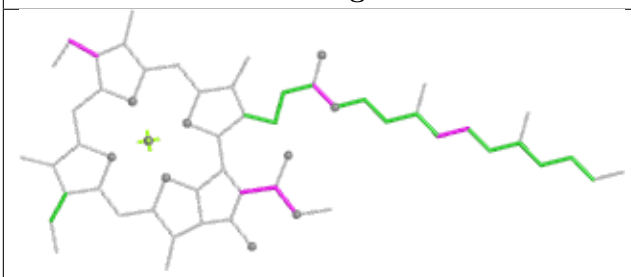
Ligand CLA G 314



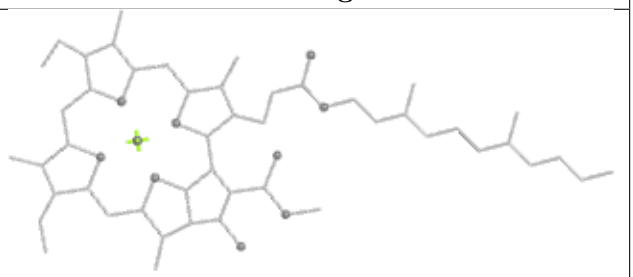
Bond lengths



Bond angles

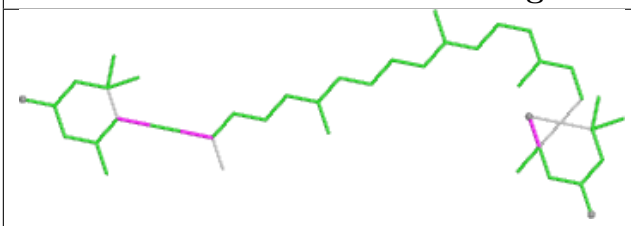


Torsions

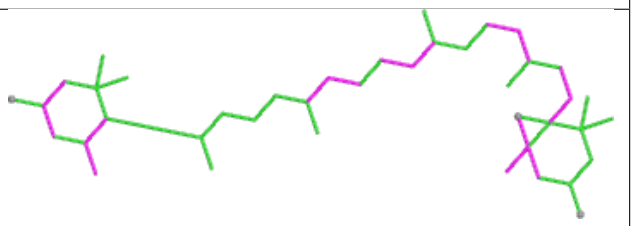


Rings

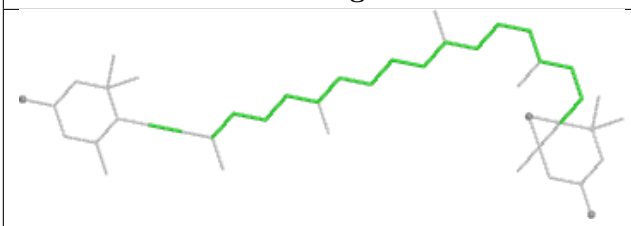
Ligand DD6 E 302



Bond lengths



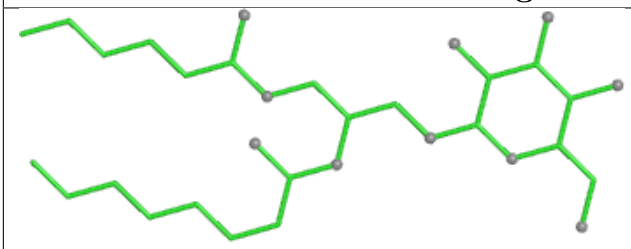
Bond angles



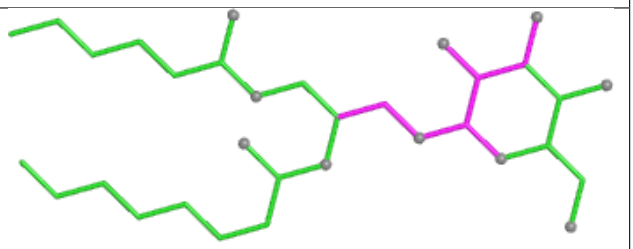
Torsions

Rings

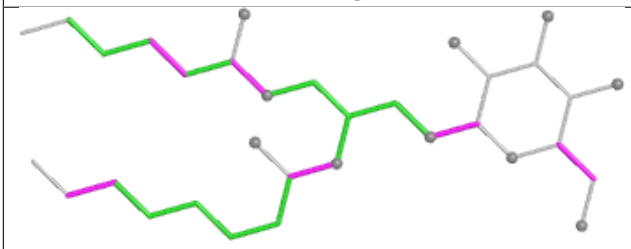
Ligand LMG M 320



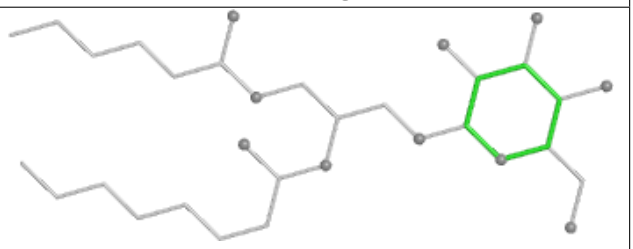
Bond lengths



Bond angles

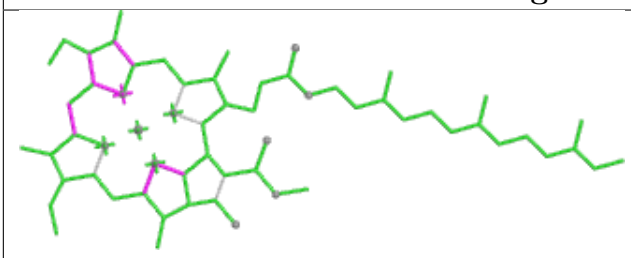


Torsions

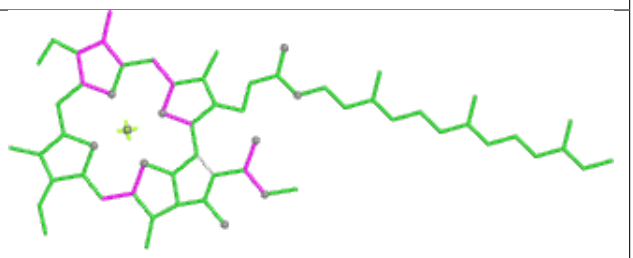


Rings

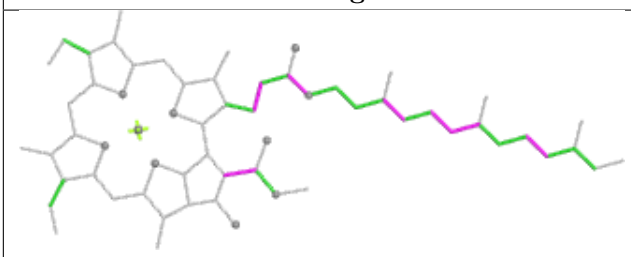
Ligand CLA I 308



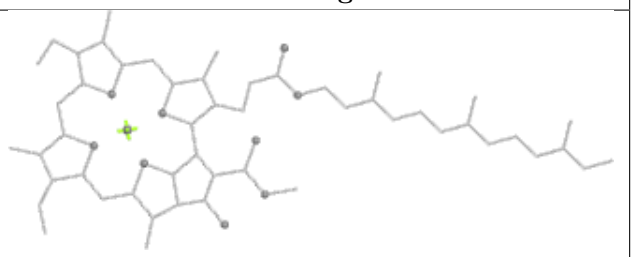
Bond lengths



Bond angles

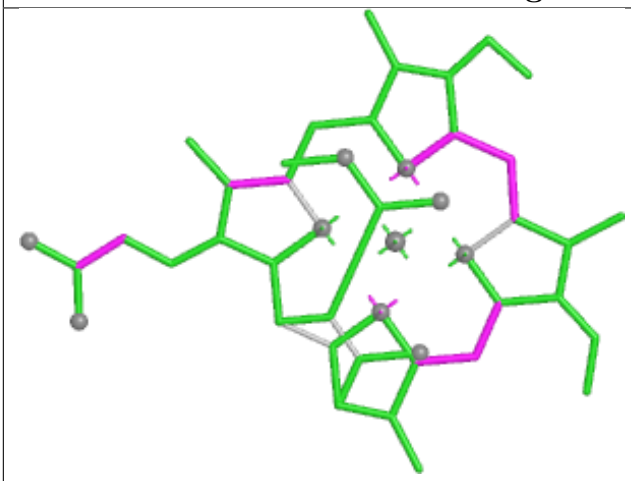


Torsions

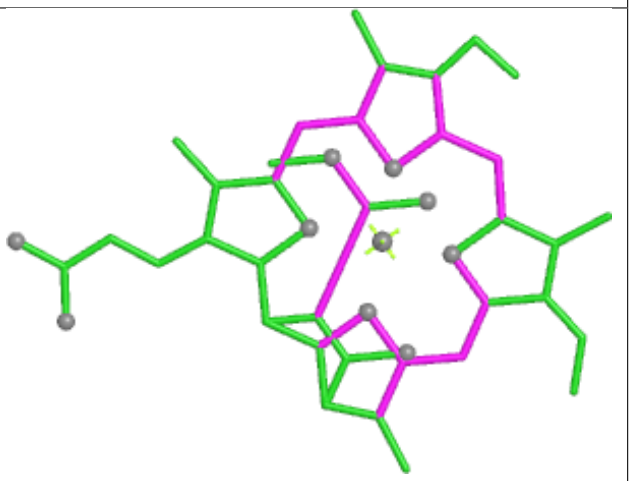


Rings

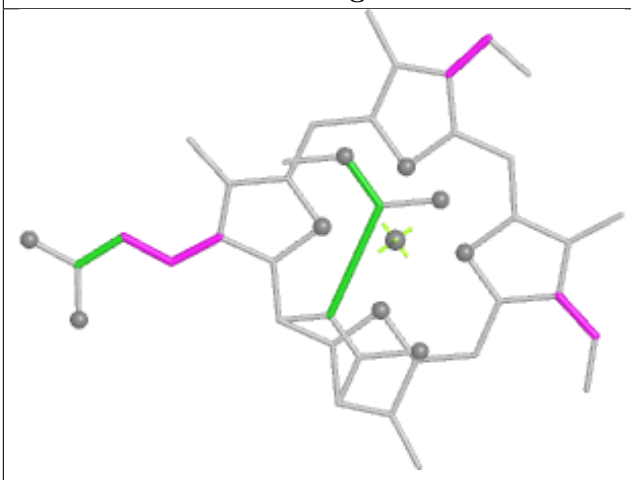
Ligand KC2 A 310



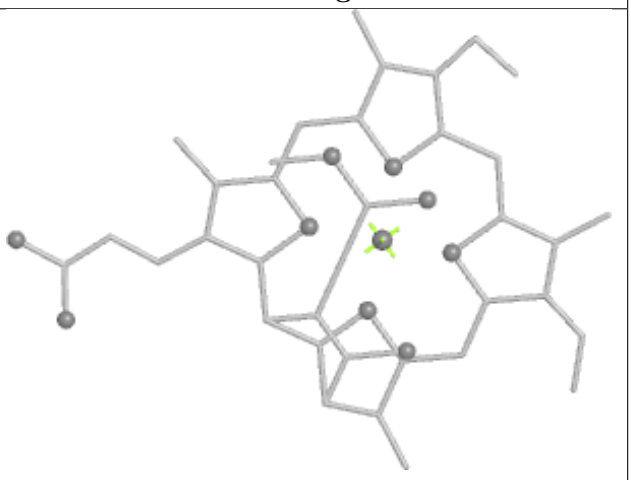
Bond lengths



Bond angles

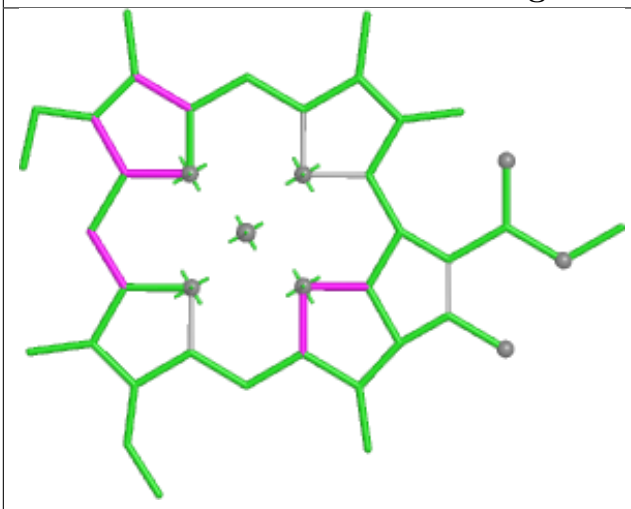


Torsions



Rings

Ligand CLA 1 316



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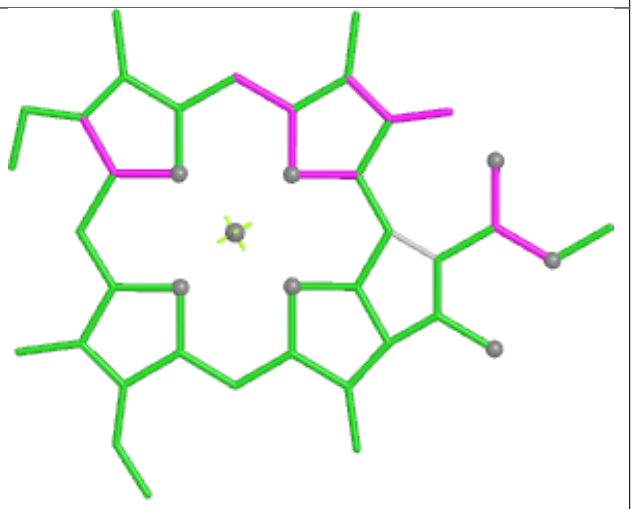
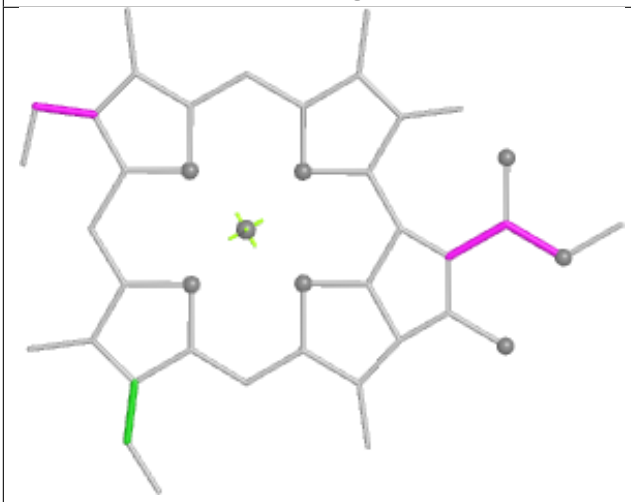


Bond angles



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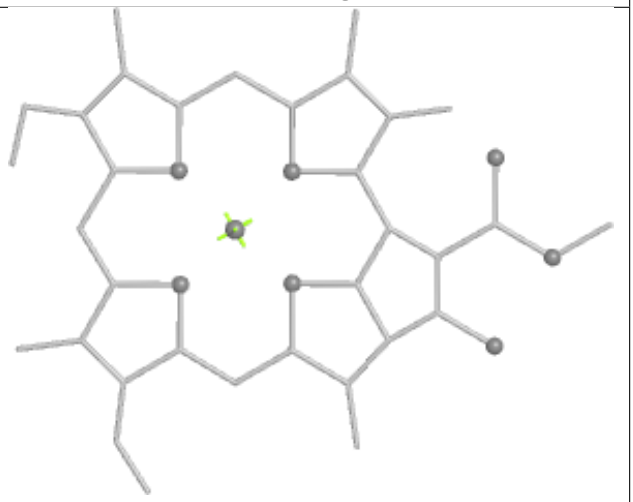
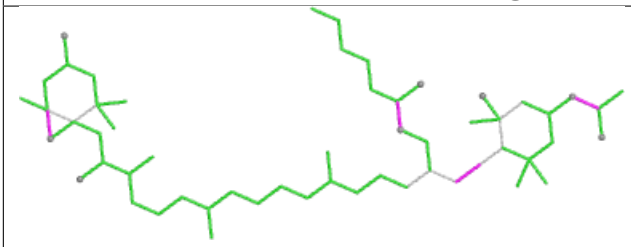


Rings

Ligand A1EB1 E 301



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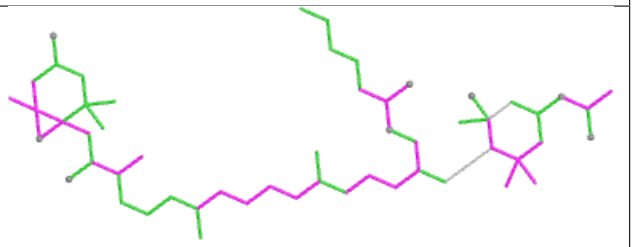
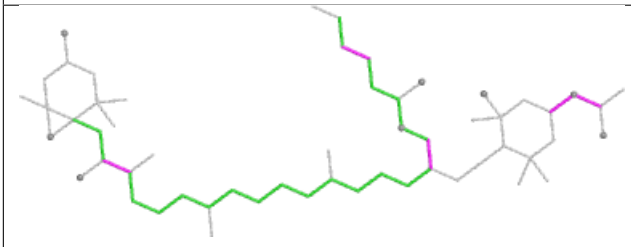


Bond angles



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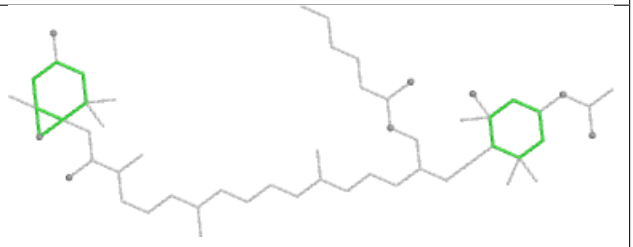
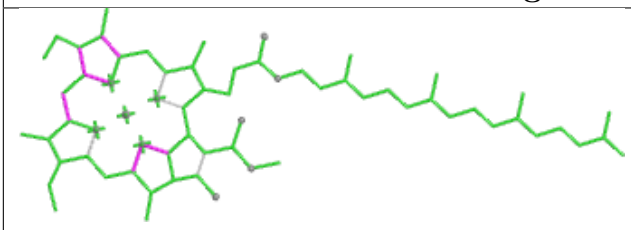
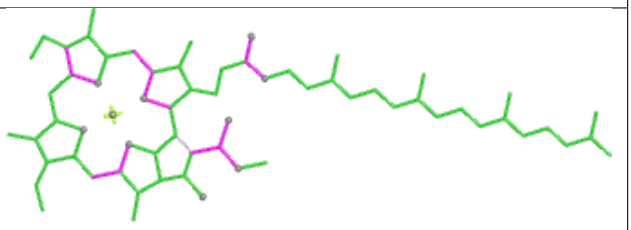


Rings

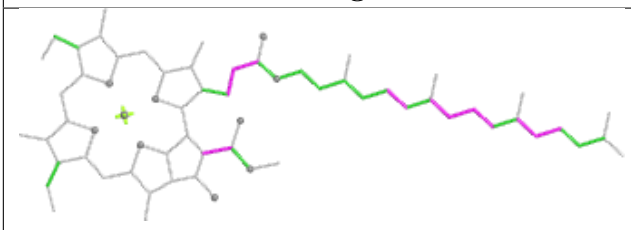
Ligand CLA R 309



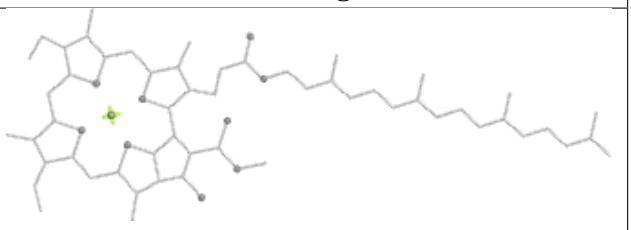
Bond lengths



Bond angles

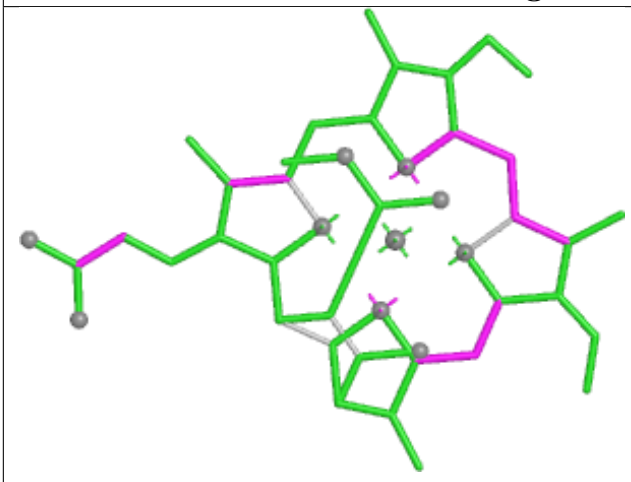


Torsions

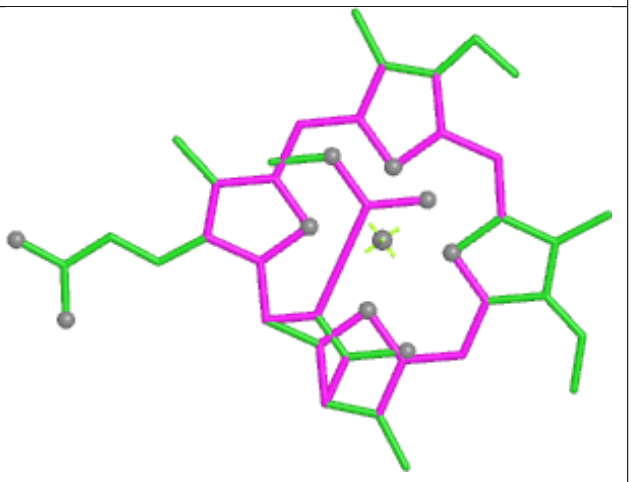


Rings

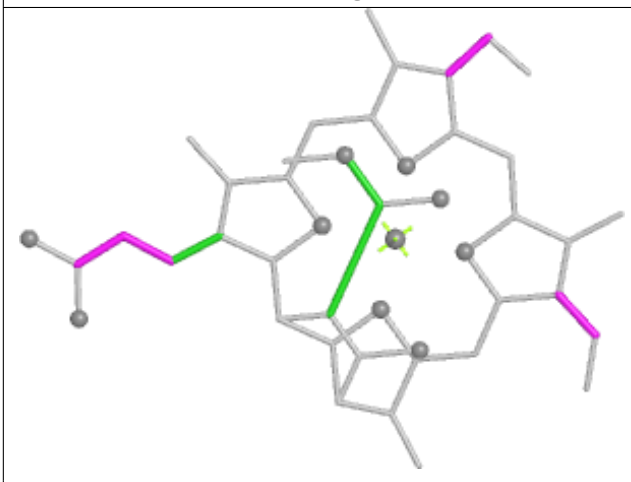
Ligand KC2 V 312



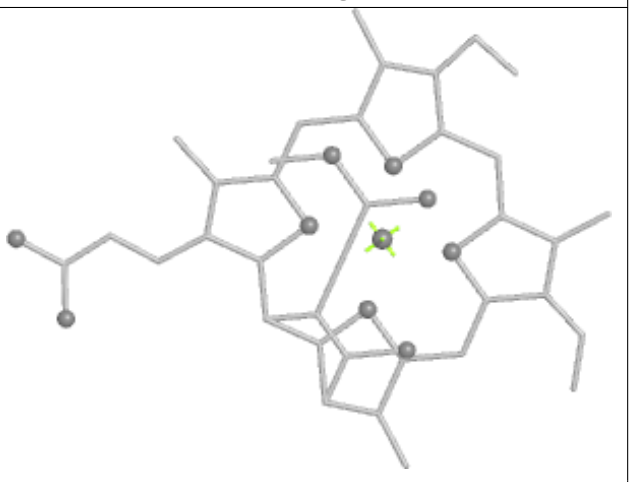
Bond lengths



Bond angles

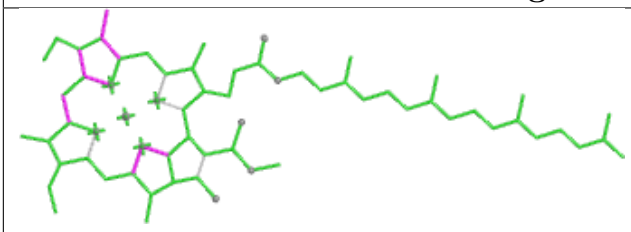


Torsions

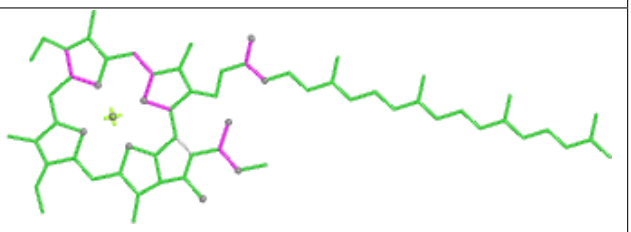


Rings

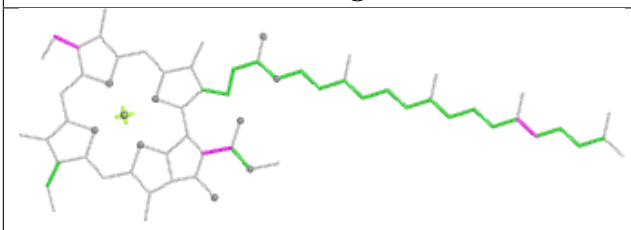
Ligand CLA a 837



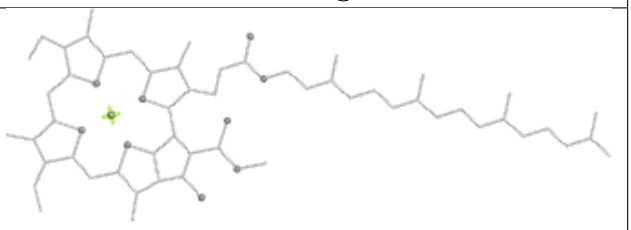
Bond lengths



Bond angles

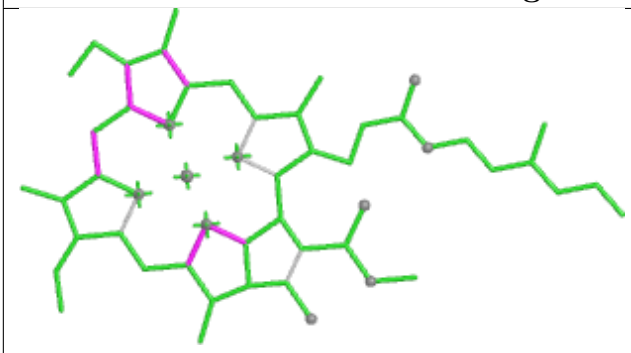


Torsions

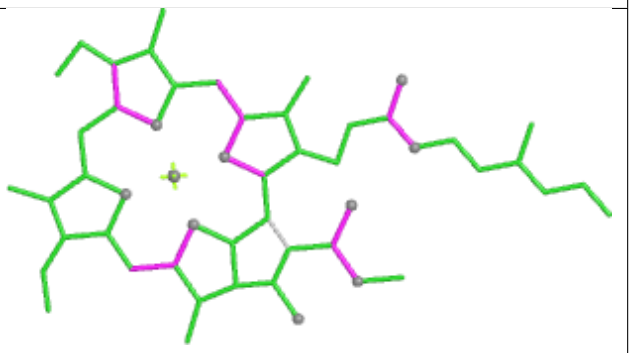


Rings

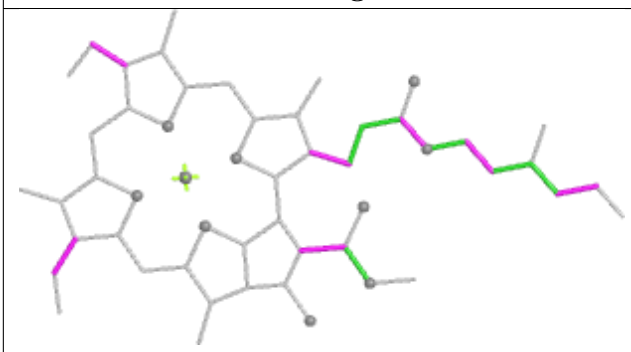
Ligand CLA G 312



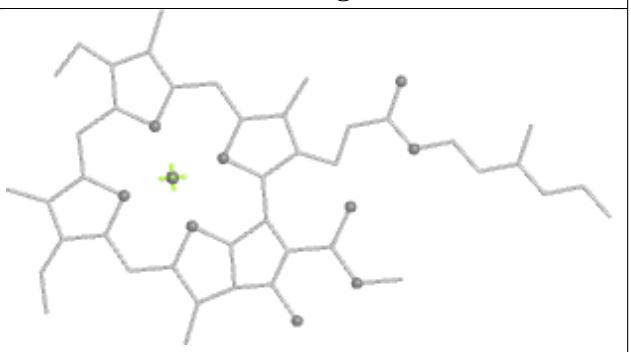
Bond lengths



Bond angles

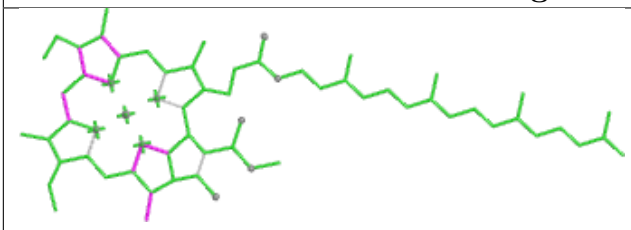


Torsions



Rings

Ligand CLA I 309



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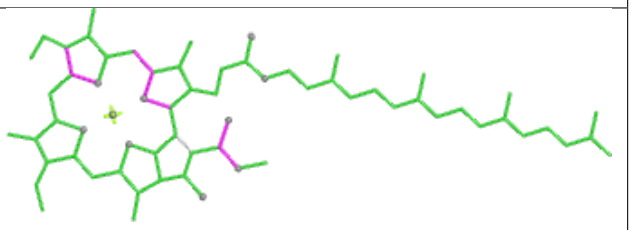
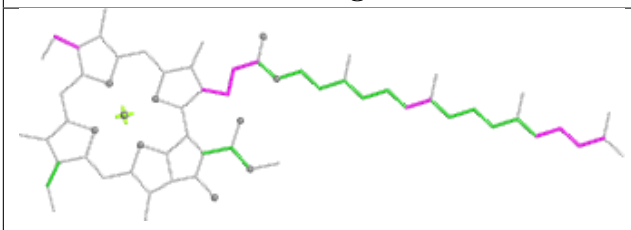
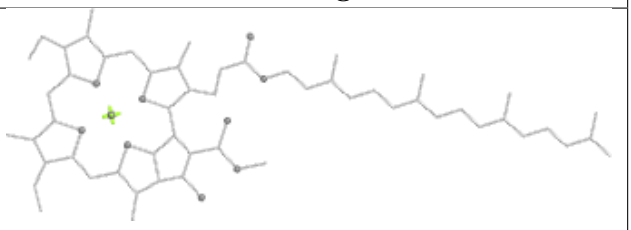


Bond angles

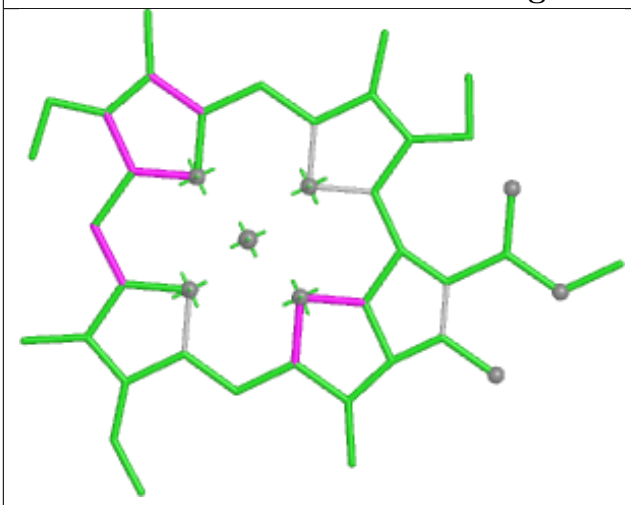


Torsions

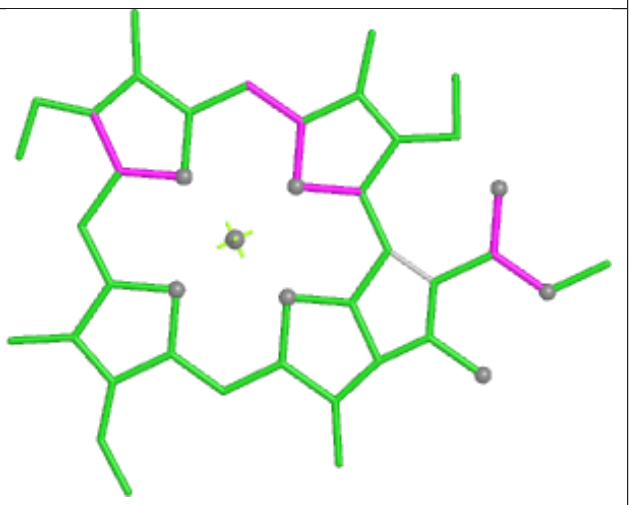


Rings

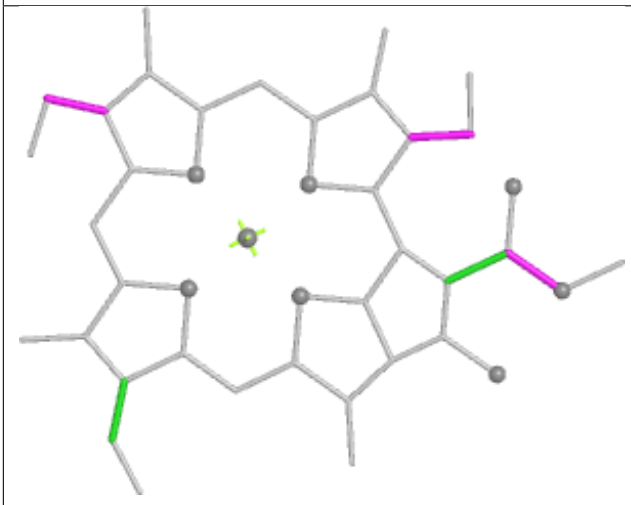
Ligand CLA 6 313



Bond lengths



Bond angles



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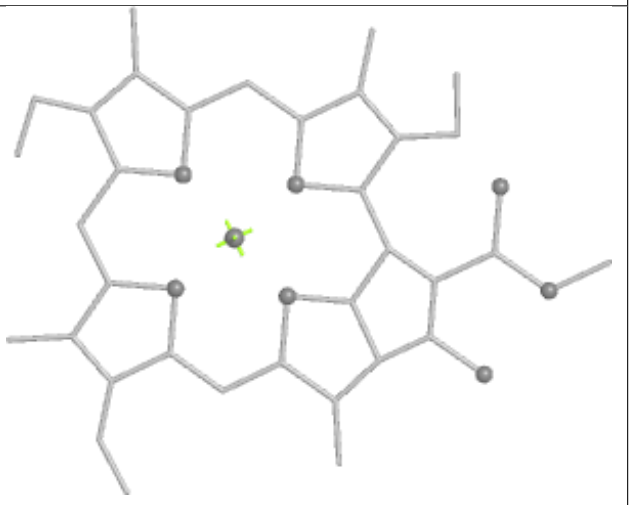
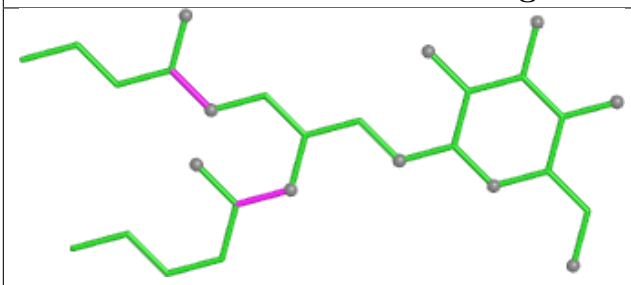


Rings

Ligand LMG Q 322



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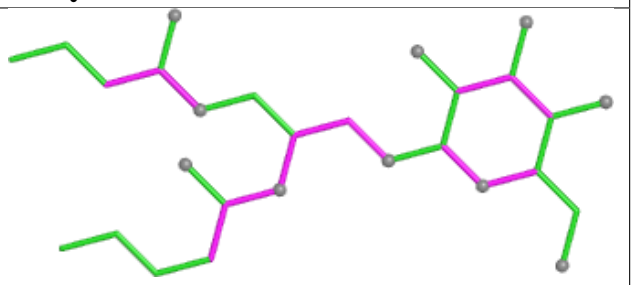
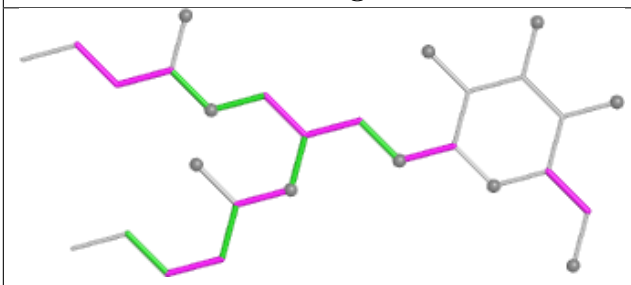


Bond angles



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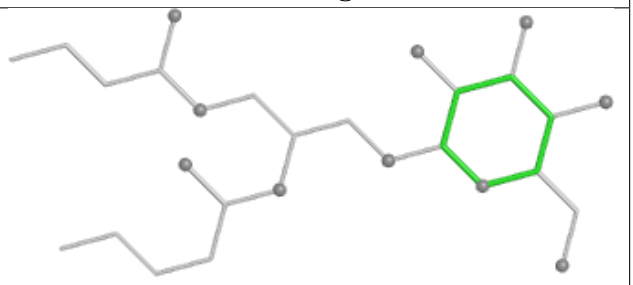
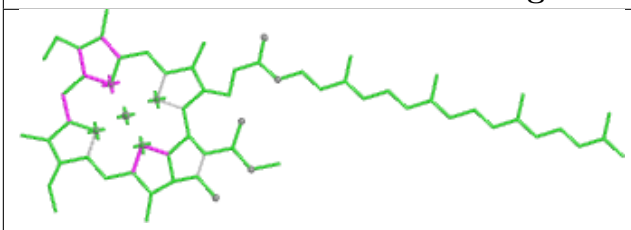


Rings

Ligand CLA b 827



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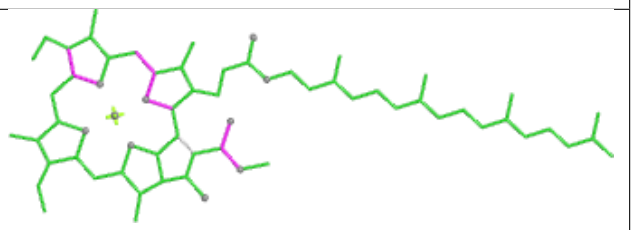
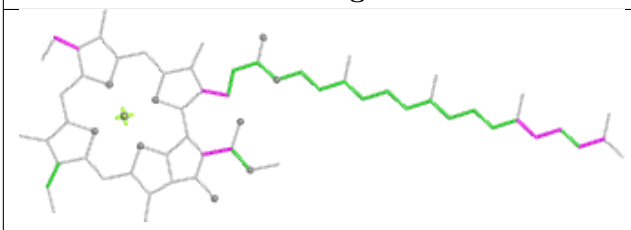
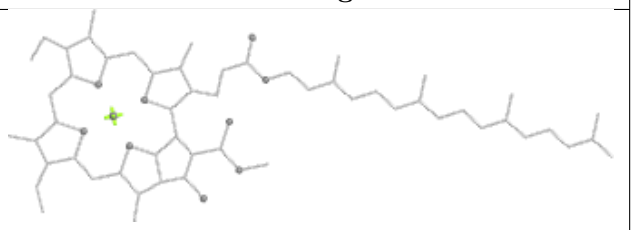


Bond angles

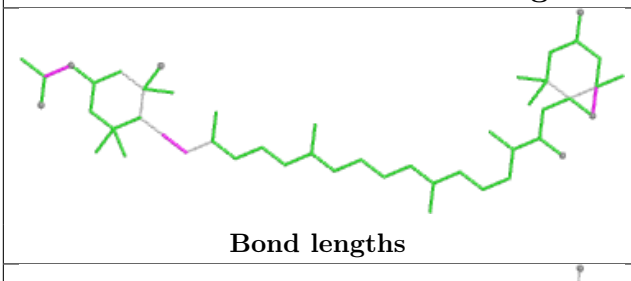


Torsions



Rings

Ligand A86 P 303



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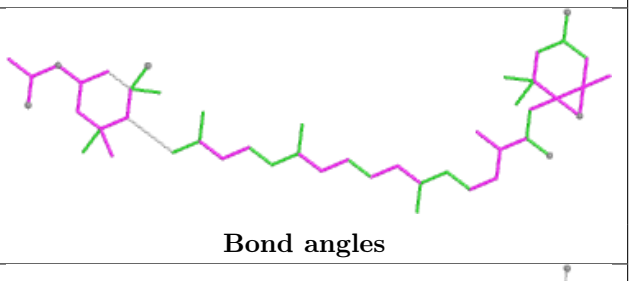
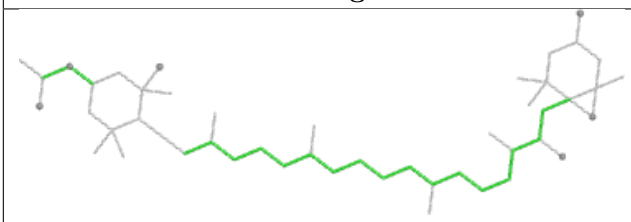


Bond angles



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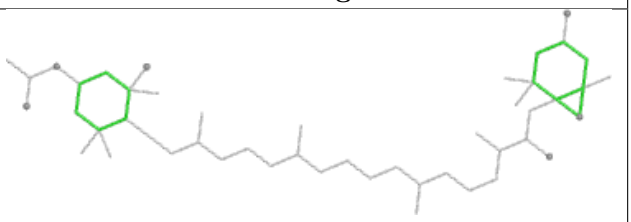
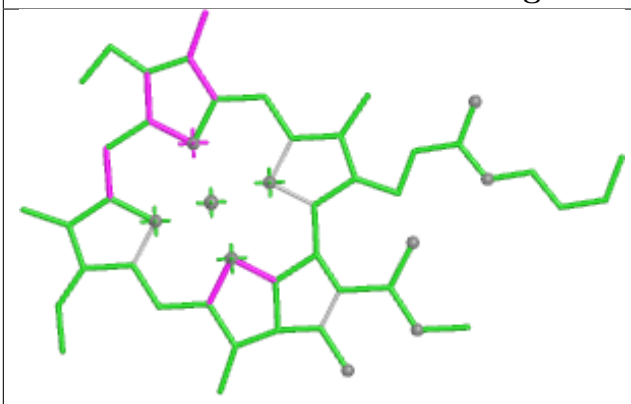


Rings

Ligand CLA D 309



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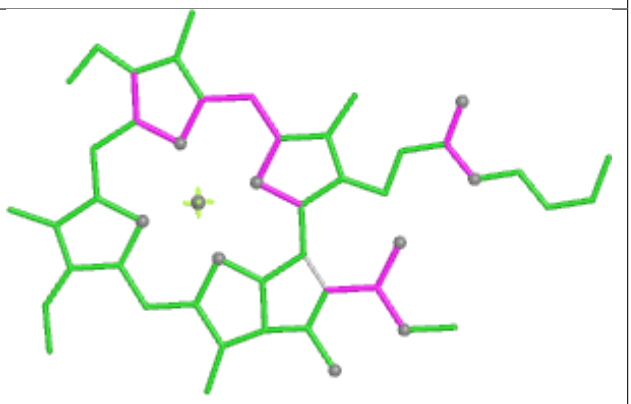

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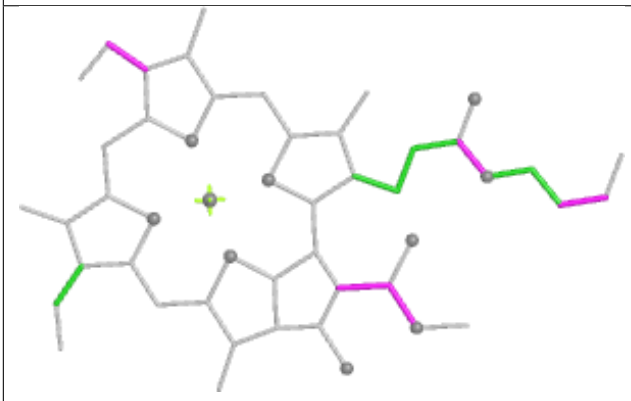

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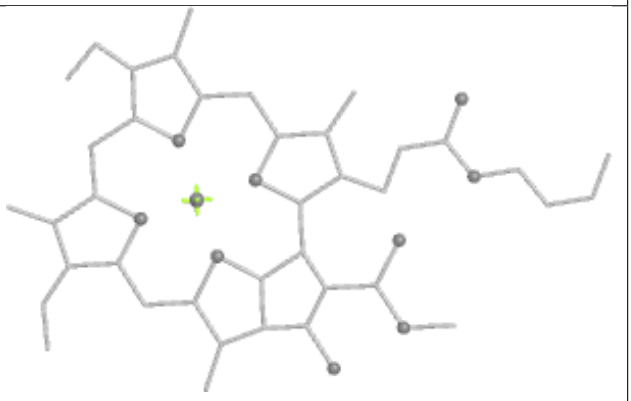
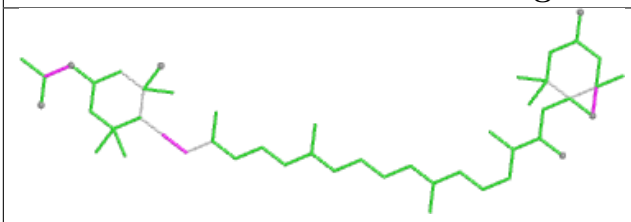


Rings

Ligand A86 7 307



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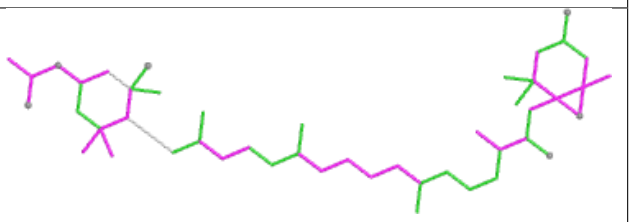

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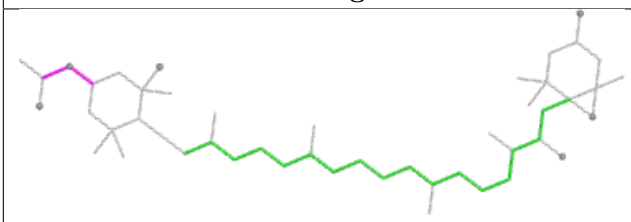

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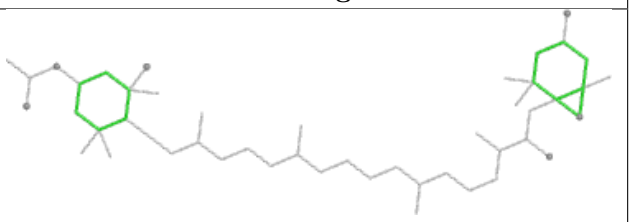
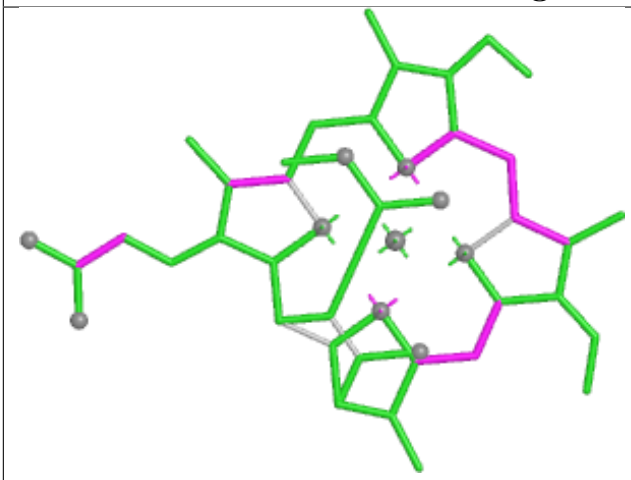


Rings

Ligand KC2 z 312



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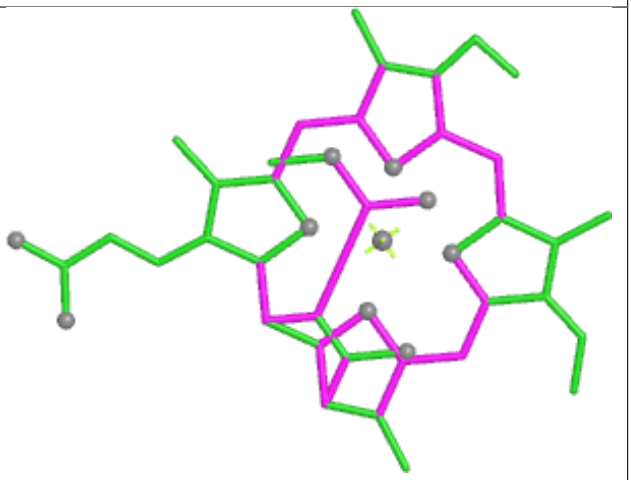
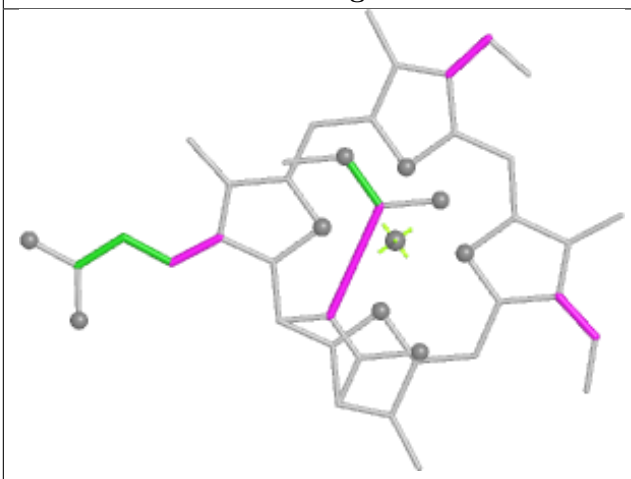


Bond angles



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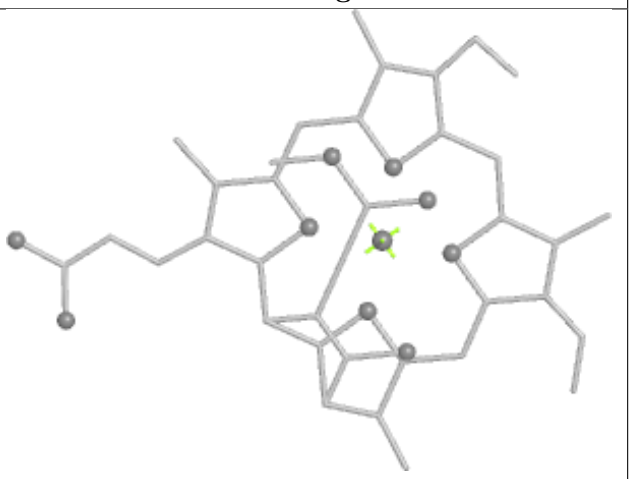
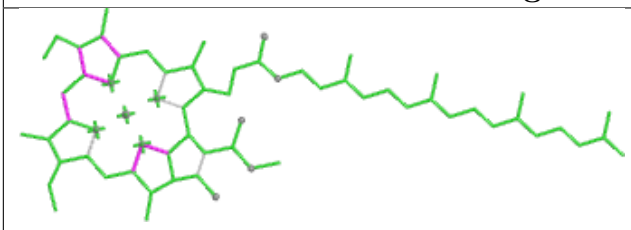
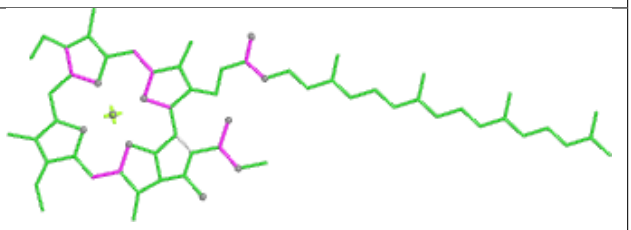
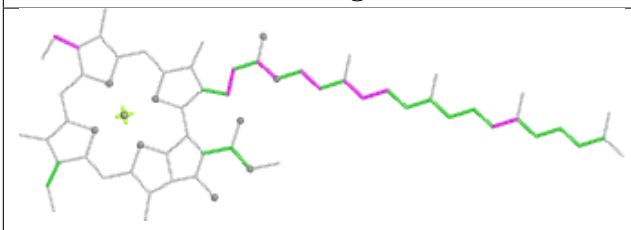
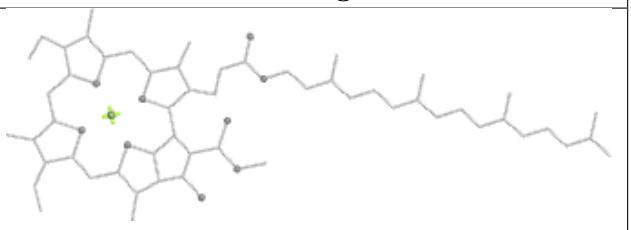
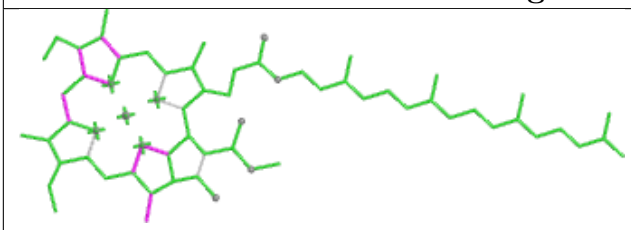
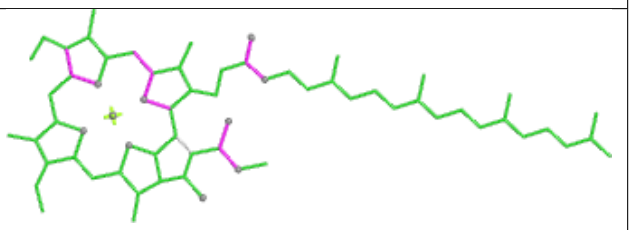
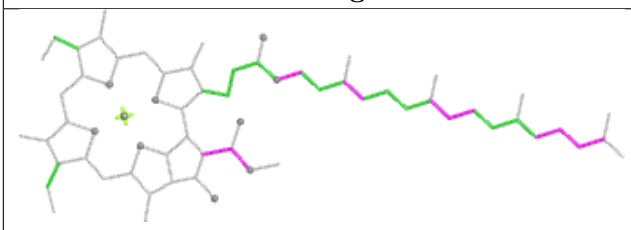
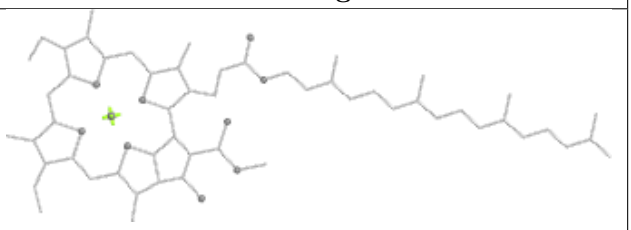
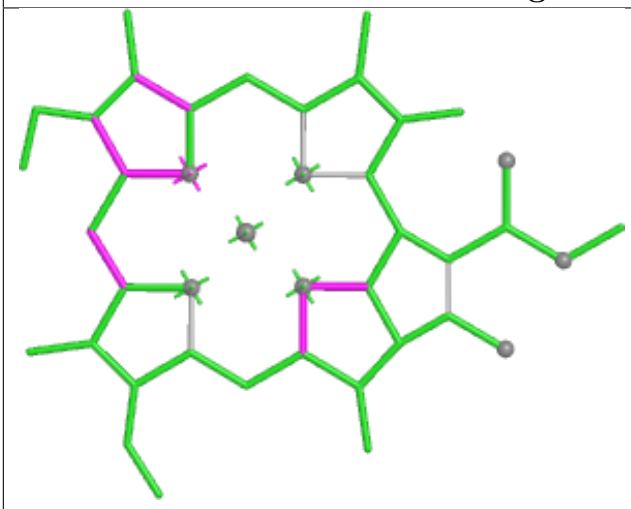


Rings

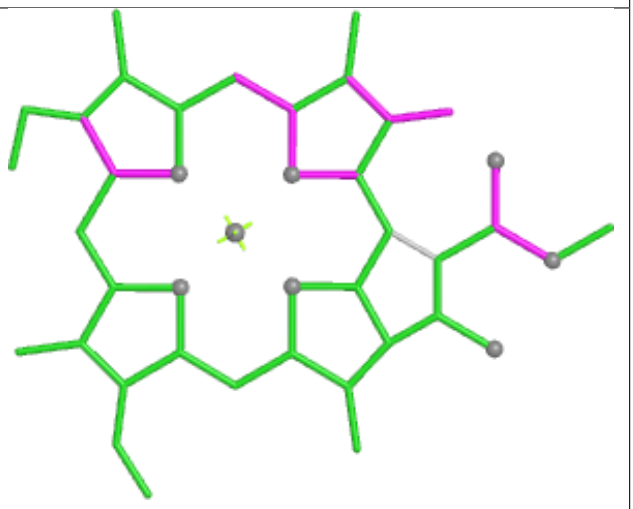
Ligand CLA X 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

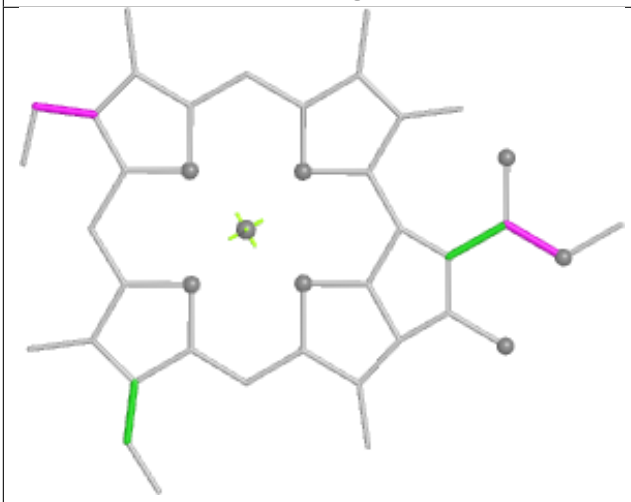
Ligand CLA 4 319



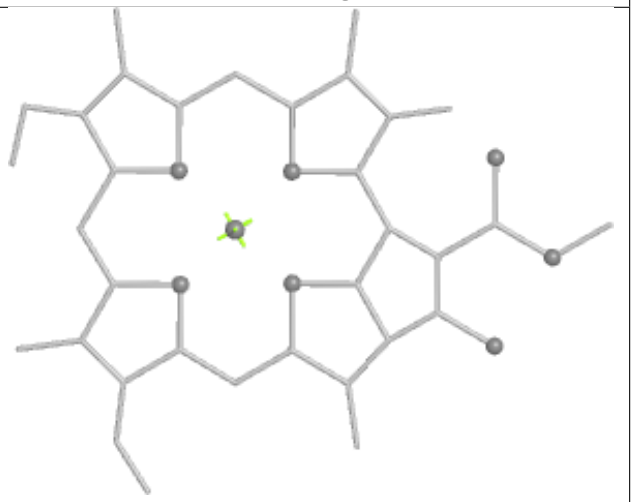
Bond lengths



Bond angles

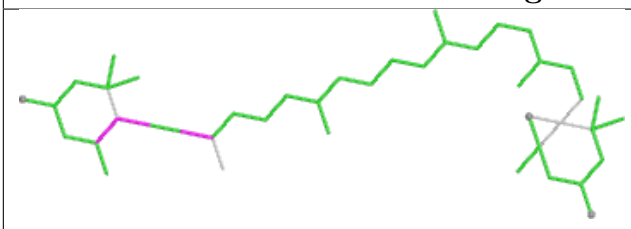


Torsions

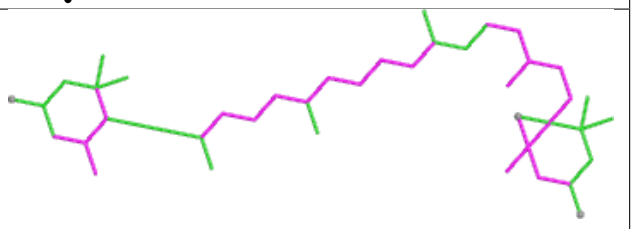


Rings

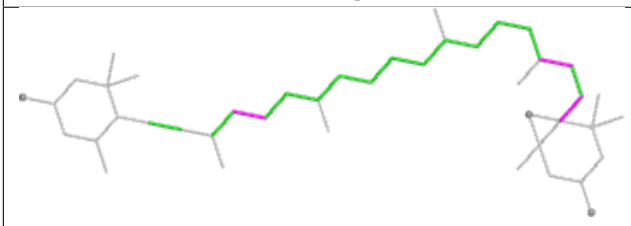
Ligand DD6 Q 303



Bond lengths



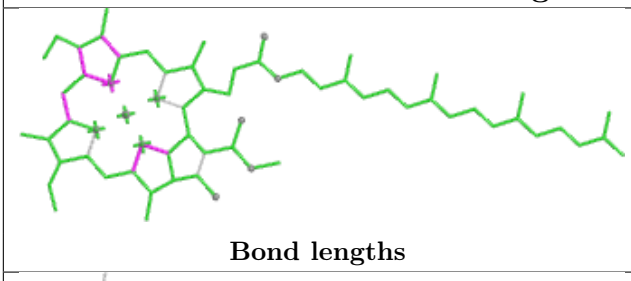
Bond angles



Torsions

Rings

Ligand CLA f 802



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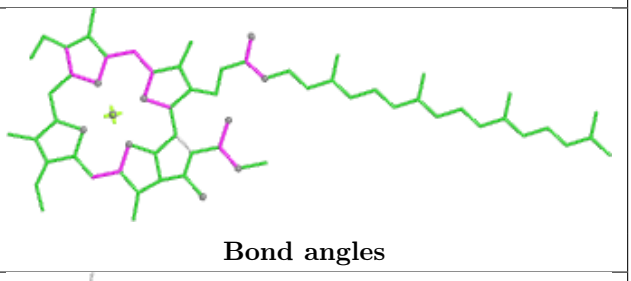

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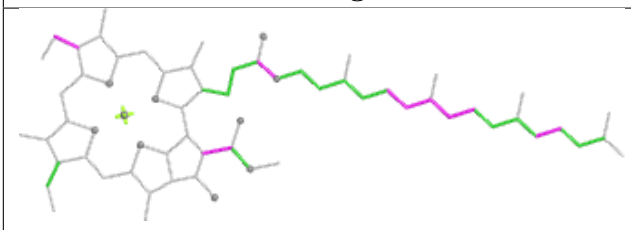
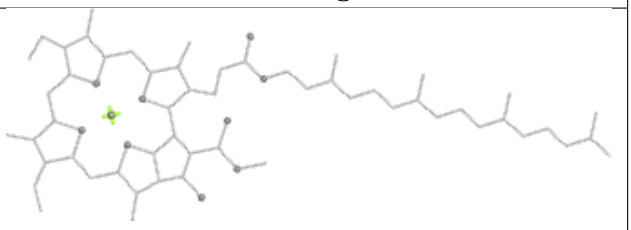
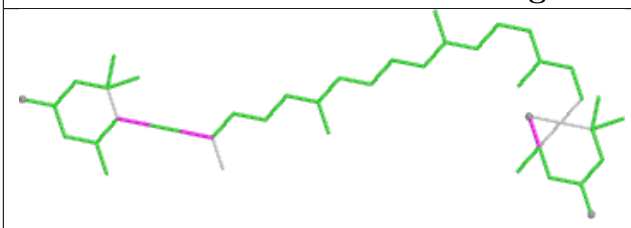


Torsions



Rings

Ligand DD6 y 303



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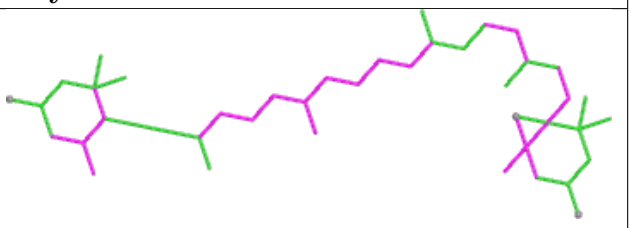
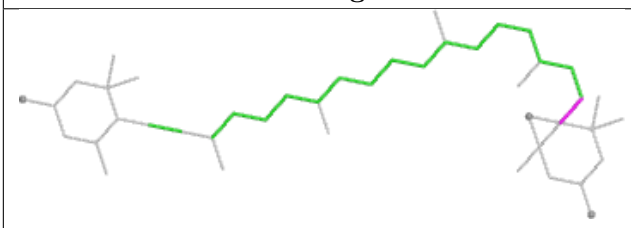


Bond angles



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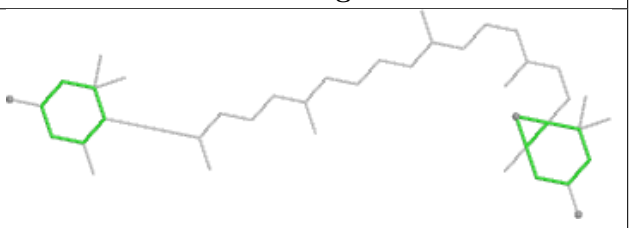
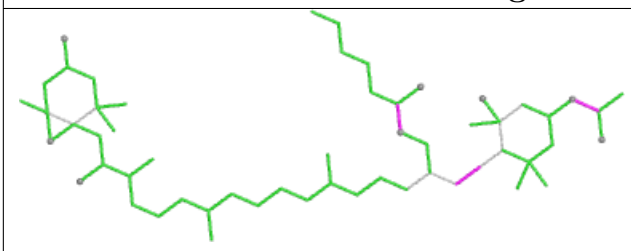


Rings

Ligand A1EB1 S 302



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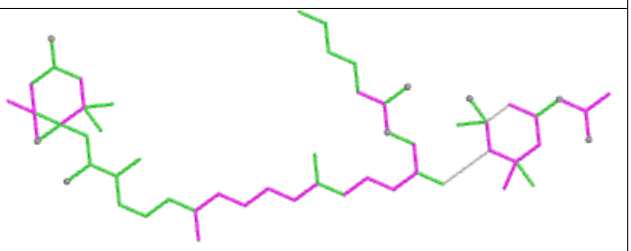
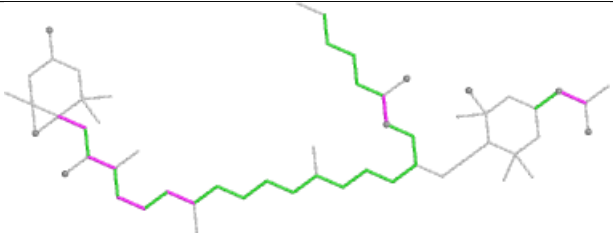


Bond angles



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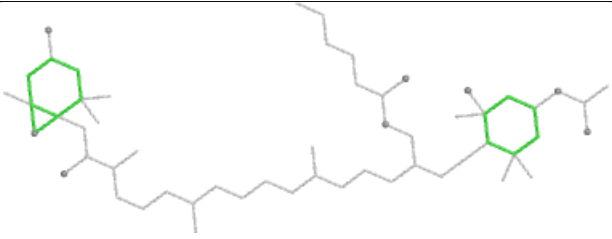
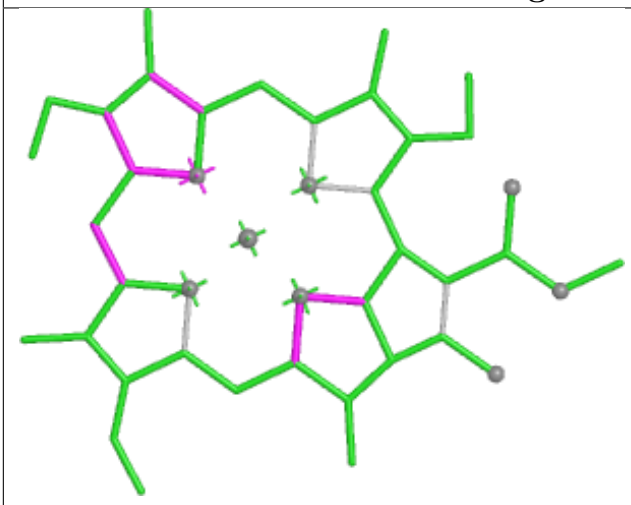


Rings

Ligand CLA 6 310



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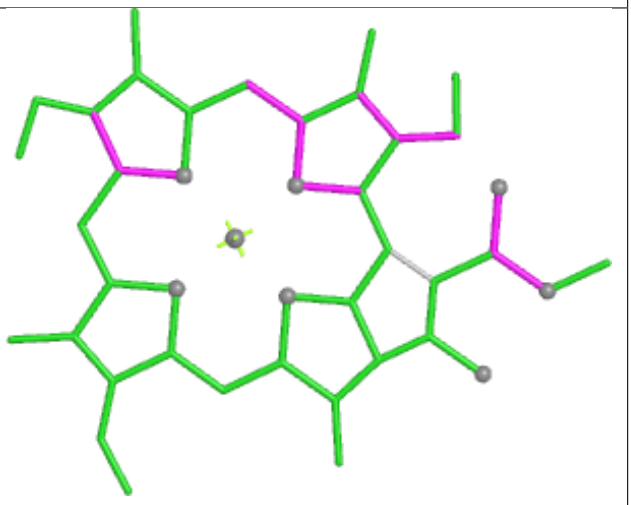
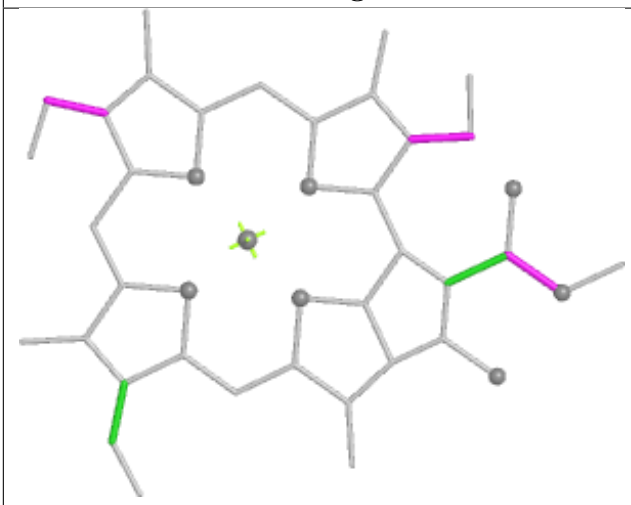
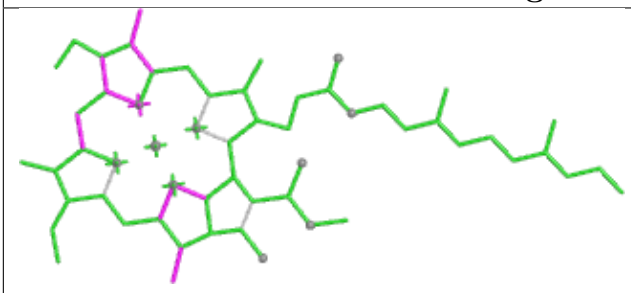
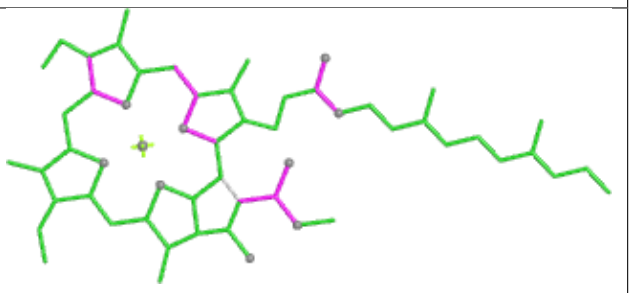
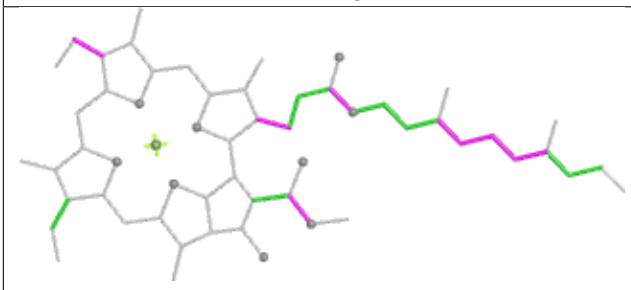
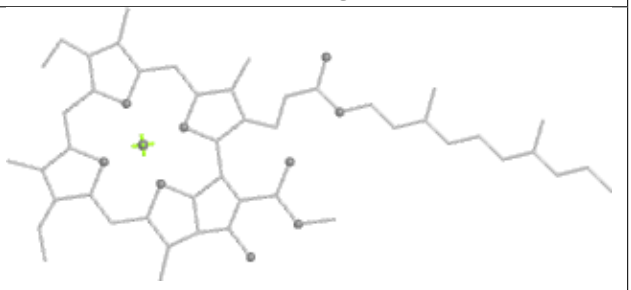


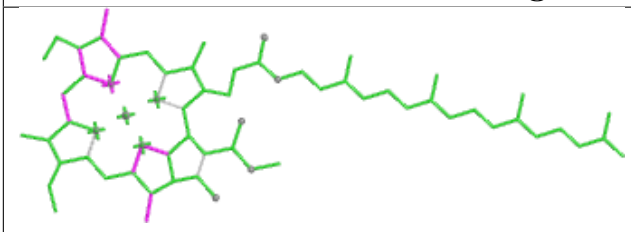
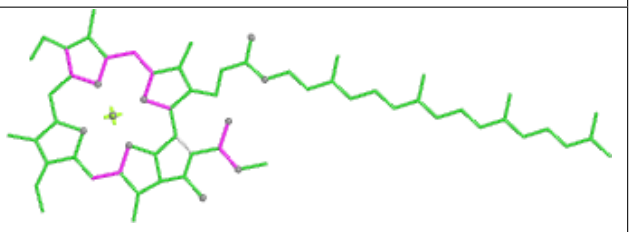
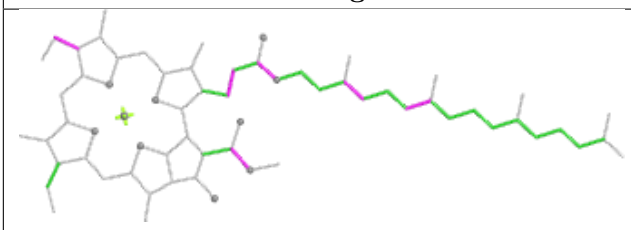
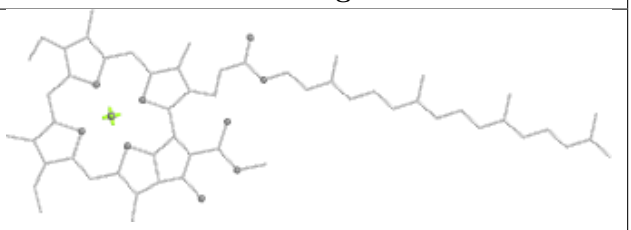
Bond angles



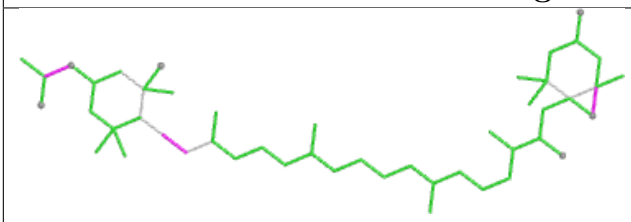
Torsions

Rings

Ligand CLA F 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 9 305



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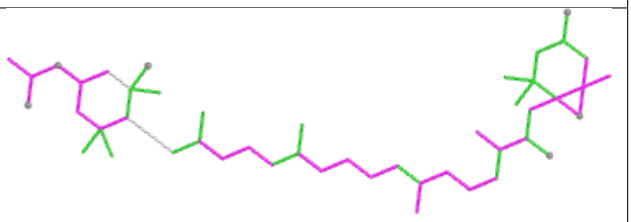

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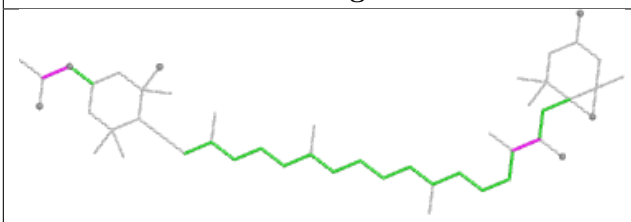
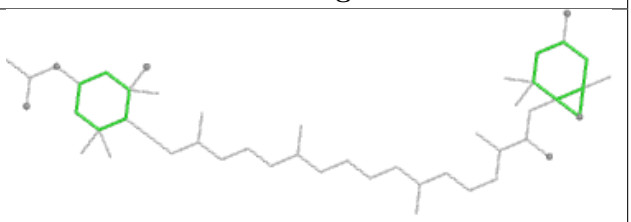
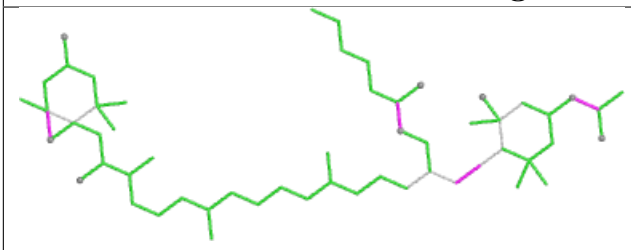


Torsions

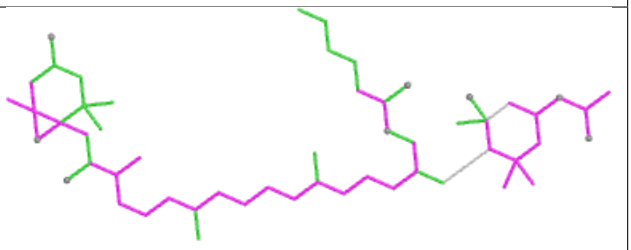


Rings

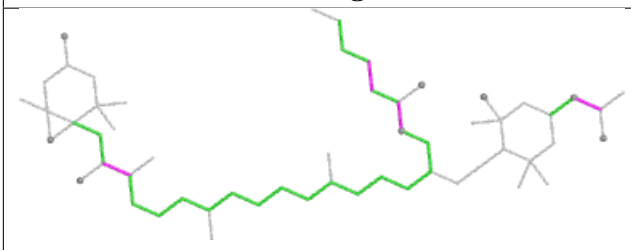
Ligand A1EB1 J 302



Bond lengths



Bond angles



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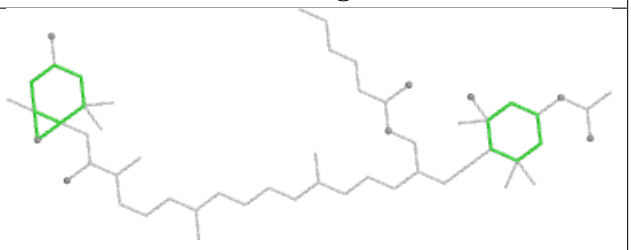
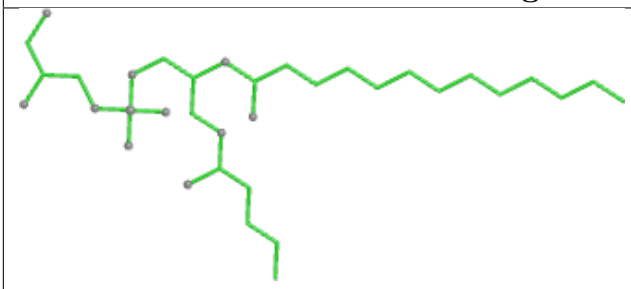


Rings

Ligand LHG H 317



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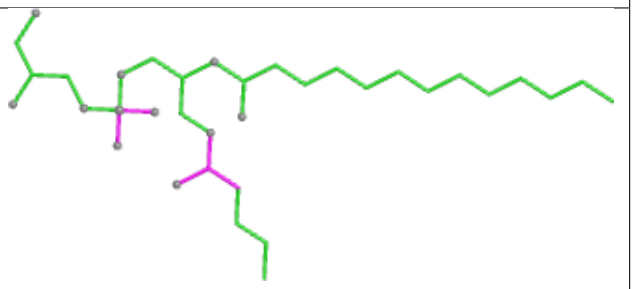
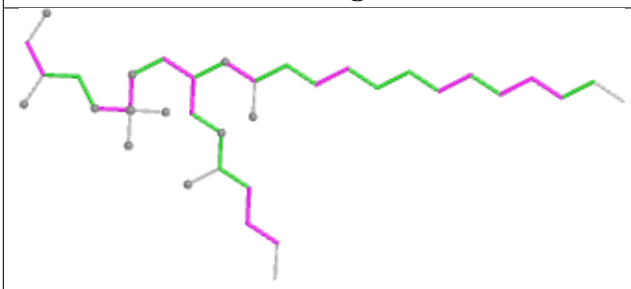
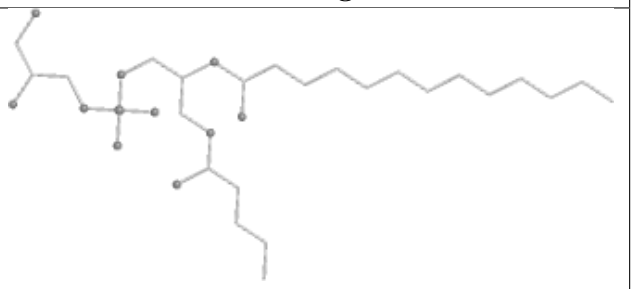


Bond angles

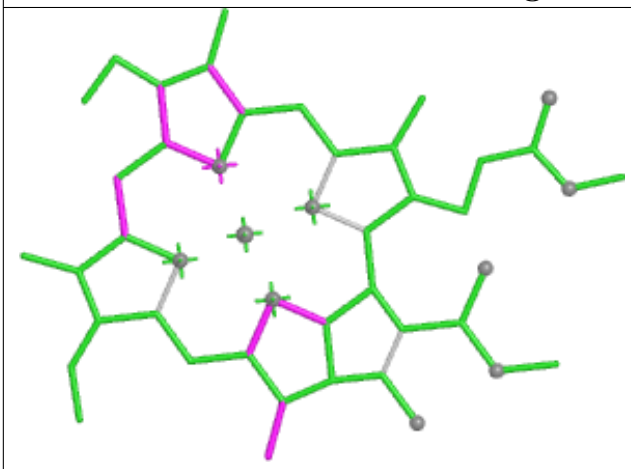


Torsions

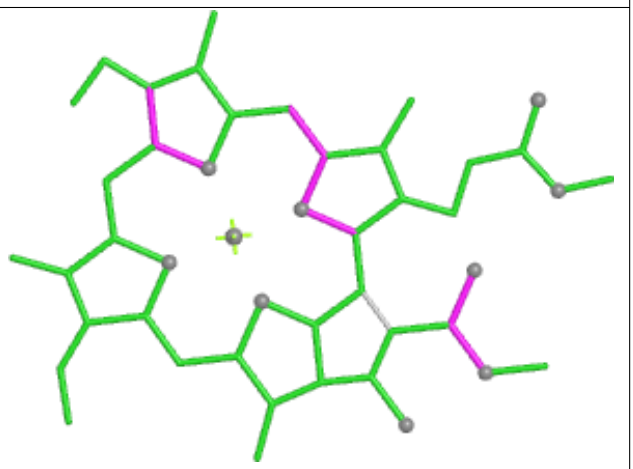


Rings

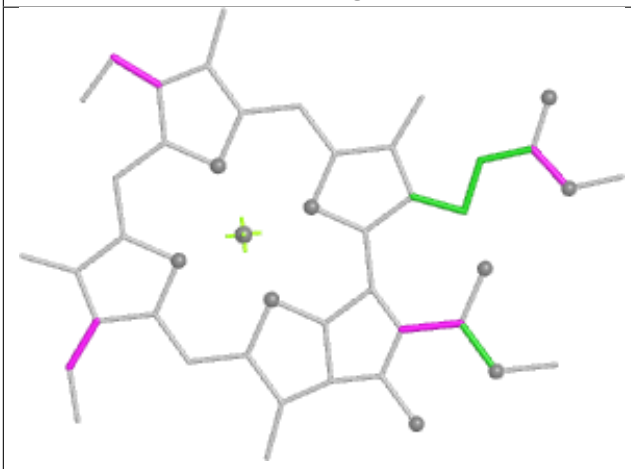
Ligand CLA O 312



Bond lengths



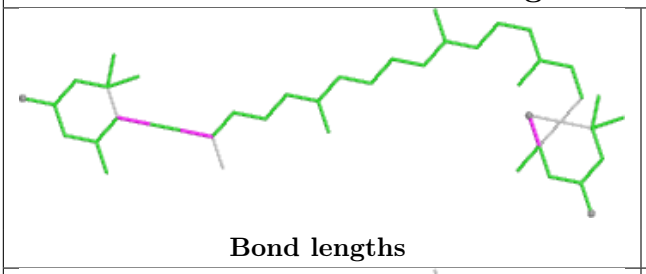
Bond angles



Torsions

Rings

Ligand DD6 Q 306



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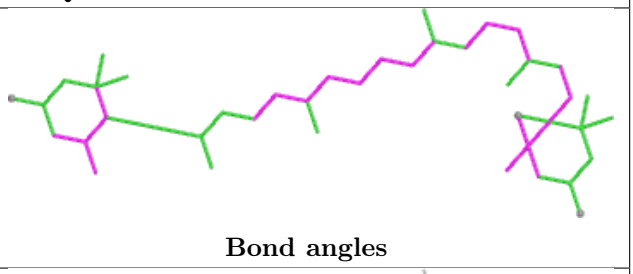
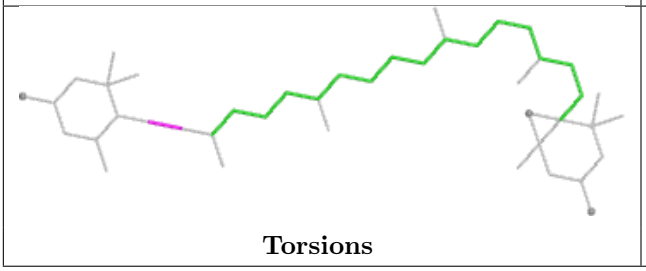
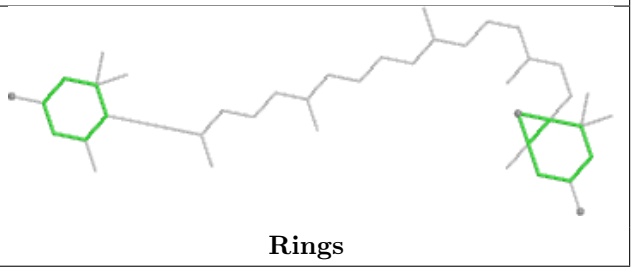


Bond angles

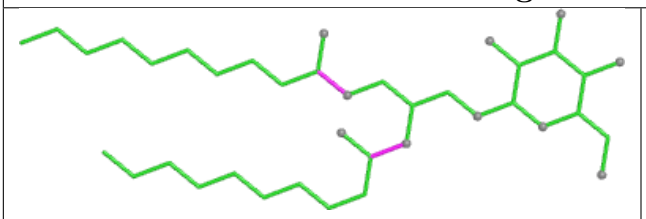


Torsions



Rings

Ligand LMG M 319



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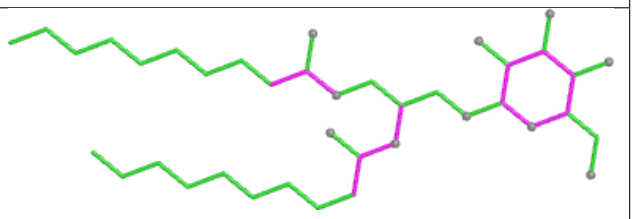
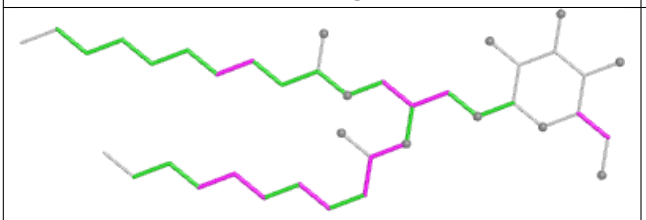
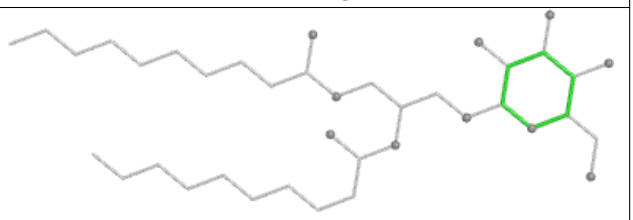


Bond angles

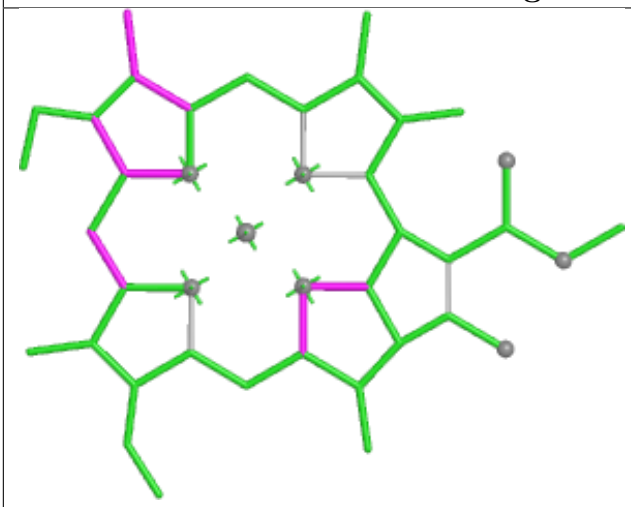


Torsions

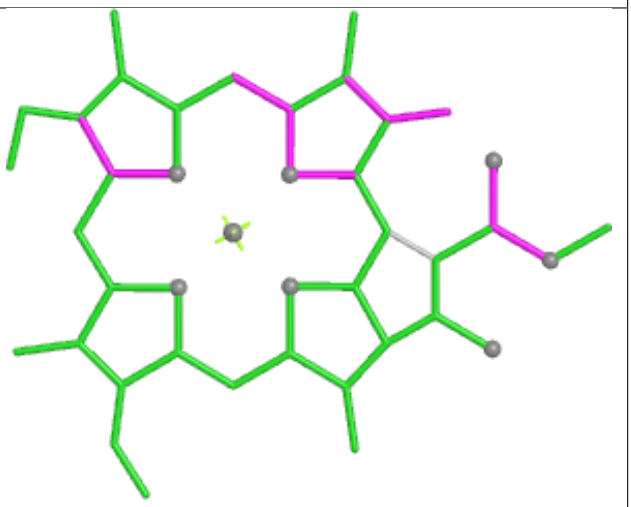


Rings

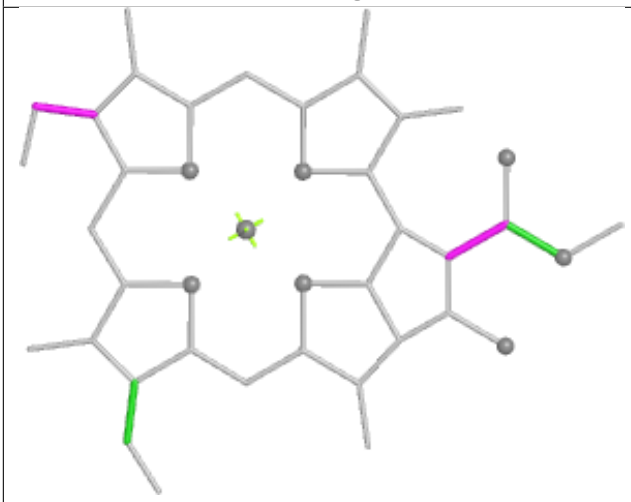
Ligand CLA Y 307



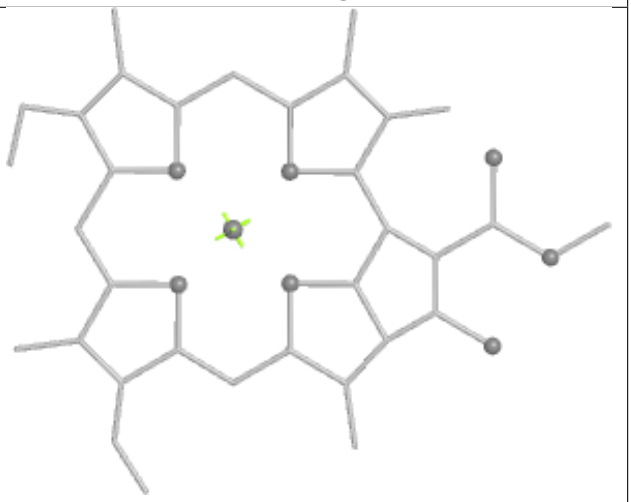
Bond lengths



Bond angles

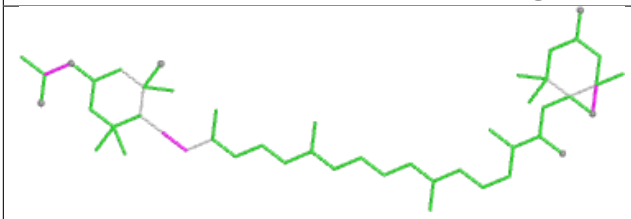


Torsions

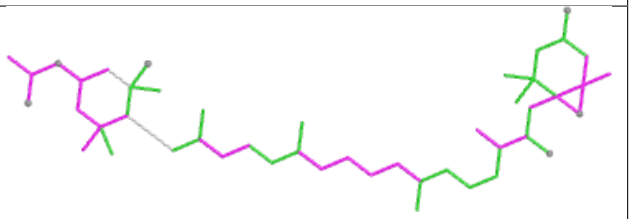


Rings

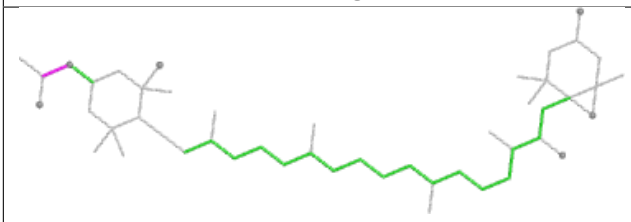
Ligand A86 R 301



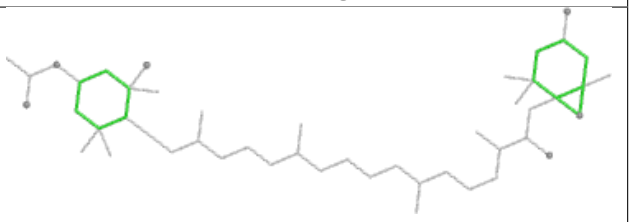
Bond lengths



Bond angles

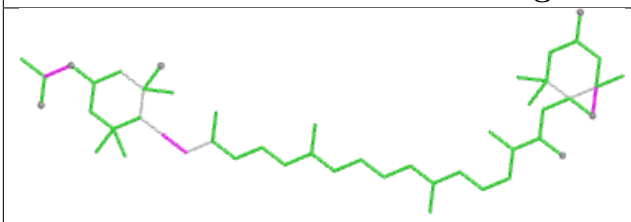


Torsions



Rings

Ligand A86 y 305



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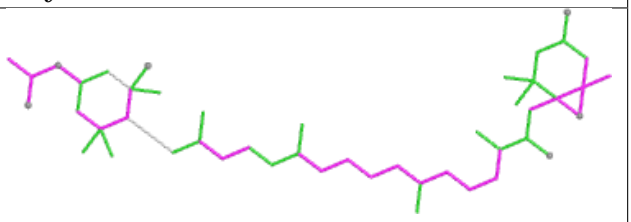

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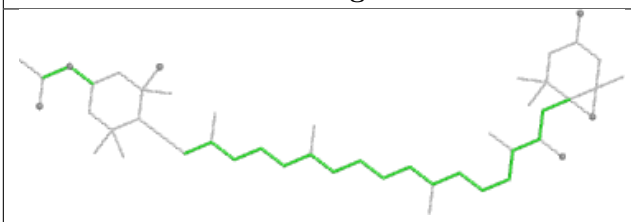

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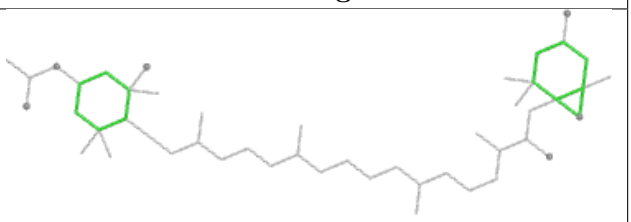
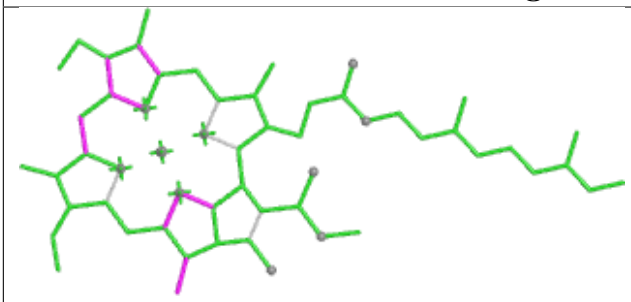


Rings

Ligand CLA T 309



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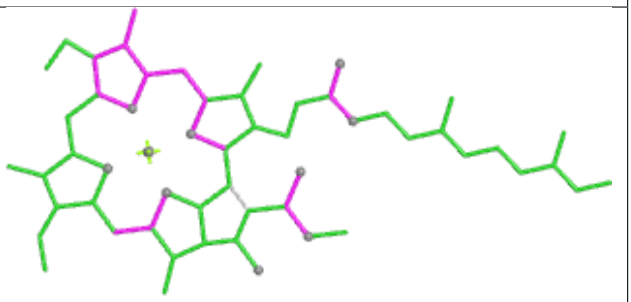
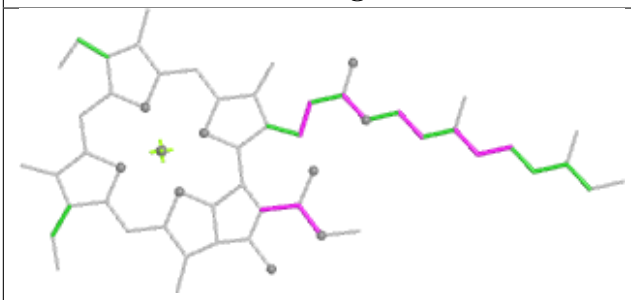


Bond angles



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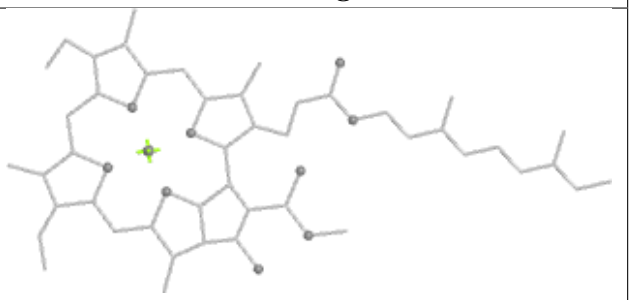
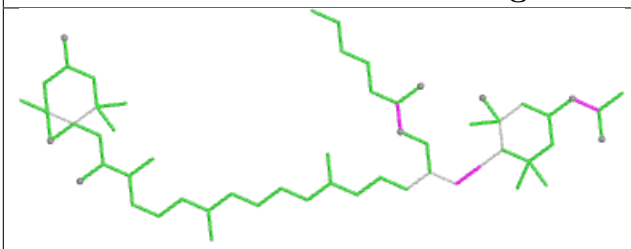


Rings

Ligand A1EB1 4 301



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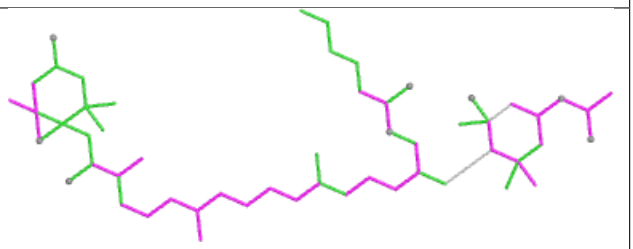
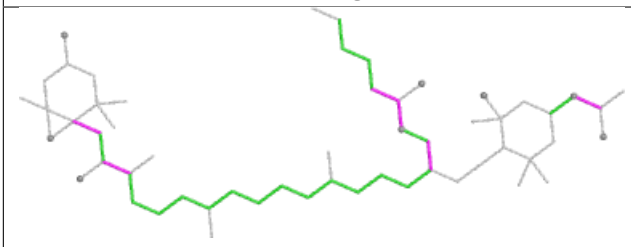


Bond angles



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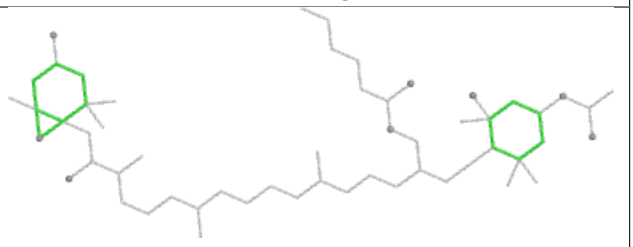
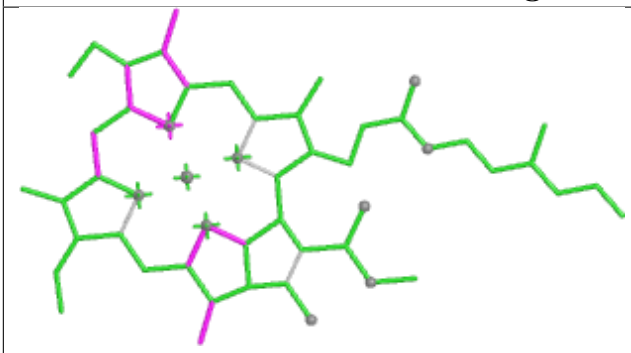


Rings

Ligand CLA X 317



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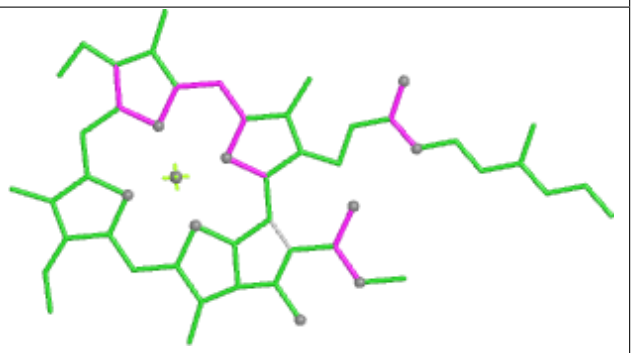
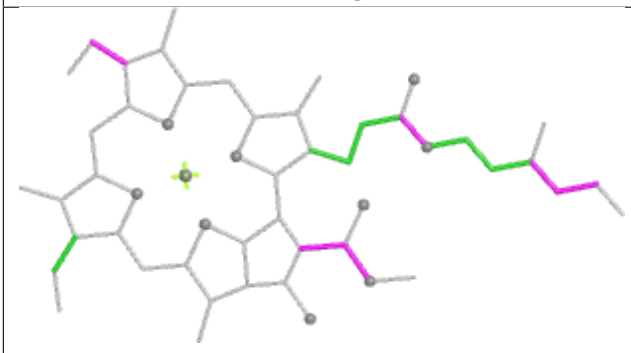


Bond angles



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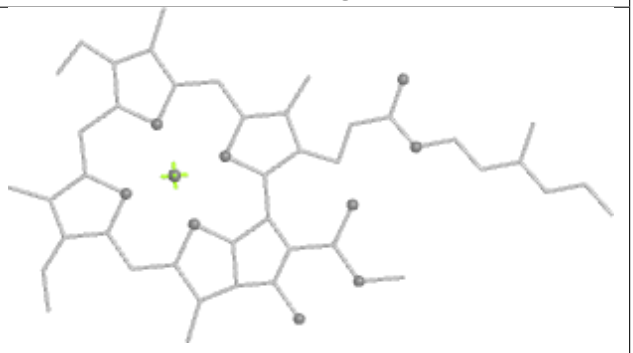
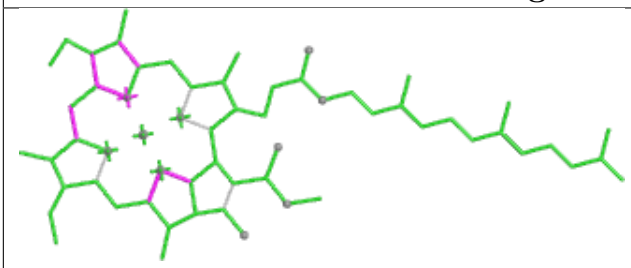


Rings

Ligand CLA 5 307



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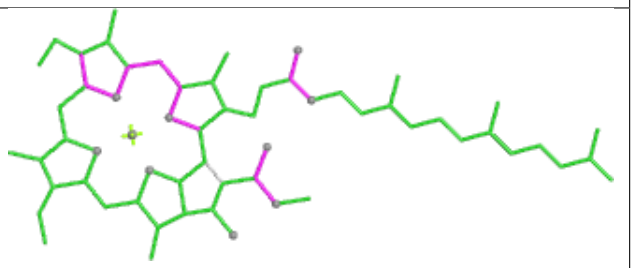
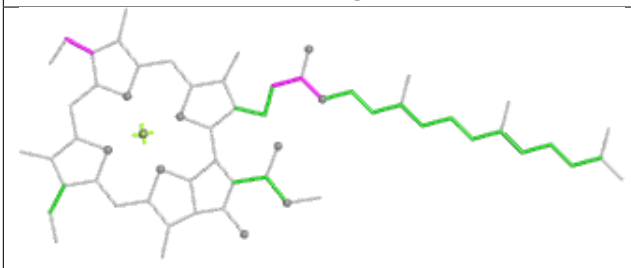


Bond angles



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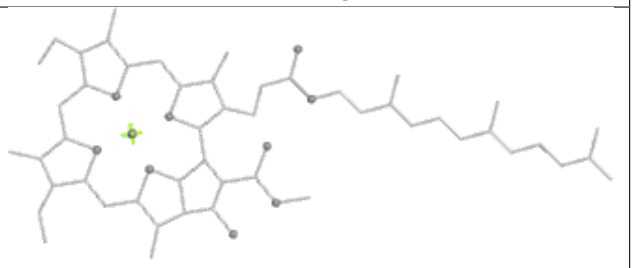
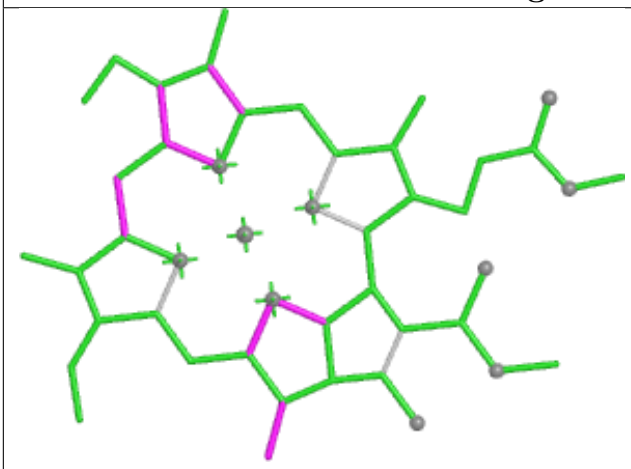


Rings

Ligand CLA y 309



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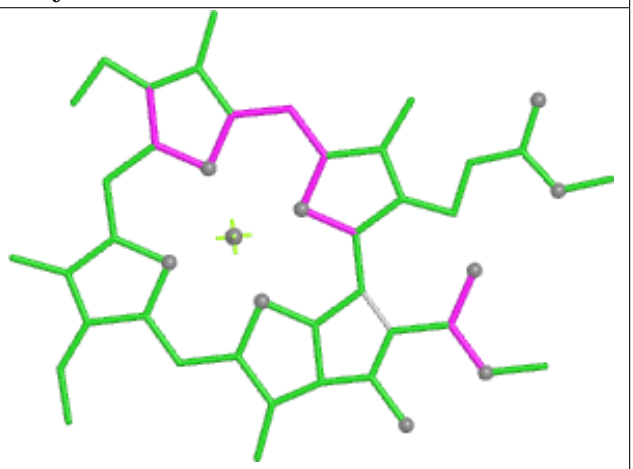

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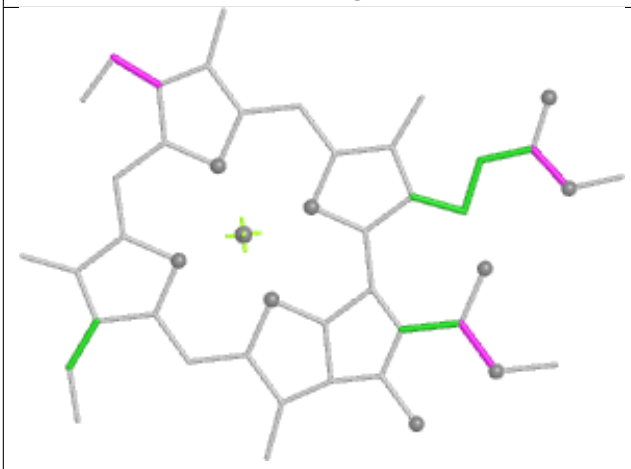
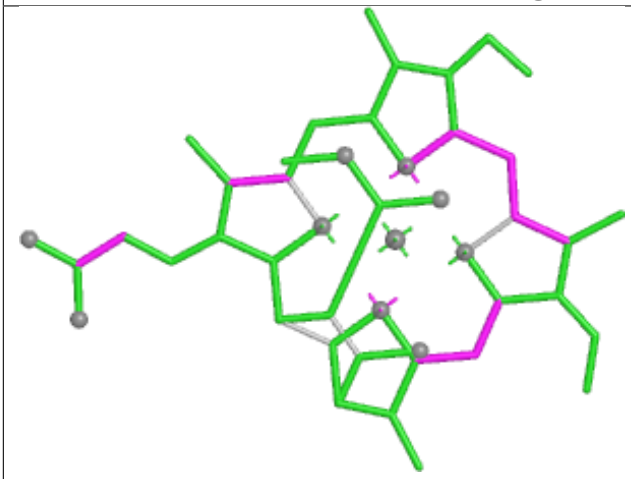


Torsions

Rings

Ligand KC2 y 316



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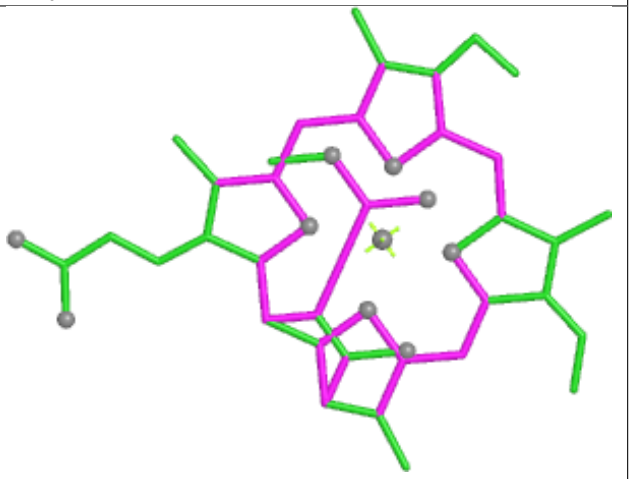
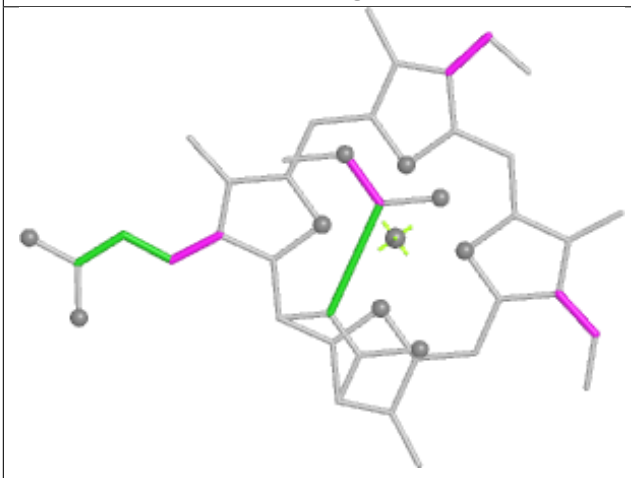
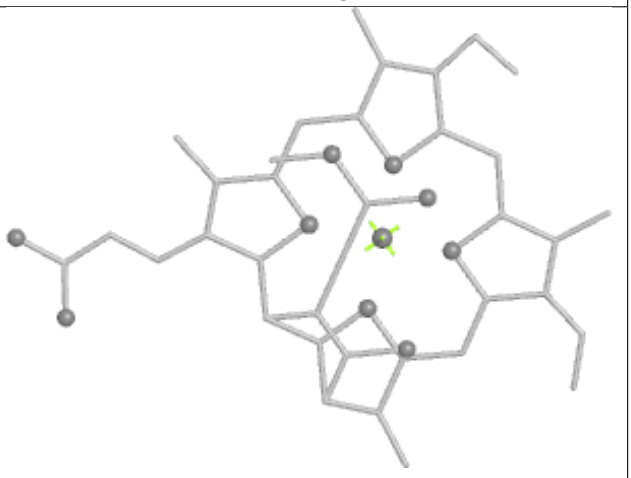


Bond angles

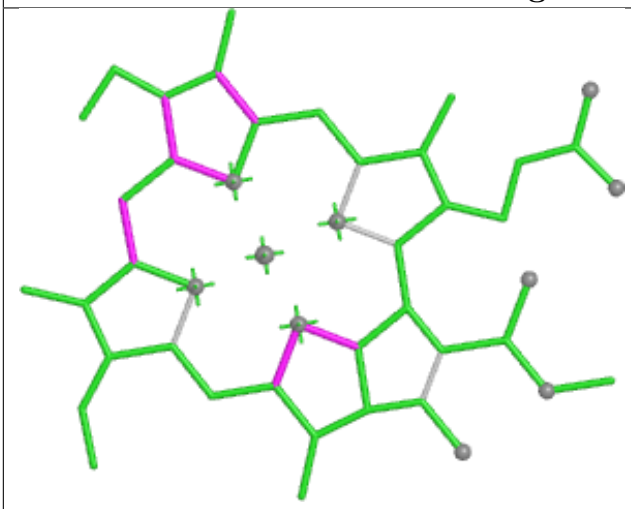


Torsions



Rings

Ligand CLA 9 319



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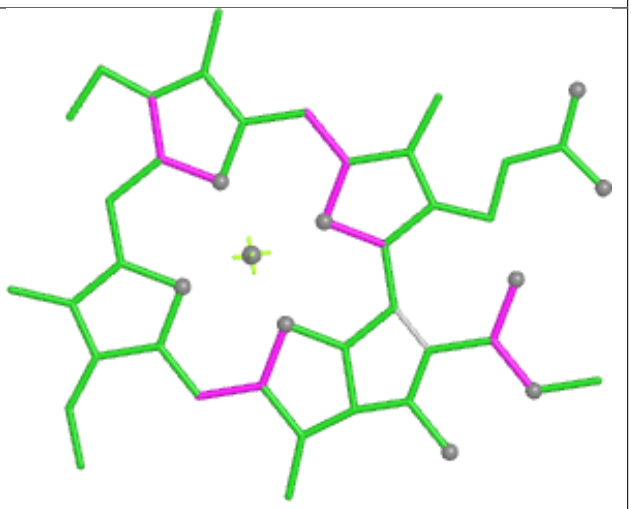
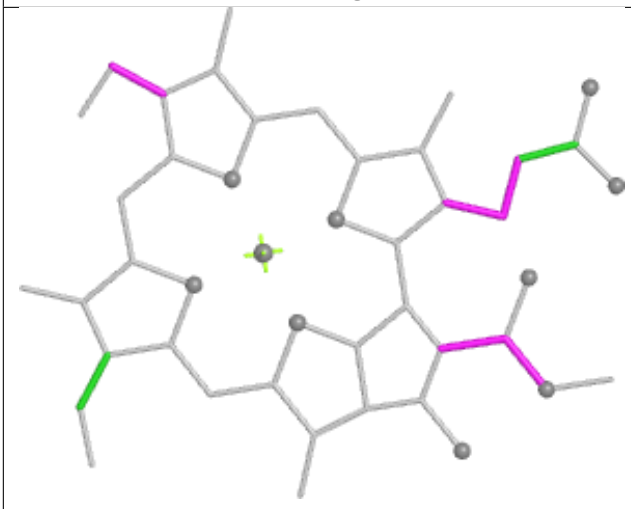


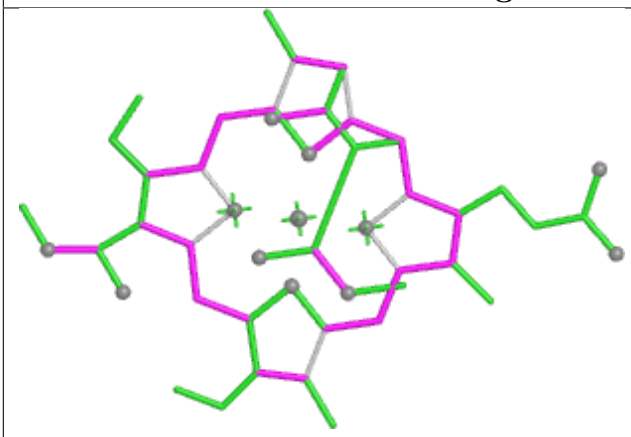
Bond angles



Torsions

Rings

Ligand A1ECV W 317



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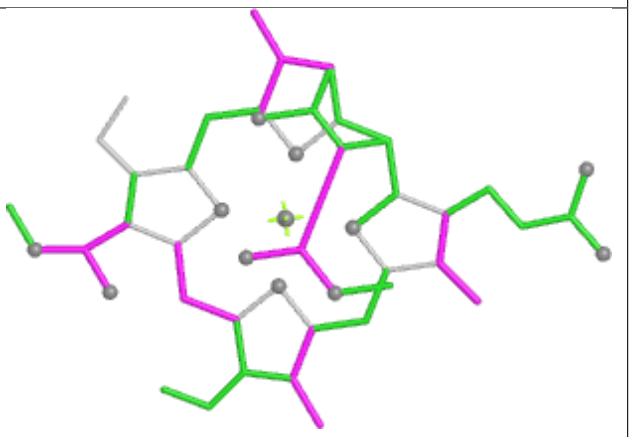
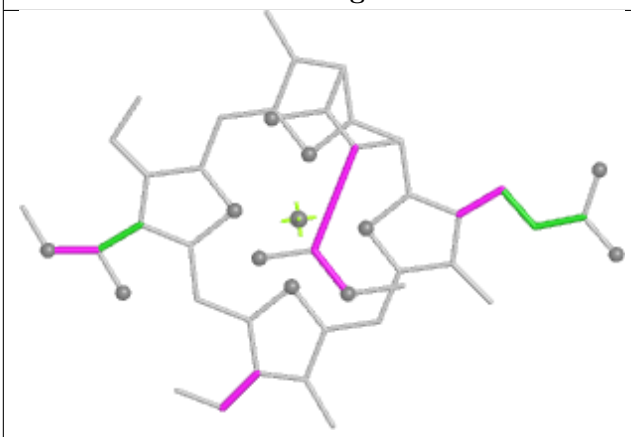
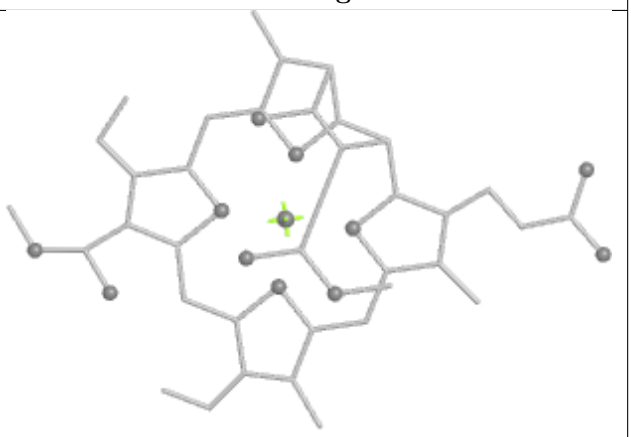


Bond angles

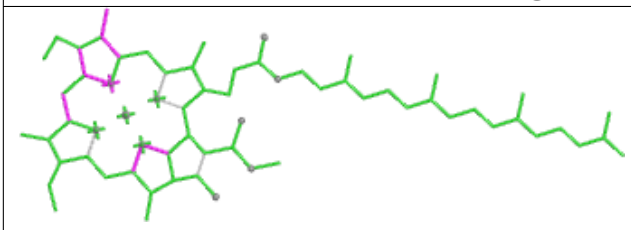


Torsions



Rings

Ligand CLA a 835



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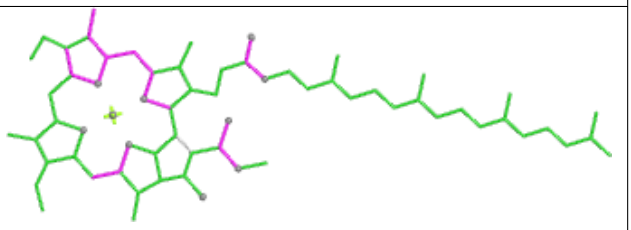
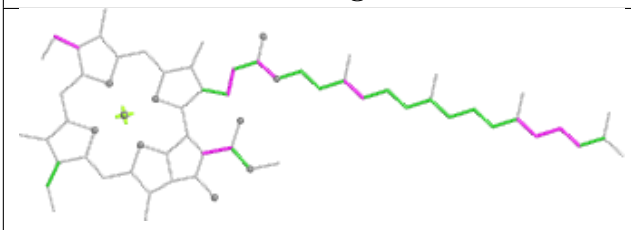


Bond angles



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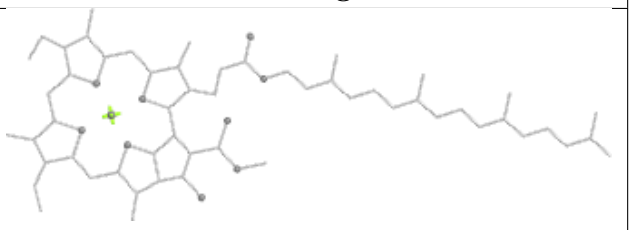
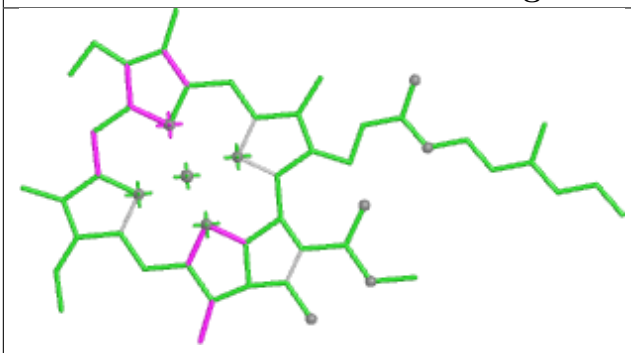


Rings

Ligand CLA H 309



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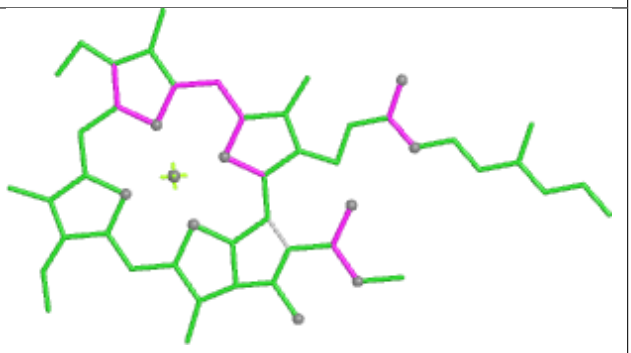
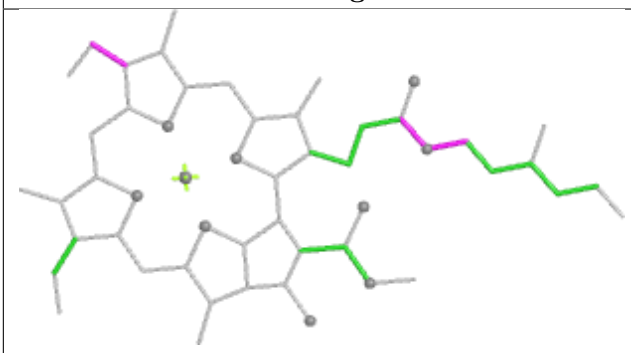


Bond angles



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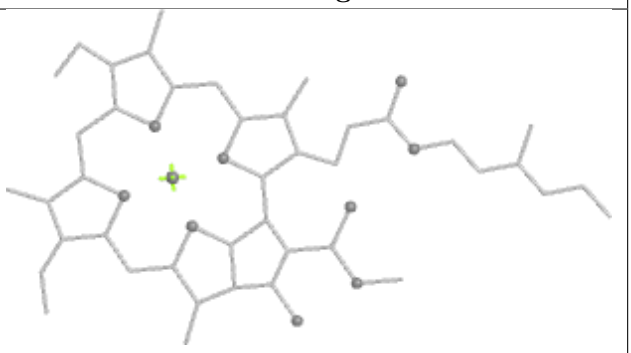
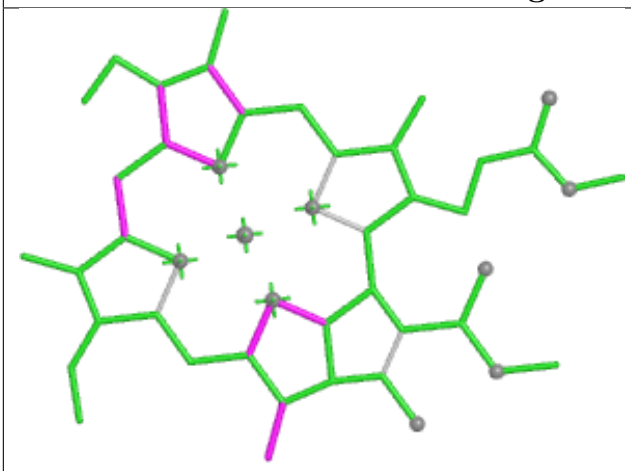


Rings

Ligand CLA J 316



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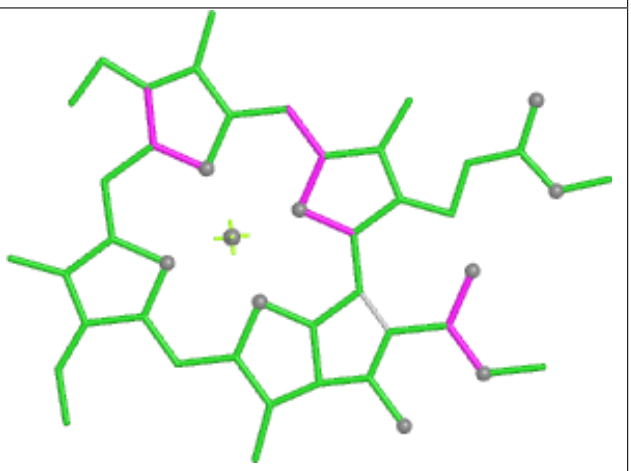
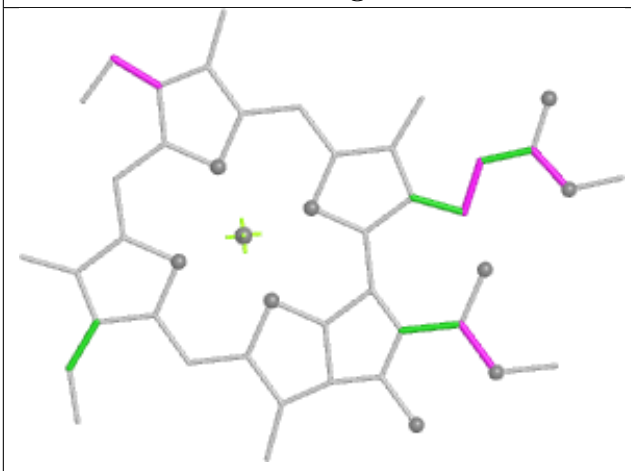


Bond angles



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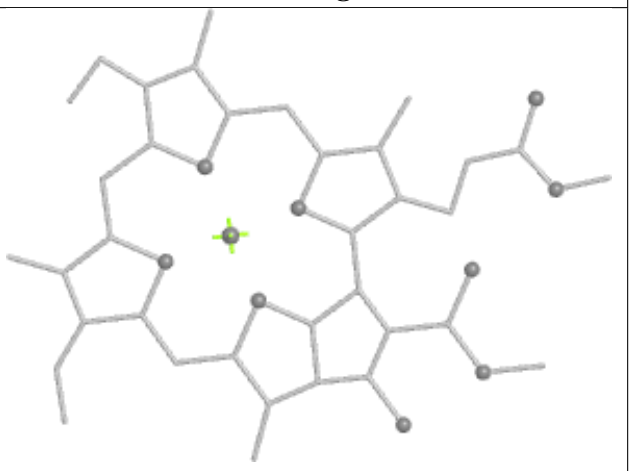
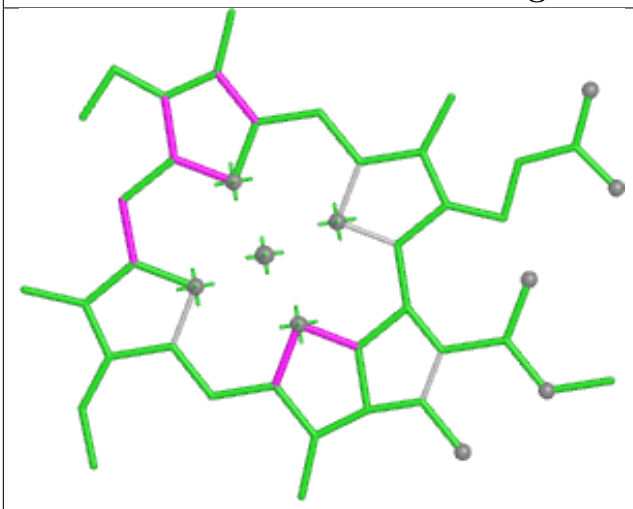


Rings

Ligand CLA 3 320



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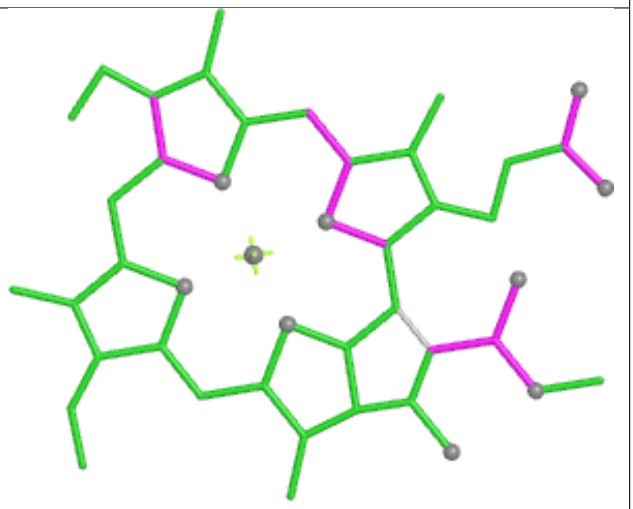
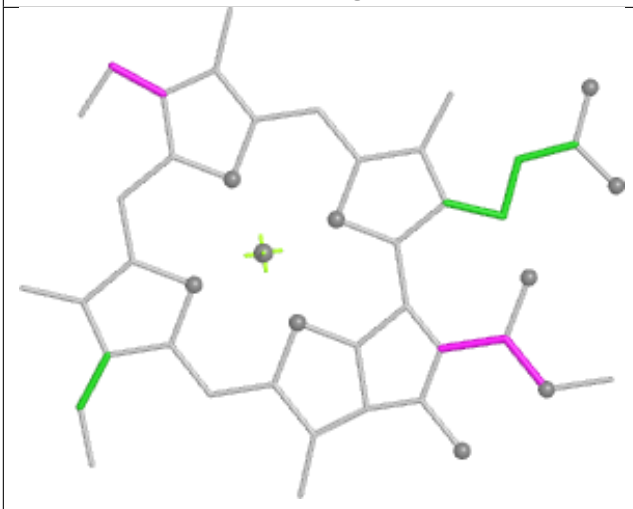


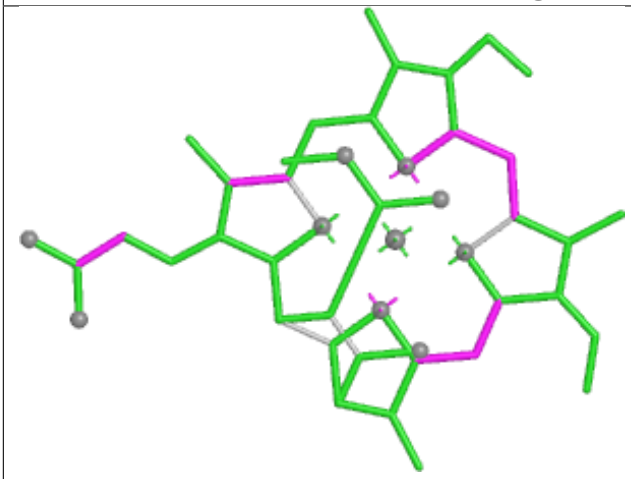
Bond angles



Torsions

Rings

Ligand KC2 y 314



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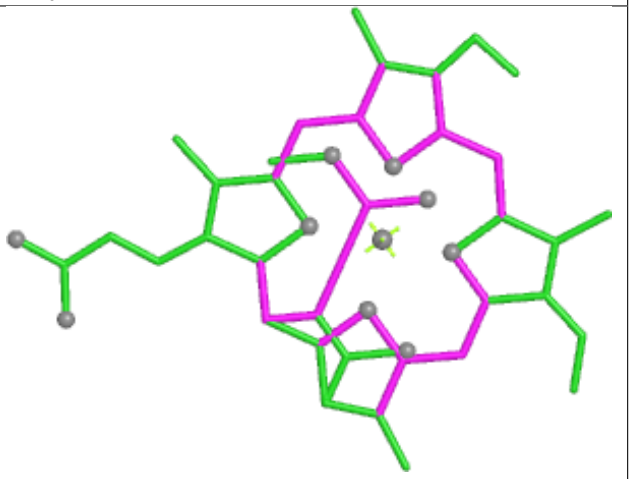
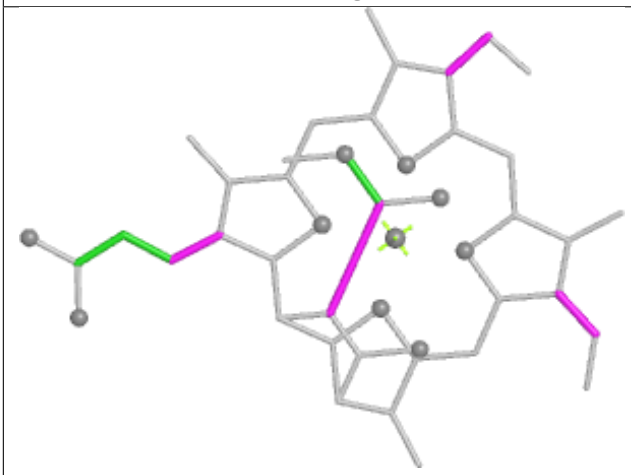
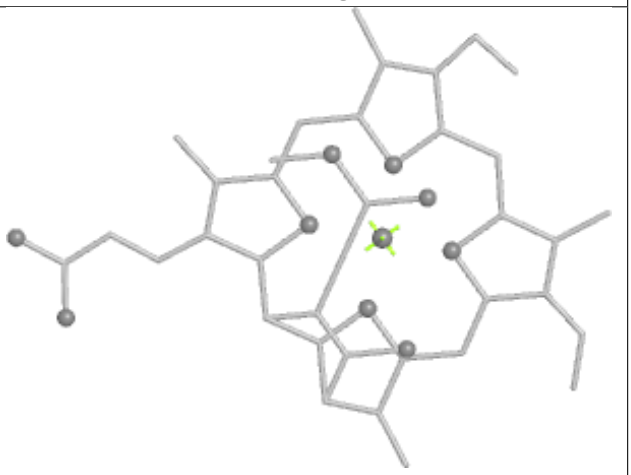


Bond angles

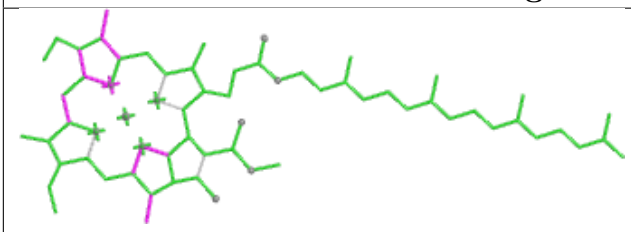


Torsions

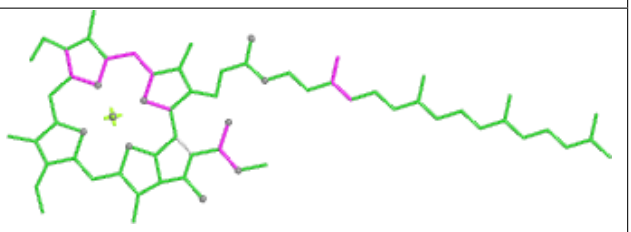


Rings

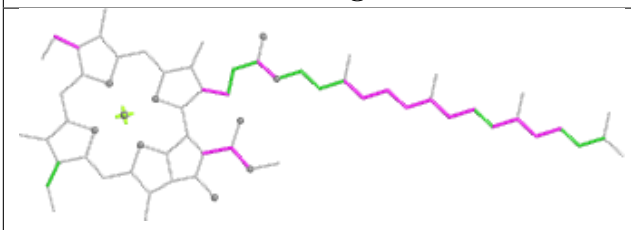
Ligand CLA E 312



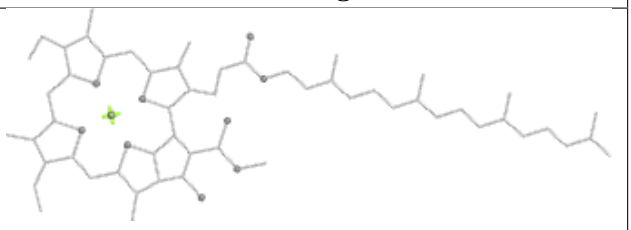
Bond lengths



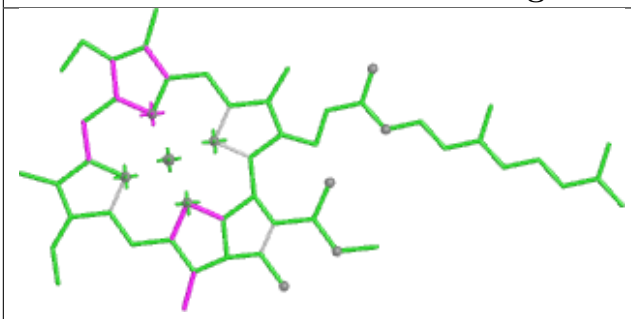
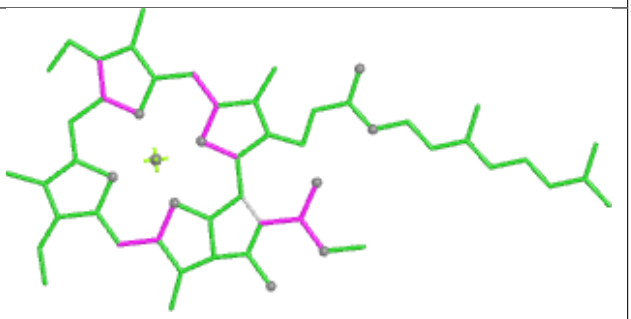
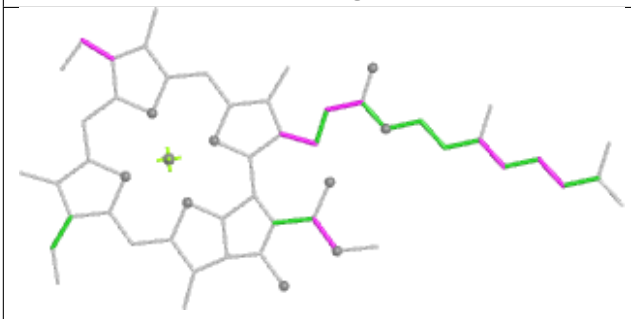
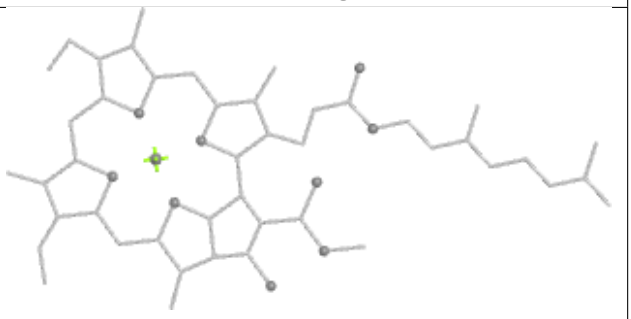
Bond angles

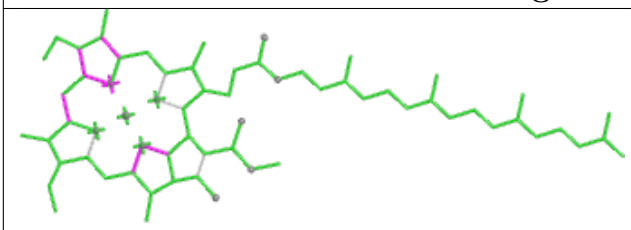
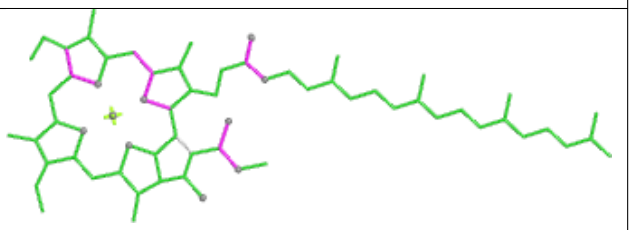
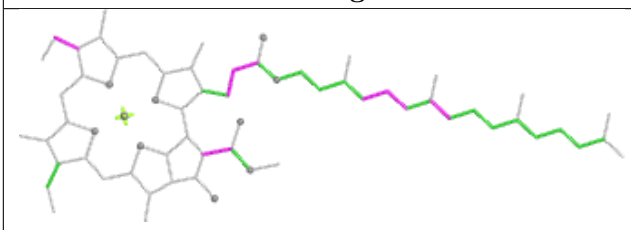
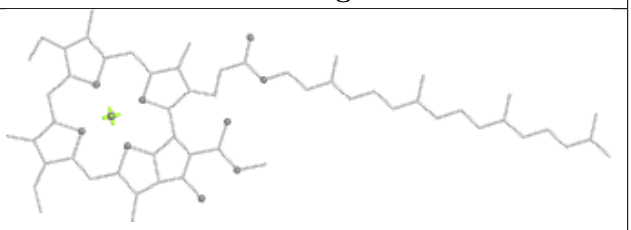


Torsions

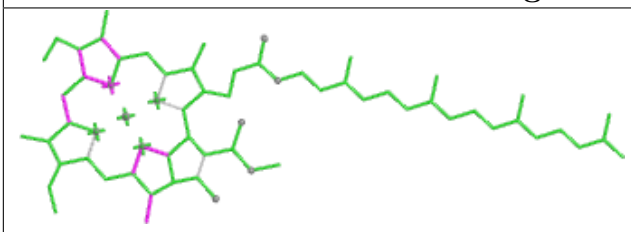


Rings

Ligand CLA h 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA i 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Q 310



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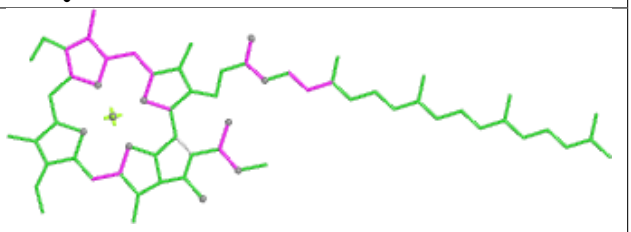
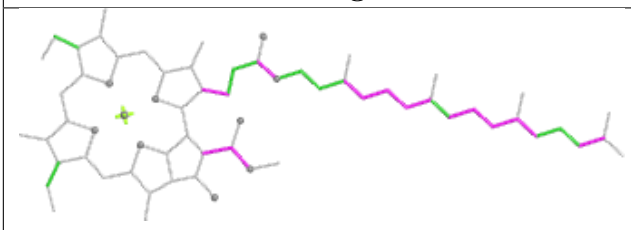
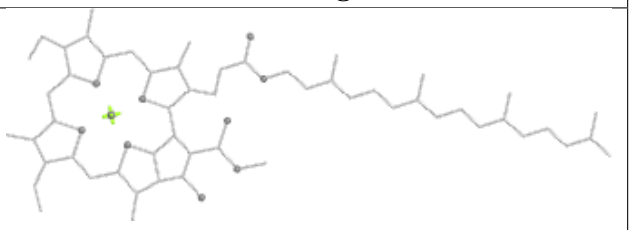


Bond angles



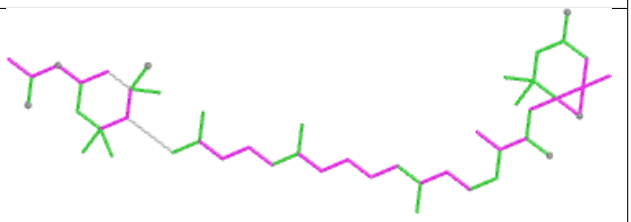
Torsions



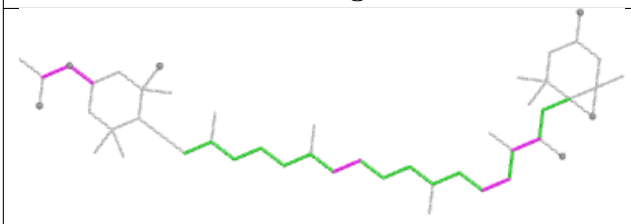
Rings

Ligand A86 9 303

Bond lengths



Bond angles



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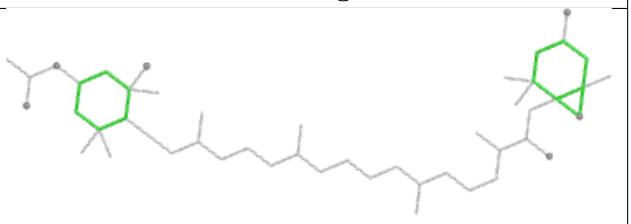
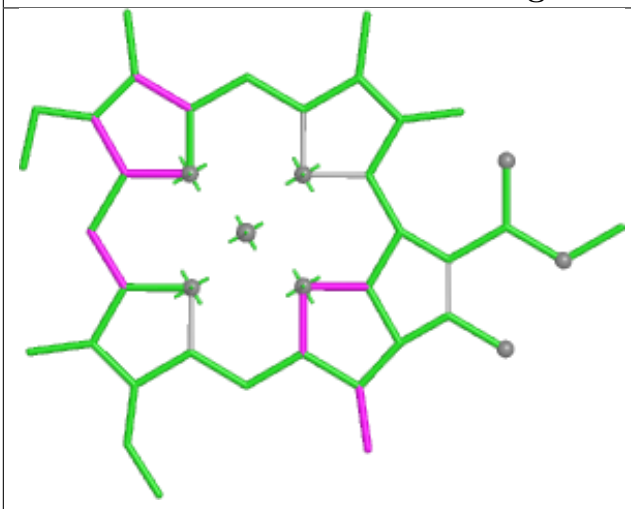


Rings

Ligand CLA y 310



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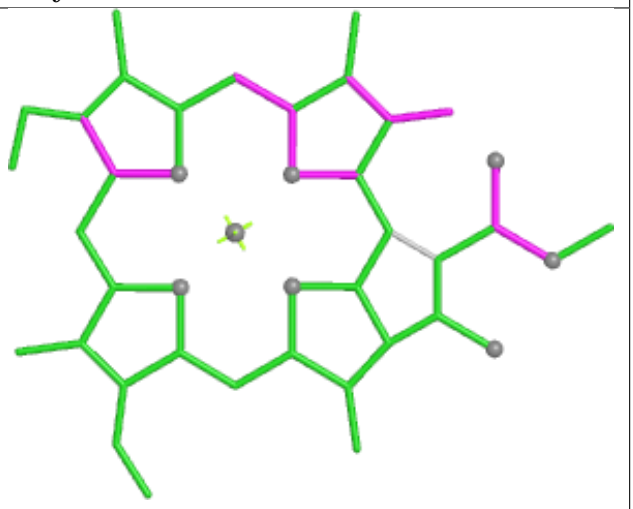
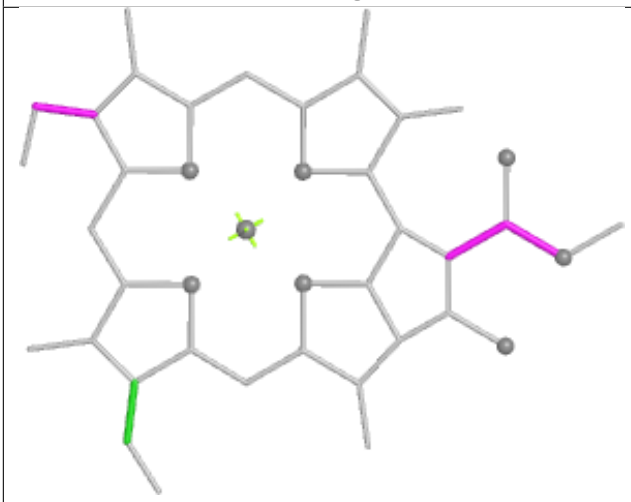


Bond angles



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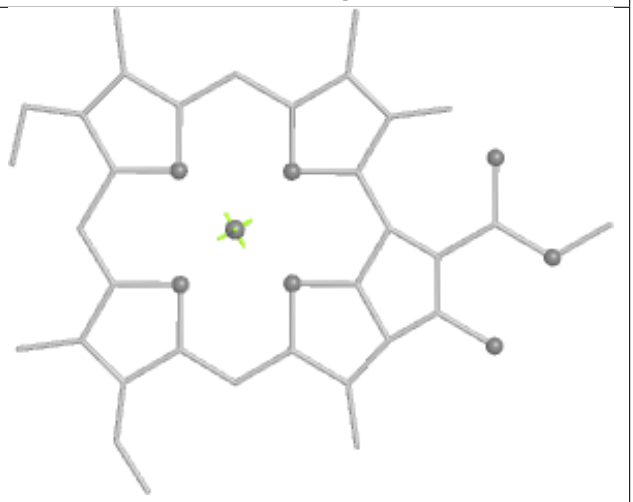
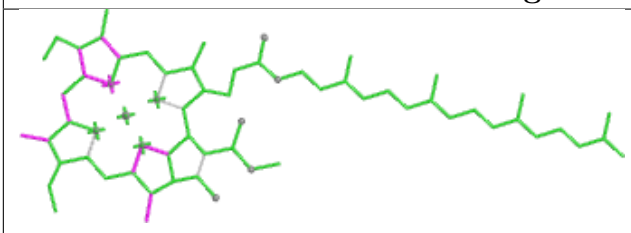


Rings

Ligand CLA A 312



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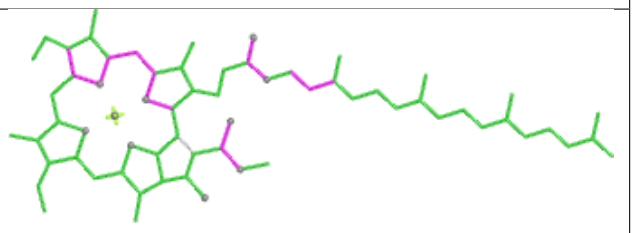
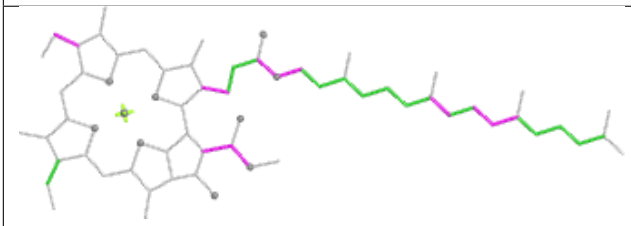


Bond angles



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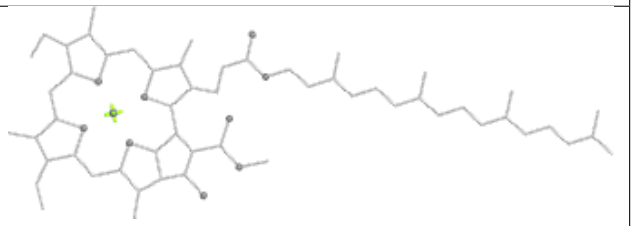
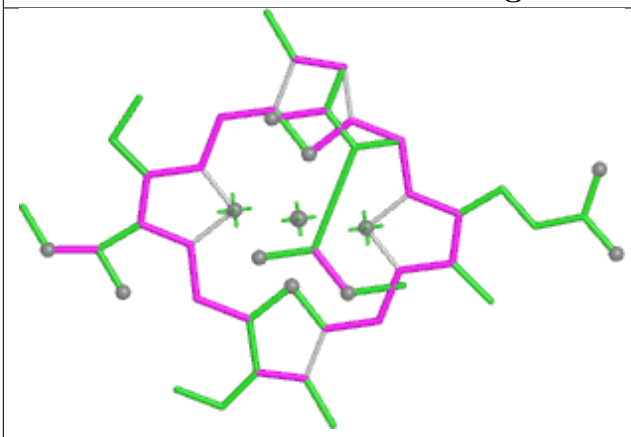


Rings

Ligand A1ECV 1 318



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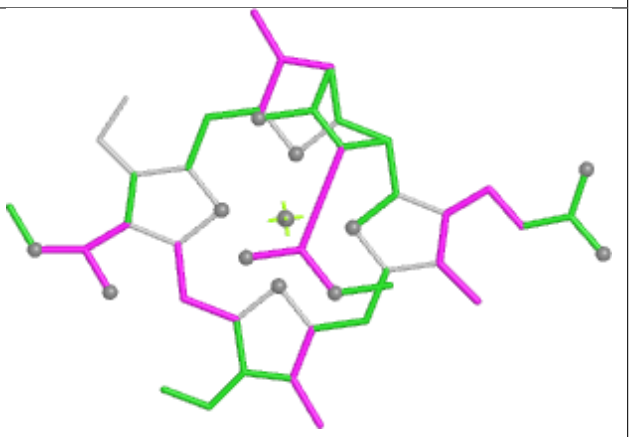
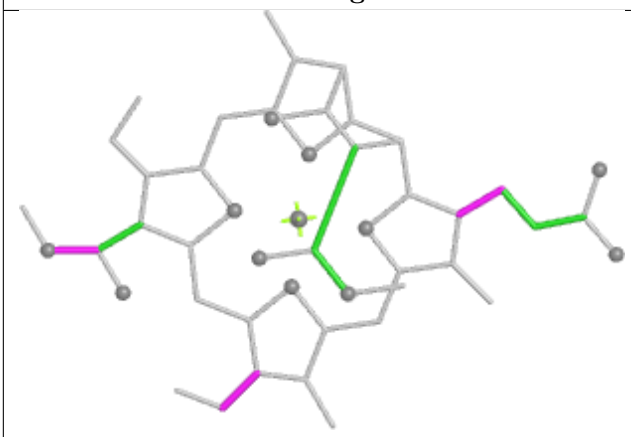


Bond angles



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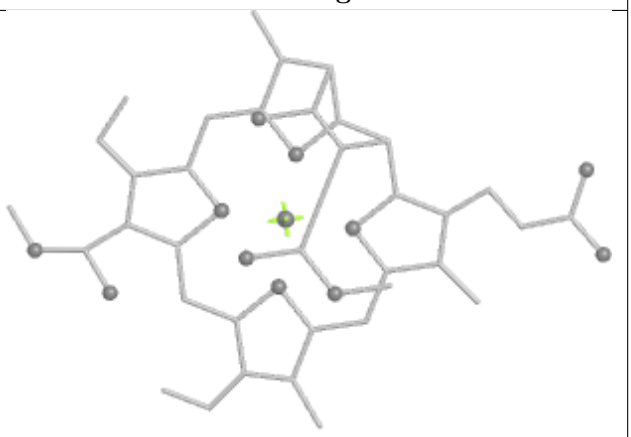
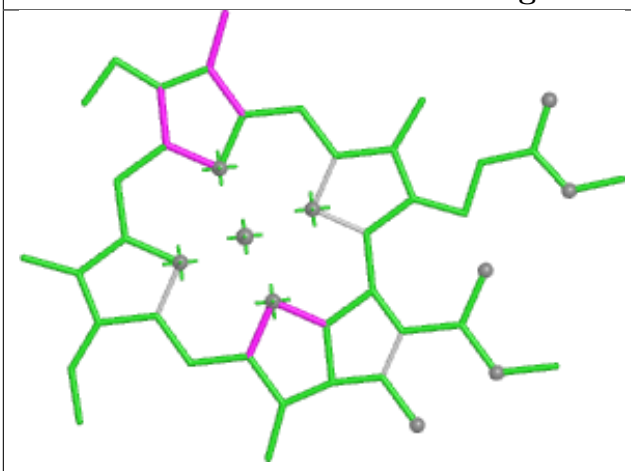


Rings

Ligand CLA W 319



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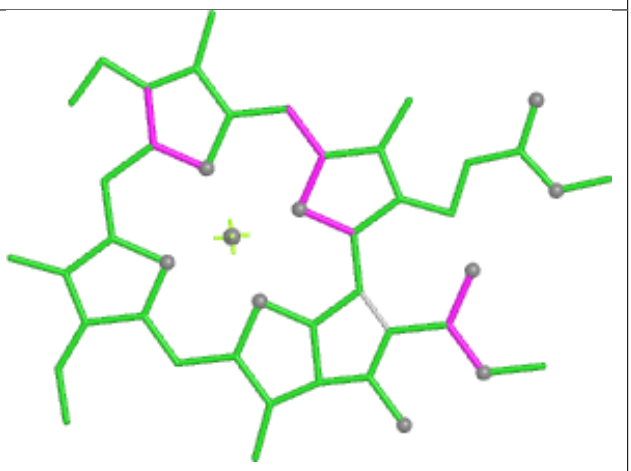
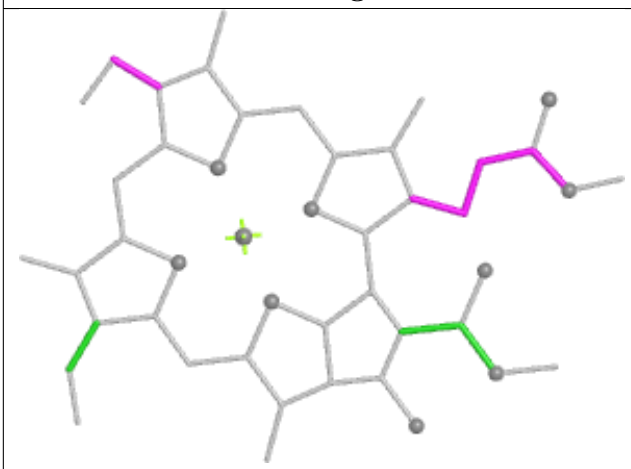


Bond angles



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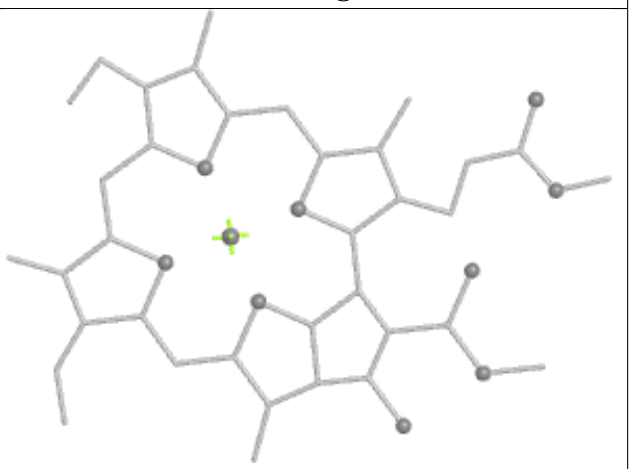
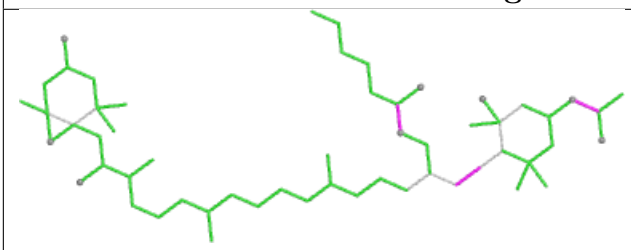


Rings

Ligand A1EB1 H 301



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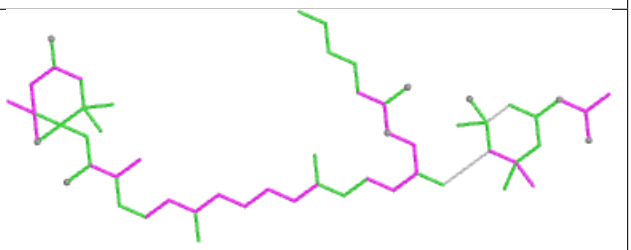
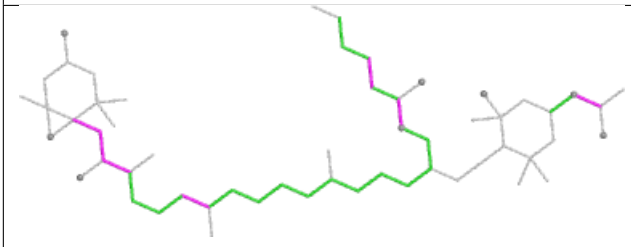


Bond angles



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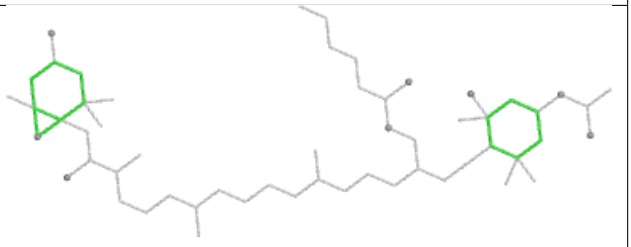
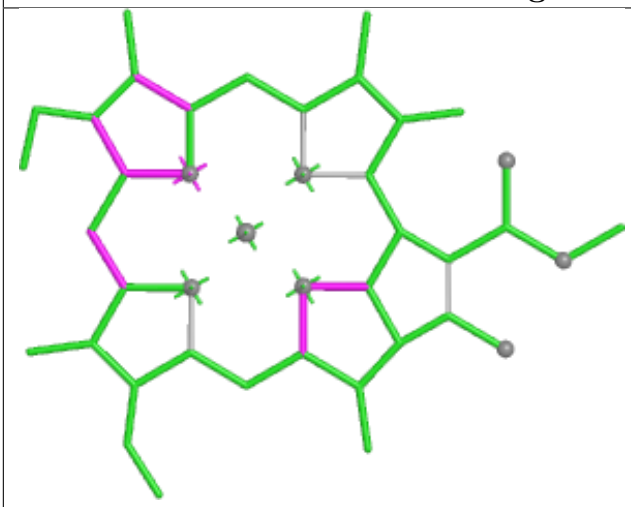


Rings

Ligand CLA 1 308



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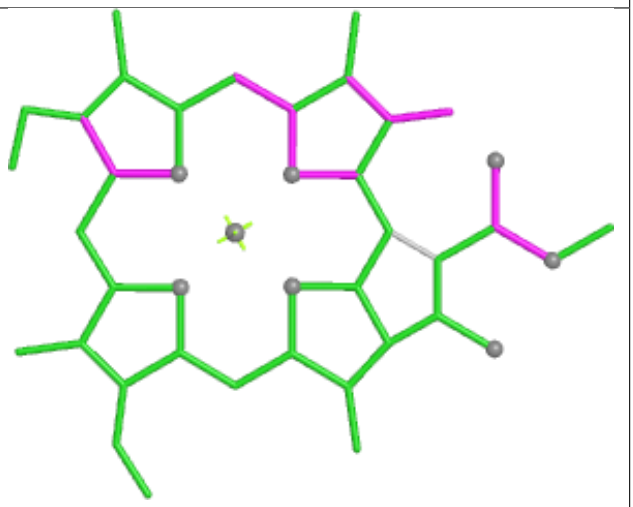
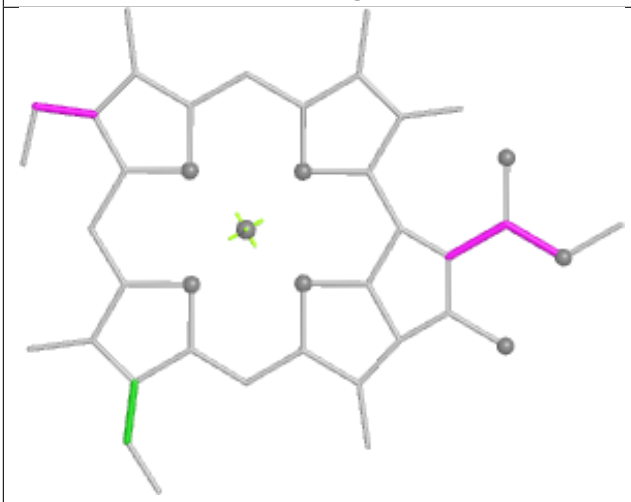
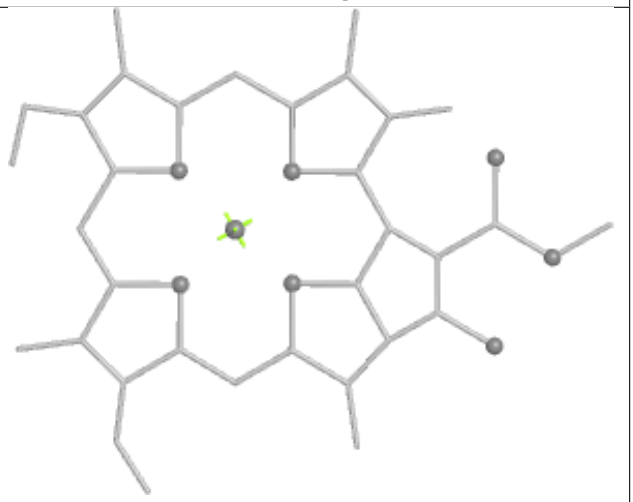


Bond angles

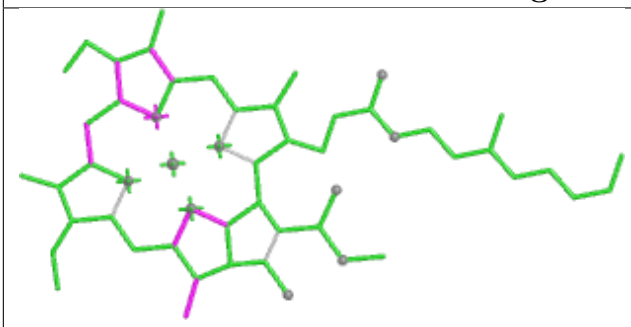


Torsions



Rings

Ligand CLA I 310



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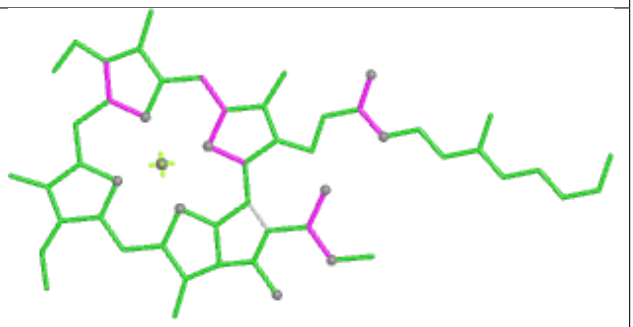
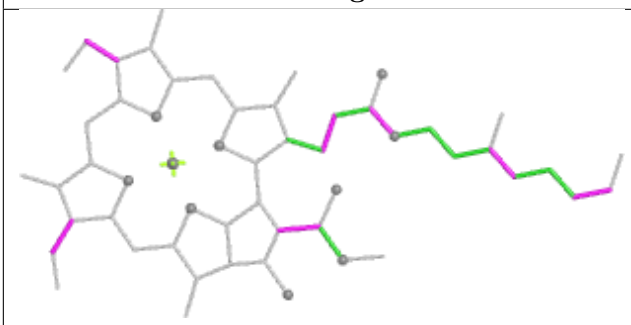


Bond angles



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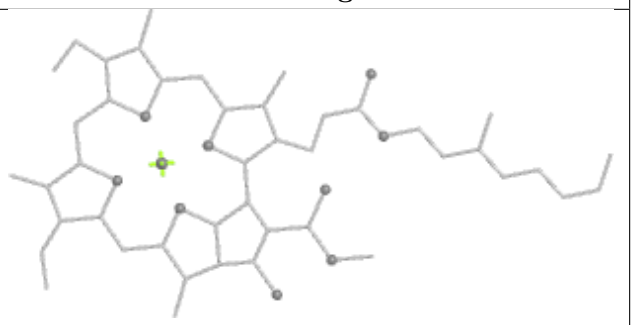
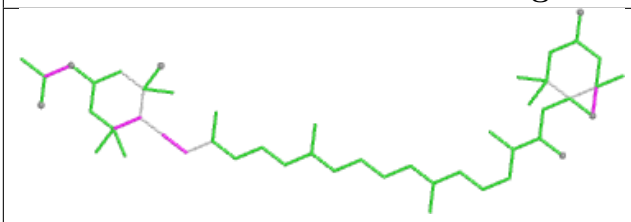
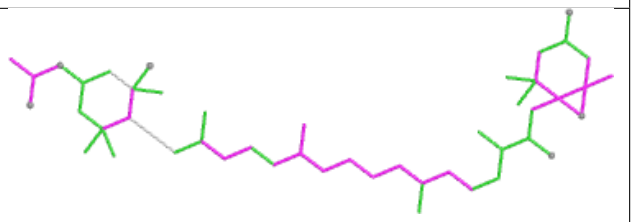


Rings

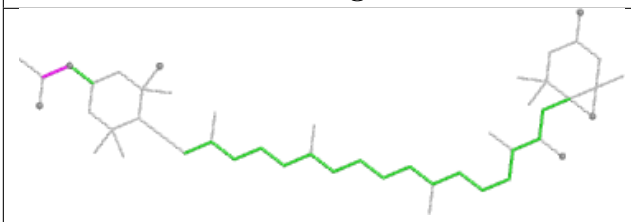
Ligand A86 F 302



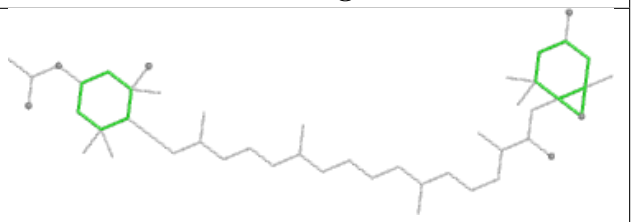
Bond lengths



Bond angles

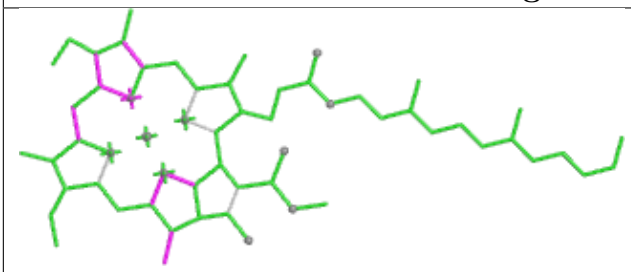


Torsions



Rings

Ligand CLA K 308



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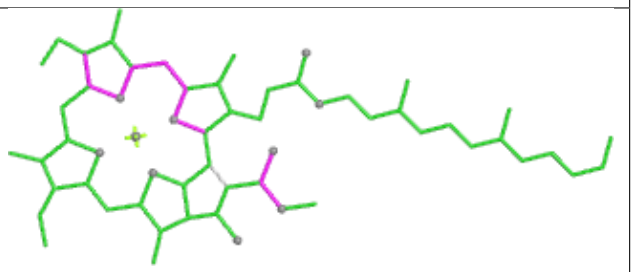
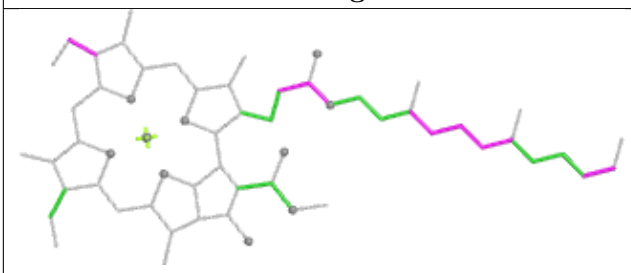
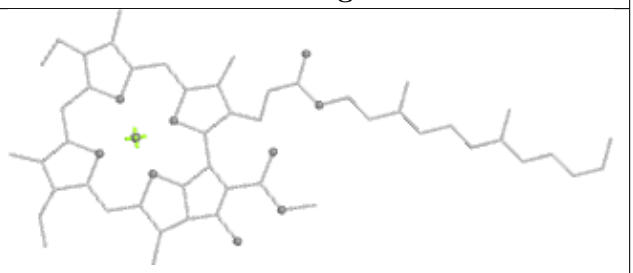


Bond angles

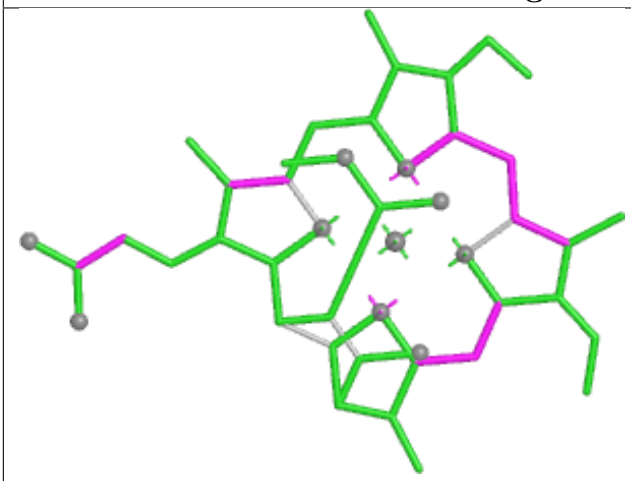


Torsions

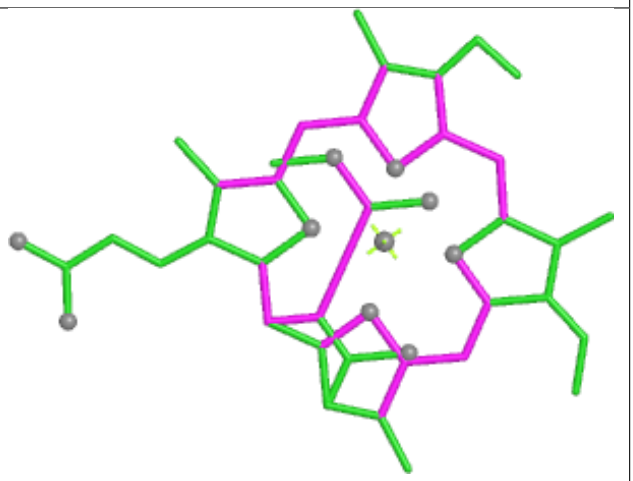


Rings

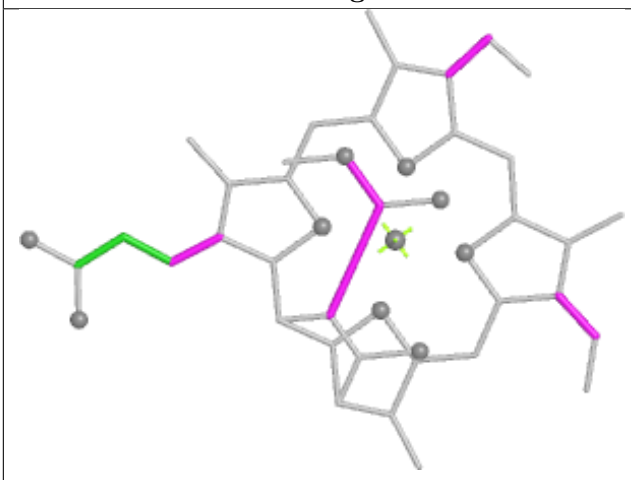
Ligand KC2 R 306



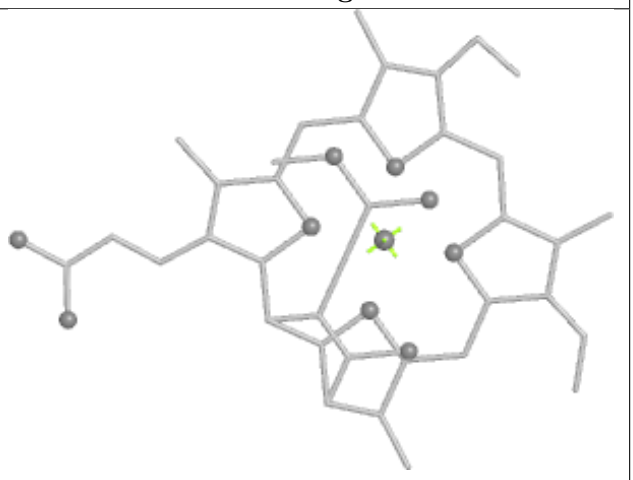
Bond lengths



Bond angles

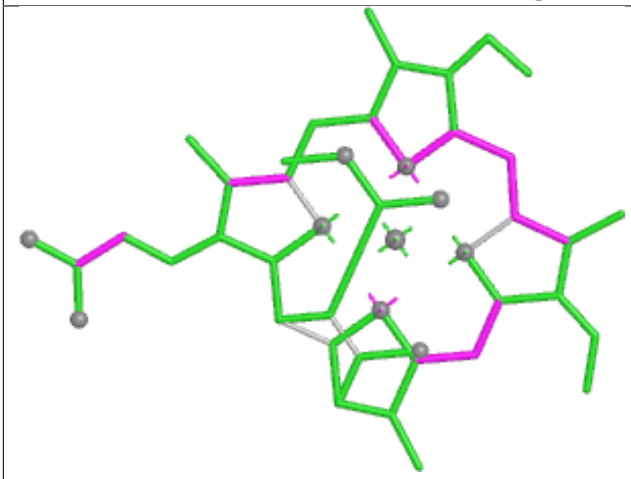


Torsions



Rings

Ligand KC2 2 317



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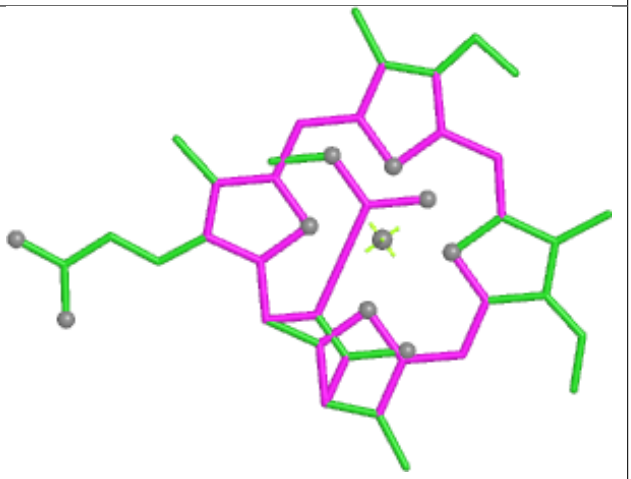
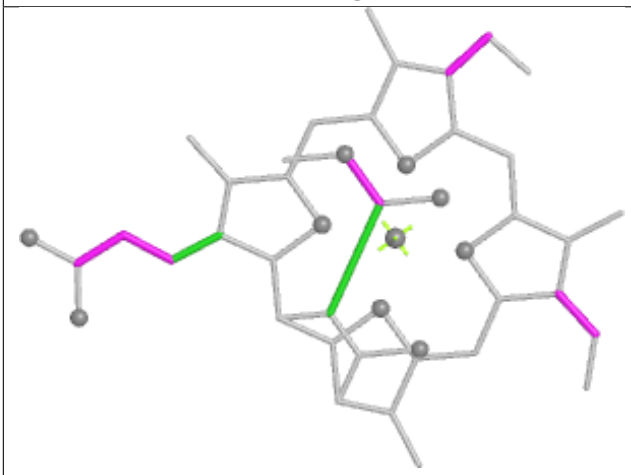
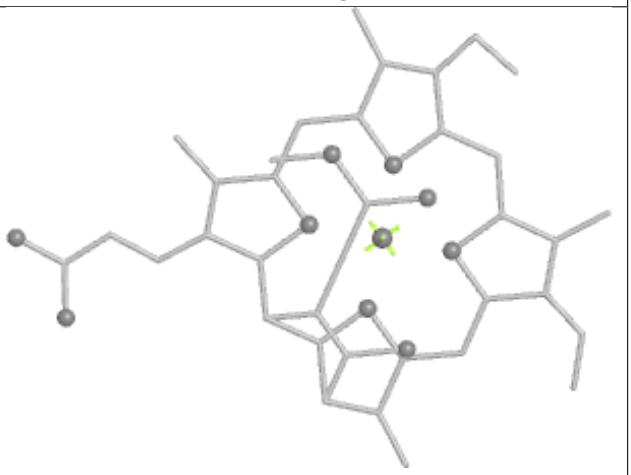


Bond angles

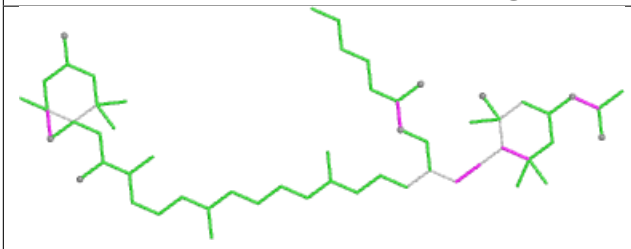


Torsions

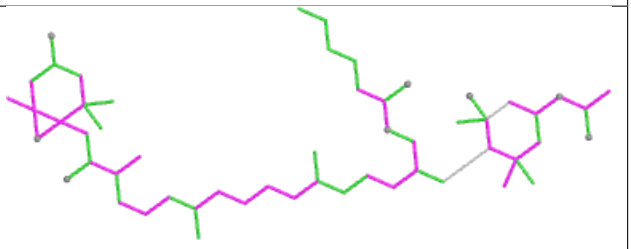


Rings

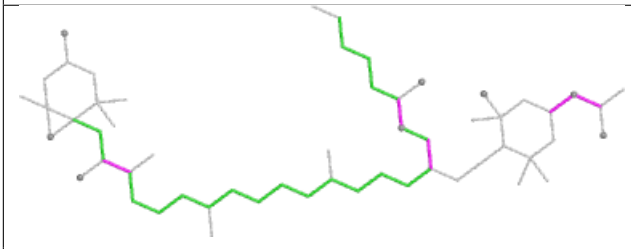
Ligand A1EB1 R 303



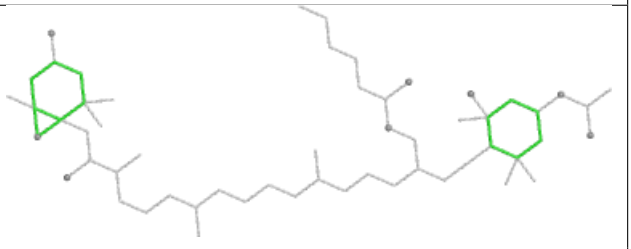
Bond lengths



Bond angles

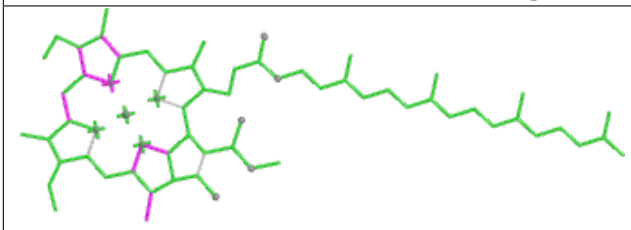


Torsions

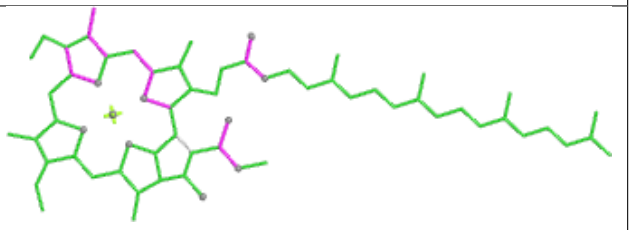


Rings

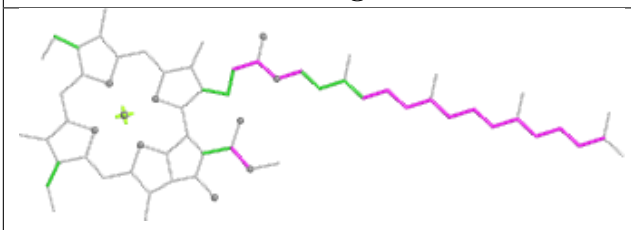
Ligand CLA P 308



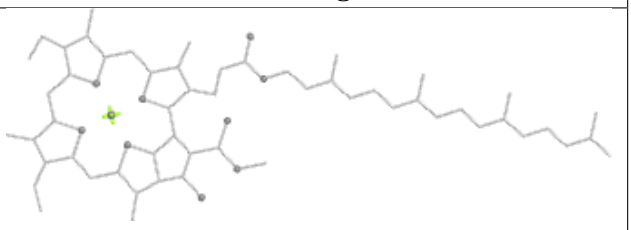
Bond lengths



Bond angles

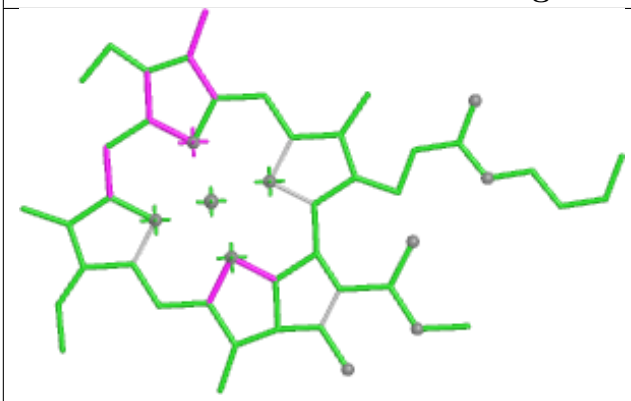


Torsions

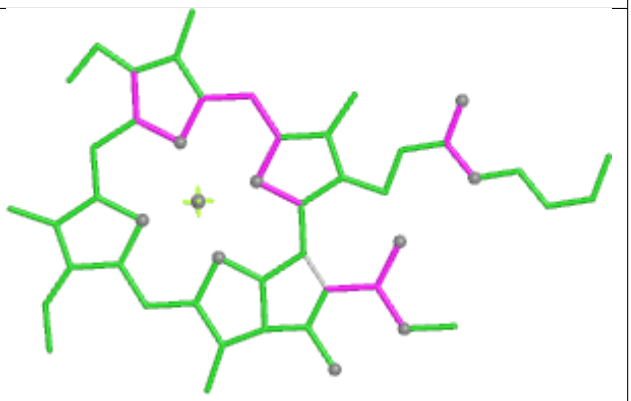


Rings

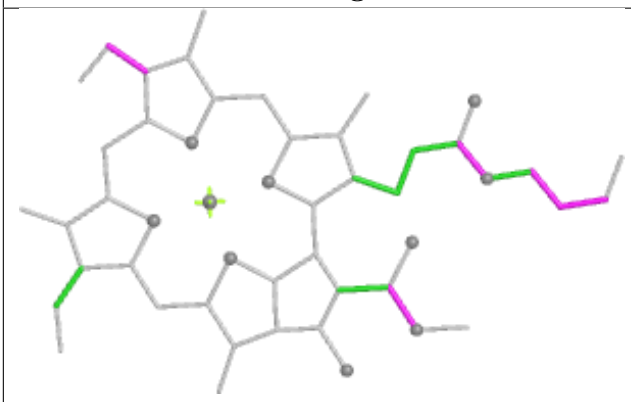
Ligand CLA l 203



Bond lengths



Bond angles



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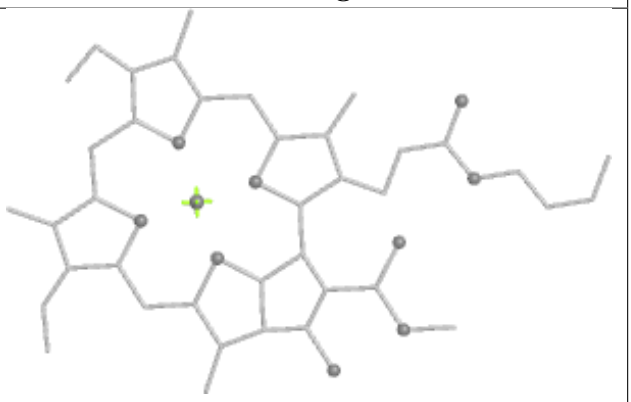
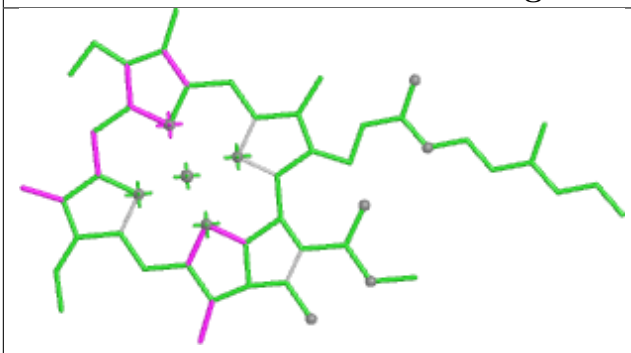


Rings

Ligand CLA T 310



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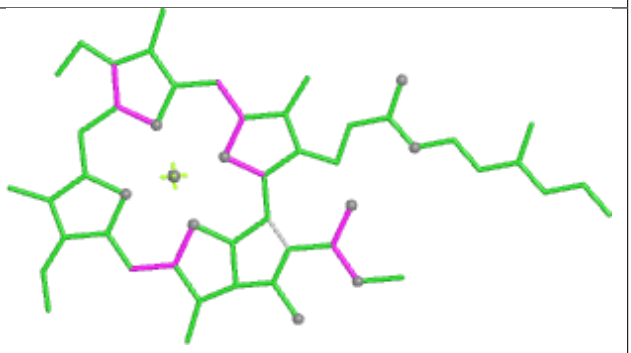
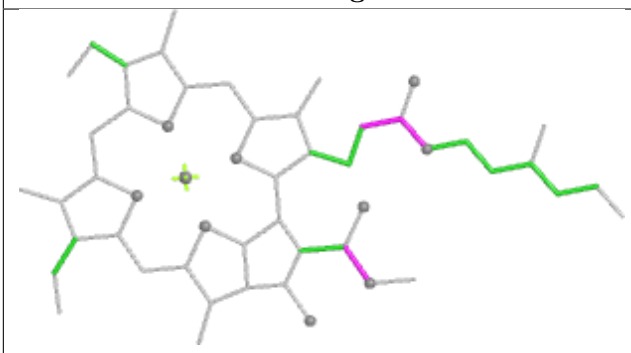
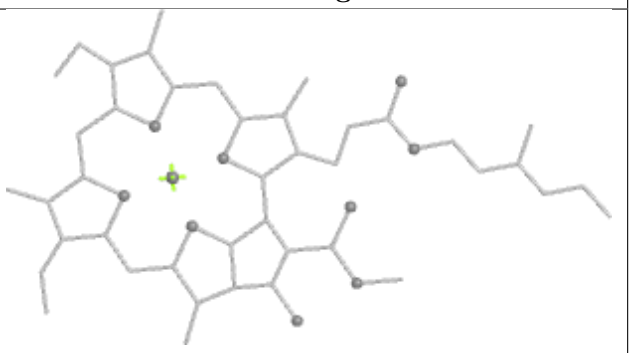


Bond angles

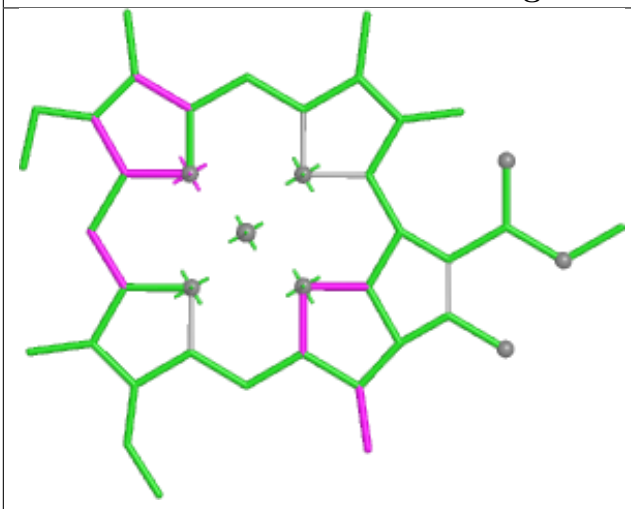


Torsions



Rings

Ligand CLA H 315



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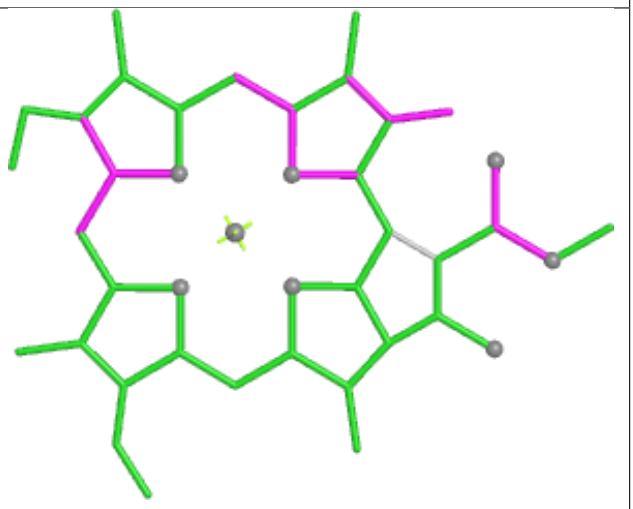
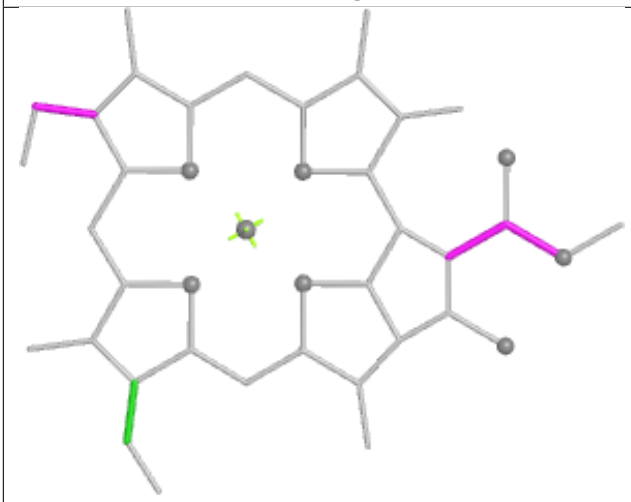


Bond angles



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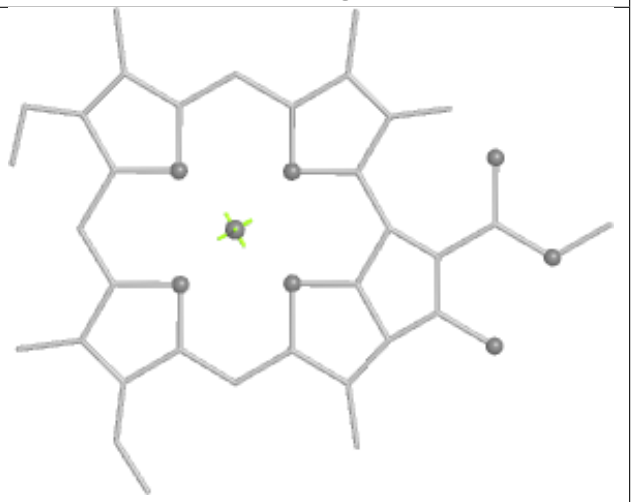
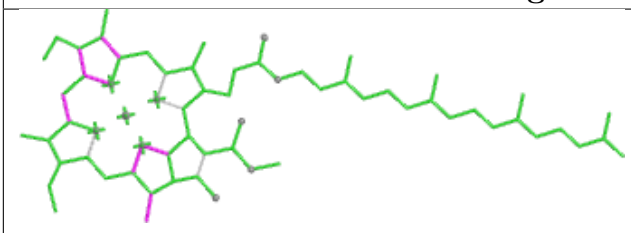
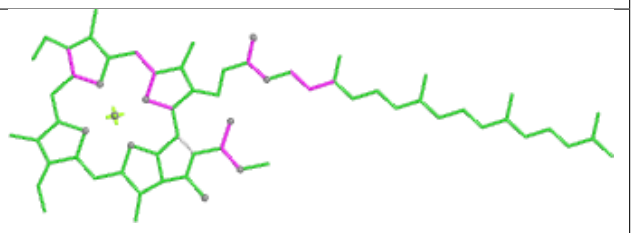


Rings

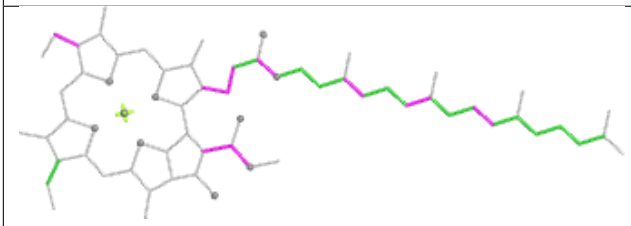
Ligand CLA b 828



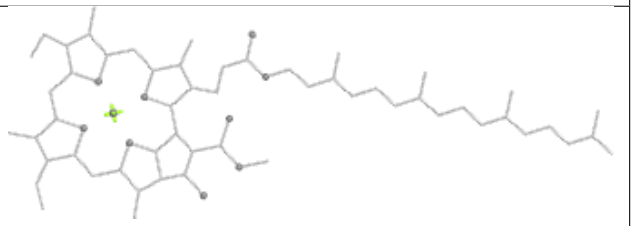
Bond lengths



Bond angles

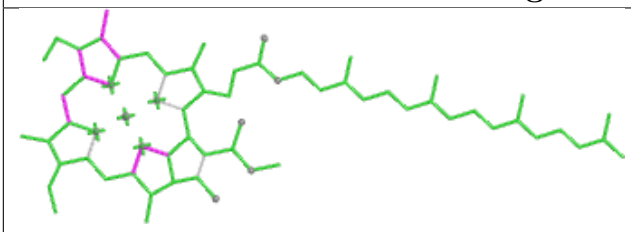


Torsions



Rings

Ligand CLA F 321



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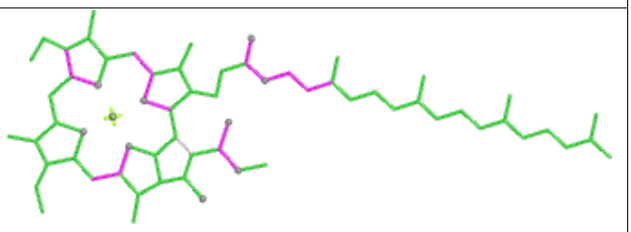
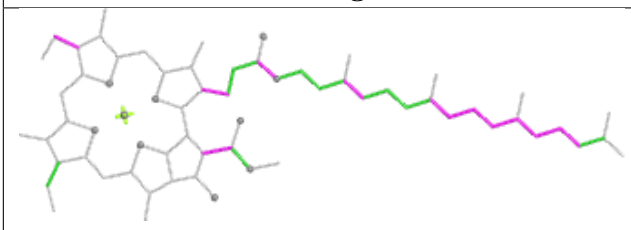


Bond angles



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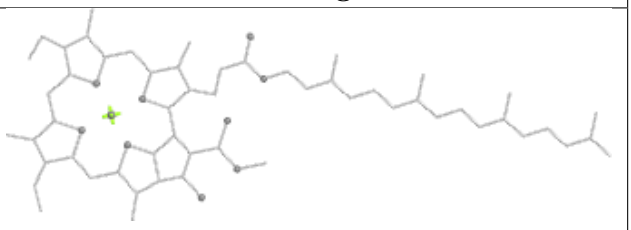
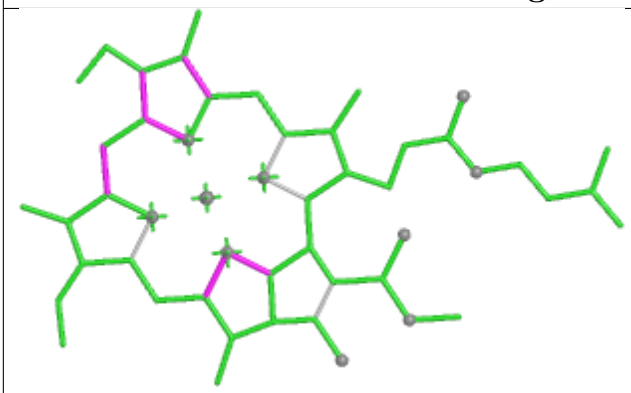


Rings

Ligand CLA J 308



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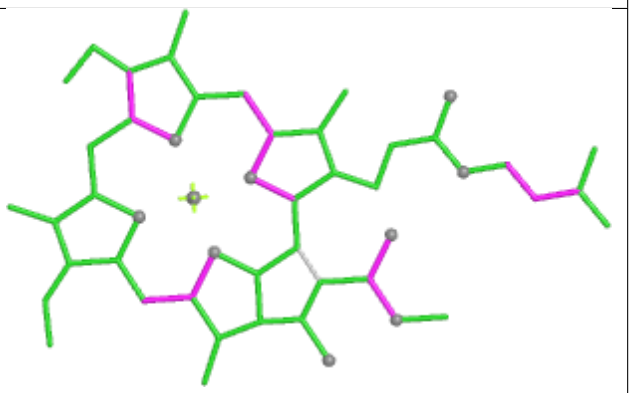
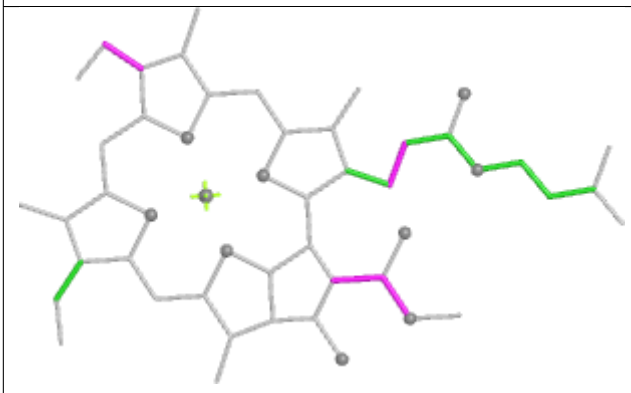
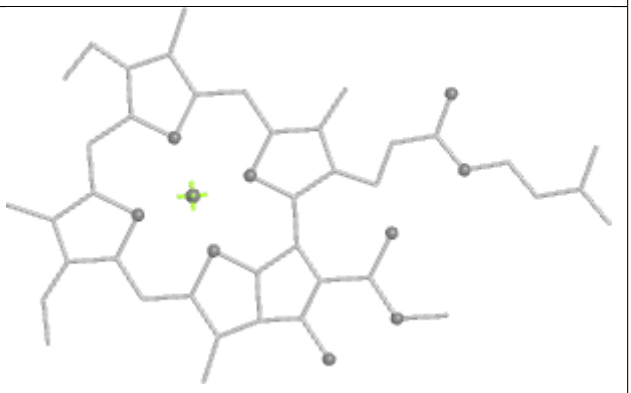


Bond angles

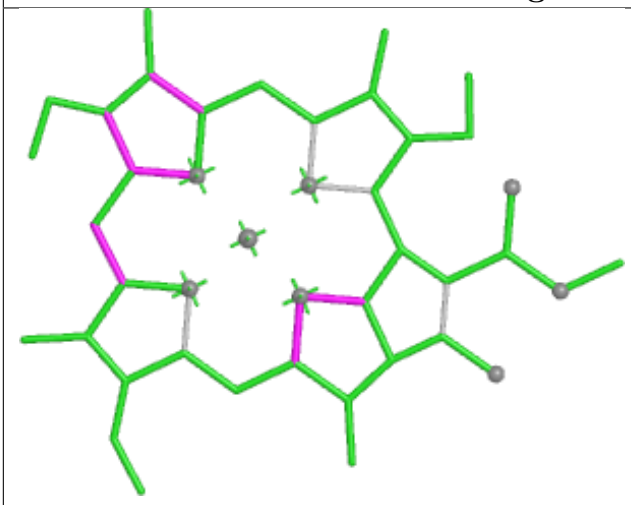


Torsions



Rings

Ligand CLA y 318



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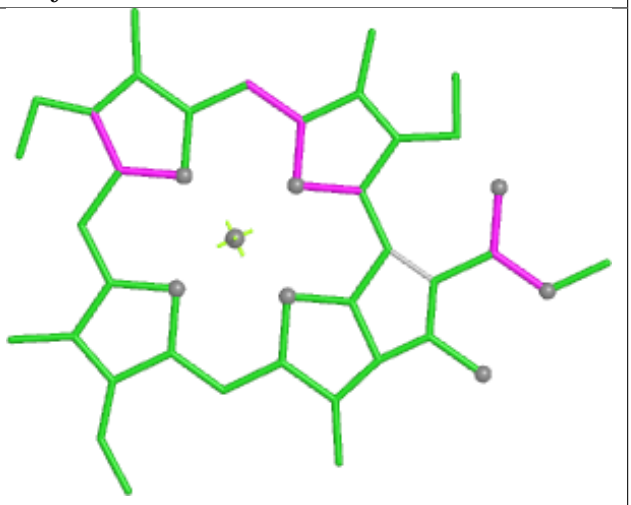
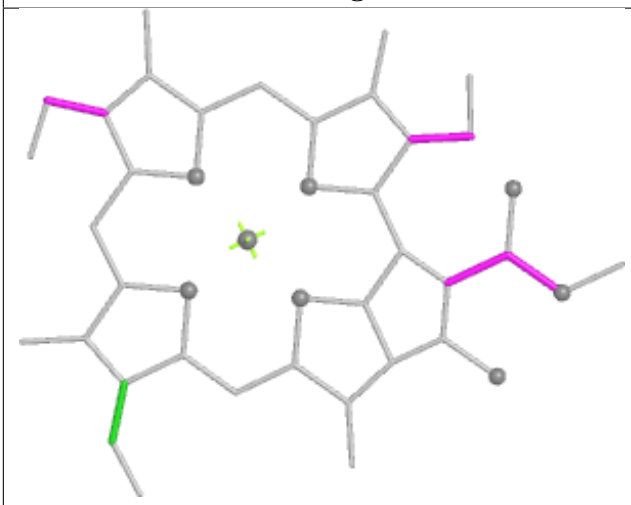


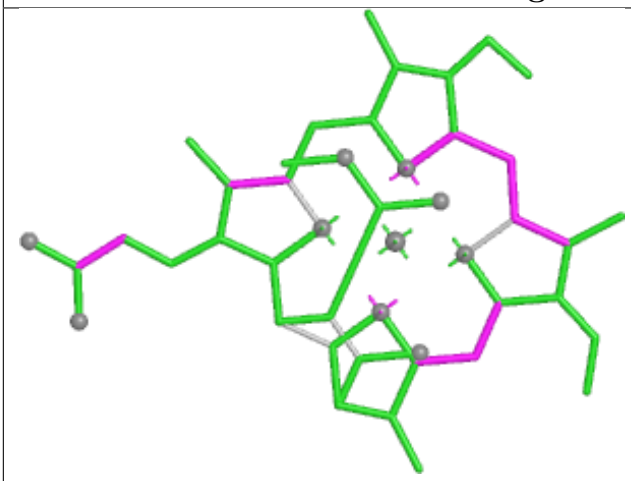
Bond angles



Torsions

Rings

Ligand KC2 Z 310



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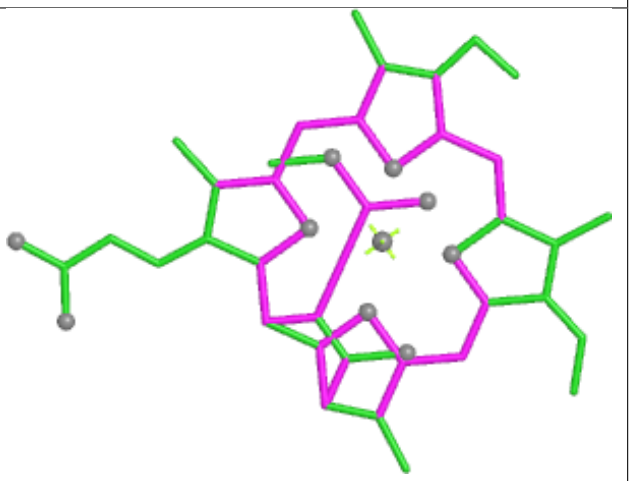
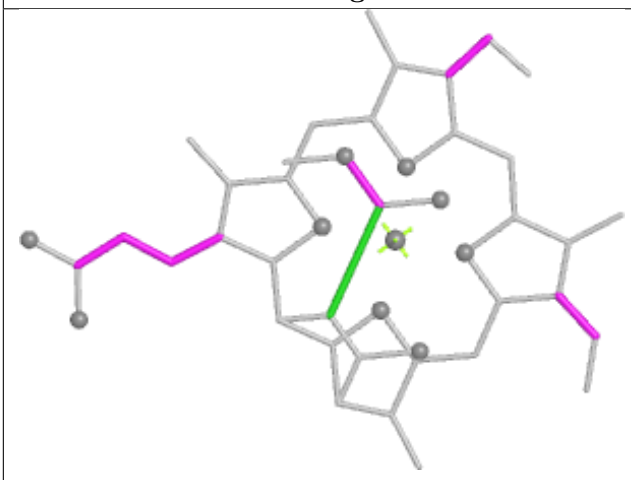
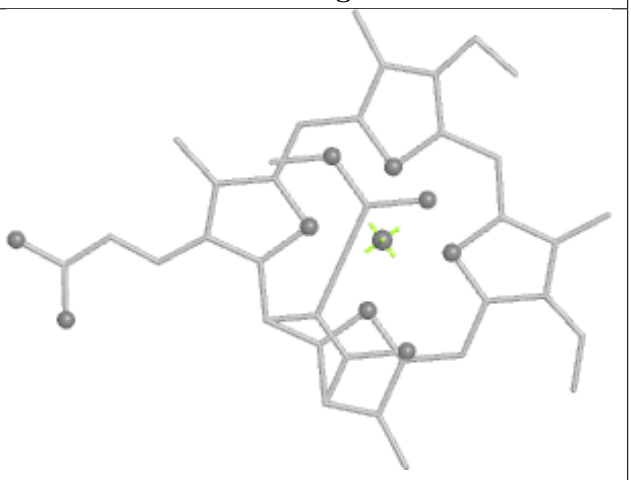


Bond angles

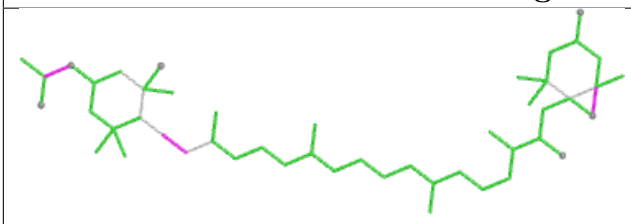


Torsions

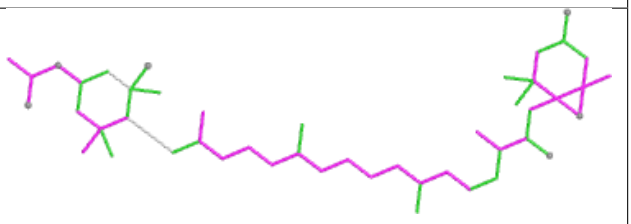


Rings

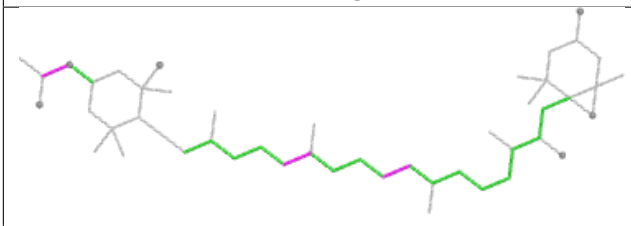
Ligand A86 8 309



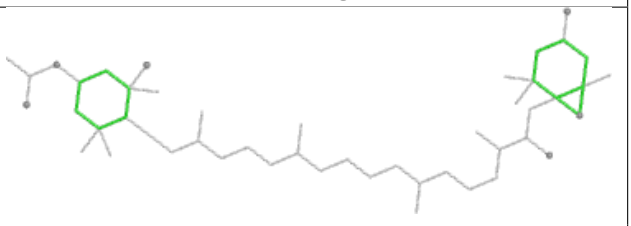
Bond lengths



Bond angles

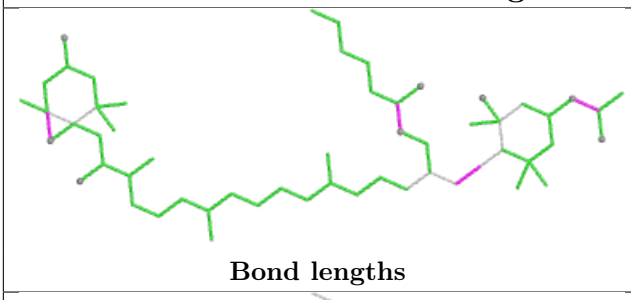


Torsions

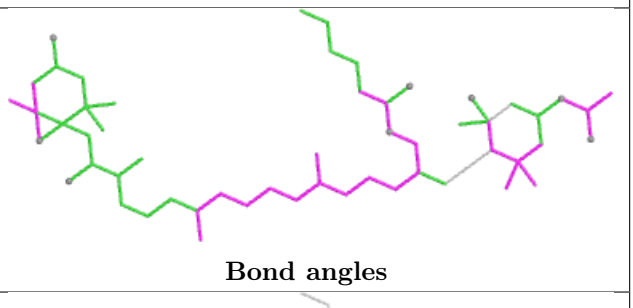


Rings

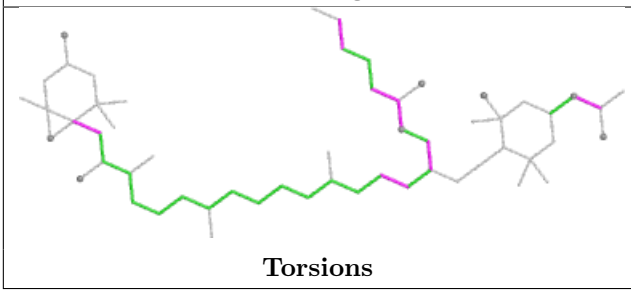
Ligand A1EB1 F 304



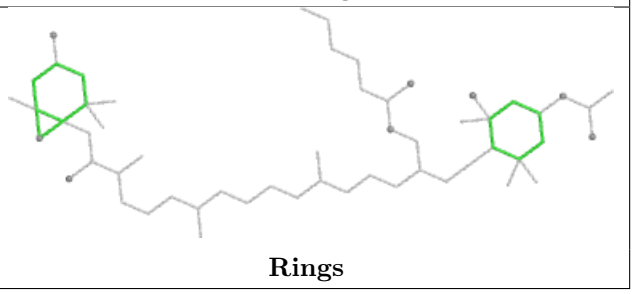
Bond lengths



Bond angles

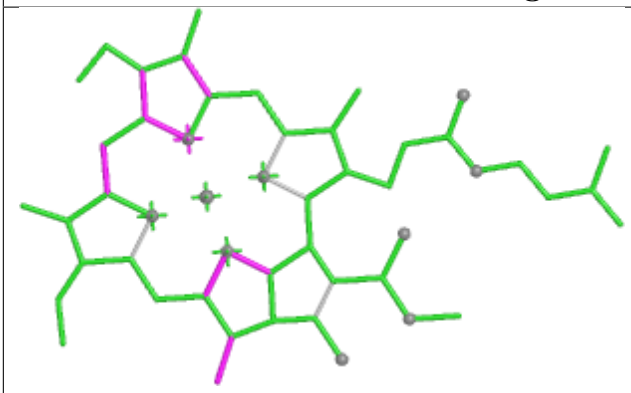


Torsions



Rings

Ligand CLA O 313



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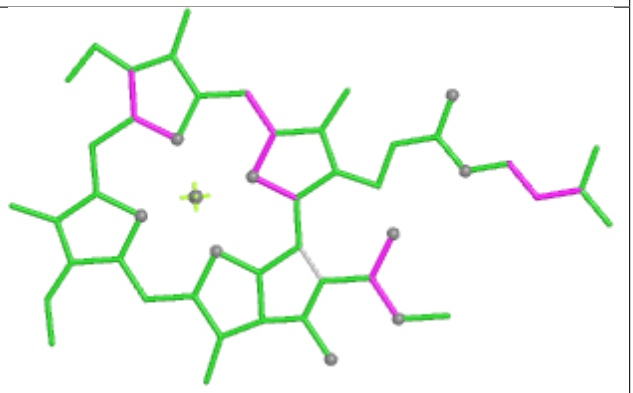
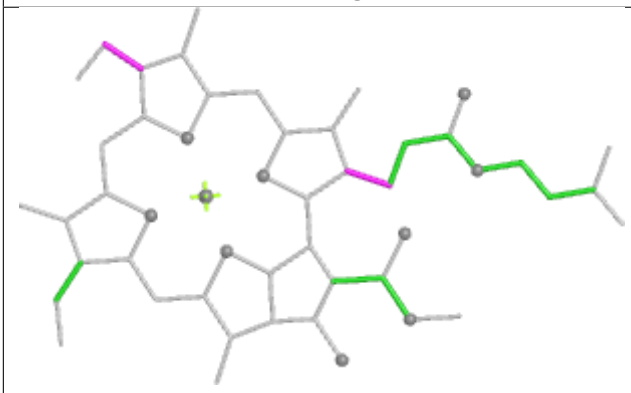
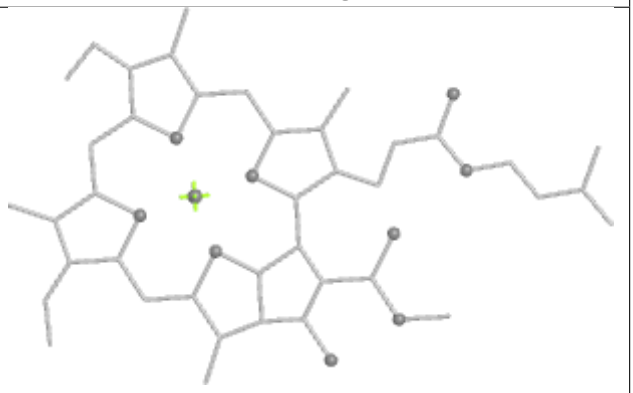


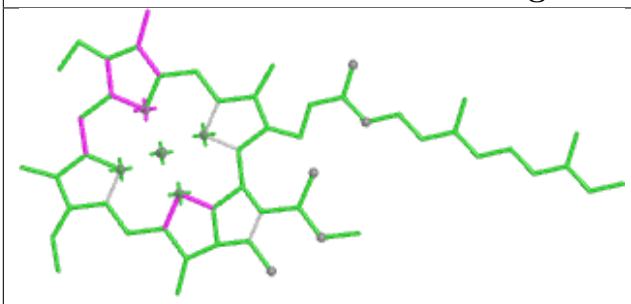
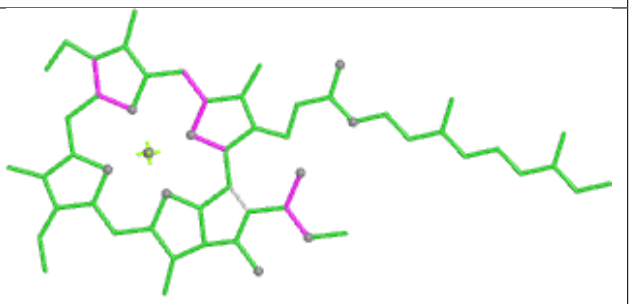
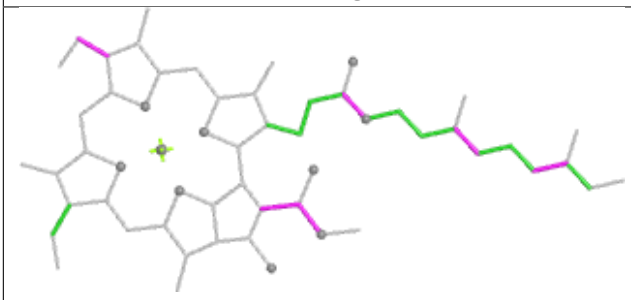
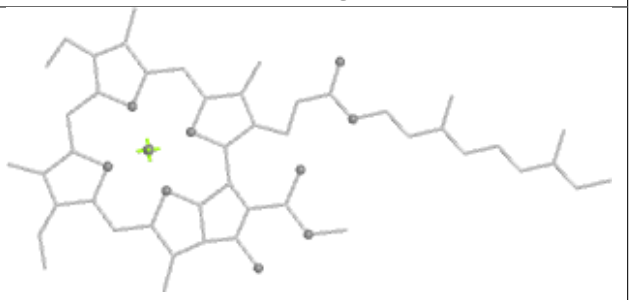
Bond angles

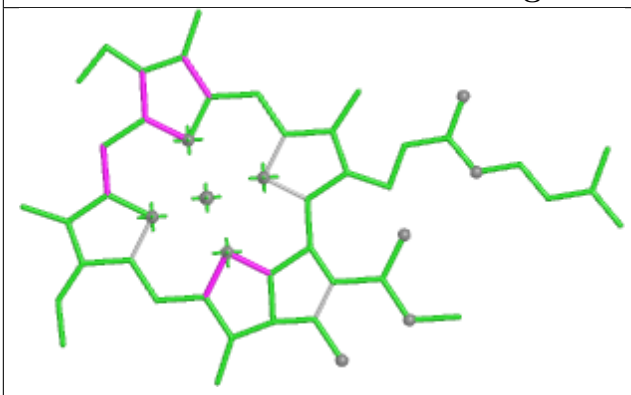
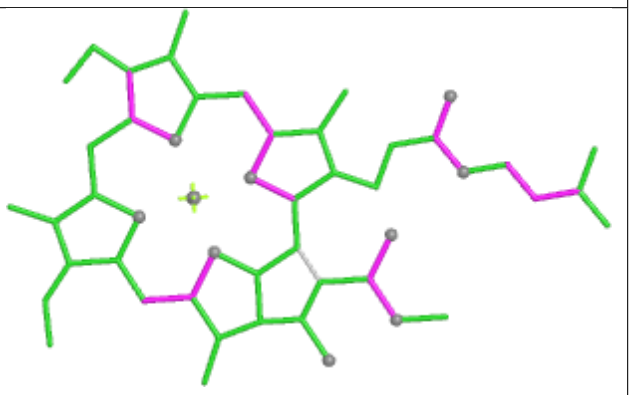
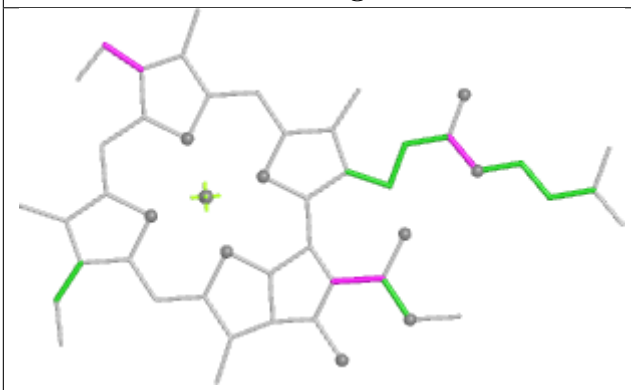
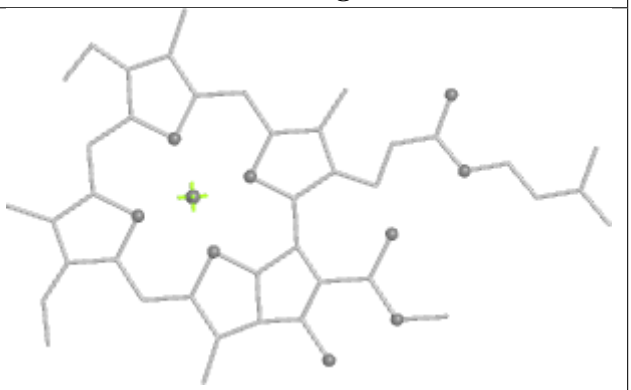


Torsions

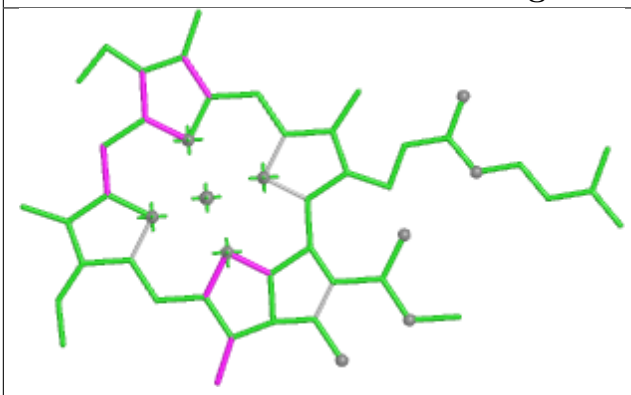


Rings

Ligand CLA a 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA X 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 0 315



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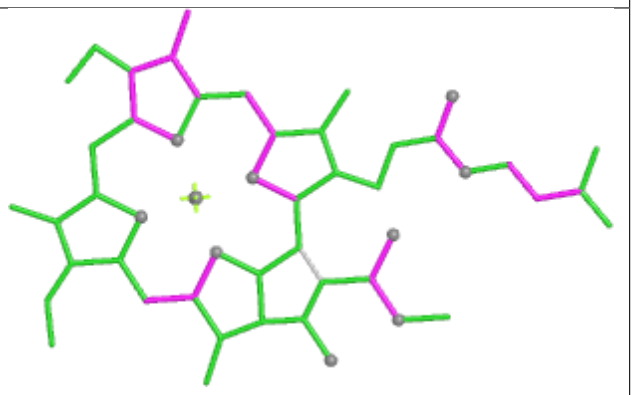
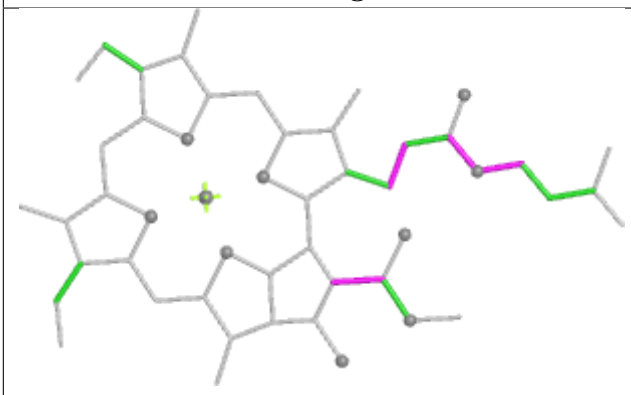
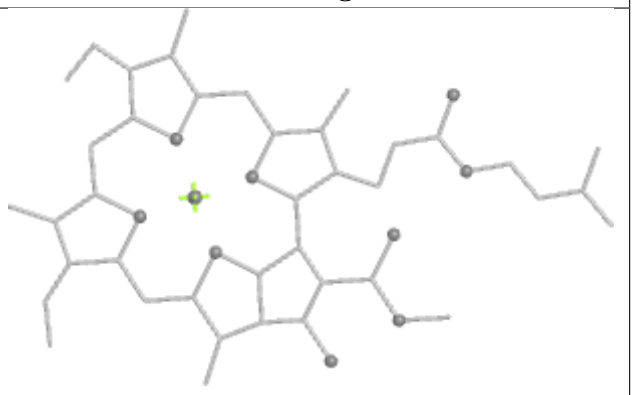


Bond angles

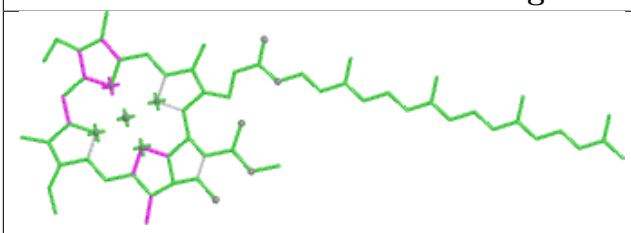


Torsions



Rings

Ligand CLA b 851



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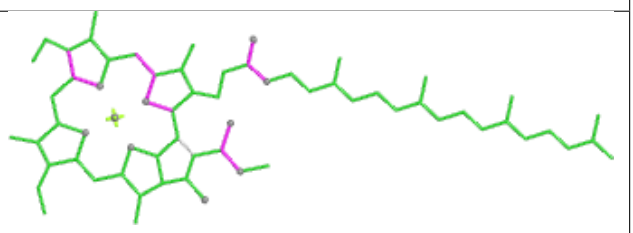
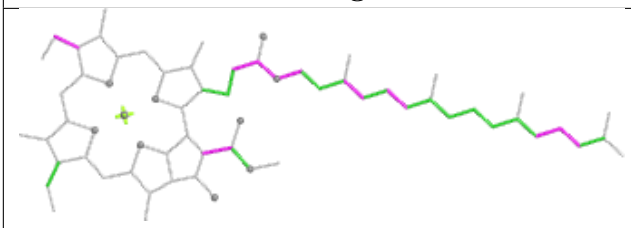


Bond angles



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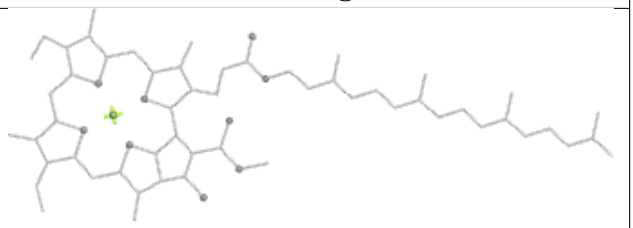
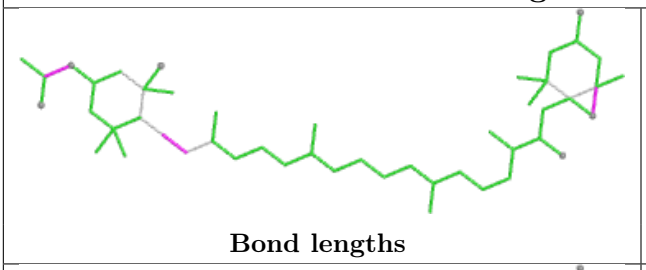


Rings

Ligand A86 U 206



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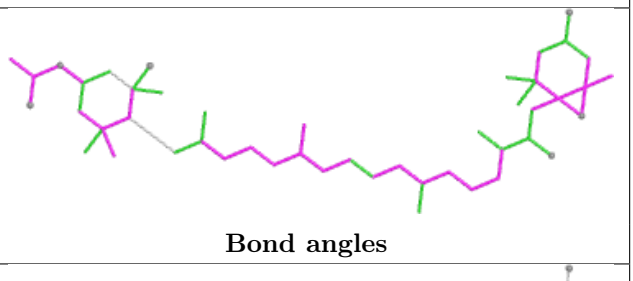
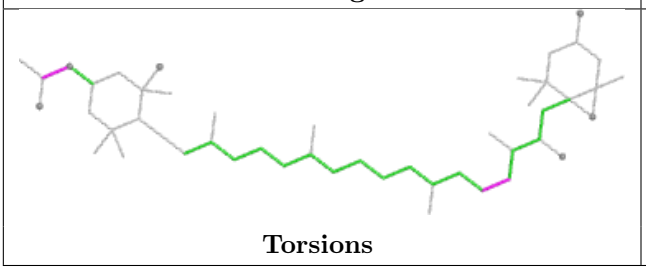


Bond angles



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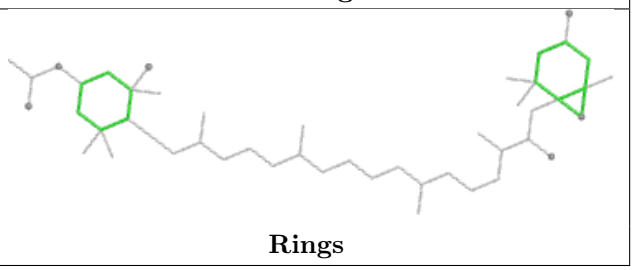
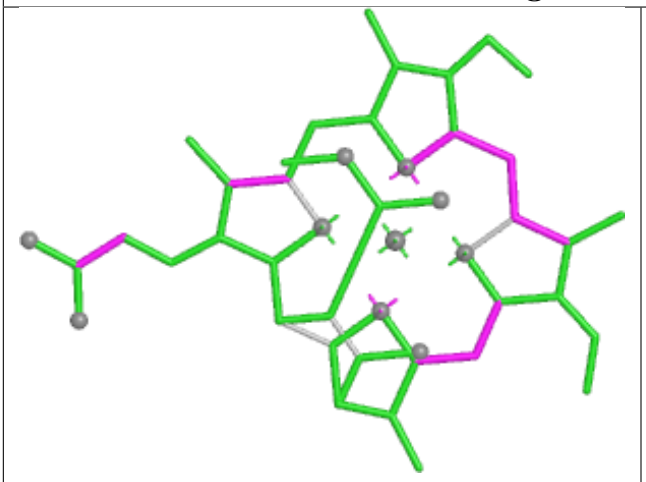


Rings

Ligand KC2 R 318



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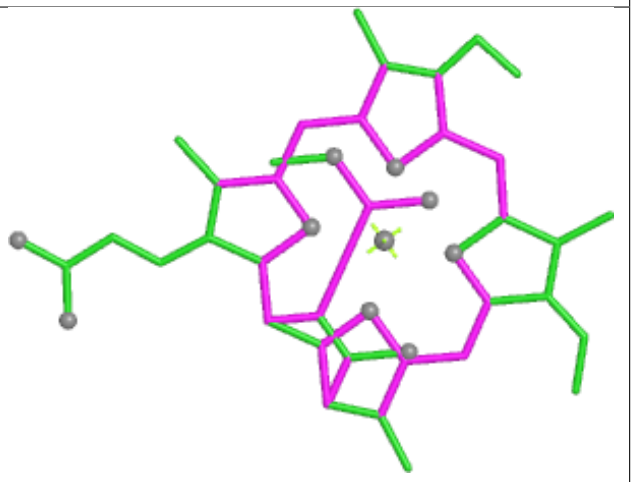
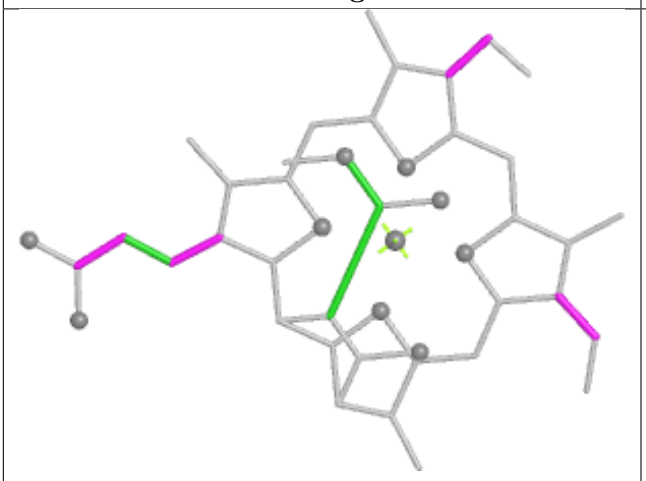


Bond angles



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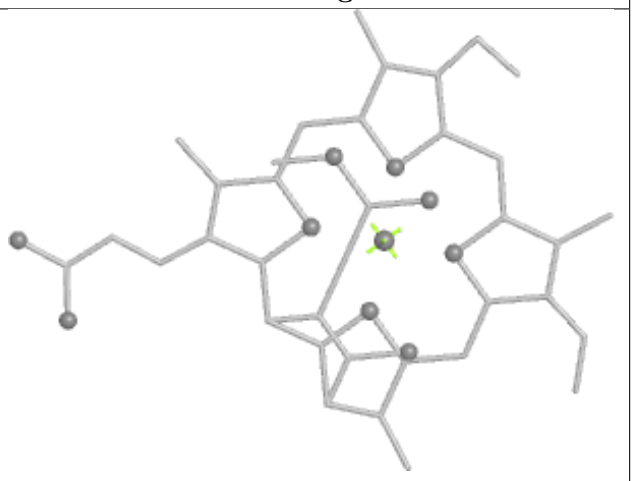
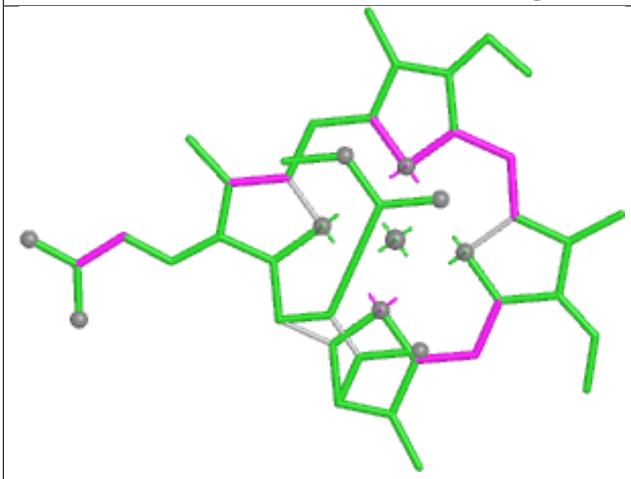


Rings

Ligand KC2 L 312



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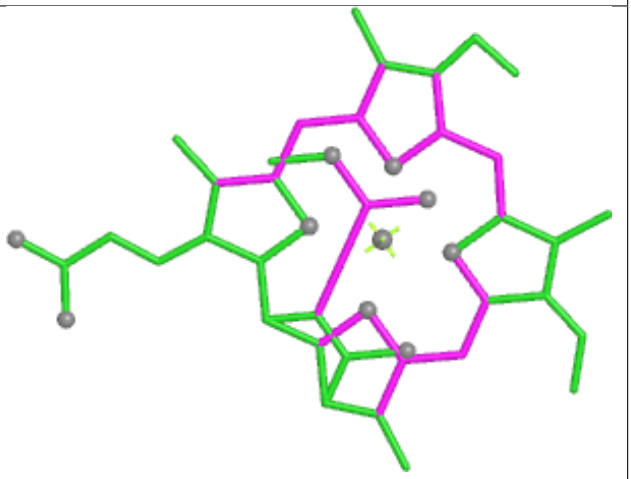
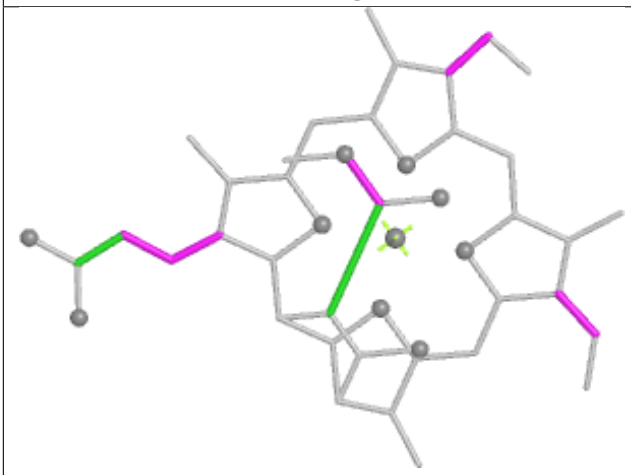
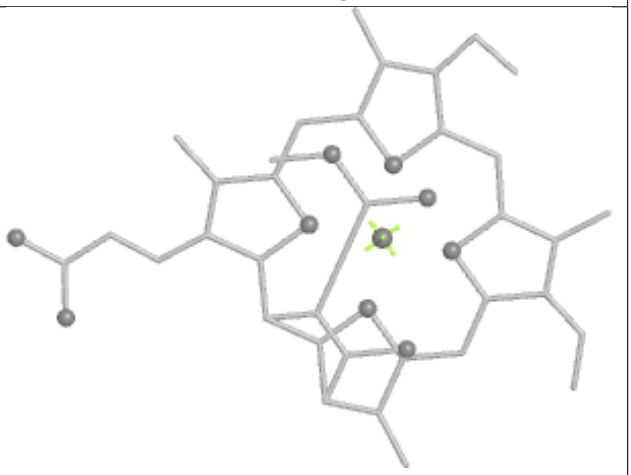


Bond angles

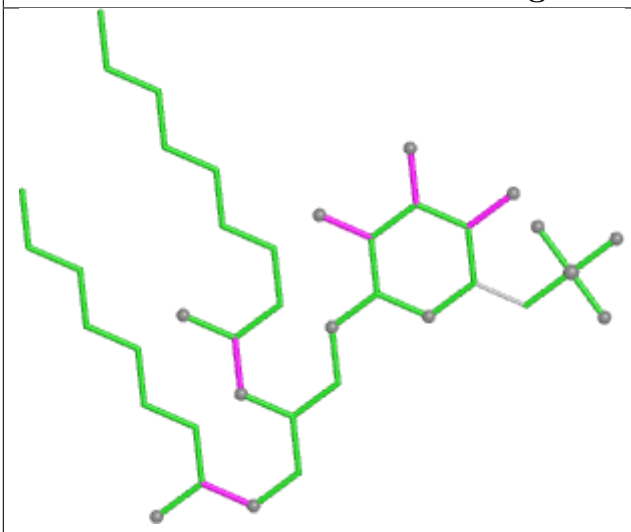


Torsions



Rings

Ligand SQD 4 327



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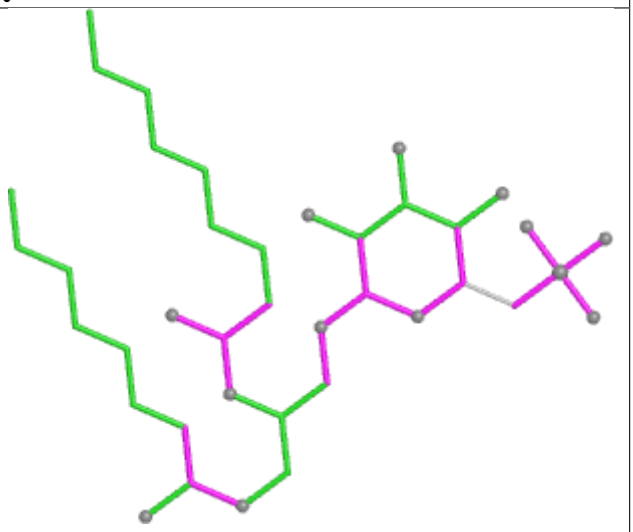
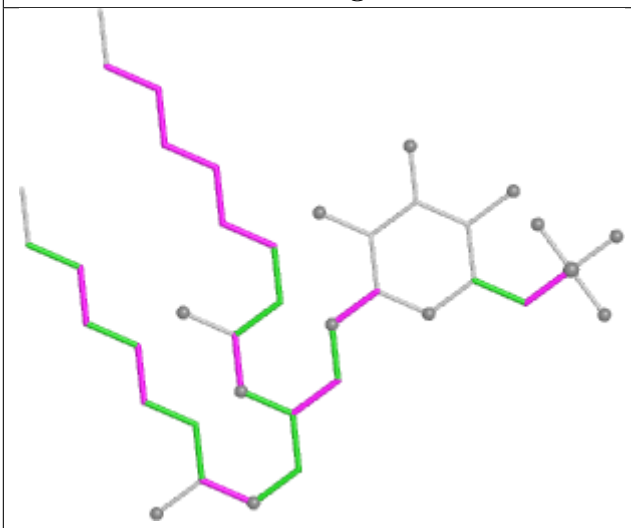


Bond angles



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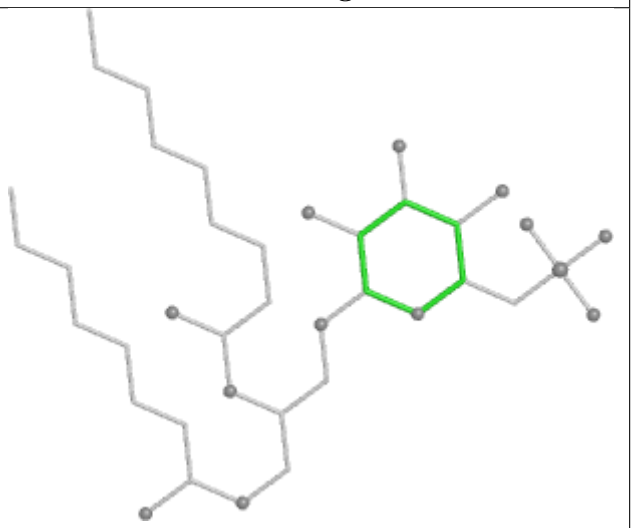
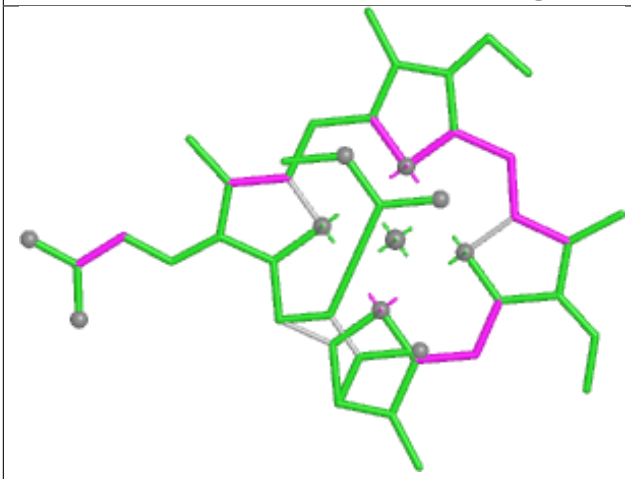


Rings

Ligand KC2 1 312



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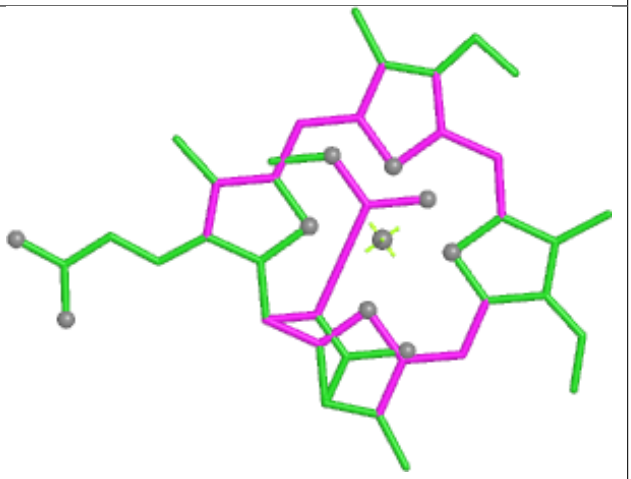
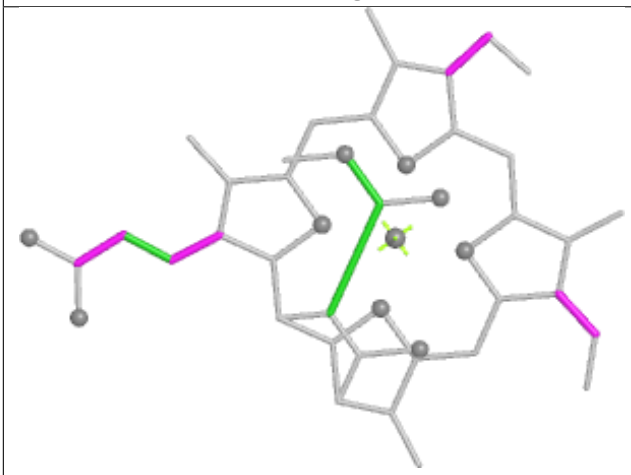


Bond angles



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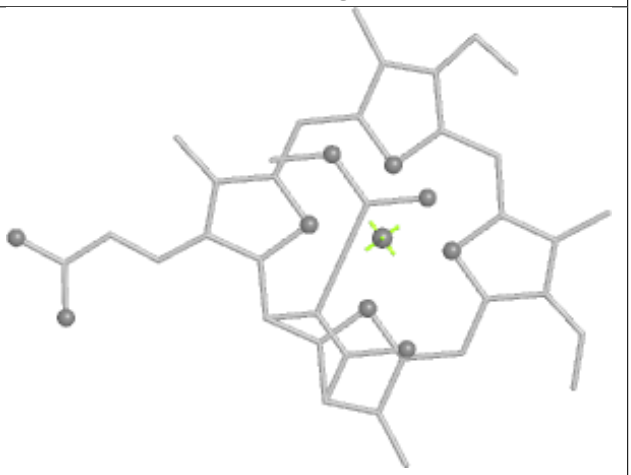
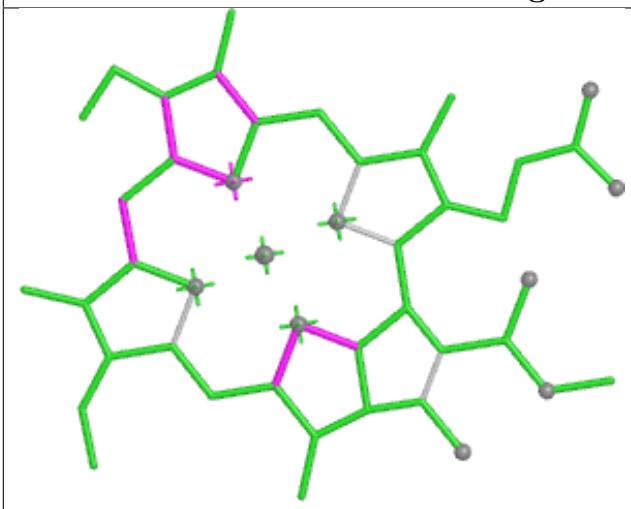


Rings

Ligand CLA 8 312



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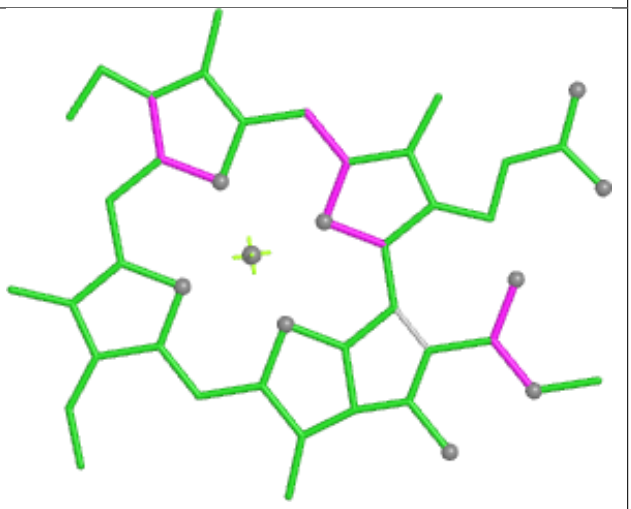
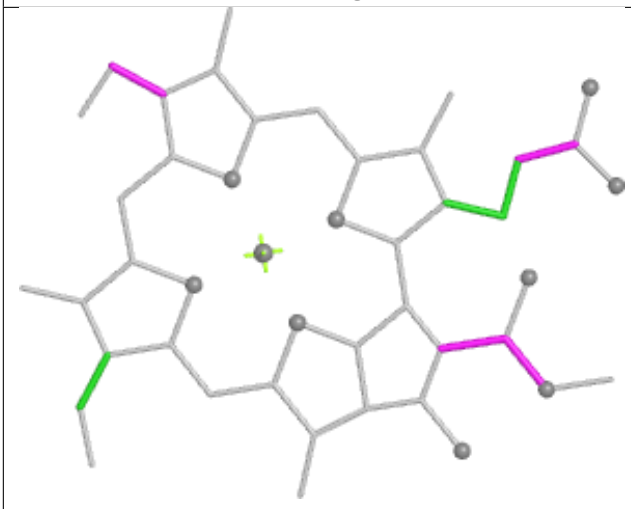


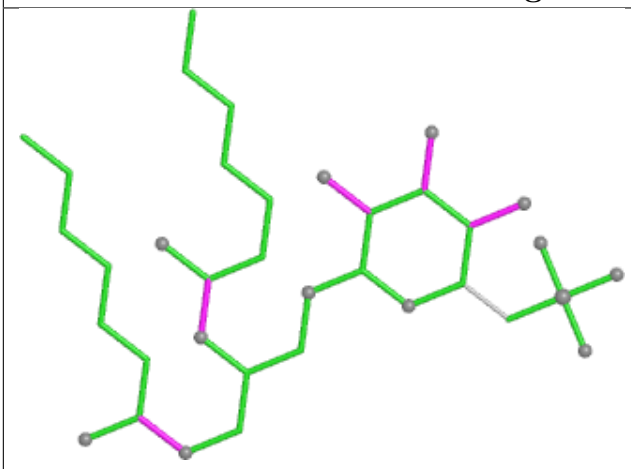
Bond angles



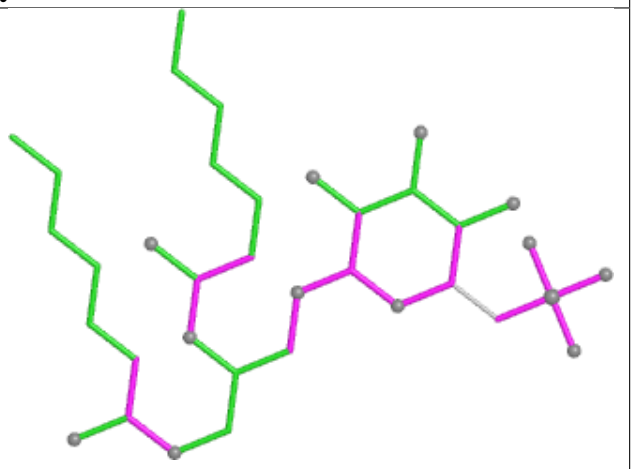
Torsions

Rings

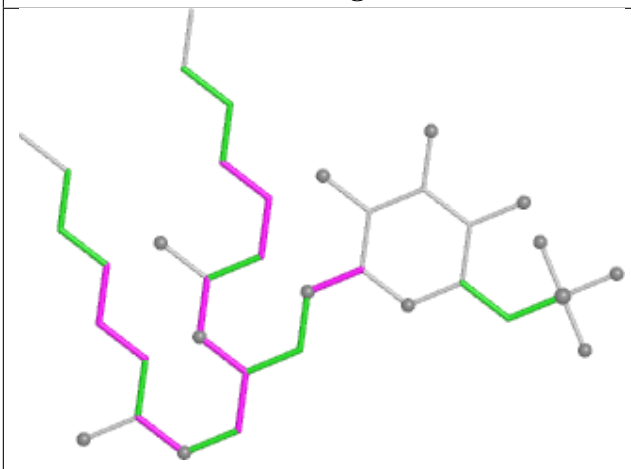
Ligand SQD T 321



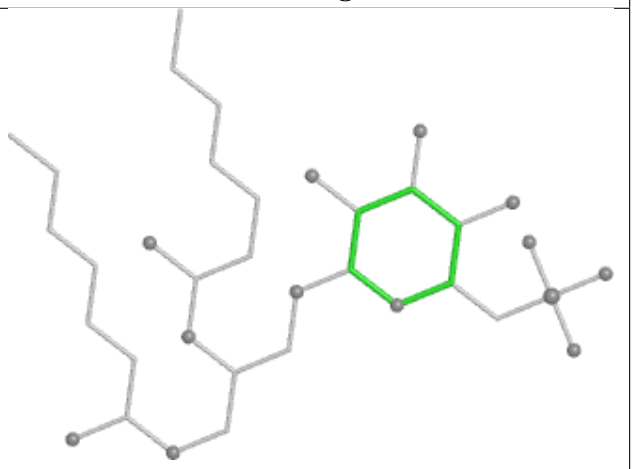
Bond lengths



Bond angles

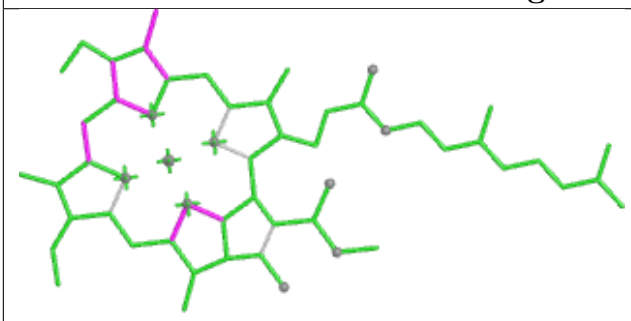


Torsions

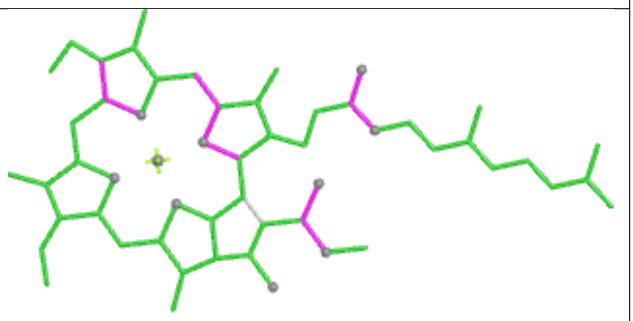


Rings

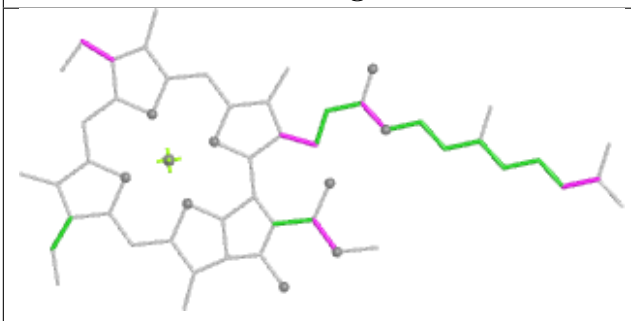
Ligand CLA k 203



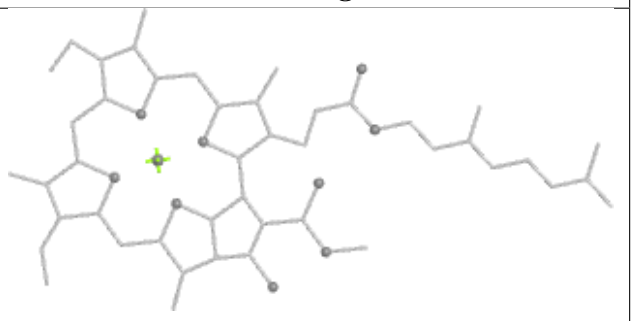
Bond lengths



Bond angles

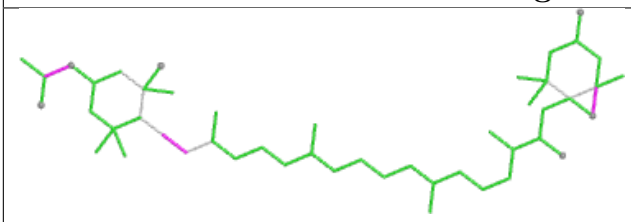


Torsions

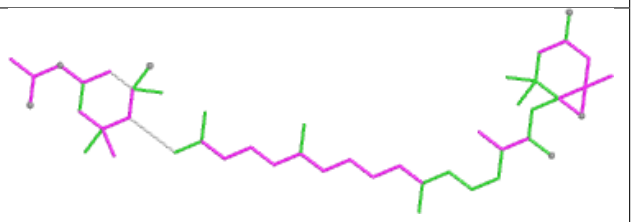


Rings

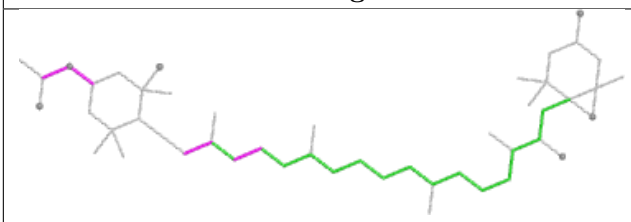
Ligand A86 3 308



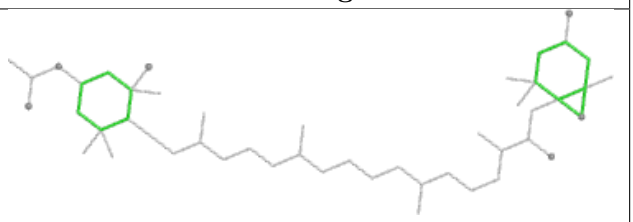
Bond lengths



Bond angles

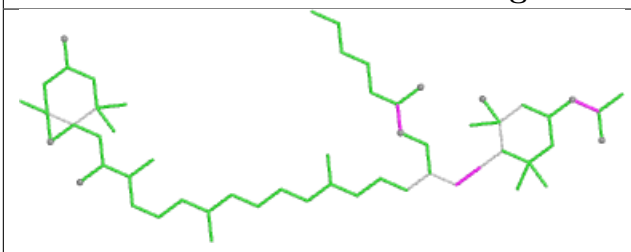


Torsions



Rings

Ligand A1EB1 0 302



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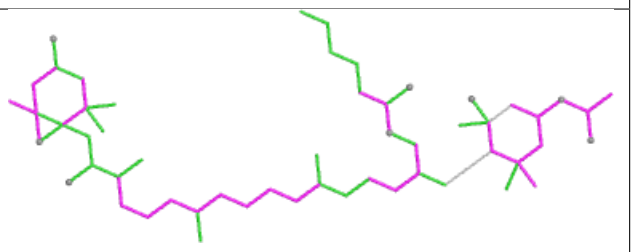

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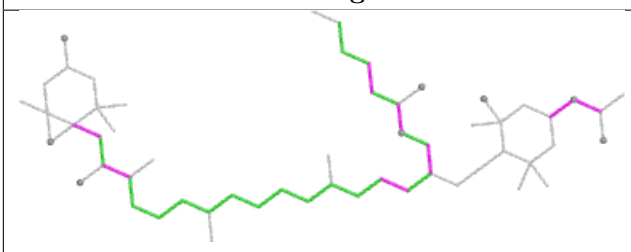

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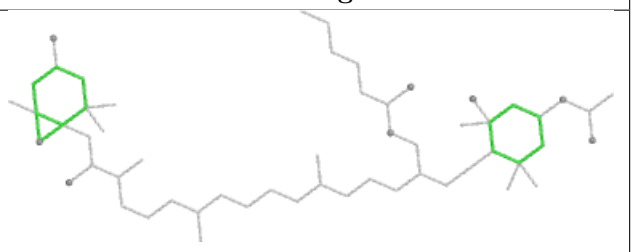
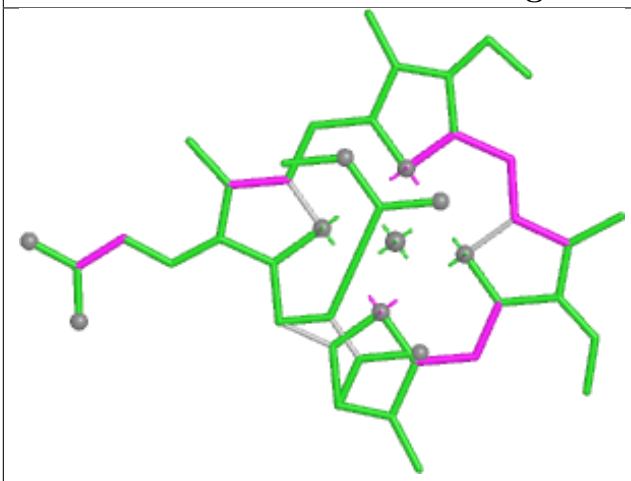


Rings

Ligand KC2 Q 315



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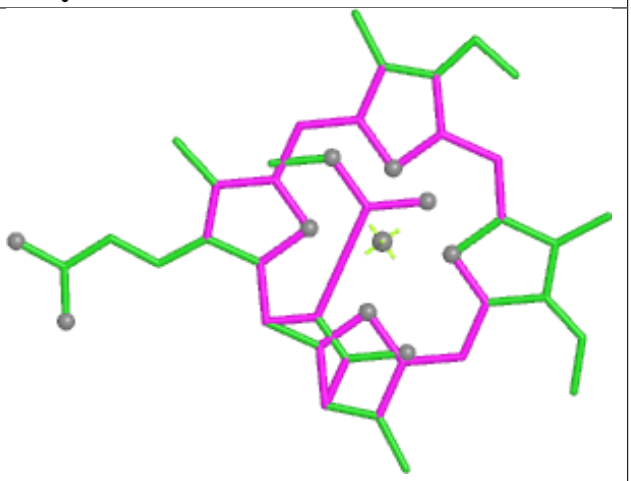

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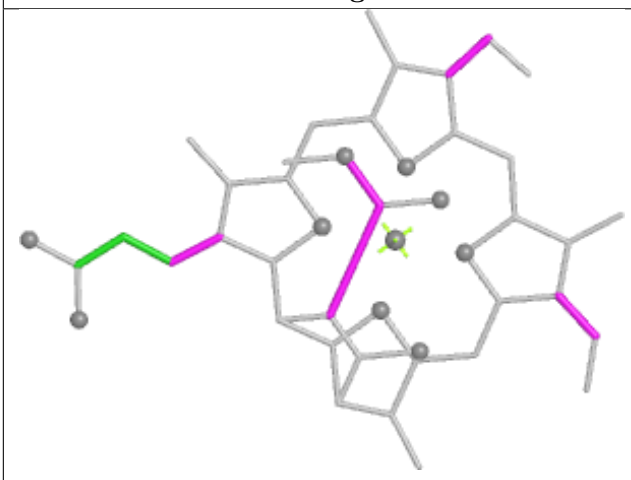

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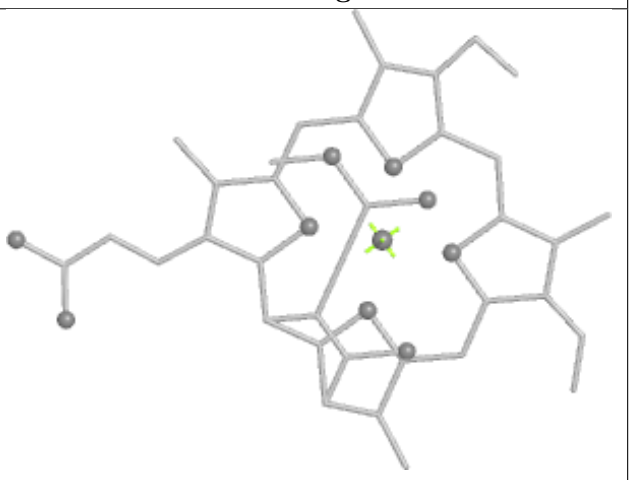
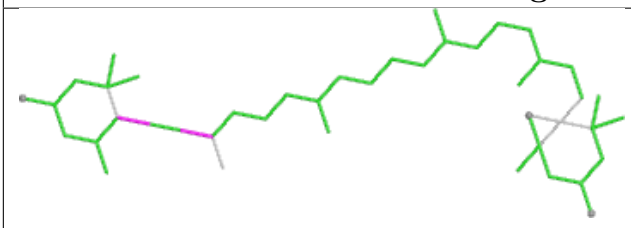


Rings

Ligand DD6 z 305



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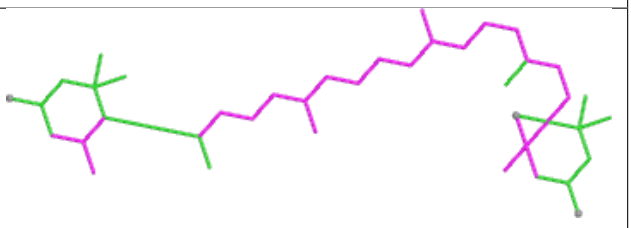

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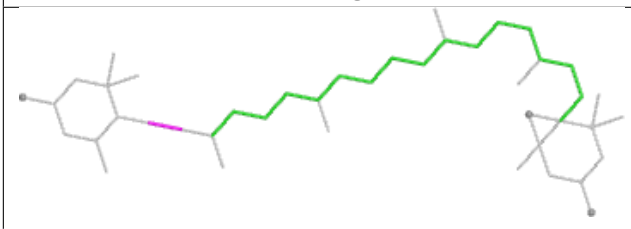
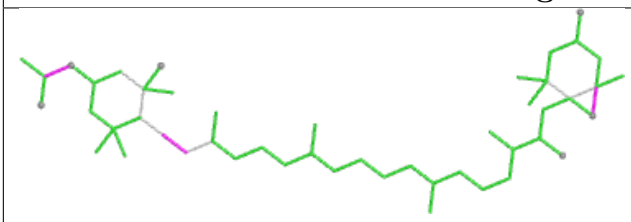


Torsions

Rings

Ligand A86 I 304



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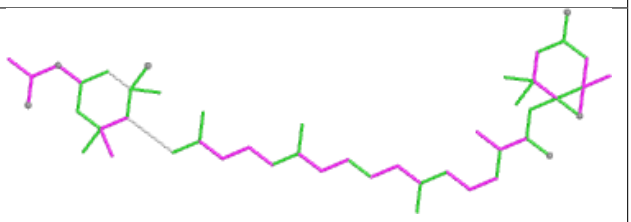
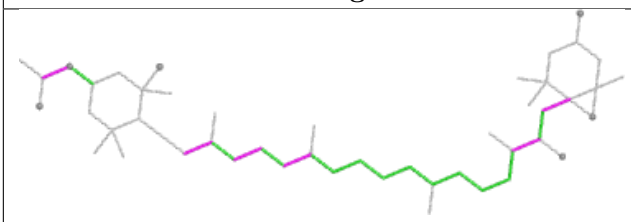


Bond angles



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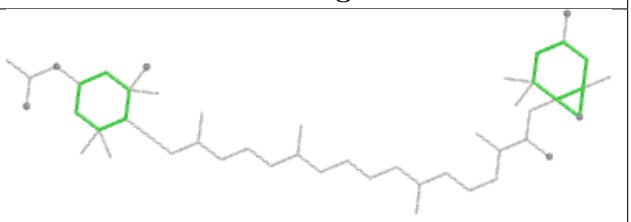
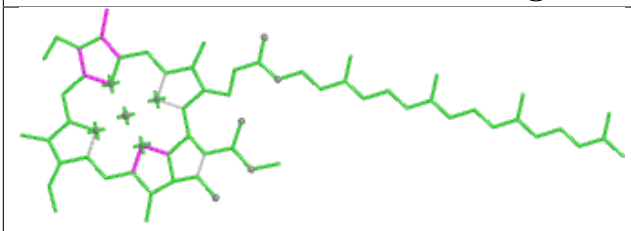


Rings

Ligand CLA b 841



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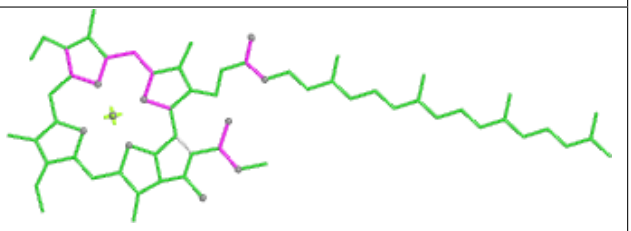
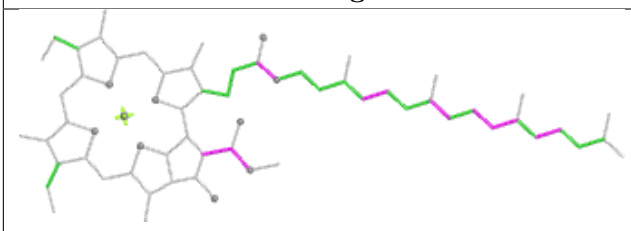


Bond angles



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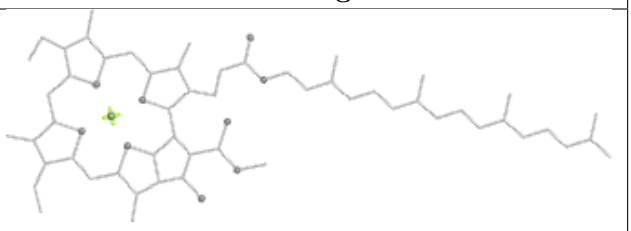
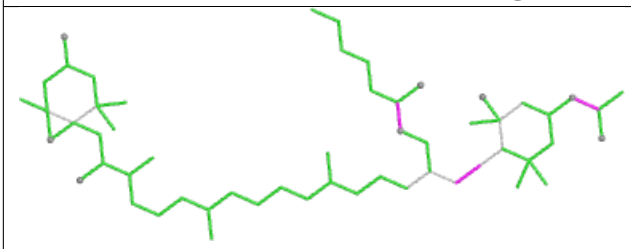


Rings

Ligand A1EB1 x 302



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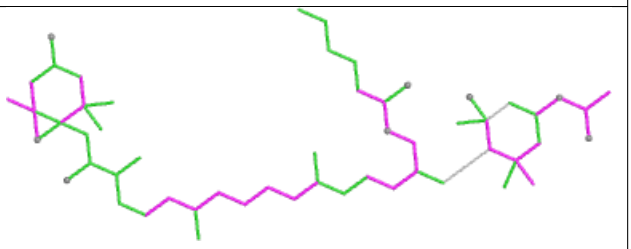

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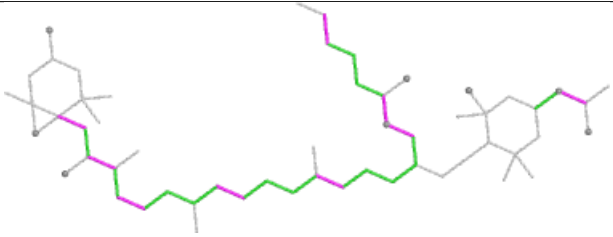

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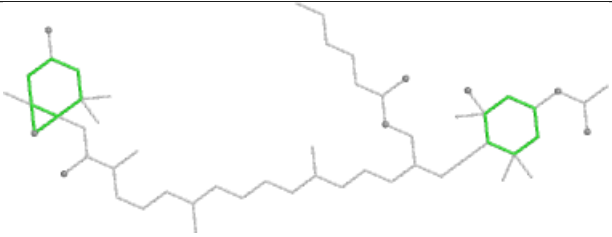
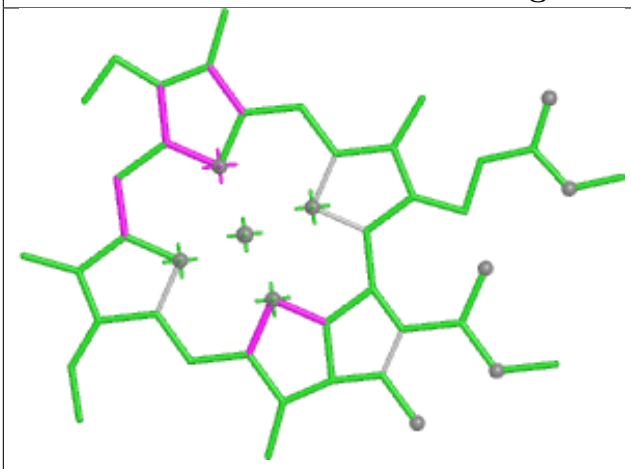


Rings

Ligand CLA z 308



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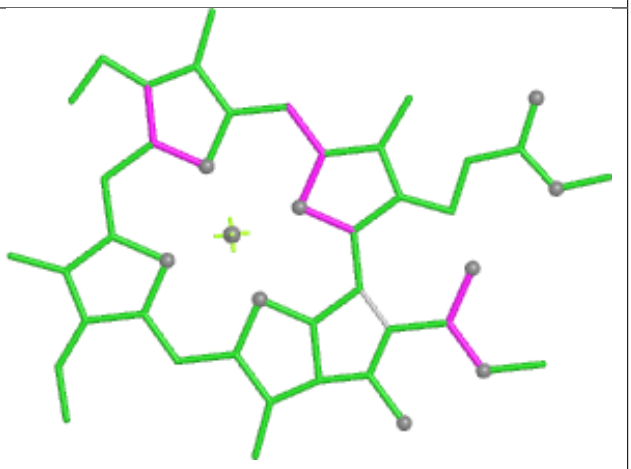

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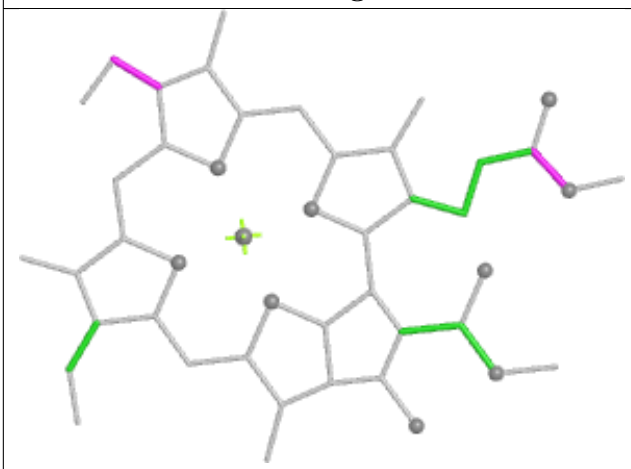

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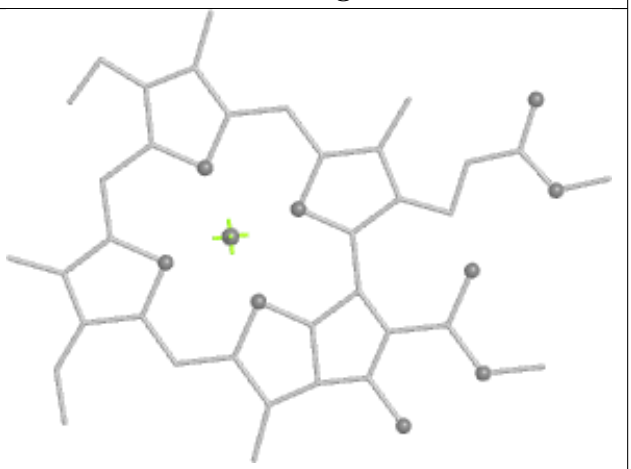
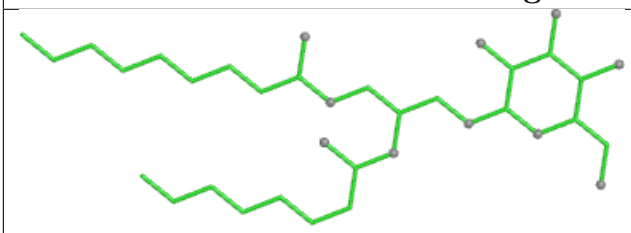


Rings

Ligand LMG 9 321



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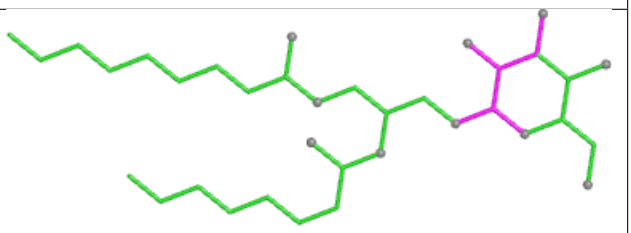

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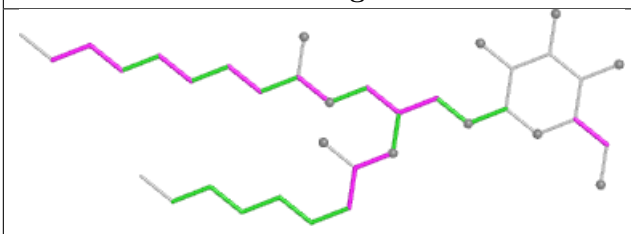

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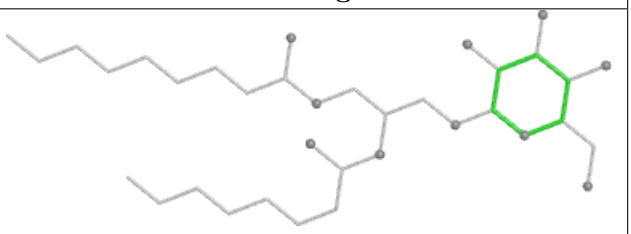
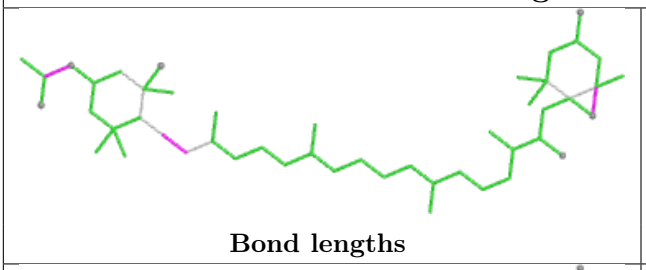


Rings

Ligand A86 Z 301



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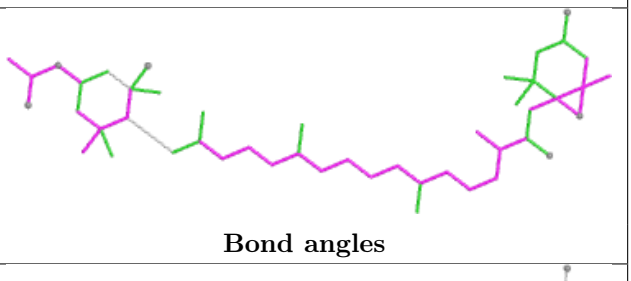
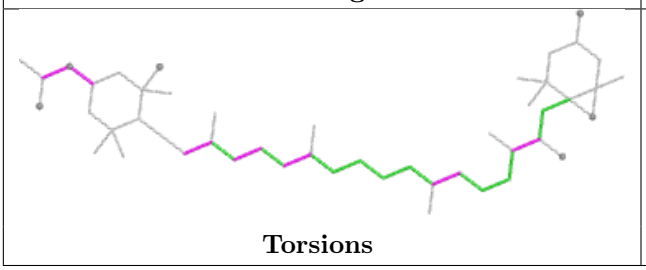


Bond angles



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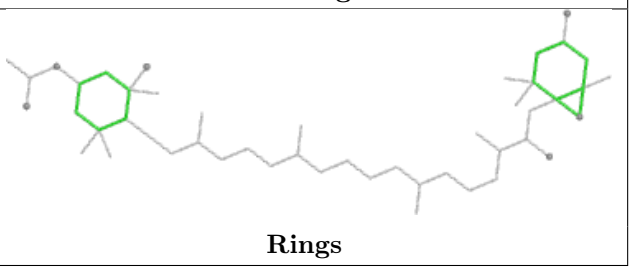
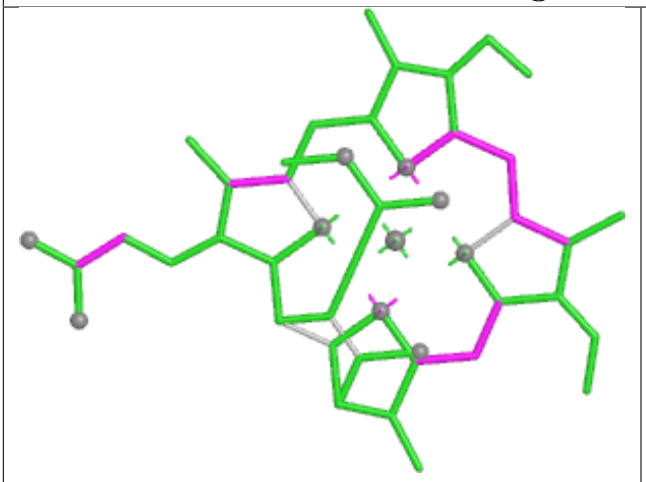


Rings

Ligand KC2 5 314



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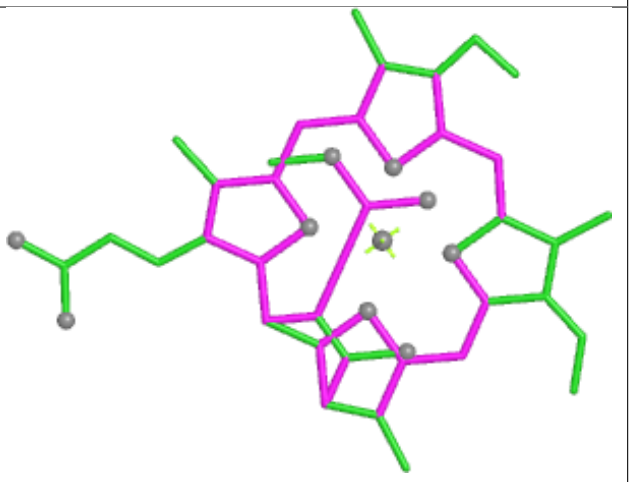
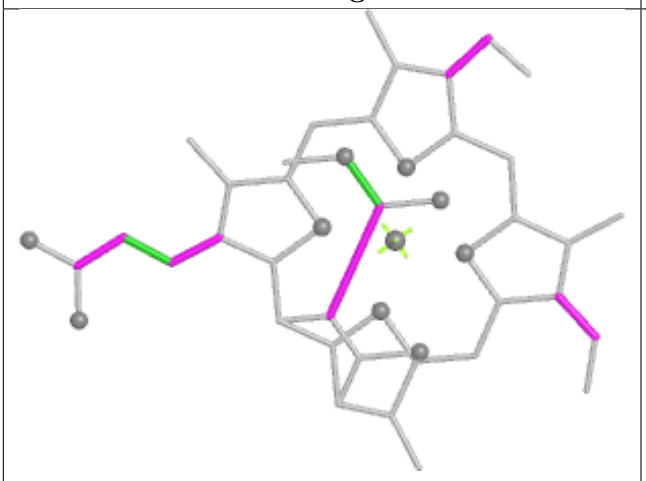


Bond angles



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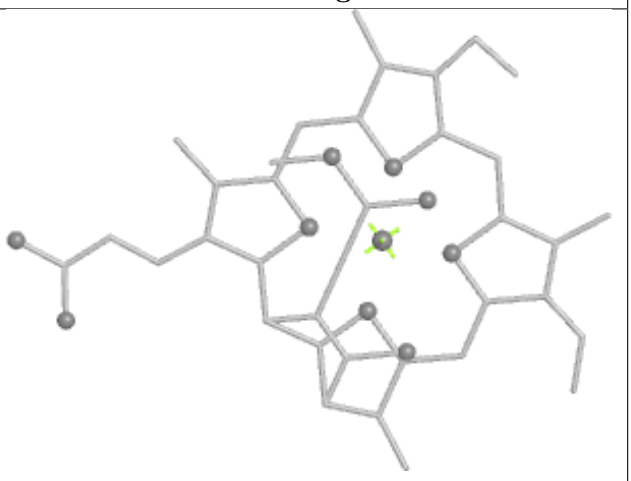
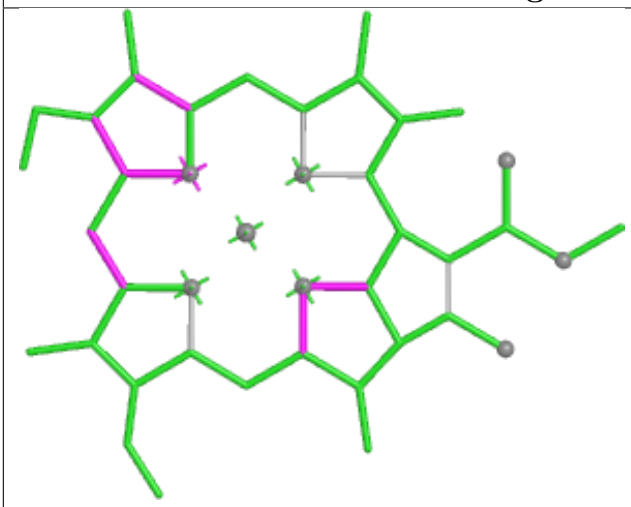


Rings

Ligand CLA L 316



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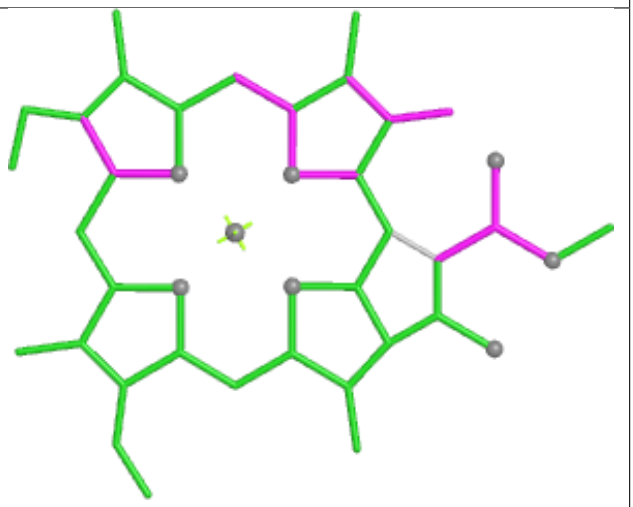
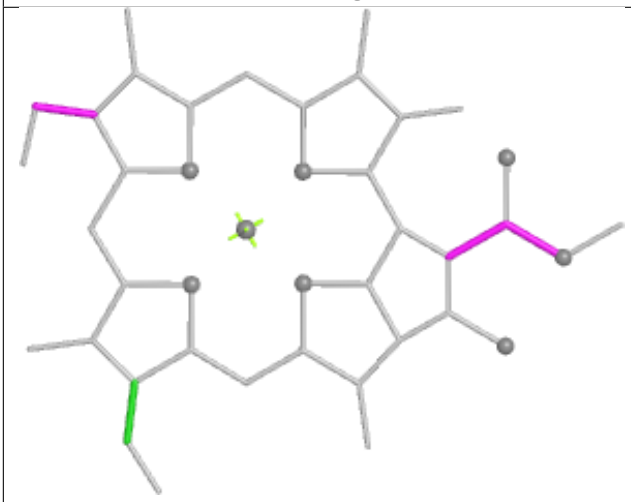
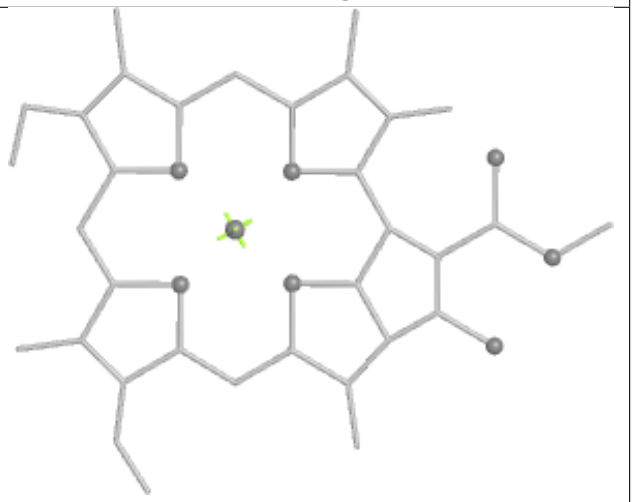


Bond angles

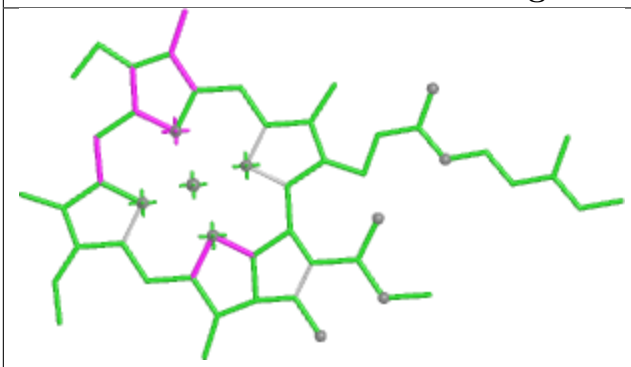


Torsions



Rings

Ligand CLA o 201



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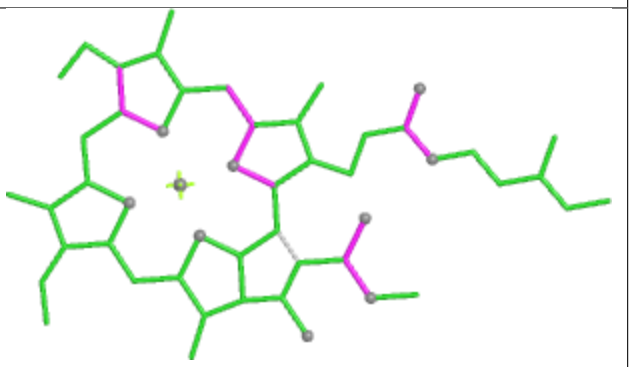
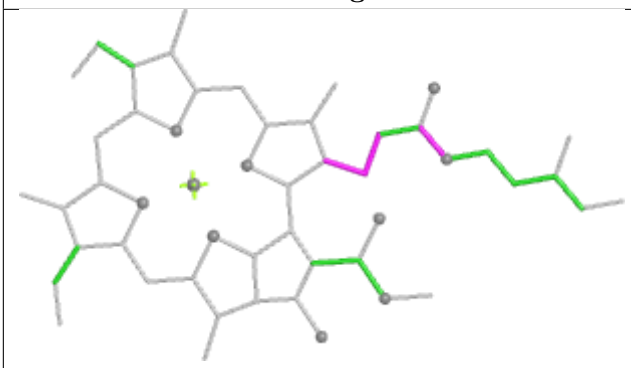
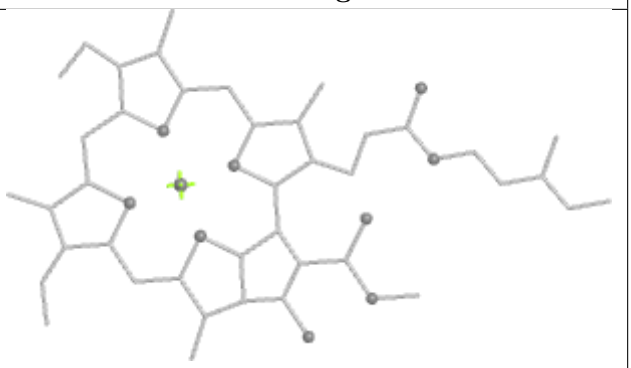


Bond angles

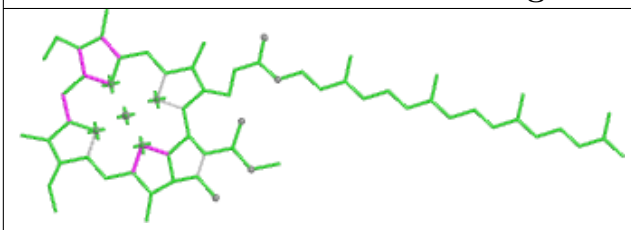


Torsions



Rings

Ligand CLA b 838



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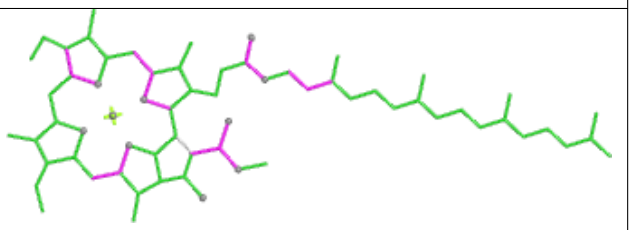
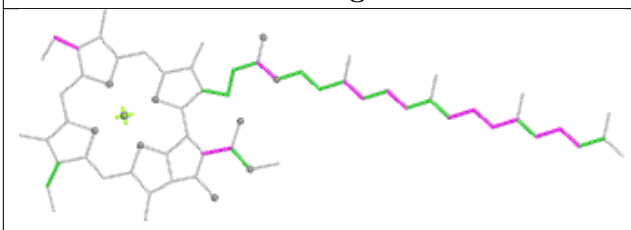
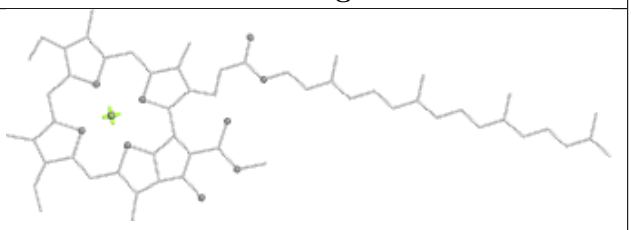


Bond angles

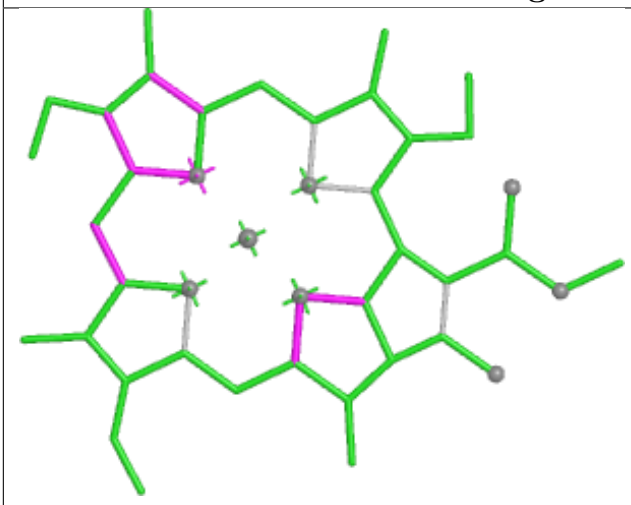


Torsions

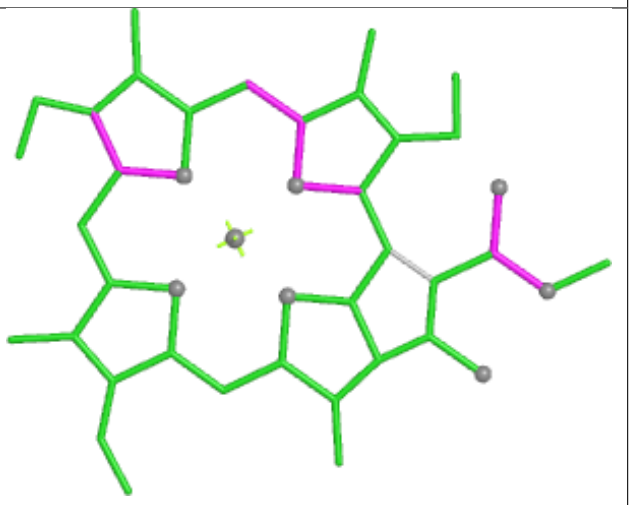


Rings

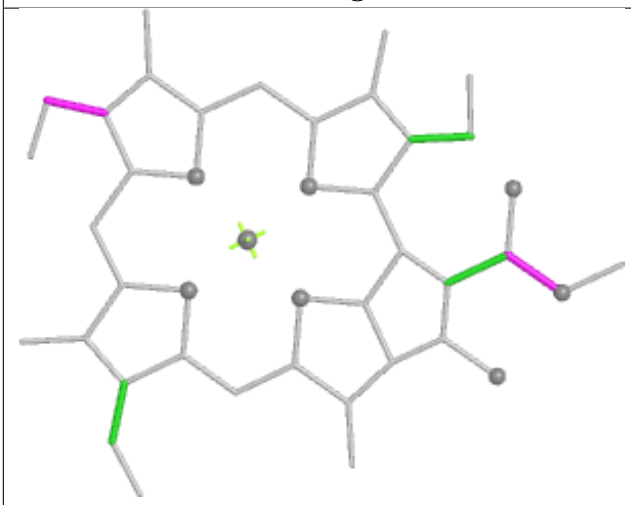
Ligand CLA 8 321



Bond lengths



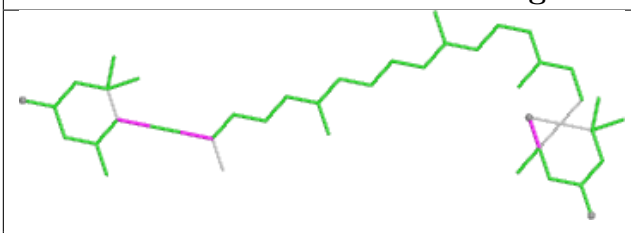
Bond angles



Torsions

Rings

Ligand DD6 y 304



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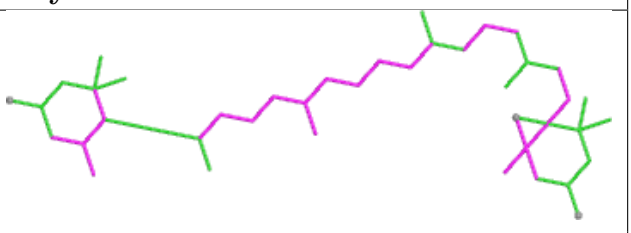
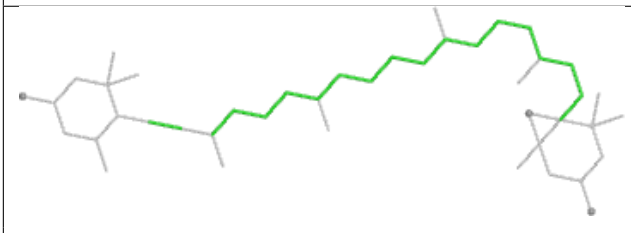


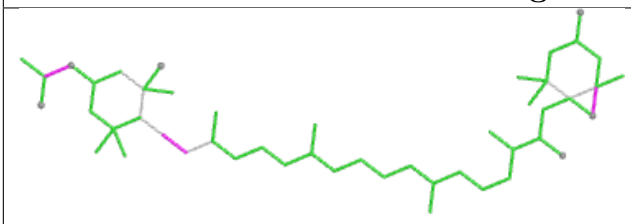
Bond angles



Torsions

Rings

Ligand A86 O 306



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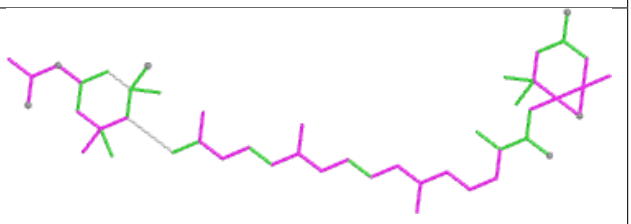
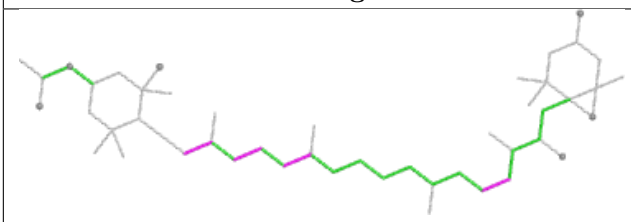
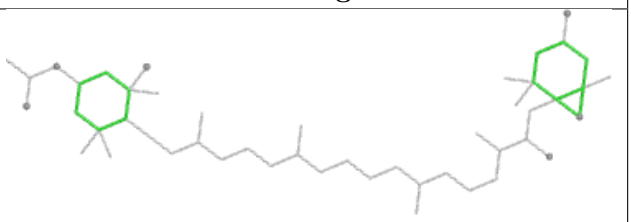


Bond angles

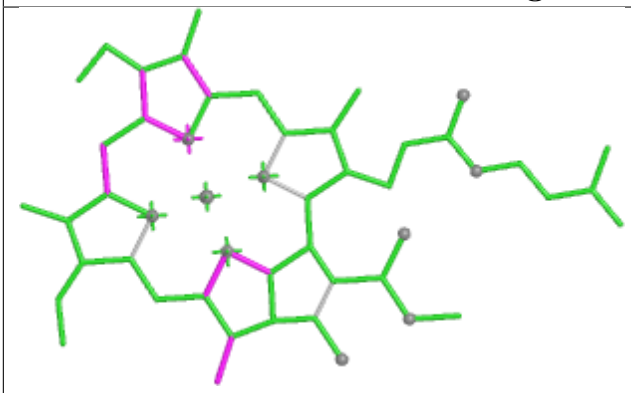


Torsions



Rings

Ligand CLA L 313



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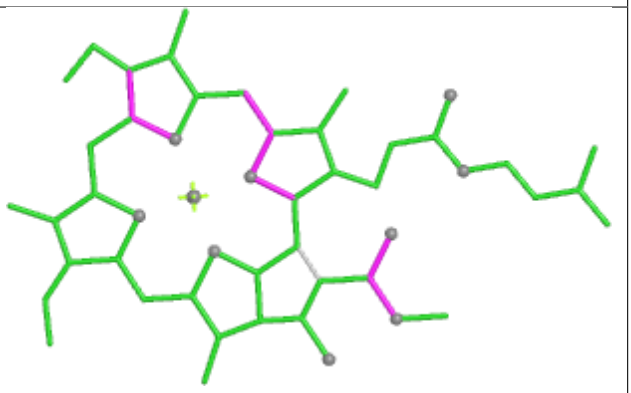
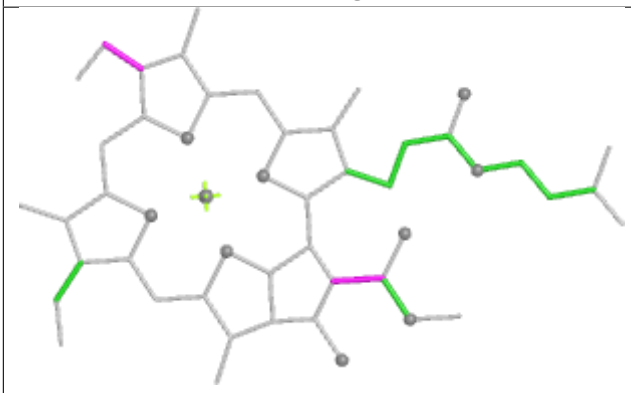
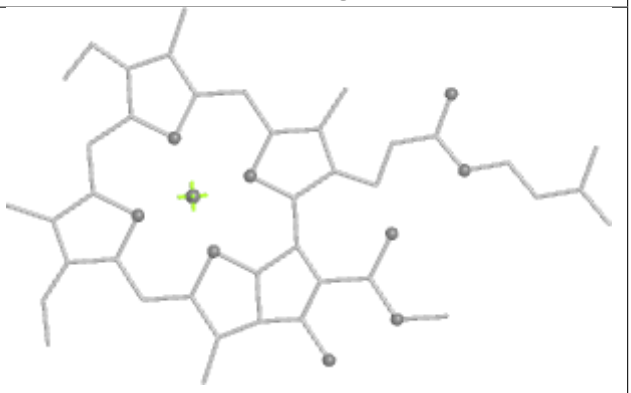


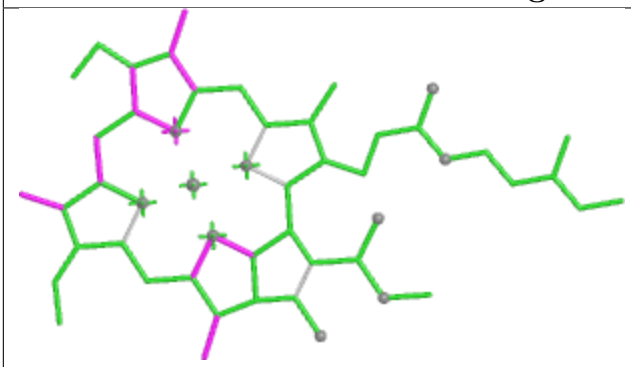
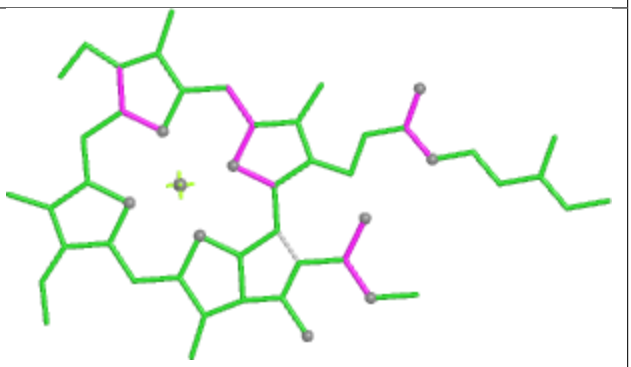
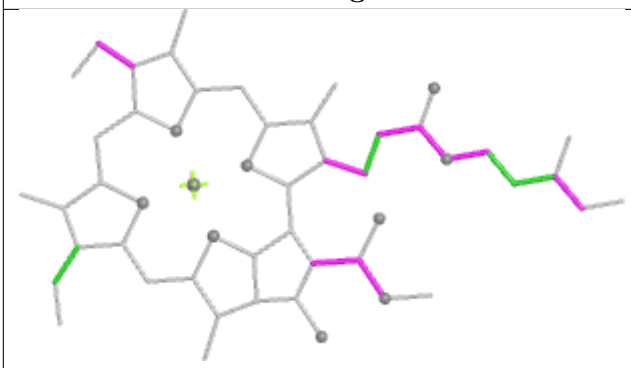
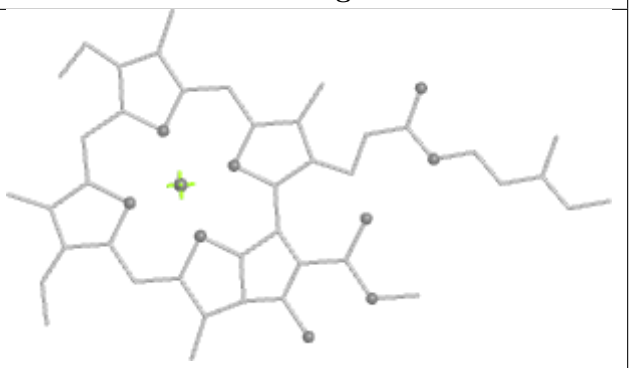
Bond angles

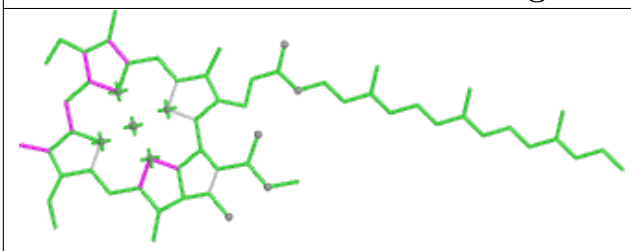
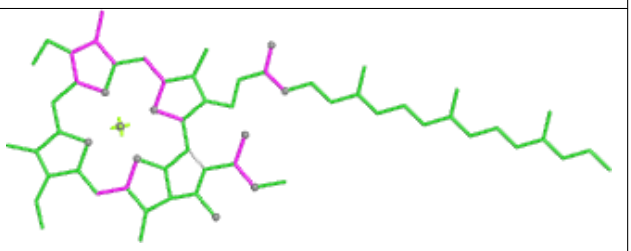
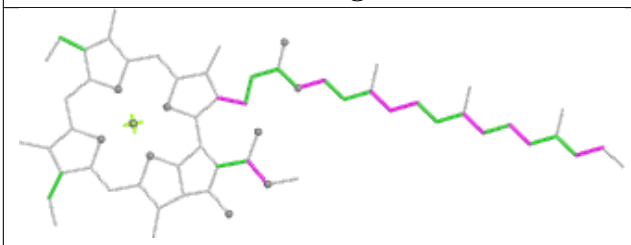
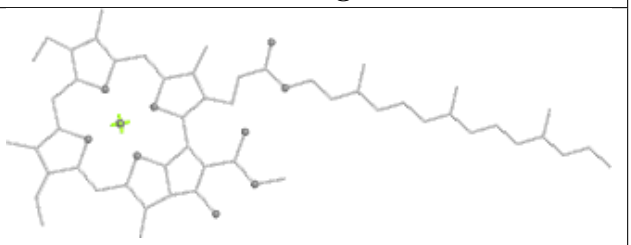


Torsions

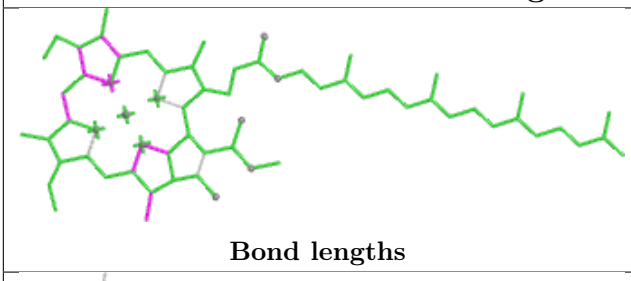


Rings

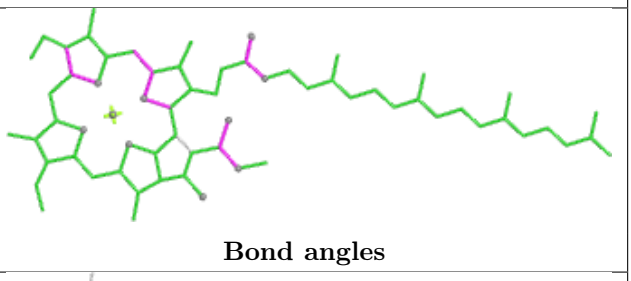
Ligand CLA 0 322	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

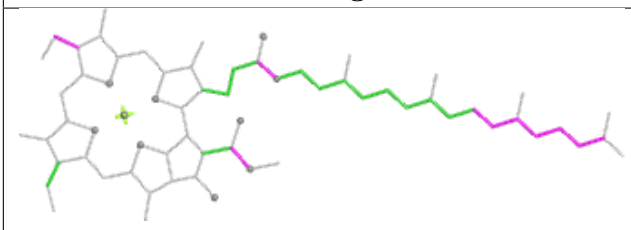
Ligand CLA b 842



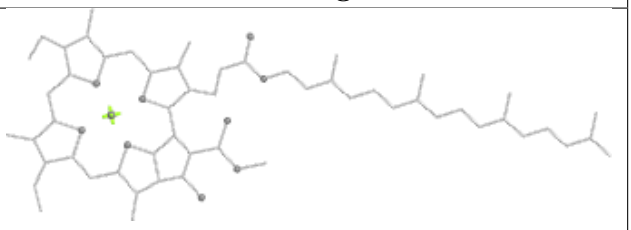
Bond lengths



Bond angles

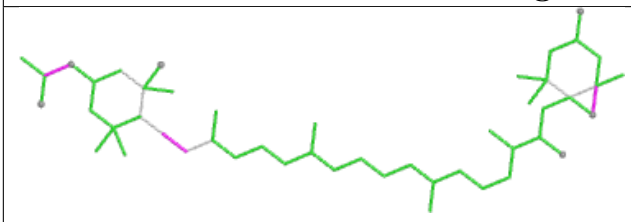


Torsions



Rings

Ligand A86 J 301



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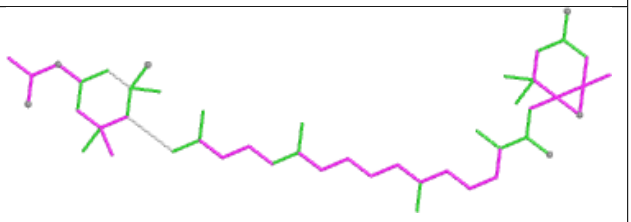

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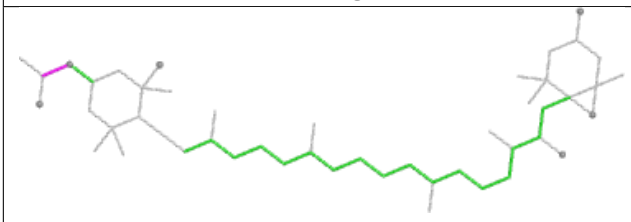
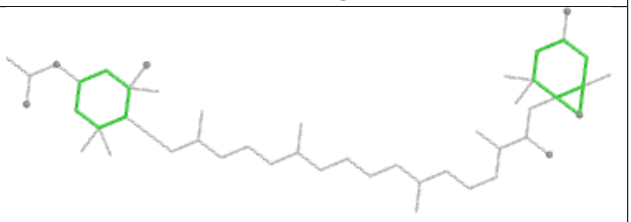
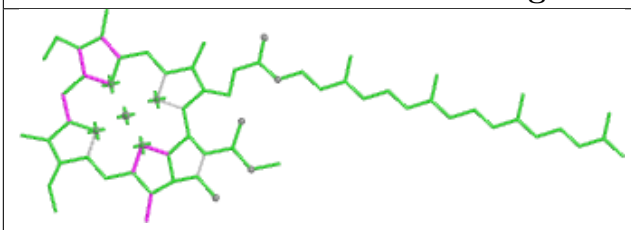


Torsions



Rings

Ligand CLA a 831



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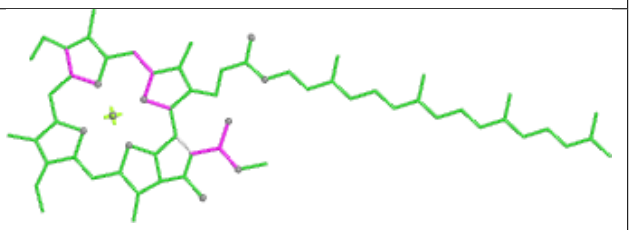
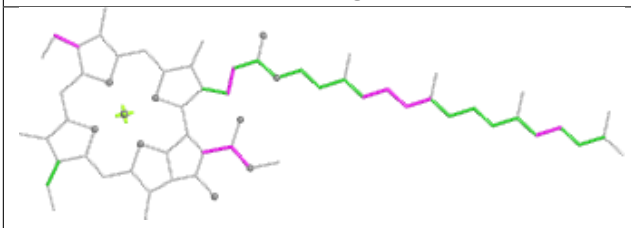
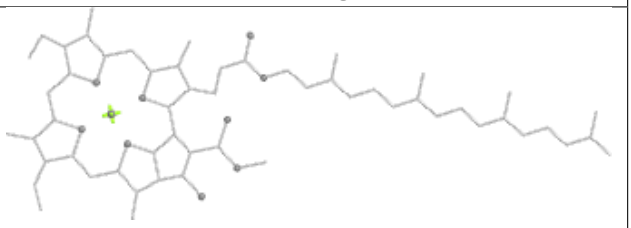


Bond angles

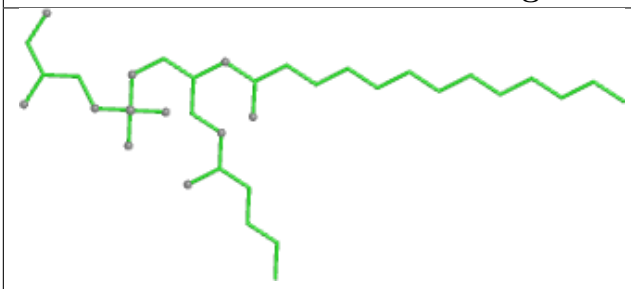


Torsions



Rings

Ligand LHG D 301



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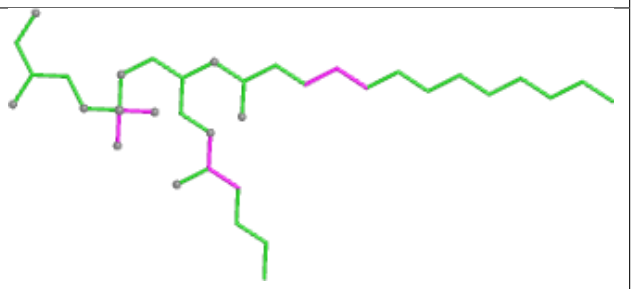

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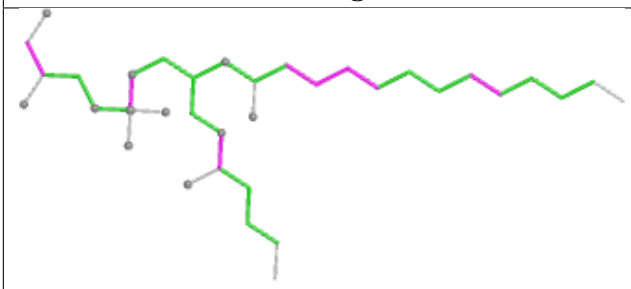
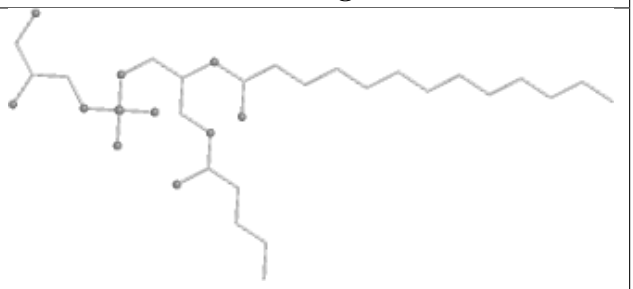
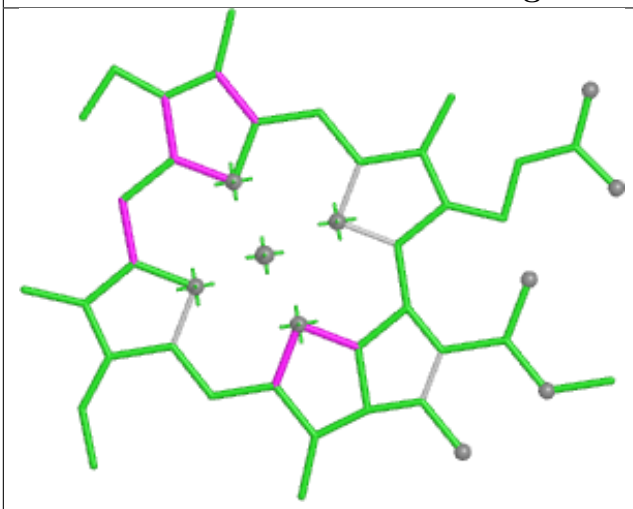


Torsions



Rings

Ligand CLA H 307



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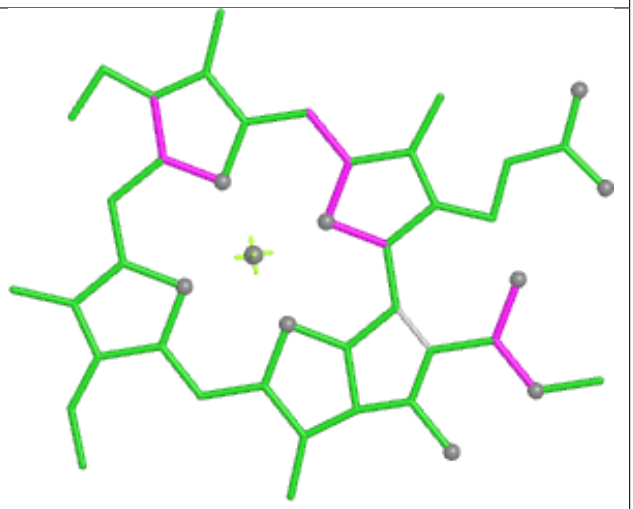
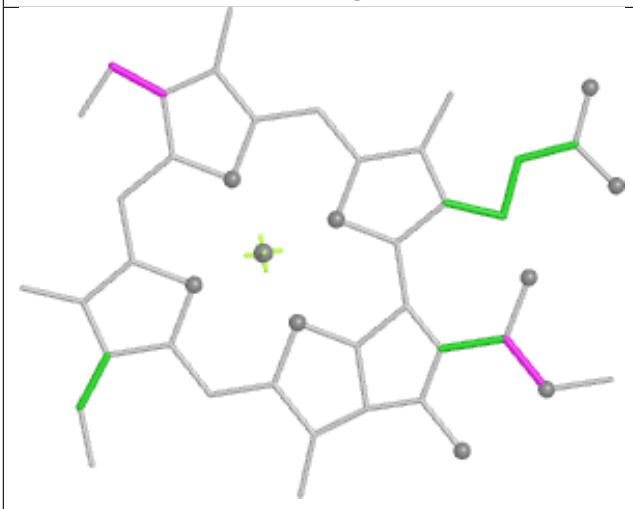


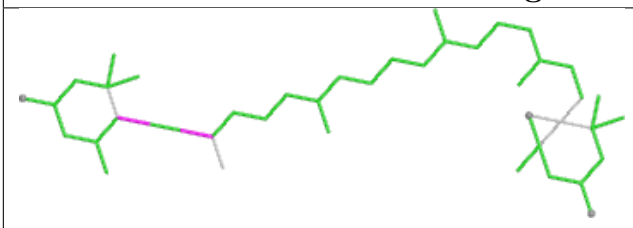
Bond angles



Torsions

Rings

Ligand DD6 O 305



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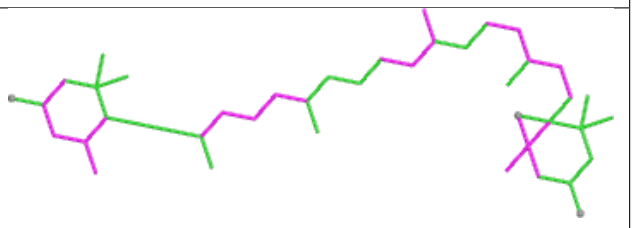
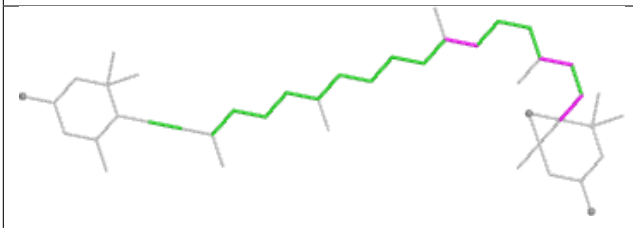


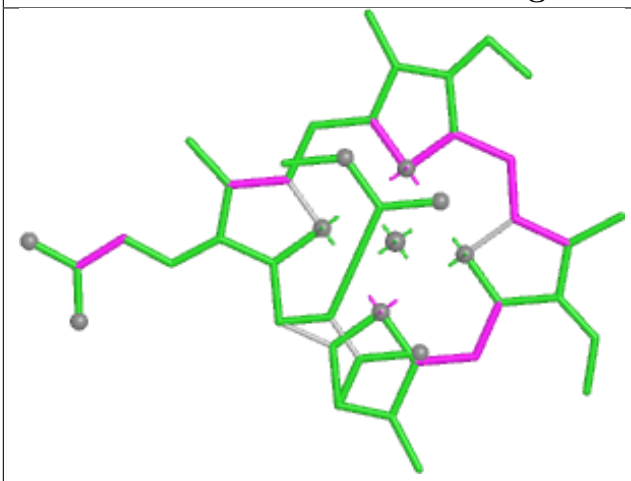
Bond angles



Torsions

Rings

Ligand KC2 L 321



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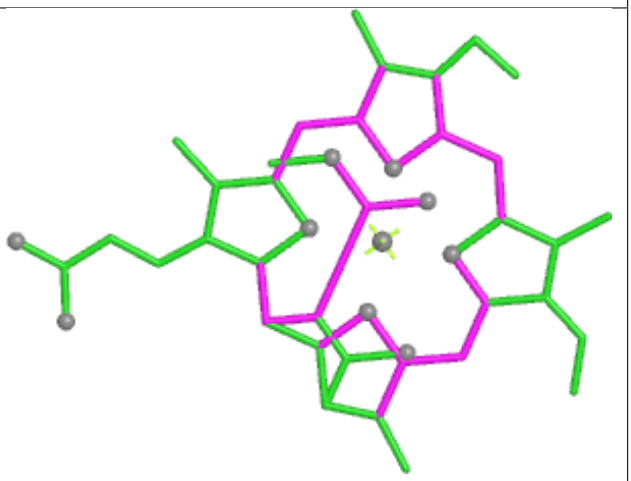
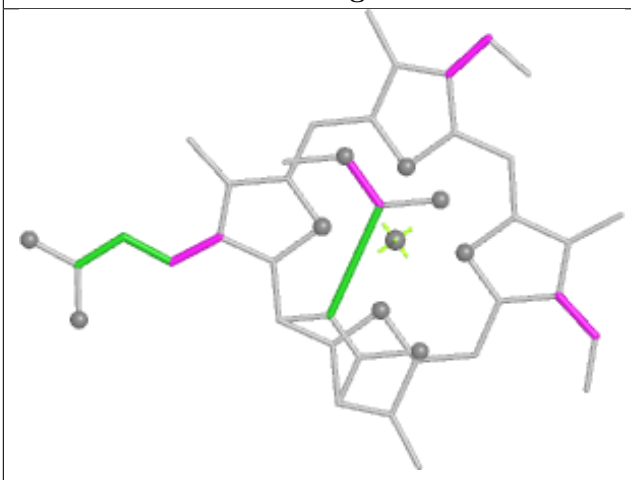
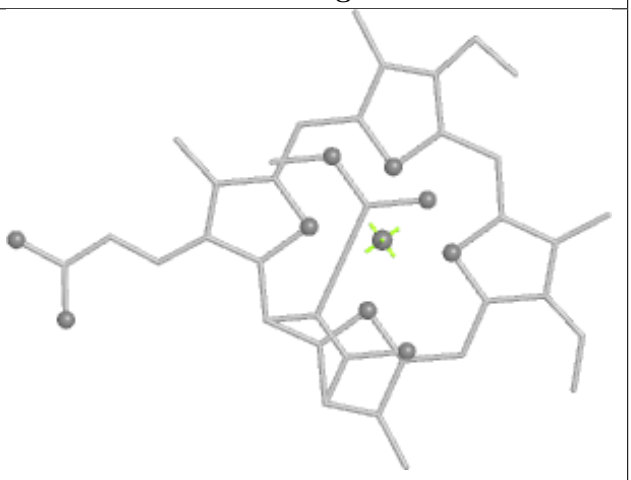


Bond angles

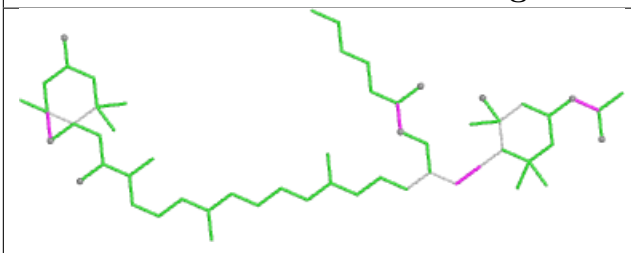


Torsions



Rings

Ligand A1EB1 8 308



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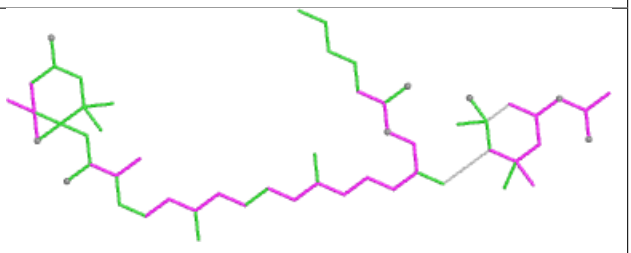
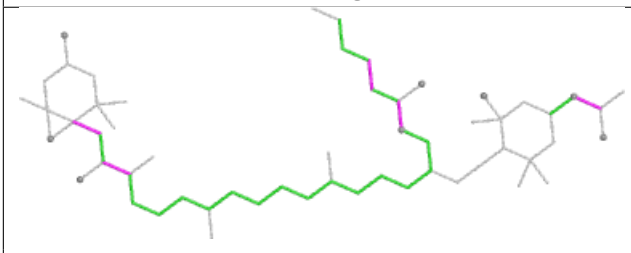
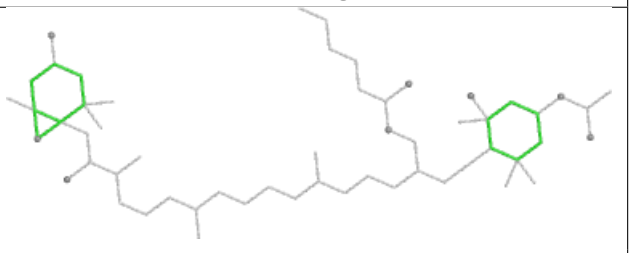


Bond angles

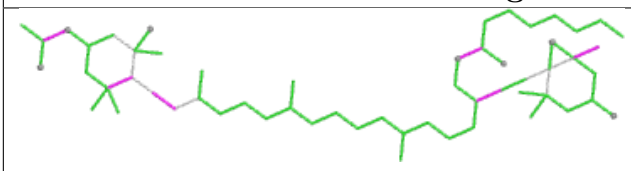


Torsions



Rings

Ligand A1EB4 P 319



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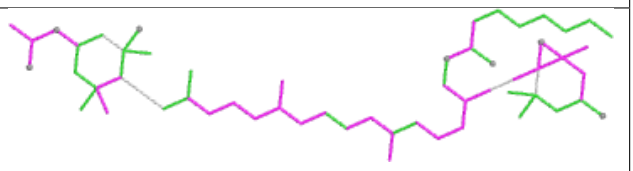
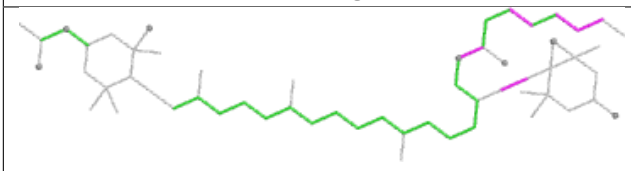
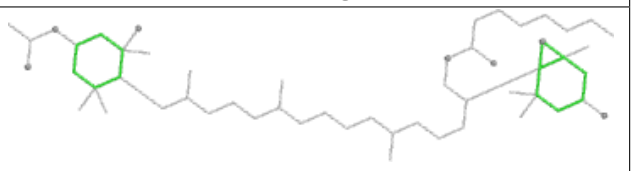


Bond angles

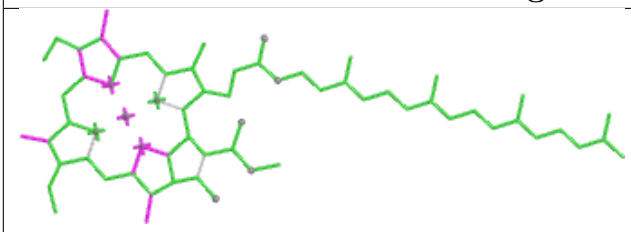


Torsions

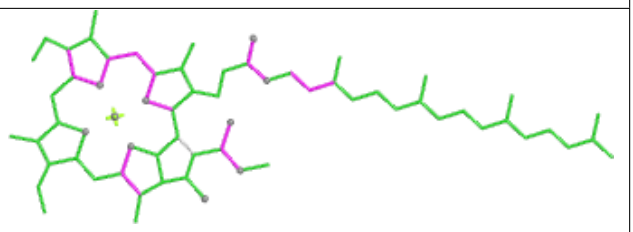


Rings

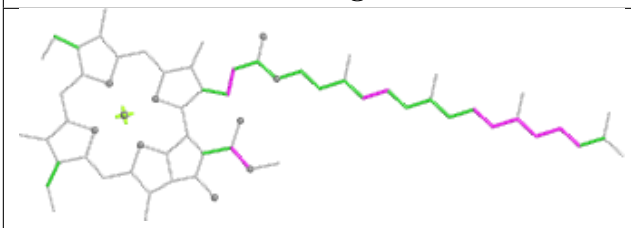
Ligand CLA b 801



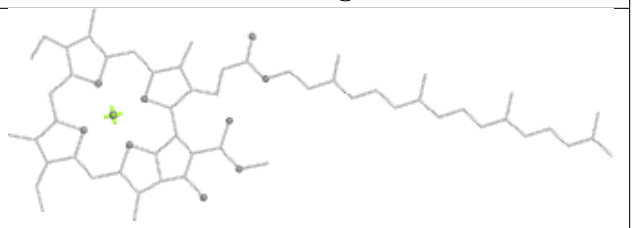
Bond lengths



Bond angles

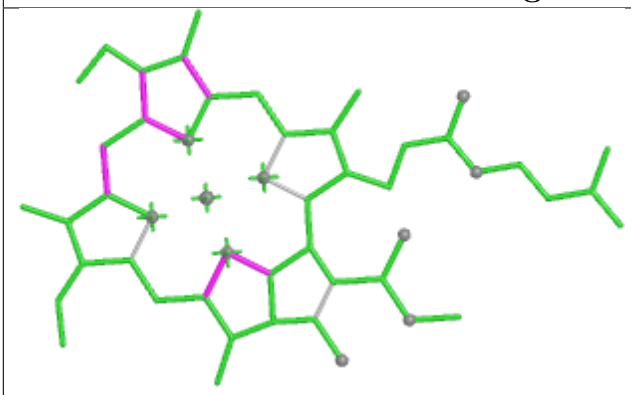


Torsions



Rings

Ligand CLA A 315



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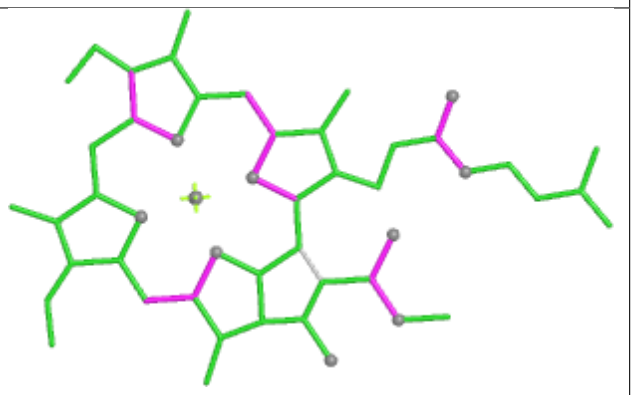
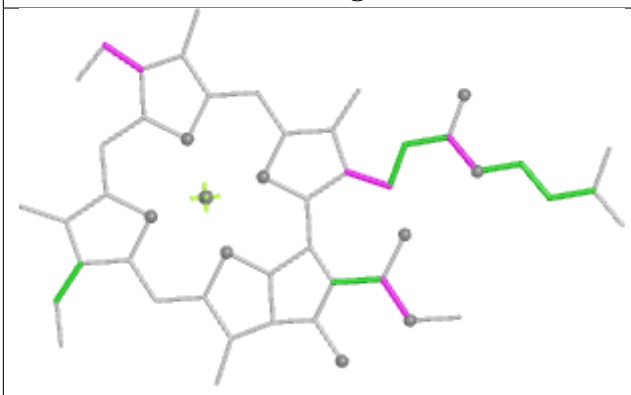
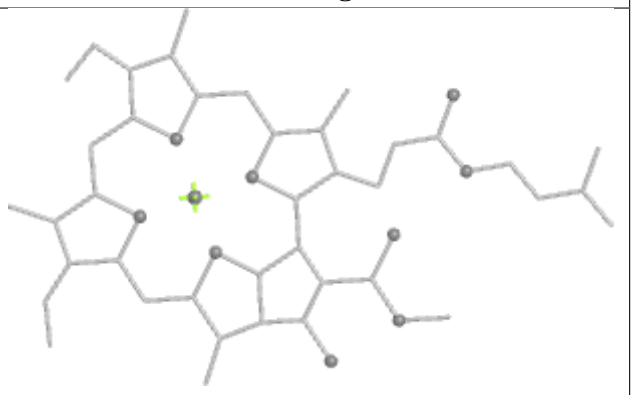


Bond angles

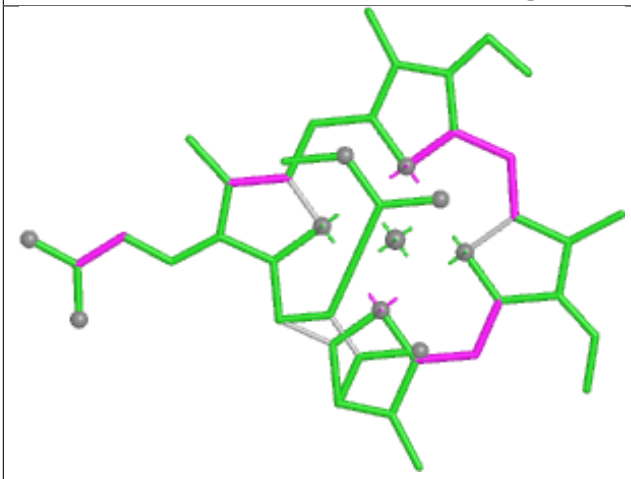


Torsions



Rings

Ligand KC2 M 314



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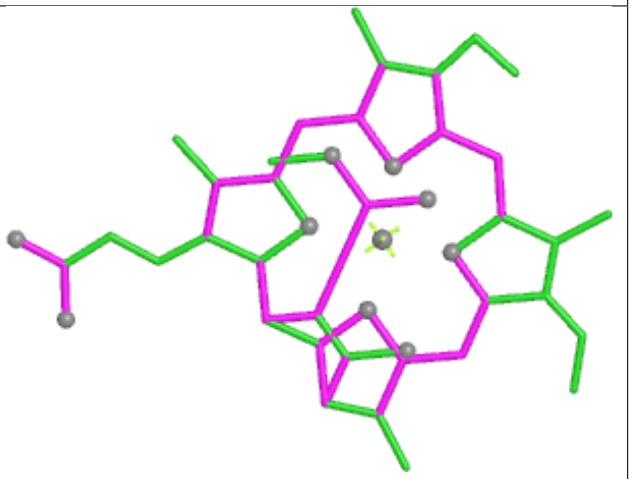
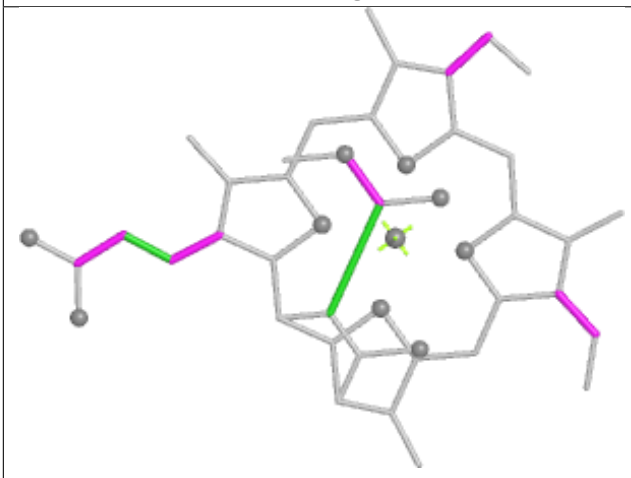


Bond angles



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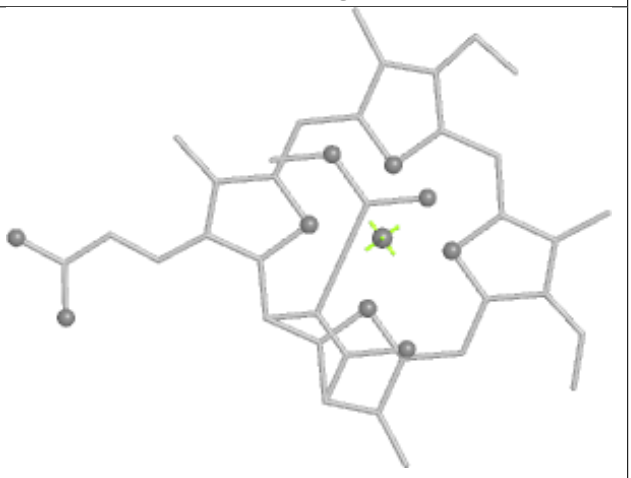
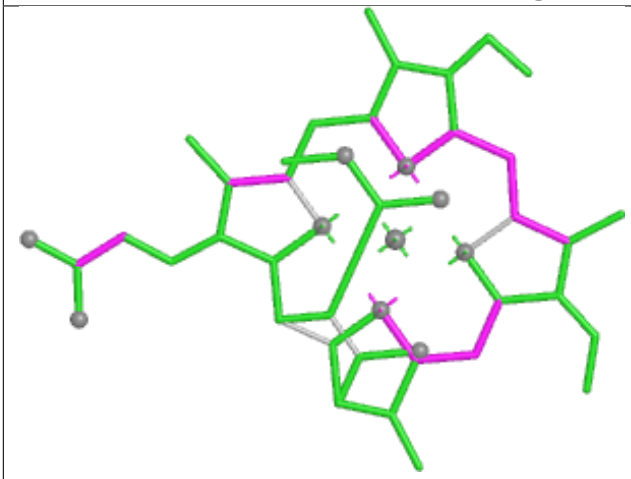


Rings

Ligand KC2 9 313



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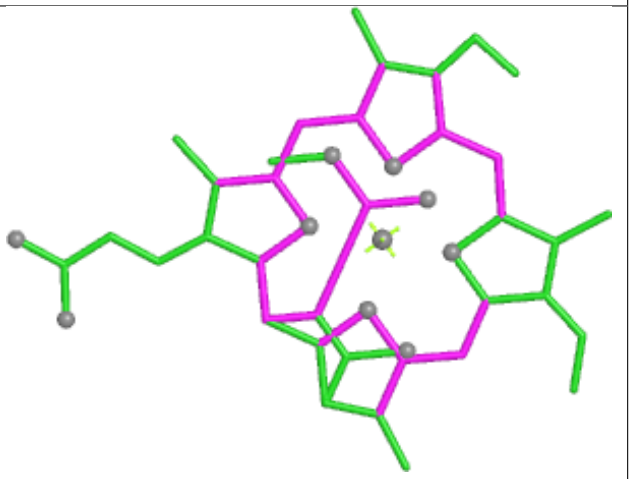
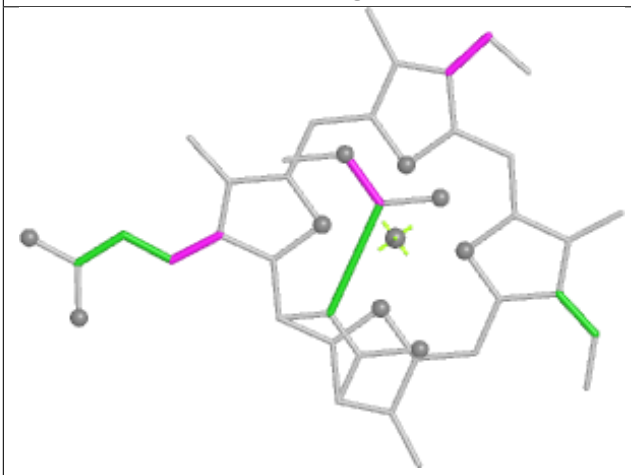


Bond angles



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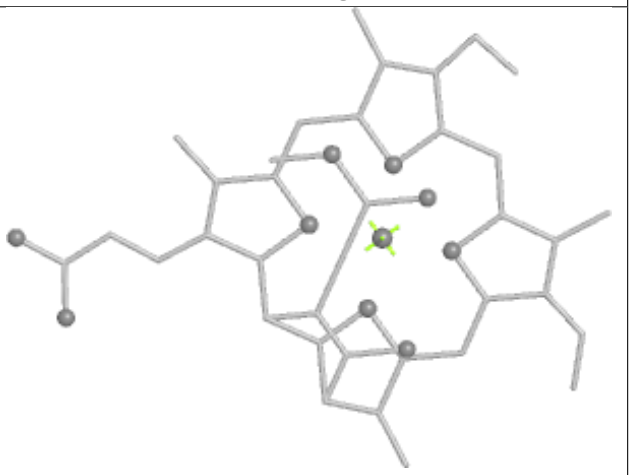
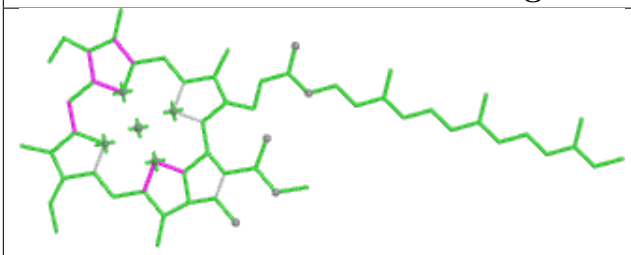


Rings

Ligand CLA C 305



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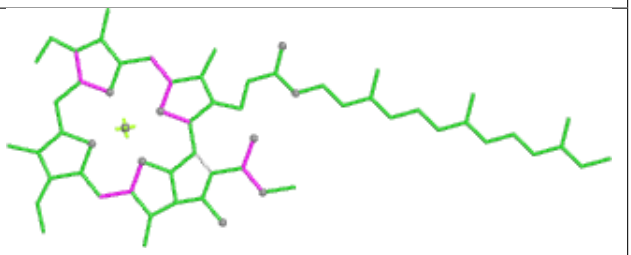
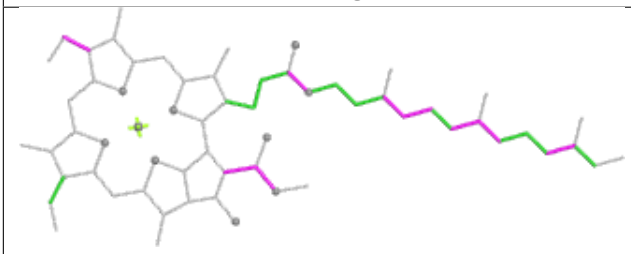


Bond angles



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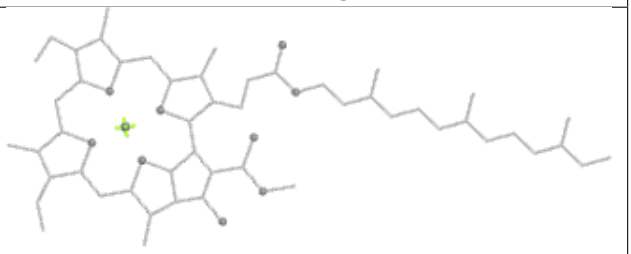
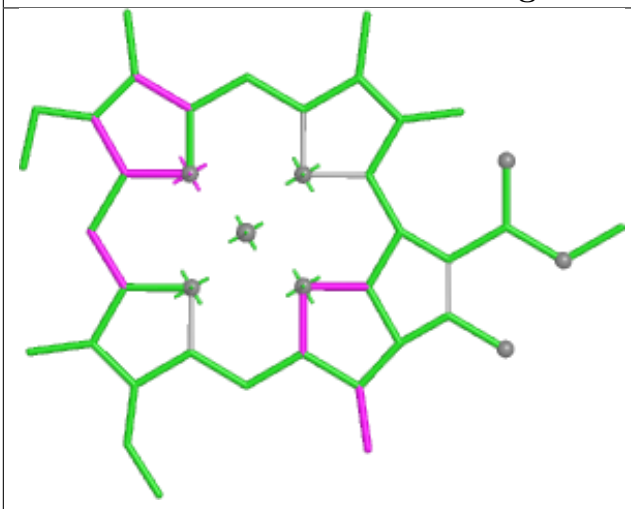


Rings

Ligand CLA W 316



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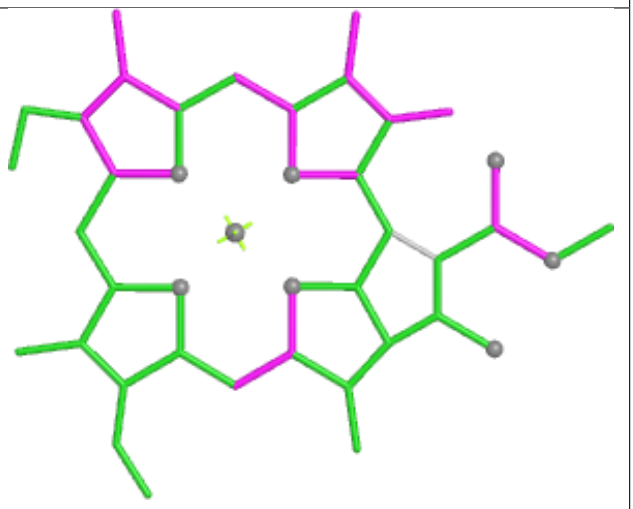
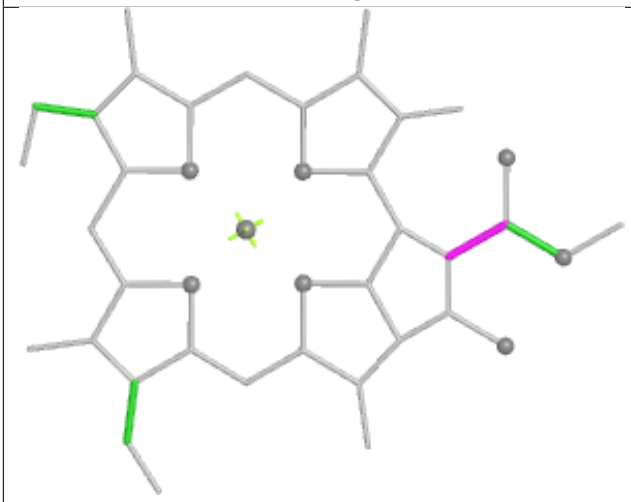


Bond angles



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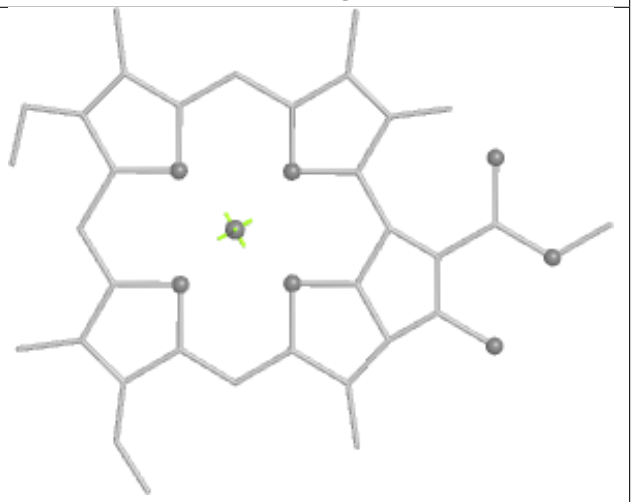
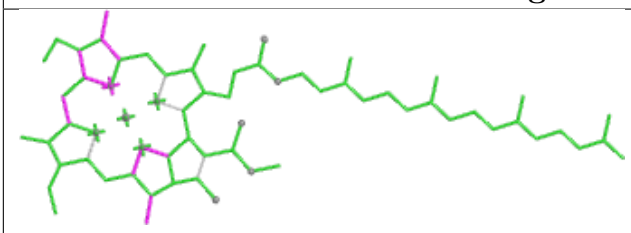


Rings

Ligand CLA a 804



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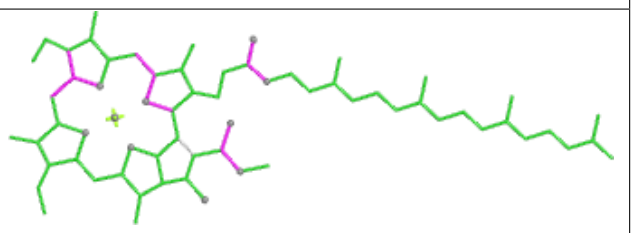
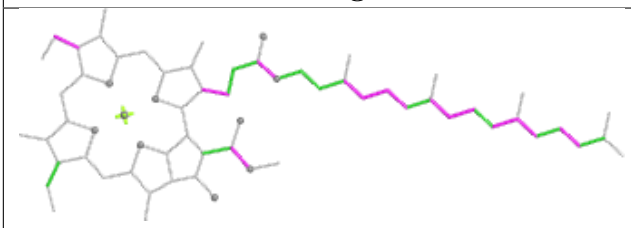


Bond angles



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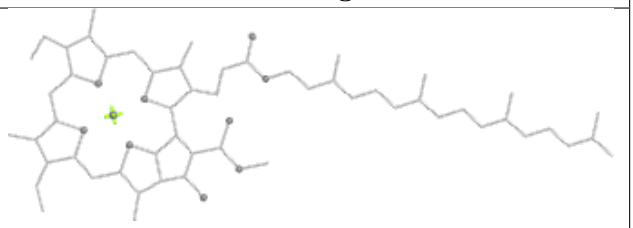
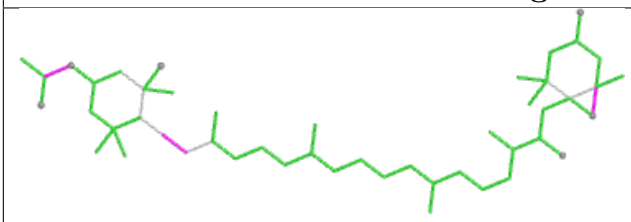


Rings

Ligand A86 B 201



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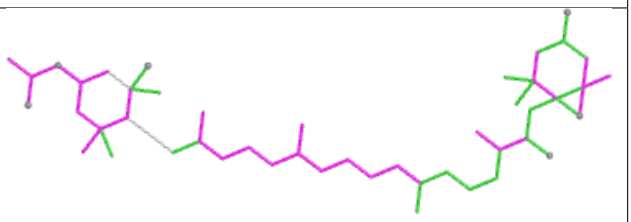
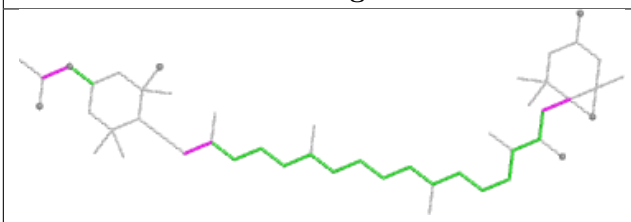


Bond angles



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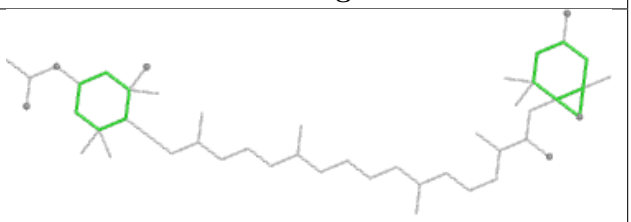
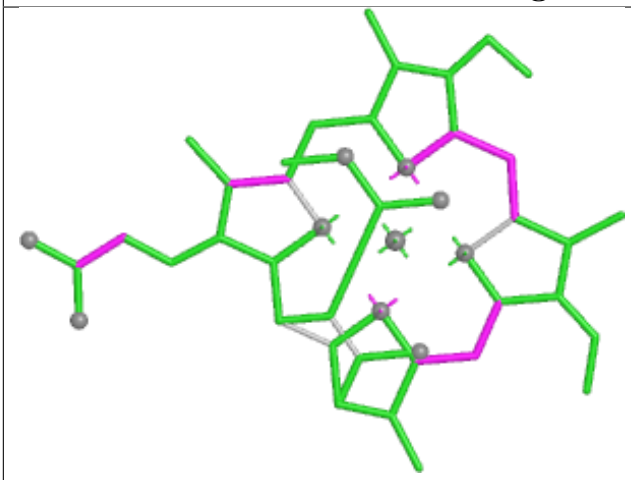


Rings

Ligand KC2 7 320



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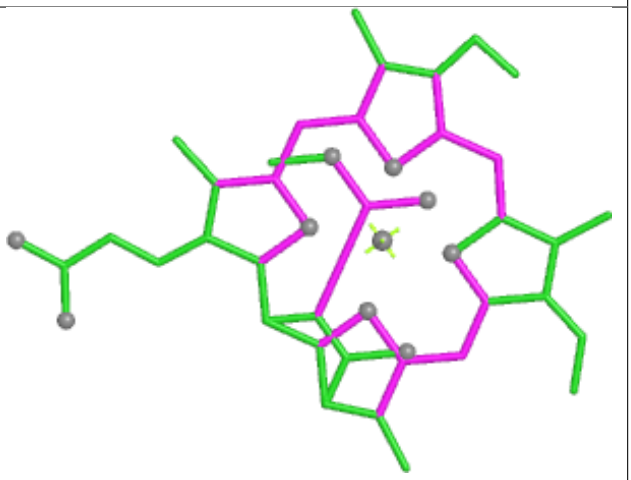
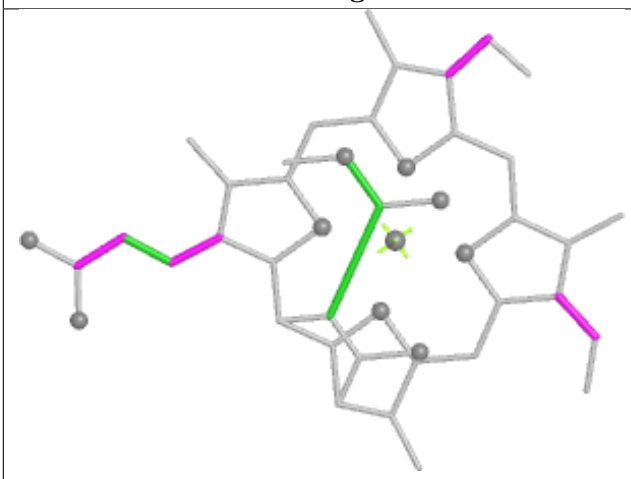


Bond angles



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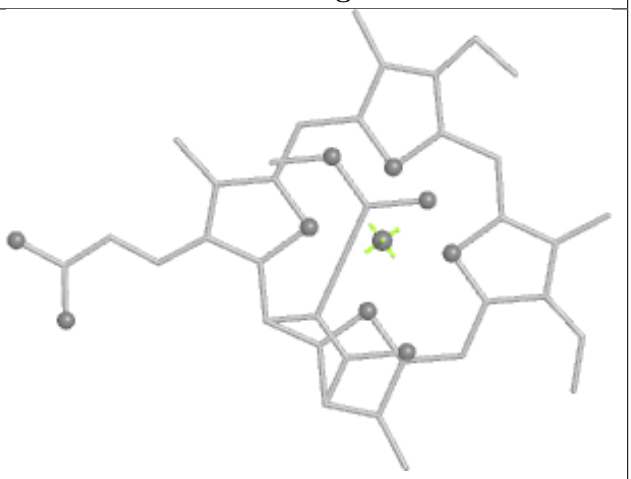
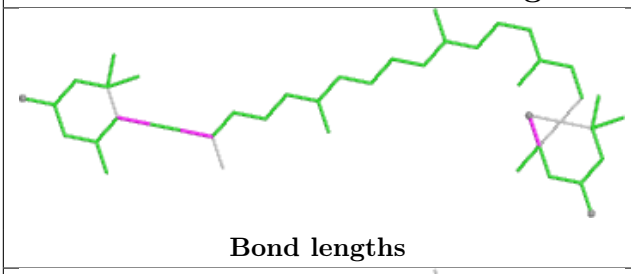


Rings

Ligand DD6 K 303



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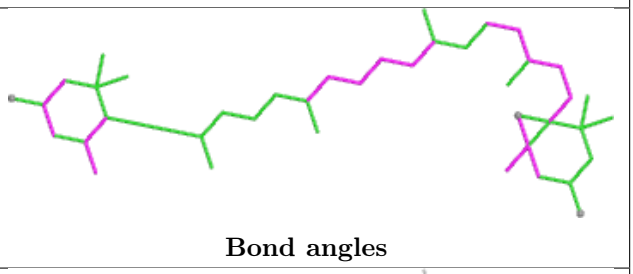
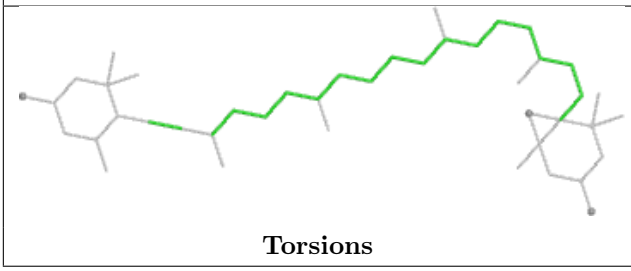


Bond angles



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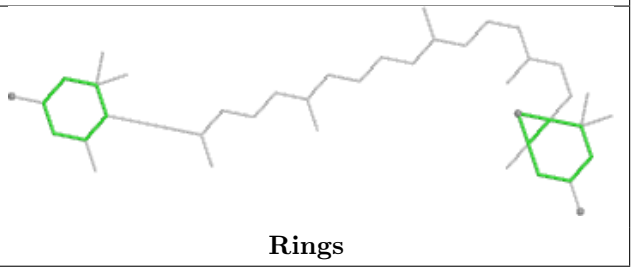
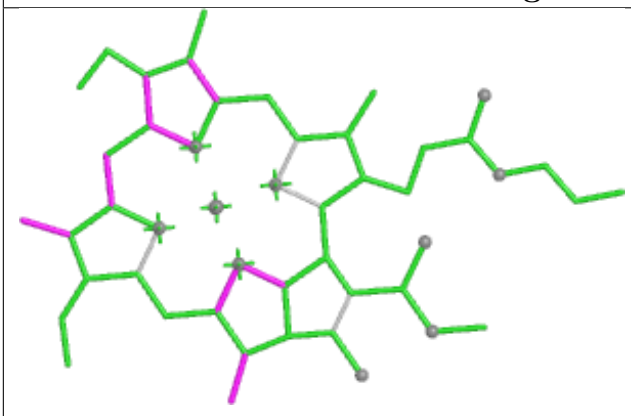


Rings

Ligand CLA H 306



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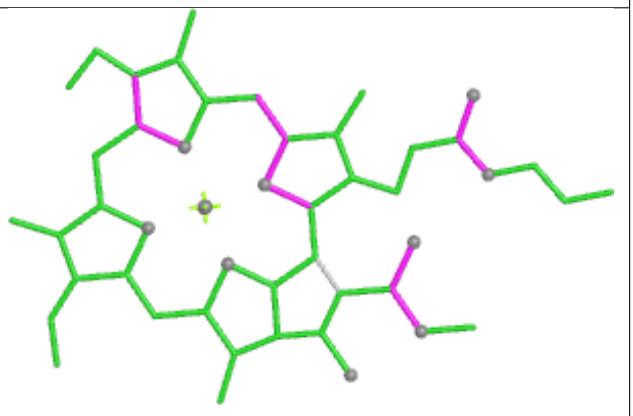
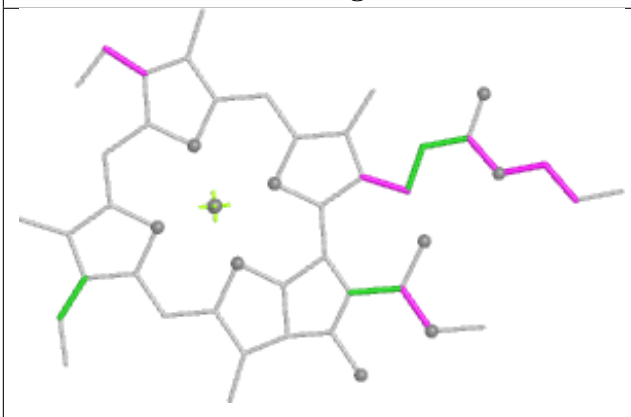


Bond angles



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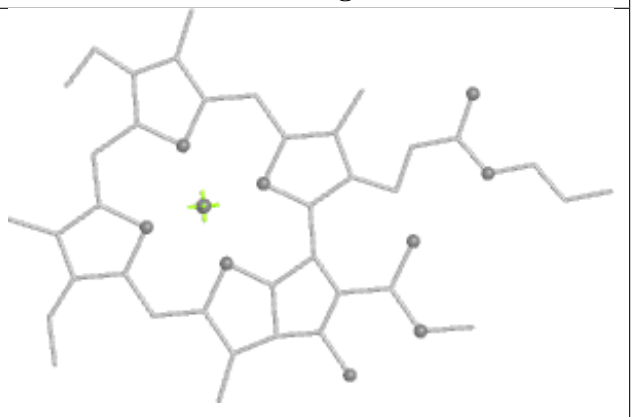
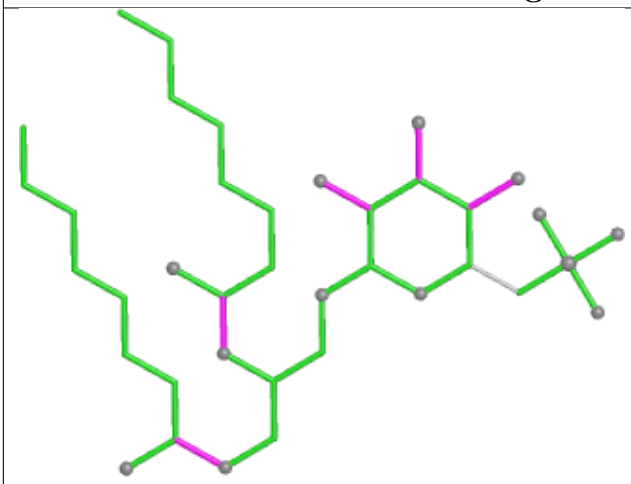


Rings

Ligand SQD P 301



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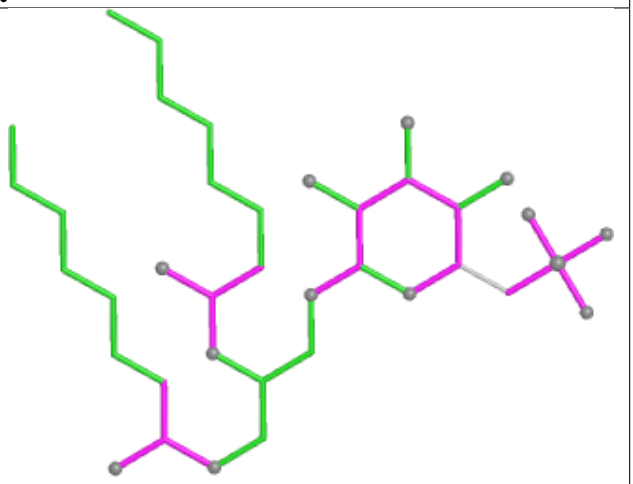
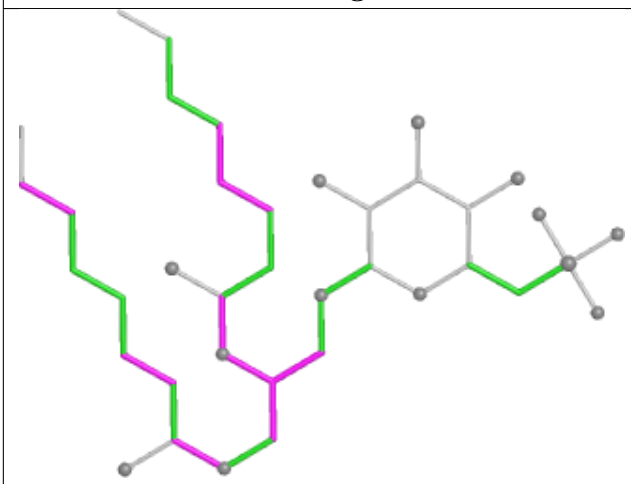


Bond angles



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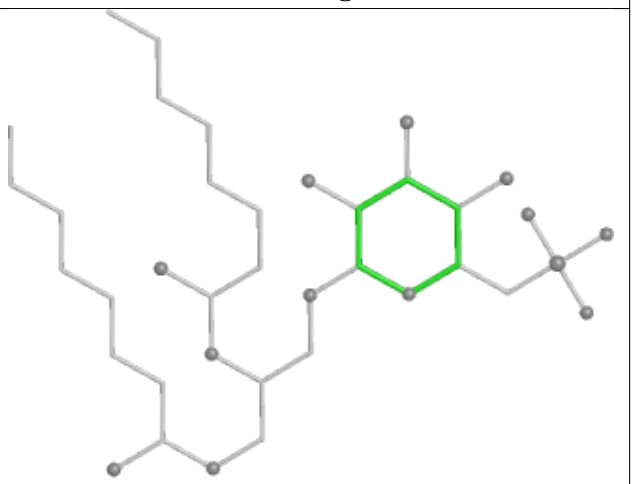
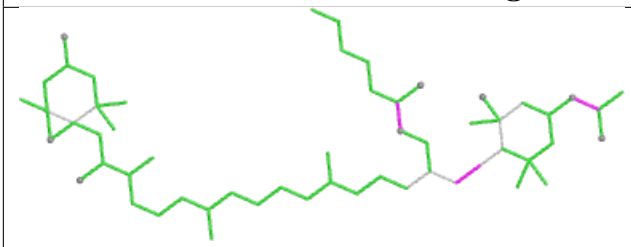


Rings

Ligand A1EB1 V 306



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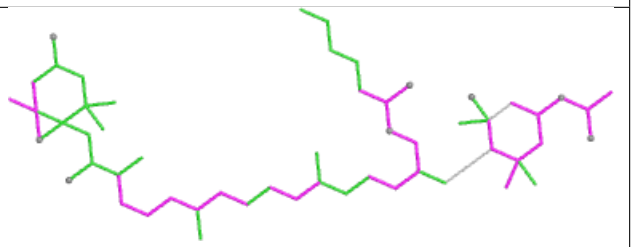
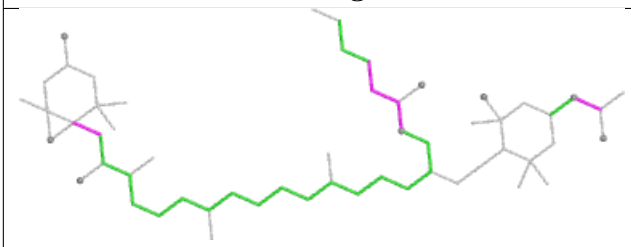


Bond angles



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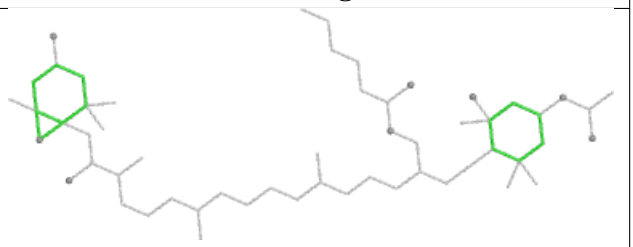
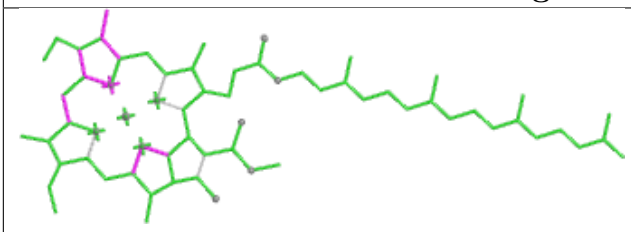
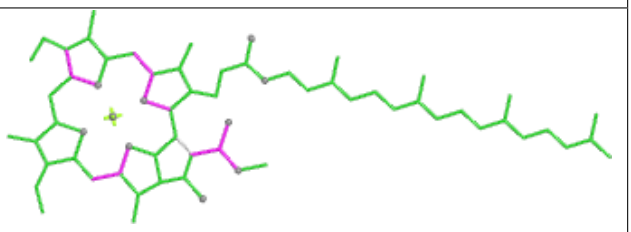


Rings

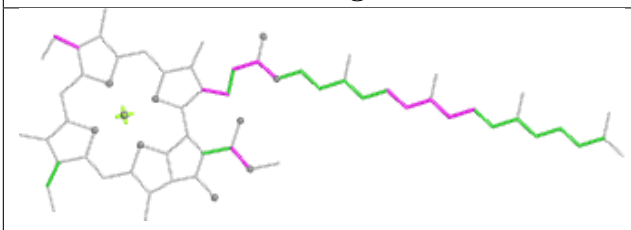
Ligand CLA l 201



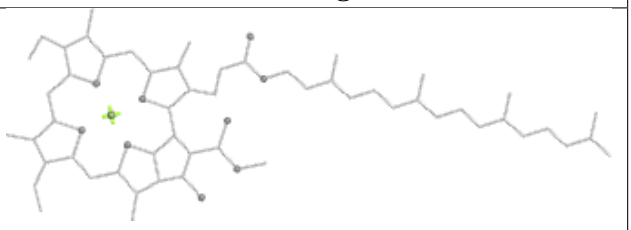
Bond lengths



Bond angles

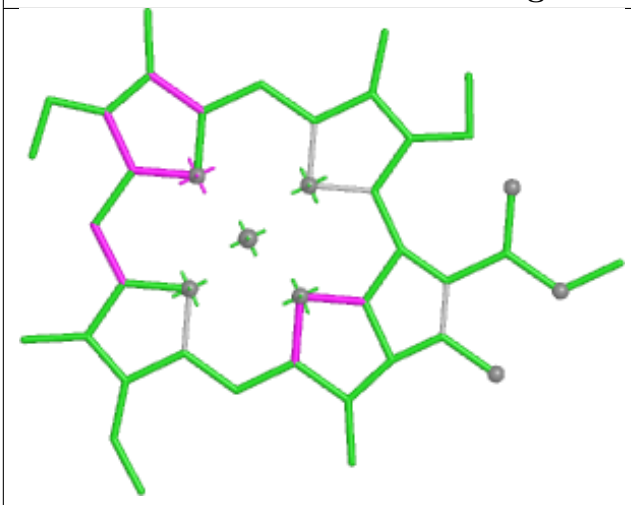


Torsions

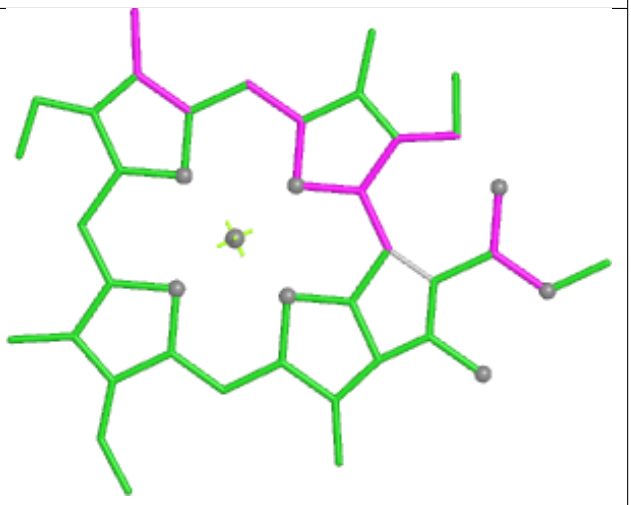


Rings

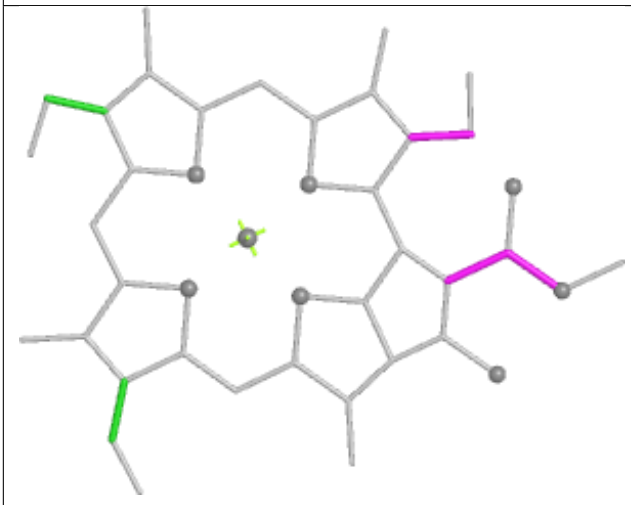
Ligand CLA S 310



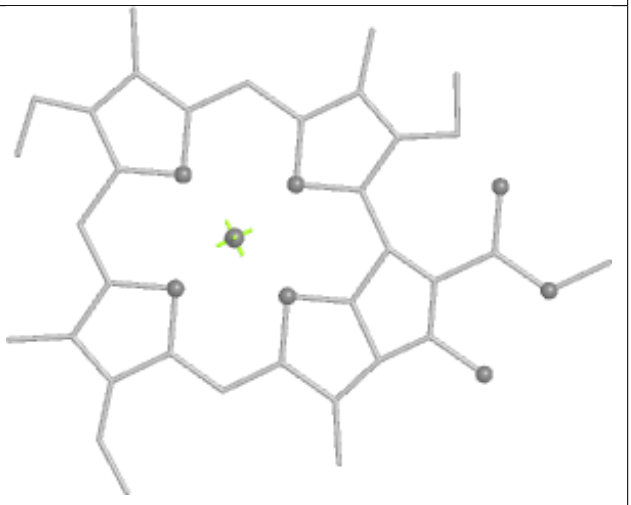
Bond lengths



Bond angles

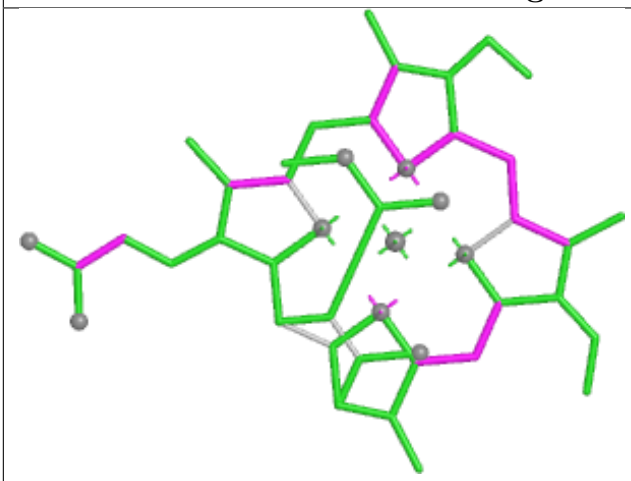


Torsions

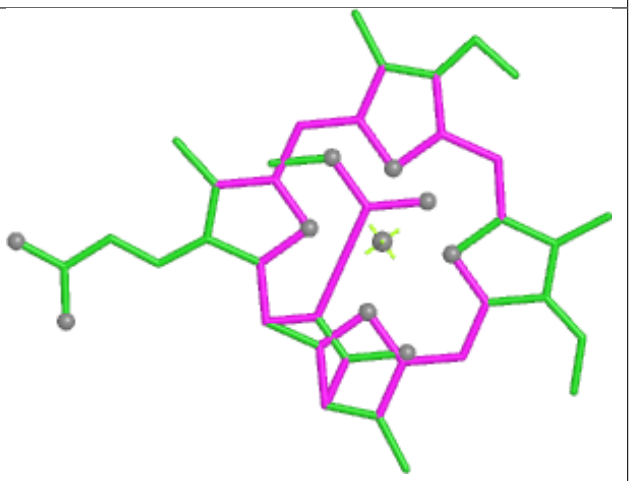


Rings

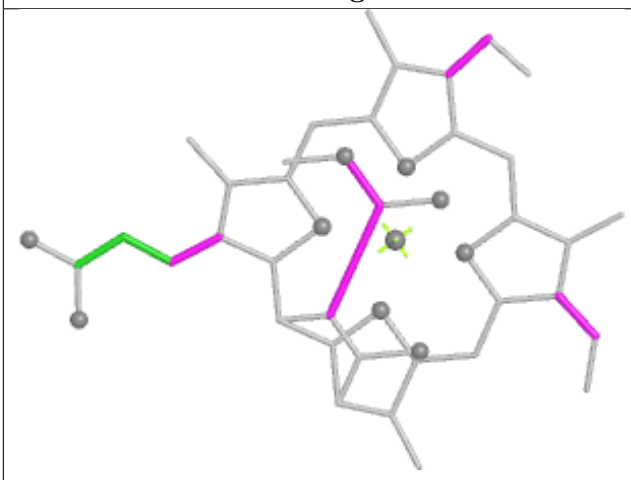
Ligand KC2 P 306



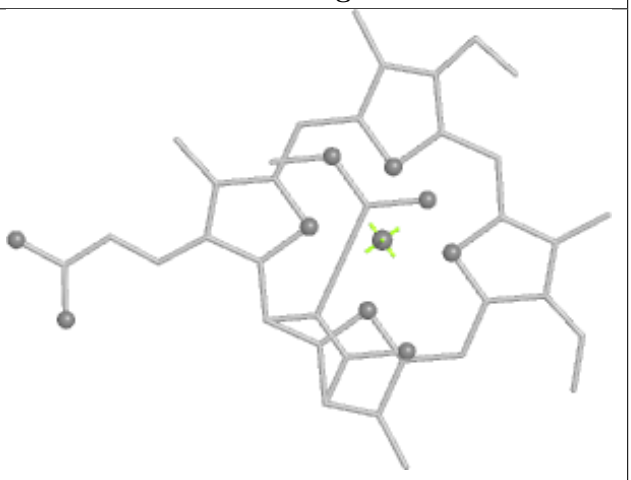
Bond lengths



Bond angles

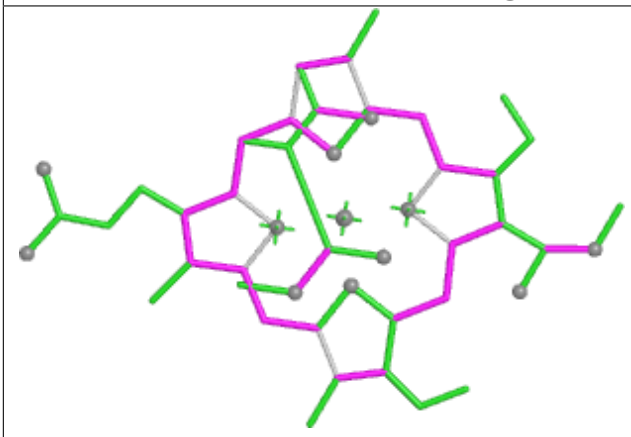


Torsions

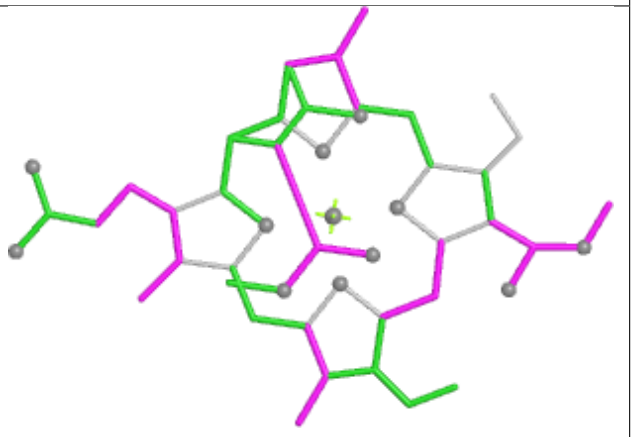


Rings

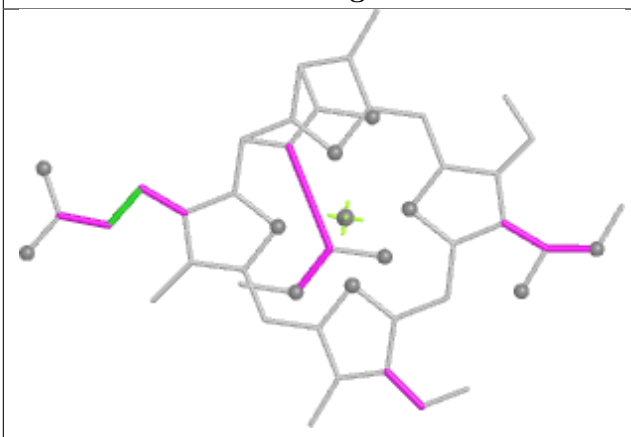
Ligand A1ECV P 315



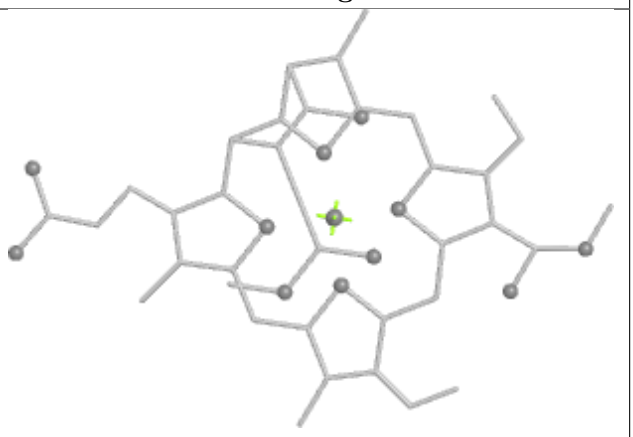
Bond lengths



Bond angles

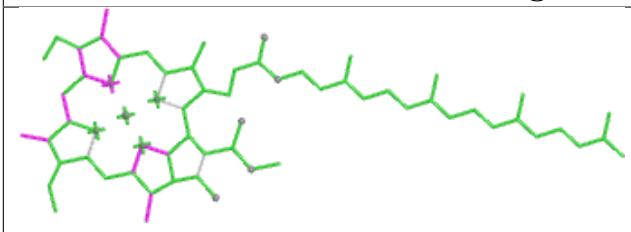


Torsions



Rings

Ligand CLA a 824



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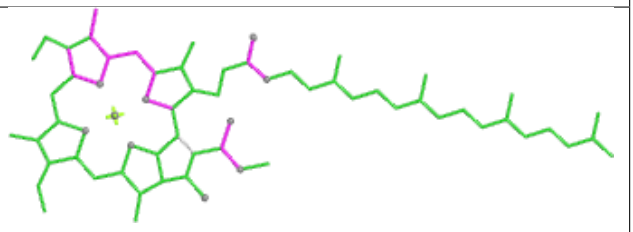
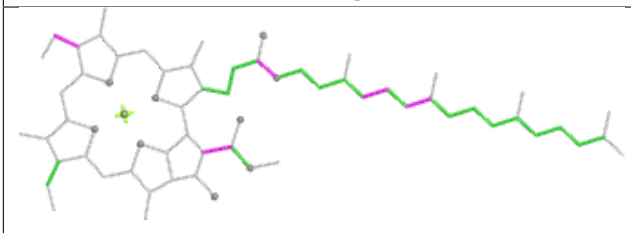
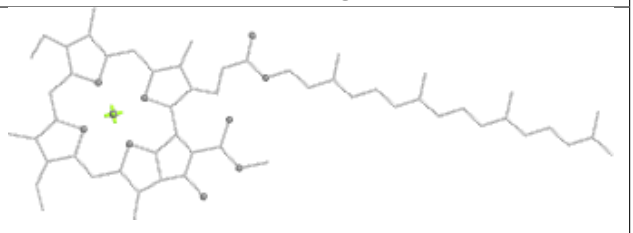


Bond angles

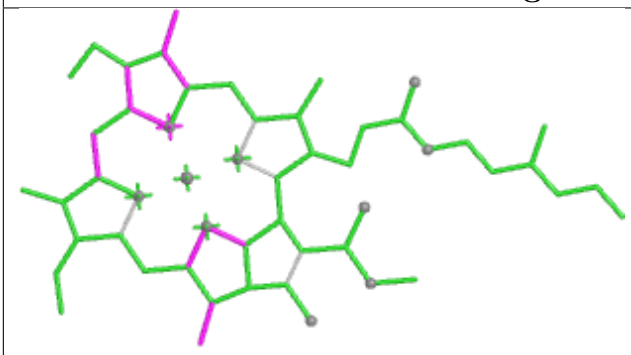


Torsions

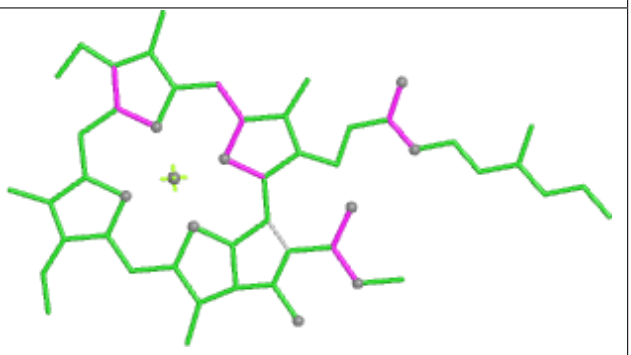


Rings

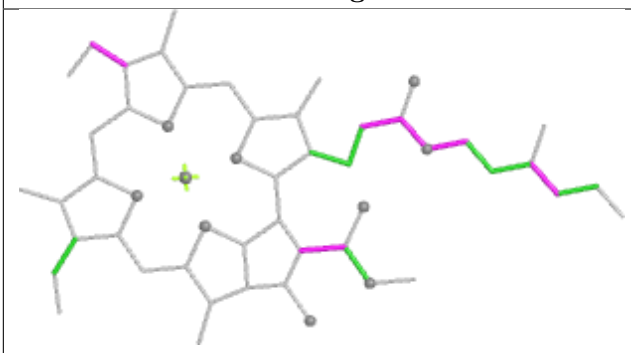
Ligand CLA R 316



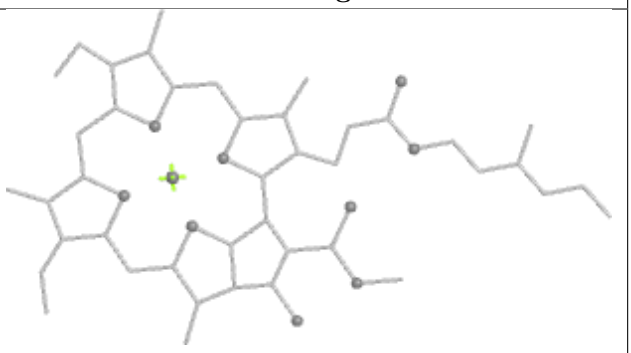
Bond lengths



Bond angles

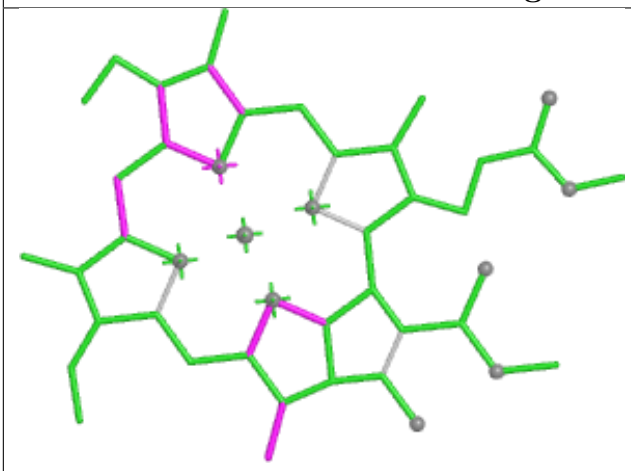


Torsions

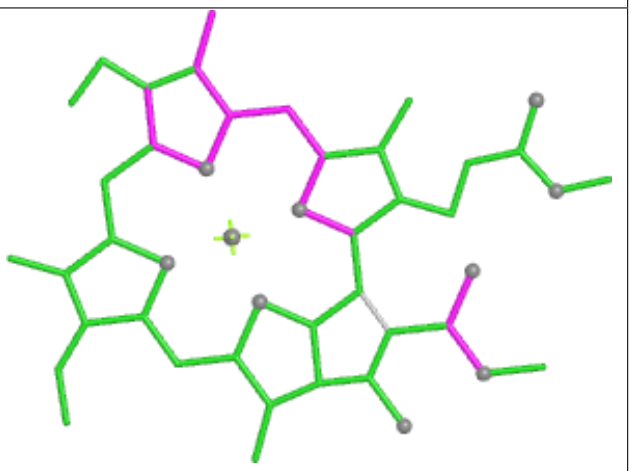


Rings

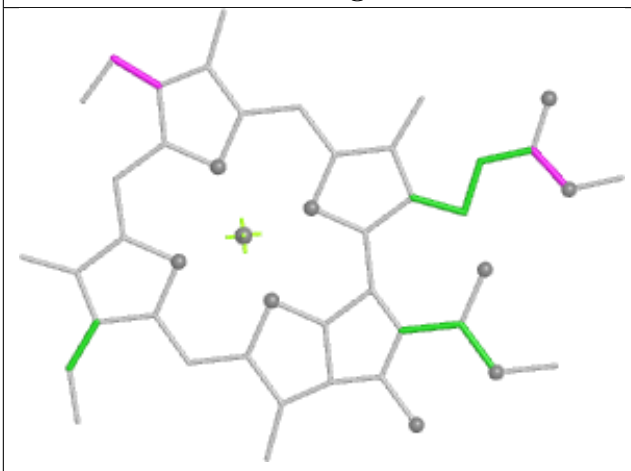
Ligand CLA B 204



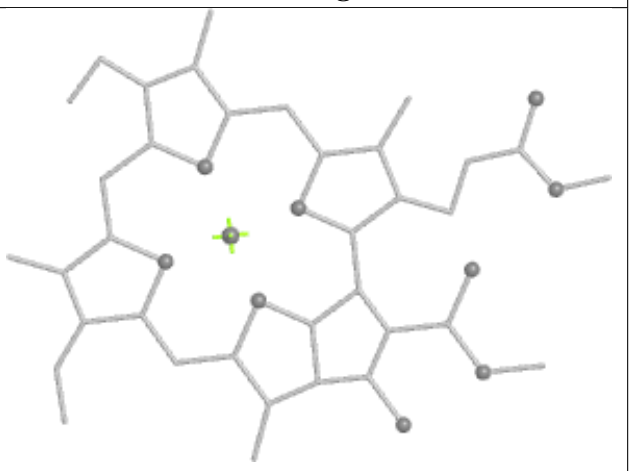
Bond lengths



Bond angles

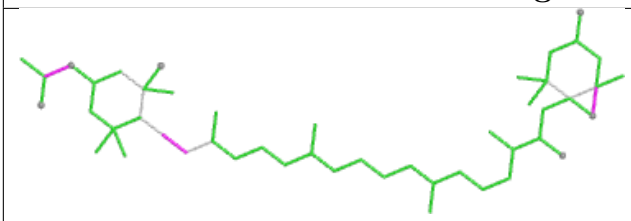


Torsions

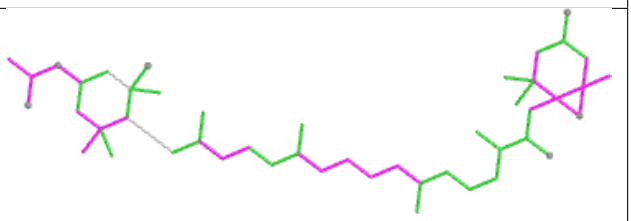


Rings

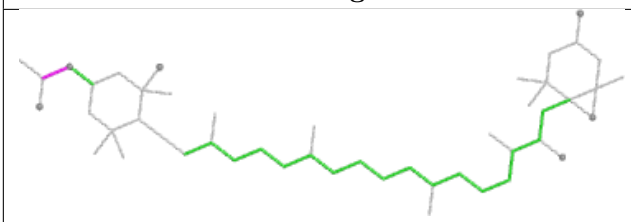
Ligand A86 6 303



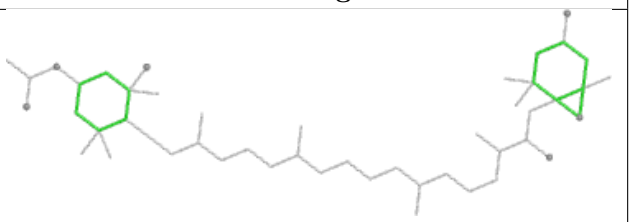
Bond lengths



Bond angles

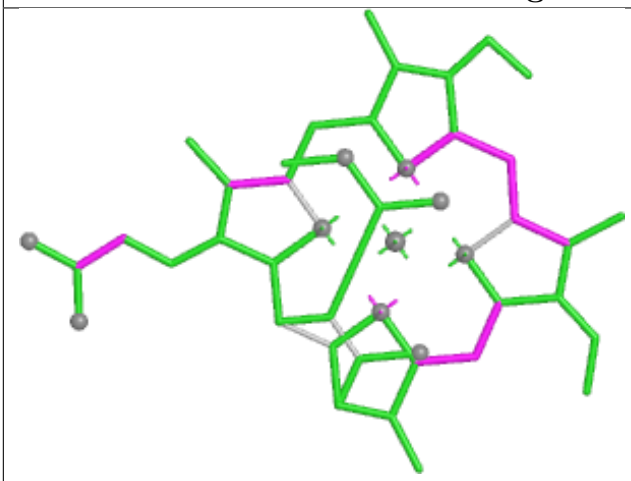


Torsions

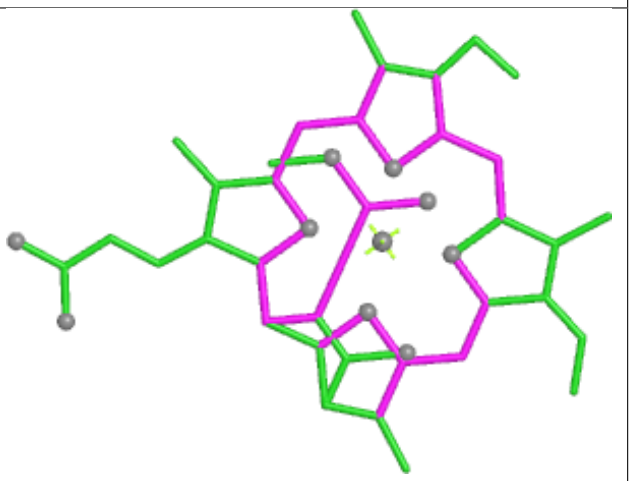


Rings

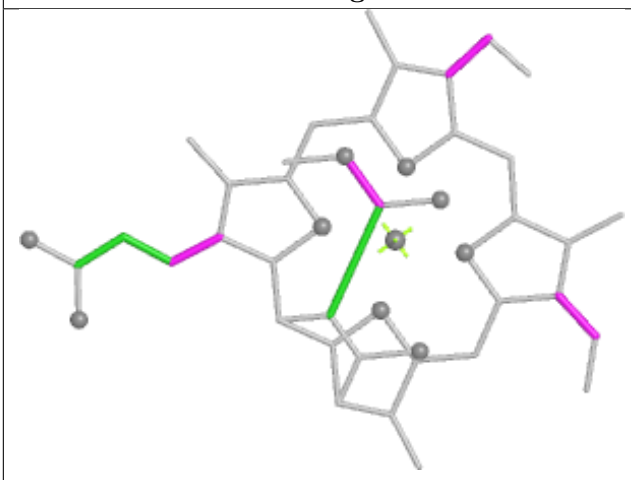
Ligand KC2 P 312



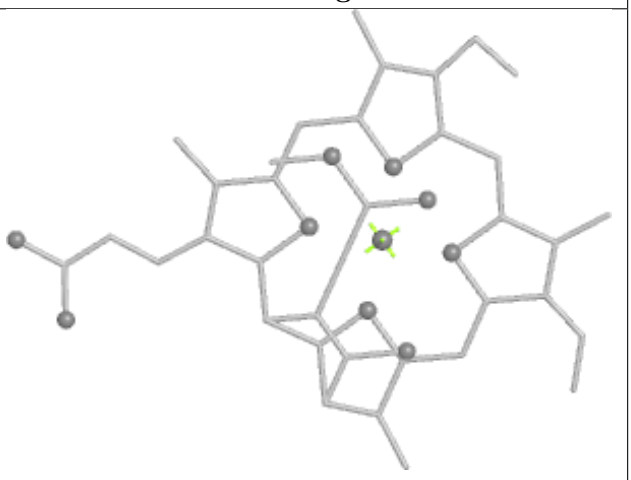
Bond lengths



Bond angles

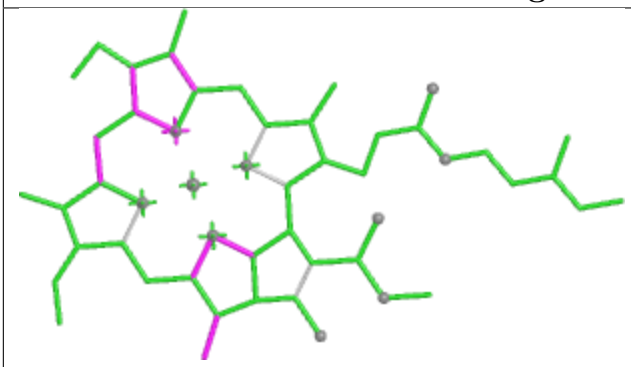


Torsions



Rings

Ligand CLA a 834



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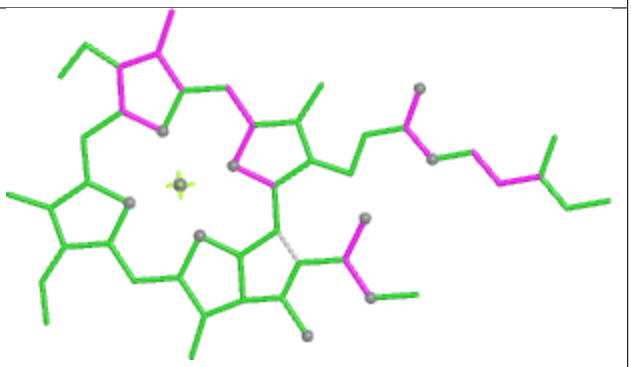
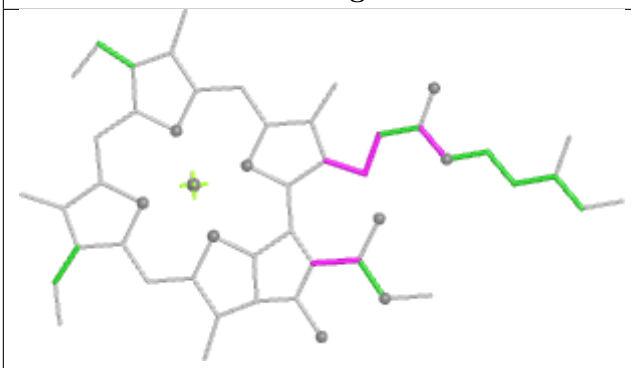
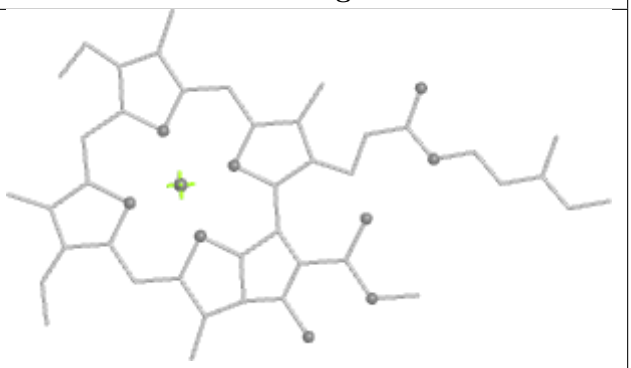


Bond angles

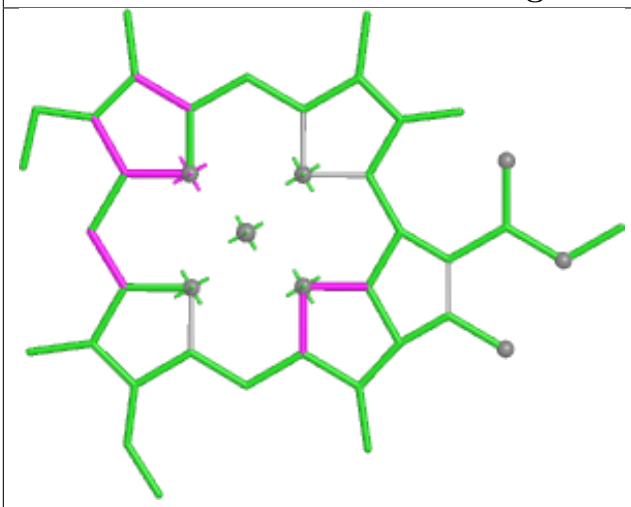


Torsions



Rings

Ligand CLA Z 315



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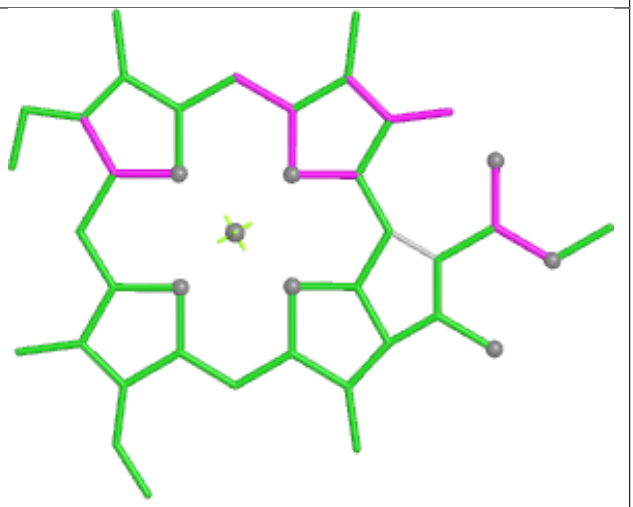
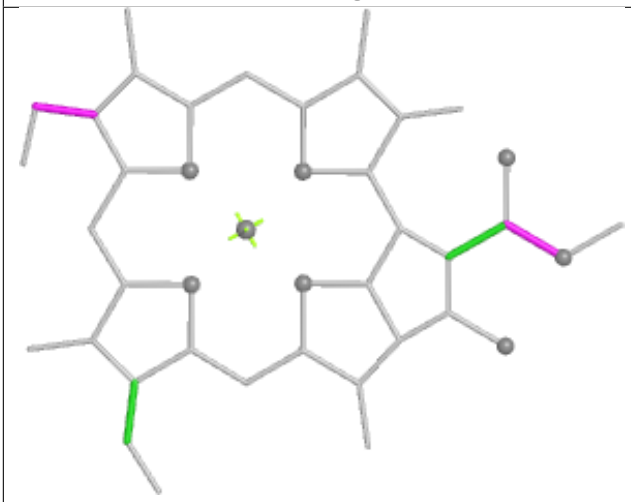
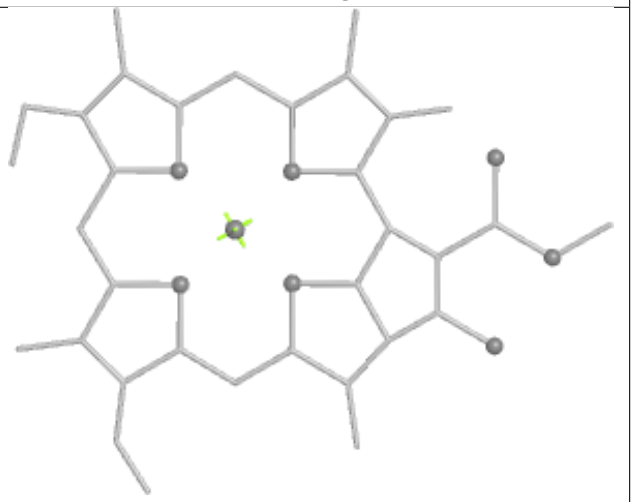


Bond angles

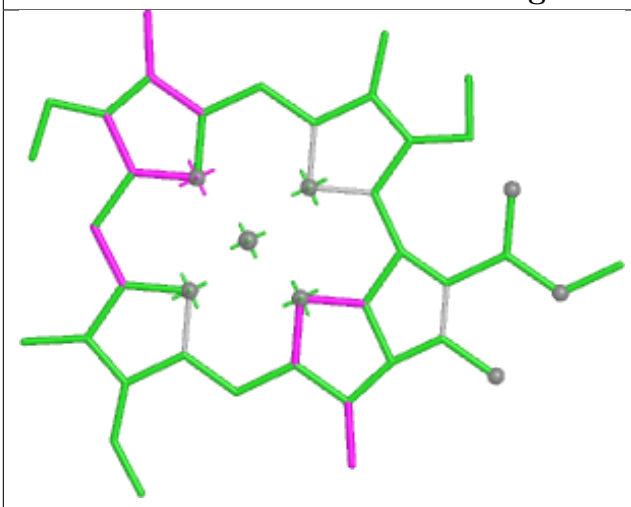


Torsions

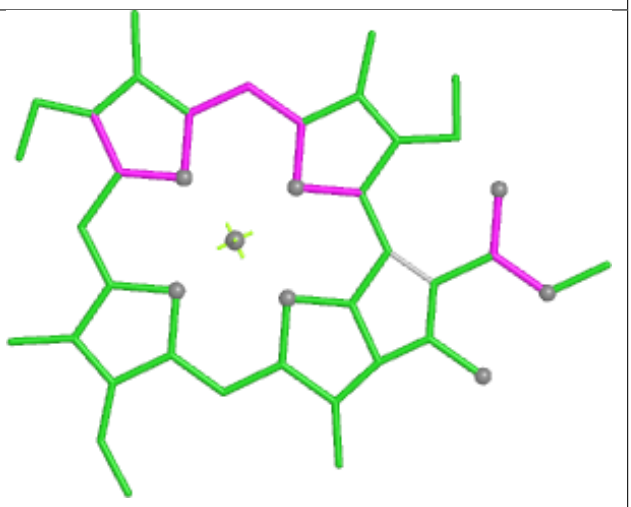


Rings

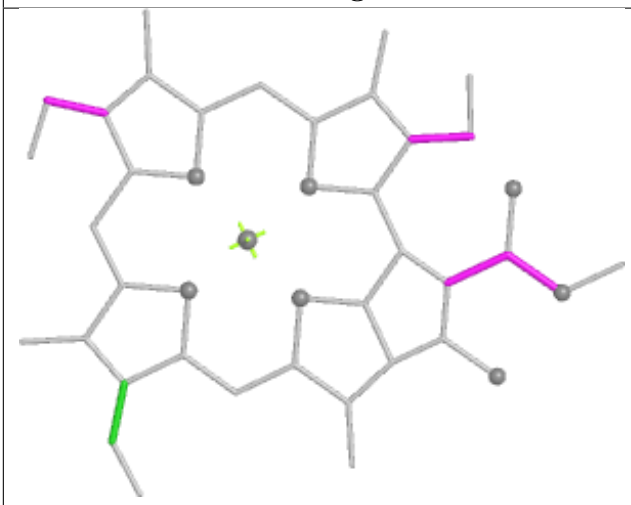
Ligand CLA 1 309



Bond lengths



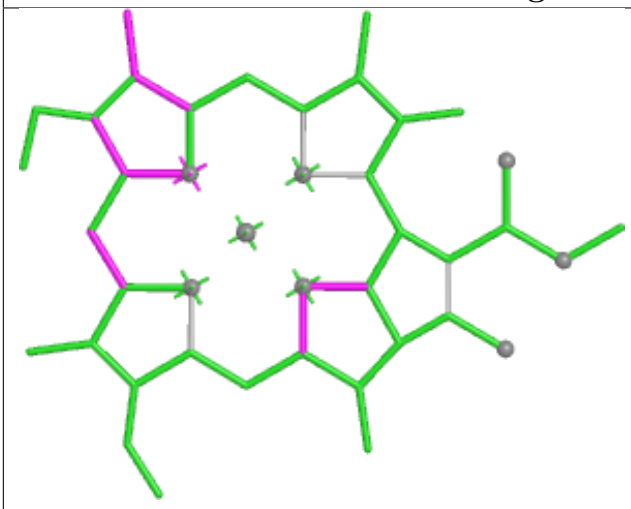
Bond angles



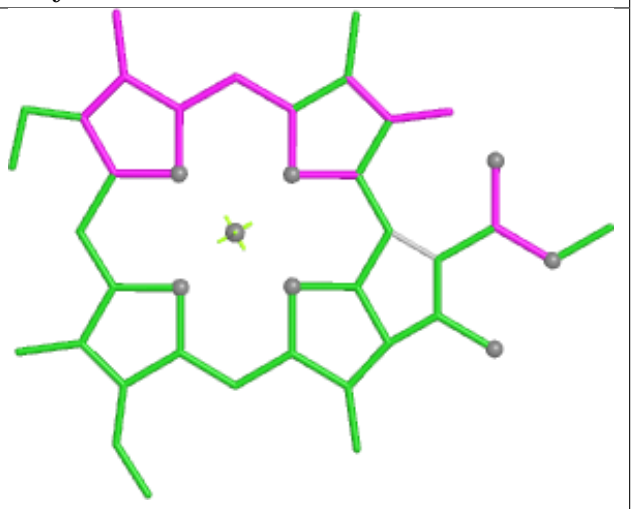
Torsions

Rings

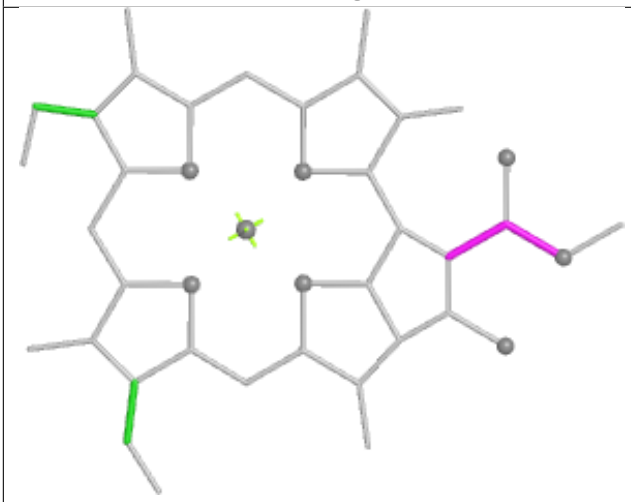
Ligand CLA y 319



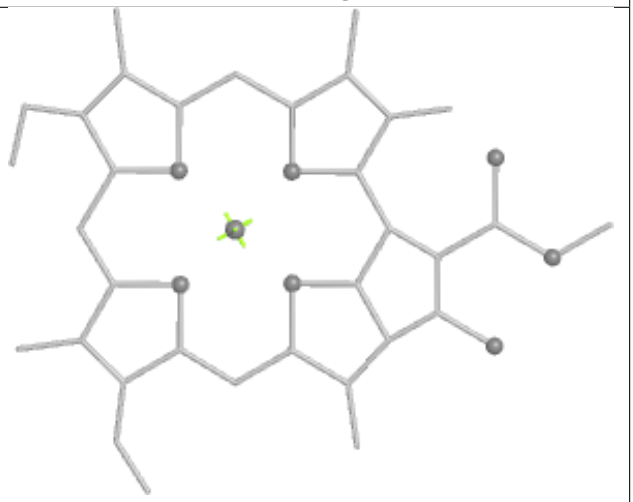
Bond lengths



Bond angles

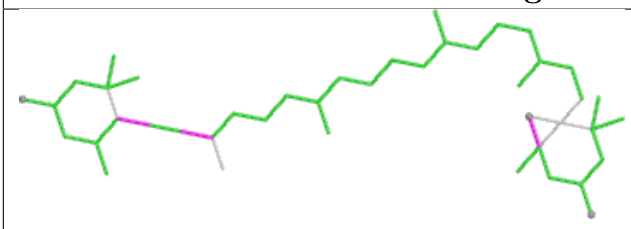


Torsions

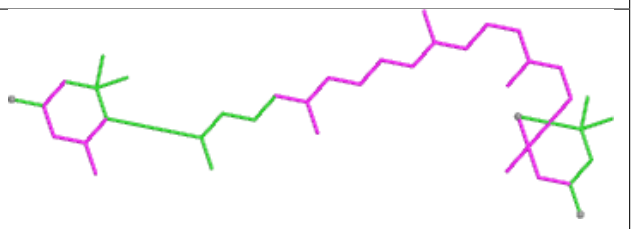


Rings

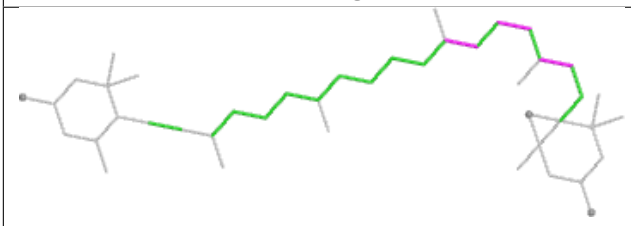
Ligand DD6 A 303



Bond lengths



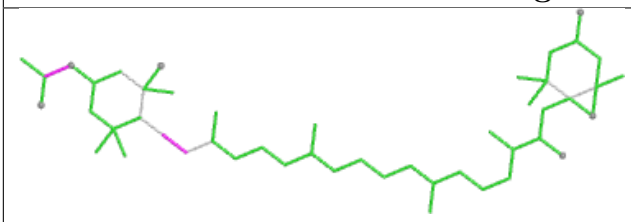
Bond angles



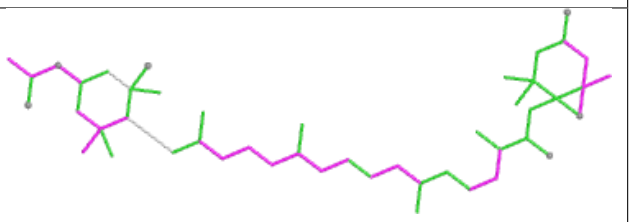
Torsions

Rings

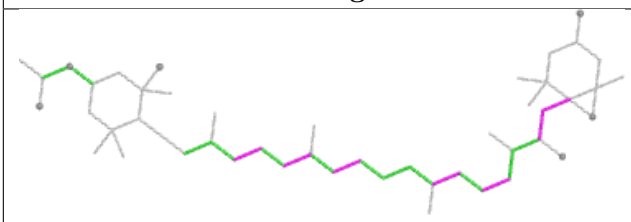
Ligand A86 1 306



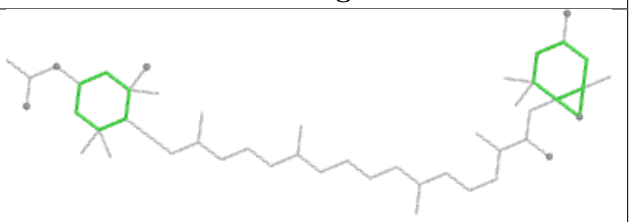
Bond lengths



Bond angles

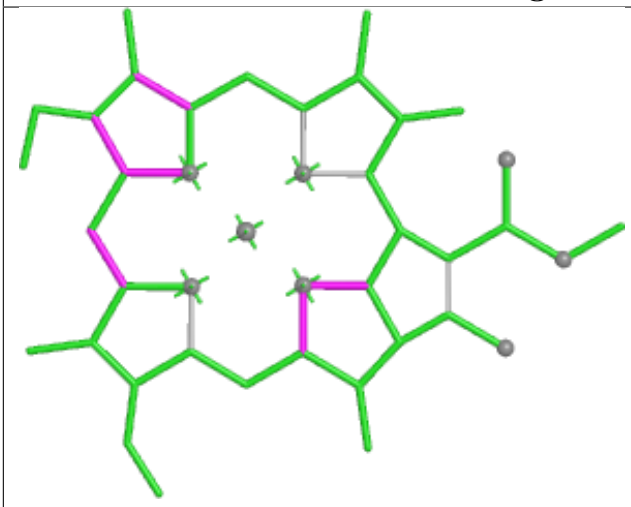


Torsions



Rings

Ligand CLA 0 318



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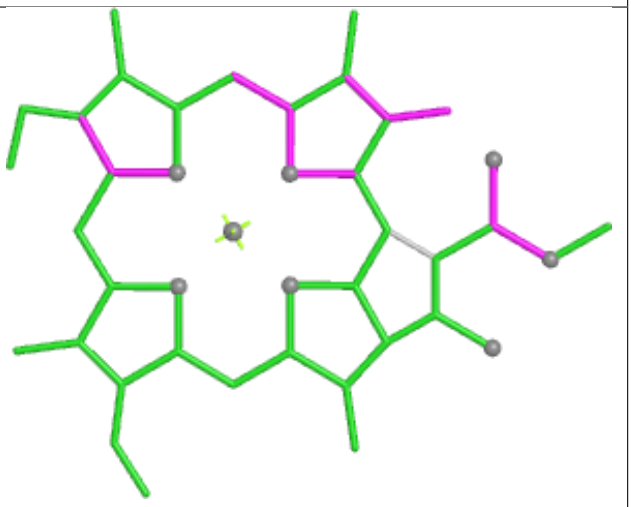

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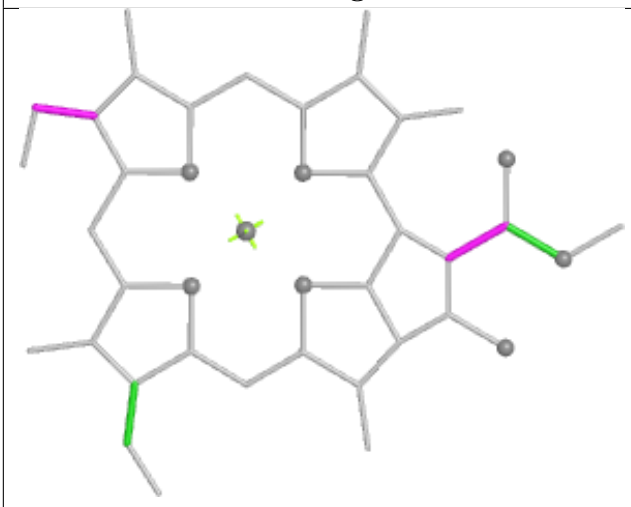

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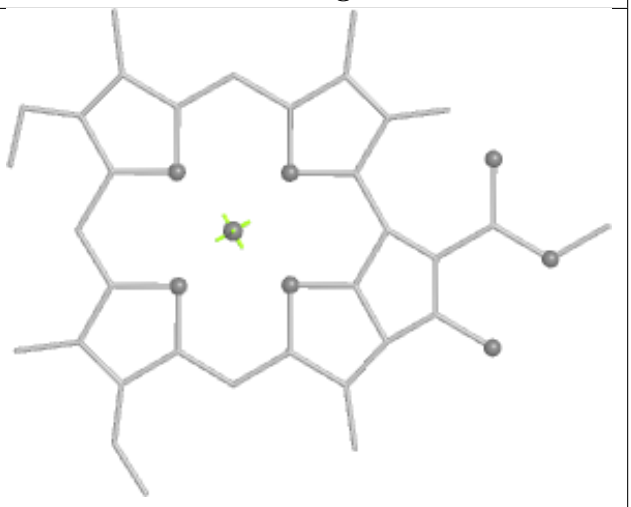
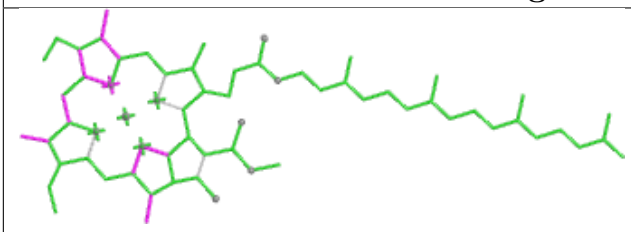


Rings

Ligand CLA a 803



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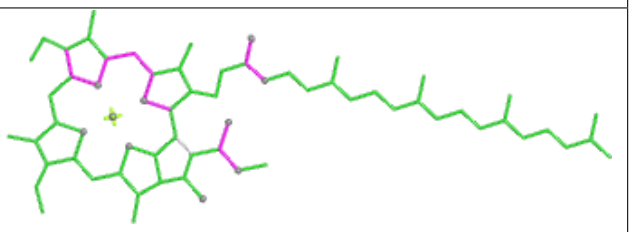

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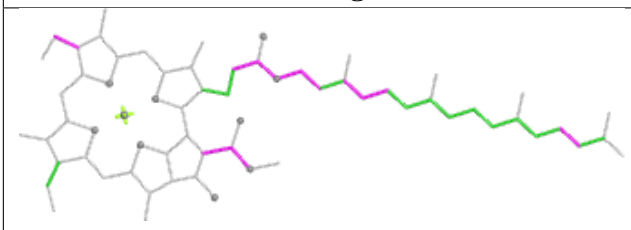

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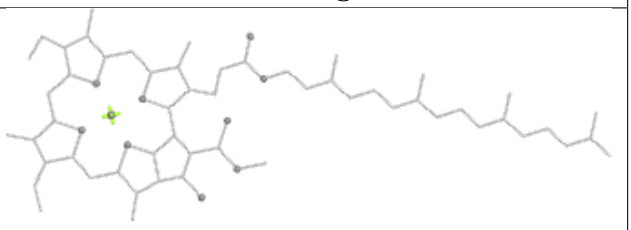
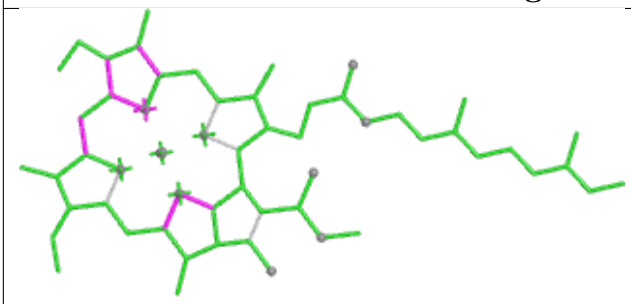


Rings

Ligand CLA T 311



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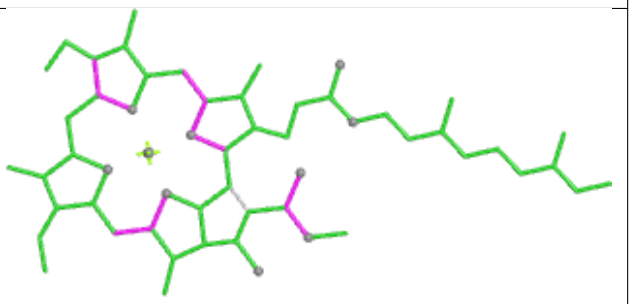
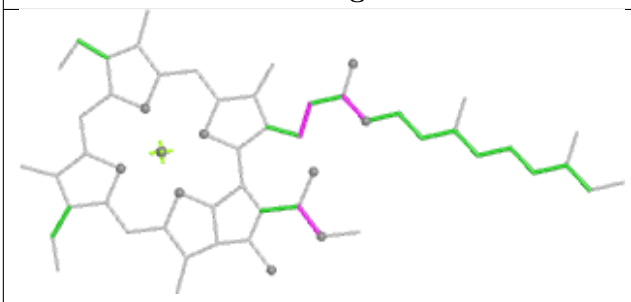


Bond angles



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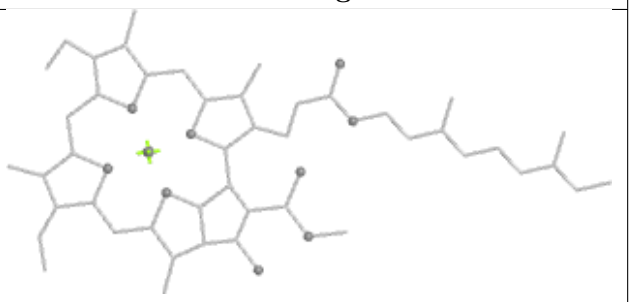
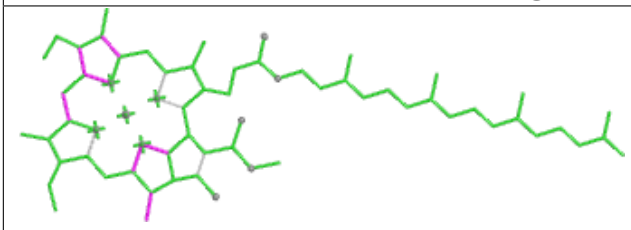


Rings

Ligand CLA J 311



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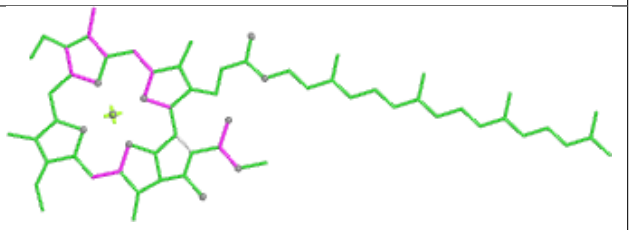
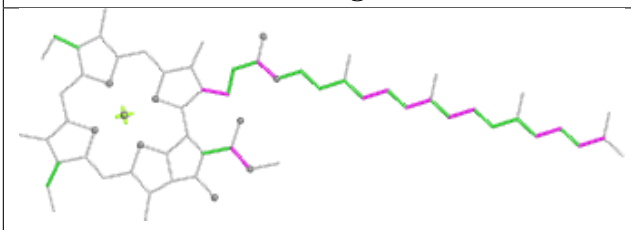


Bond angles



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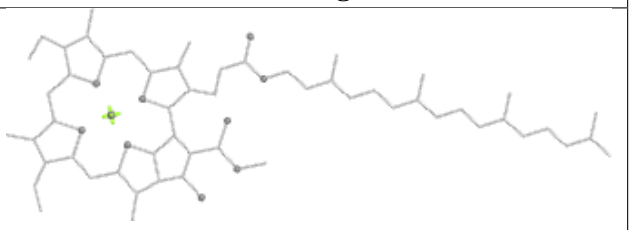
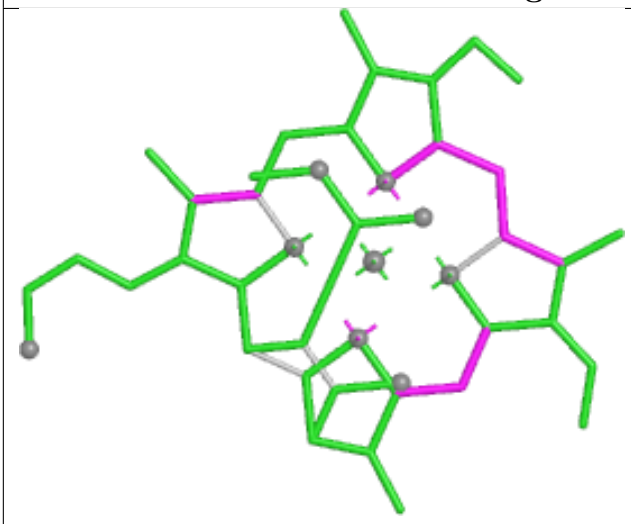


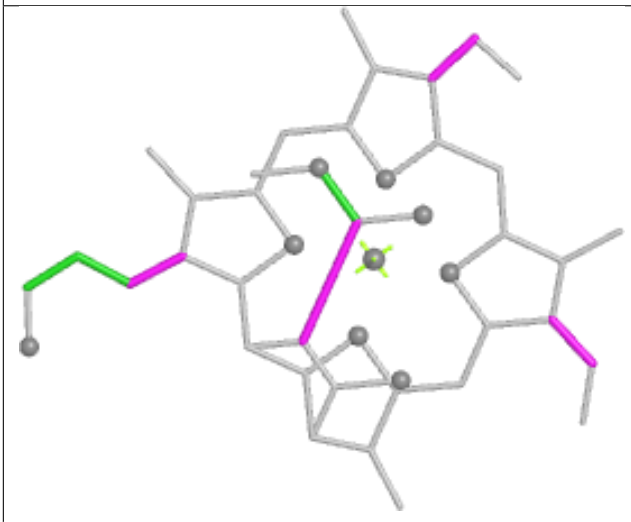
Rings

Ligand KC2 X 314



Bond lengths

Bond angles



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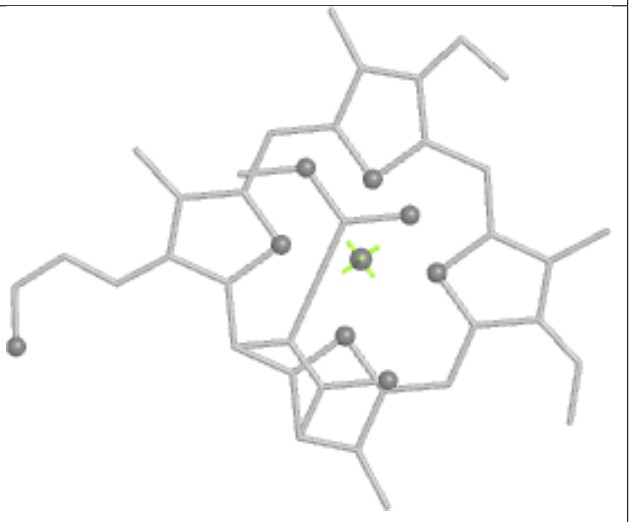
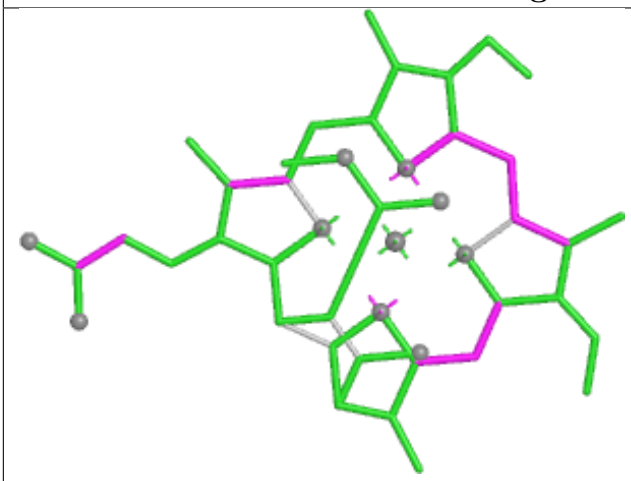


Rings

Ligand KC2 1 314



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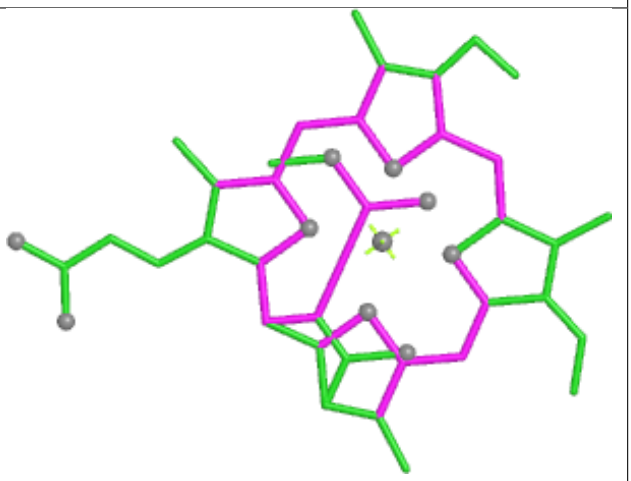
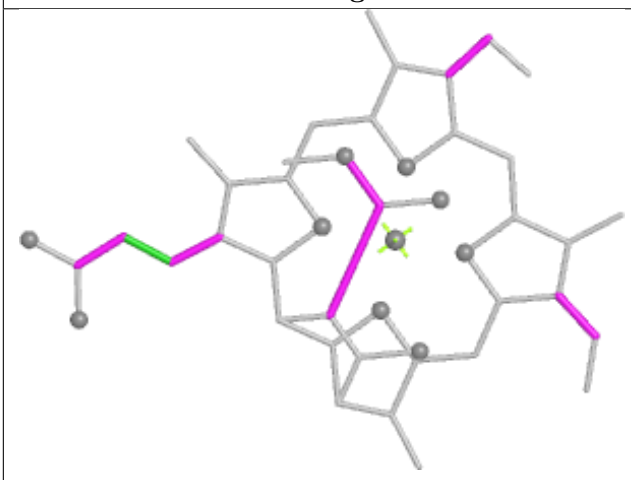


Bond angles



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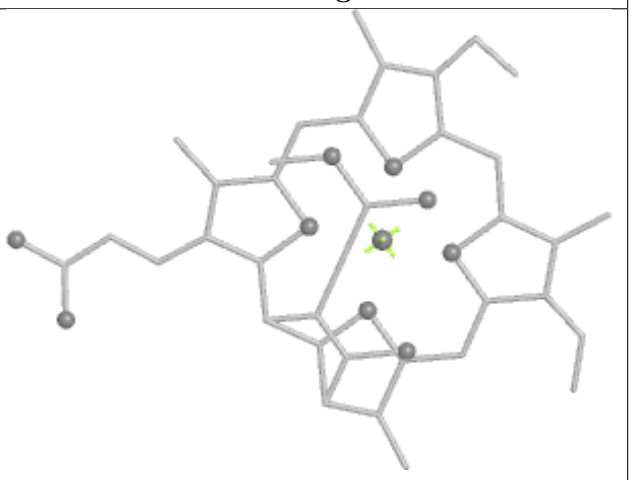
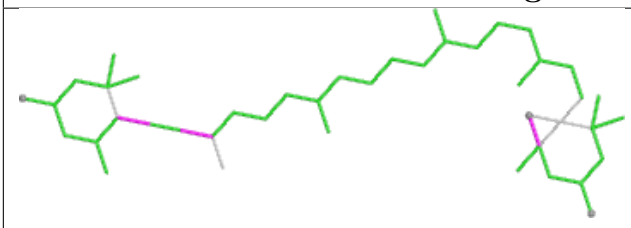


Rings

Ligand DD6 V 303



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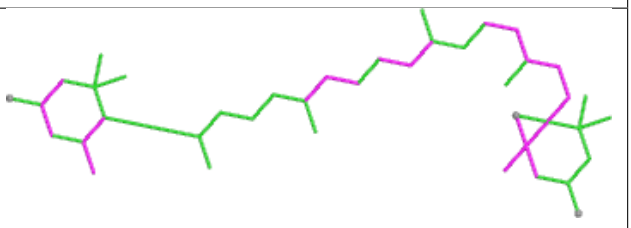

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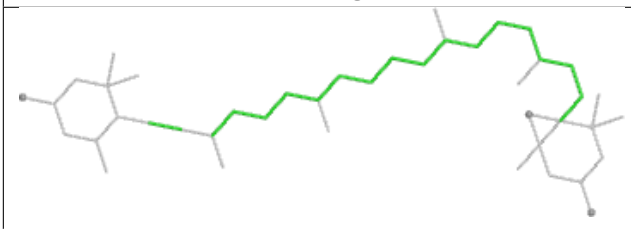
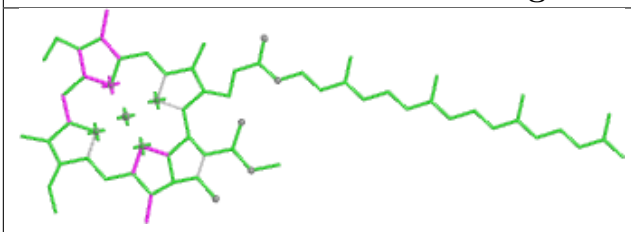


Torsions

Rings

Ligand CLA a 847



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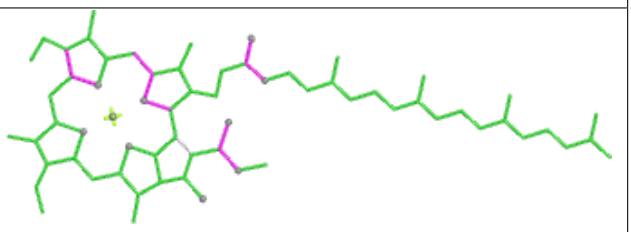
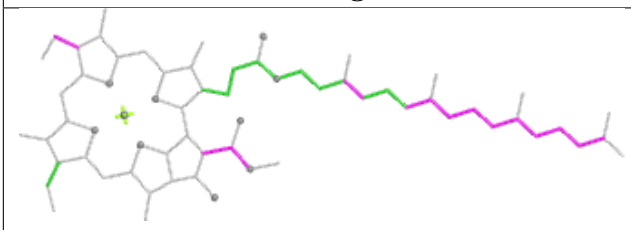


Bond angles



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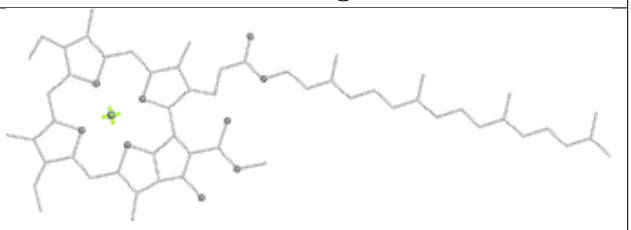
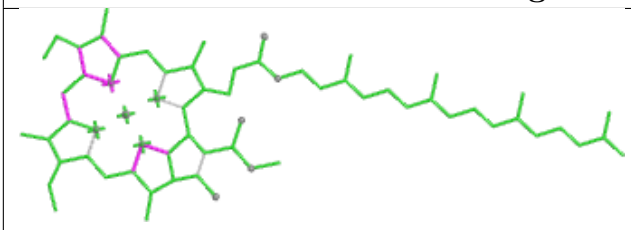


Rings

Ligand CLA 3 314



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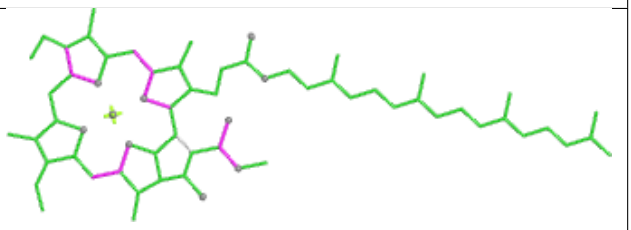
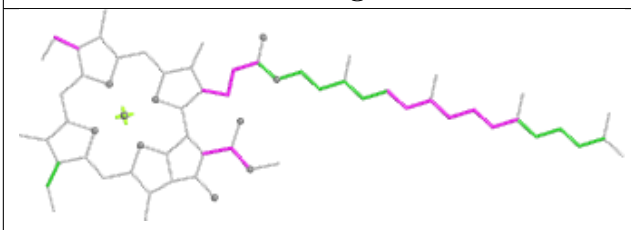


Bond angles



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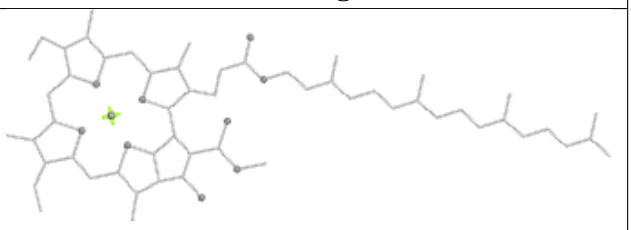
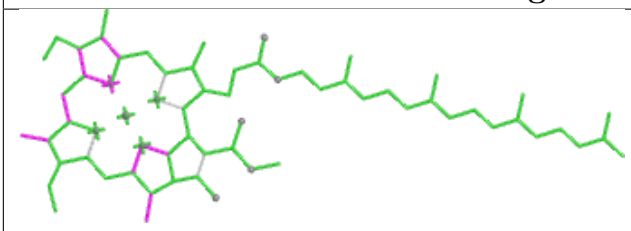


Rings

Ligand CLA 4 316



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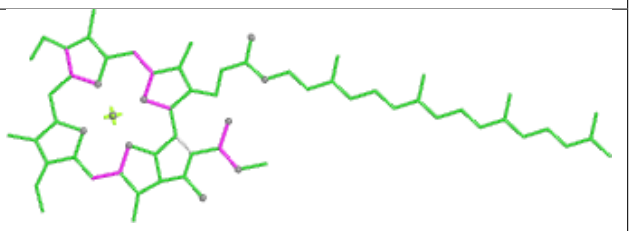
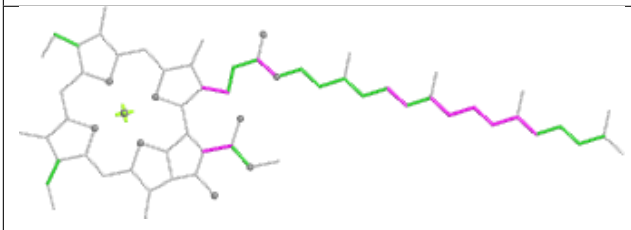


Bond angles



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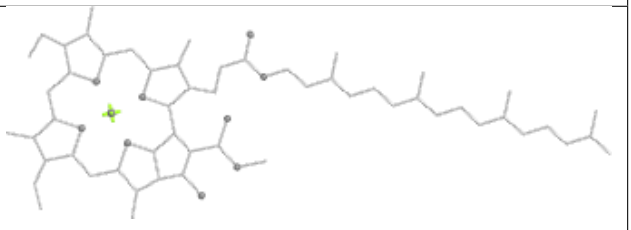
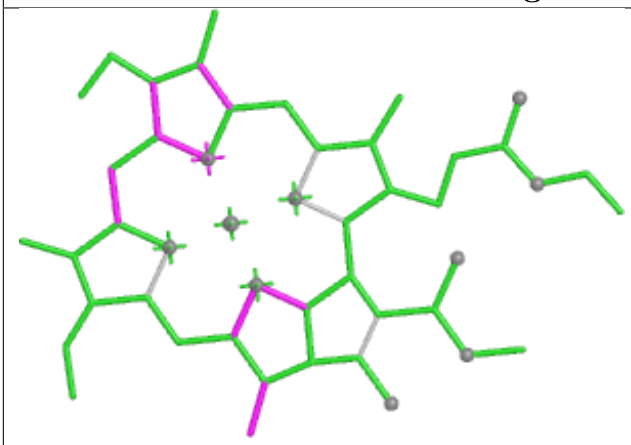


Rings

Ligand CLA X 316



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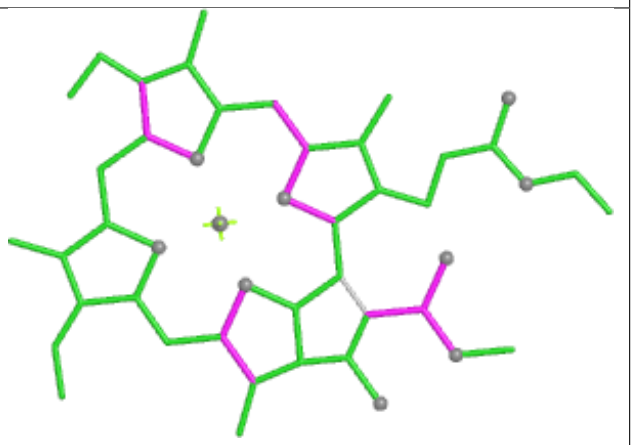
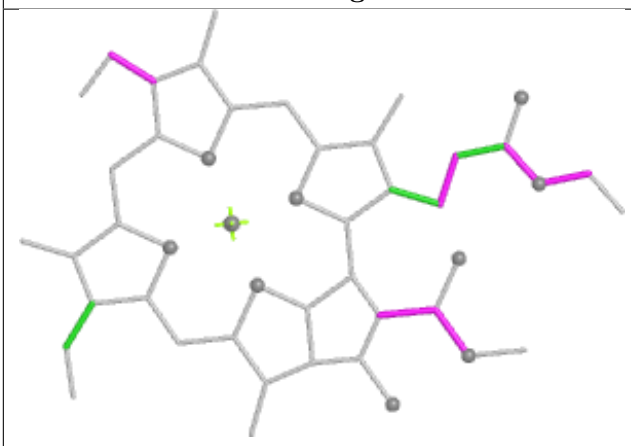


Bond angles



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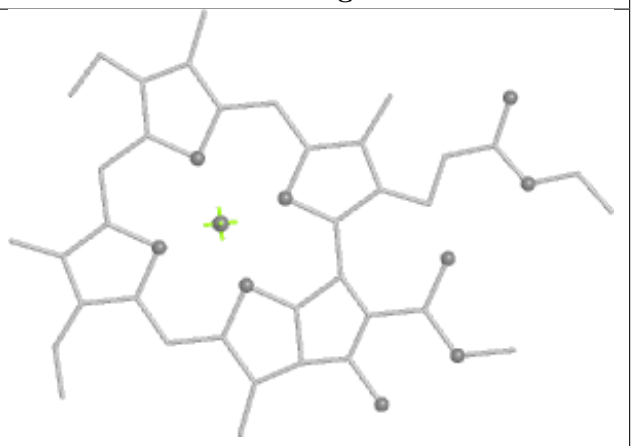
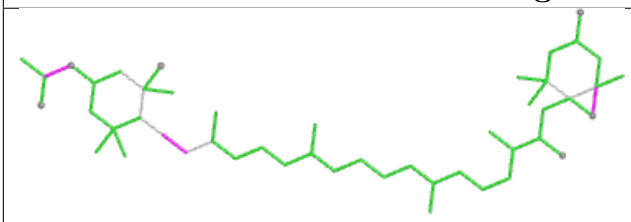


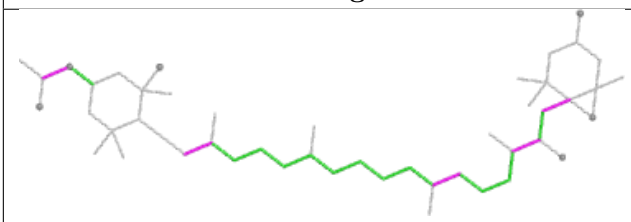
Rings

Ligand A86 8 305

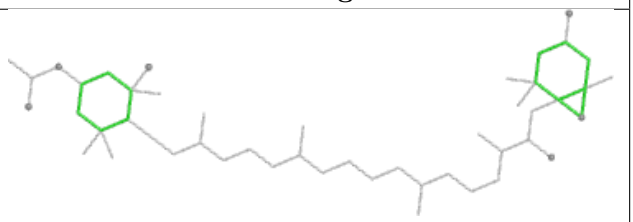


Bond lengths

Bond angles

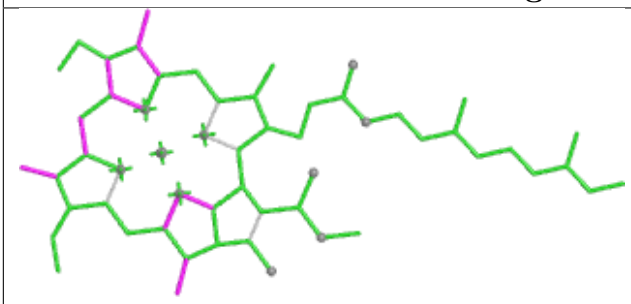


Torsions



Rings

Ligand CLA E 314



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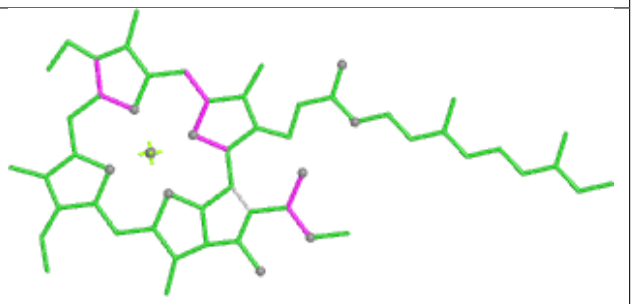
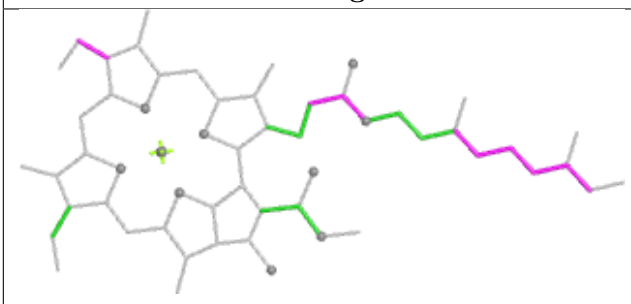
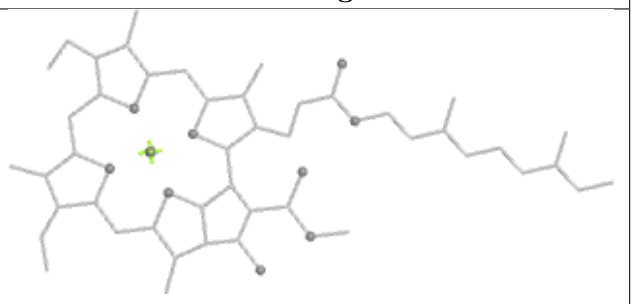


Bond angles

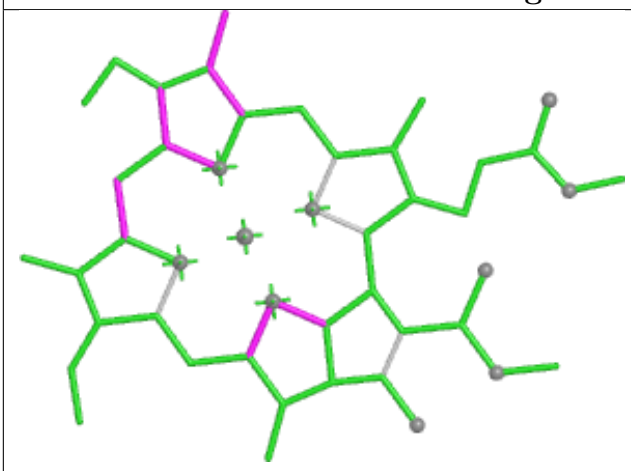


Torsions

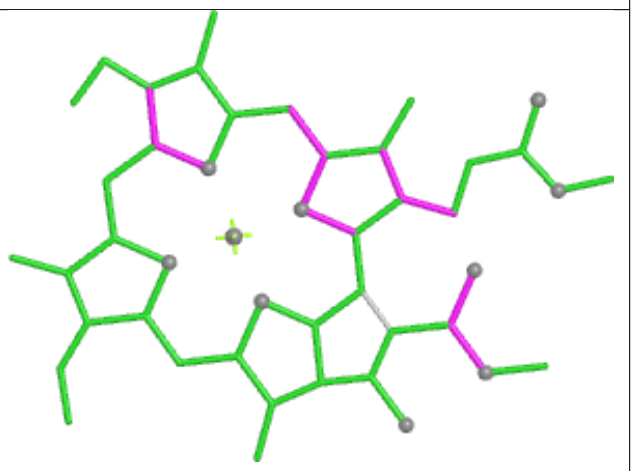


Rings

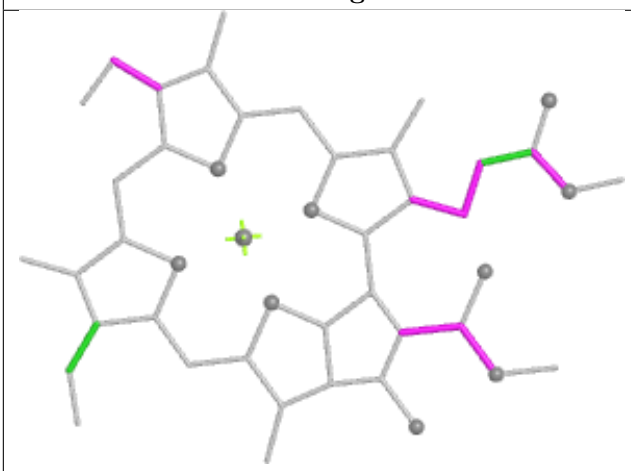
Ligand CLA T 319



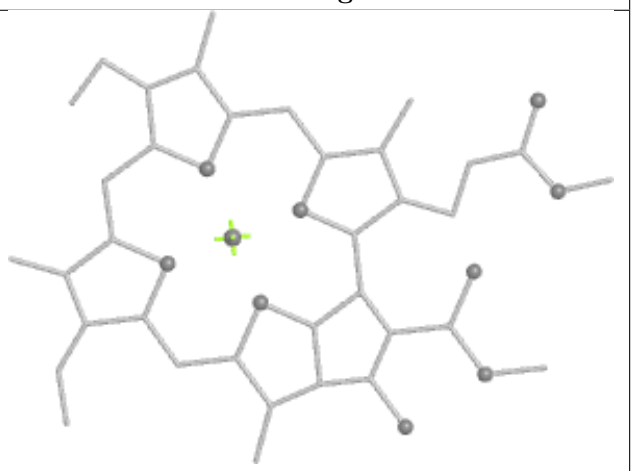
Bond lengths



Bond angles

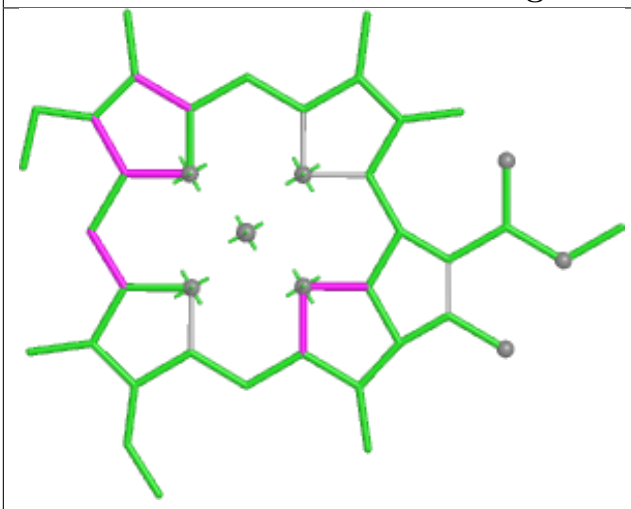


Torsions

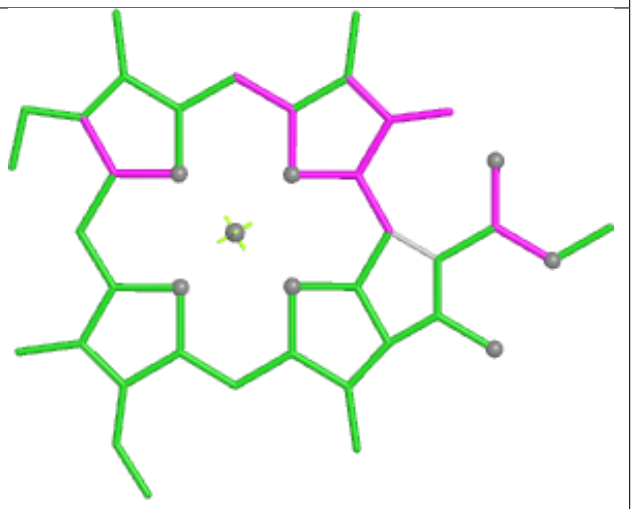


Rings

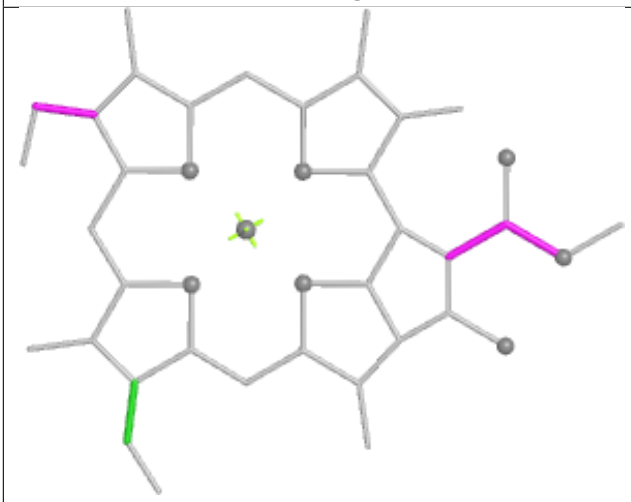
Ligand CLA Z 316



Bond lengths



Bond angles



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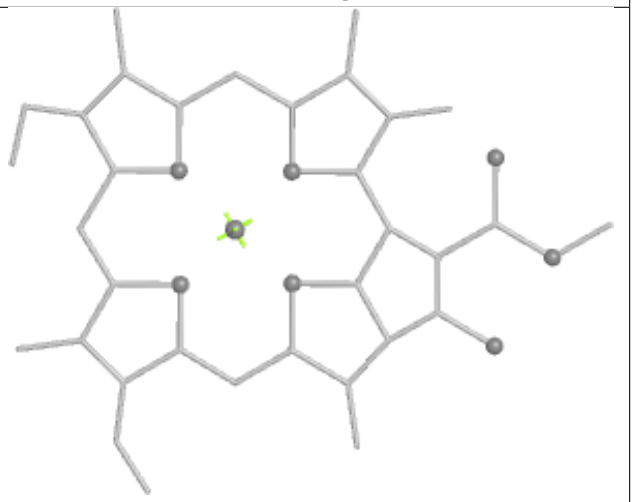
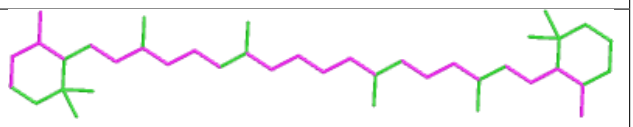


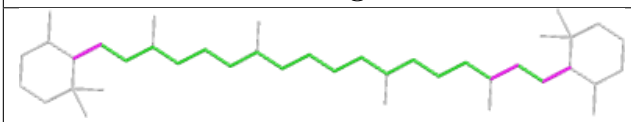
Rings

Ligand BCR l 206

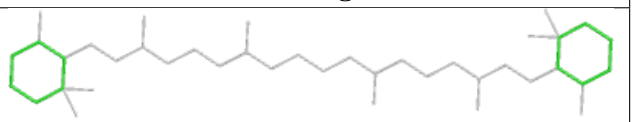
Bond lengths



Bond angles

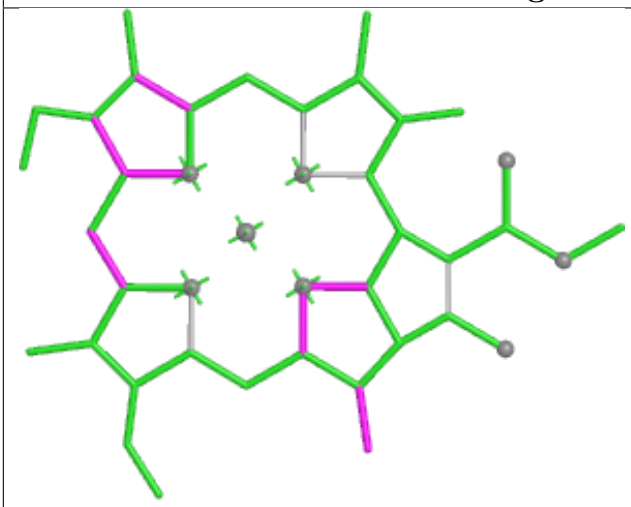


Torsions



Rings

Ligand CLA x 307



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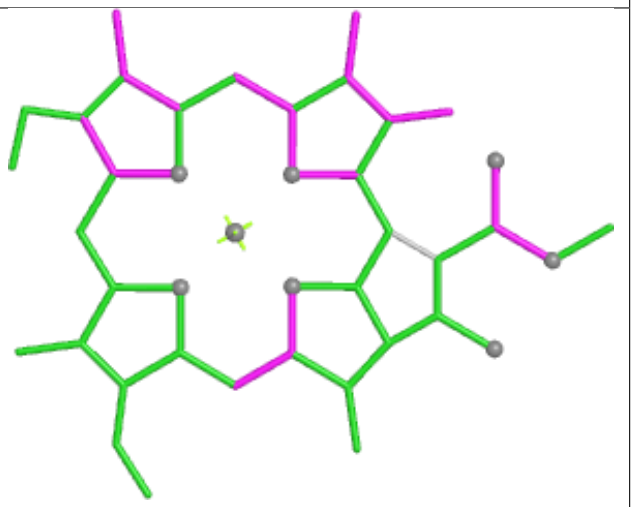
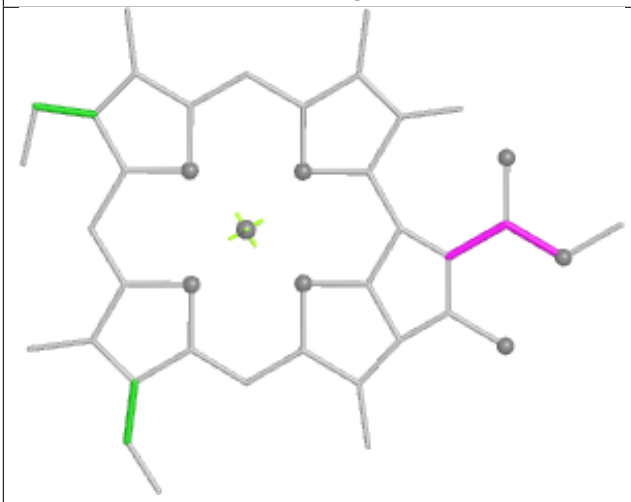
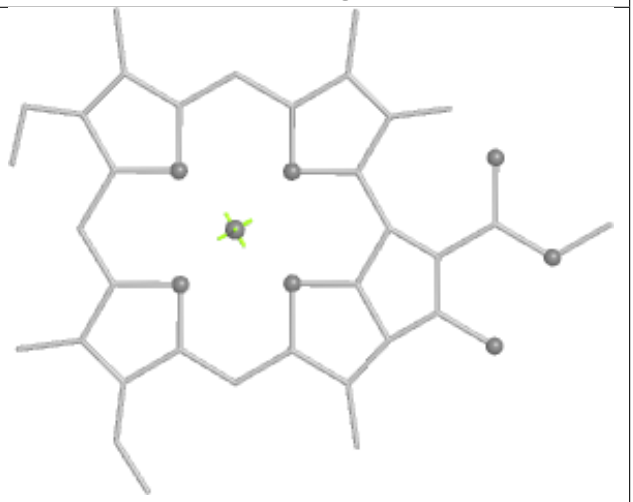


Bond angles

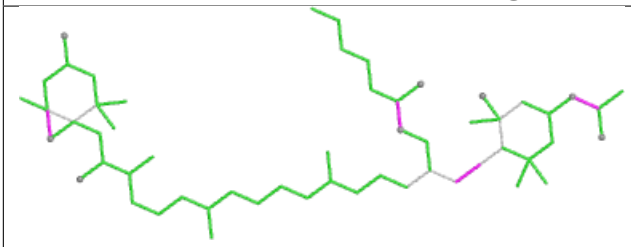


Torsions



Rings

Ligand A1EB1 V 302



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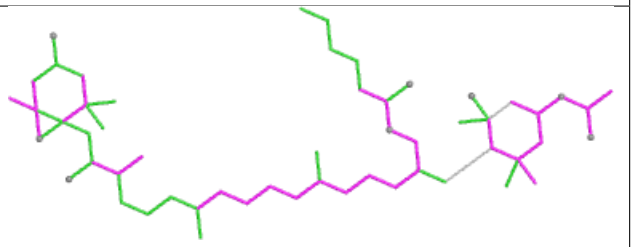
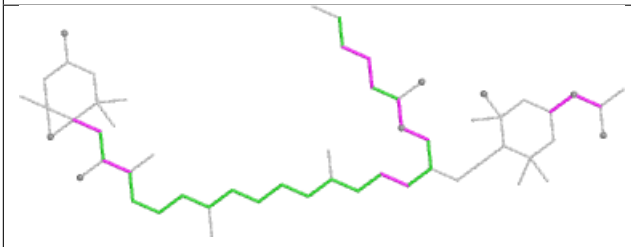


Bond angles



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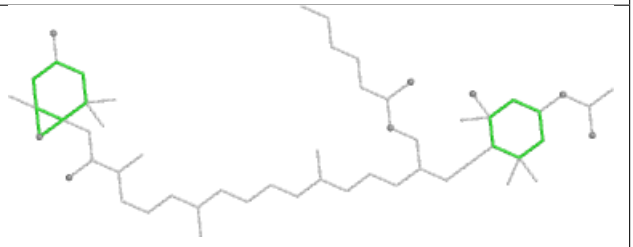
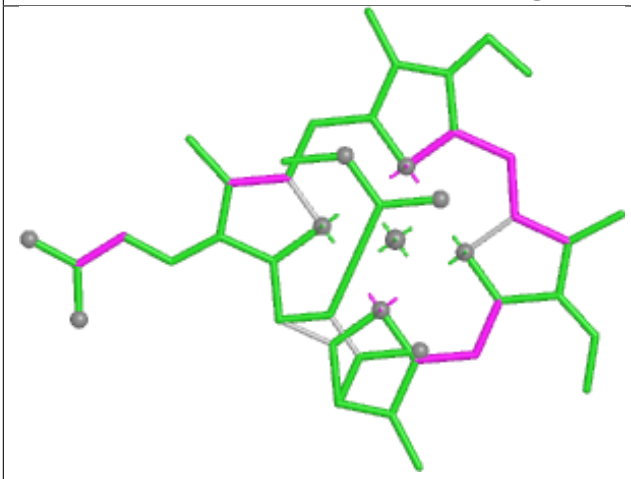


Rings

Ligand KC2 L 315



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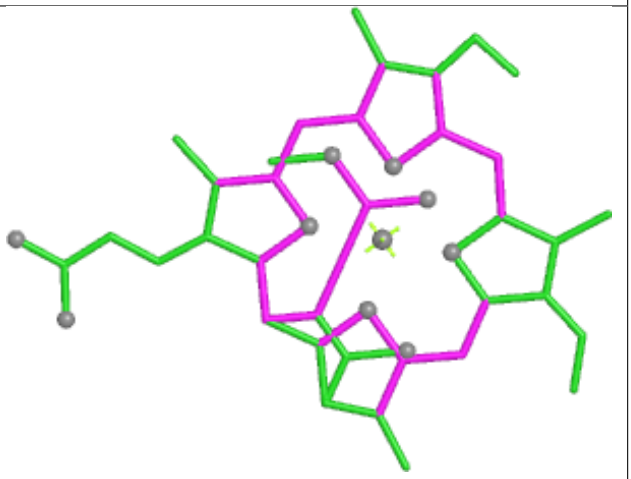
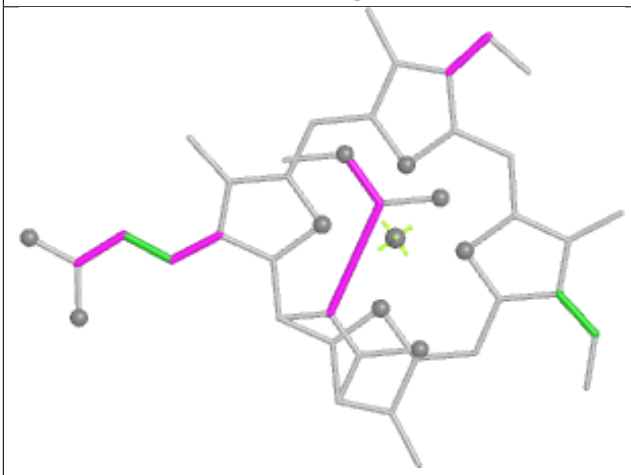


Bond angles



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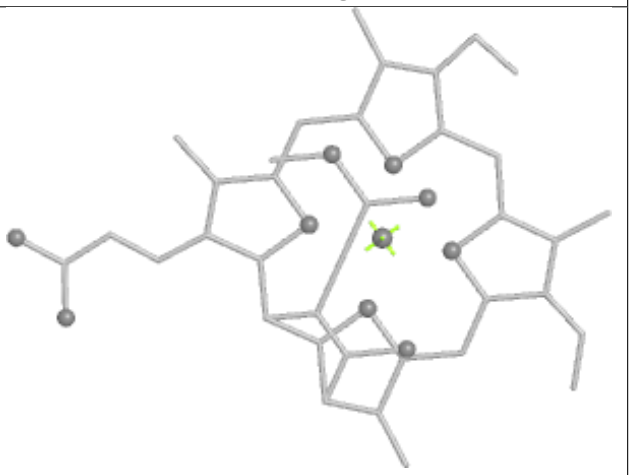
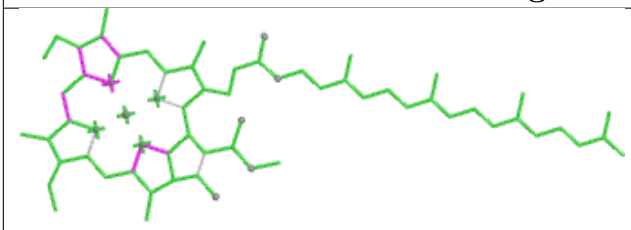


Rings

Ligand CLA 5 308



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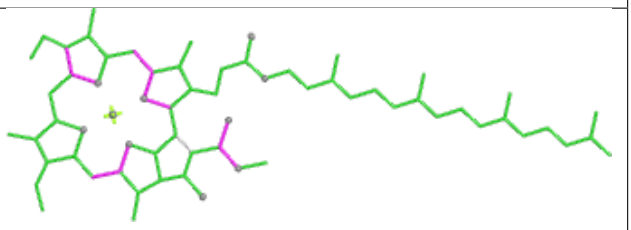
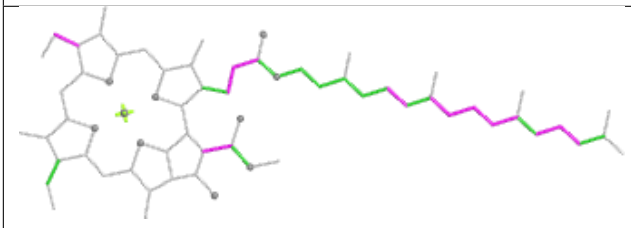


Bond angles



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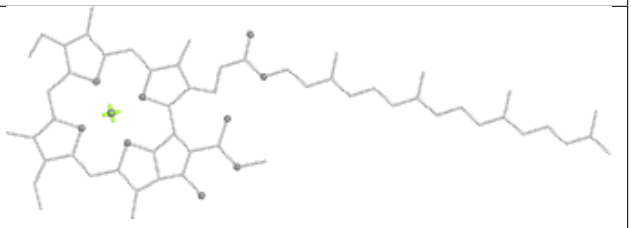
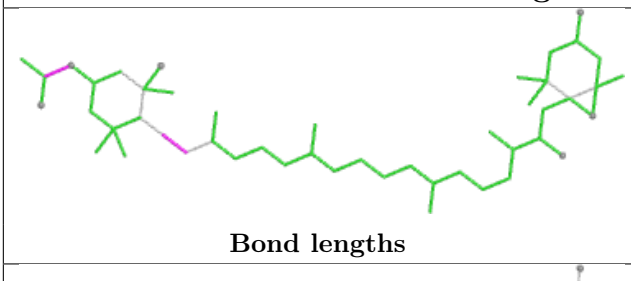


Rings

Ligand A86 S 304



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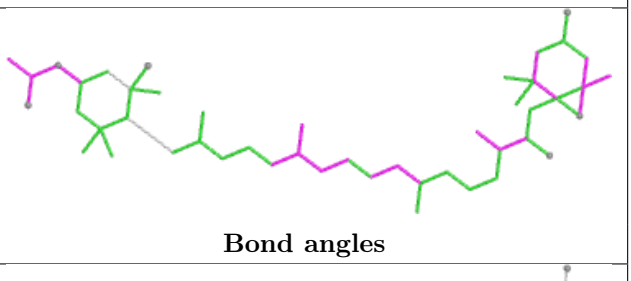
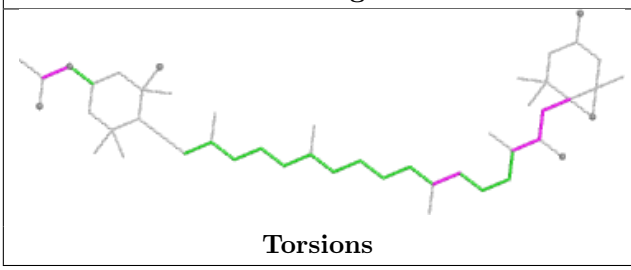


Bond angles



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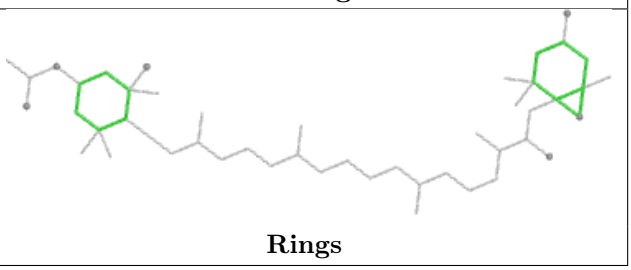
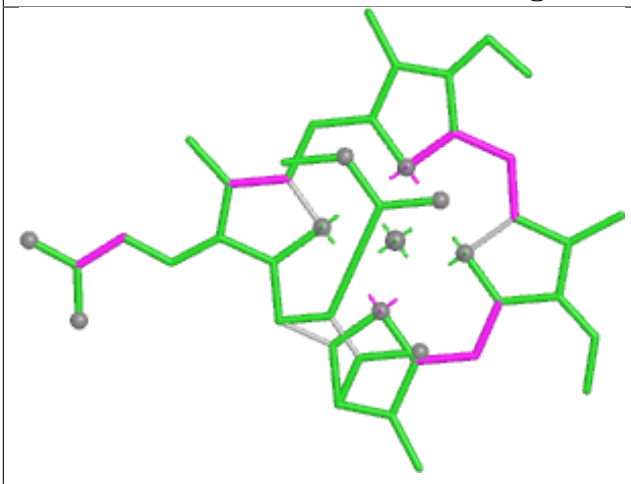
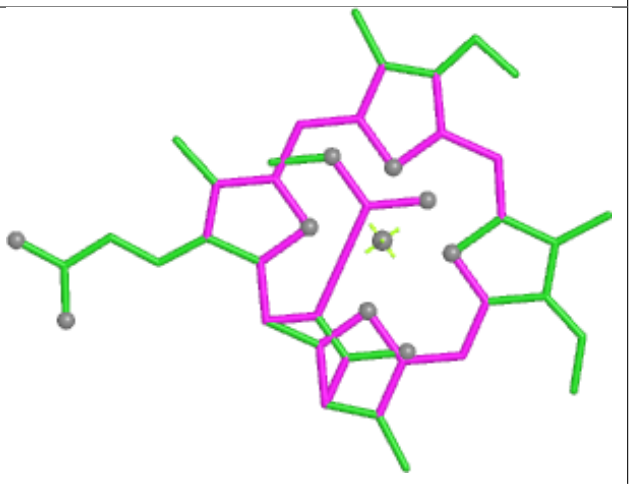


Rings

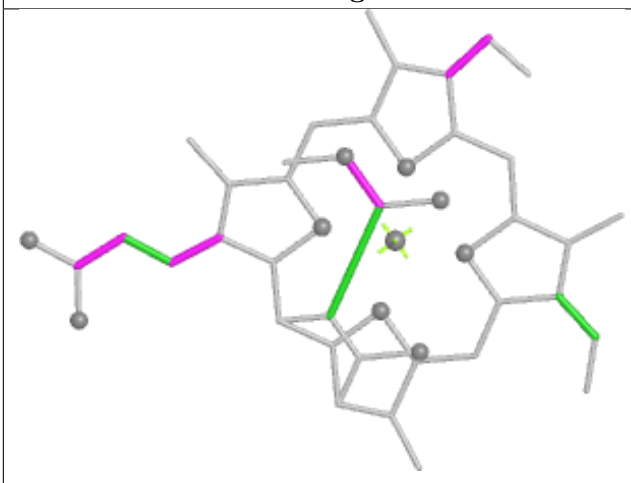
Ligand KC2 L 314



Bond lengths



Bond angles



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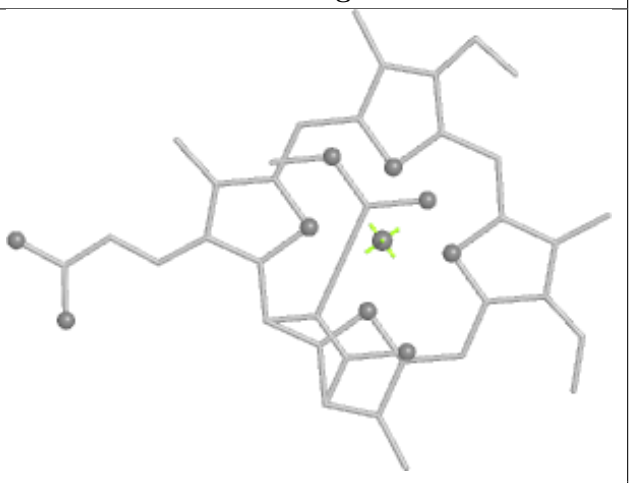
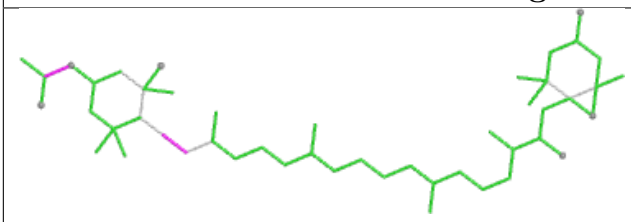


Rings

Ligand A86 G 301



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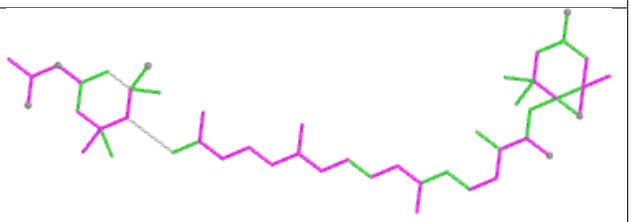
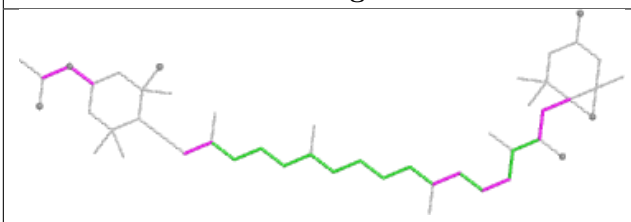


Bond angles



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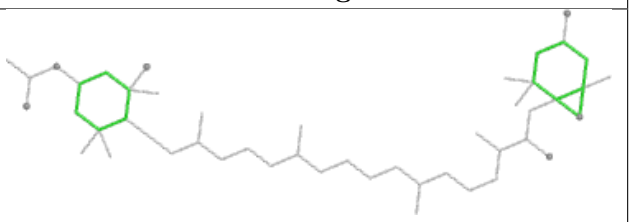
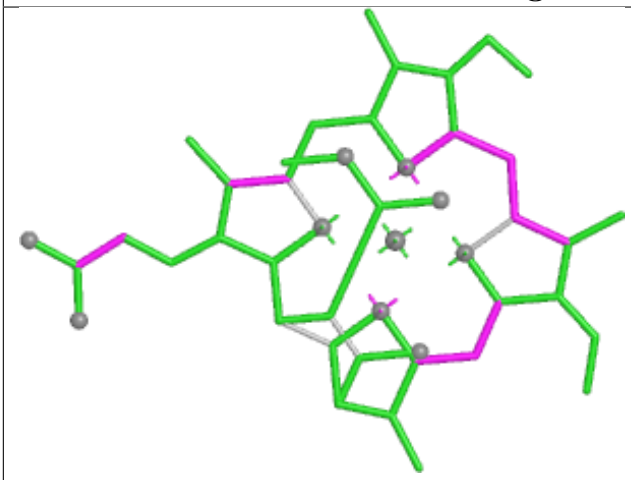


Rings

Ligand KC2 P 320



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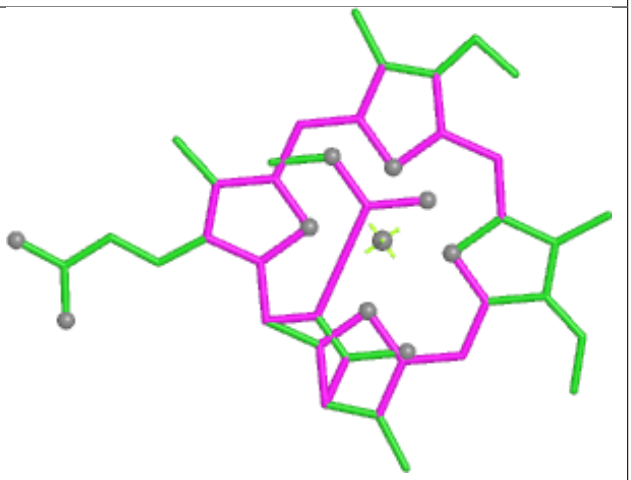
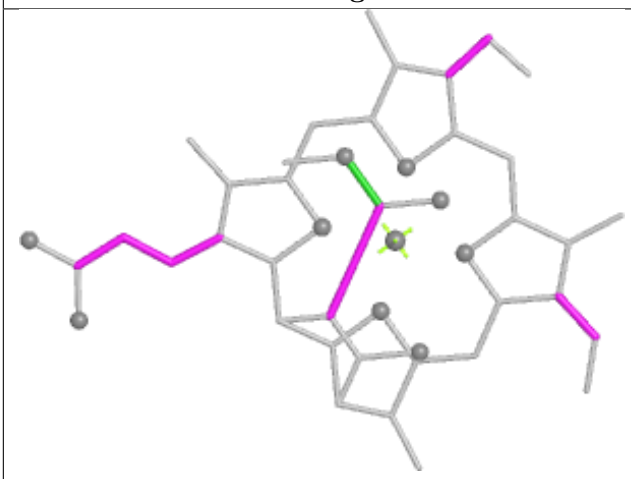


Bond angles



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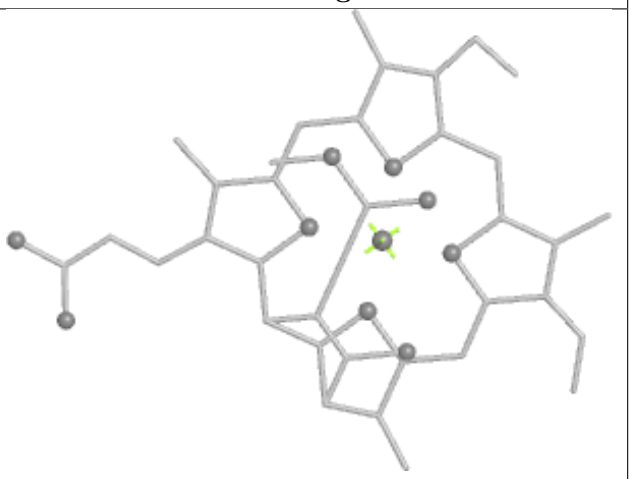
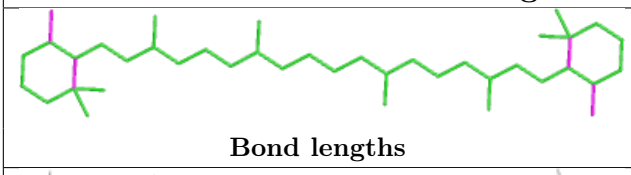


Rings

Ligand BCR m 101



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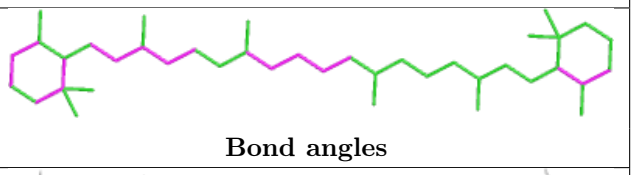
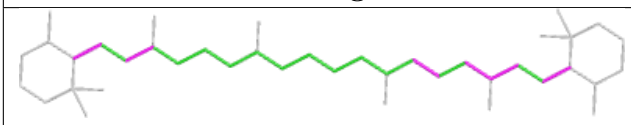
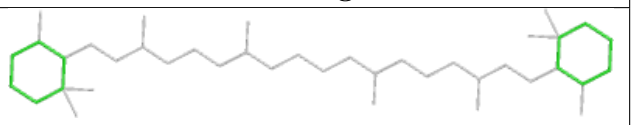


Bond angles

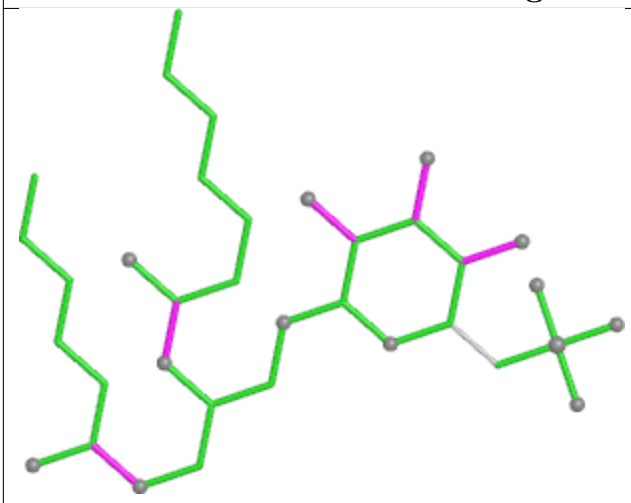


Torsions



Rings

Ligand SQD E 320



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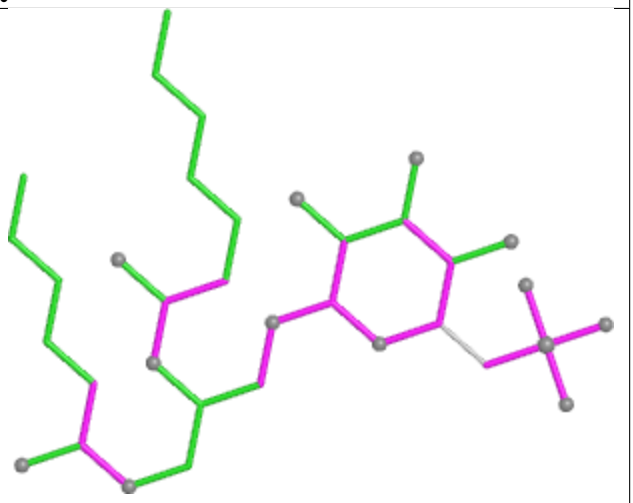
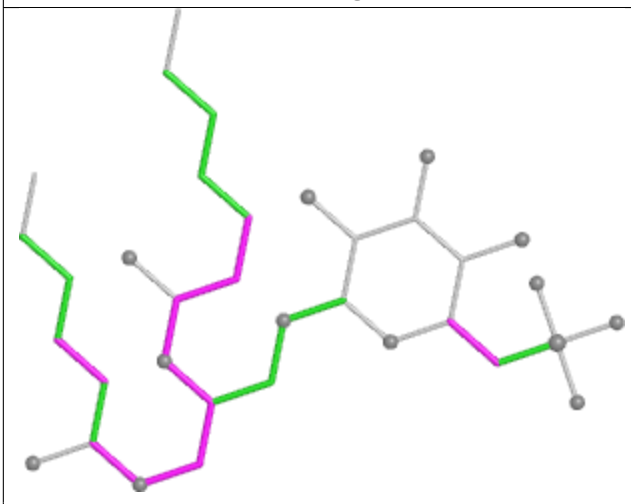
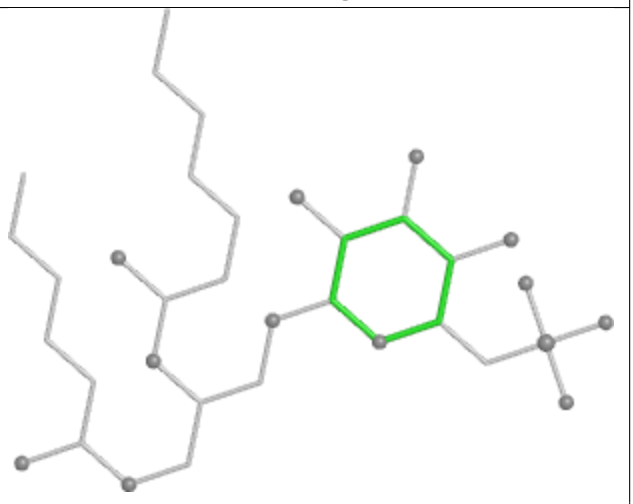


Bond angles

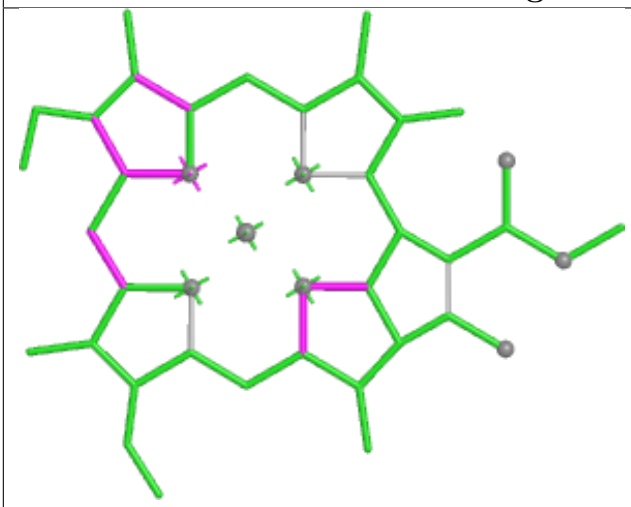


Torsions

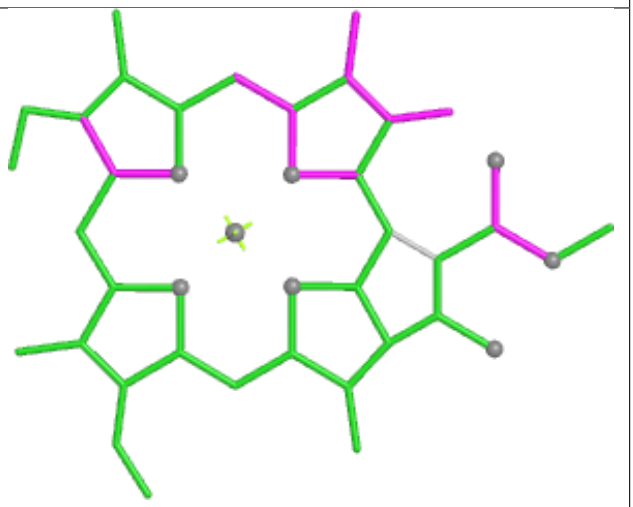


Rings

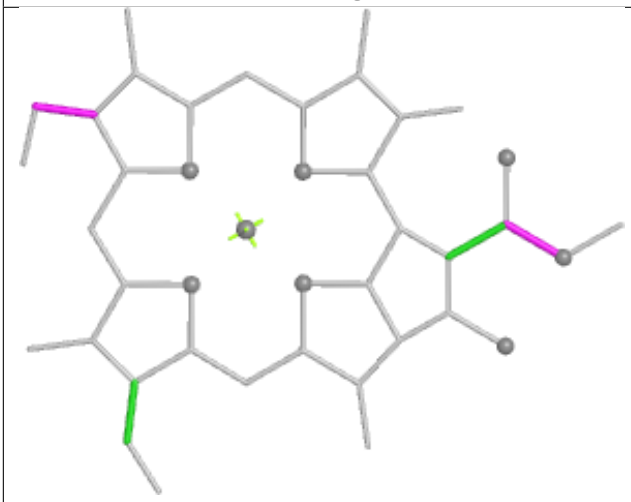
Ligand CLA Z 305



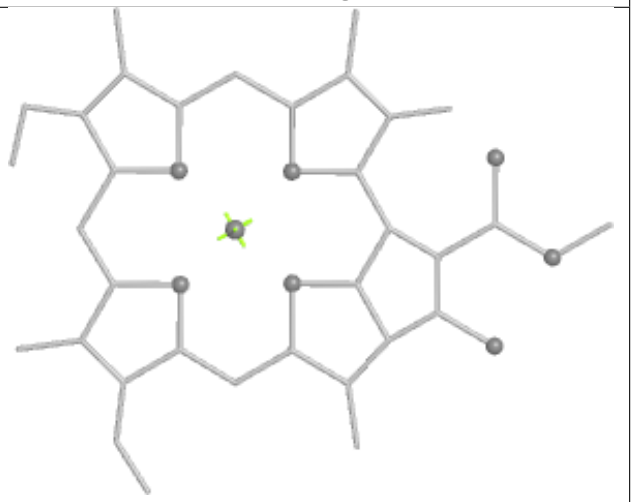
Bond lengths



Bond angles

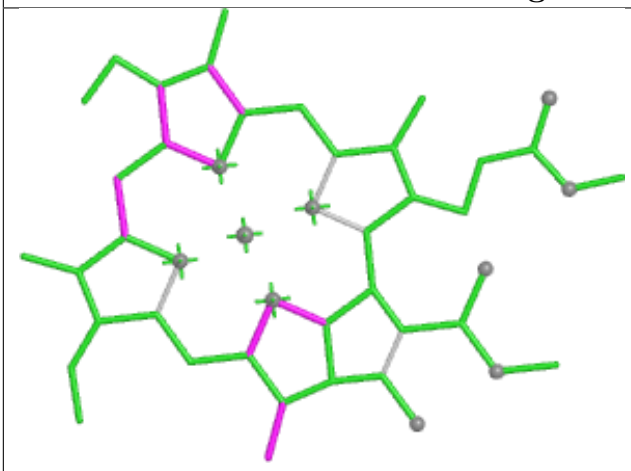


Torsions

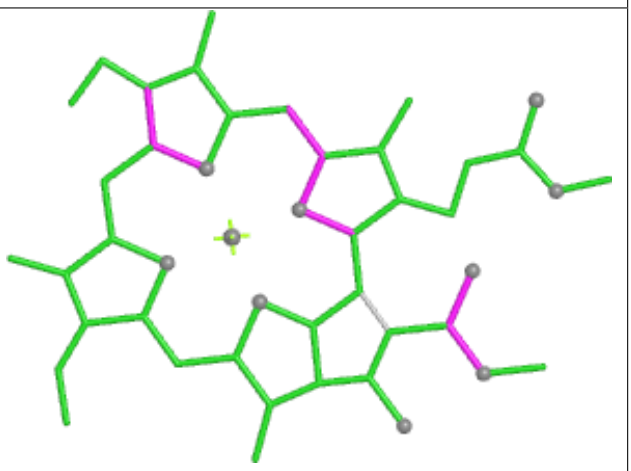


Rings

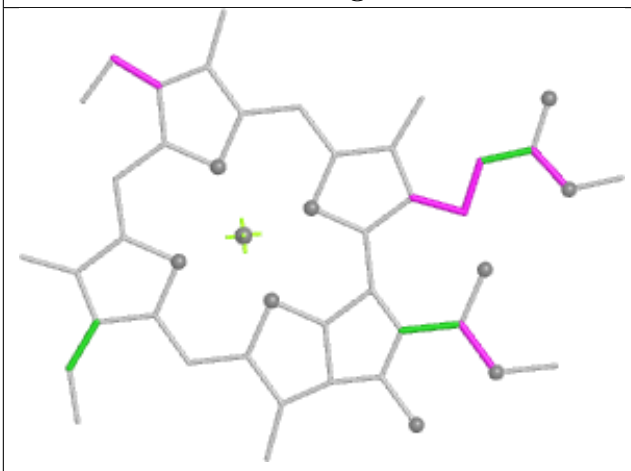
Ligand CLA J 313



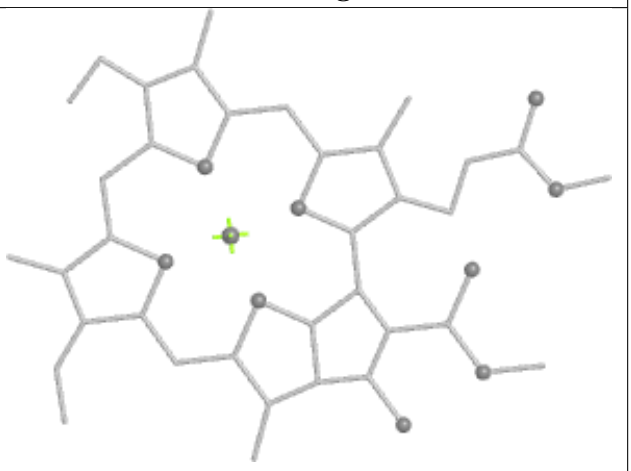
Bond lengths



Bond angles

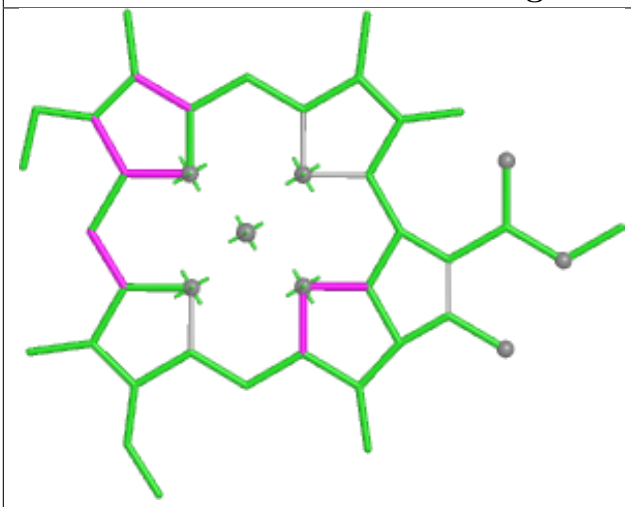


Torsions



Rings

Ligand CLA F 315



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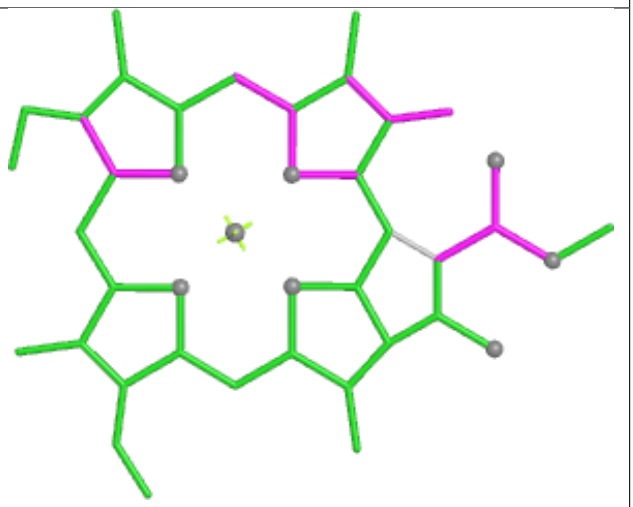
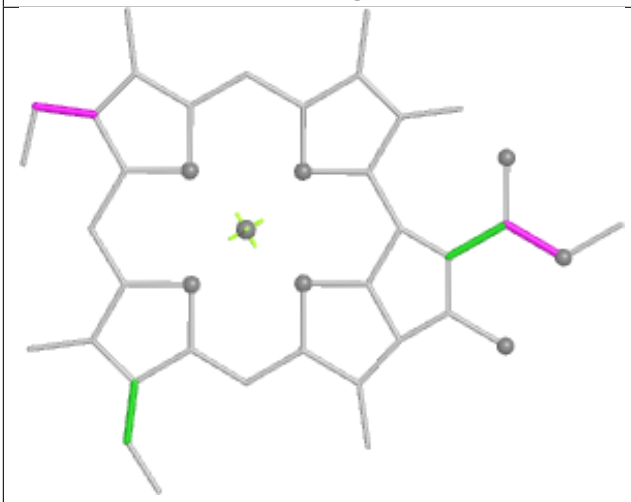
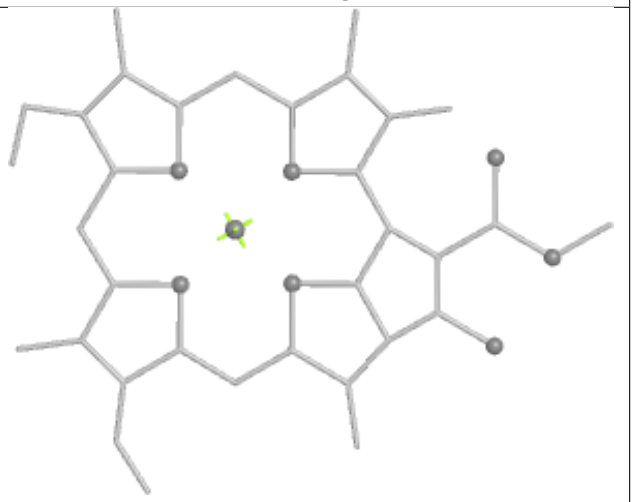


Bond angles

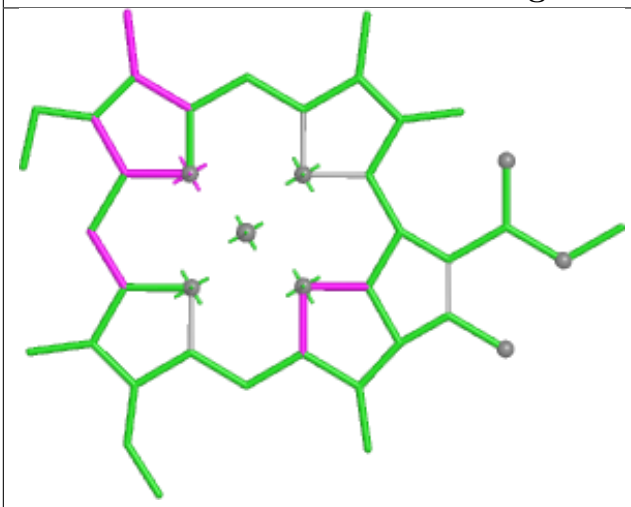


Torsions



Rings

Ligand CLA 9 315



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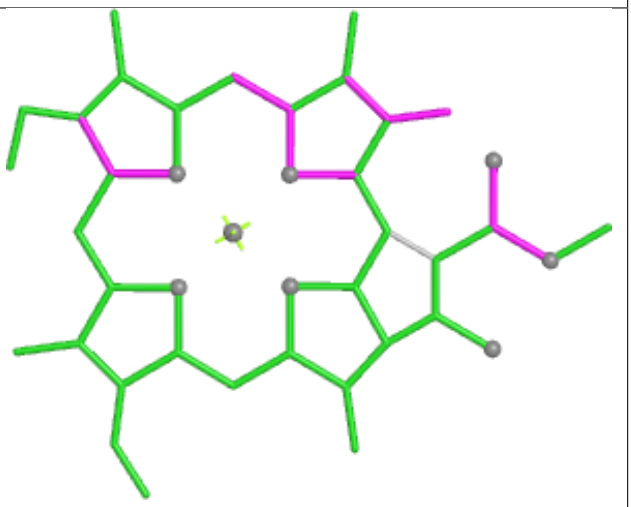
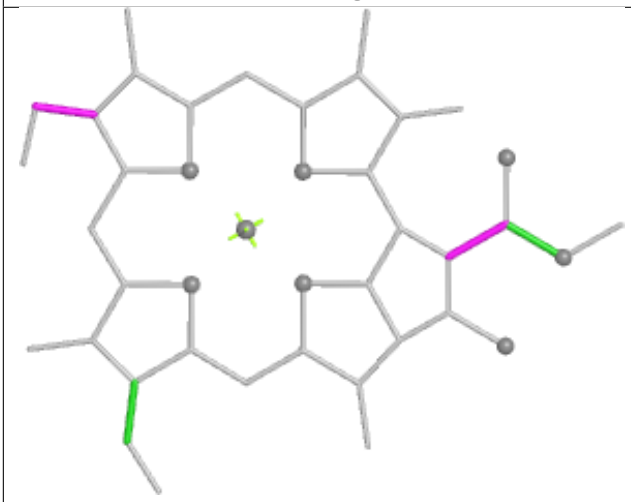


Bond angles



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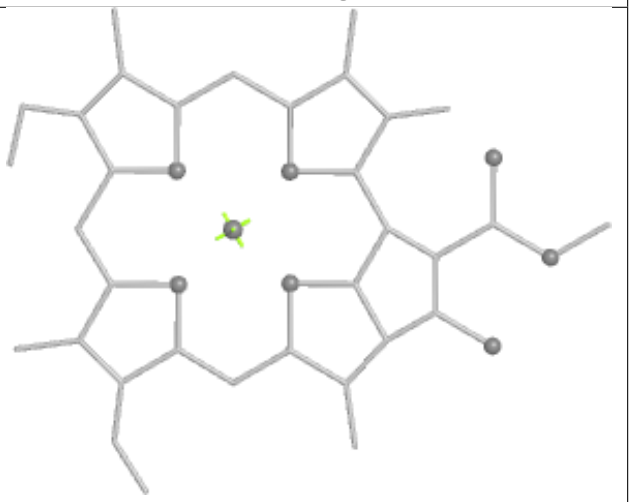
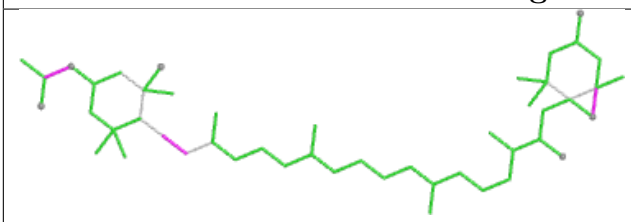


Rings

Ligand A86 Q 304



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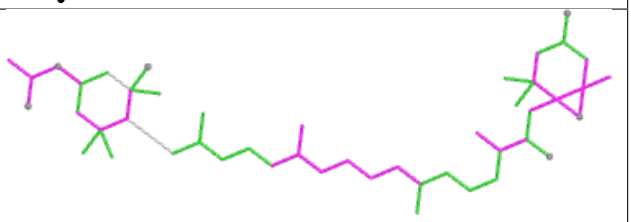
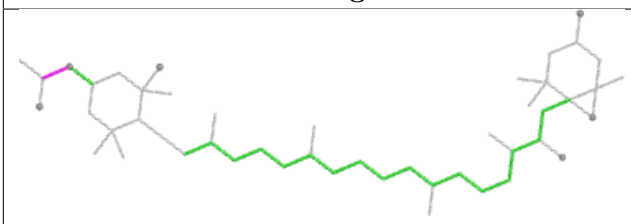


Bond angles



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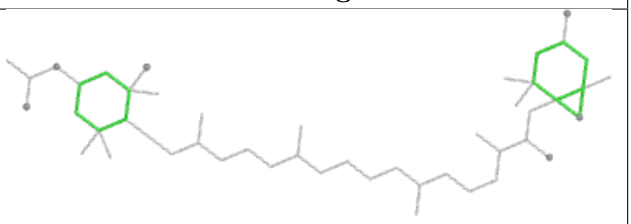
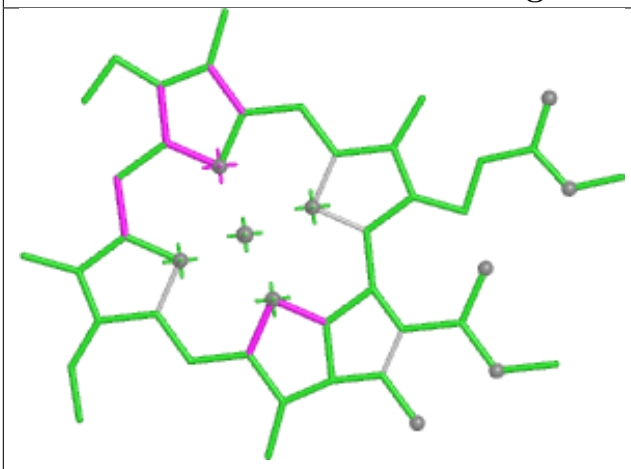


Rings

Ligand CLA Z 306



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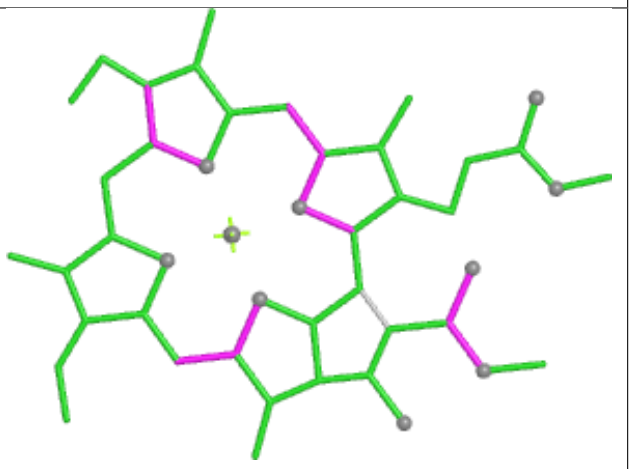
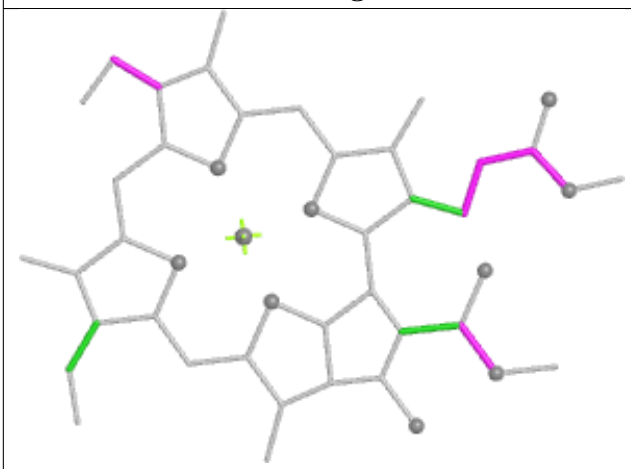


Bond angles



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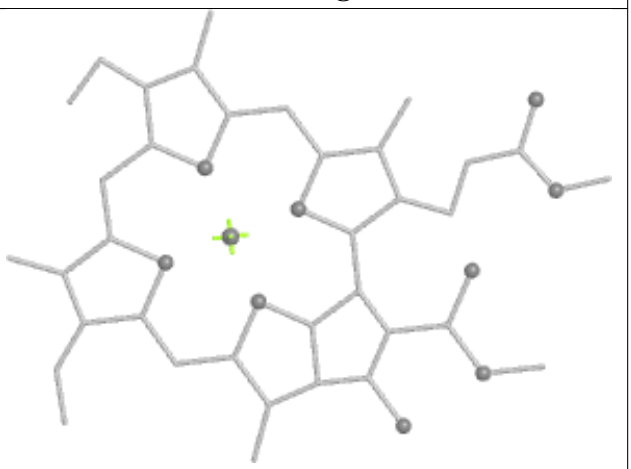
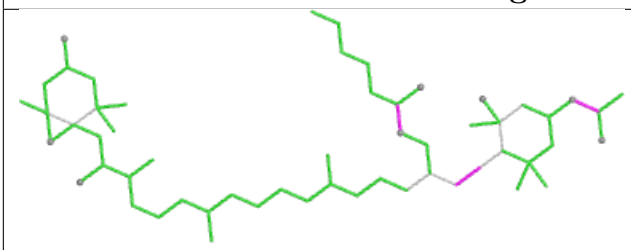


Rings

Ligand A1EB1 3 324



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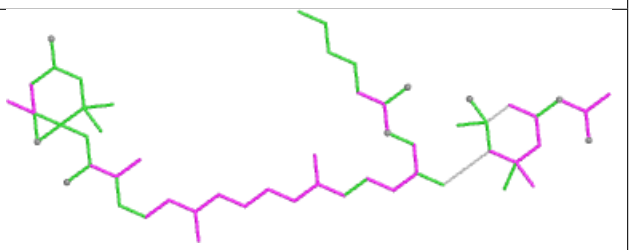
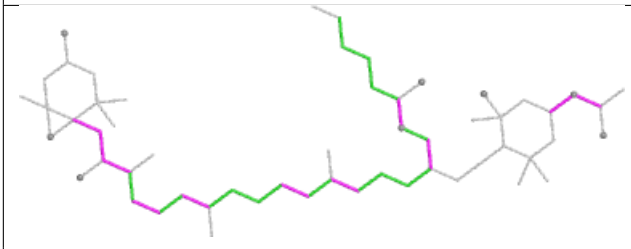


Bond angles



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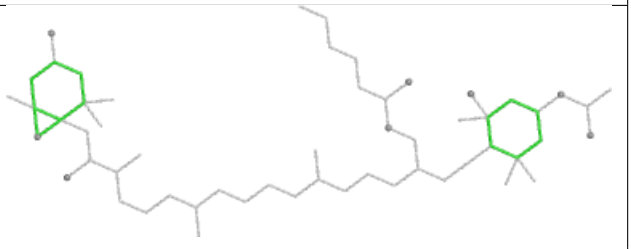
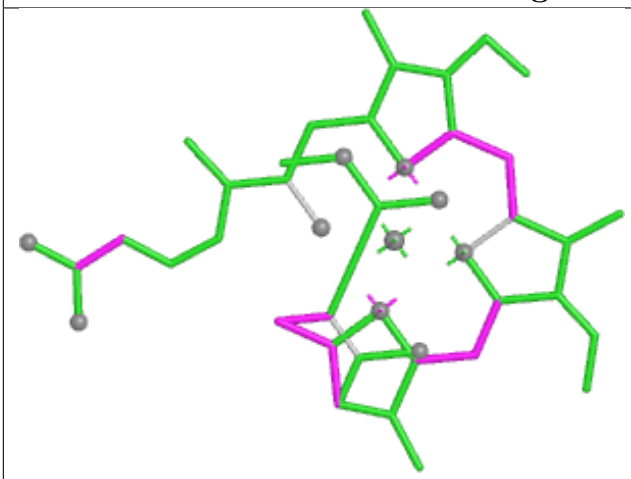


Rings

Ligand KC2 z 313



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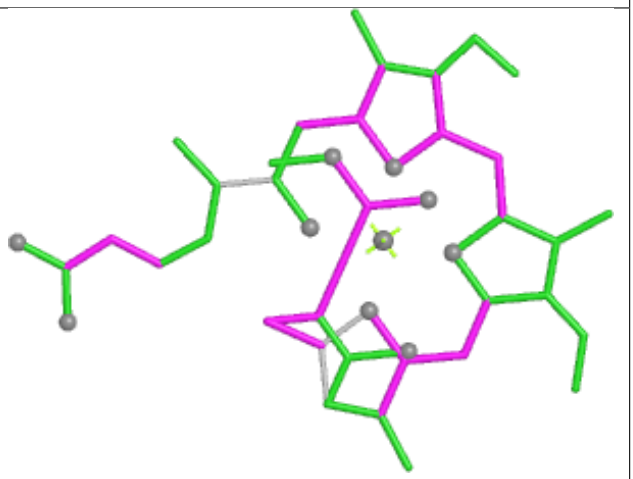
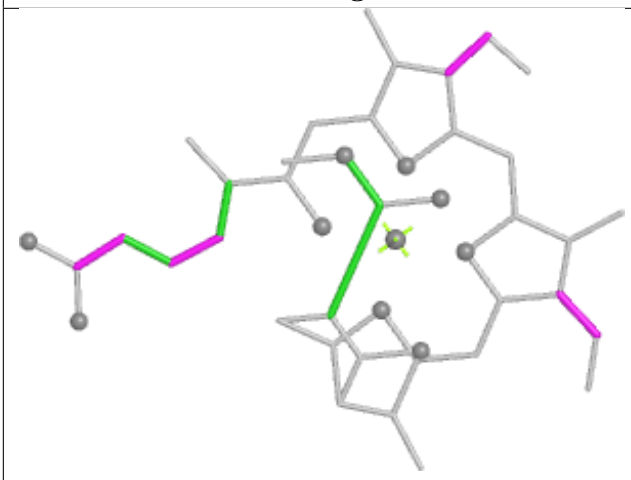


Bond angles



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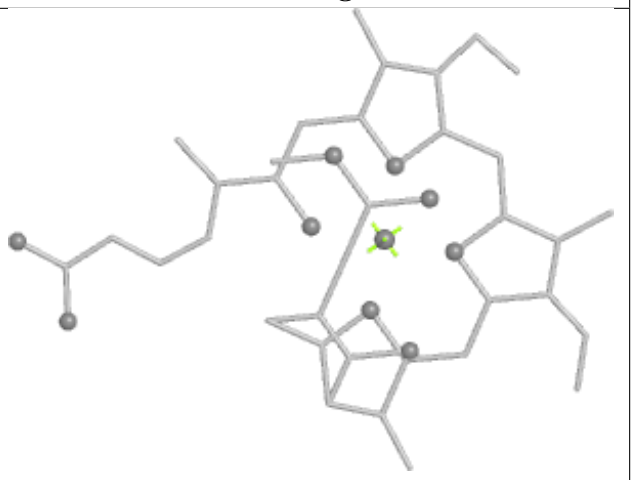
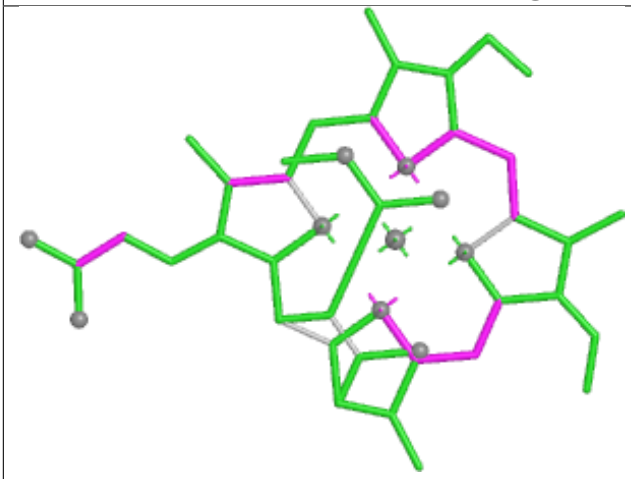


Rings

Ligand KC2 P 313



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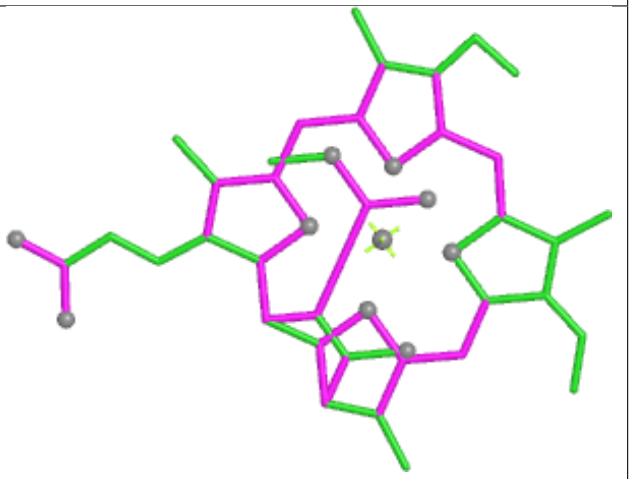
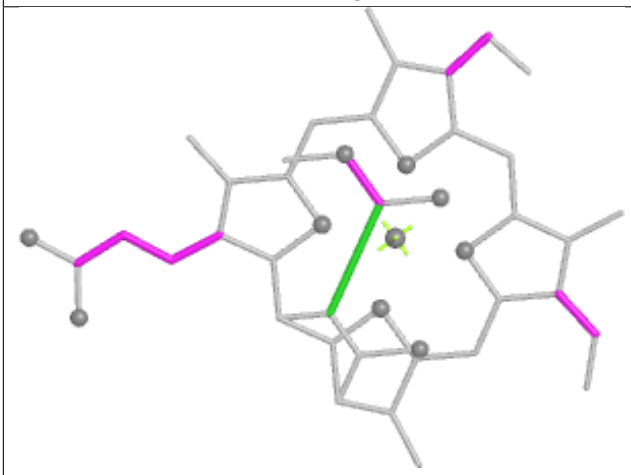


Bond angles



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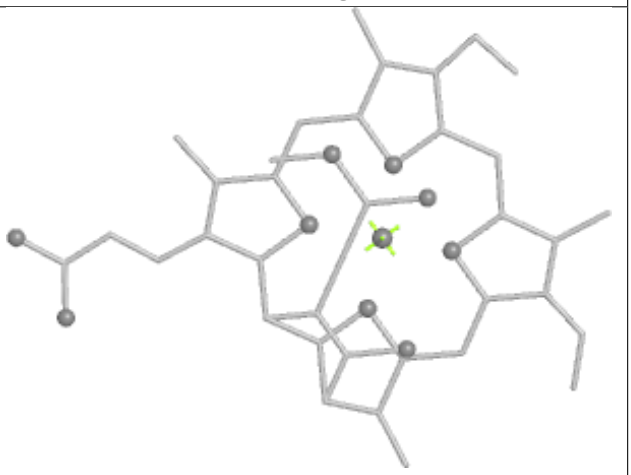
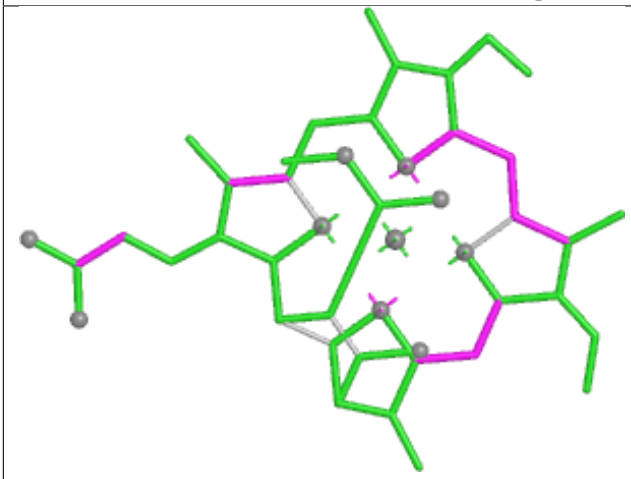


Rings

Ligand KC2 9 316



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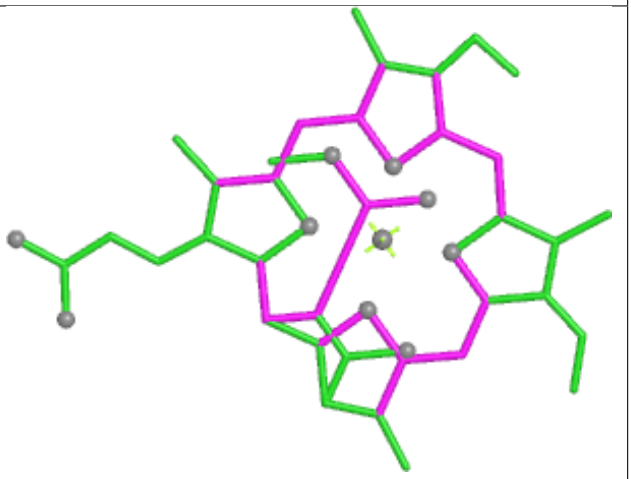

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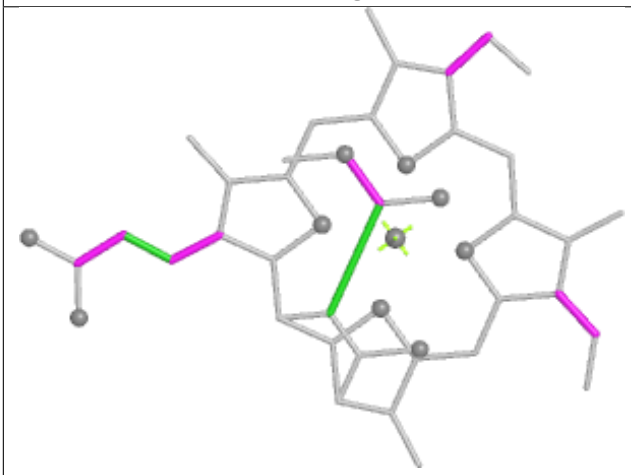
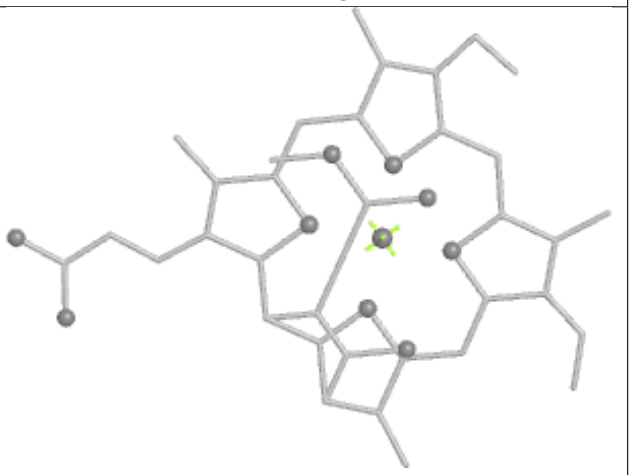
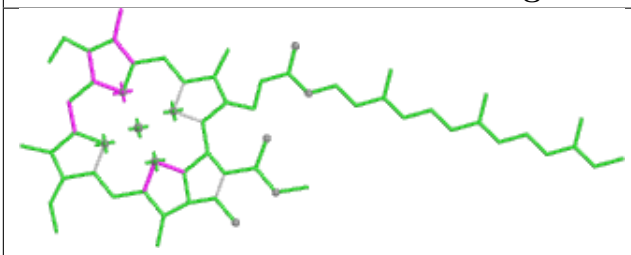


Torsions



Rings

Ligand CLA D 310



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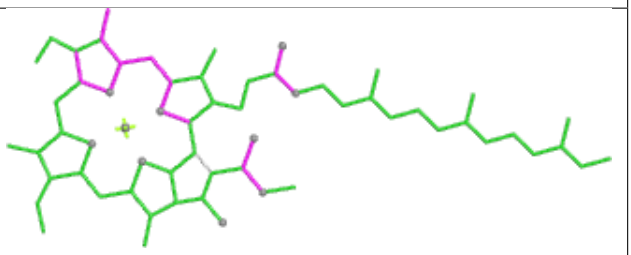
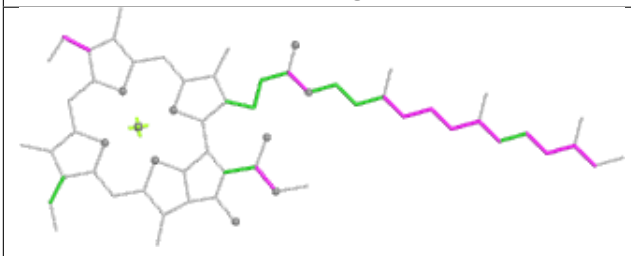


Bond angles



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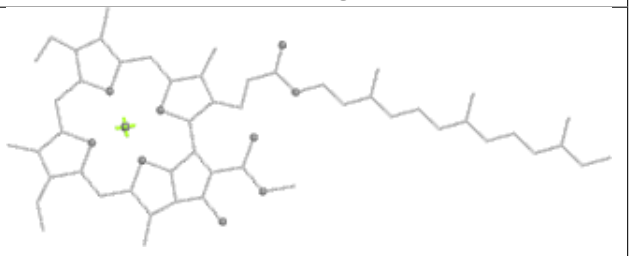
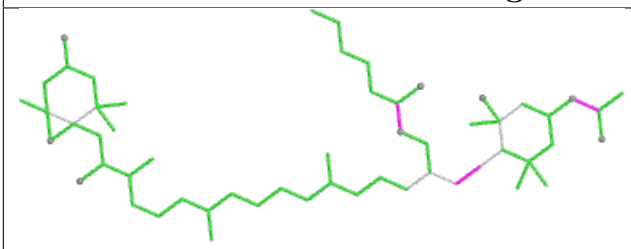


Rings

Ligand A1EB1 C 302



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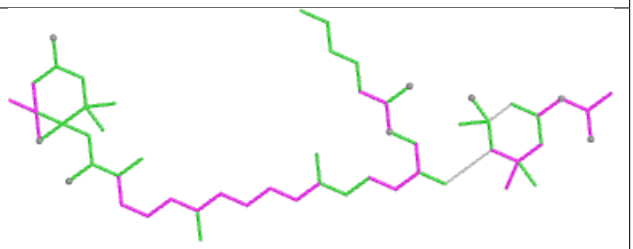
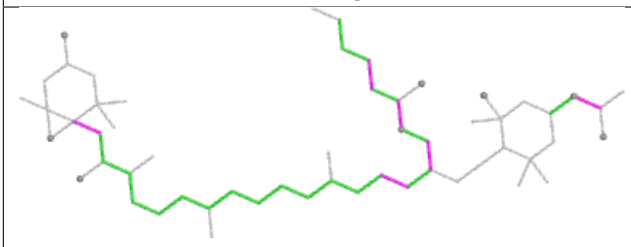
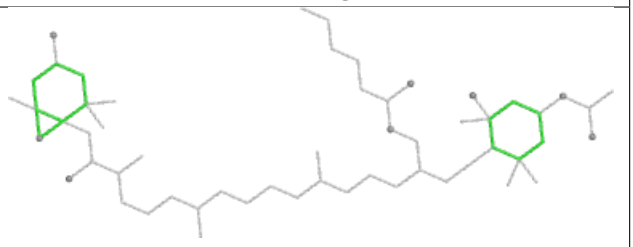


Bond angles

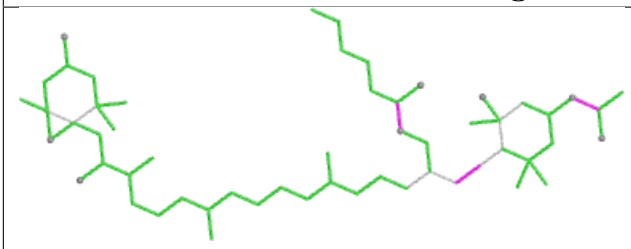


Torsions



Rings

Ligand A1EB1 5 302



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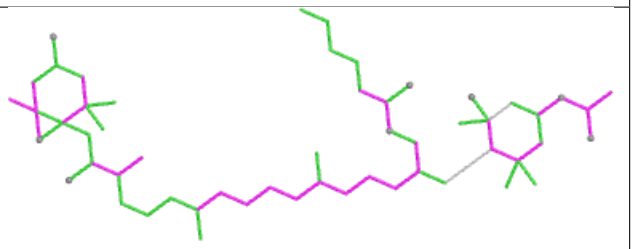
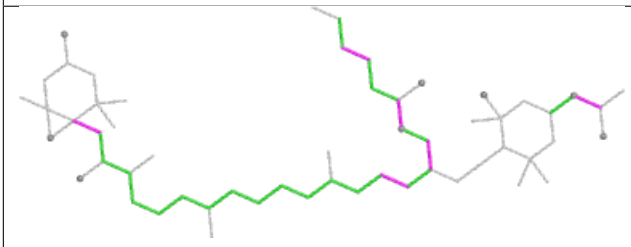


Bond angles



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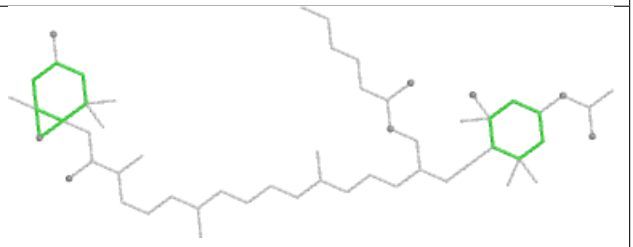
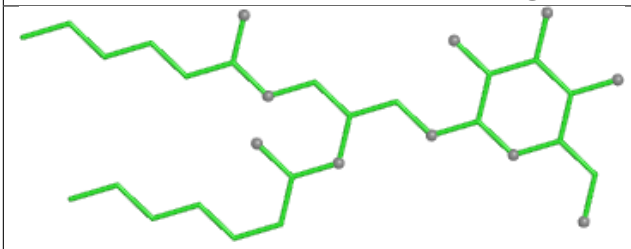
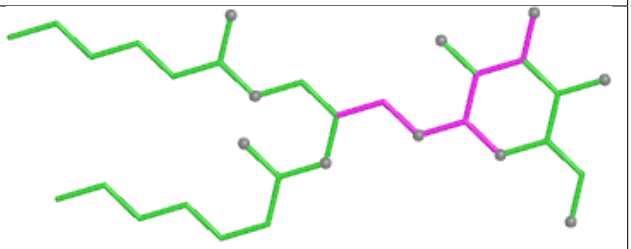


Rings

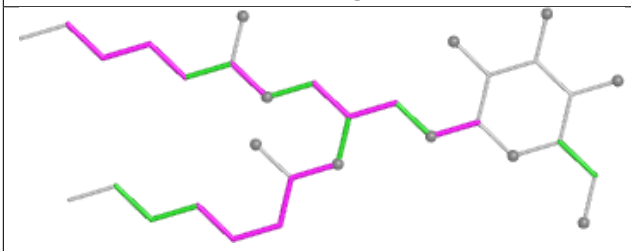
Ligand LMG 4 325



Bond lengths



Bond angles



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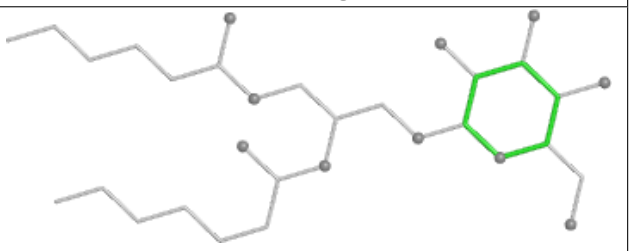
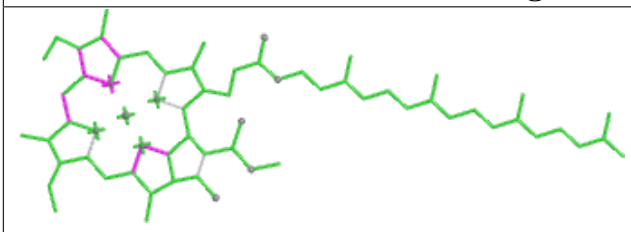


Rings

Ligand CLA L 310



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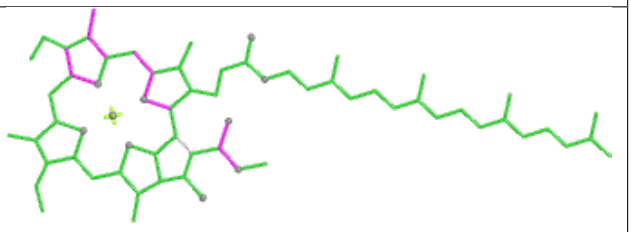
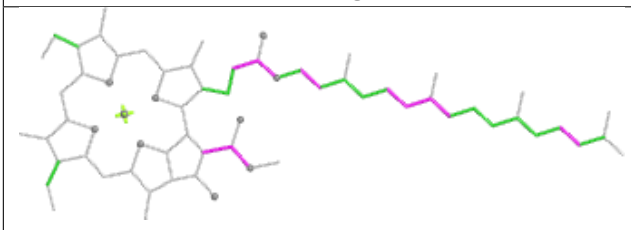
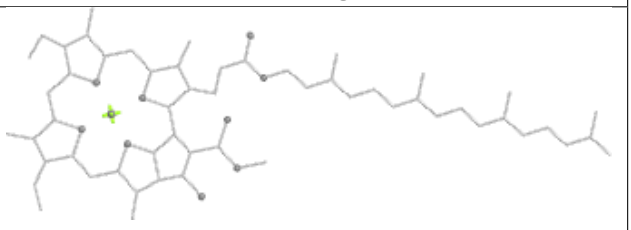


Bond angles

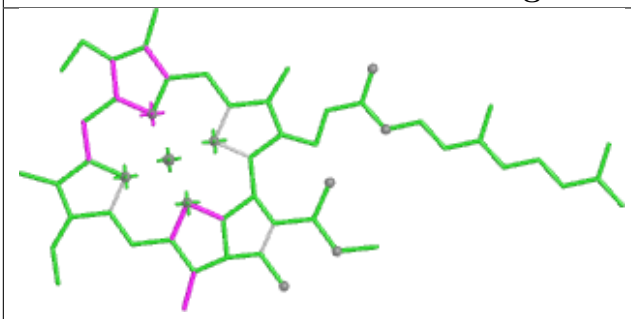


Torsions

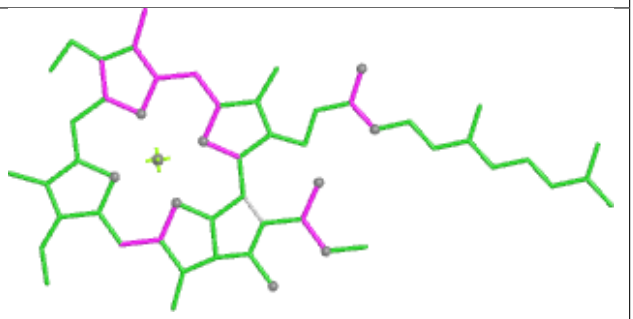


Rings

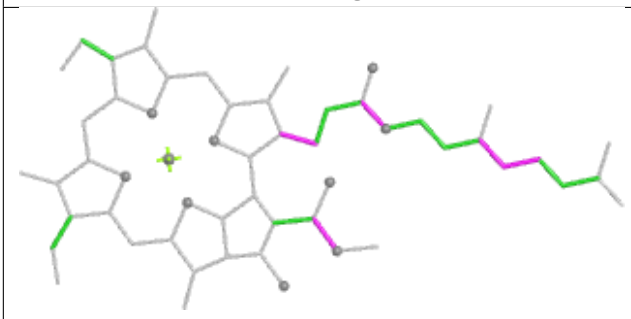
Ligand CLA D 312



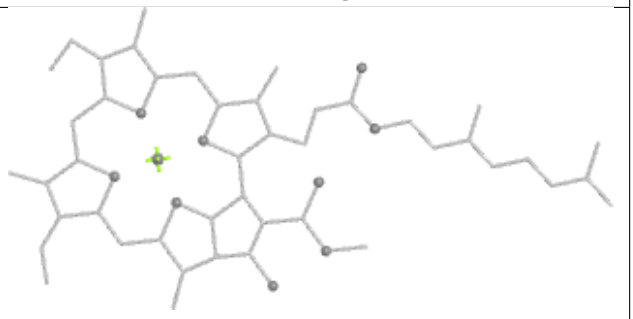
Bond lengths



Bond angles

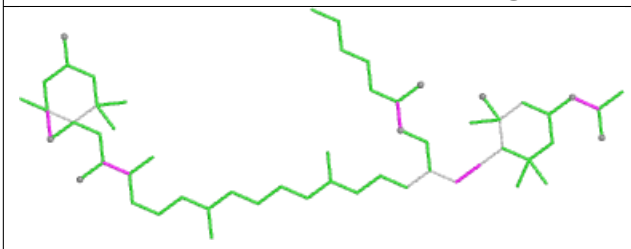


Torsions



Rings

Ligand A1EB1 Q 307



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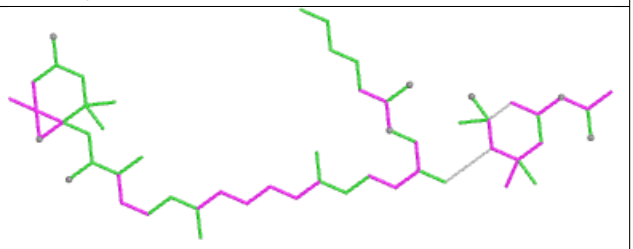

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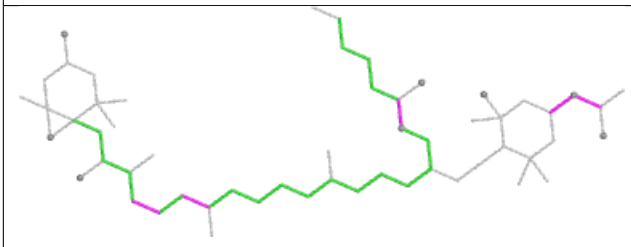

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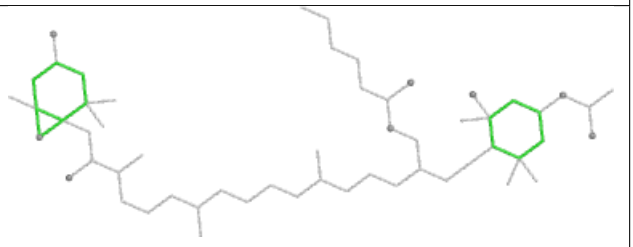
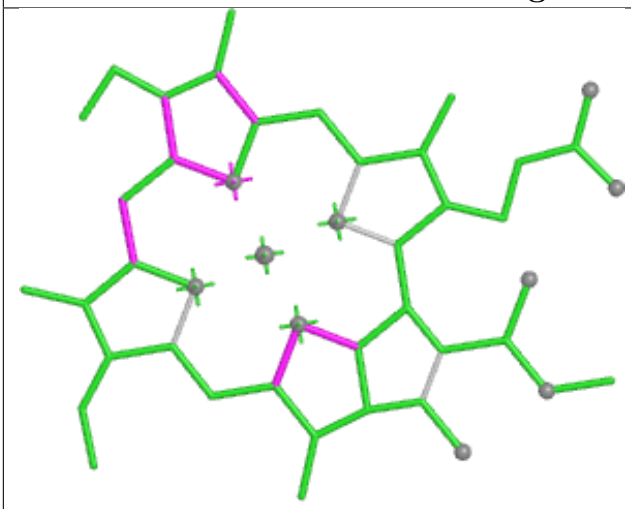


Rings

Ligand CLA 1 310



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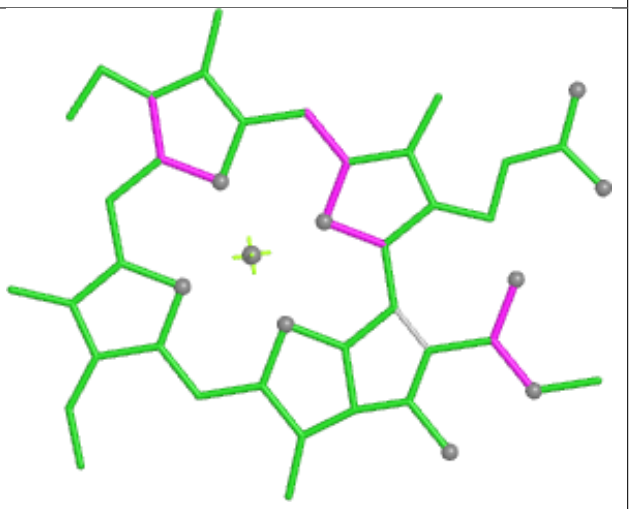
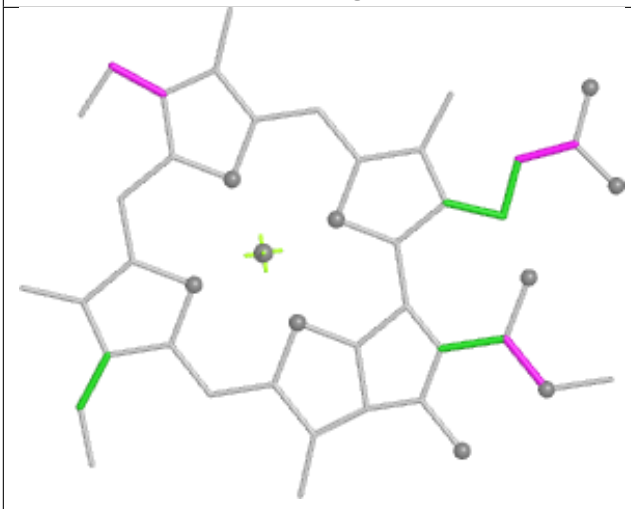


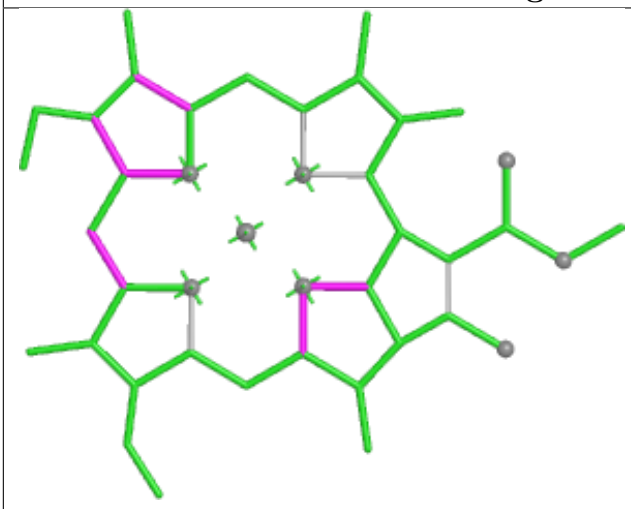
Bond angles



Torsions

Rings

Ligand CLA Z 309



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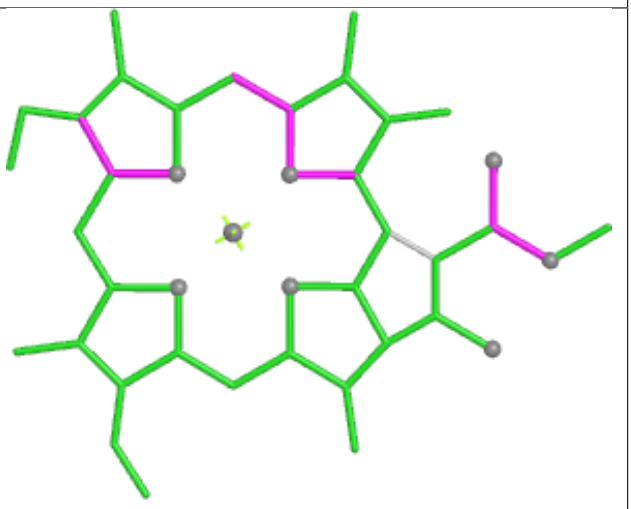

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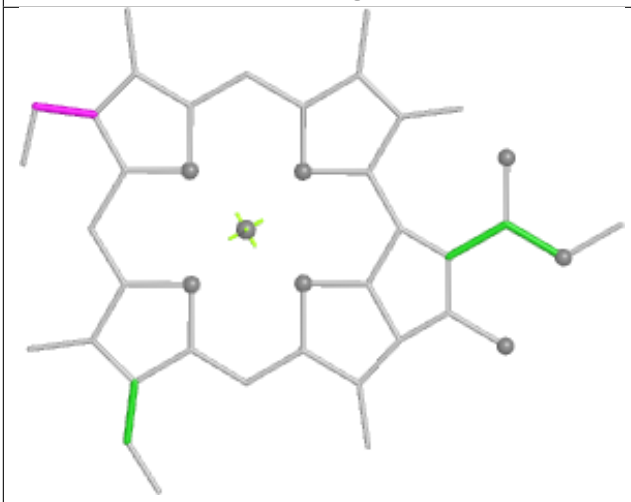

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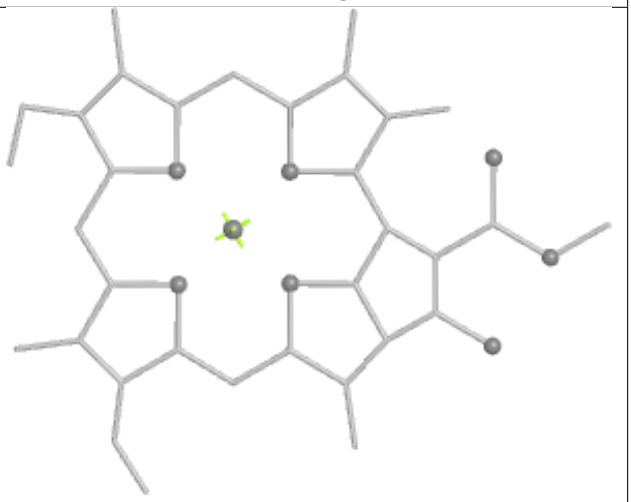
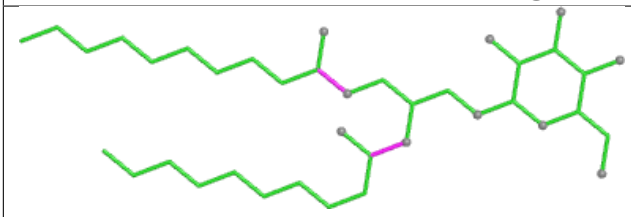


Rings

Ligand LMG l 208



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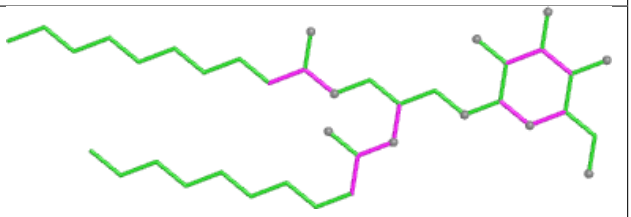
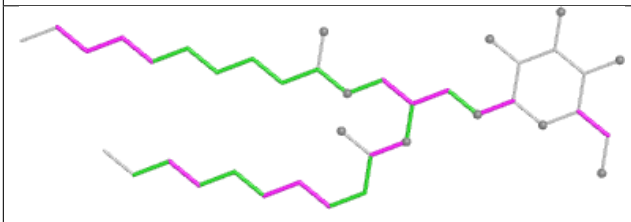


Bond angles



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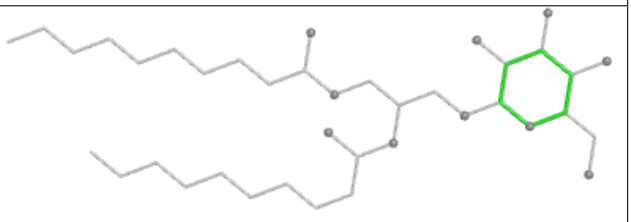
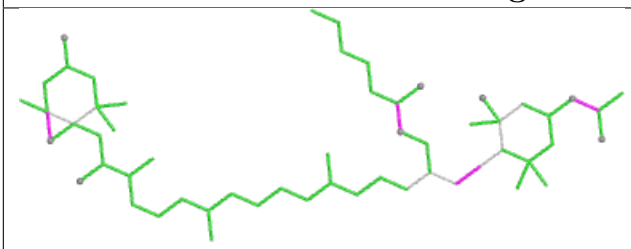


Rings

Ligand A1EB1 h 203



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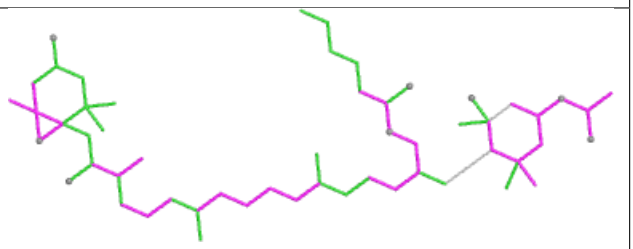
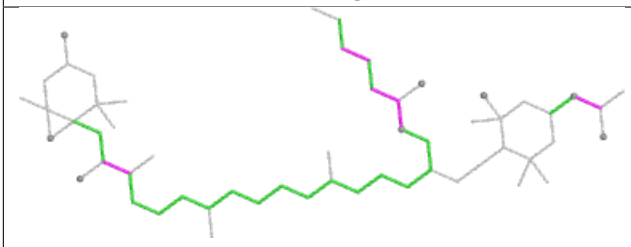


Bond angles



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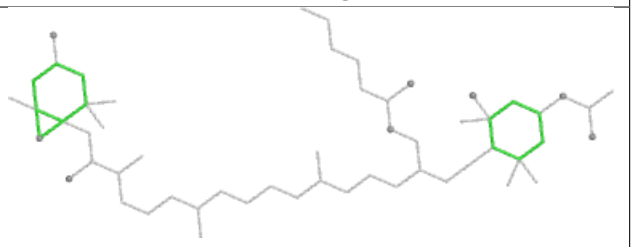
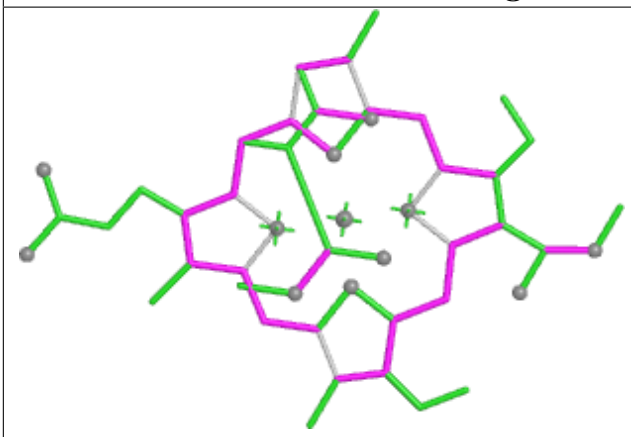


Rings

Ligand A1ECV y 317



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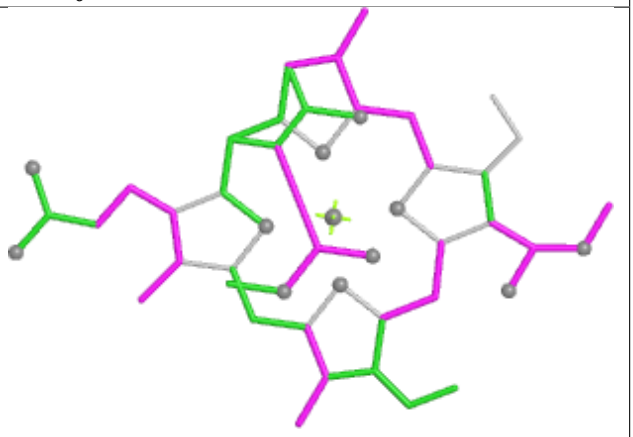

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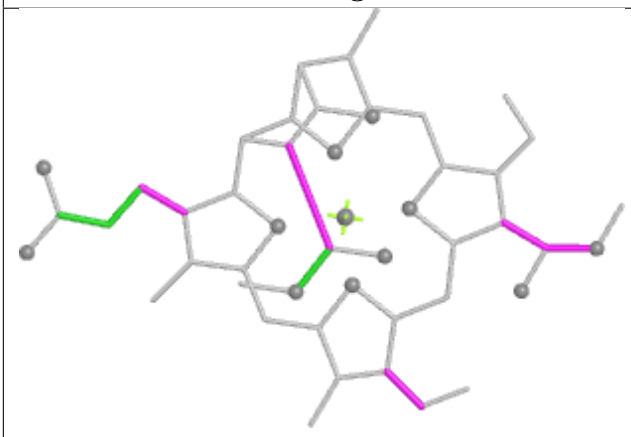

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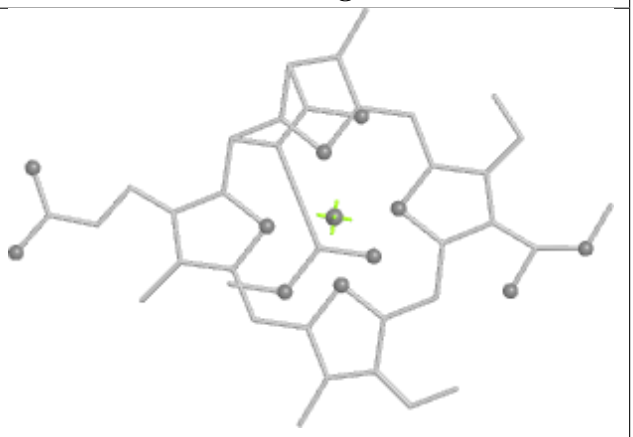
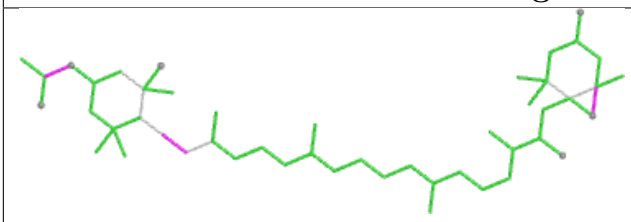


Rings

Ligand A86 L 301



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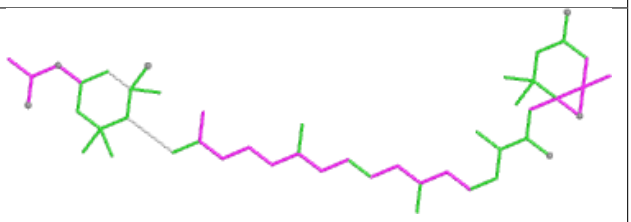
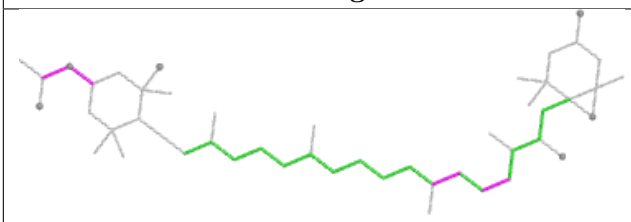


Bond angles



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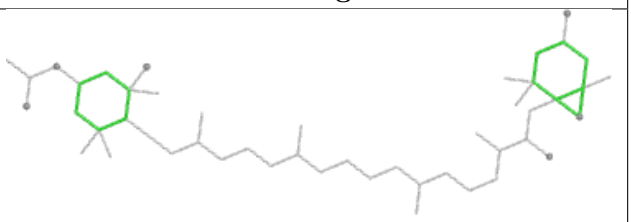
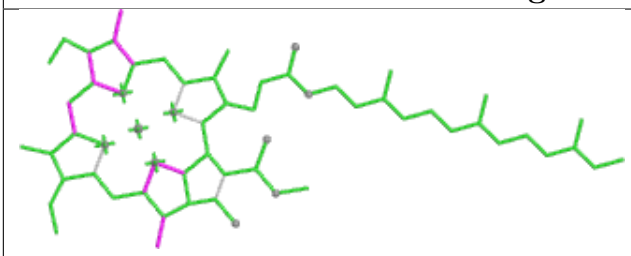


Rings

Ligand CLA 0 310



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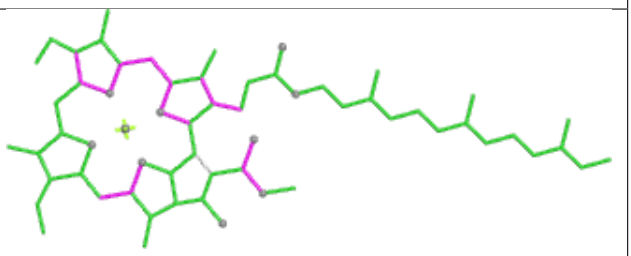

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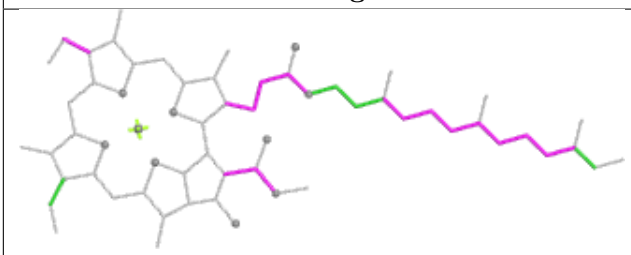

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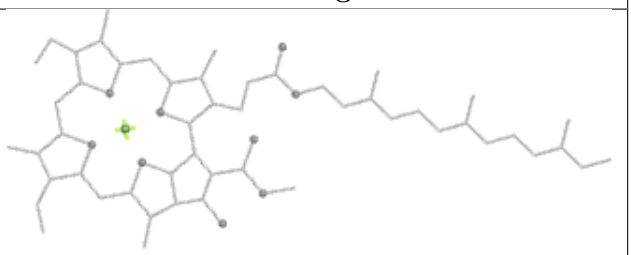
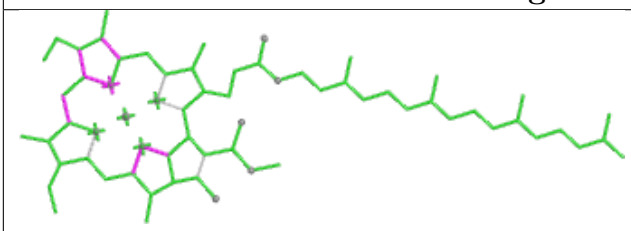


Rings

Ligand CLA a 836



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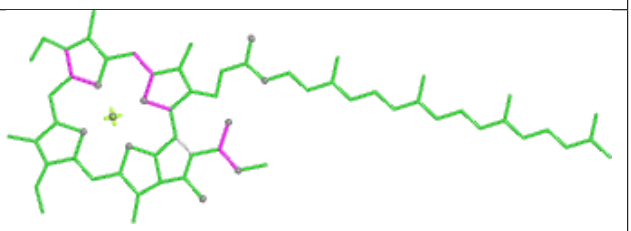

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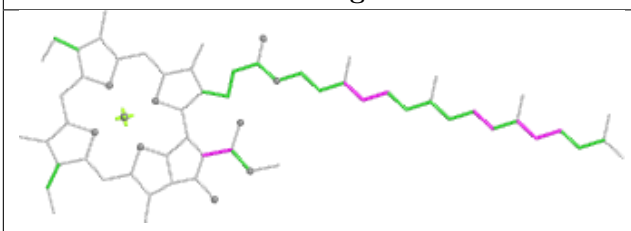

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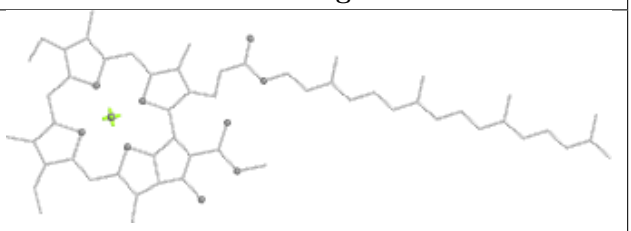
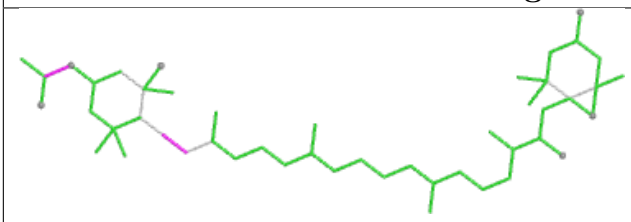


Rings

Ligand A86 W 303



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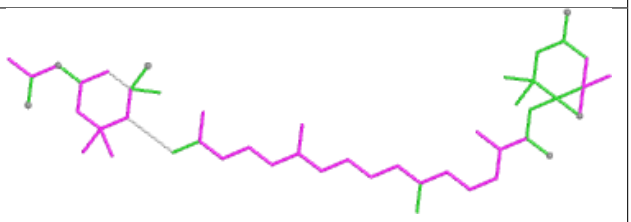

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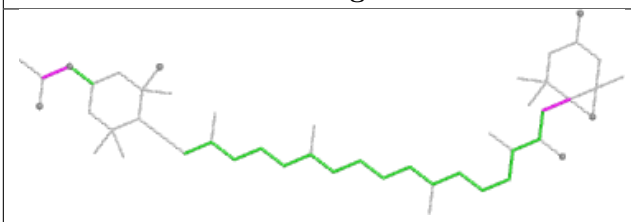

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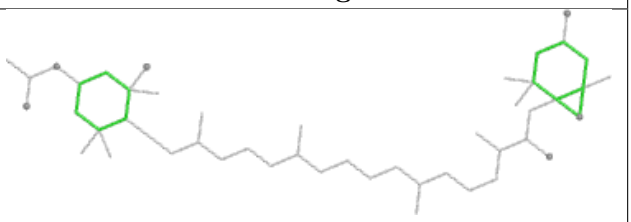
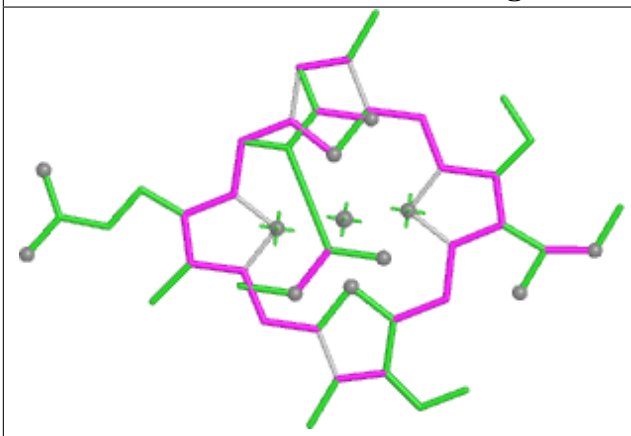


Rings

Ligand A1ECV z 310



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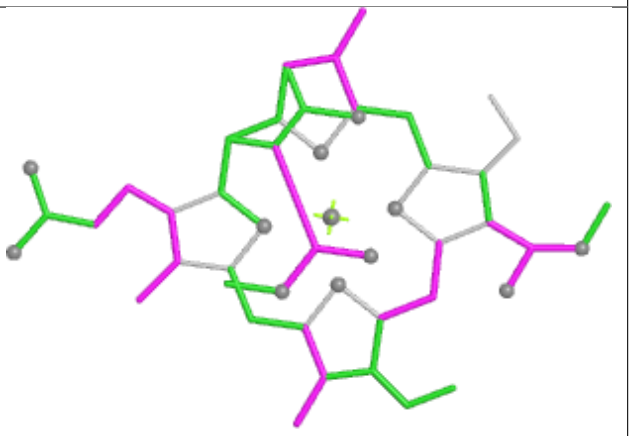
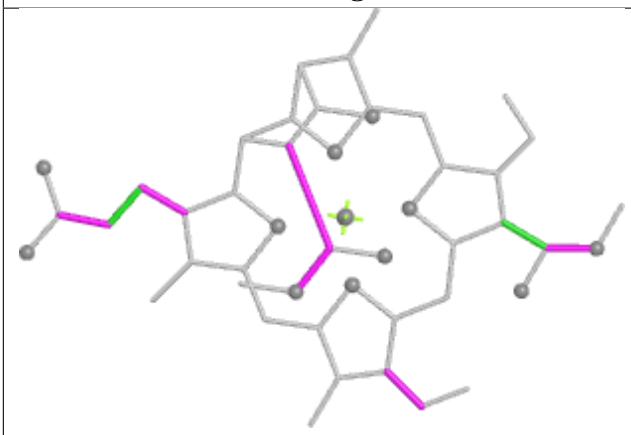


Bond angles



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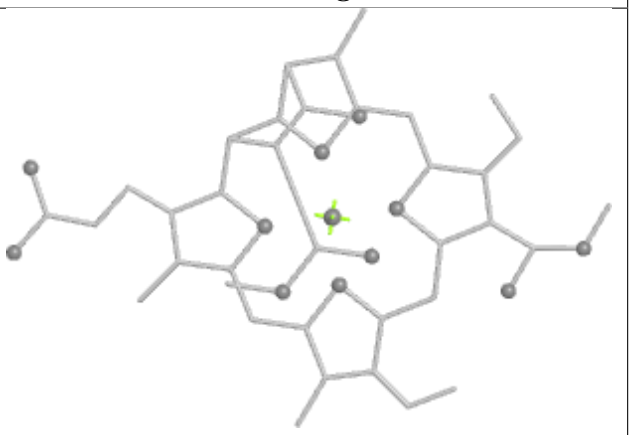
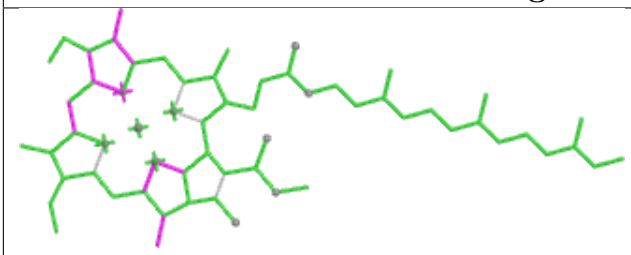


Rings

Ligand CLA 4 311



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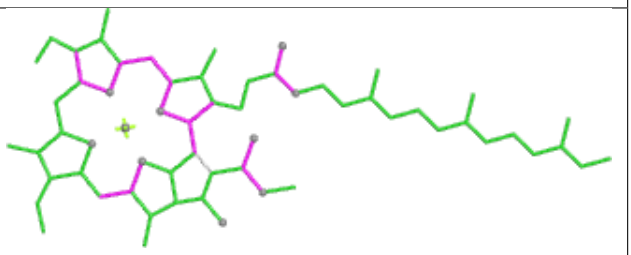
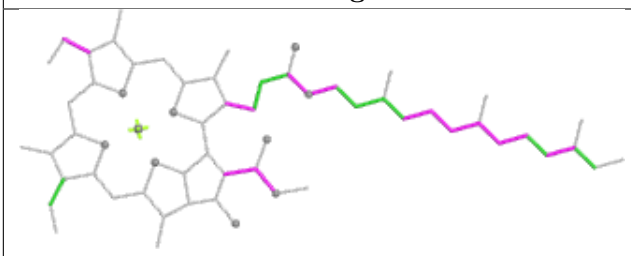


Bond angles



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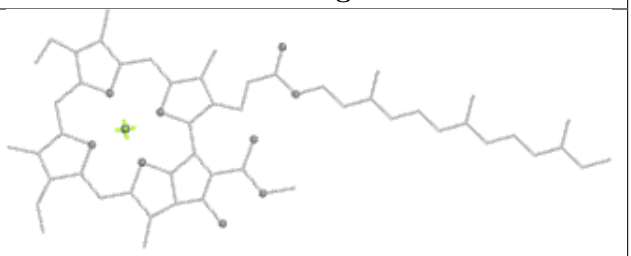
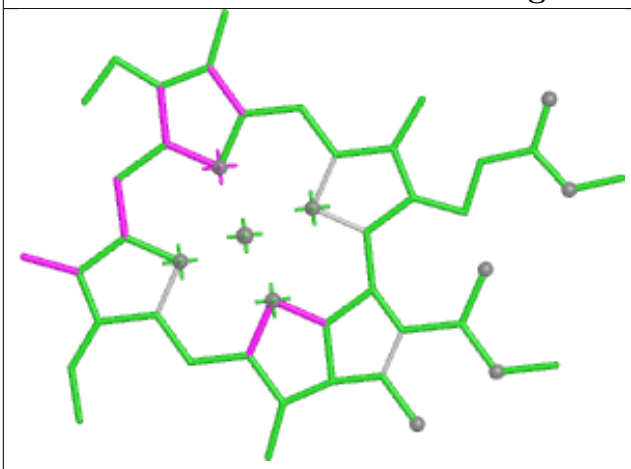


Rings

Ligand CLA 3 323



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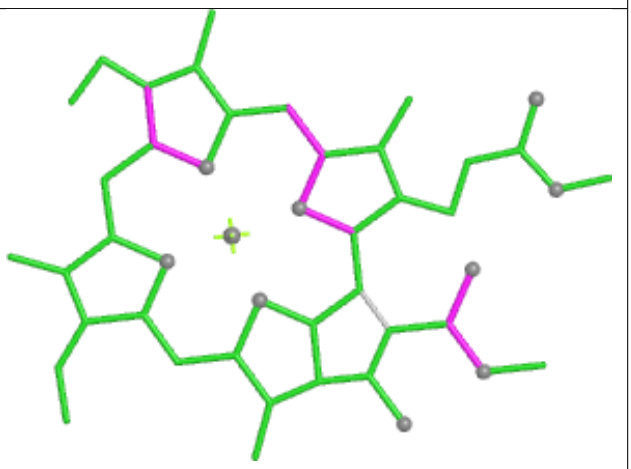
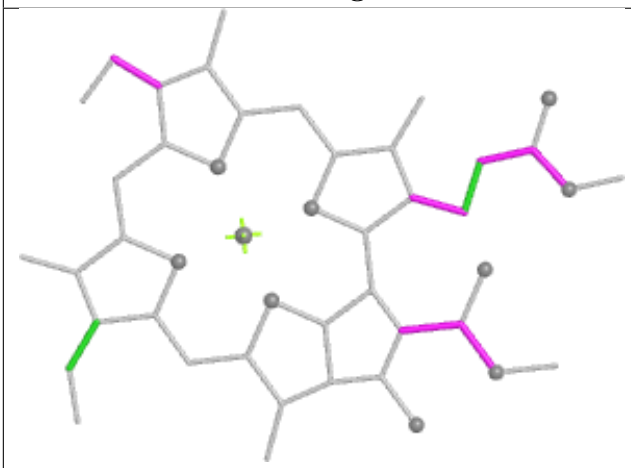


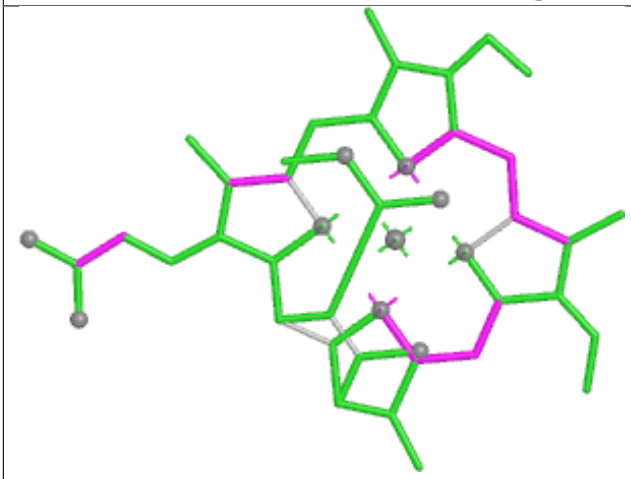
Bond angles



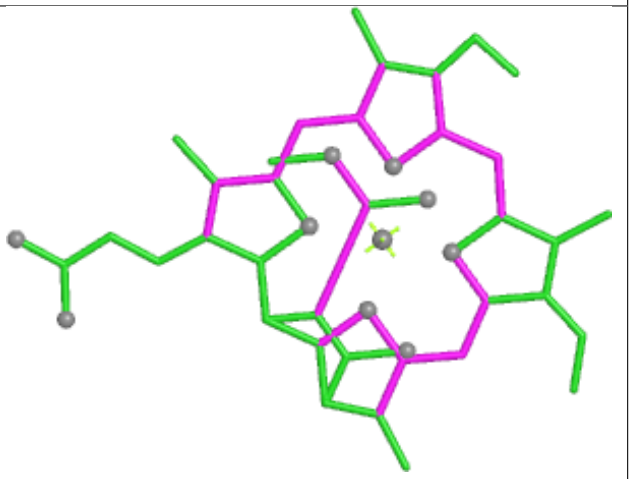
Torsions

Rings

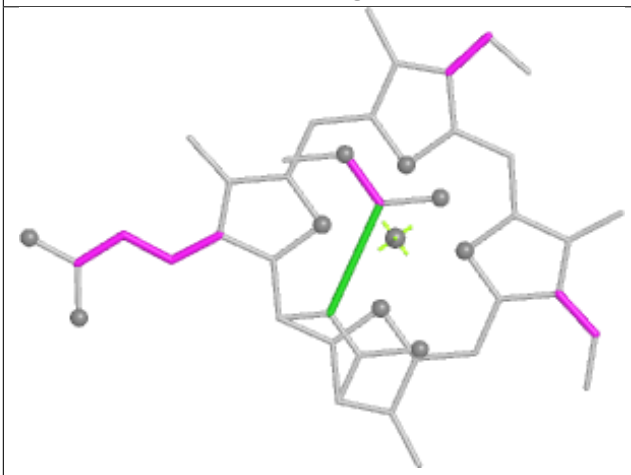
Ligand KC2 6 319



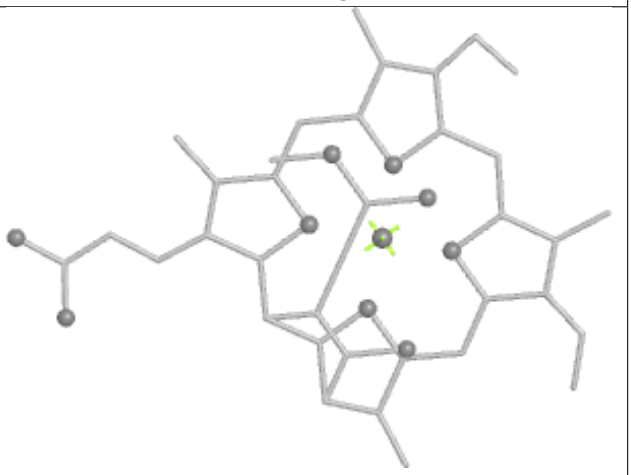
Bond lengths



Bond angles

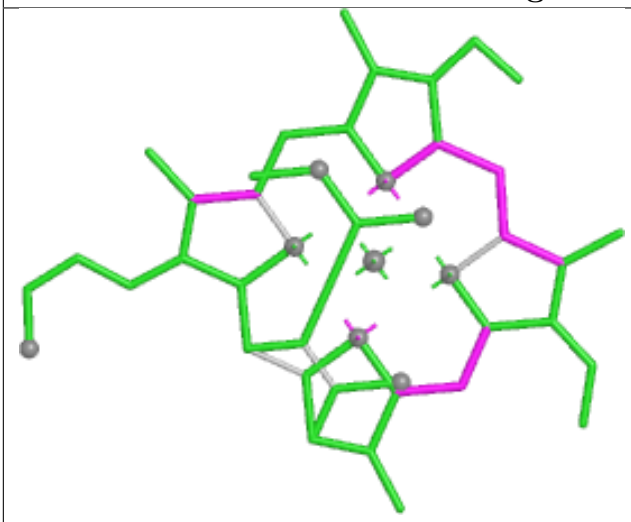


Torsions



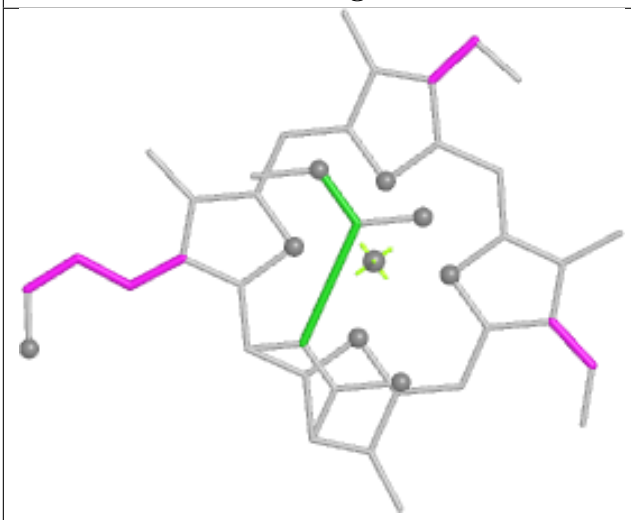
Rings

Ligand KC2 P 310



Bond lengths

Bond angles



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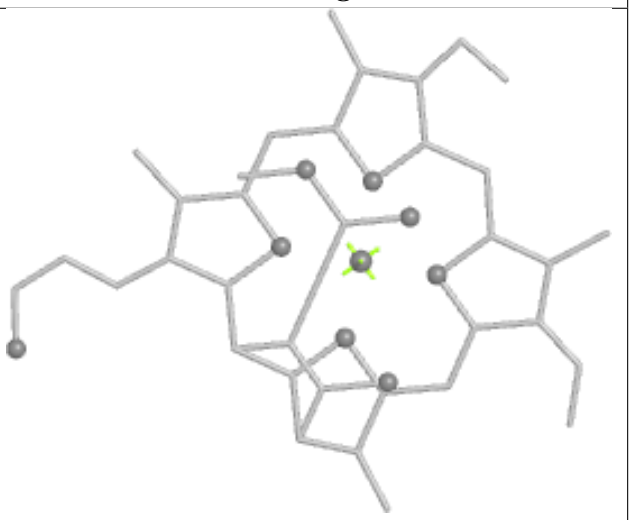
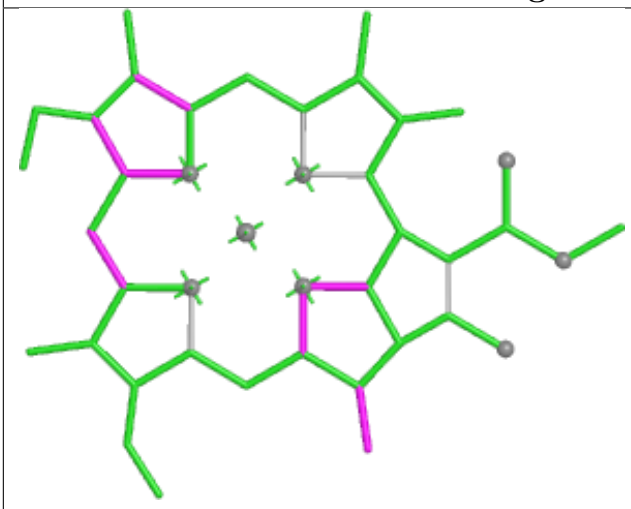


Rings

Ligand CLA 1 311



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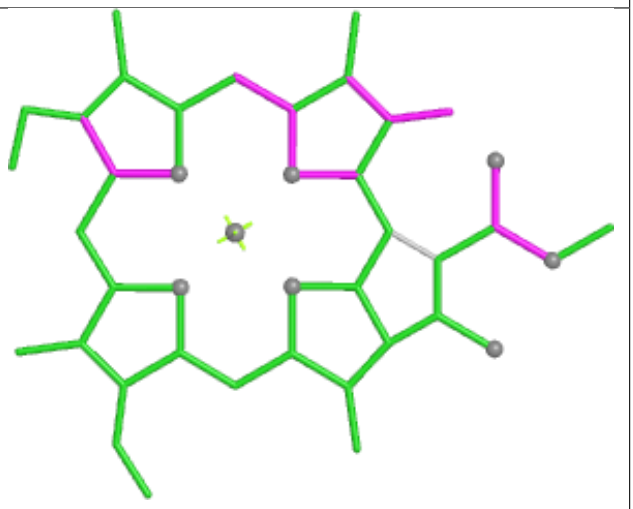

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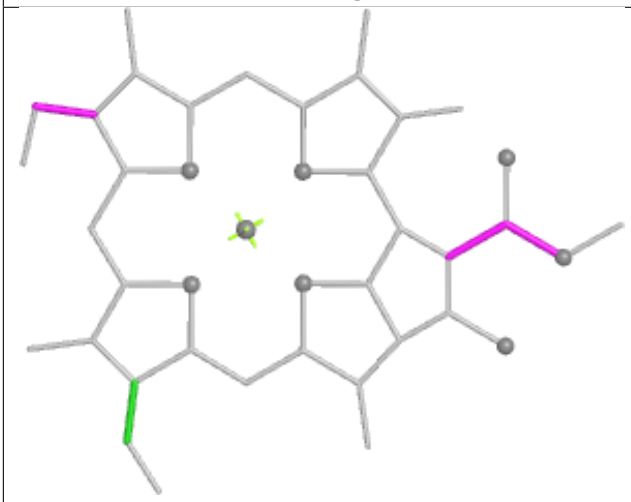

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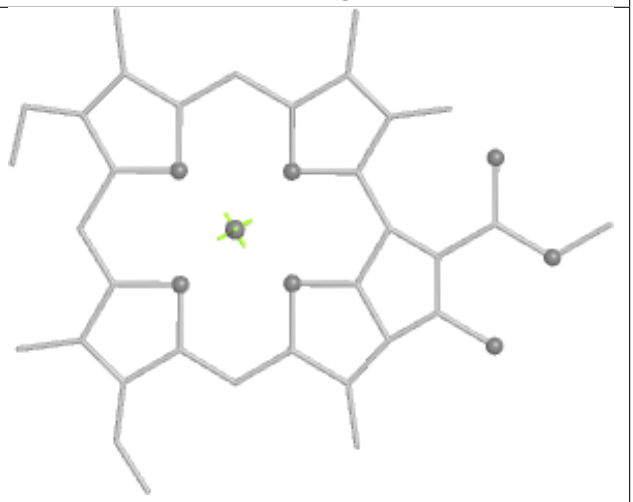
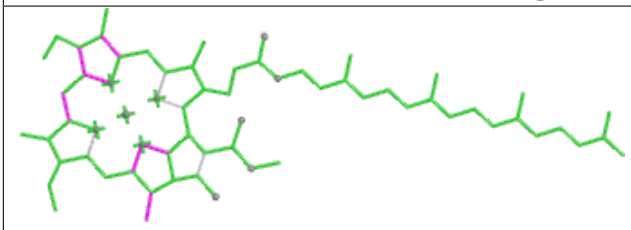


Rings

Ligand CLA j 101



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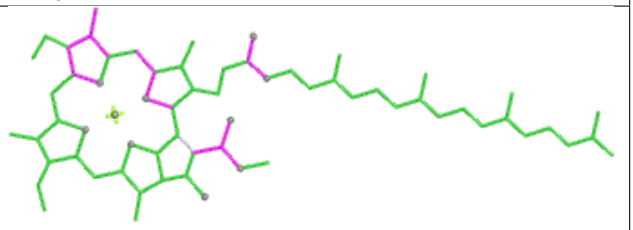
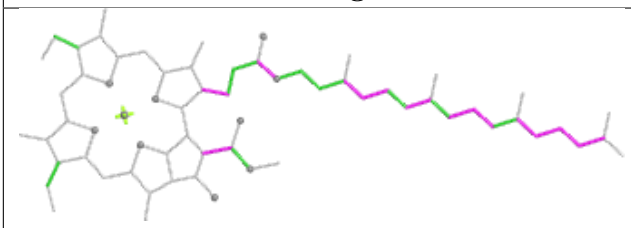


Bond angles



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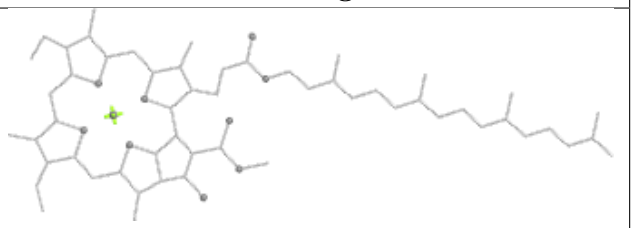
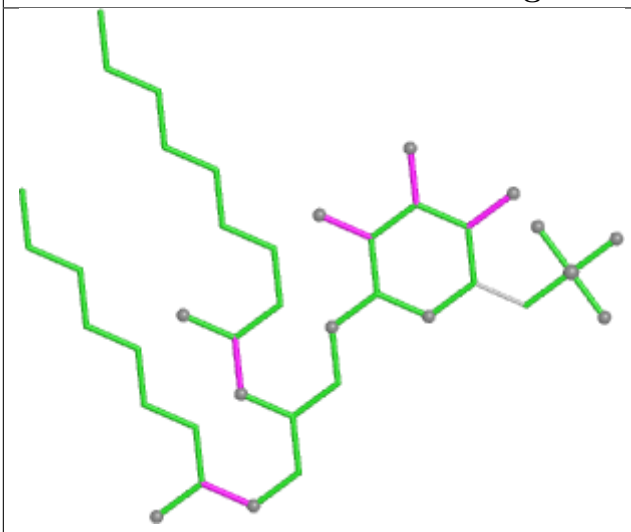


Rings

Ligand SQD D 321



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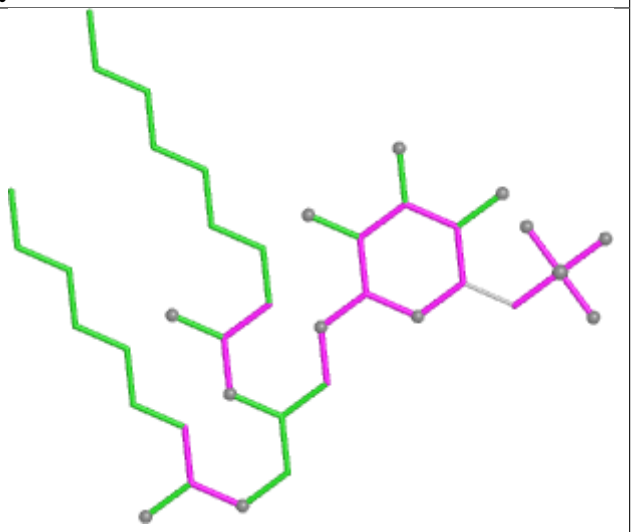

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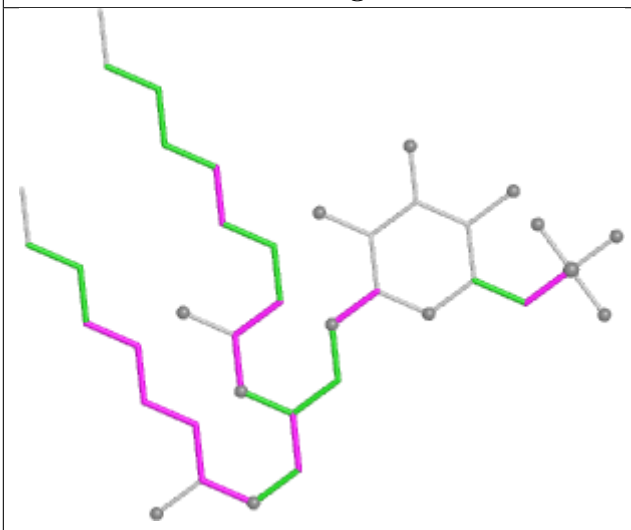

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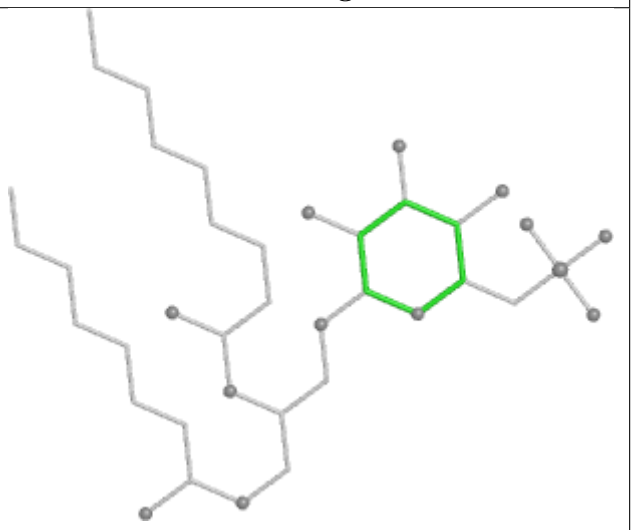
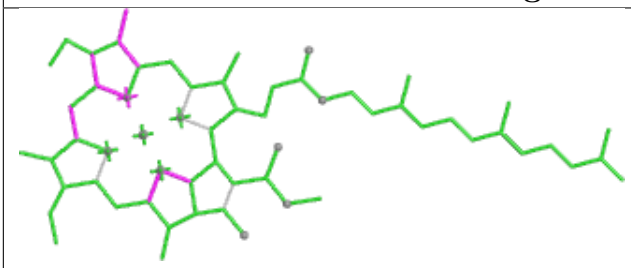
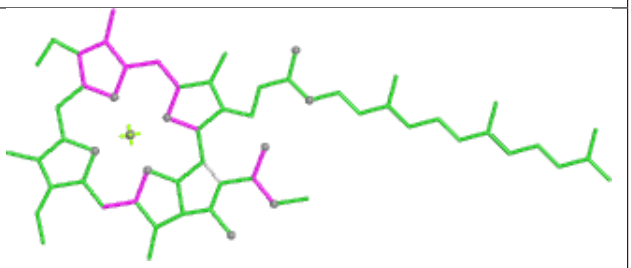
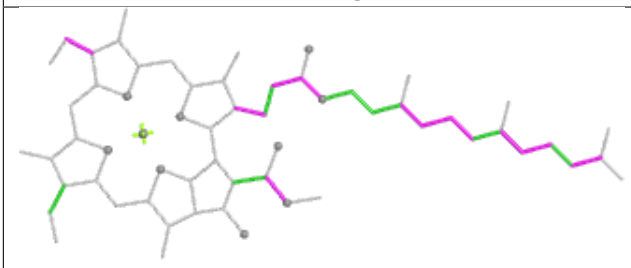
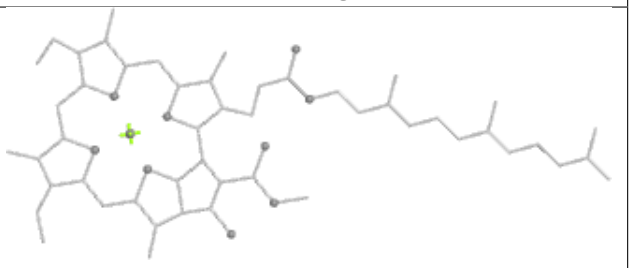
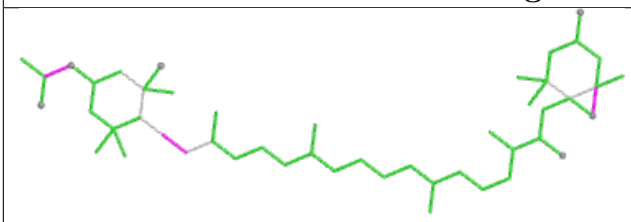
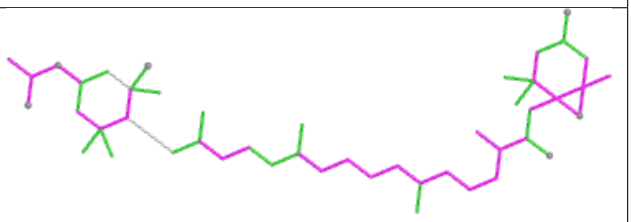
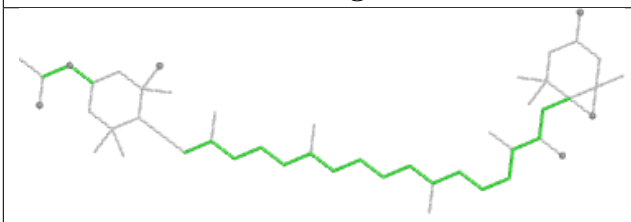
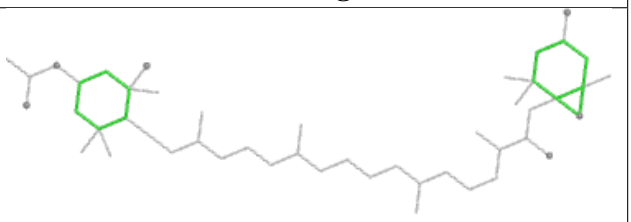
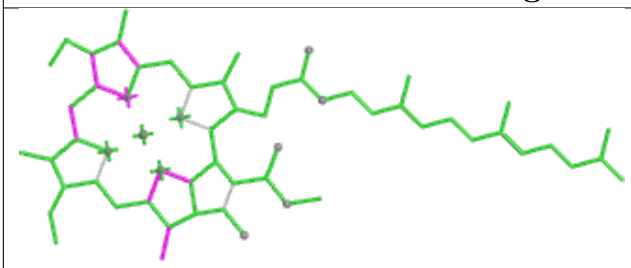


Rings

Ligand CLA X 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 W 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 207



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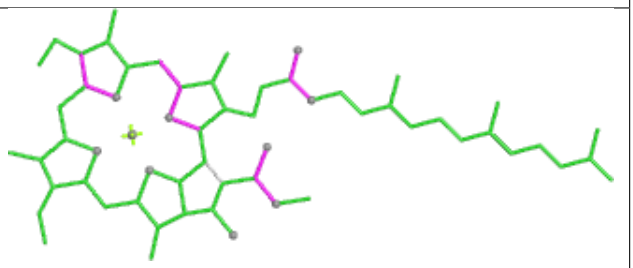
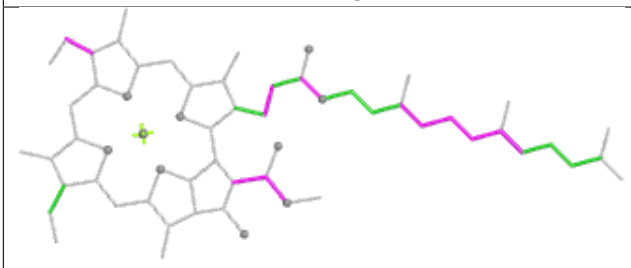


Bond angles



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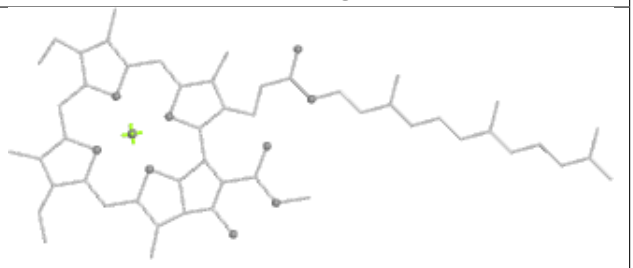
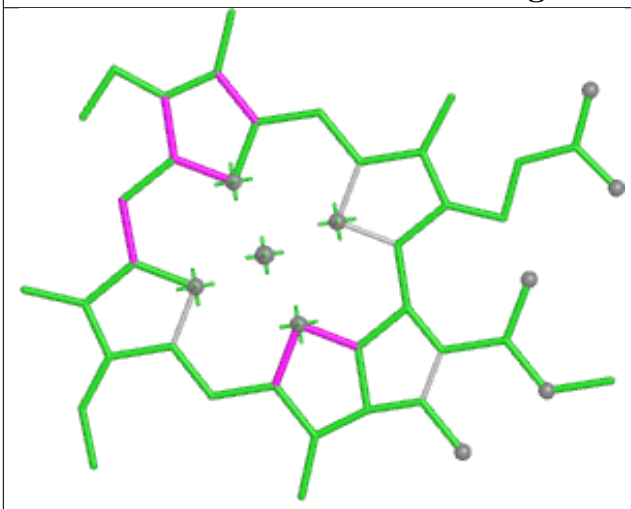


Rings

Ligand CLA x 311



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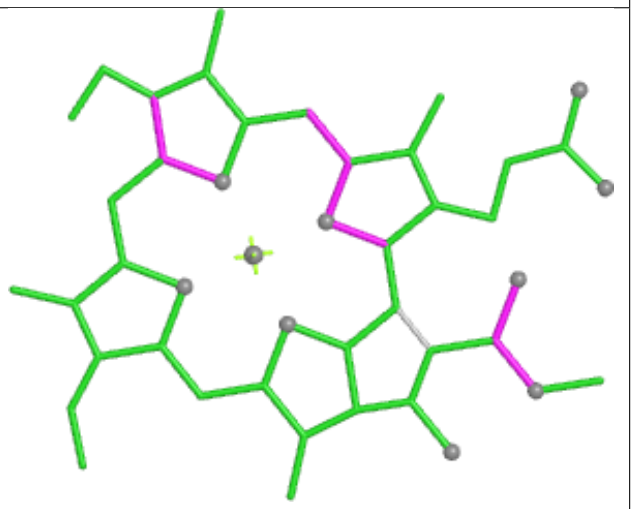
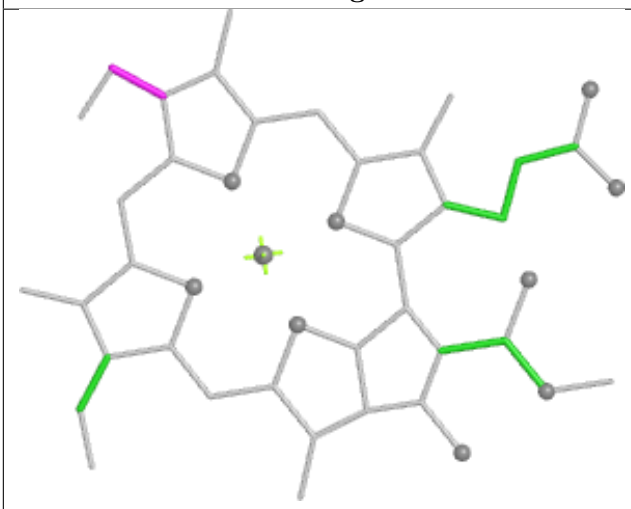


Bond angles



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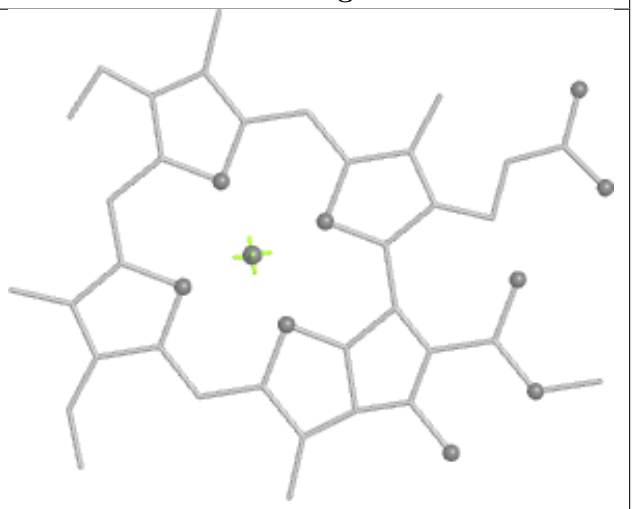
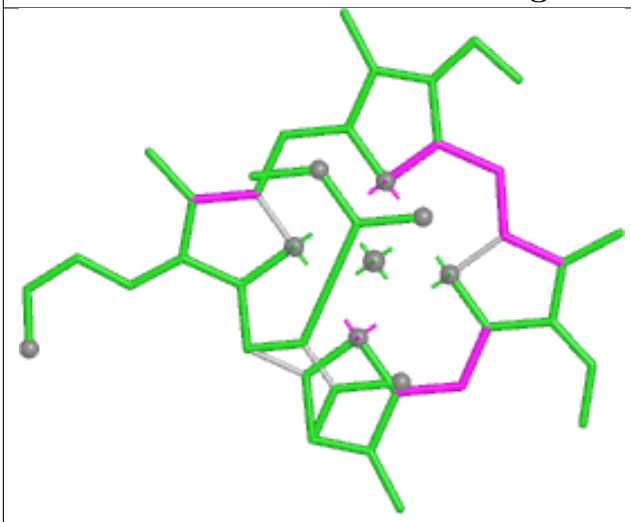


Rings

Ligand KC2 0 314



Bond lengths

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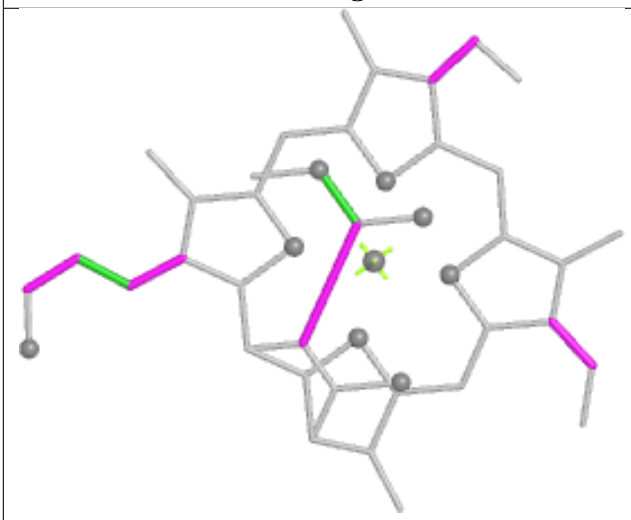

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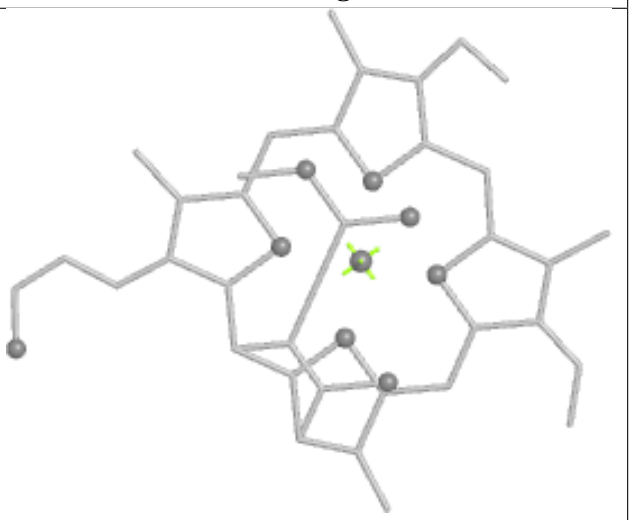
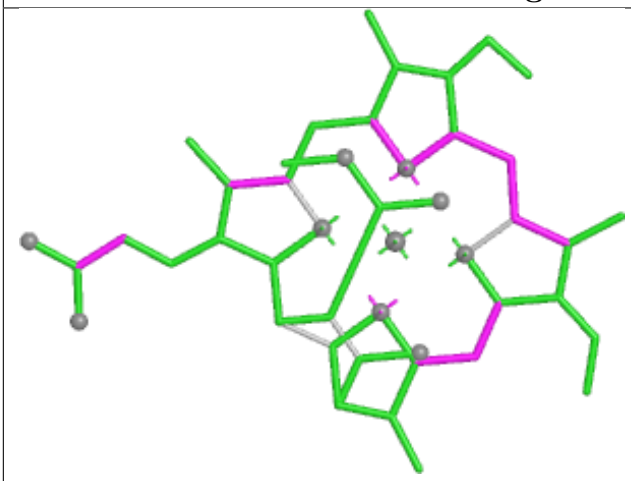


Rings

Ligand KC2 V 315



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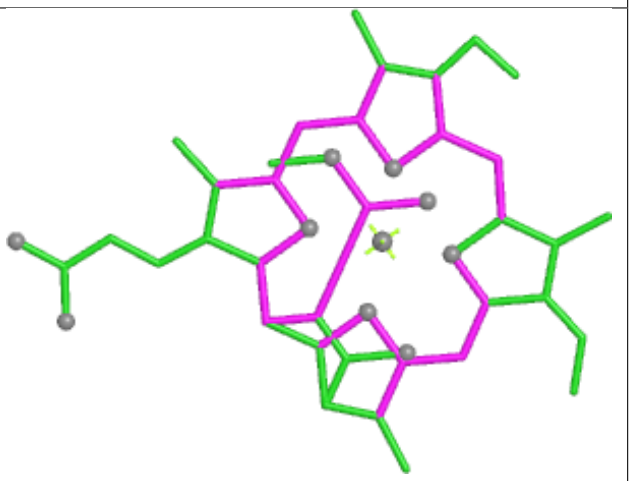
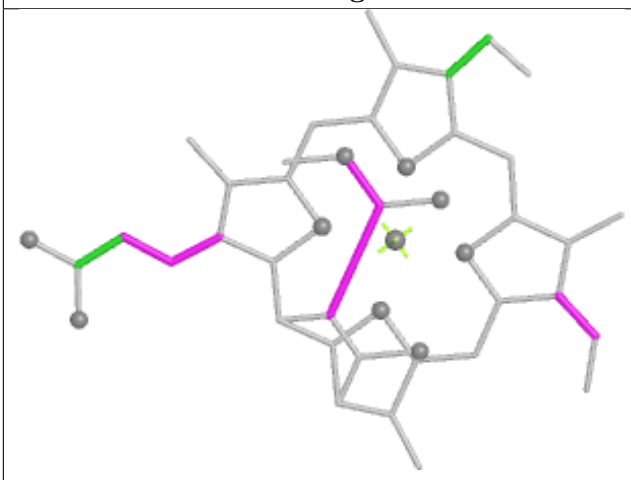


Bond angles



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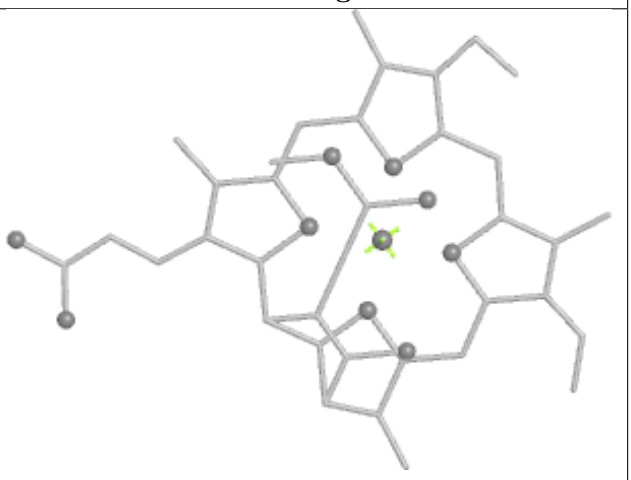
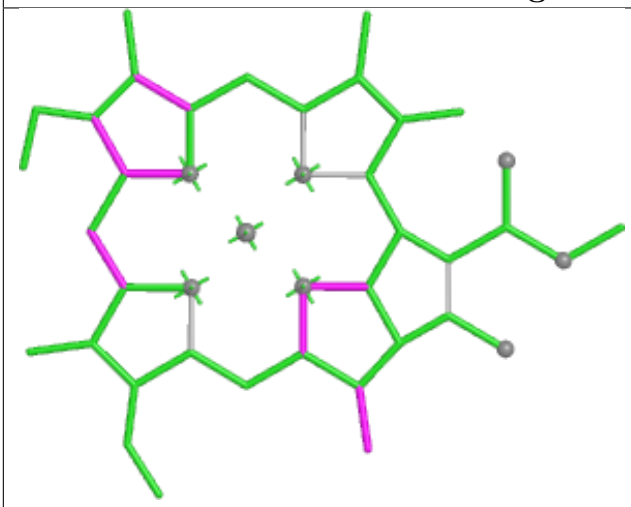


Rings

Ligand CLA 2 307



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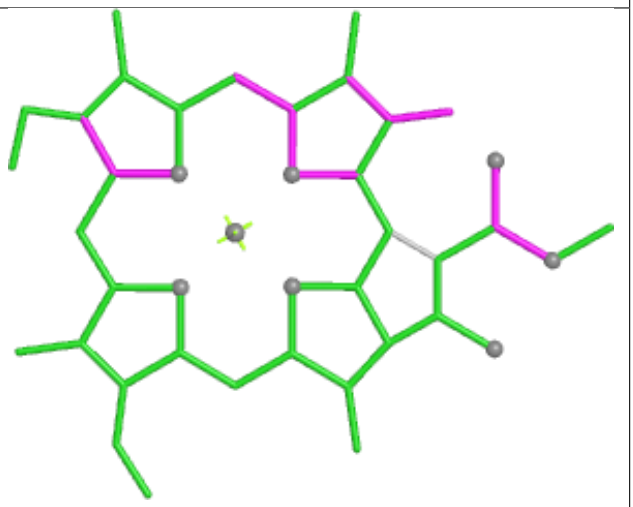
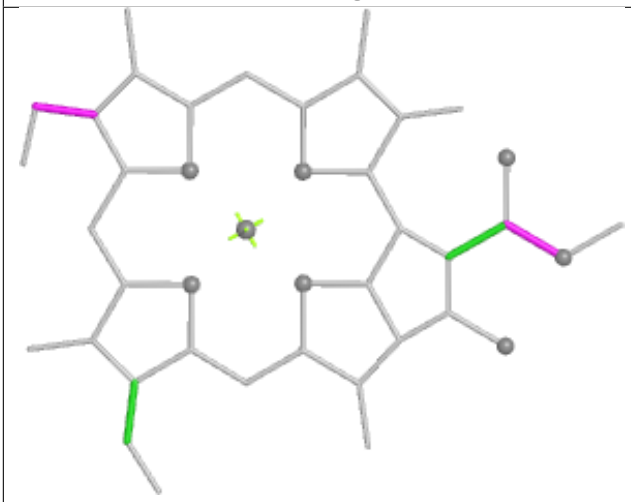


Bond angles



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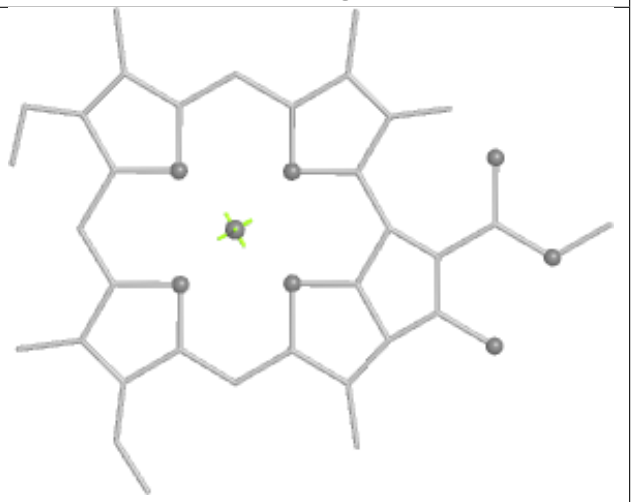
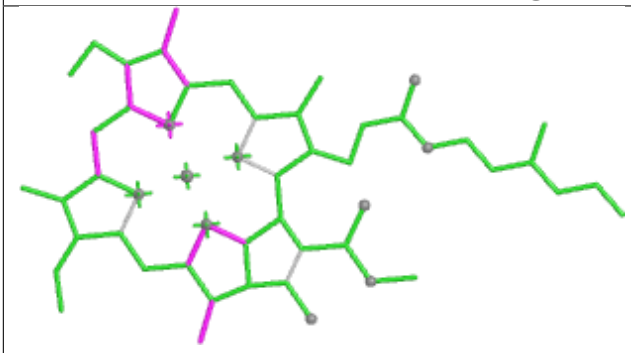


Rings

Ligand CLA S 319



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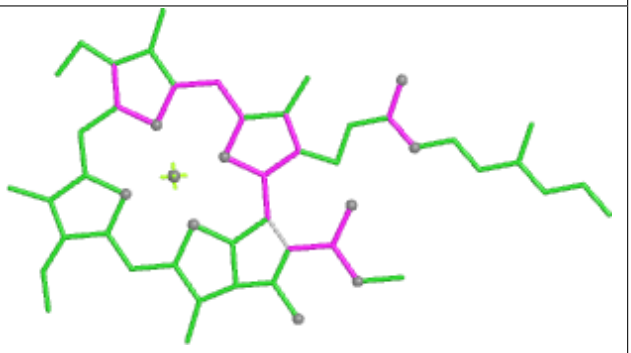
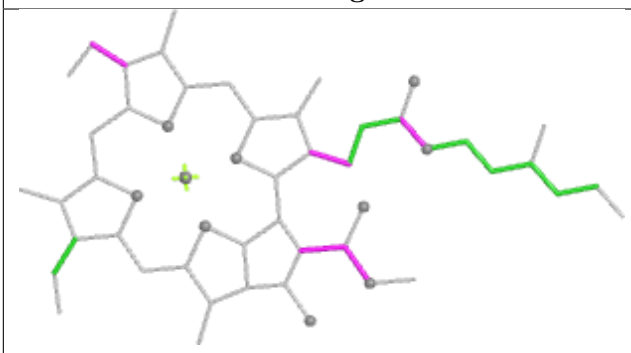


Bond angles



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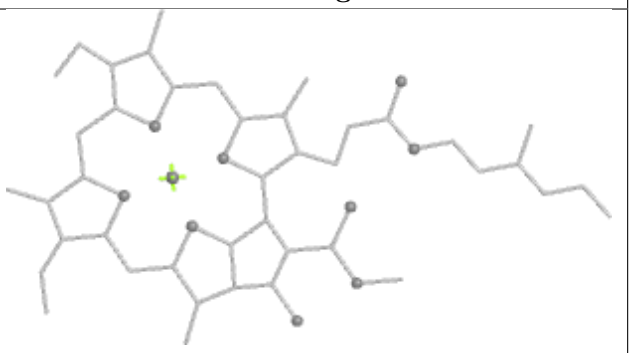
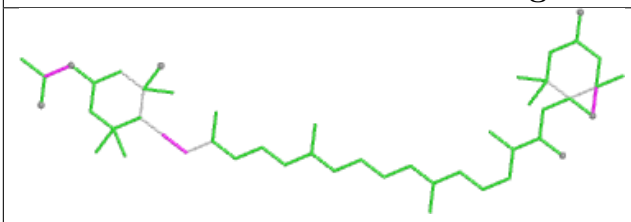


Rings

Ligand A86 X 303



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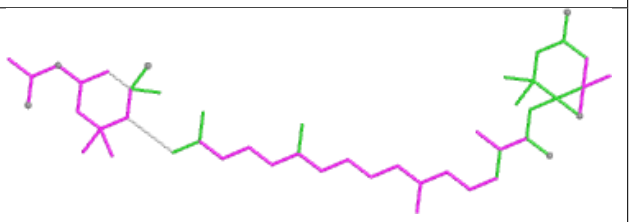
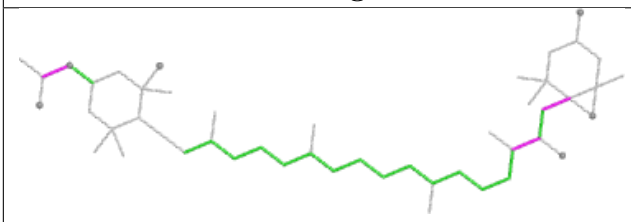
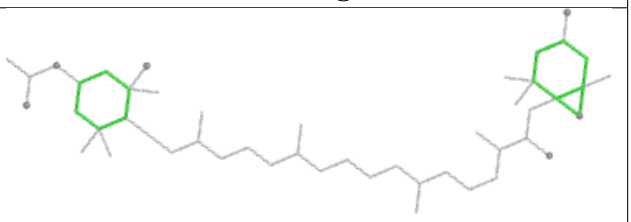


Bond angles

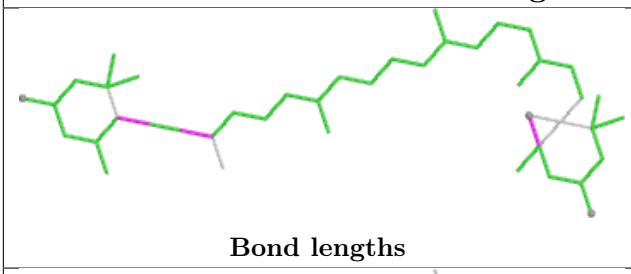


Torsions

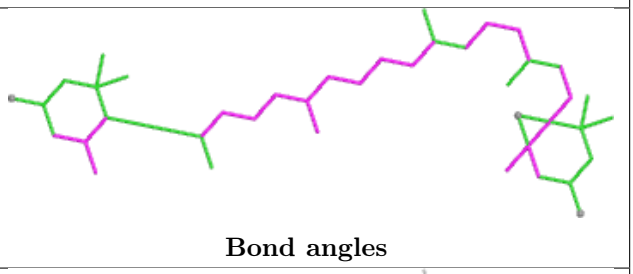


Rings

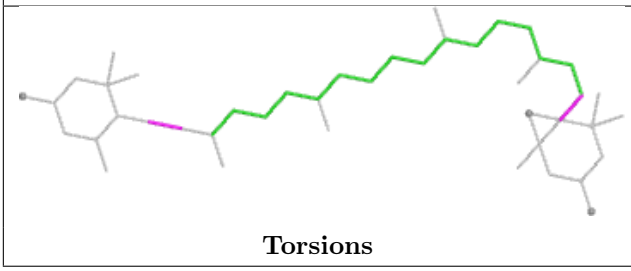
Ligand DD6 3 301



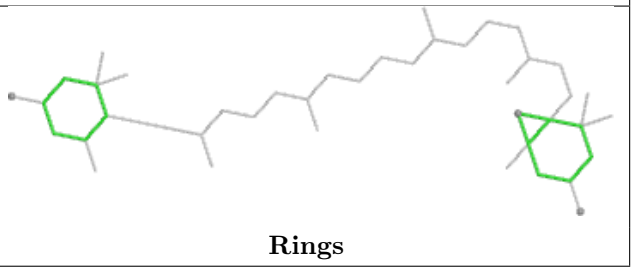
Bond lengths



Bond angles

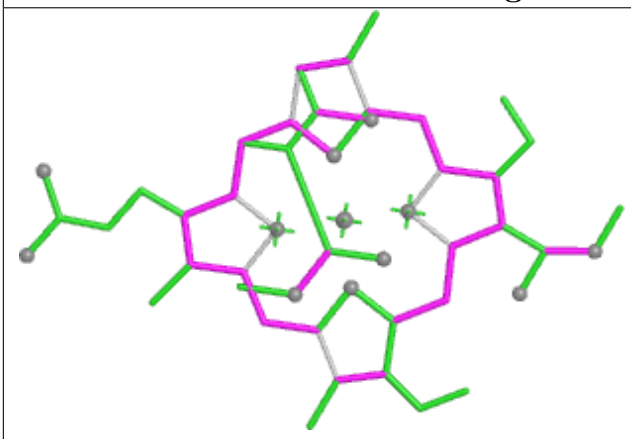


Torsions

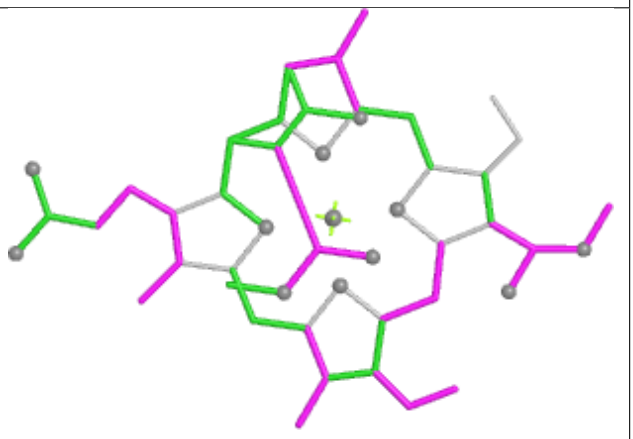


Rings

Ligand A1ECV 7 317



Bond lengths



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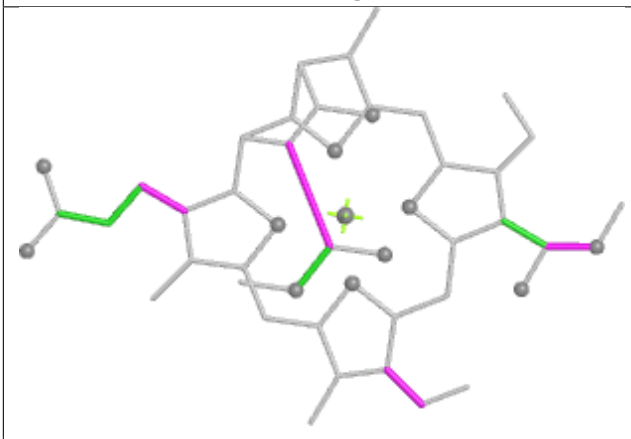

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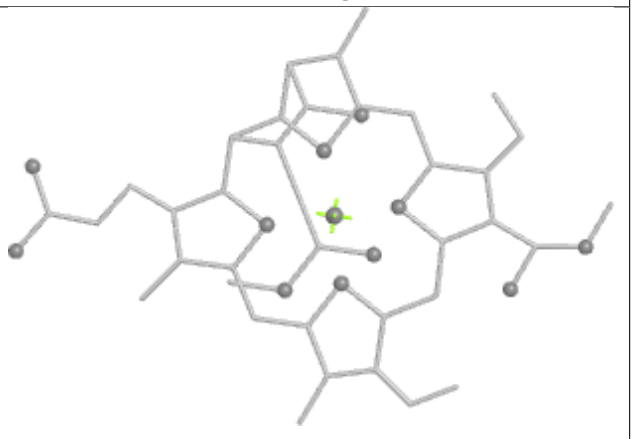
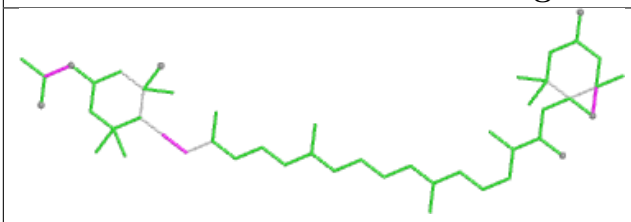


Rings

Ligand A86 6 307



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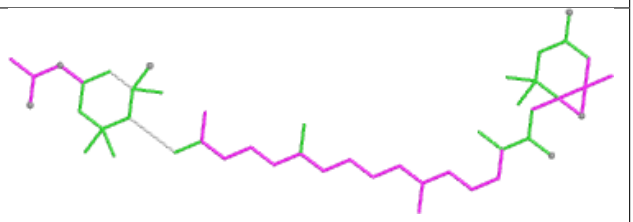

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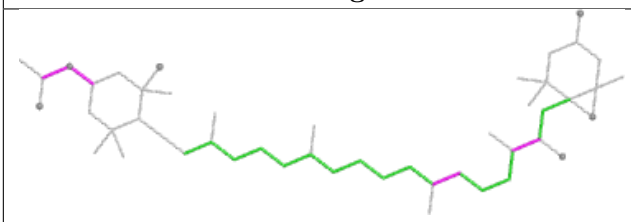

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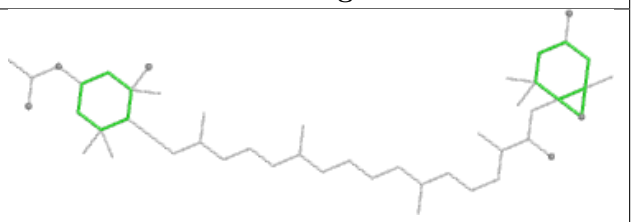
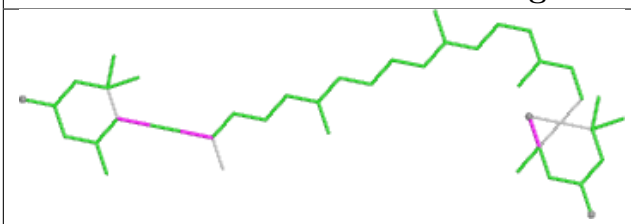


Rings

Ligand DD6 4 308



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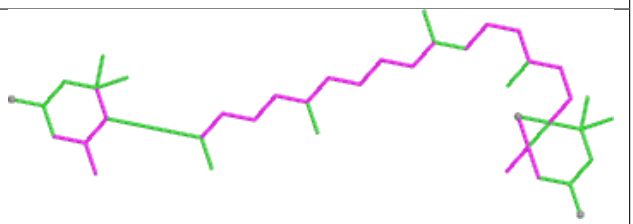
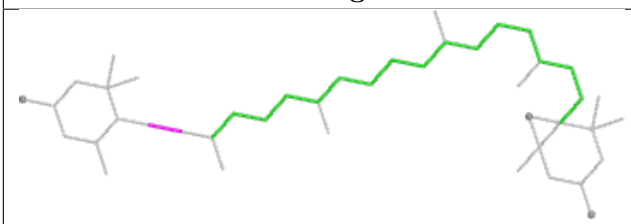


Bond angles



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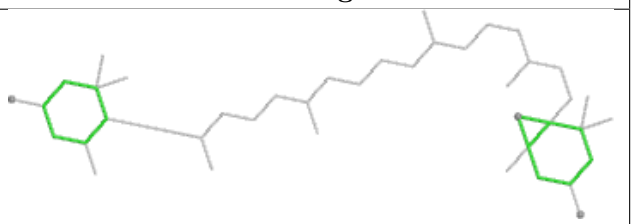
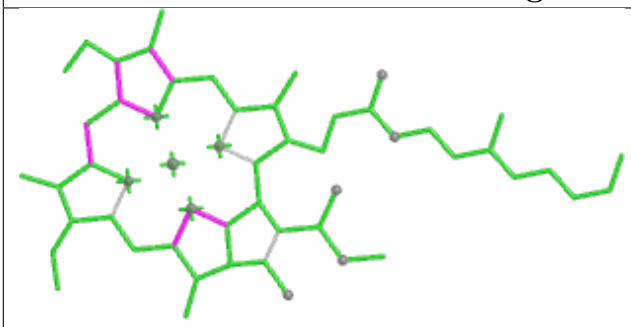


Rings

Ligand CLA F 310



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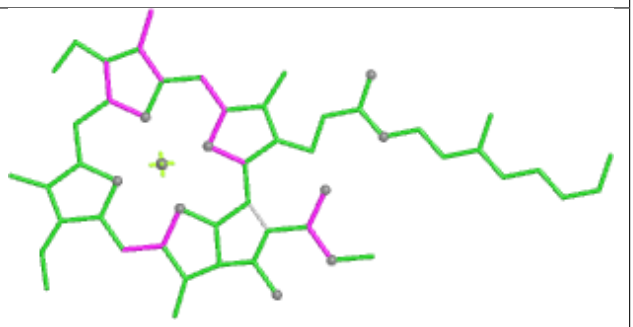

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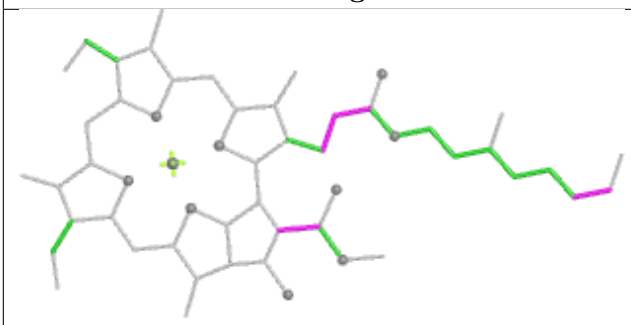

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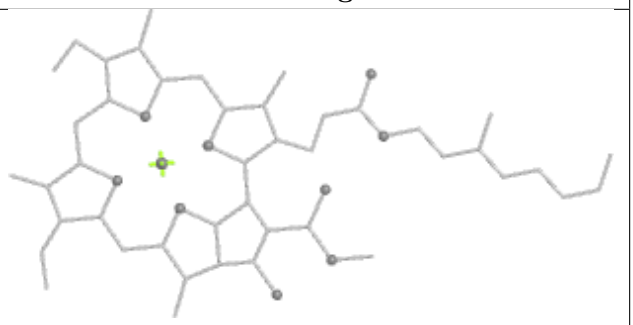
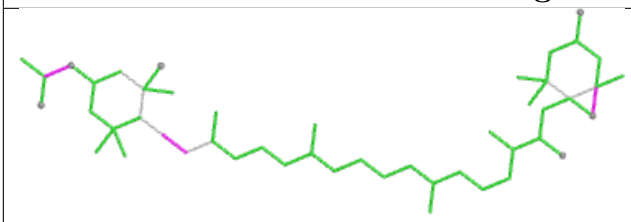


Rings

Ligand A86 1 307



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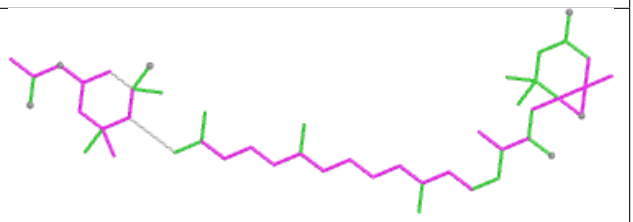

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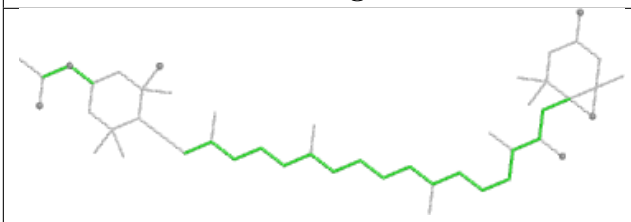

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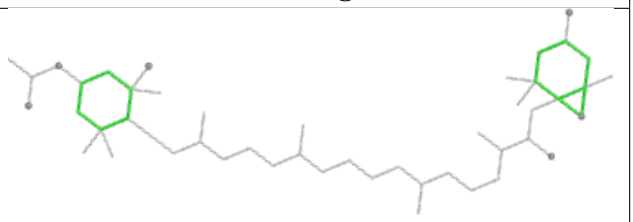
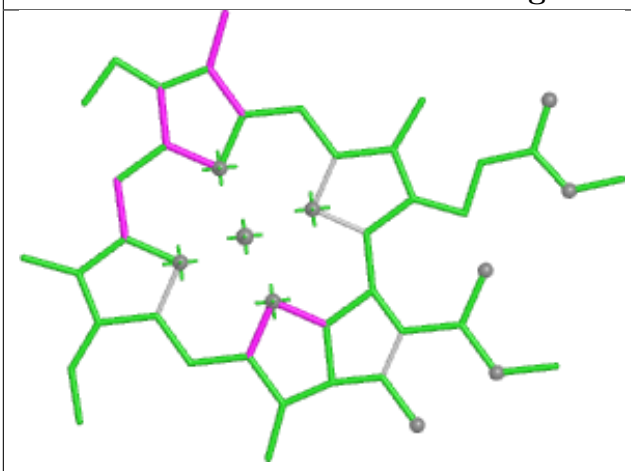


Rings

Ligand CLA 4 313



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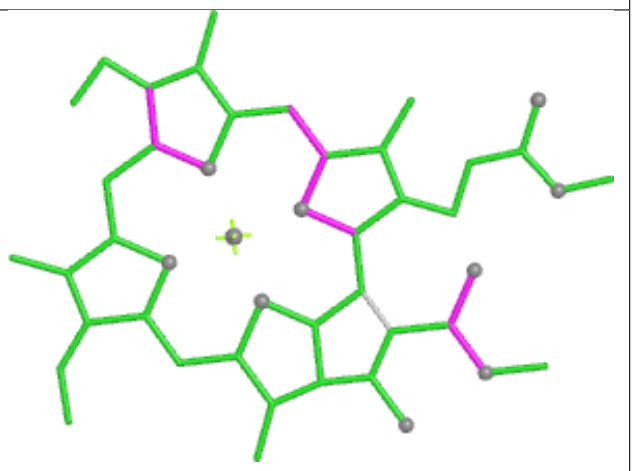

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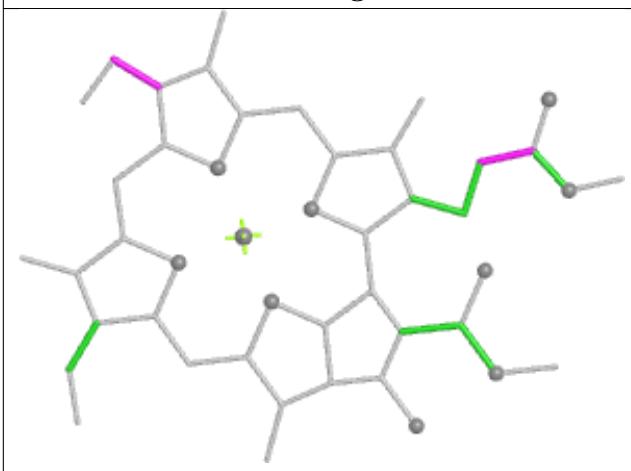

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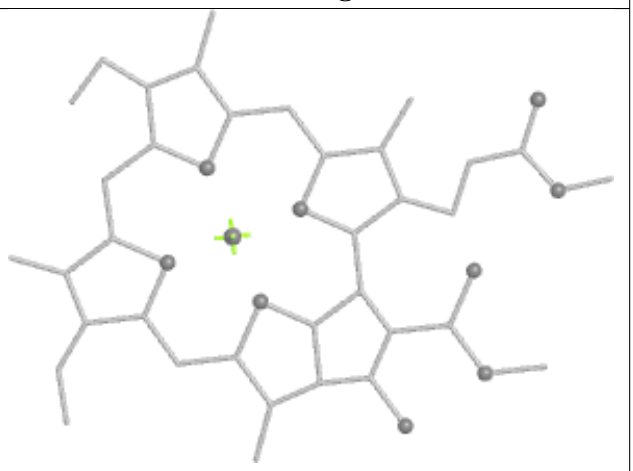
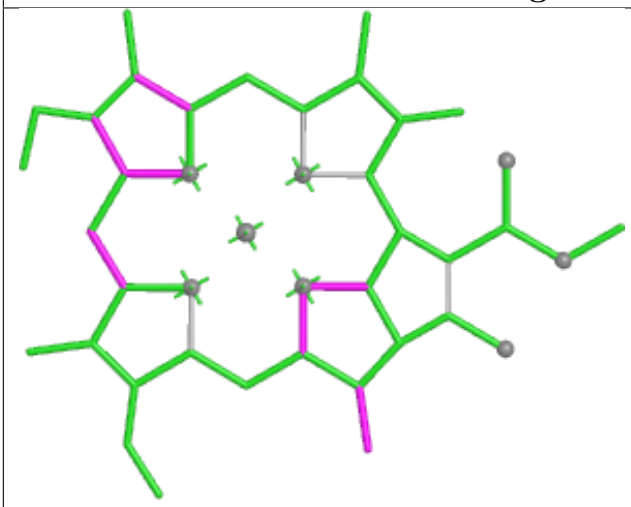


Rings

Ligand CLA z 309



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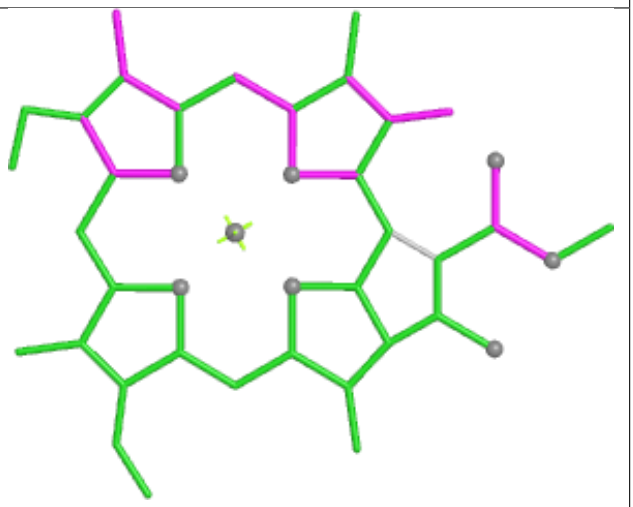

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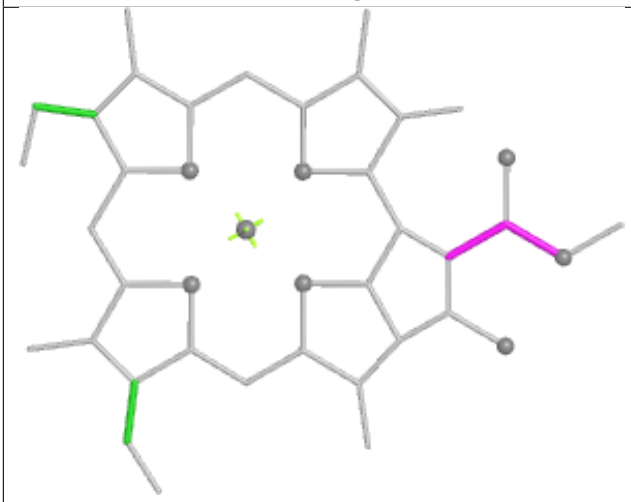

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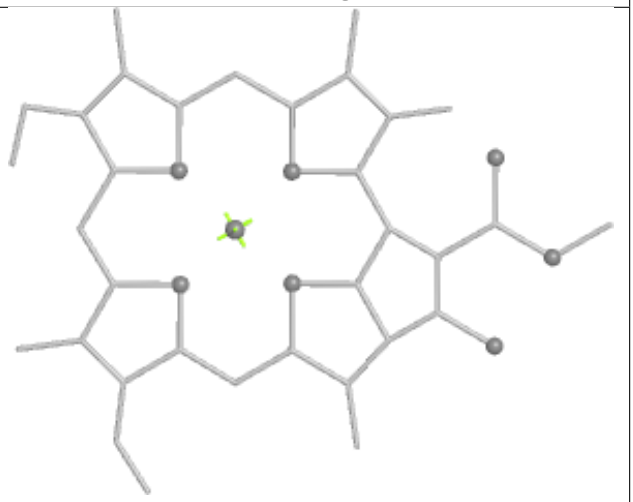
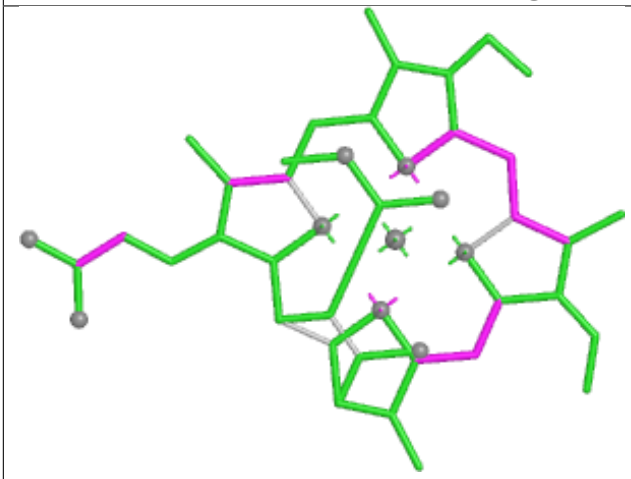


Rings

Ligand KC2 A 313



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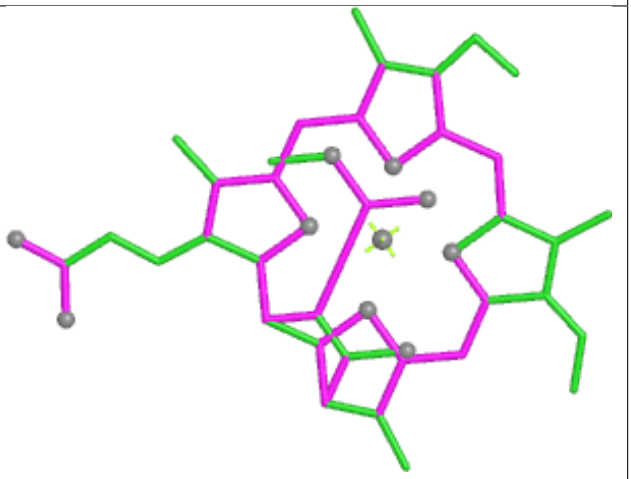

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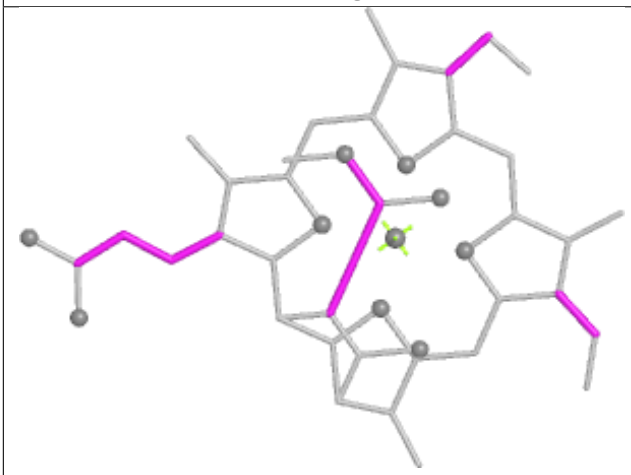

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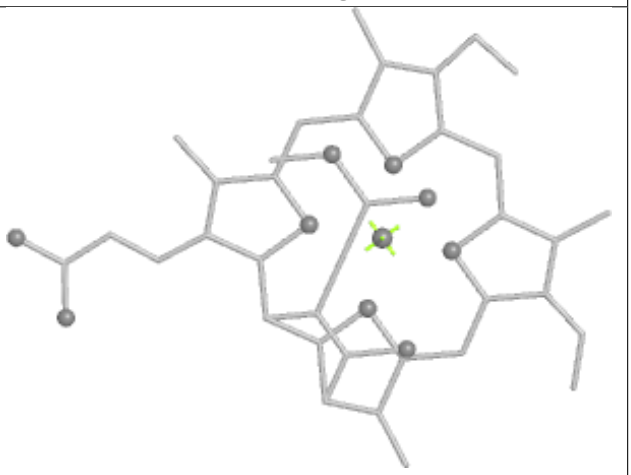
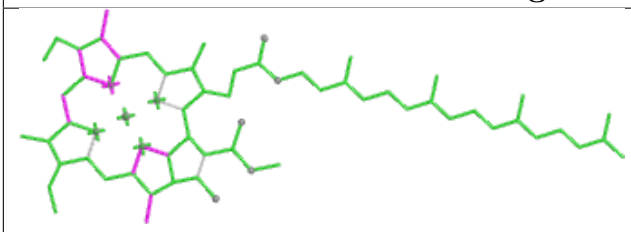


Rings

Ligand CLA 4 323



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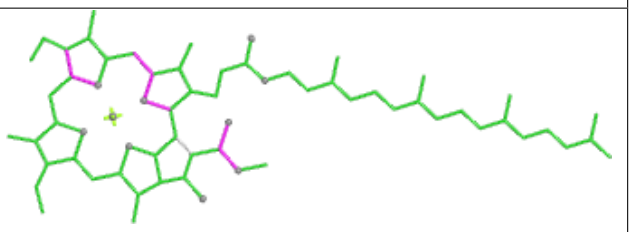
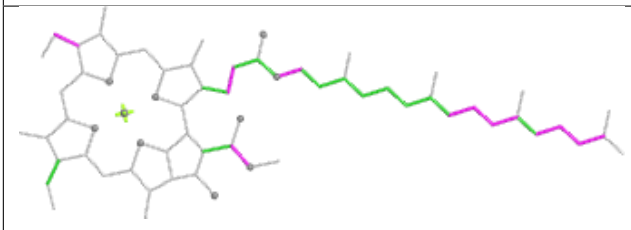


Bond angles



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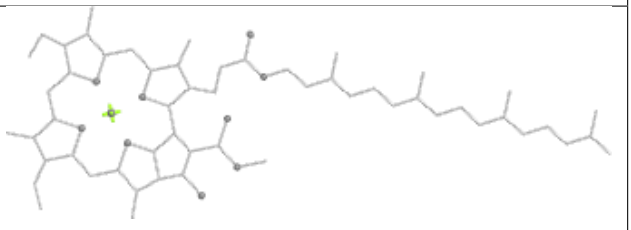
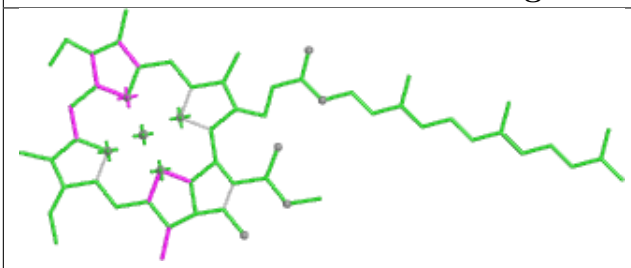
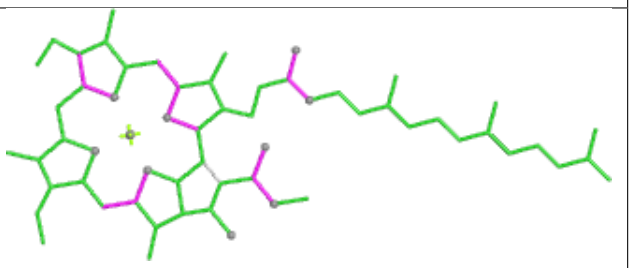
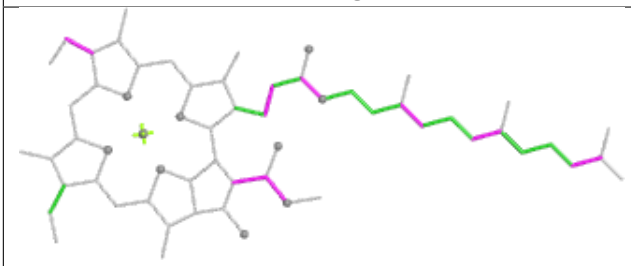
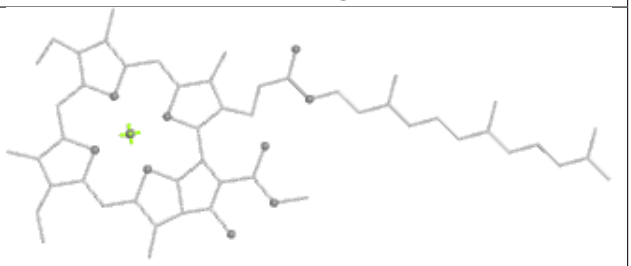
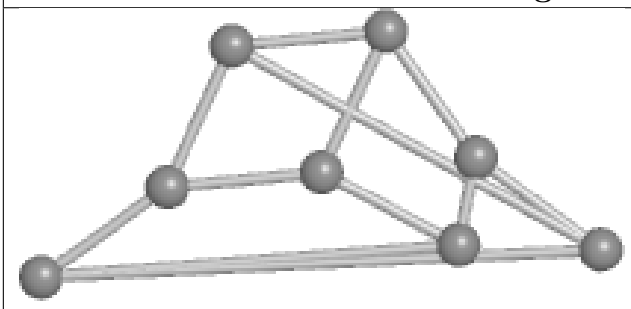
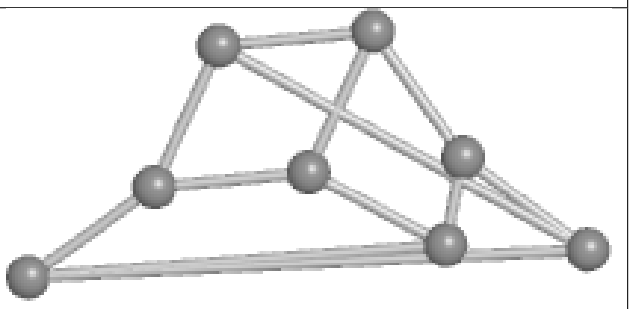
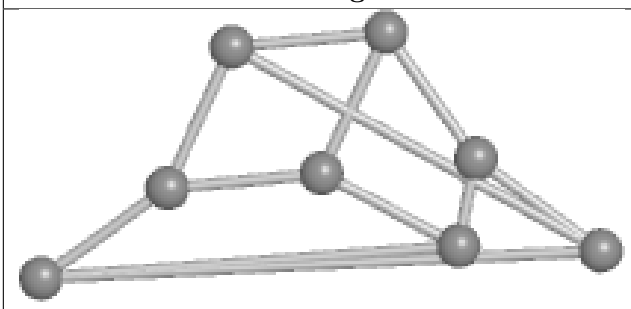
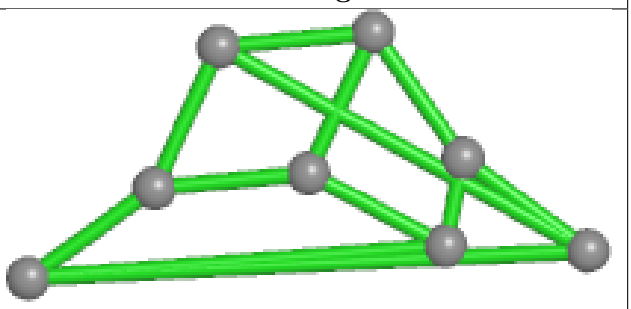
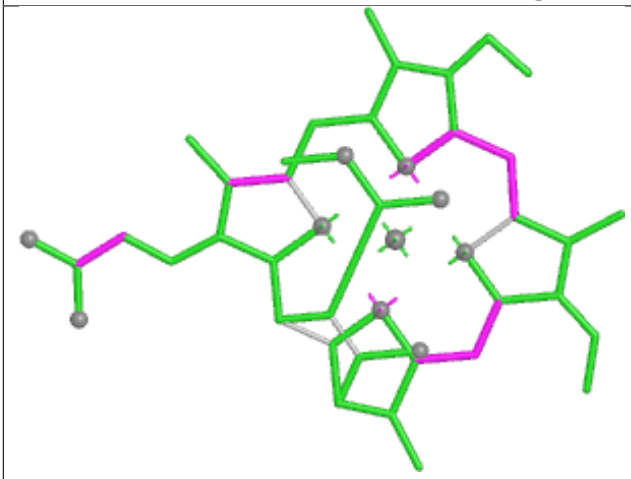


Rings

Ligand CLA C 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SF4 b 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand KC2 6 317



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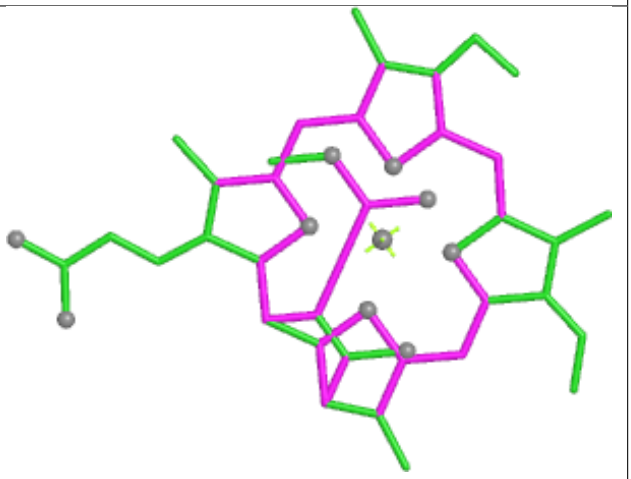
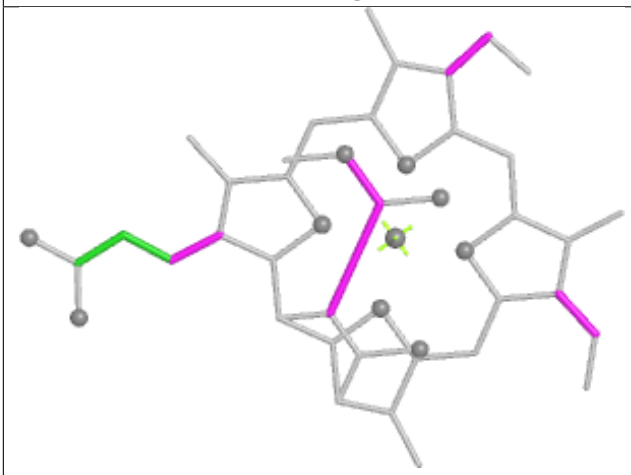
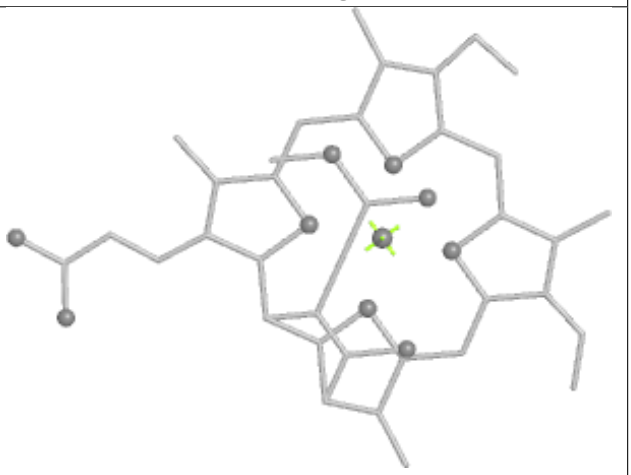


Bond angles

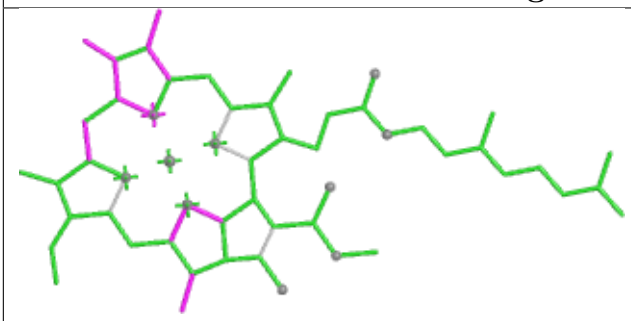


Torsions

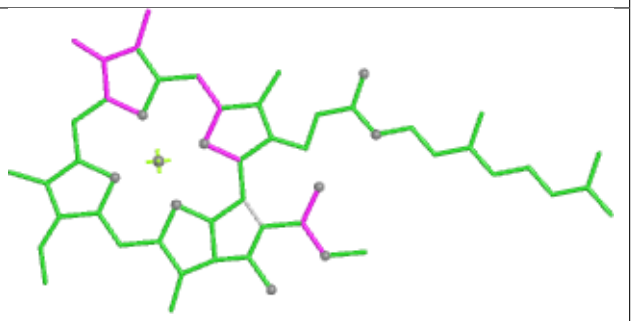


Rings

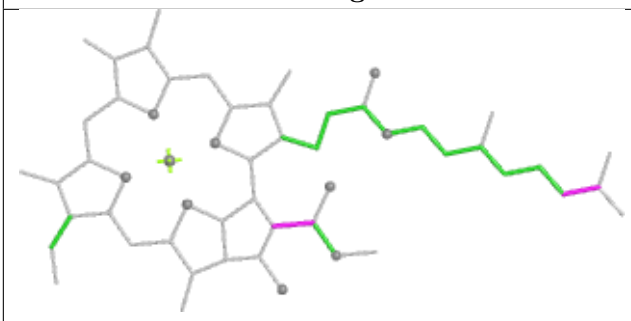
Ligand CLA b 813



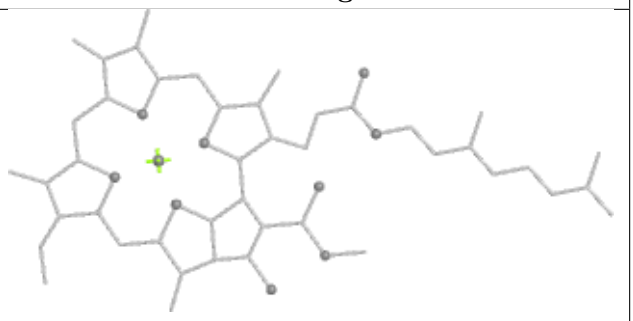
Bond lengths



Bond angles

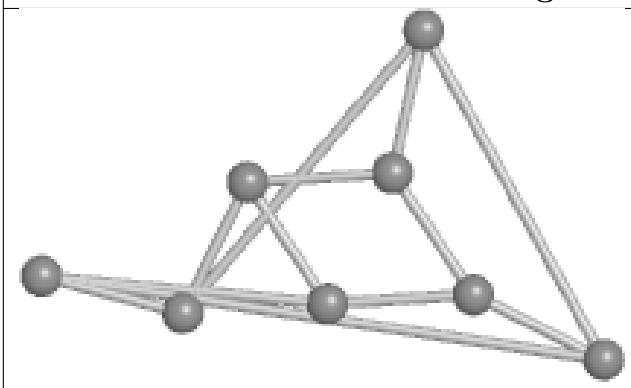


Torsions

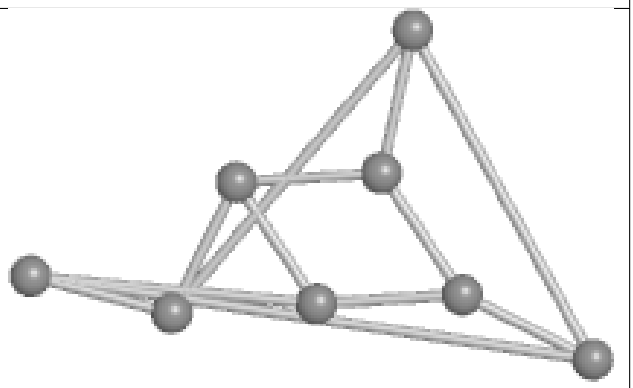


Rings

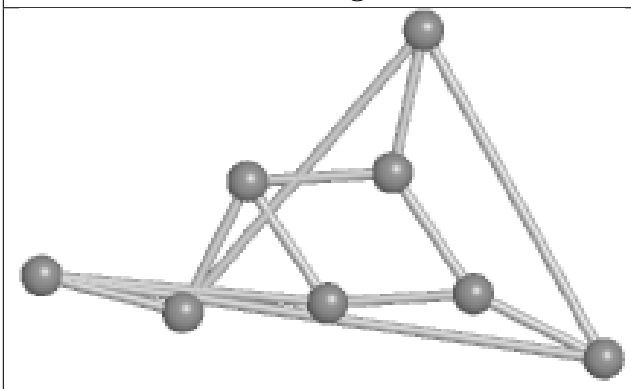
Ligand SF4 c 101



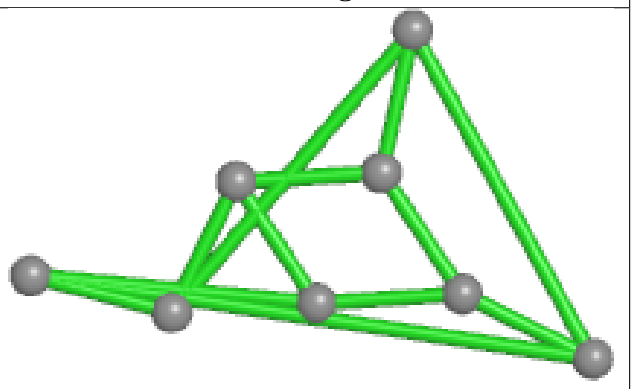
Bond lengths



Bond angles

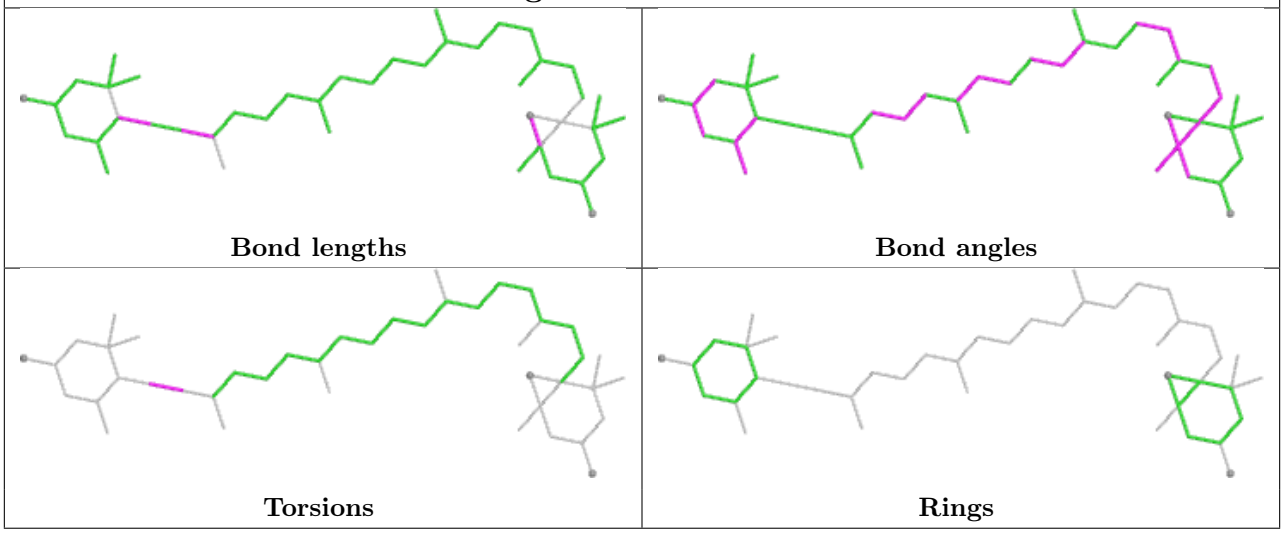


Torsions

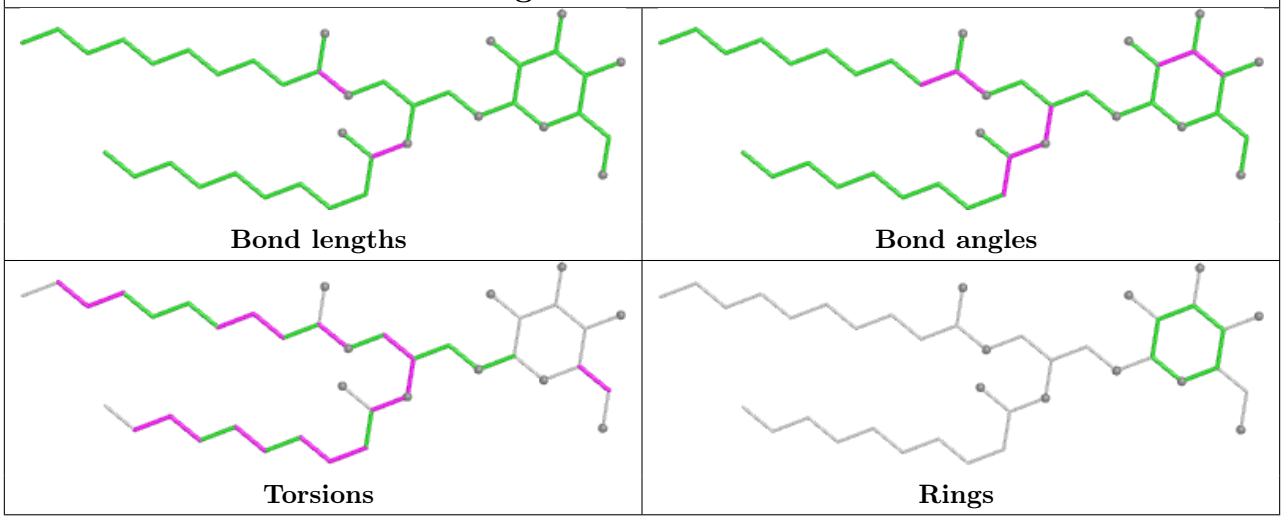


Rings

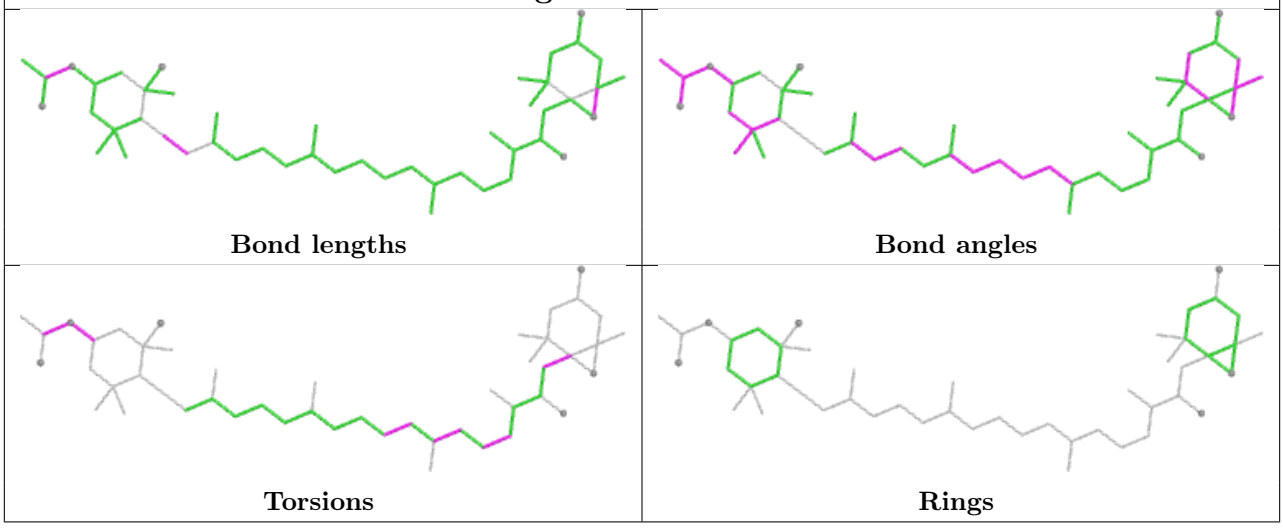
Ligand DD6 H 303



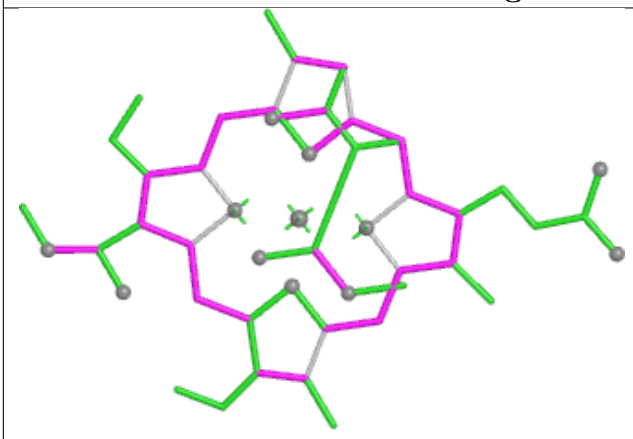
Ligand LMG W 302



Ligand A86 3 306



Ligand A1ECV 7 323



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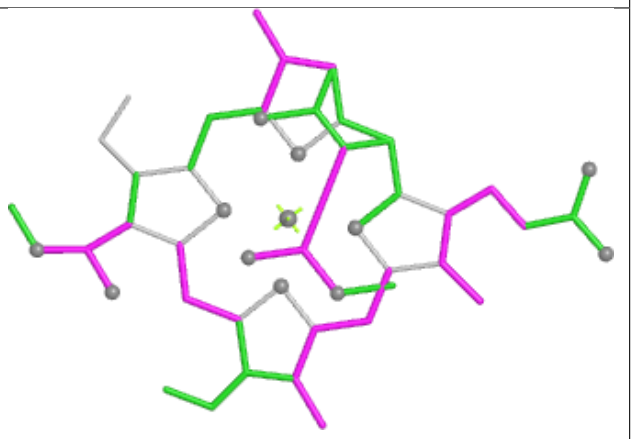

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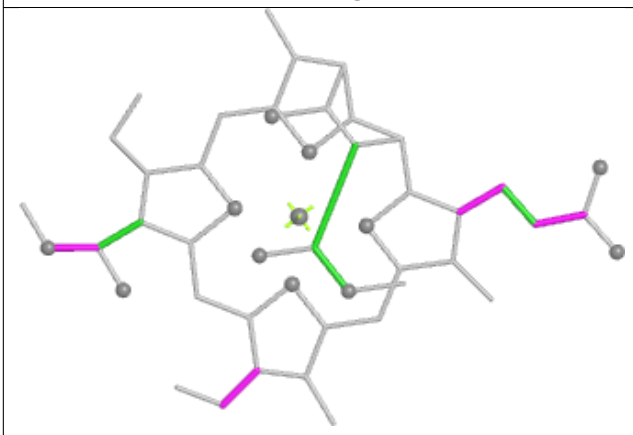
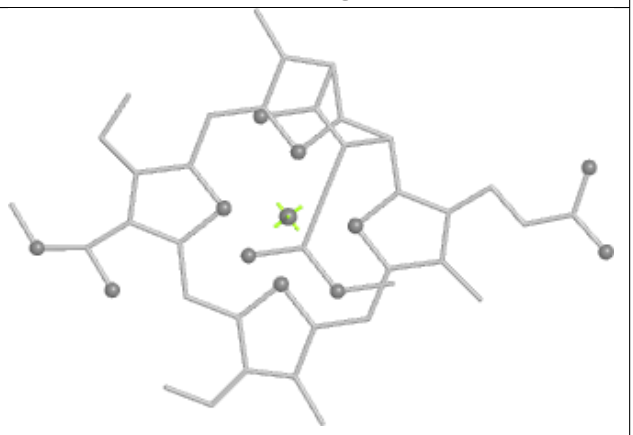
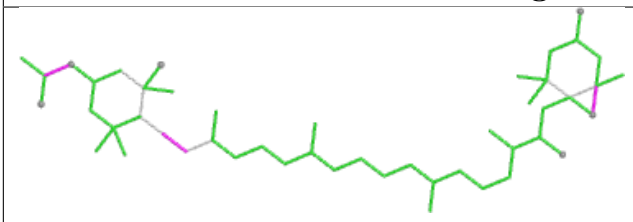


Torsions



Rings

Ligand A86 T 301



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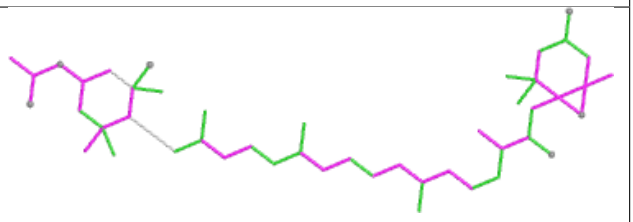

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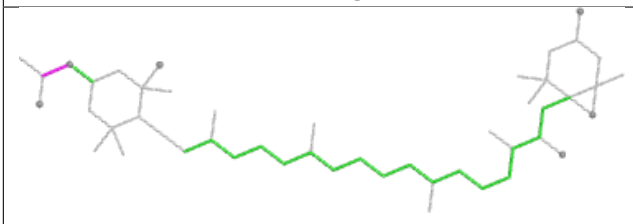

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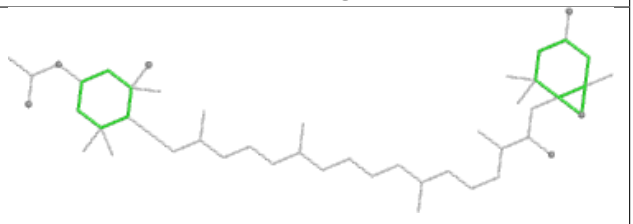
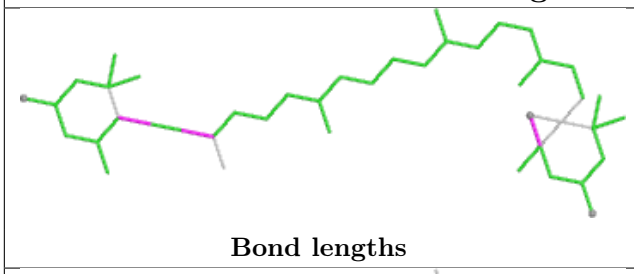


Rings

Ligand DD6 5 303



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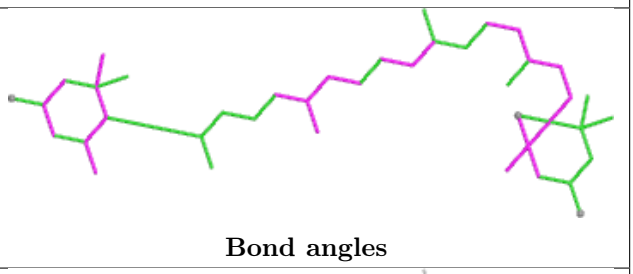
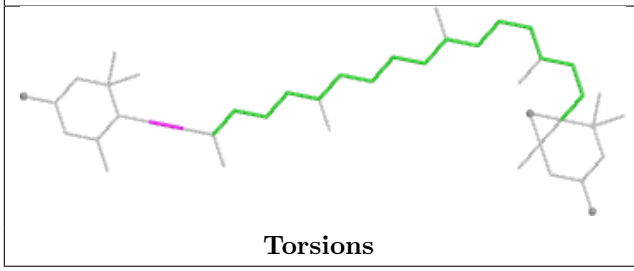


Bond angles



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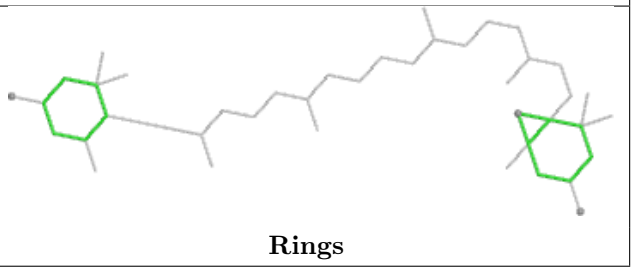
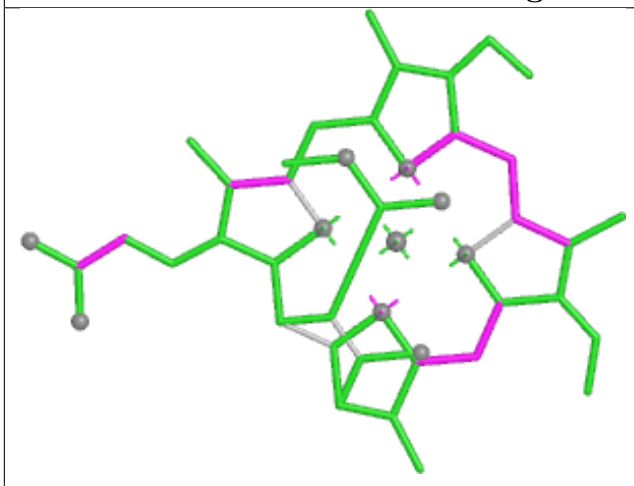


Rings

Ligand KC2 G 313



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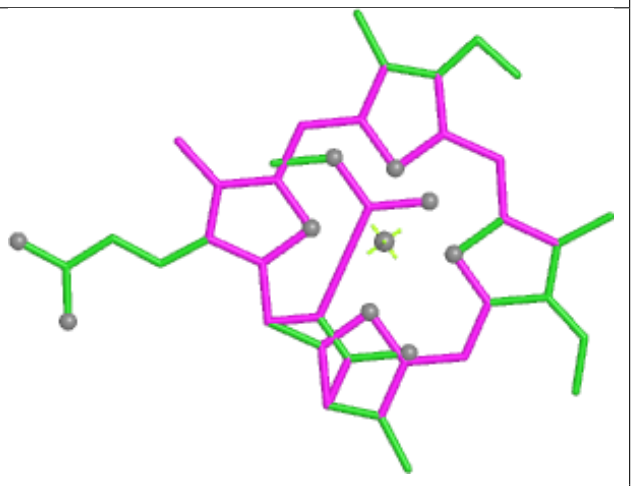

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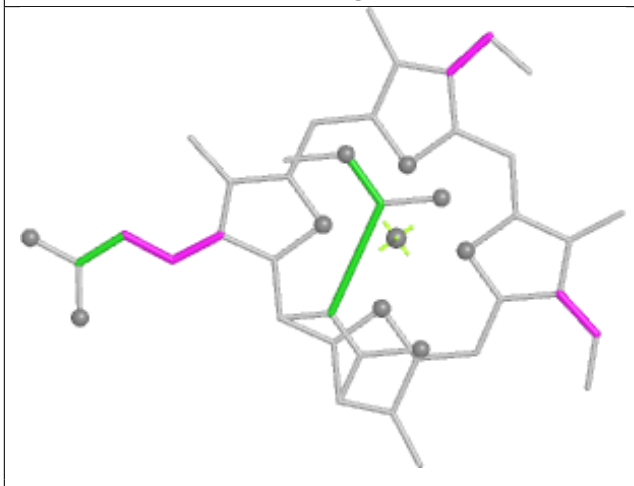

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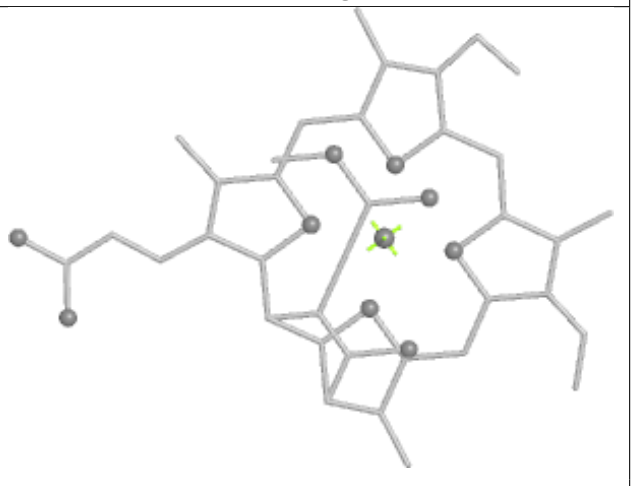
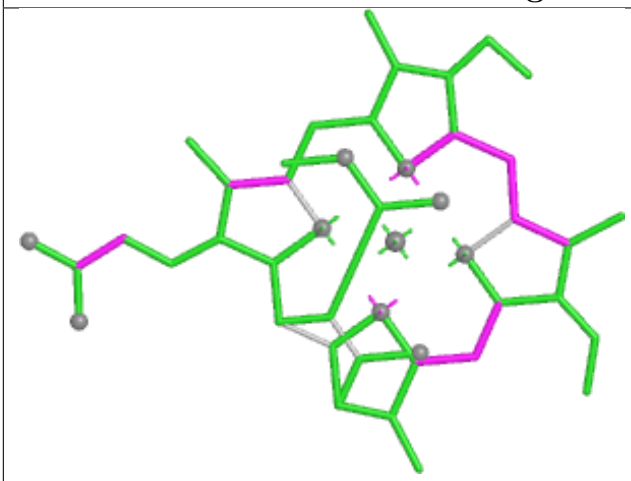


Rings

Ligand KC2 B 208



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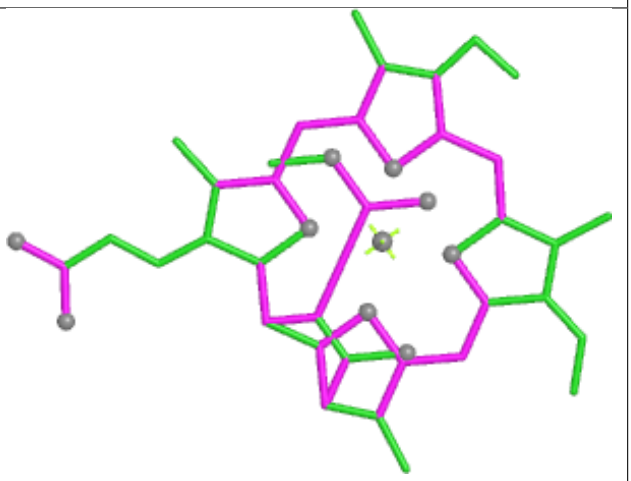

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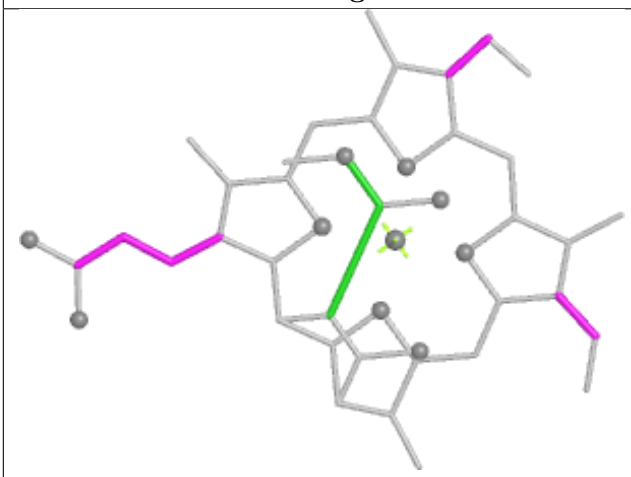
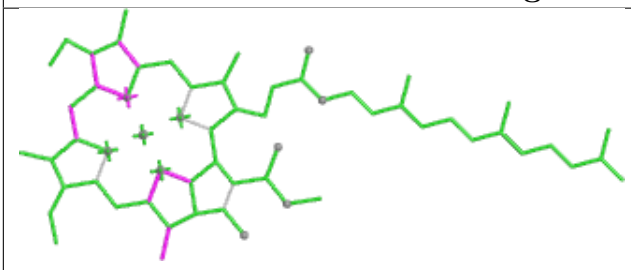


Torsions

Rings

Ligand CLA V 310



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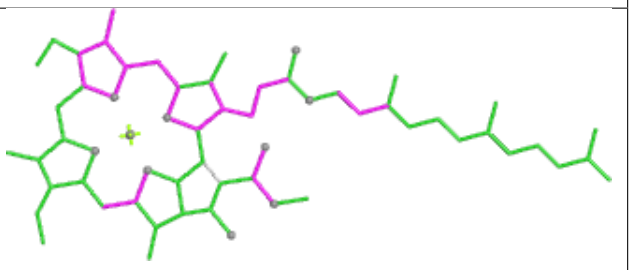

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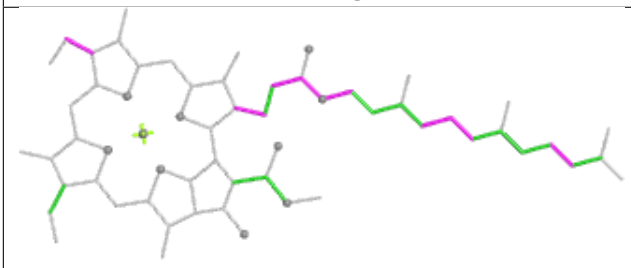

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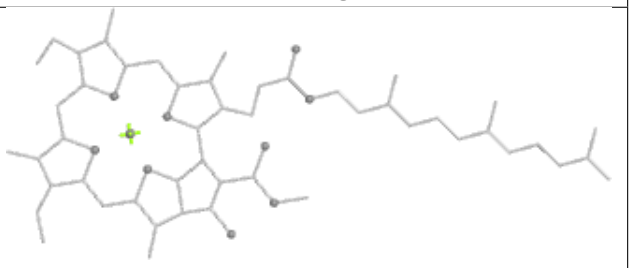
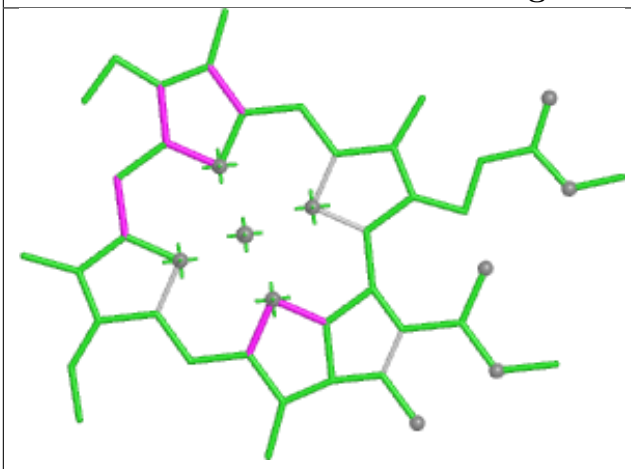


Rings

Ligand CLA 6 322



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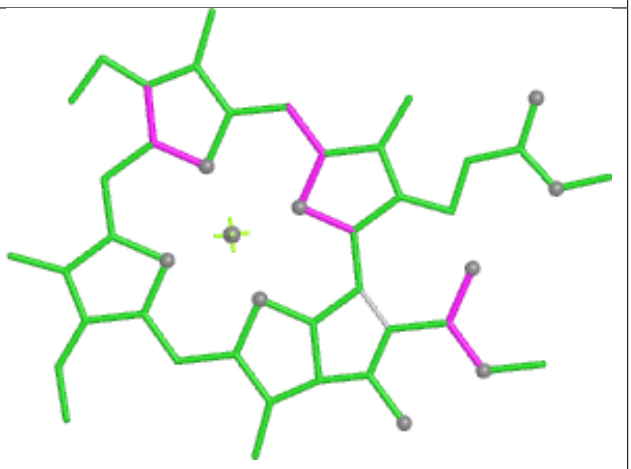
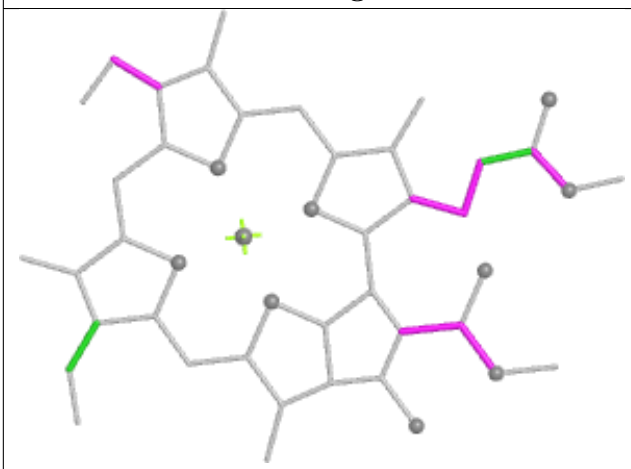


Bond angles



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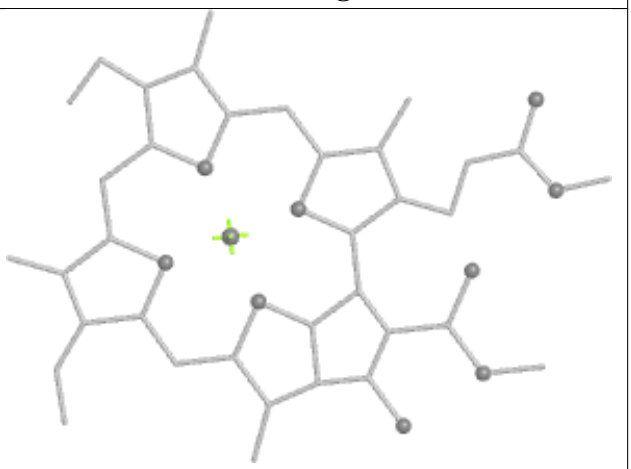
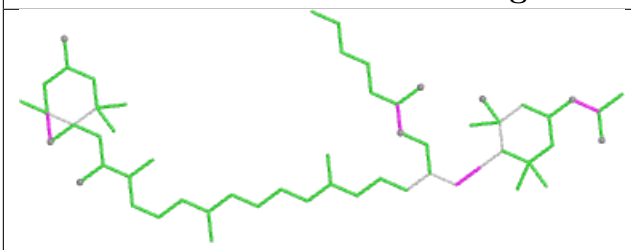


Rings

Ligand A1EB1 3 303



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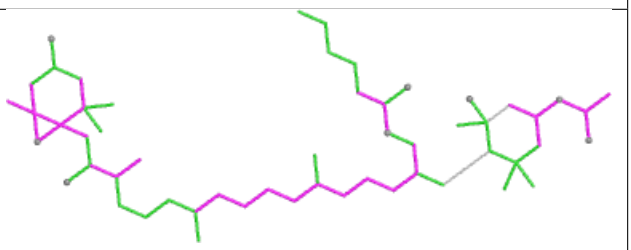

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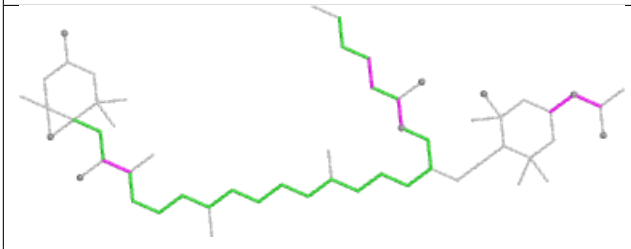

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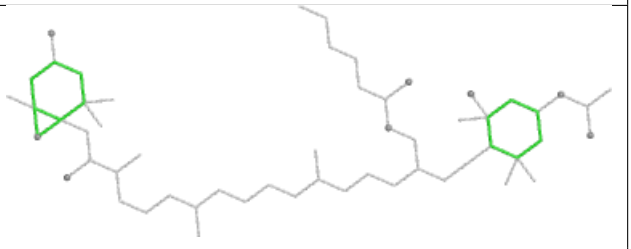
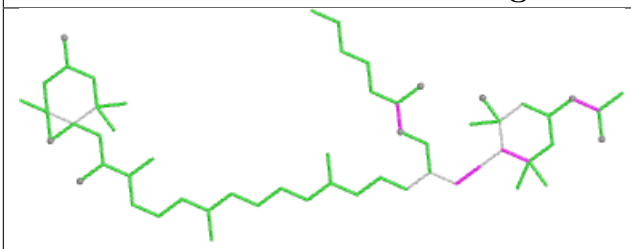


Rings

Ligand A1EB1 8 301



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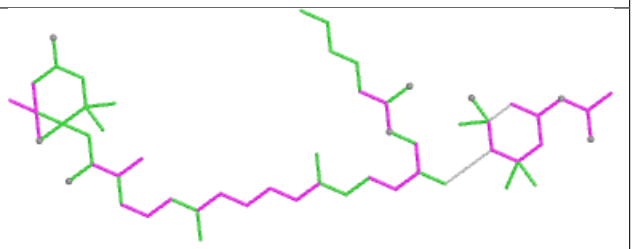
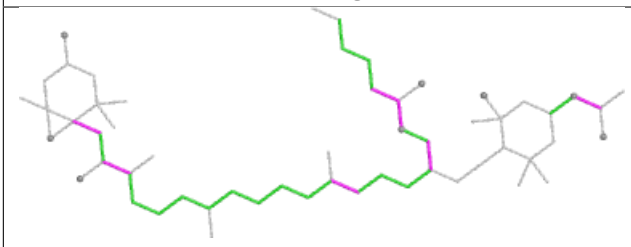


Bond angles



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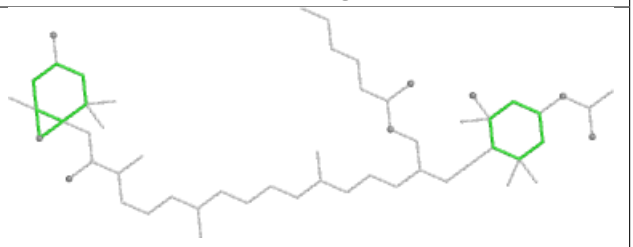
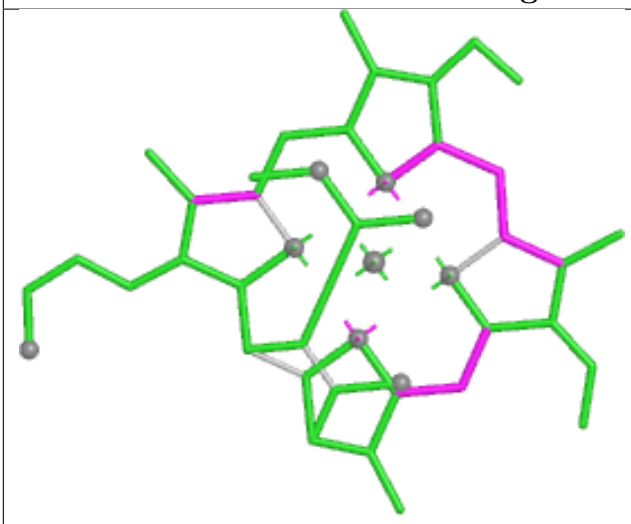


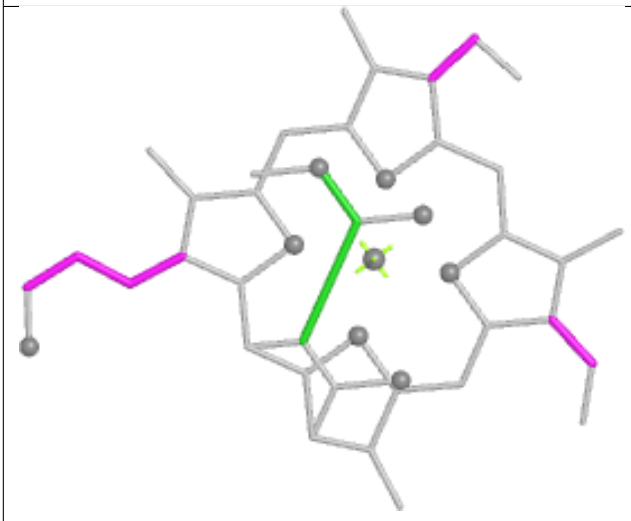
Rings

Ligand KC2 W 312



Bond lengths

Bond angles



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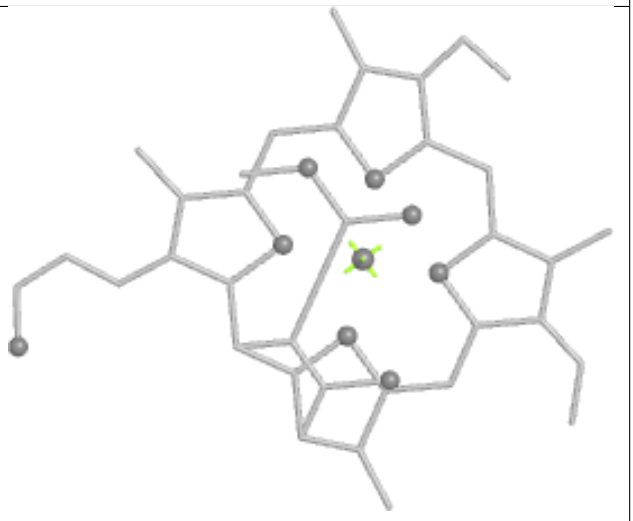
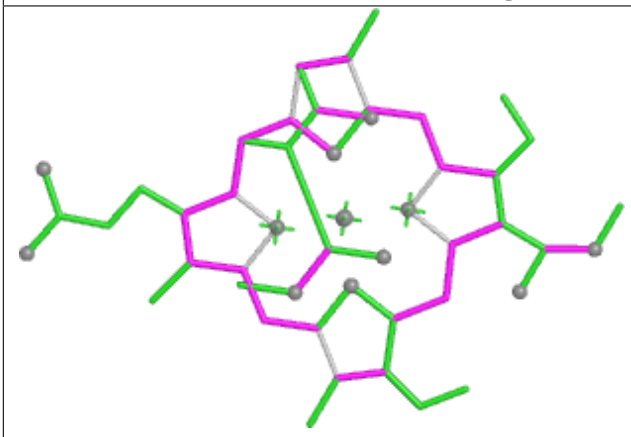


Rings

Ligand A1ECV X 310



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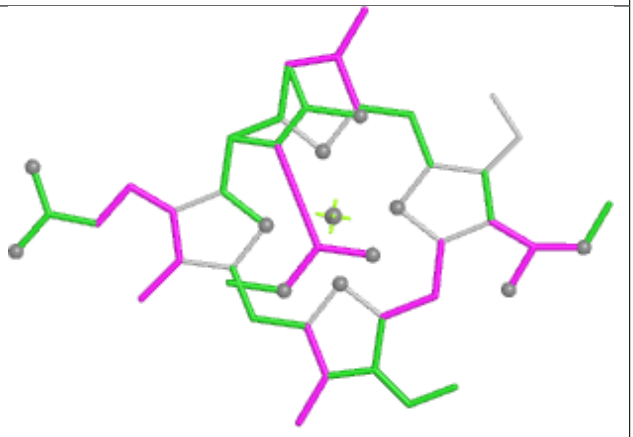
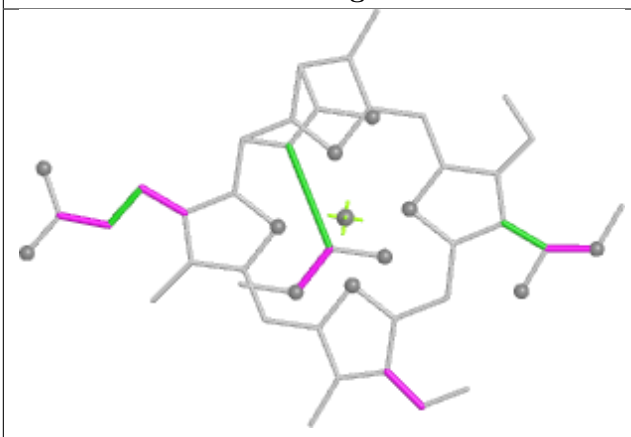


Bond angles



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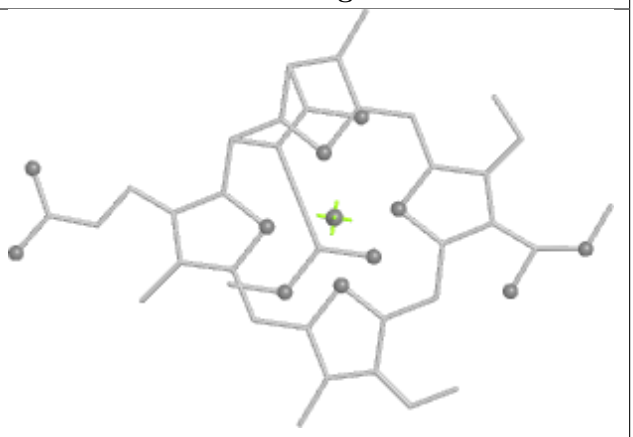
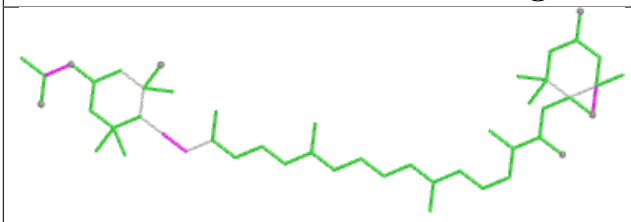


Rings

Ligand A86 Y 301



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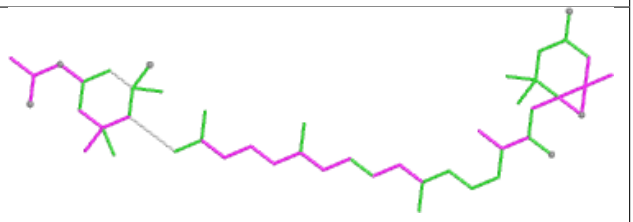
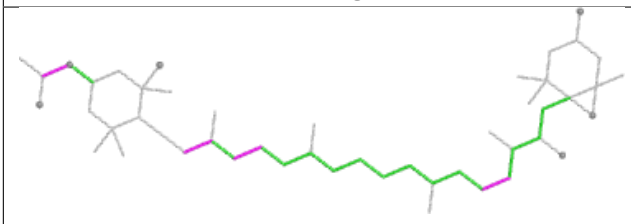


Bond angles



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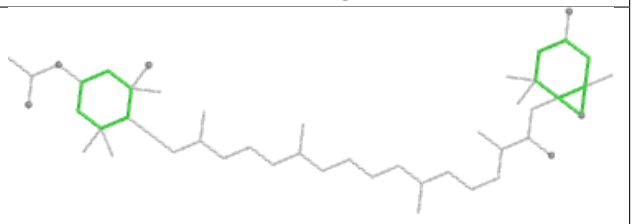
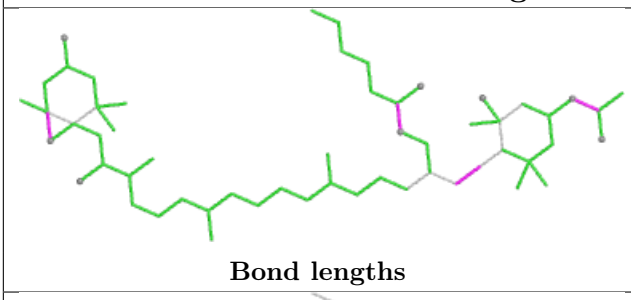


Rings

Ligand A1EB1 1 305



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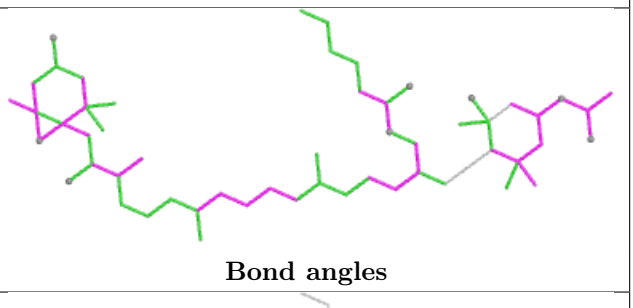
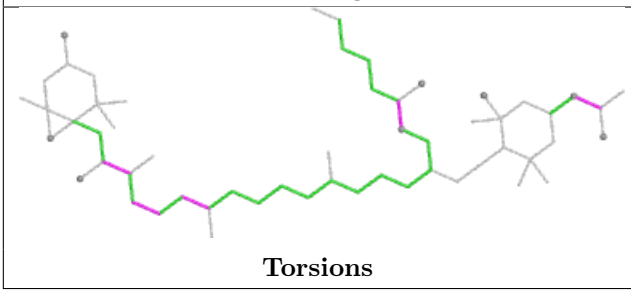
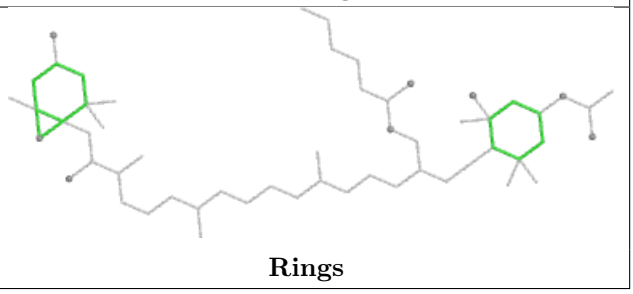


Bond angles

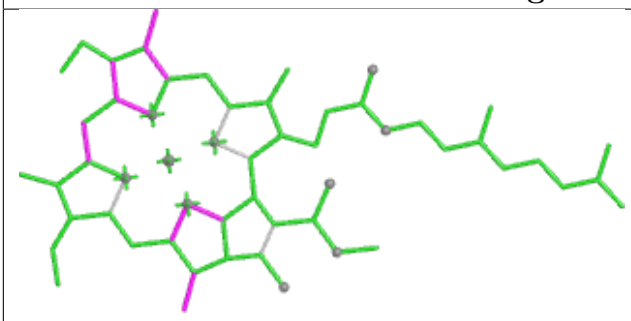


Torsions

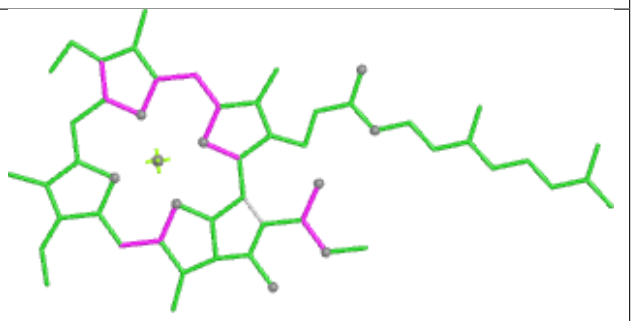


Rings

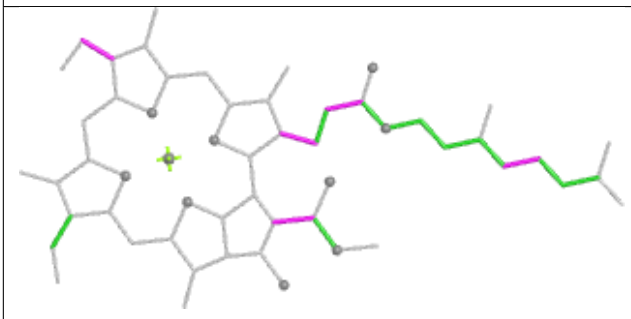
Ligand CLA b 814



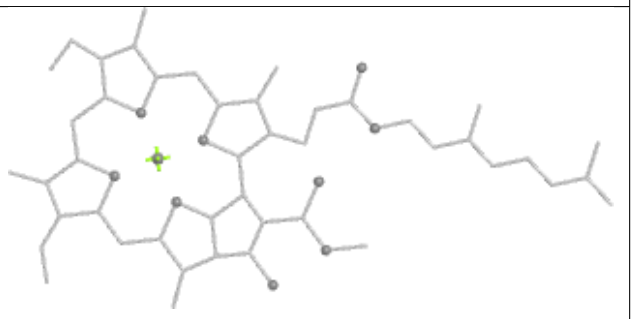
Bond lengths



Bond angles

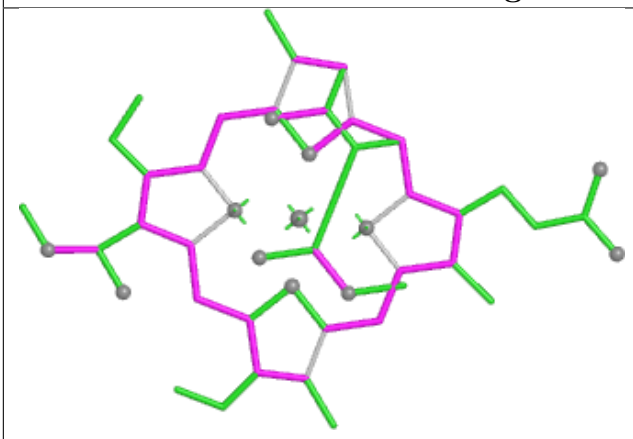


Torsions



Rings

Ligand A1ECV x 310



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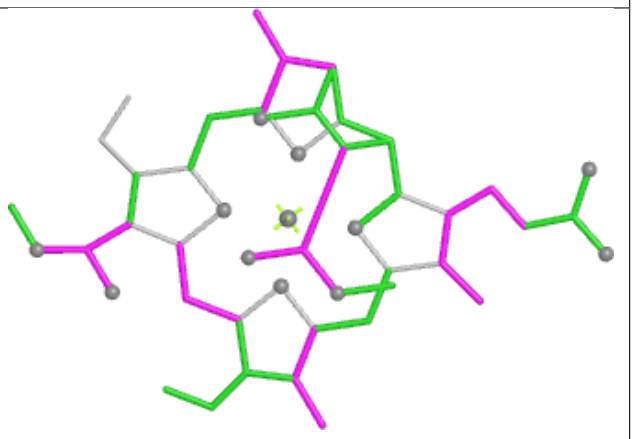
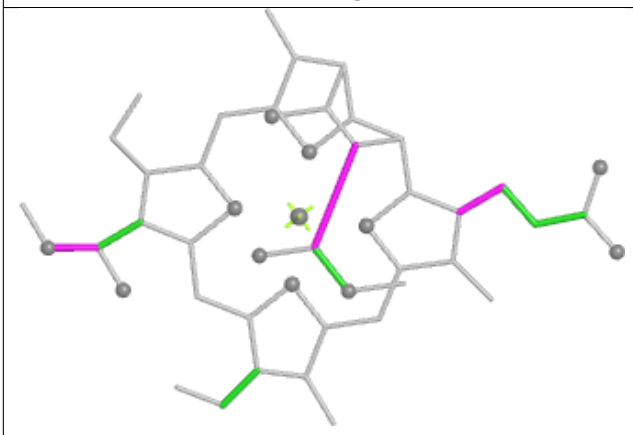
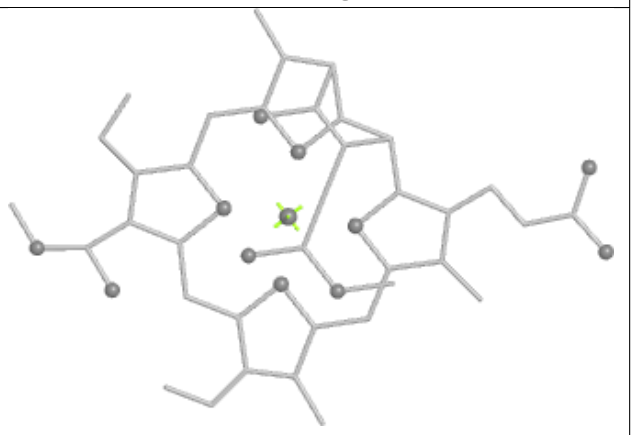


Bond angles

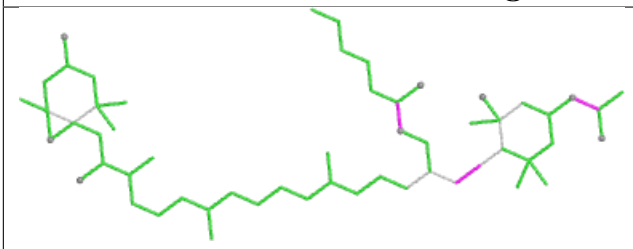


Torsions

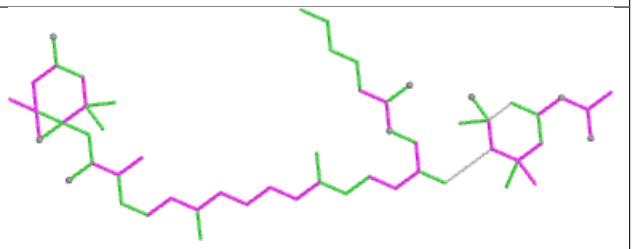


Rings

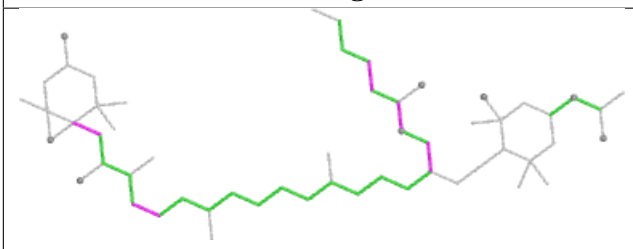
Ligand A1EB1 K 305



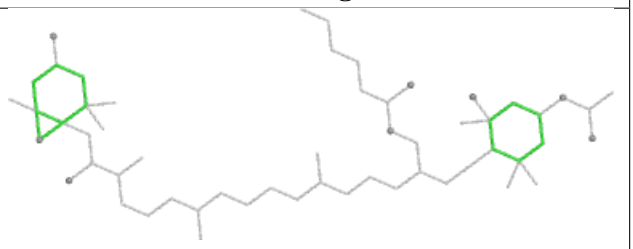
Bond lengths



Bond angles

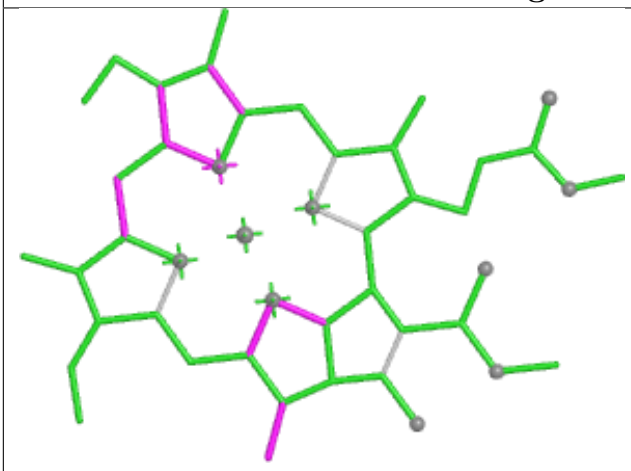


Torsions



Rings

Ligand CLA J 312



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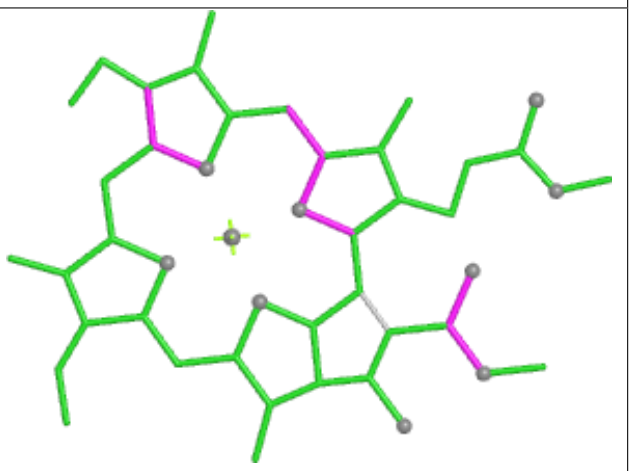
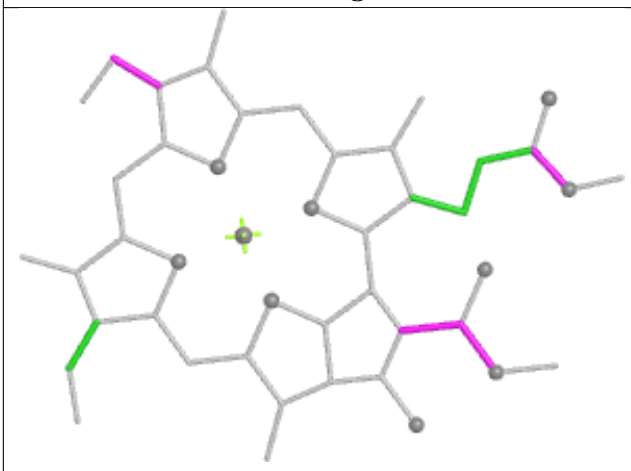


Bond angles



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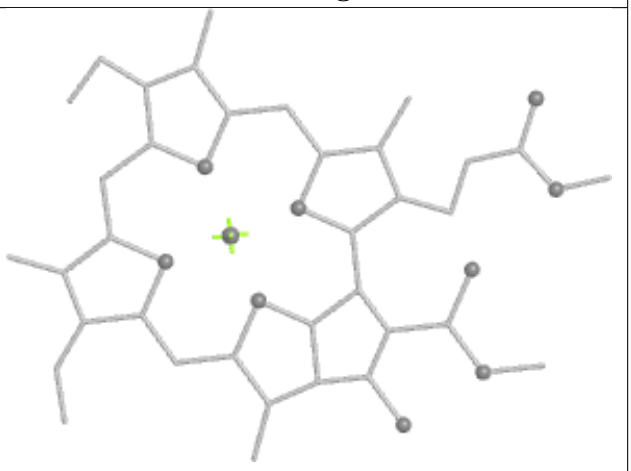
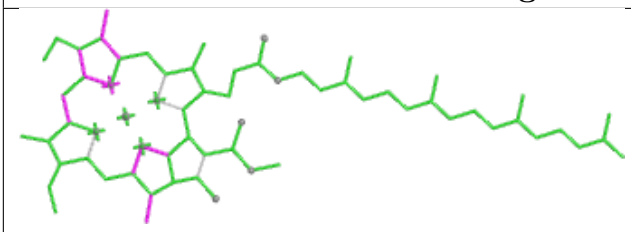


Rings

Ligand CLA W 309



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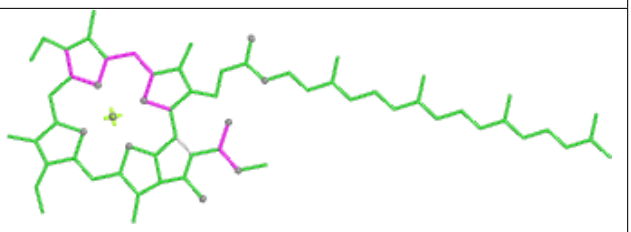
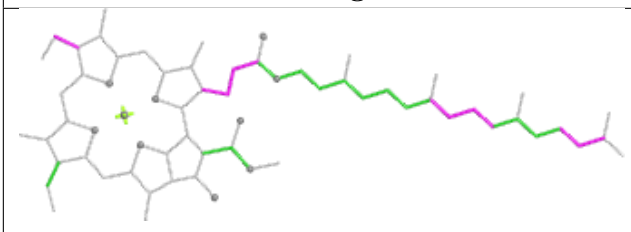


Bond angles



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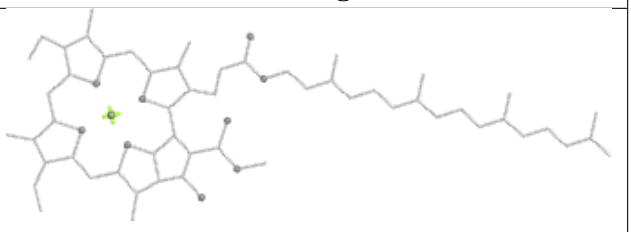
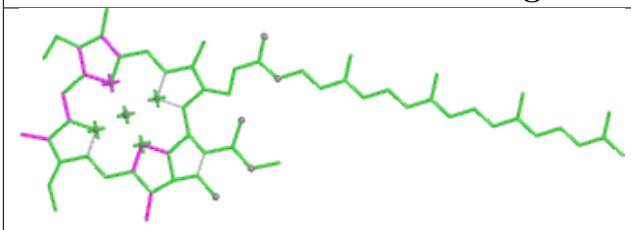


Rings

Ligand CLA D 311



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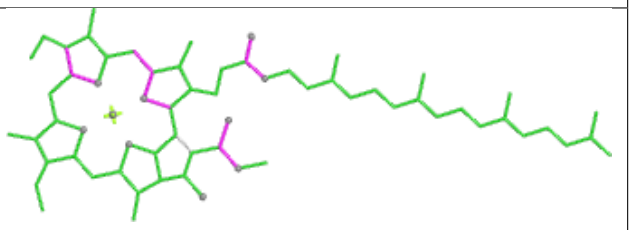
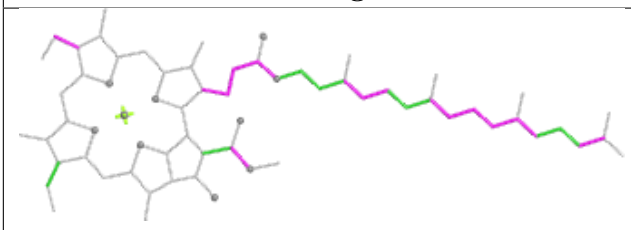


Bond angles



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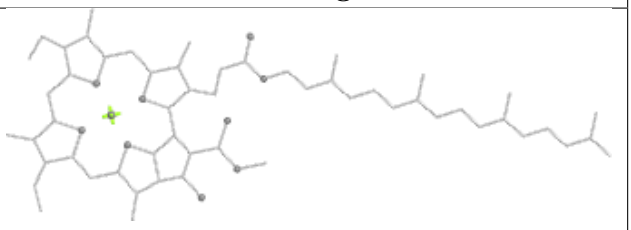
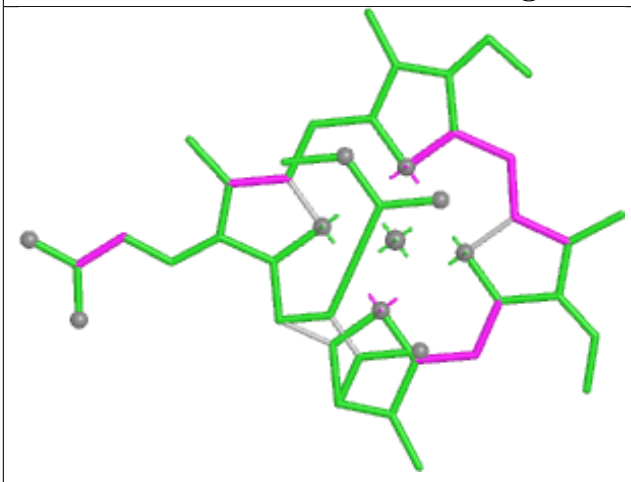


Rings

Ligand KC2 W 308



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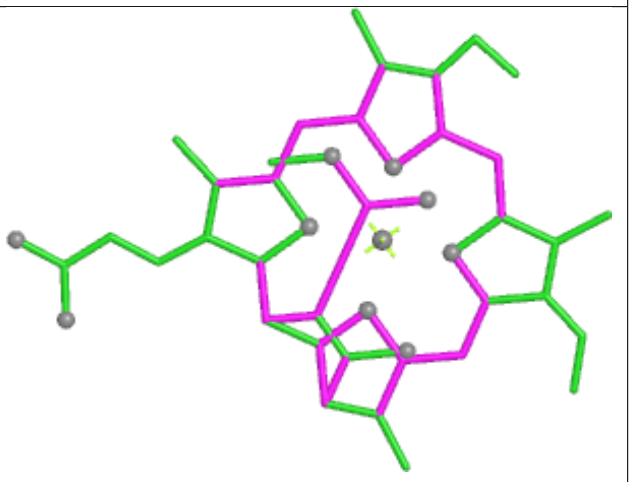
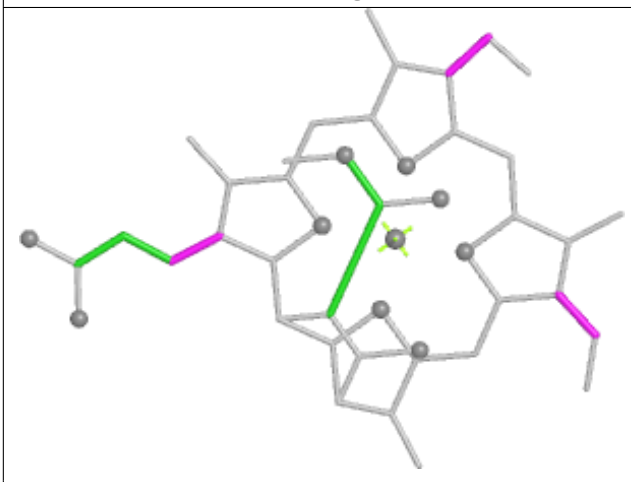


Bond angles



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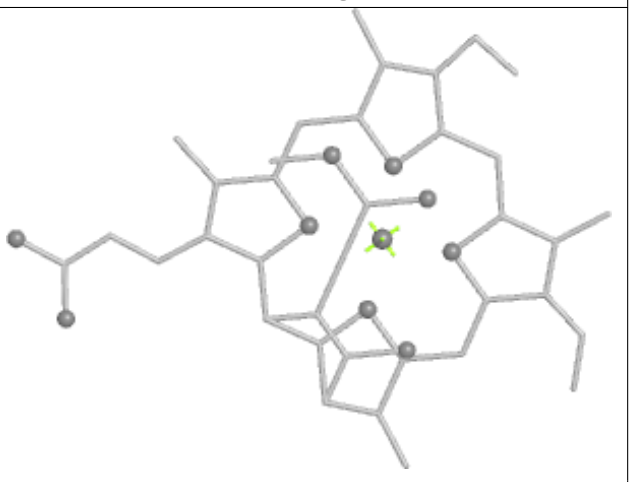
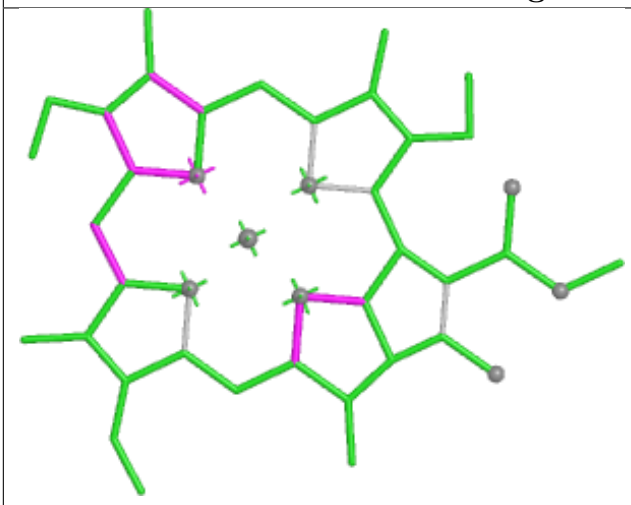
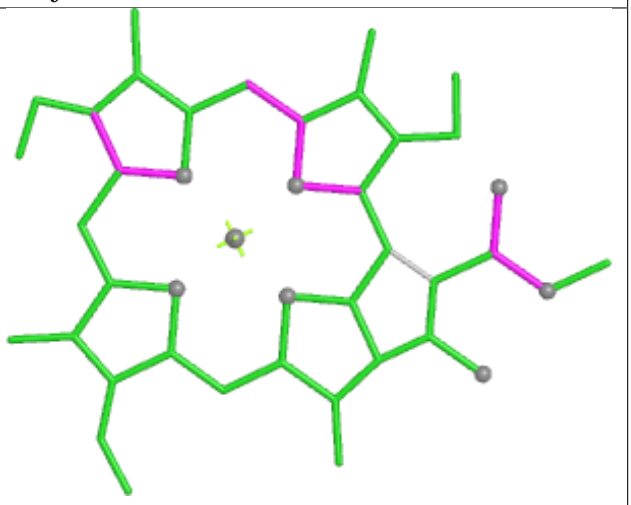


Rings

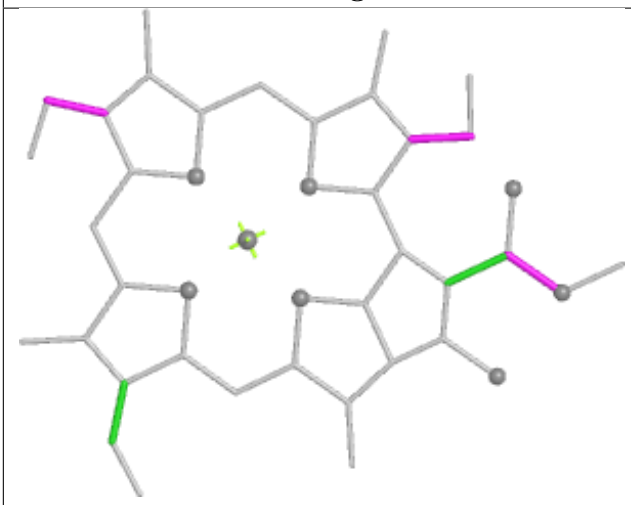
Ligand CLA y 312



Bond lengths



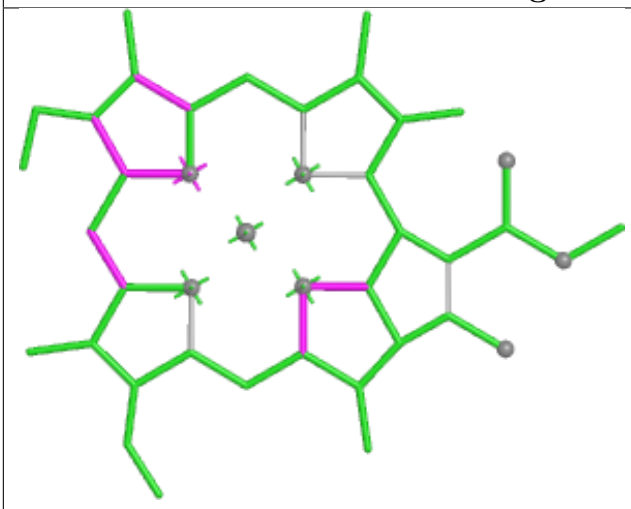
Bond angles



Torsions

Rings

Ligand CLA z 311



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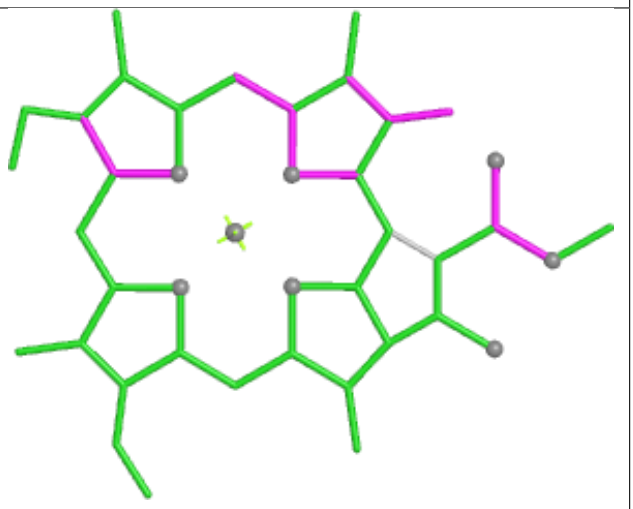
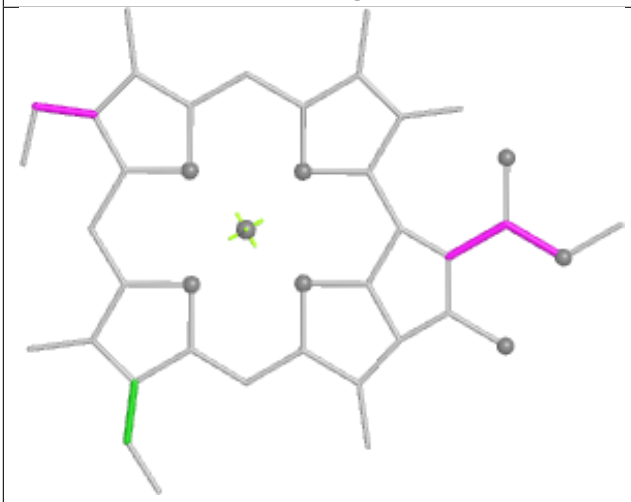


Bond angles



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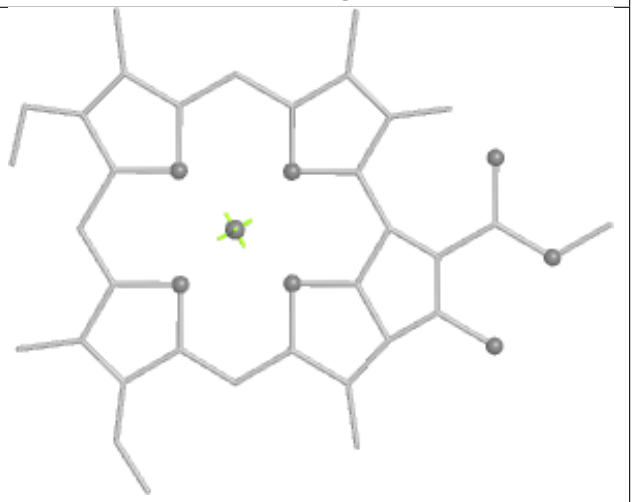
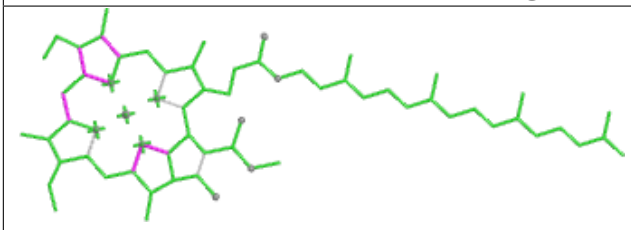


Rings

Ligand CLA D 319



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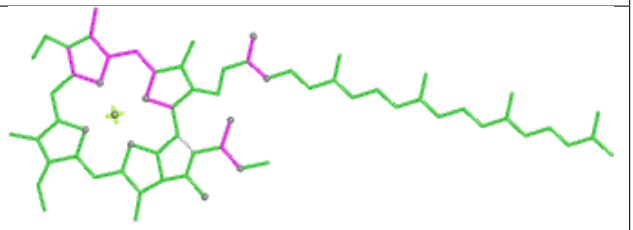
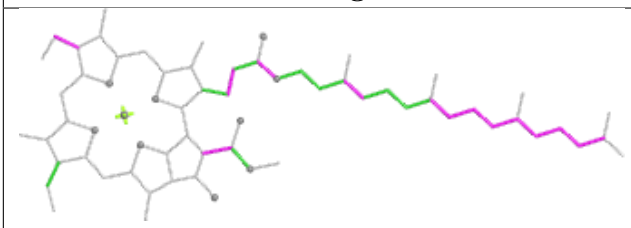


Bond angles



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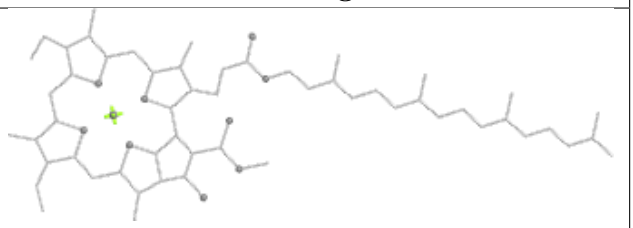
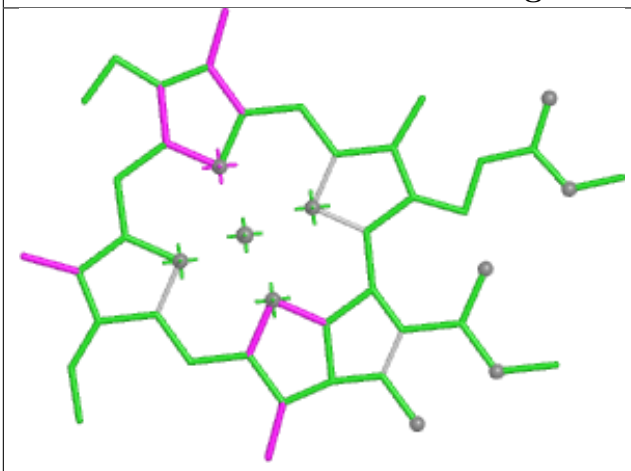


Rings

Ligand CLA T 308



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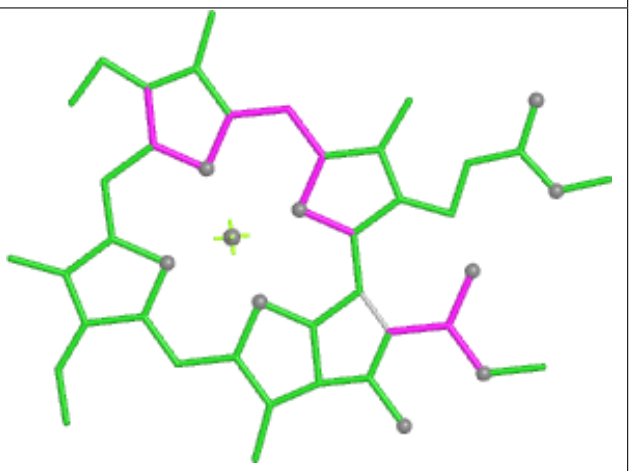
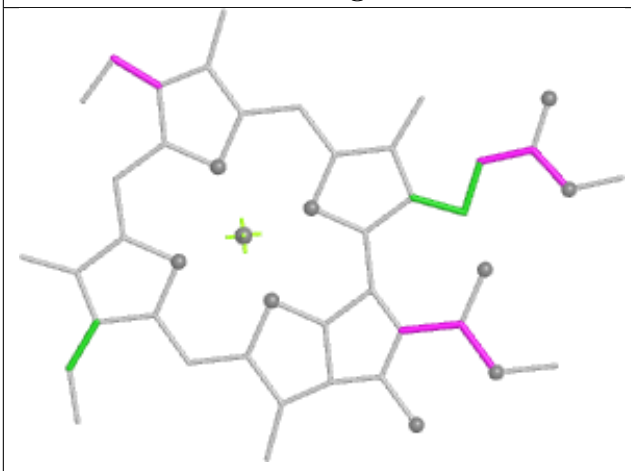
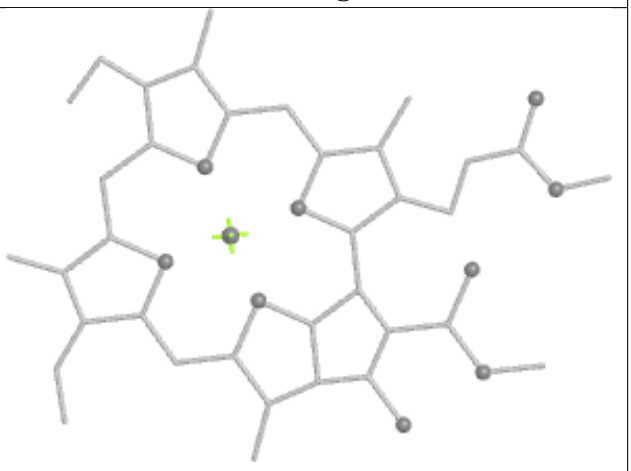


Bond angles

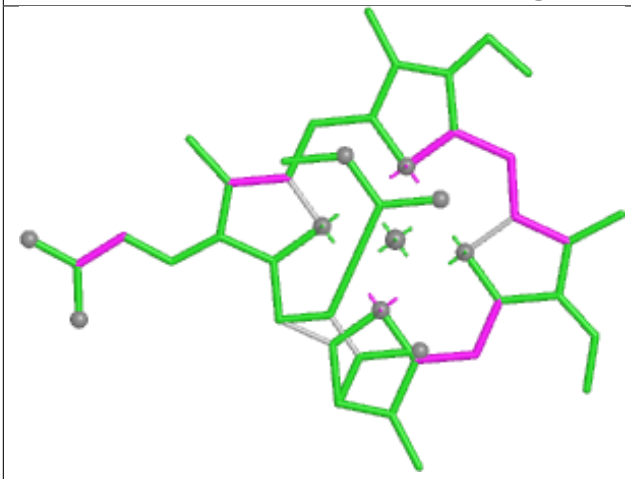


Torsions

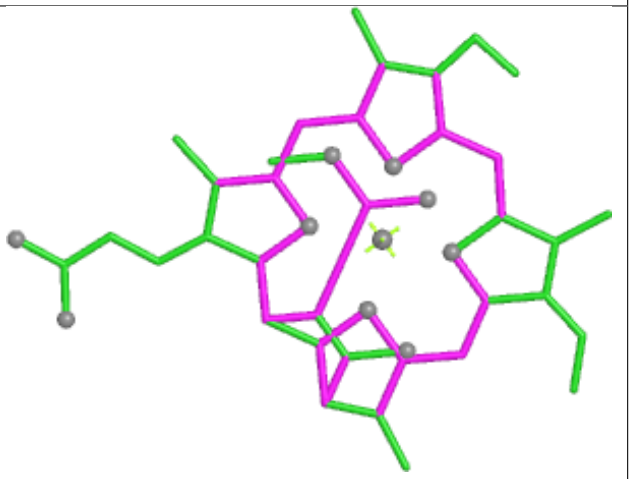


Rings

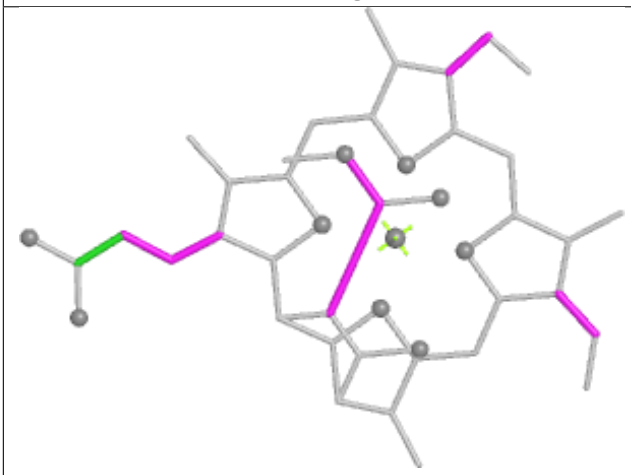
Ligand KC2 2 314



Bond lengths



Bond angles



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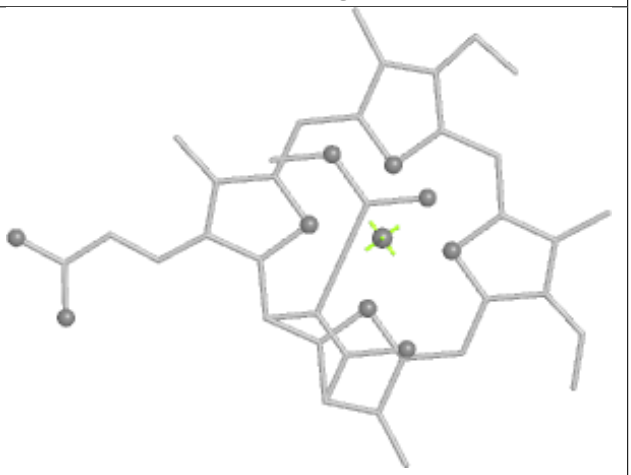
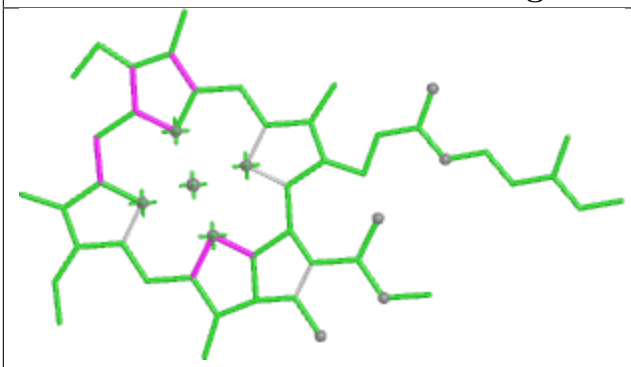
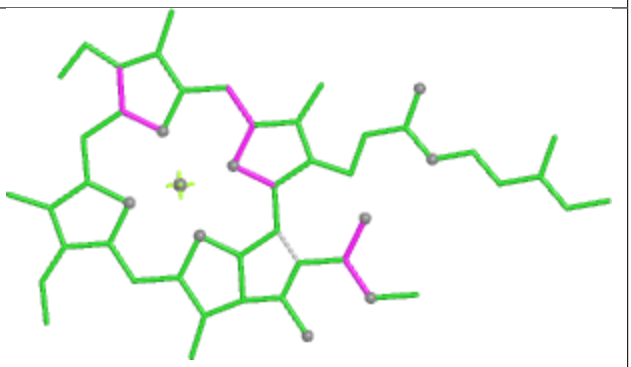


Rings

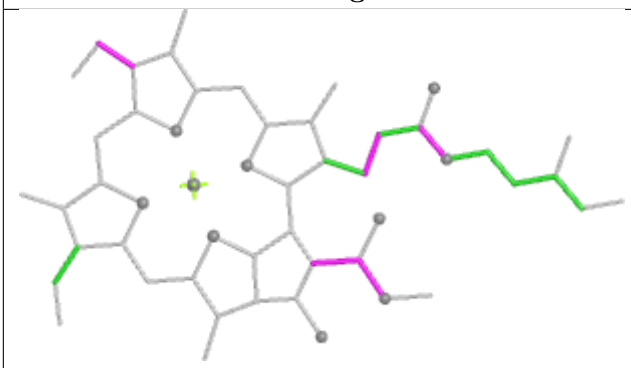
Ligand CLA L 319



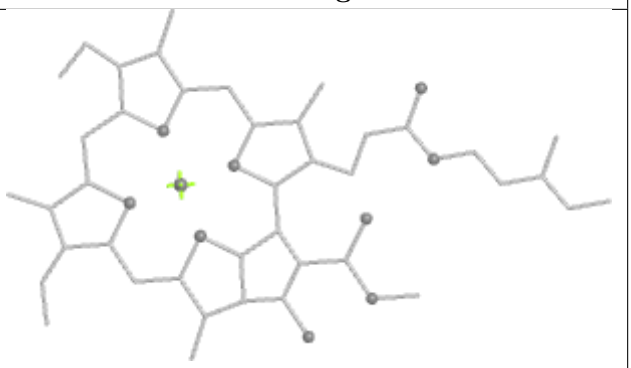
Bond lengths



Bond angles

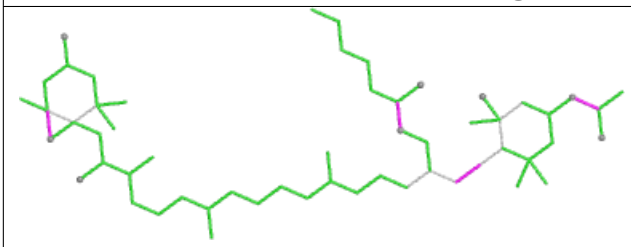


Torsions

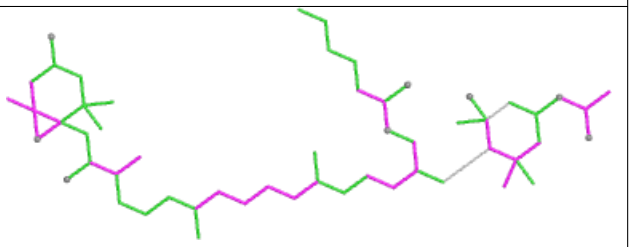


Rings

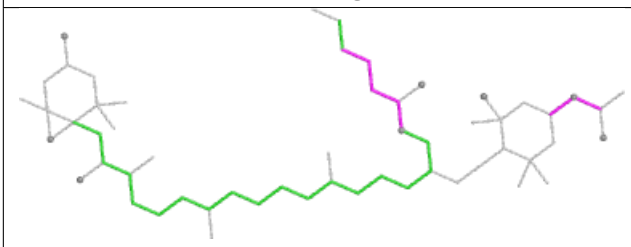
Ligand A1EB1 3 309



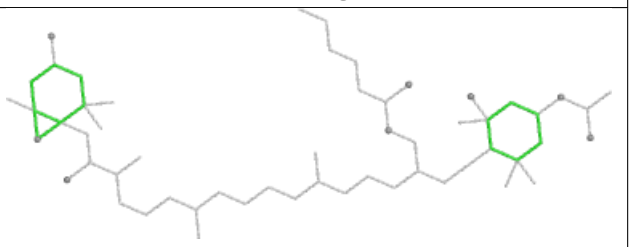
Bond lengths



Bond angles

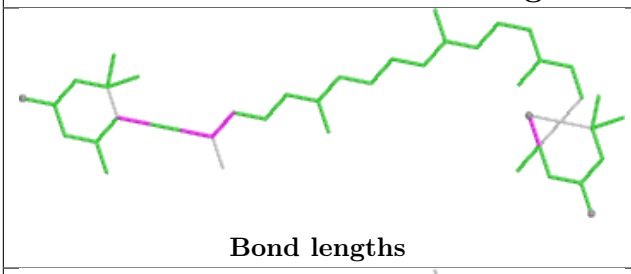


Torsions



Rings

Ligand DD6 R 304



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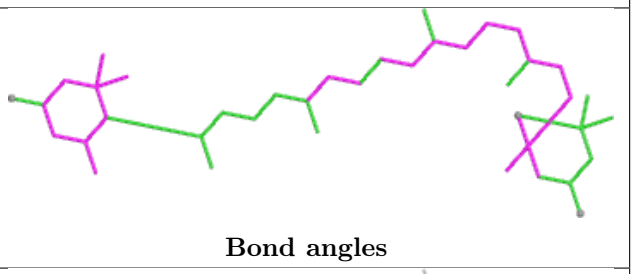
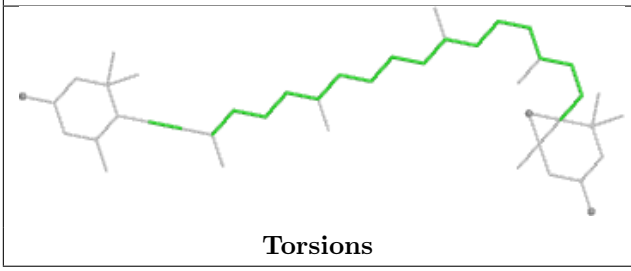


Bond angles



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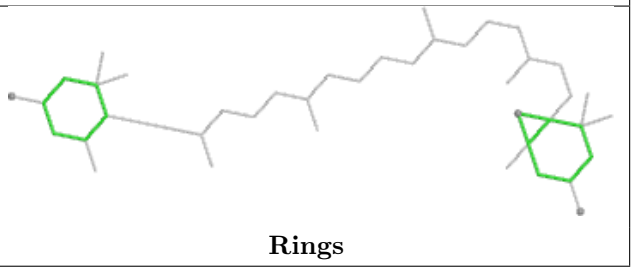
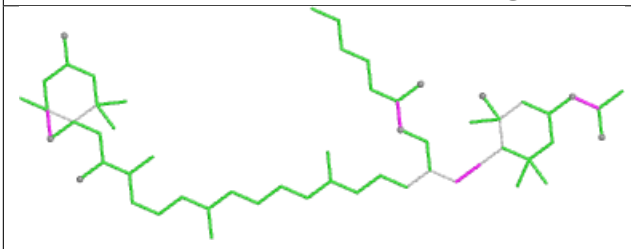


Rings

Ligand A1EB1 G 304



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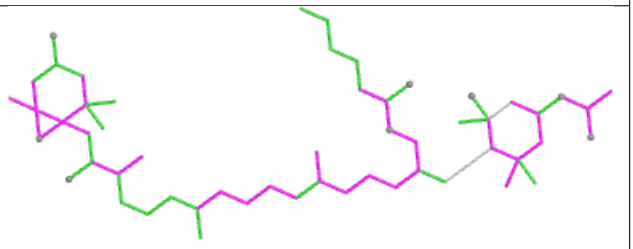
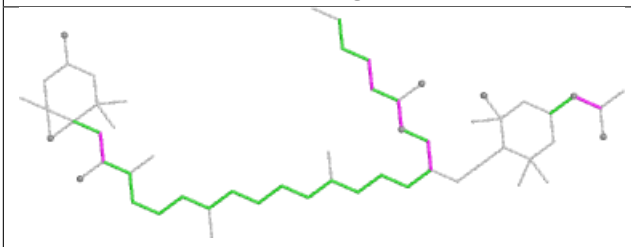
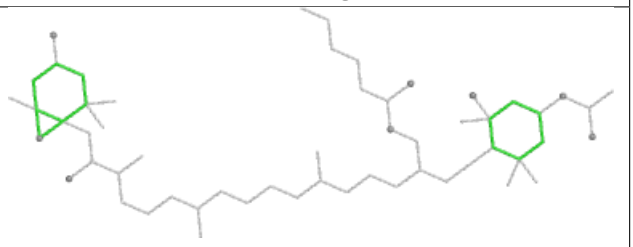


Bond angles

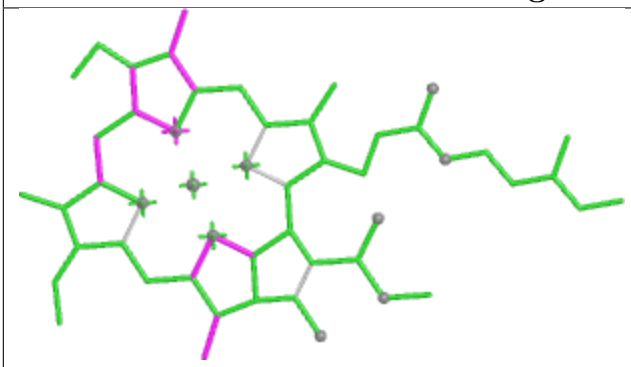


Torsions

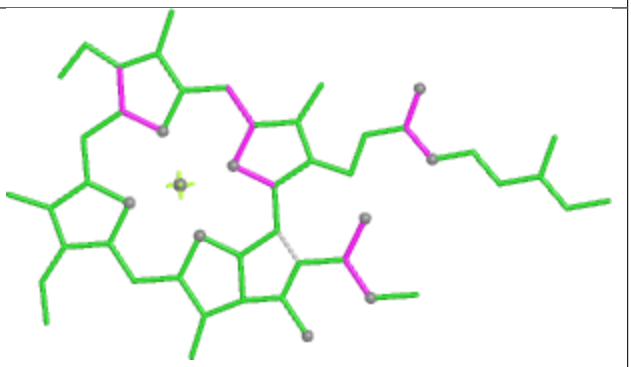


Rings

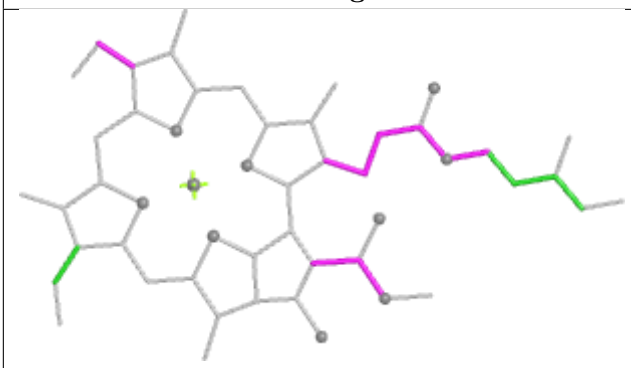
Ligand CLA 1 319



Bond lengths



Bond angles



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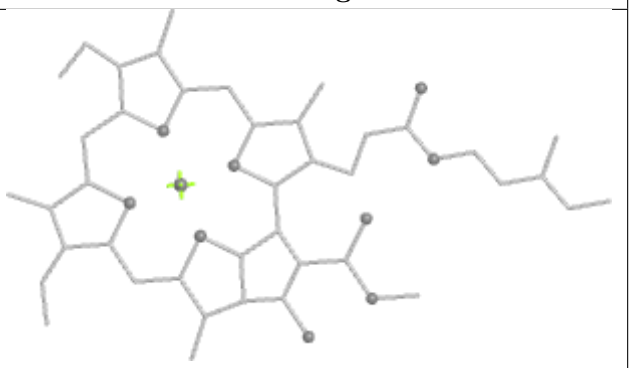
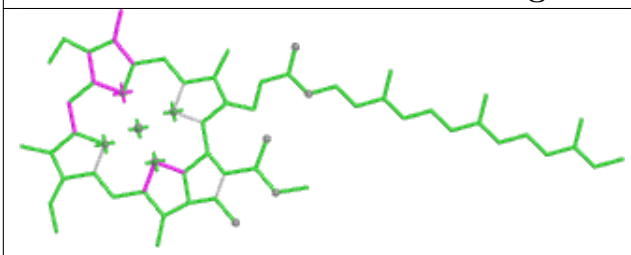


Rings

Ligand CLA 7 313



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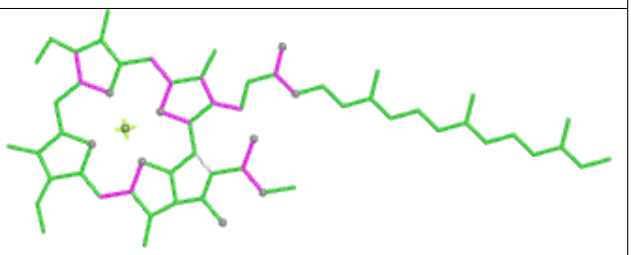
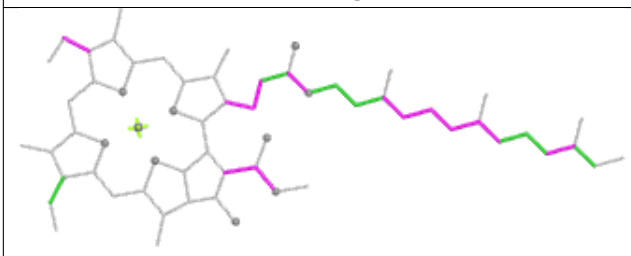


Bond angles



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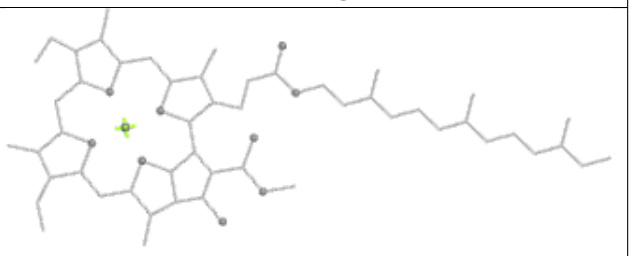
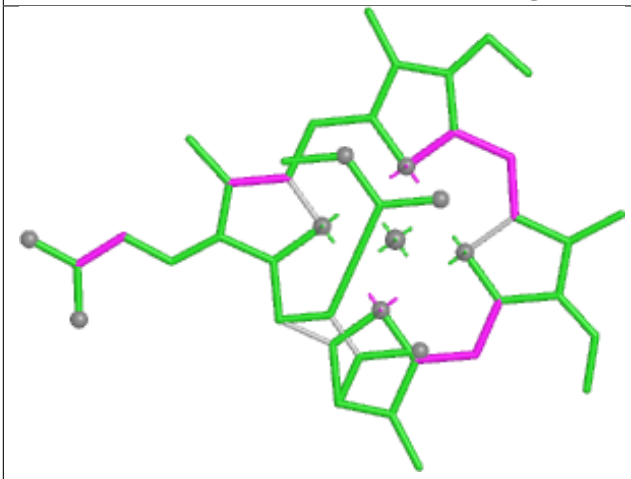


Rings

Ligand KC2 X 312



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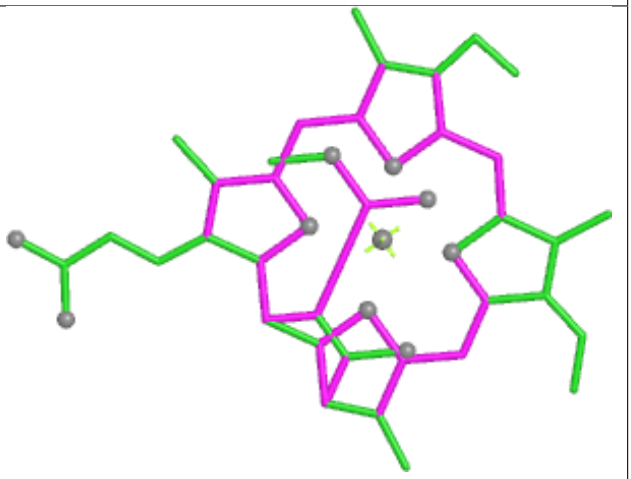
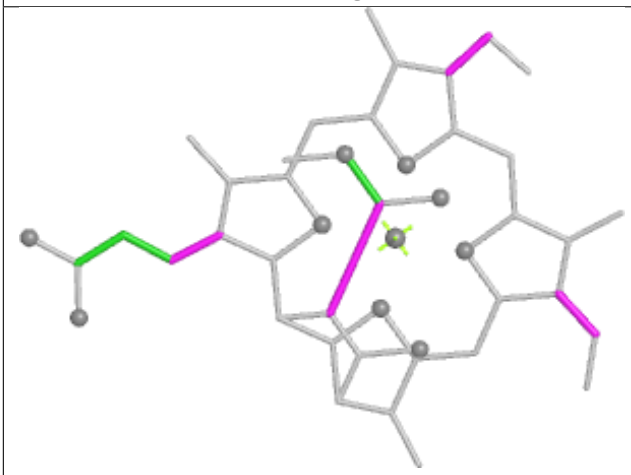


Bond angles



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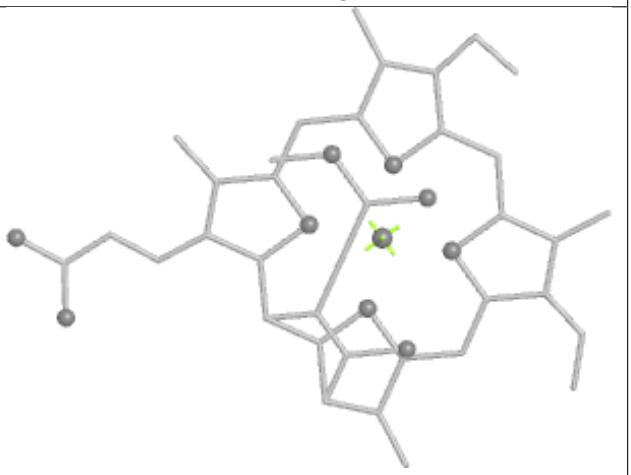
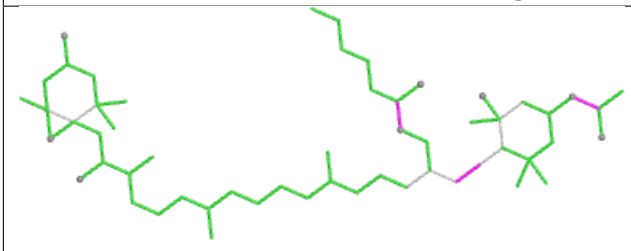


Rings

Ligand A1EB1 0 305



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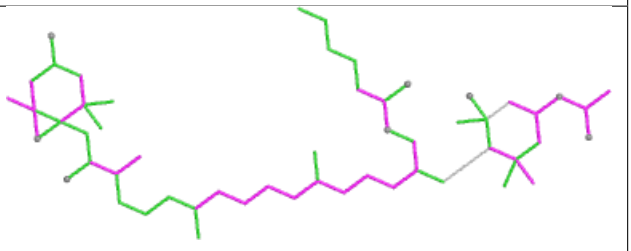
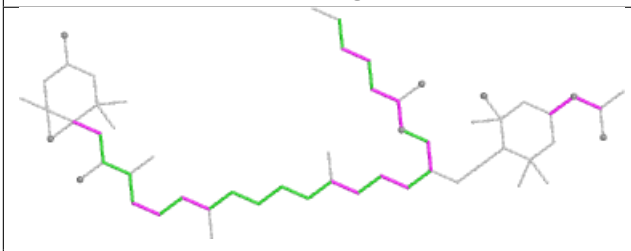


Bond angles



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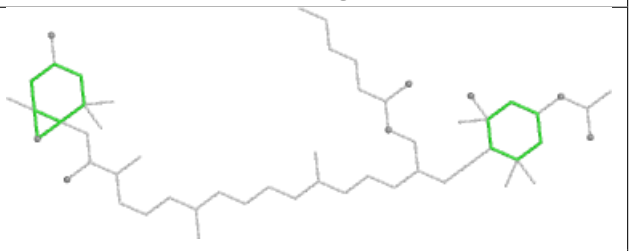
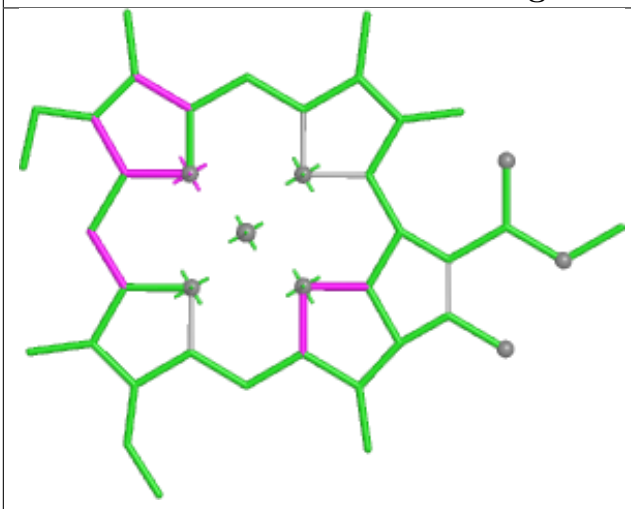


Rings

Ligand CLA 2 316



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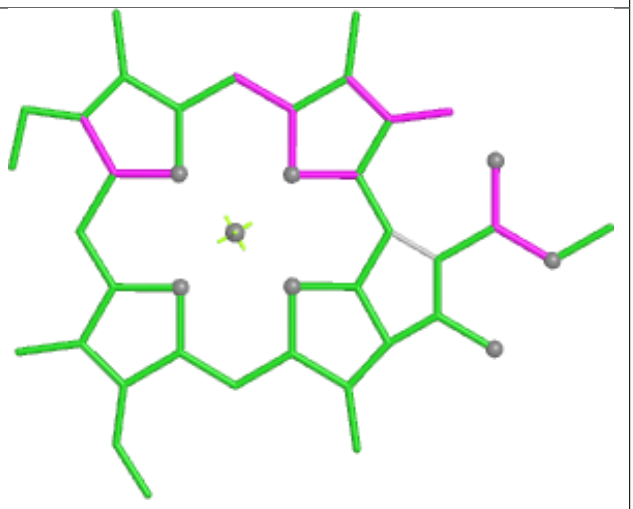
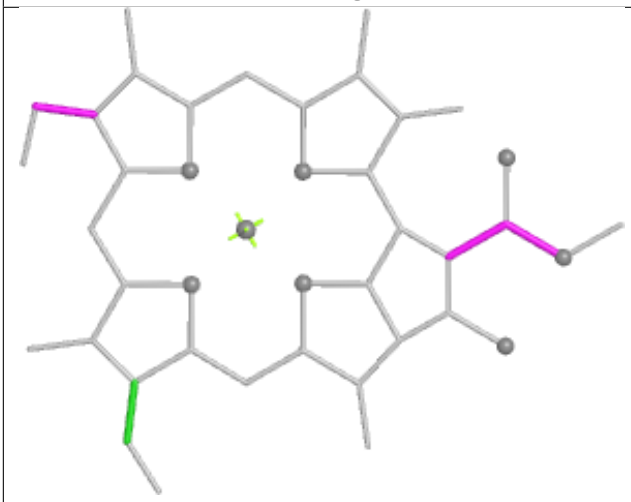


Bond angles



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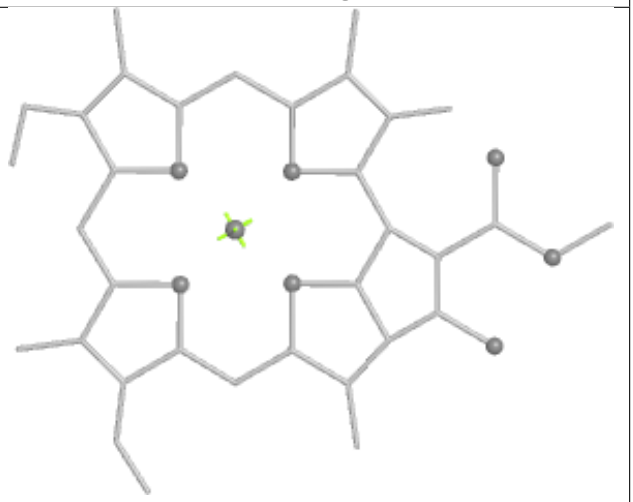
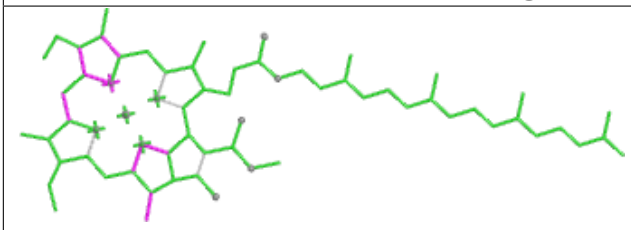


Rings

Ligand CLA M 310



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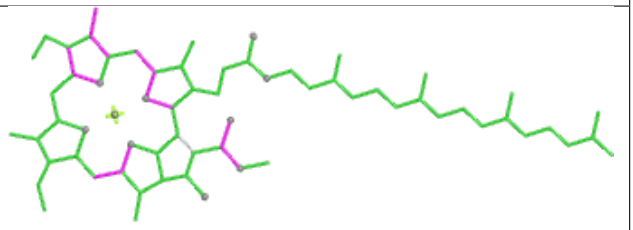
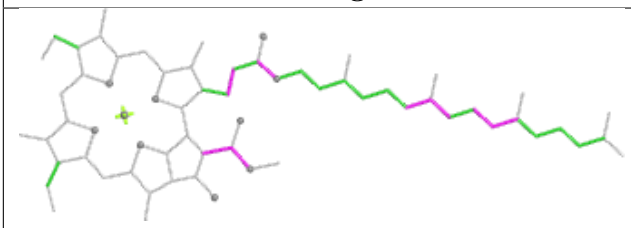
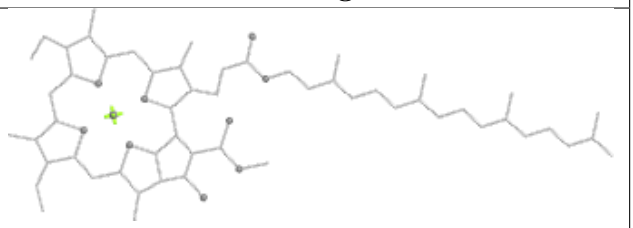


Bond angles

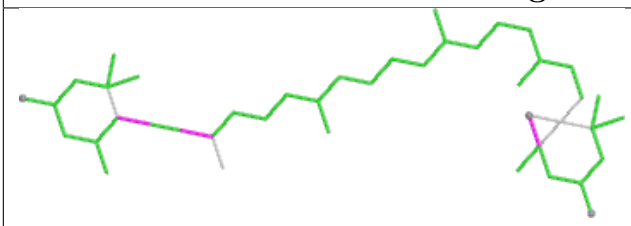


Torsions



Rings

Ligand DD6 J 305



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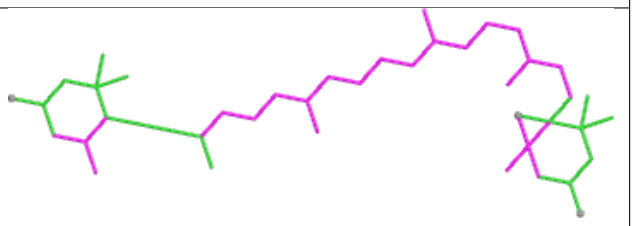
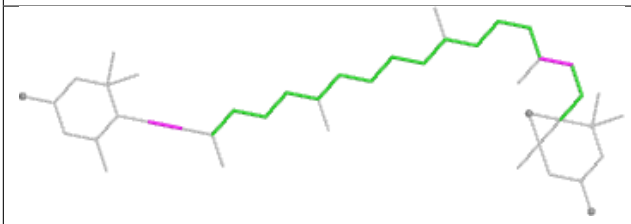
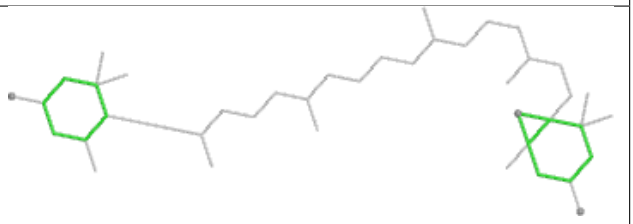


Bond angles

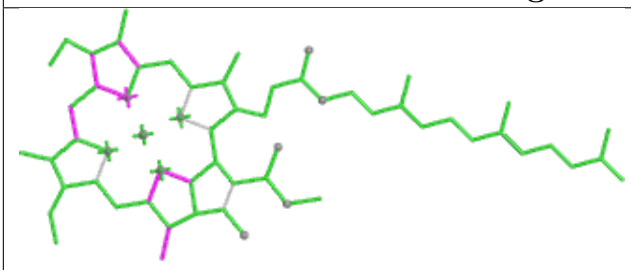


Torsions



Rings

Ligand CLA b 816



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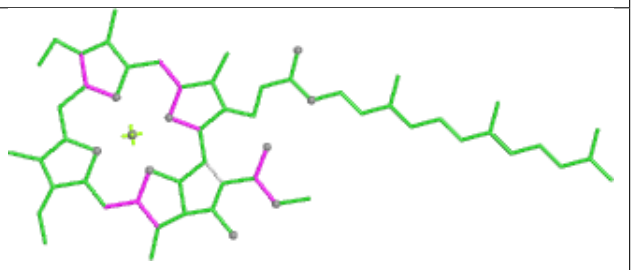
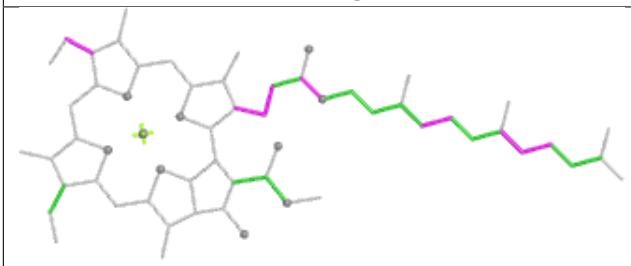
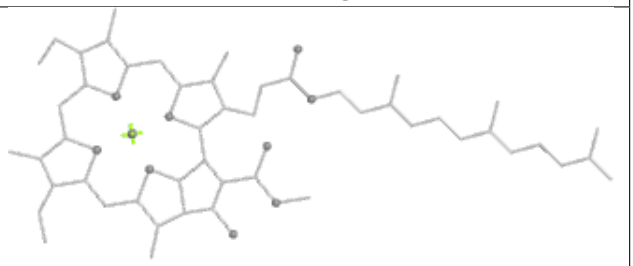


Bond angles

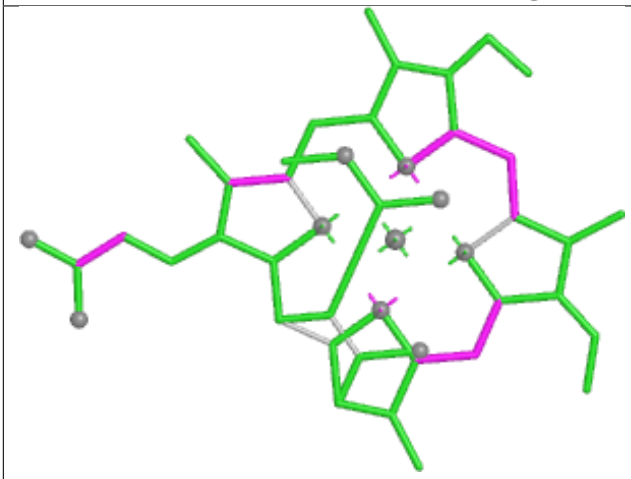


Torsions



Rings

Ligand KC2 V 318



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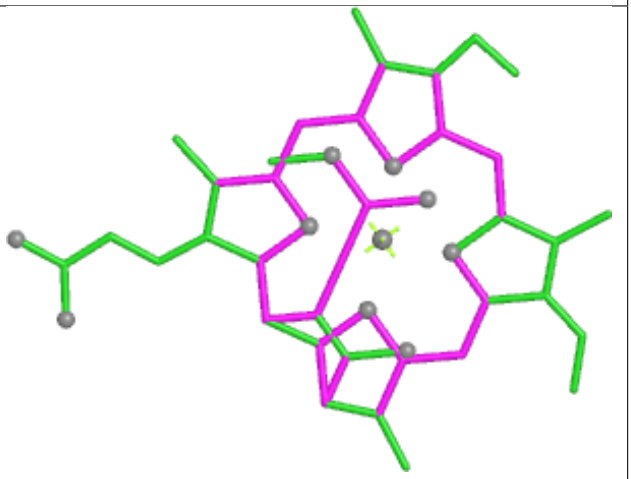
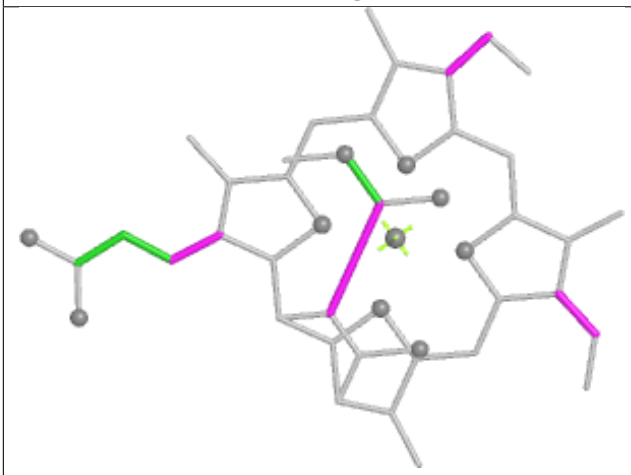
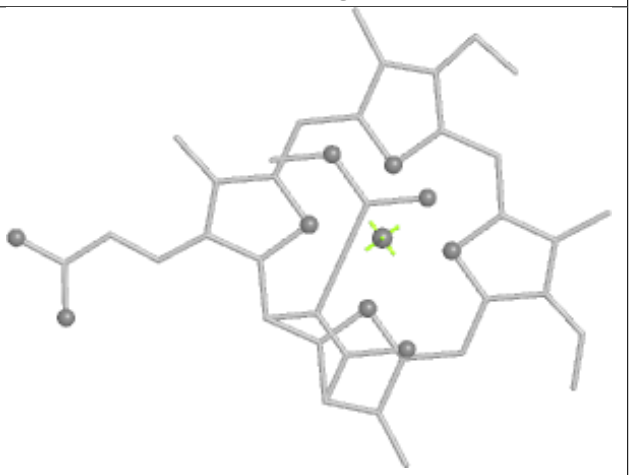


Bond angles

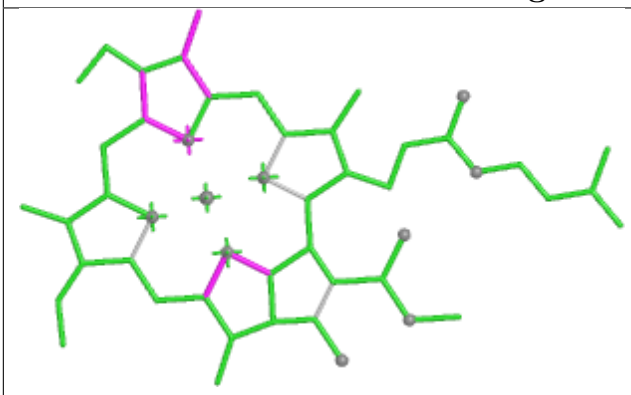


Torsions



Rings

Ligand CLA a 832



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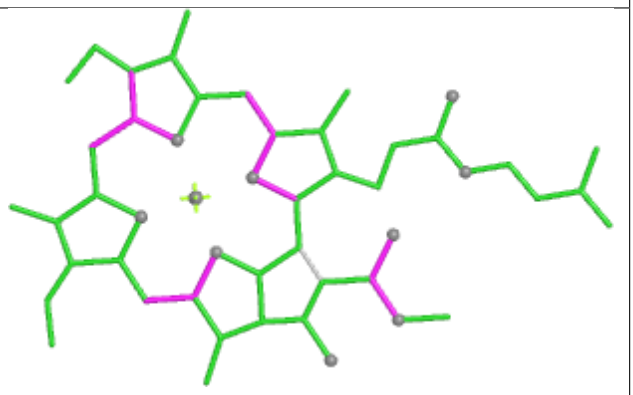
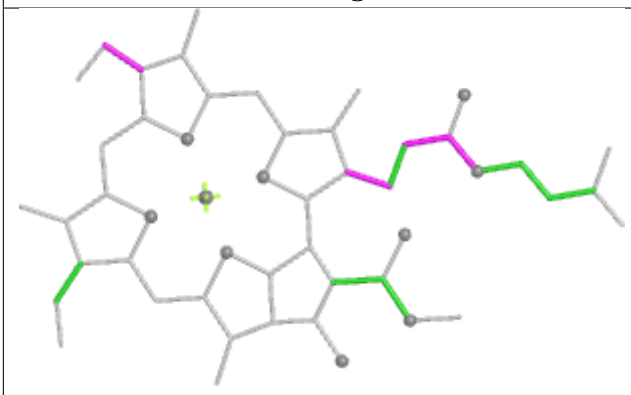


Bond angles



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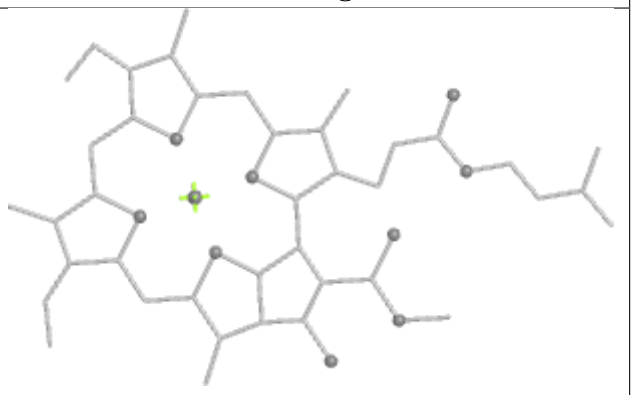
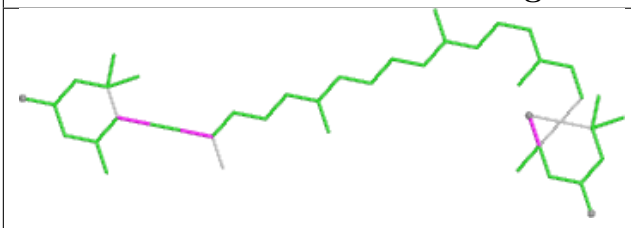


Rings

Ligand DD6 A 301



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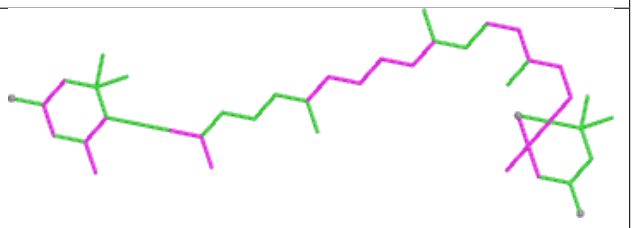
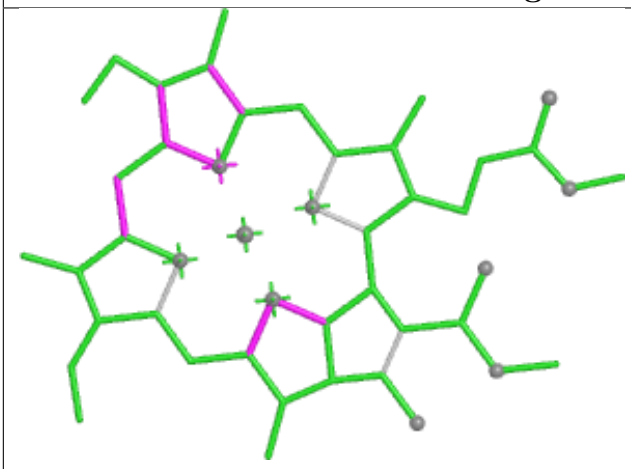


Bond angles

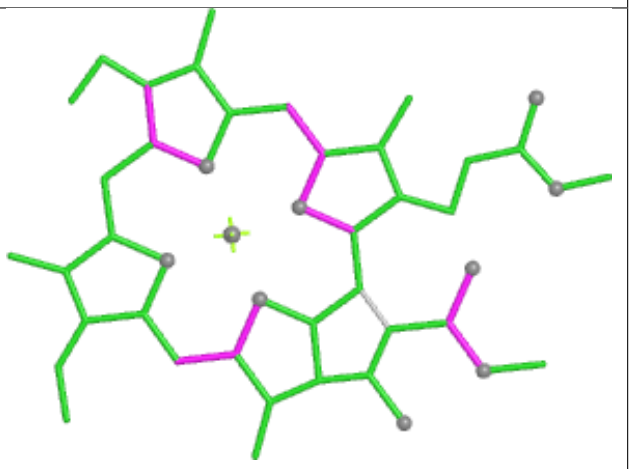
Torsions

Rings

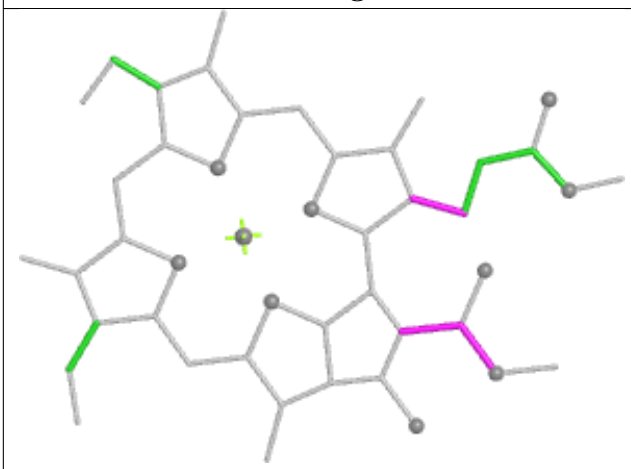
Ligand CLA B 203



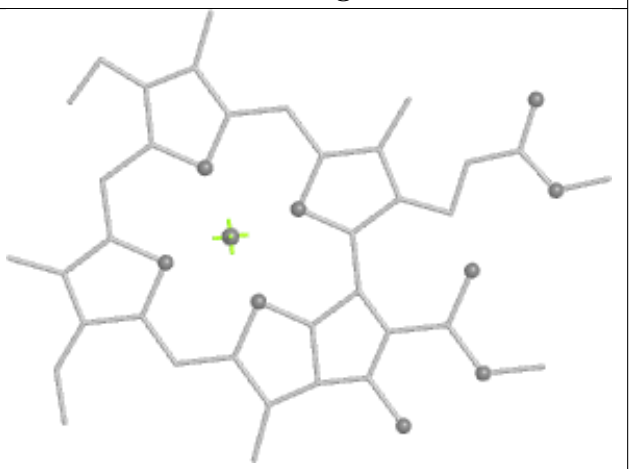
Bond lengths



Bond angles

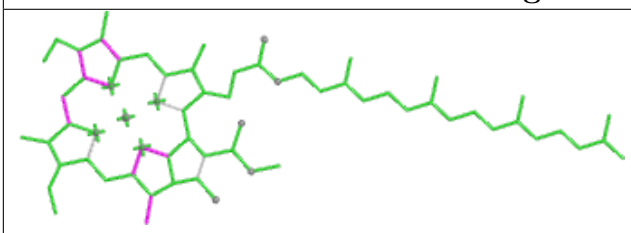


Torsions



Rings

Ligand CLA D 313



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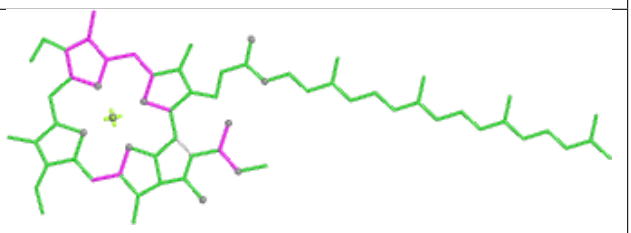

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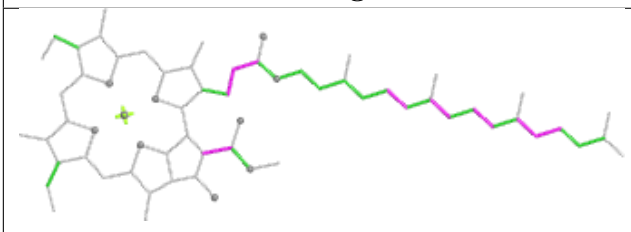

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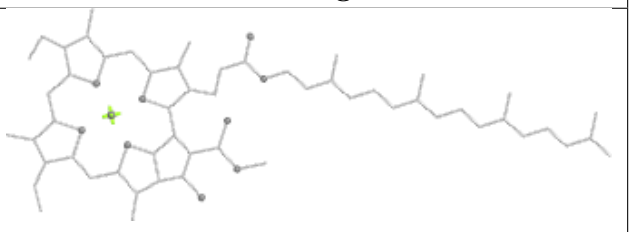
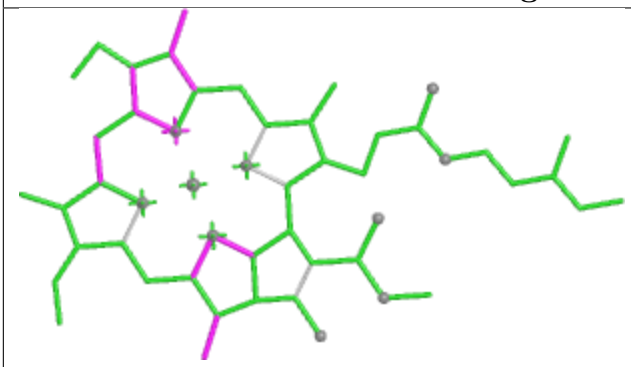


Rings

Ligand CLA M 317



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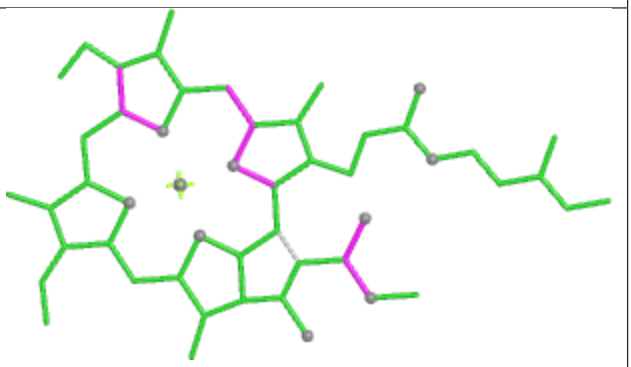
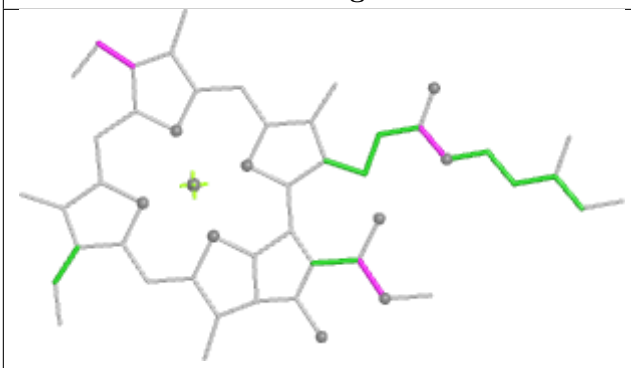


Bond angles



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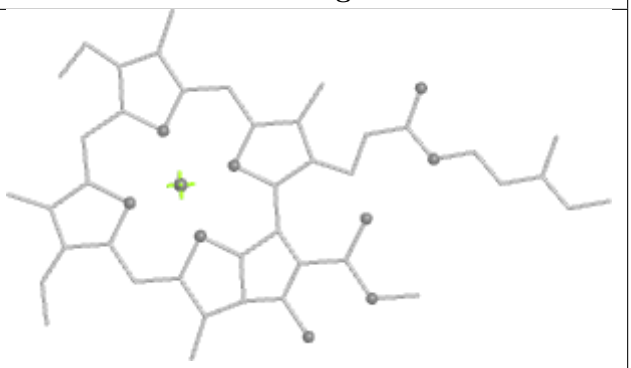
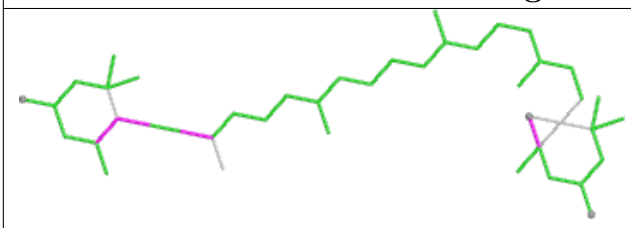


Rings

Ligand DD6 U 204



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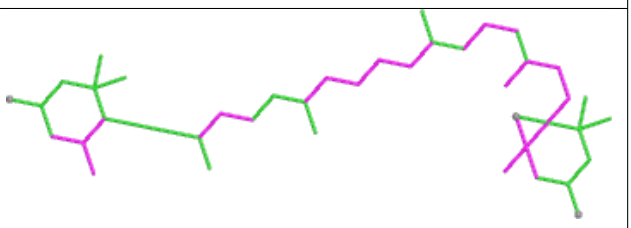
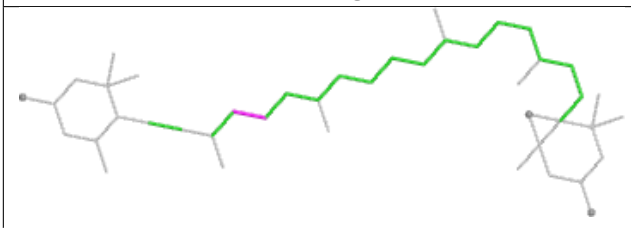


Bond angles



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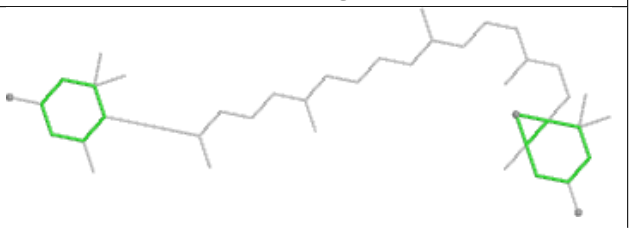
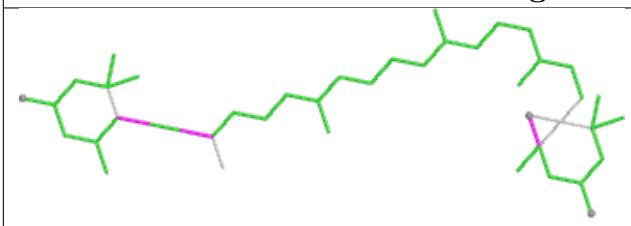


Rings

Ligand DD6 7 309



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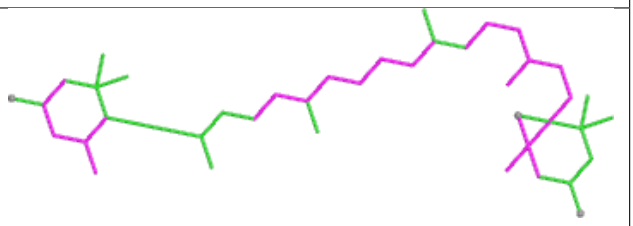
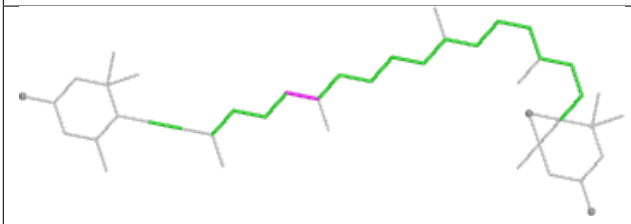


Bond angles



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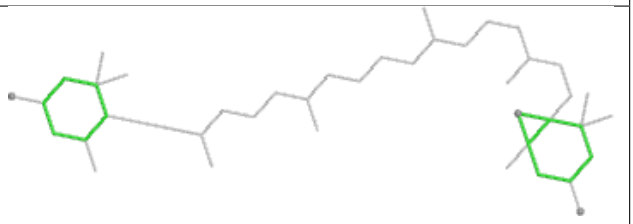
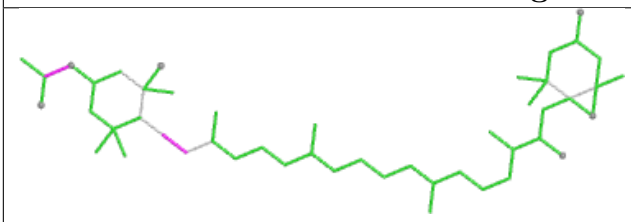


Rings

Ligand A86 T 306



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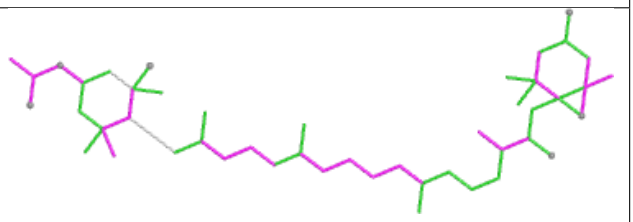
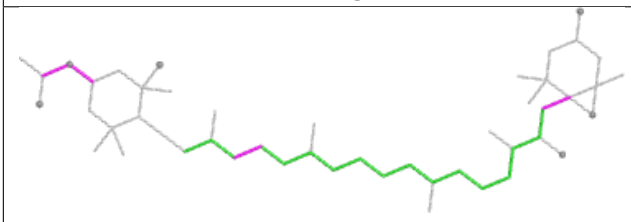


Bond angles



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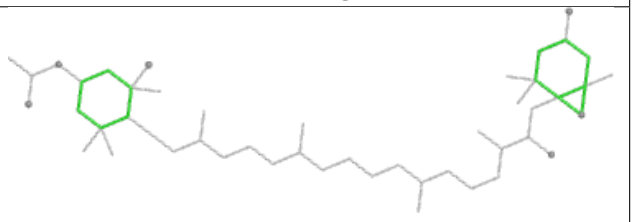
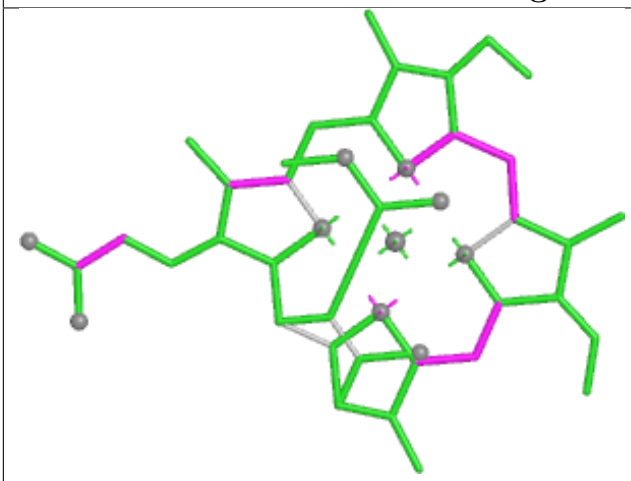


Rings

Ligand KC2 5 305



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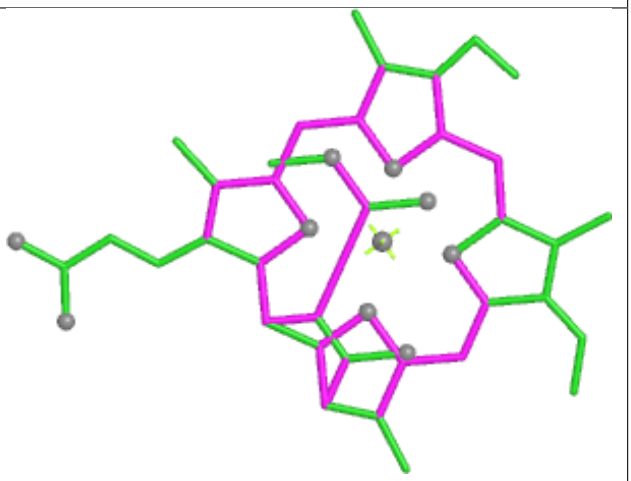
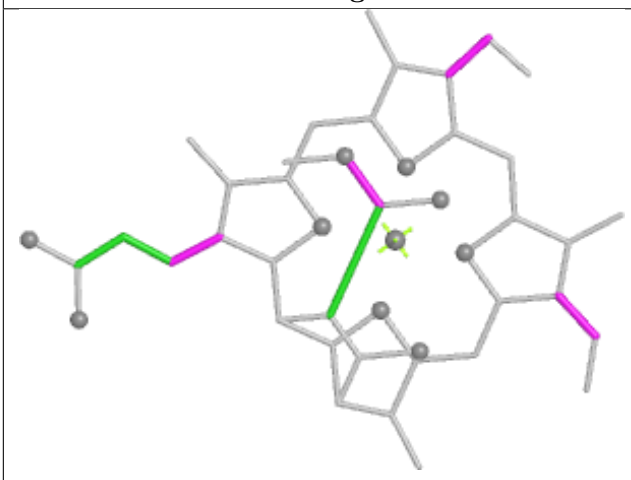
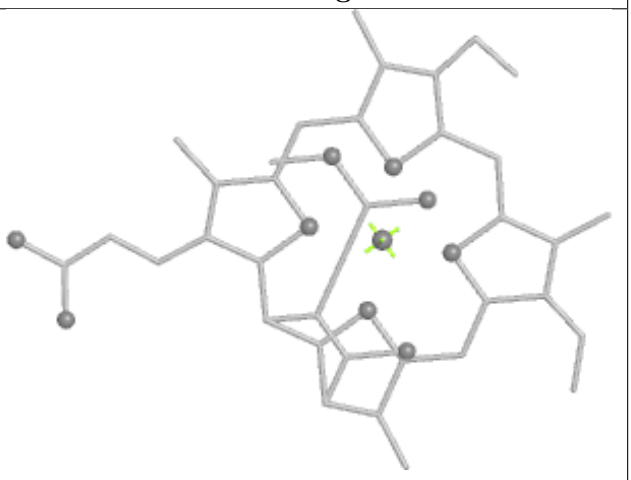


Bond angles

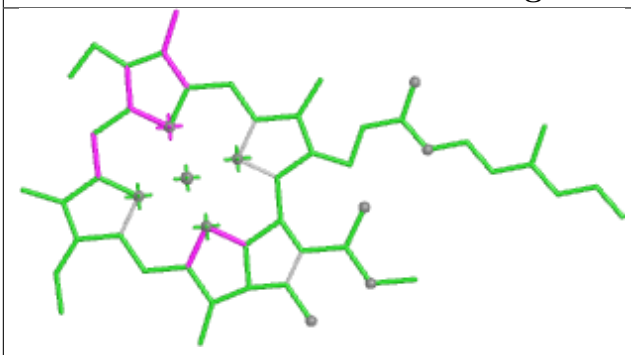


Torsions



Rings

Ligand CLA T 320



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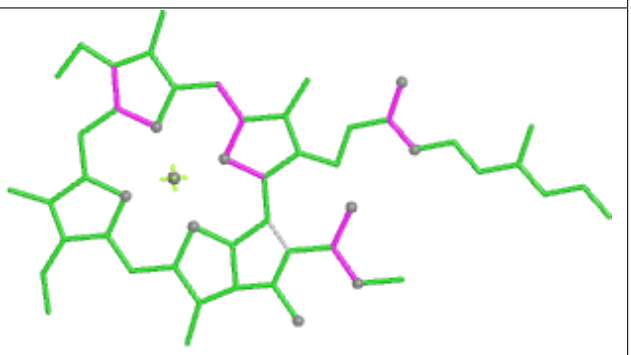
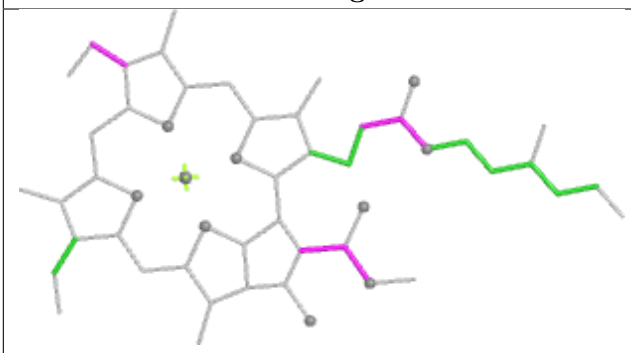


Bond angles



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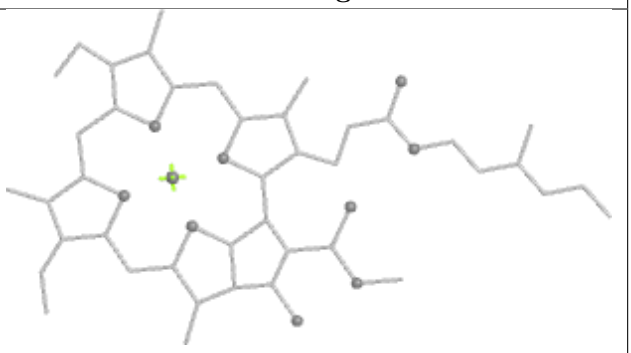
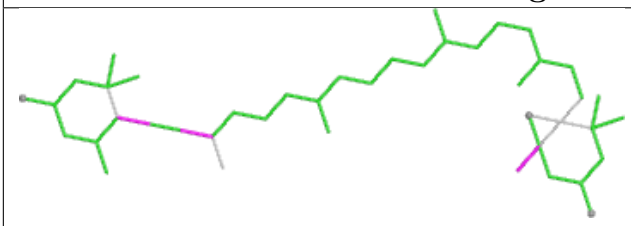


Rings

Ligand DD6 1 304



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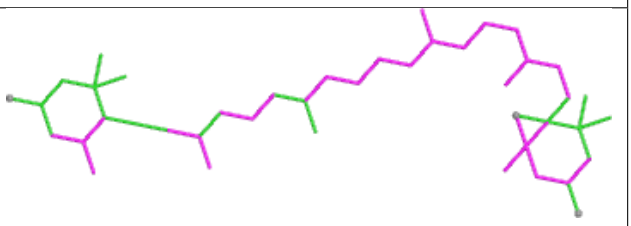
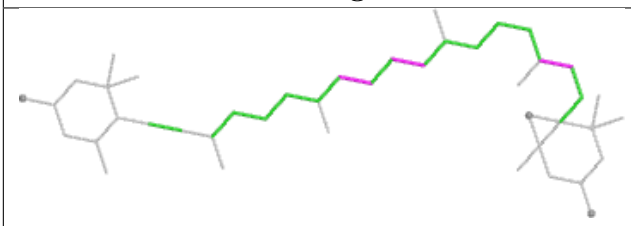
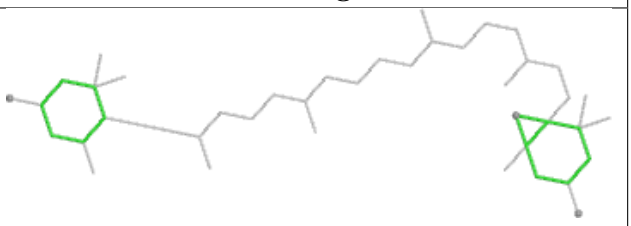


Bond angles

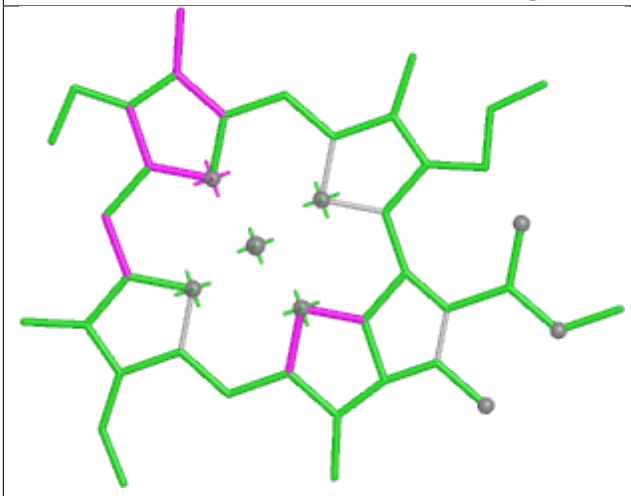


Torsions



Rings

Ligand CLA C 304



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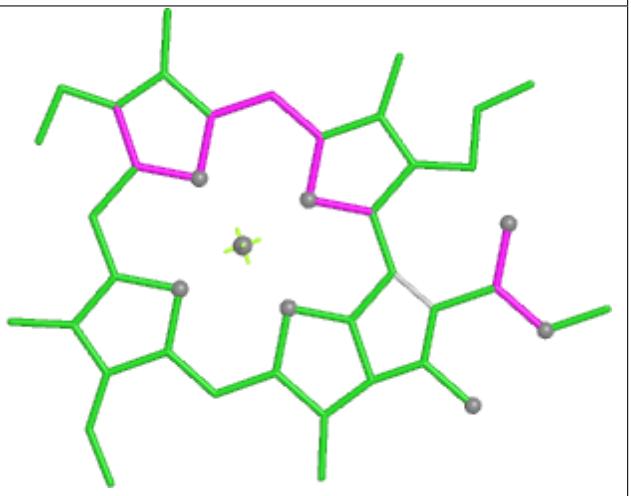
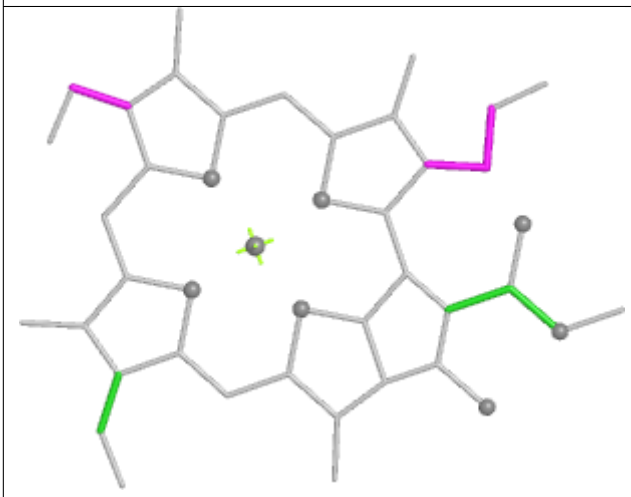


Bond angles



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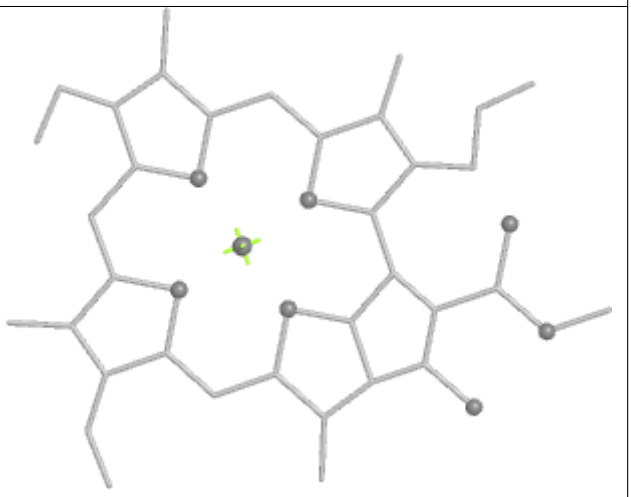
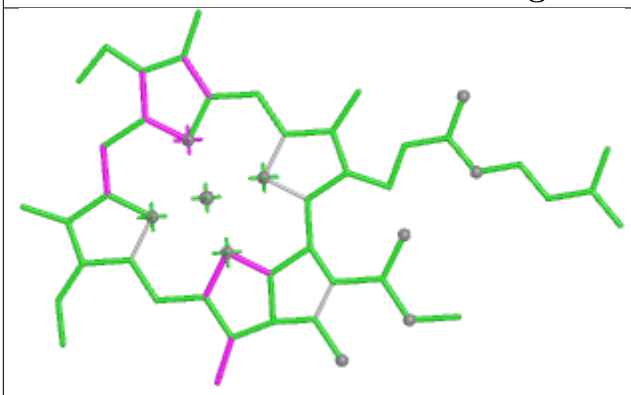


Rings

Ligand CLA 3 316



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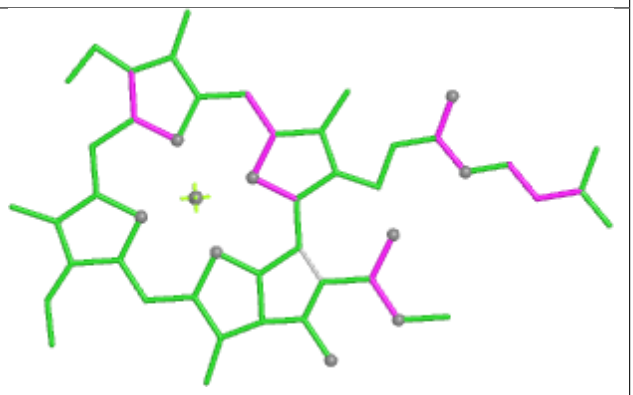
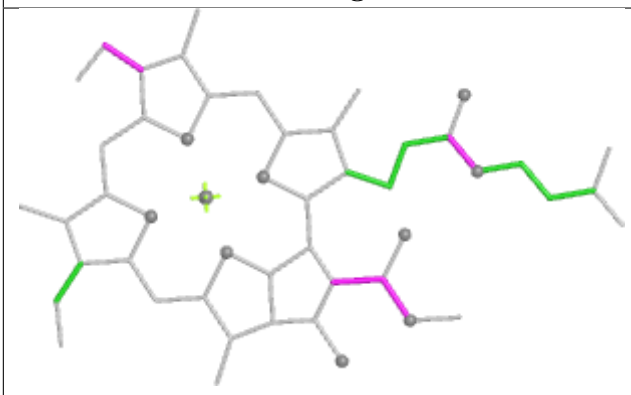


Bond angles



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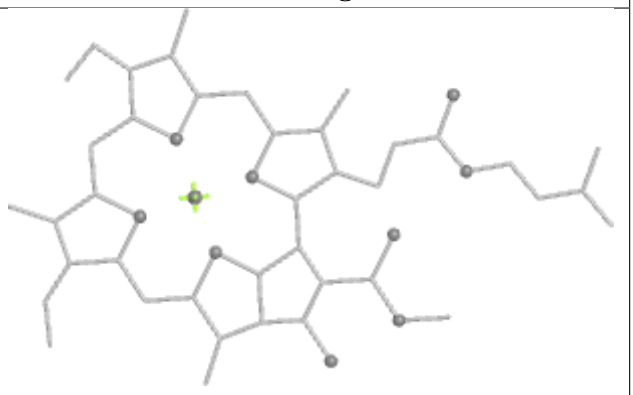
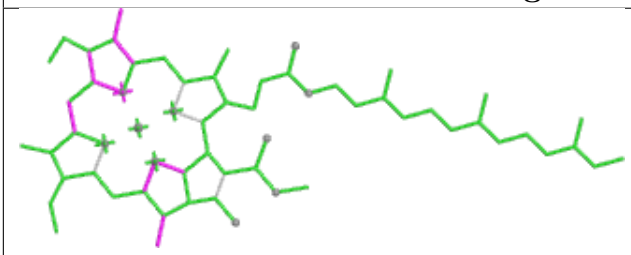


Rings

Ligand CLA A 306



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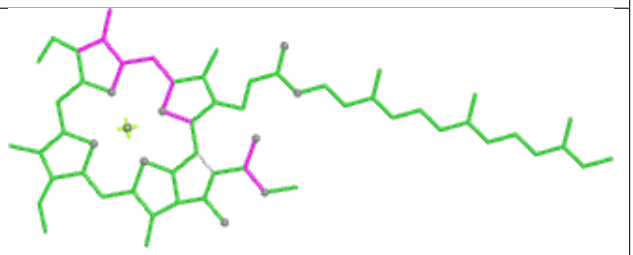
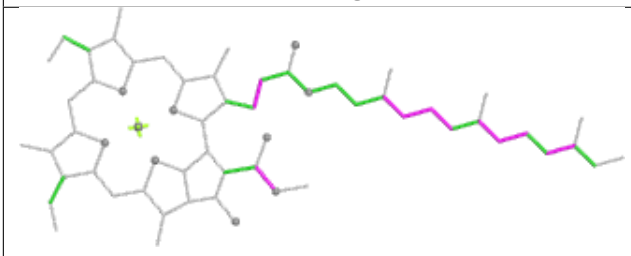
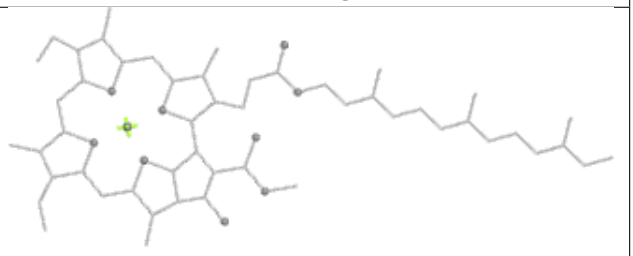


Bond angles

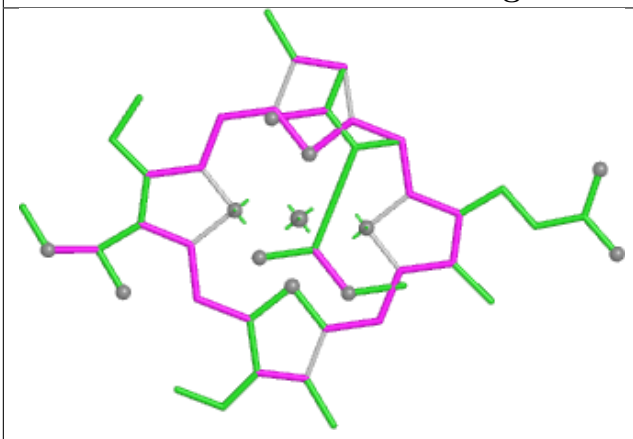


Torsions



Rings

Ligand A1ECV L 318



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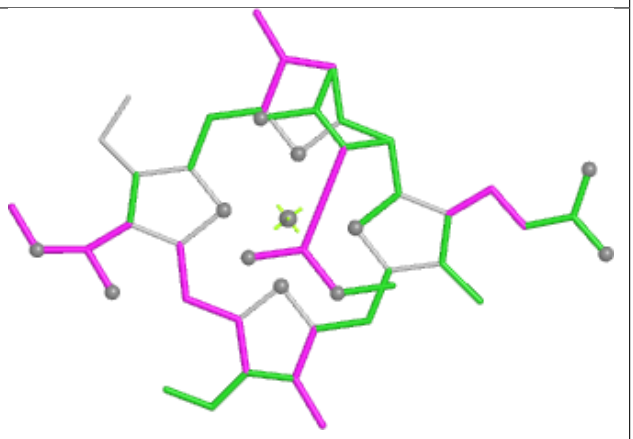
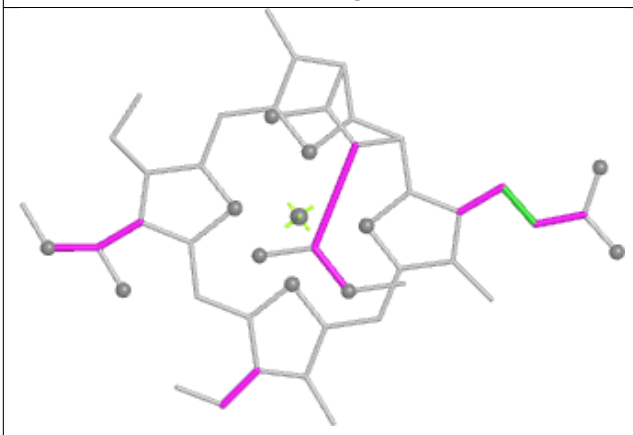
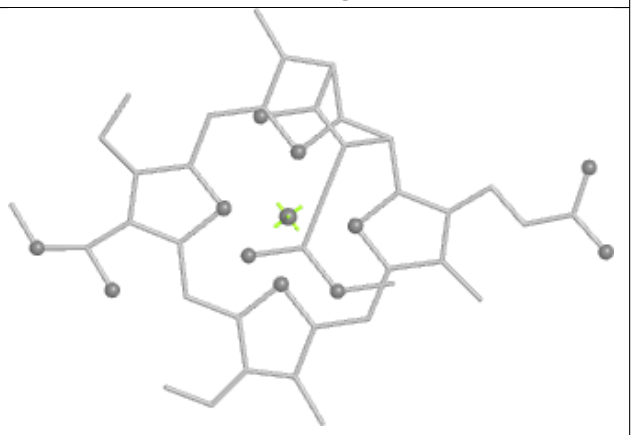


Bond angles

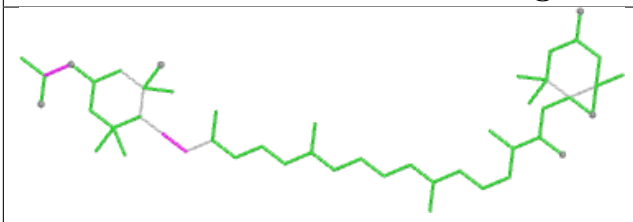


Torsions



Rings

Ligand A86 5 301



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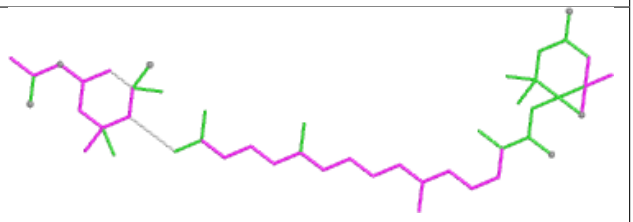
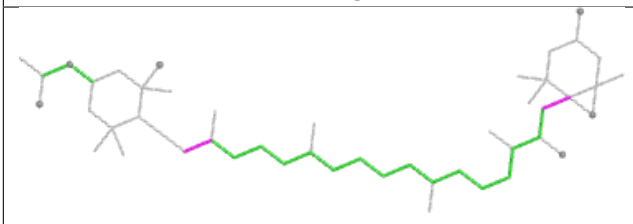
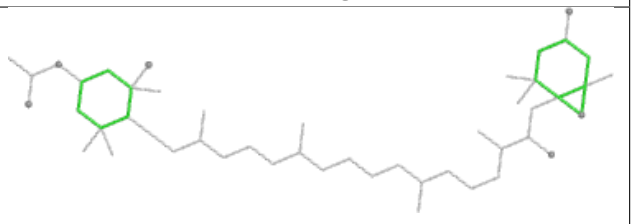


Bond angles

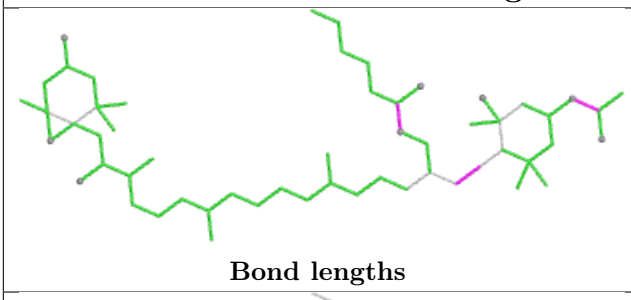


Torsions

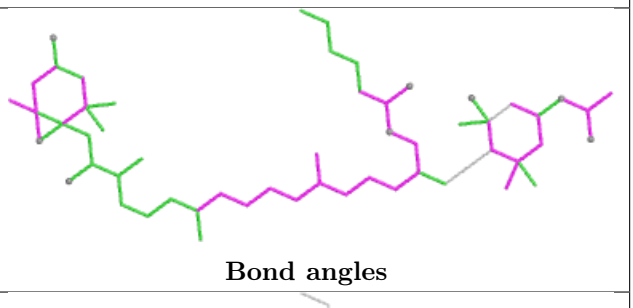


Rings

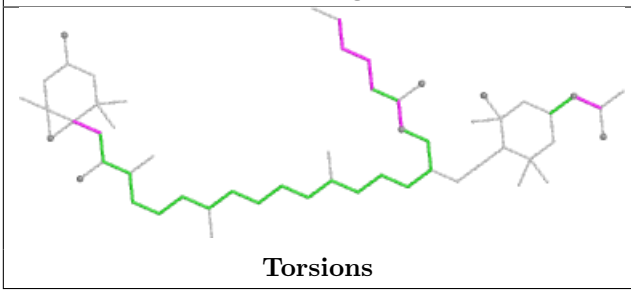
Ligand A1EB1 D 308



Bond lengths



Bond angles



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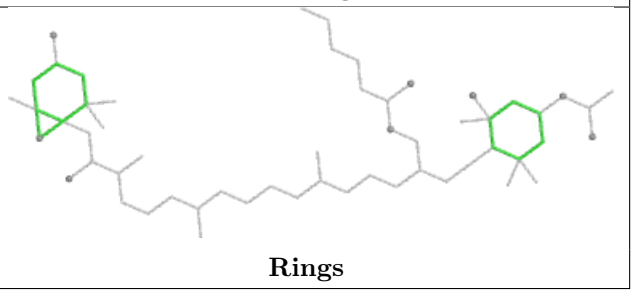
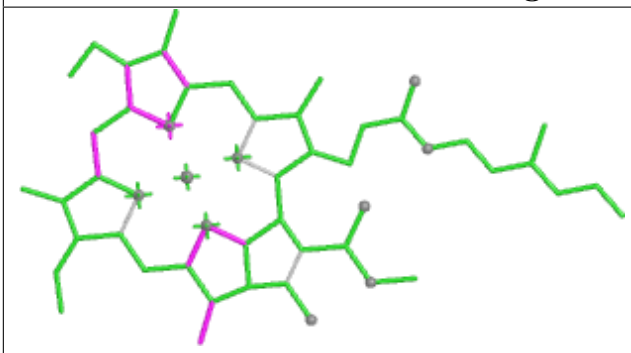


Rings

Ligand CLA U 209



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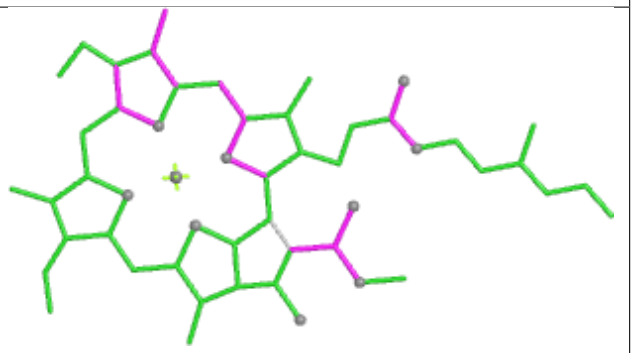
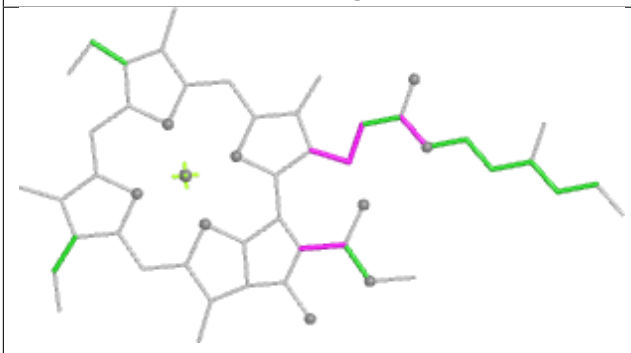


Bond angles



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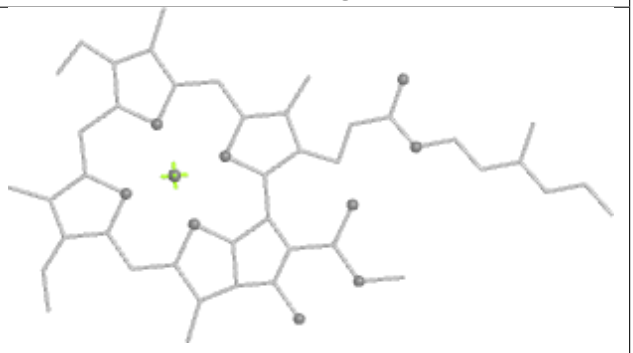
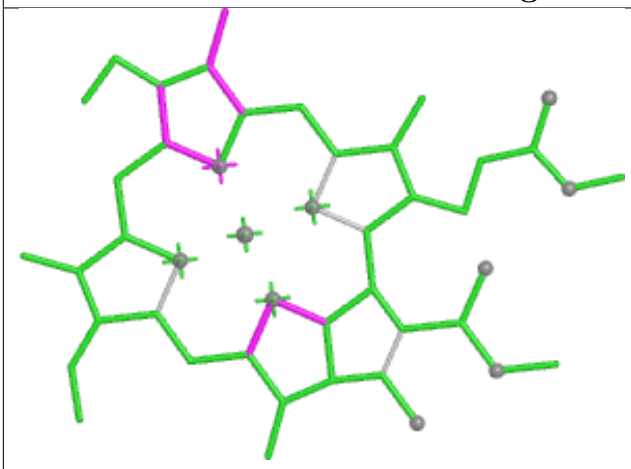


Rings

Ligand CLA M 318



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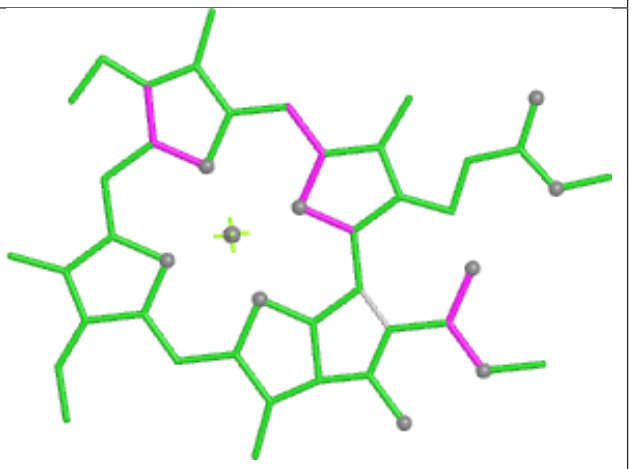
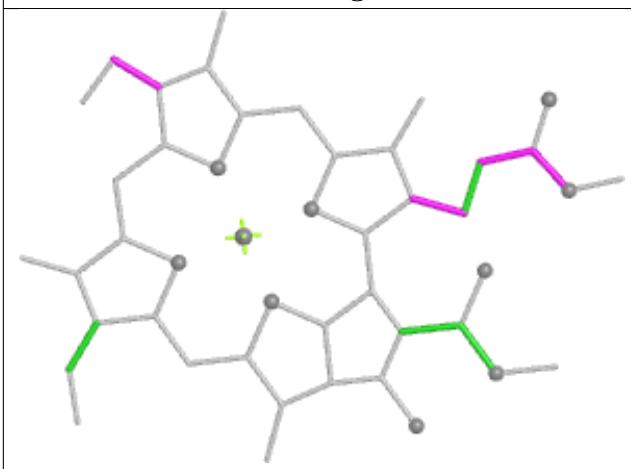


Bond angles



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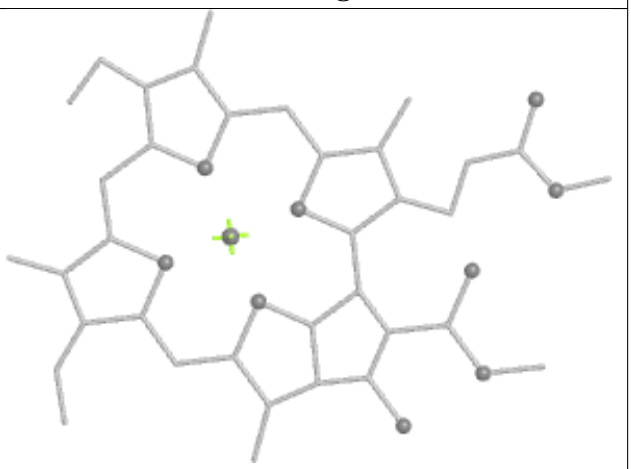
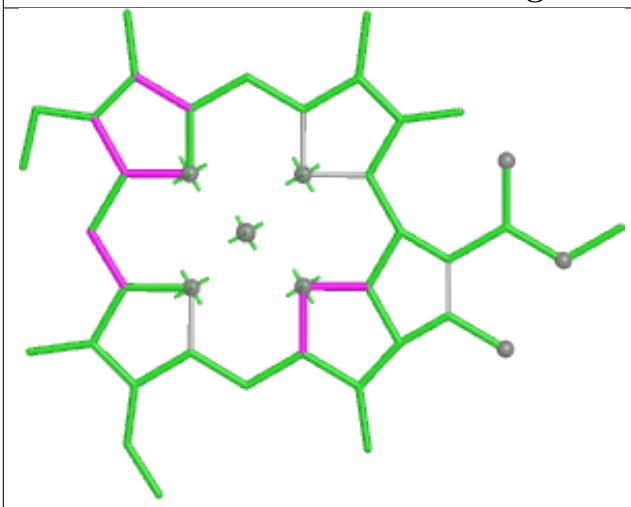


Rings

Ligand CLA Z 312



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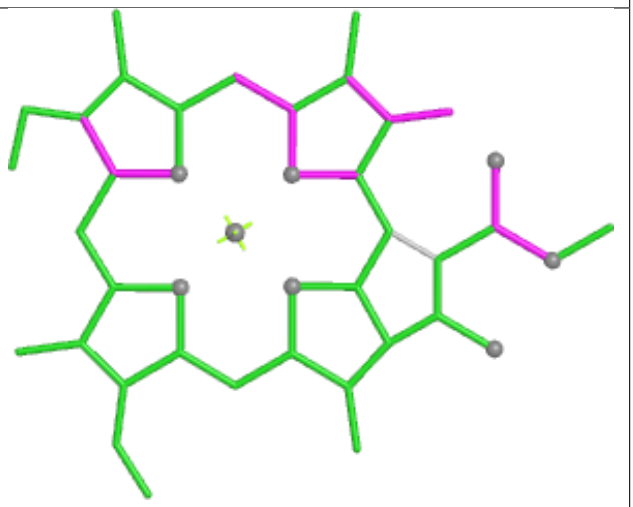

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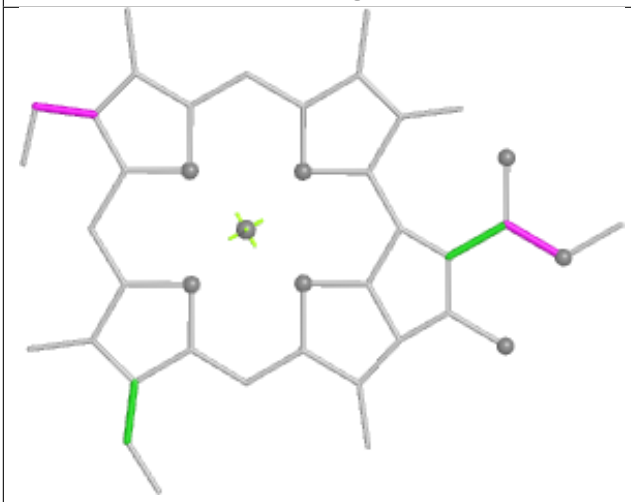

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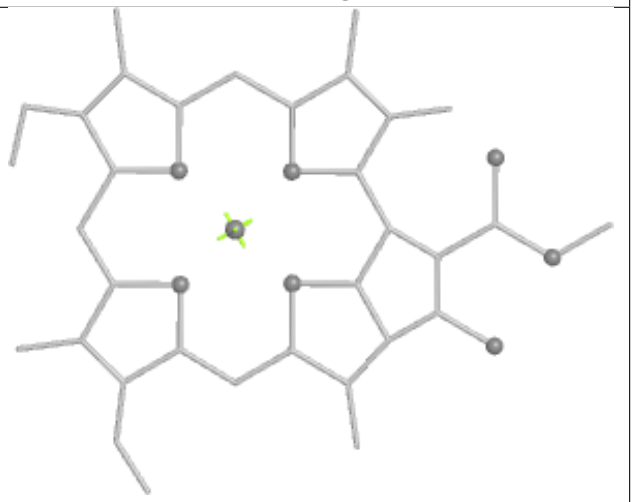
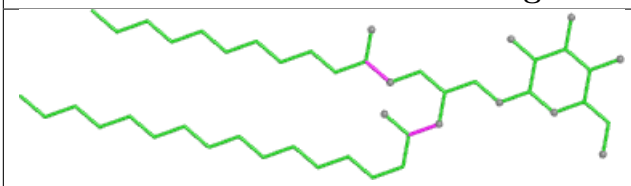


Rings

Ligand LMG 7 301



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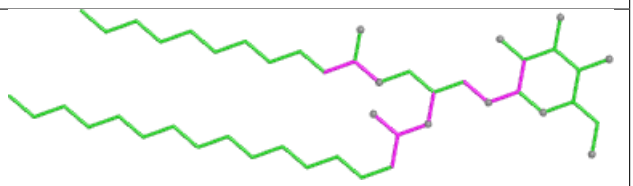

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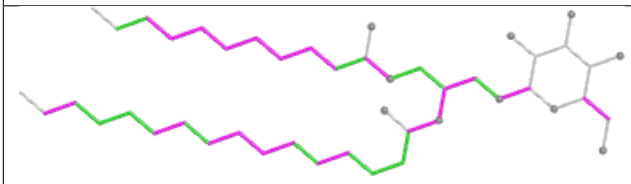

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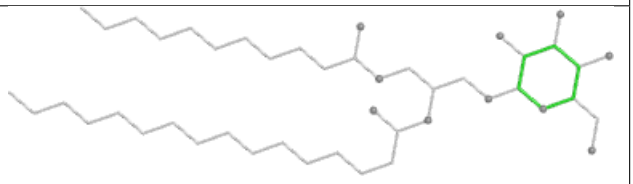
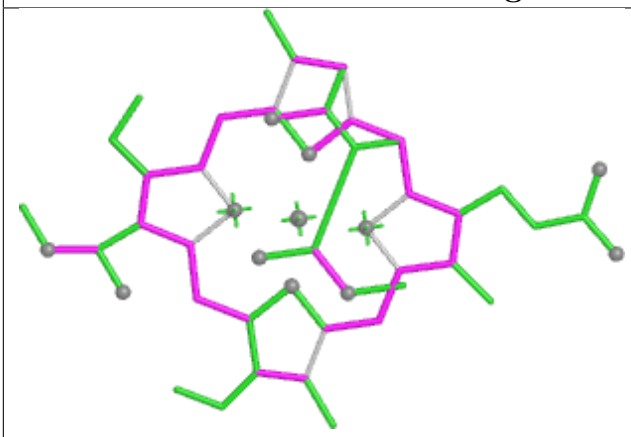


Rings

Ligand A1ECV 4 321



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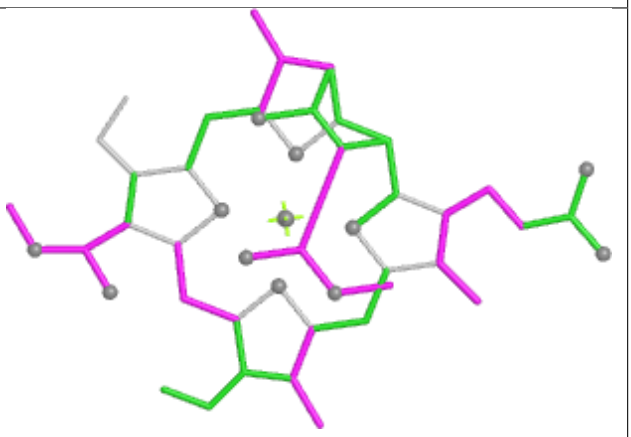

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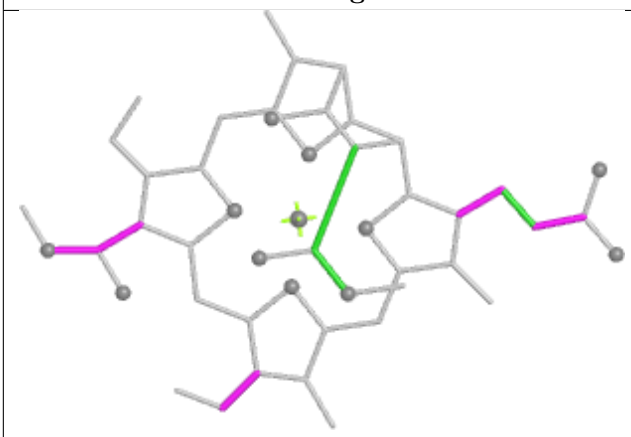

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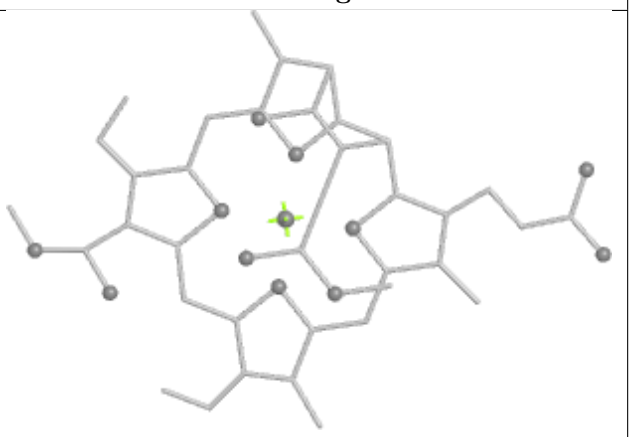
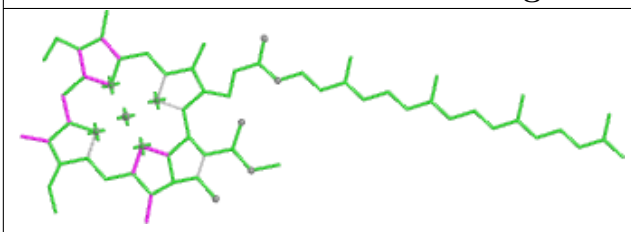


Rings

Ligand CLA D 317



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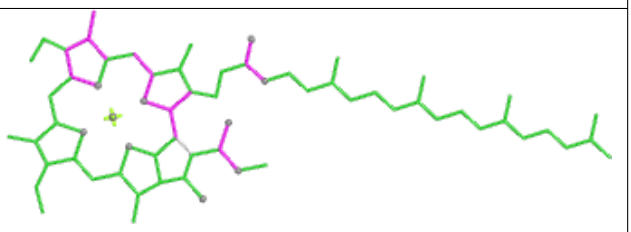

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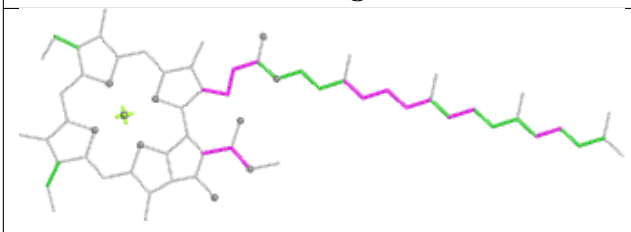

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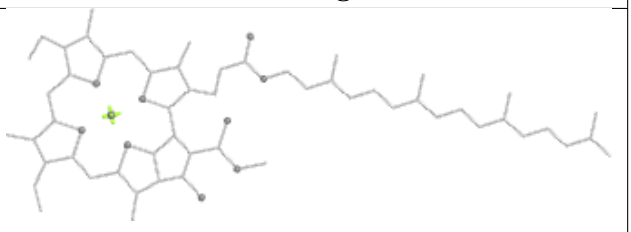
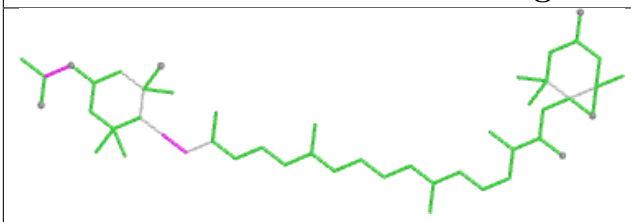


Rings

Ligand A86 6 305



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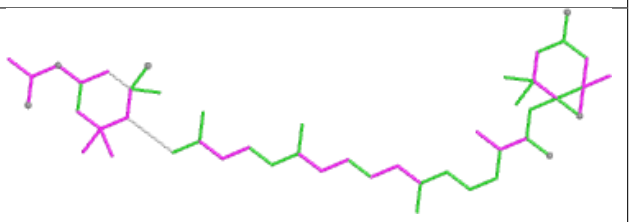

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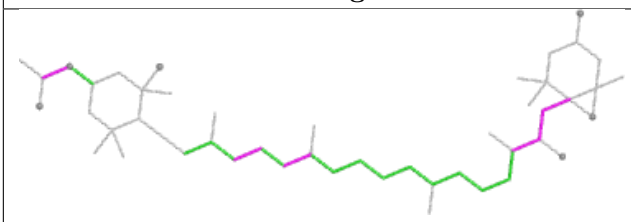

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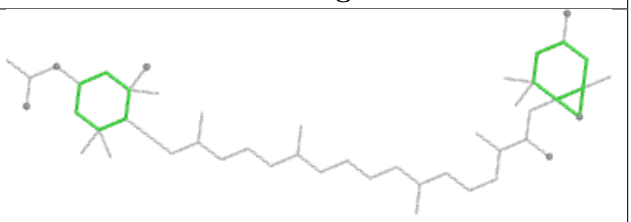
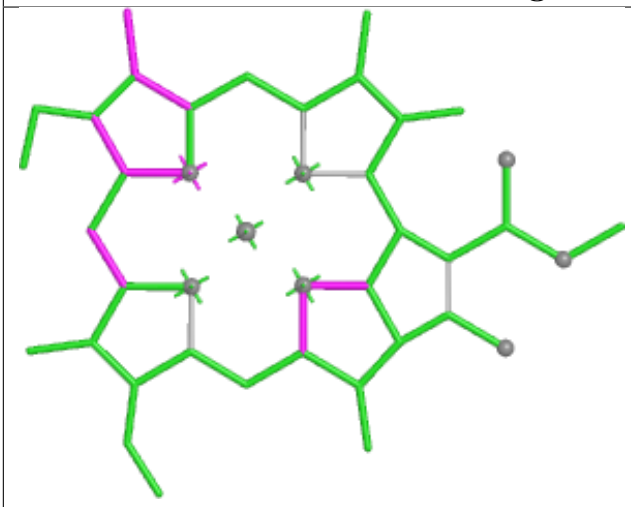


Rings

Ligand CLA 9 307



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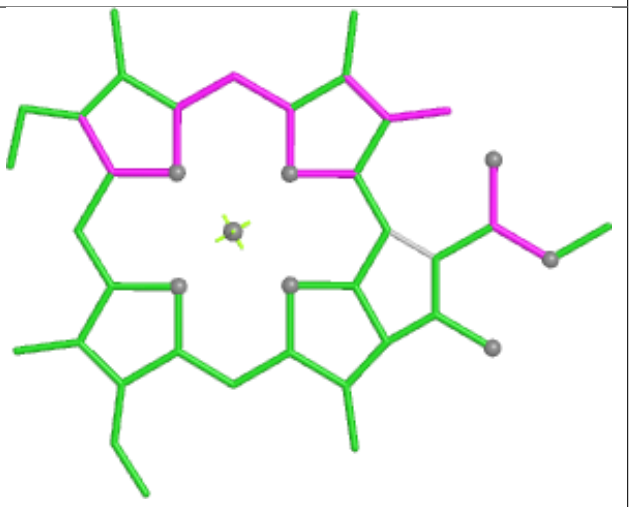

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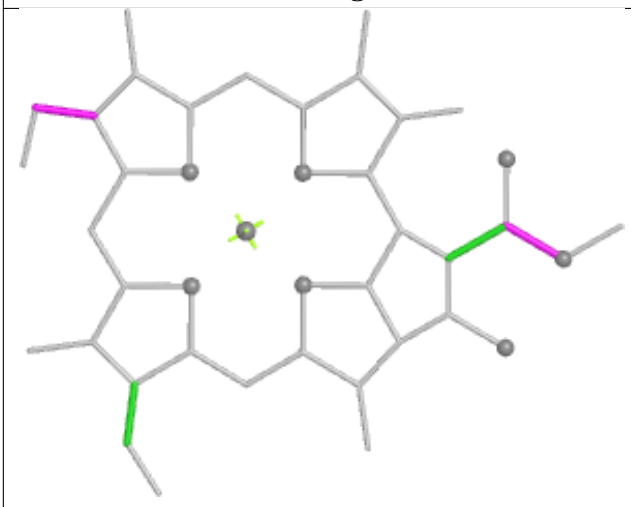

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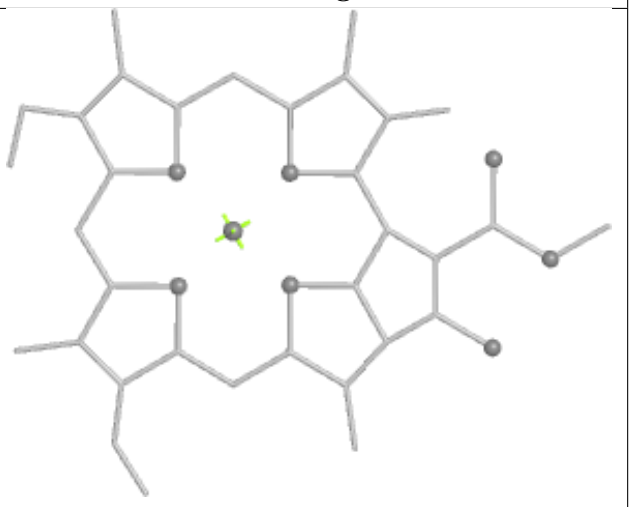
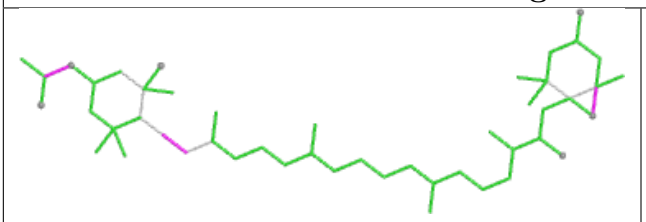


Rings

Ligand A86 Q 301



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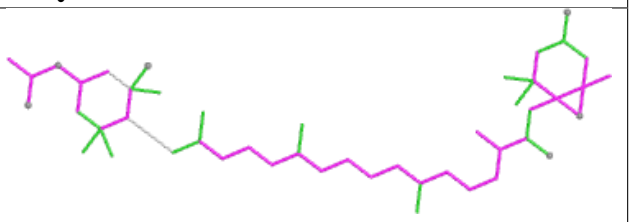
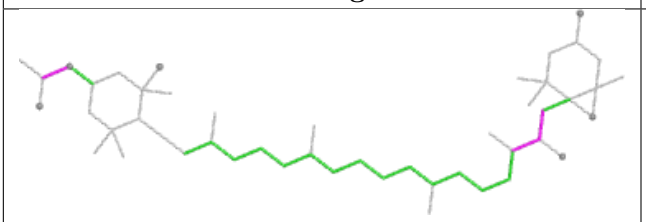


Bond angles



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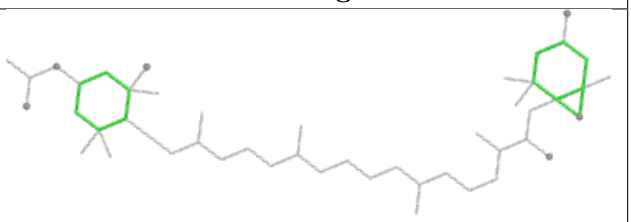
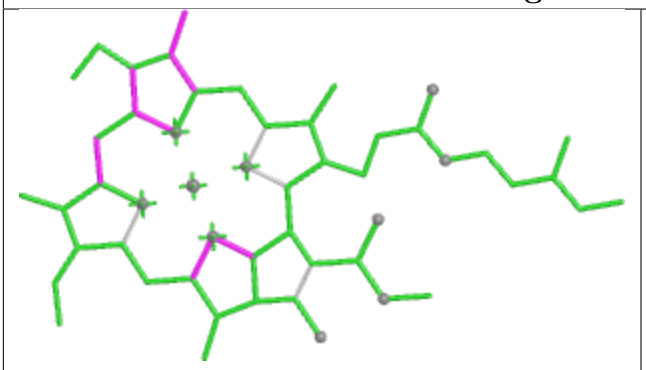


Rings

Ligand CLA T 313



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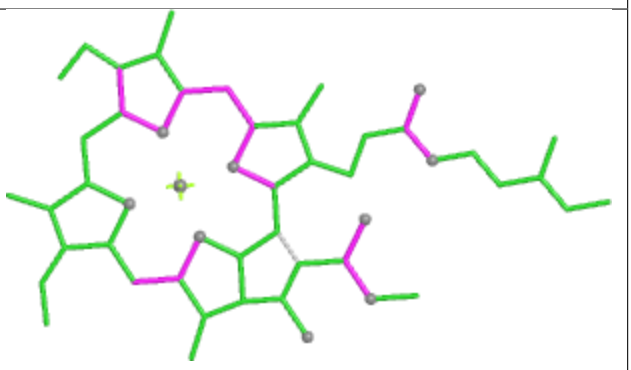

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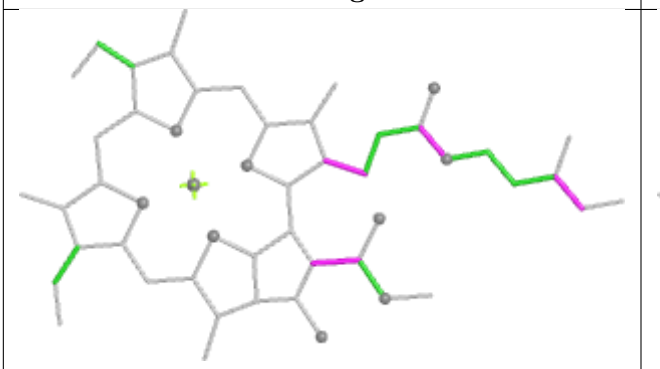

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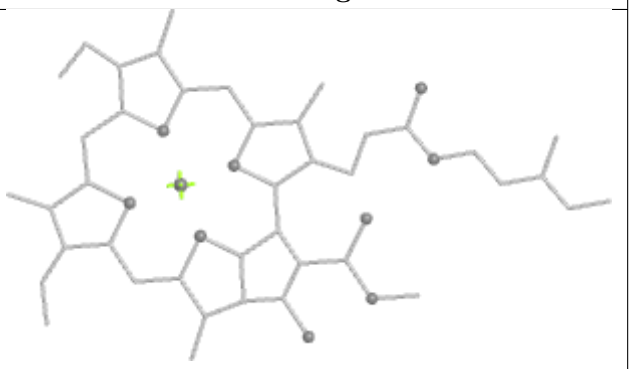
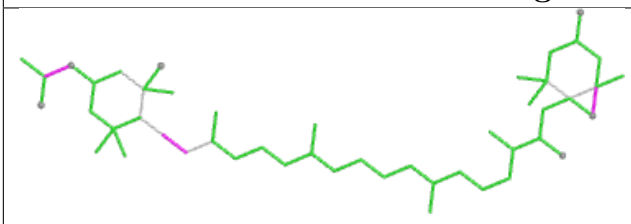


Rings

Ligand A86 8 307



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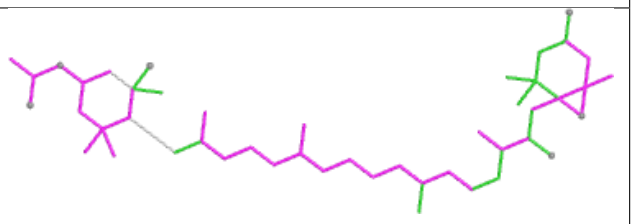
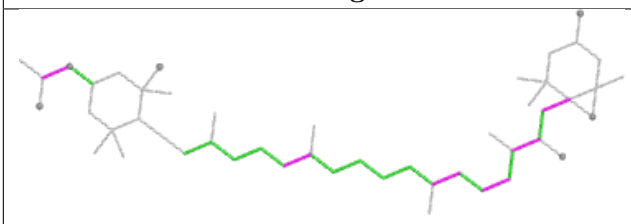


Bond angles



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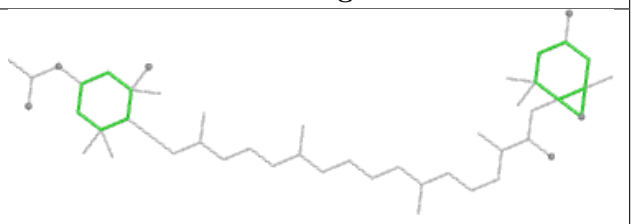
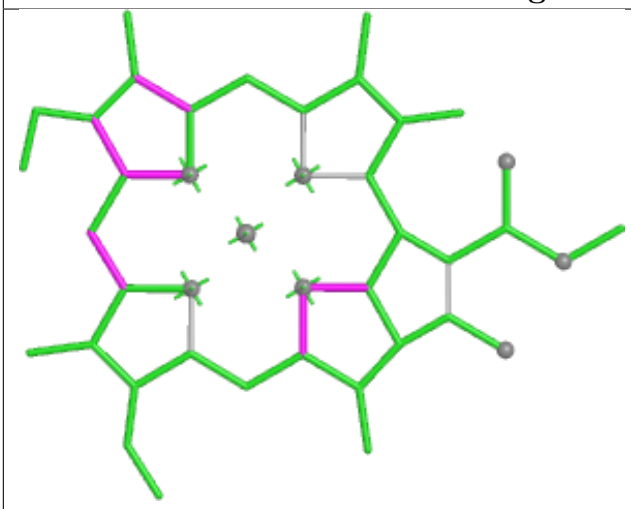


Rings

Ligand CLA 1 317



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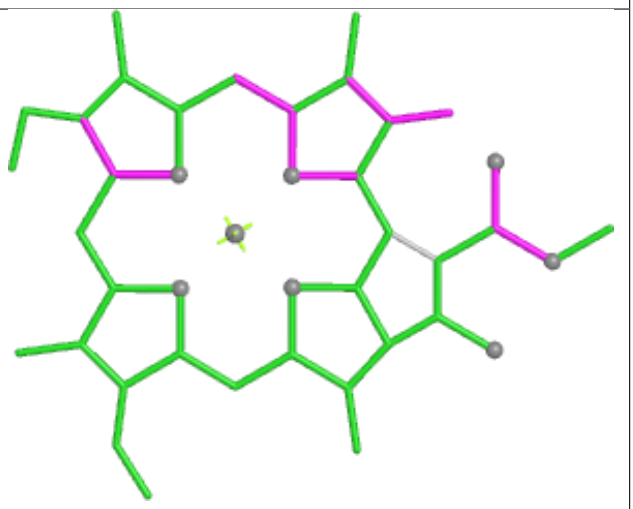
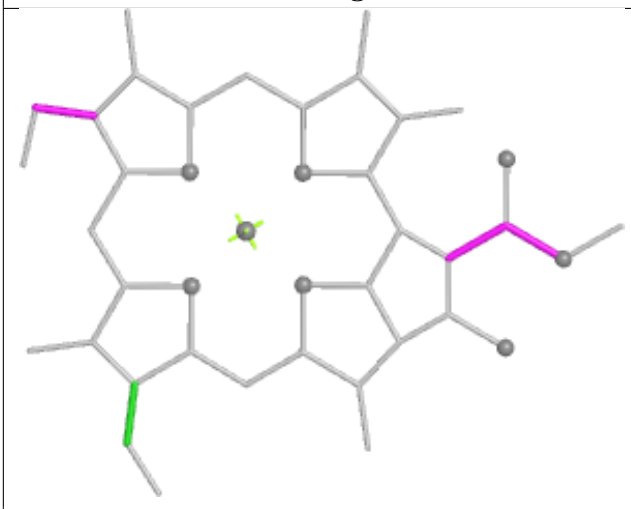


Bond angles



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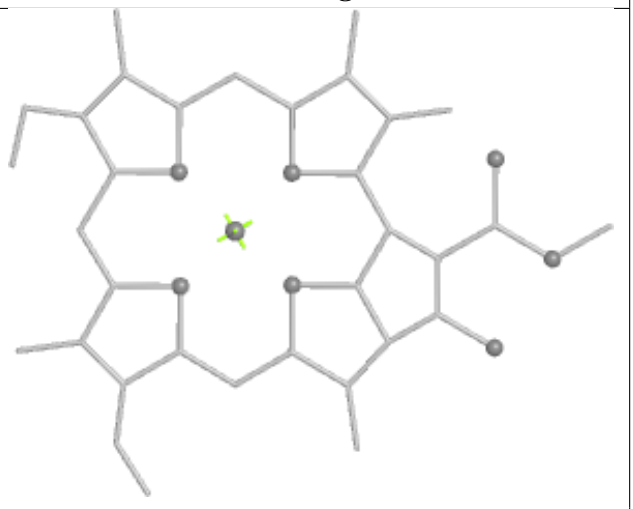
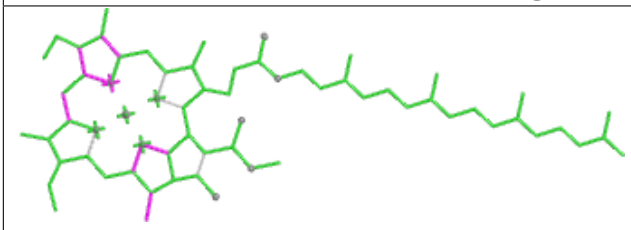
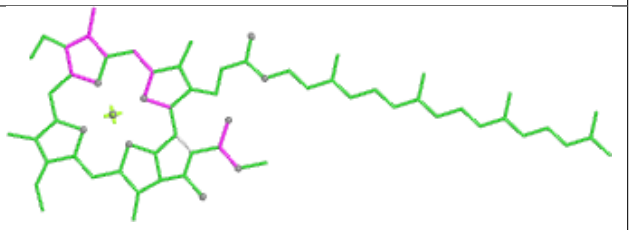


Rings

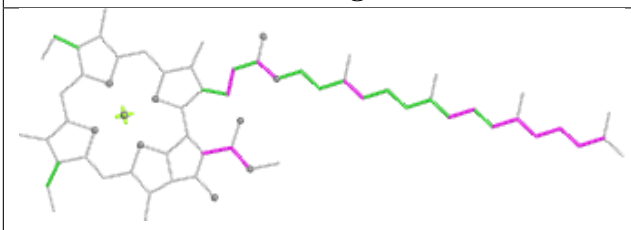
Ligand CLA a 826



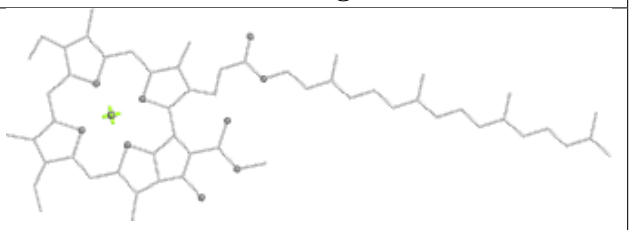
Bond lengths



Bond angles

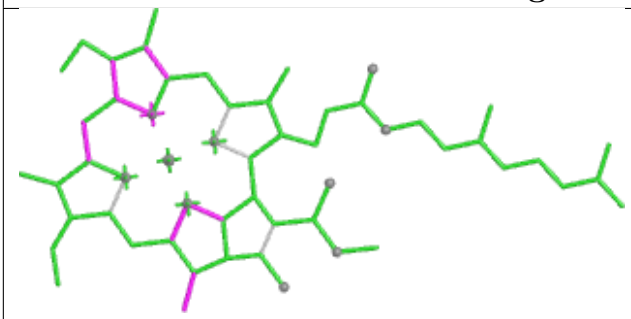


Torsions

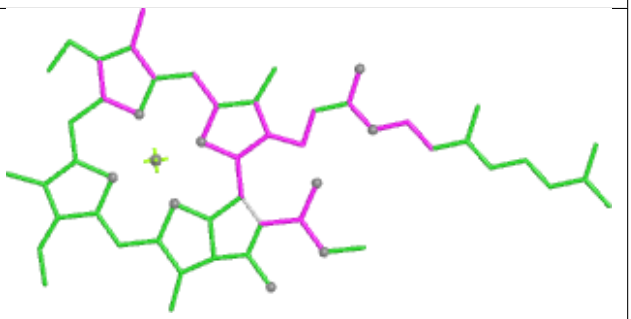


Rings

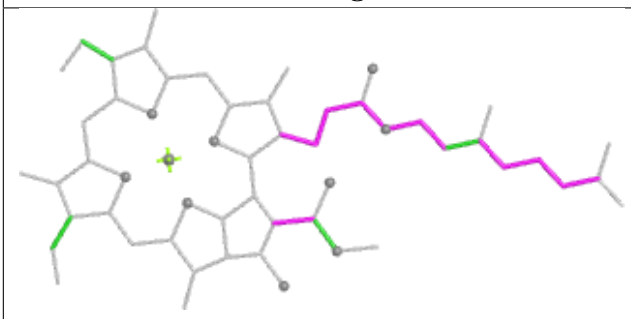
Ligand CLA 9 308



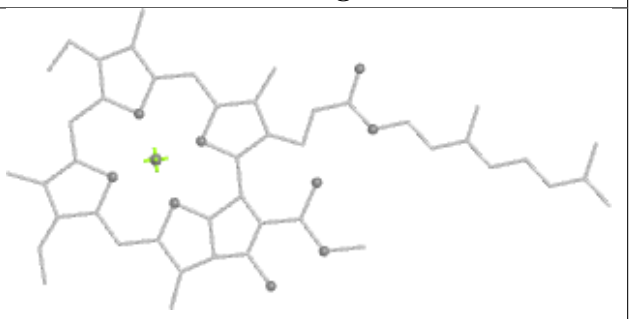
Bond lengths



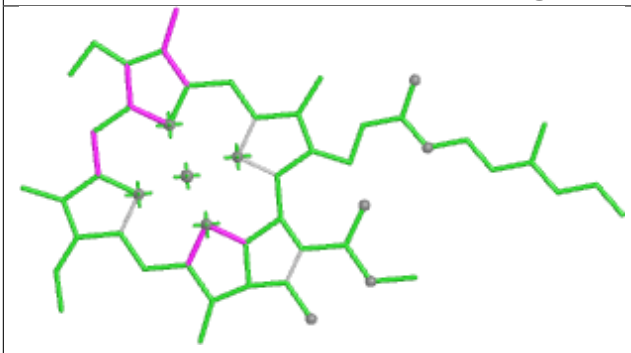
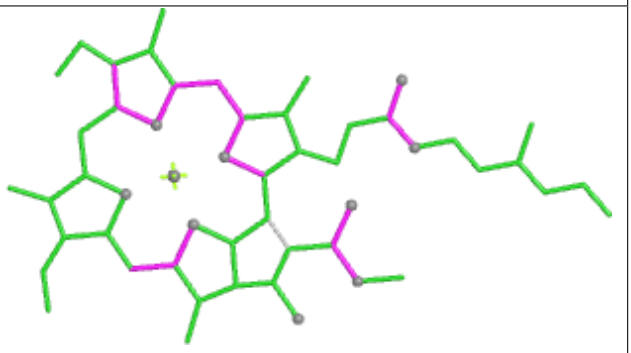
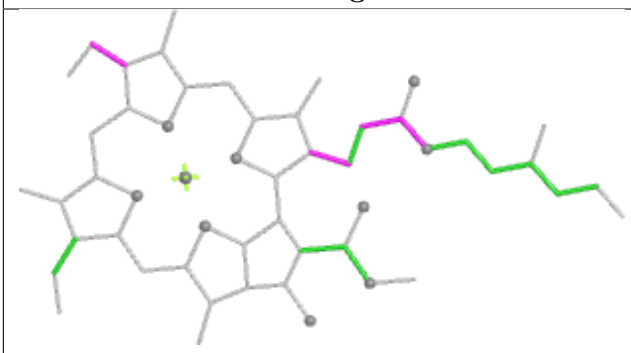
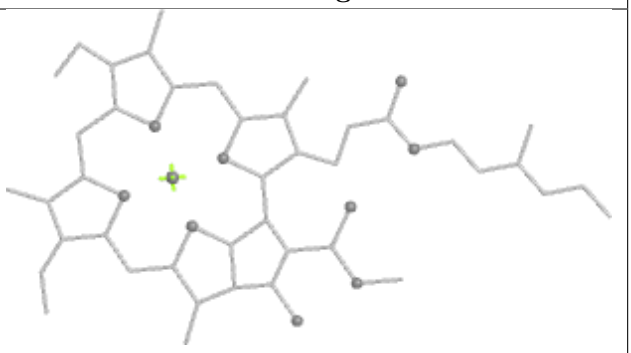
Bond angles

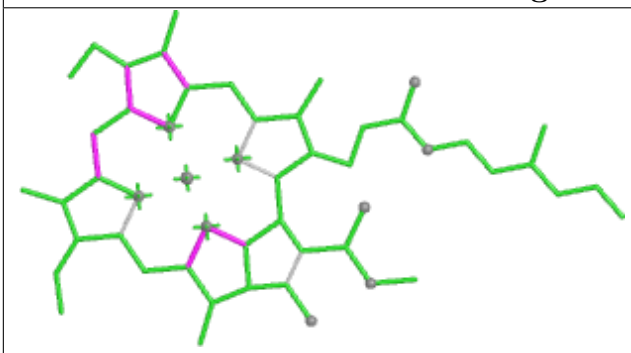
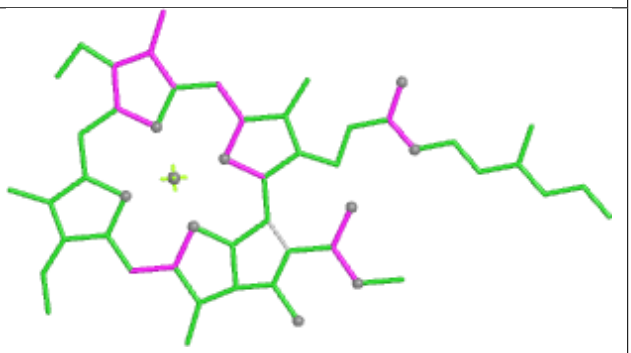
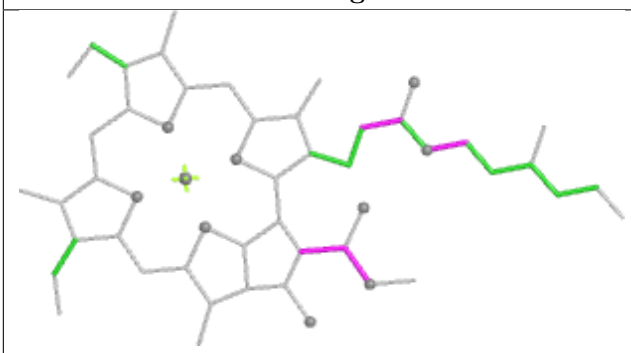
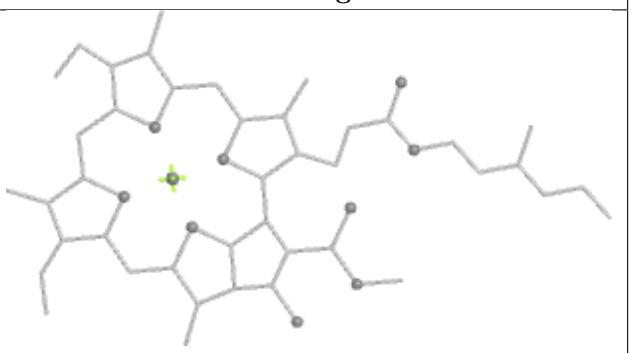


Torsions

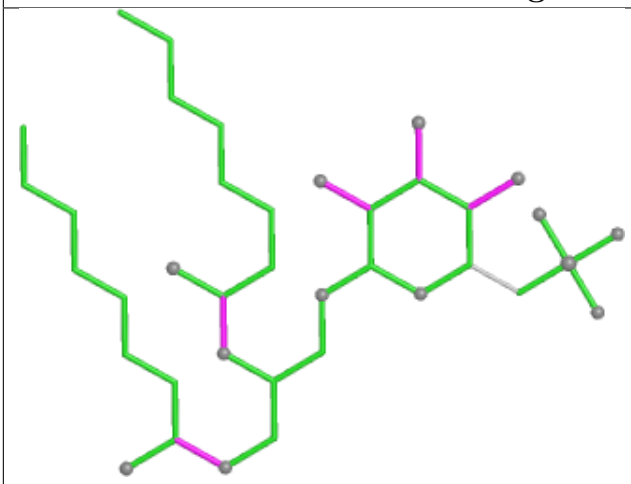


Rings

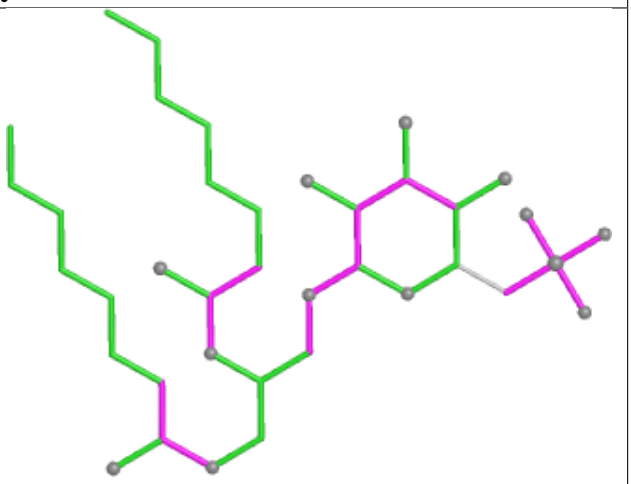
Ligand CLA I 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA I 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

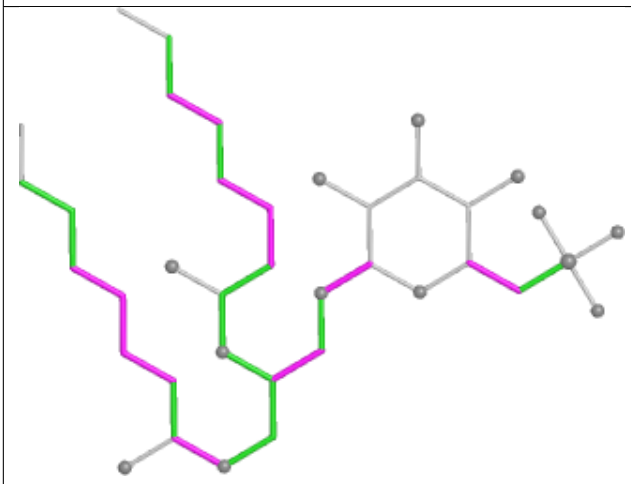
Ligand SQD k 205



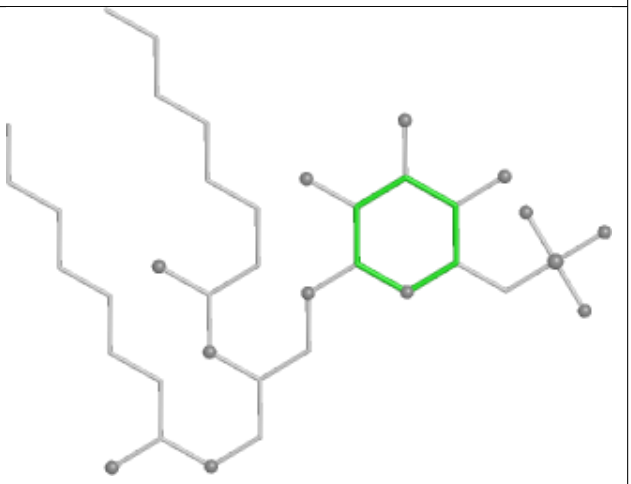
Bond lengths



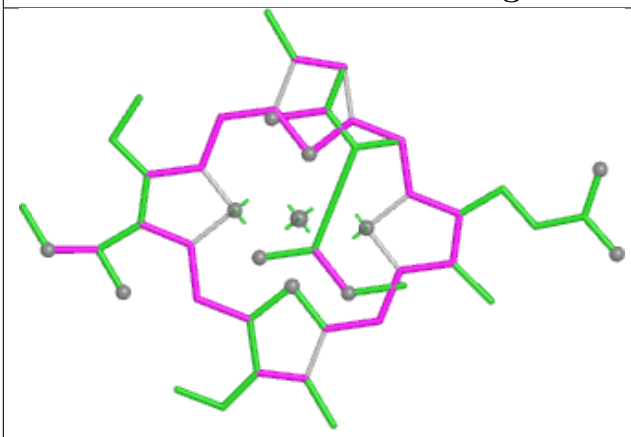
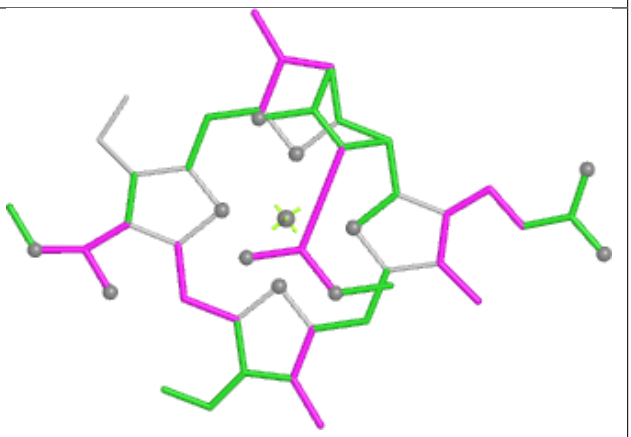
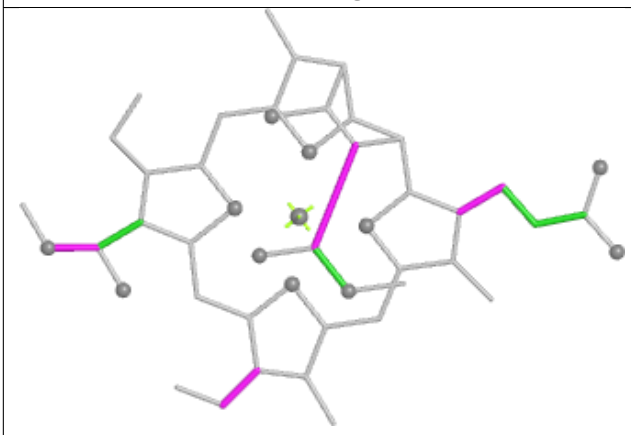
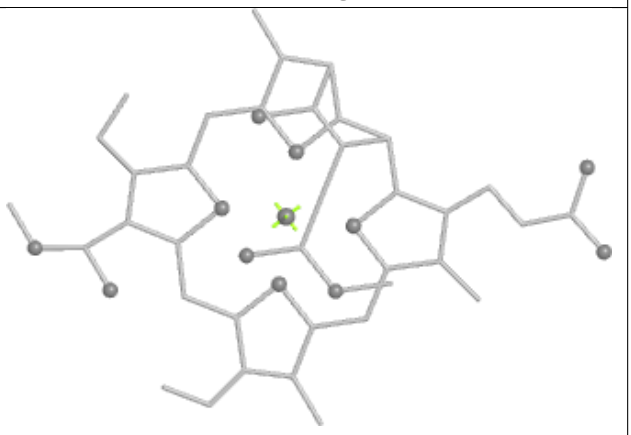
Bond angles



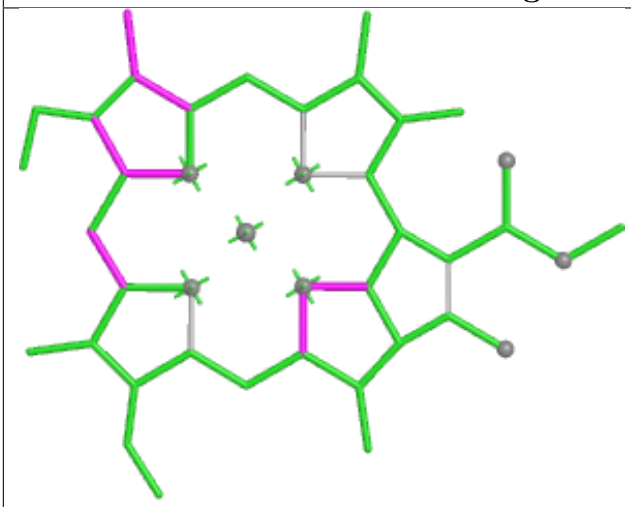
Torsions



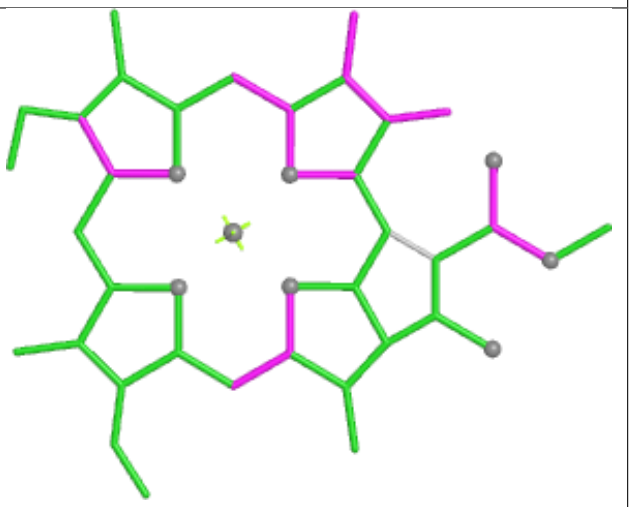
Rings

Ligand A1ECV Z 314	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

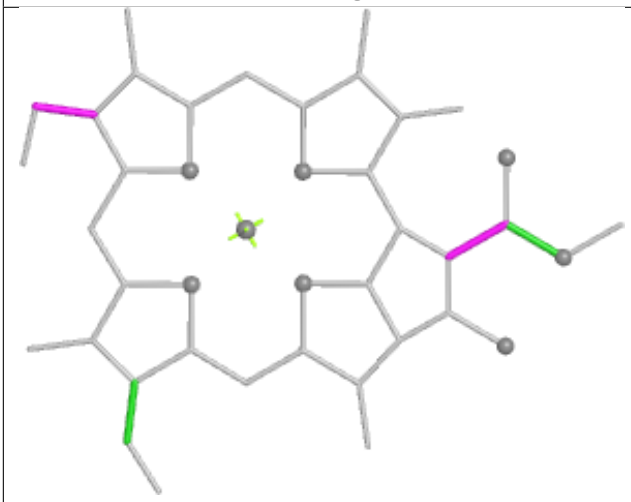
Ligand CLA K 314



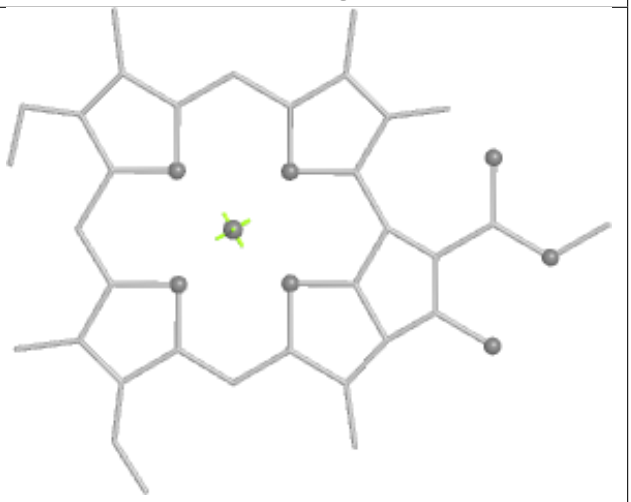
Bond lengths



Bond angles

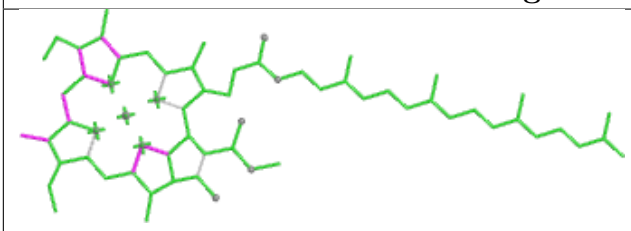


Torsions



Rings

Ligand CLA H 313



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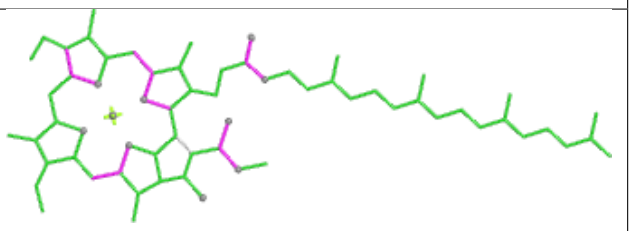
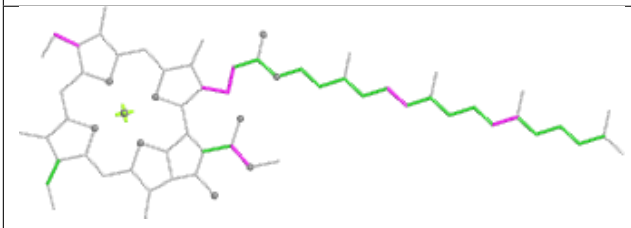


Bond angles



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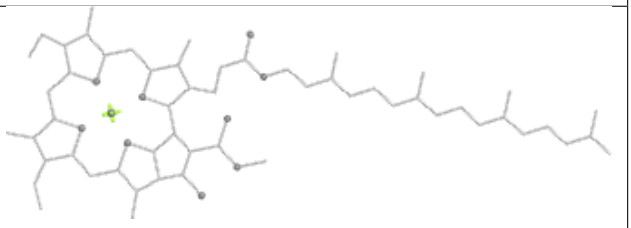
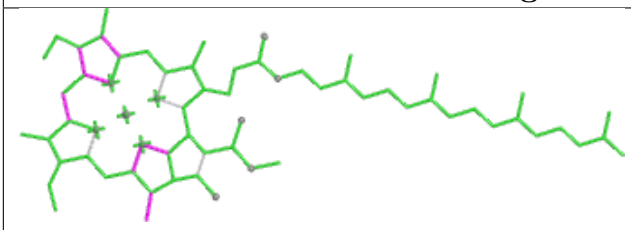
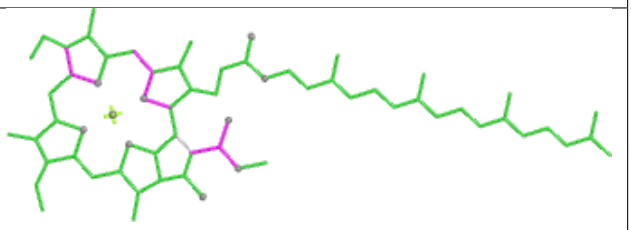


Rings

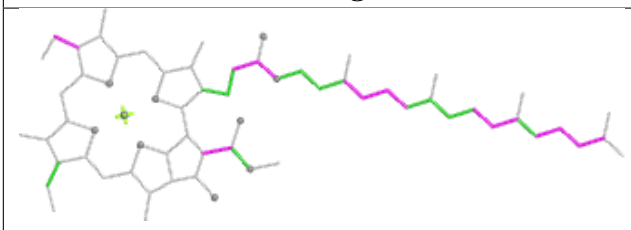
Ligand CLA M 309



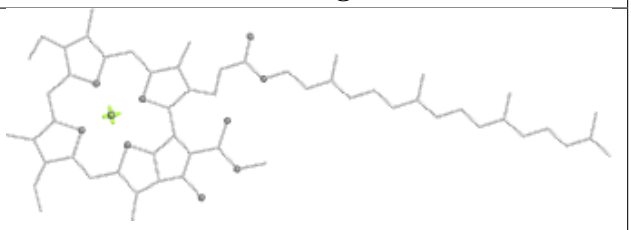
Bond lengths



Bond angles

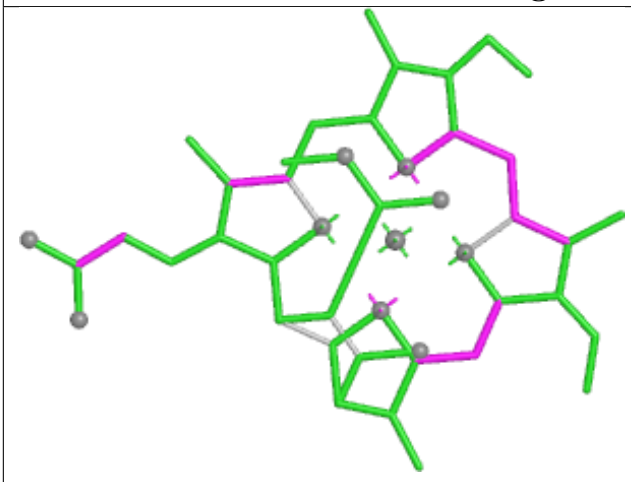


Torsions



Rings

Ligand KC2 6 314



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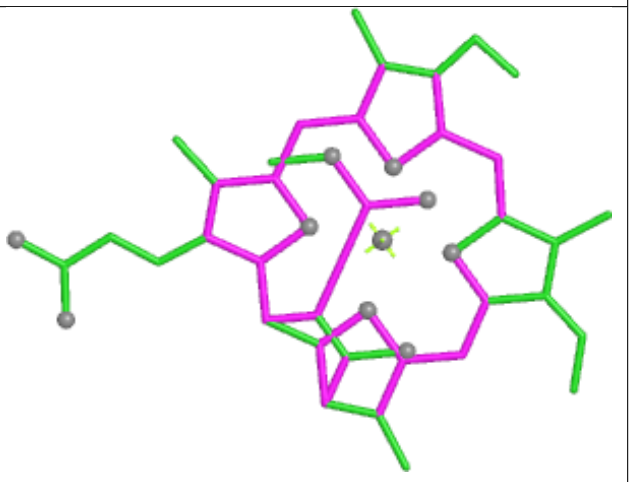
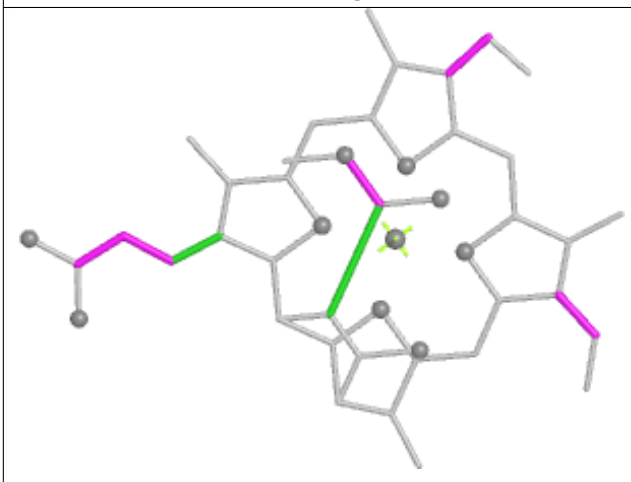


Bond angles



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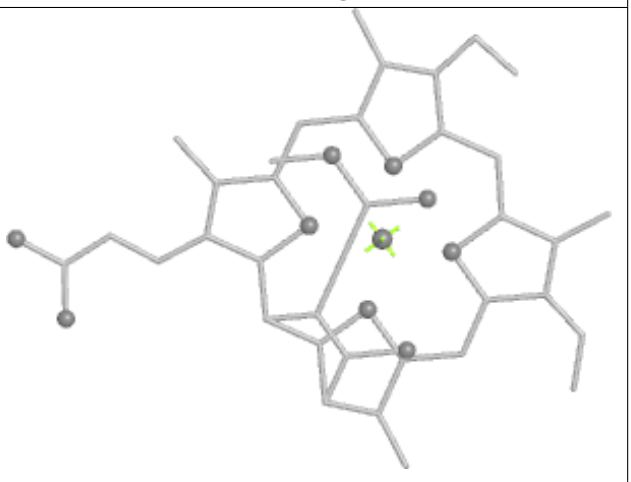
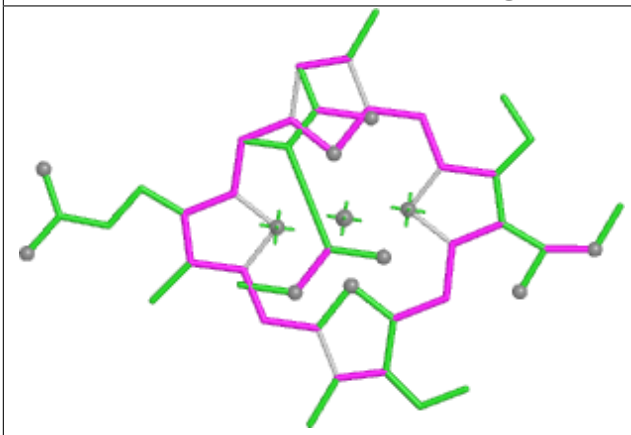


Rings

Ligand A1ECV O 315



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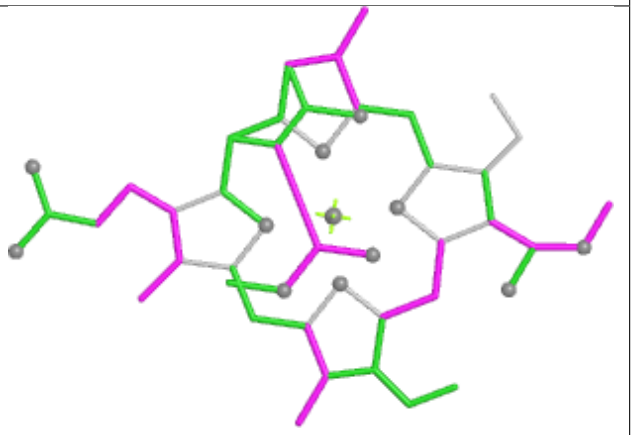
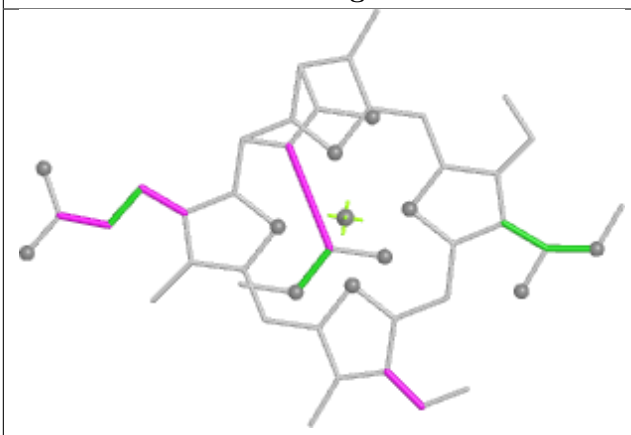


Bond angles



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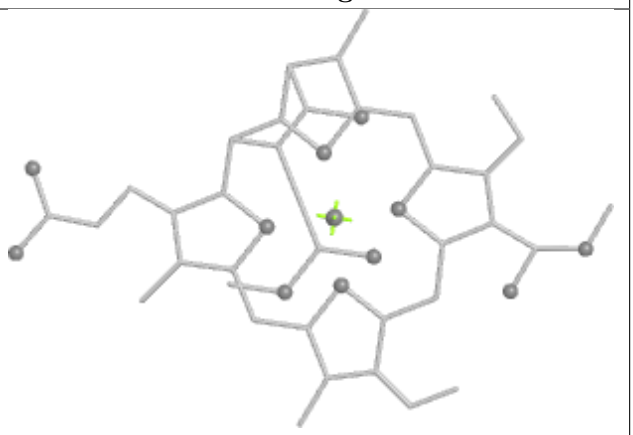
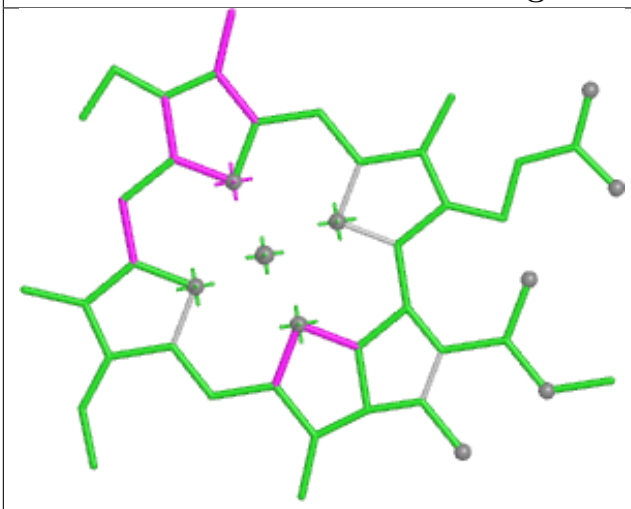


Rings

Ligand CLA b 836



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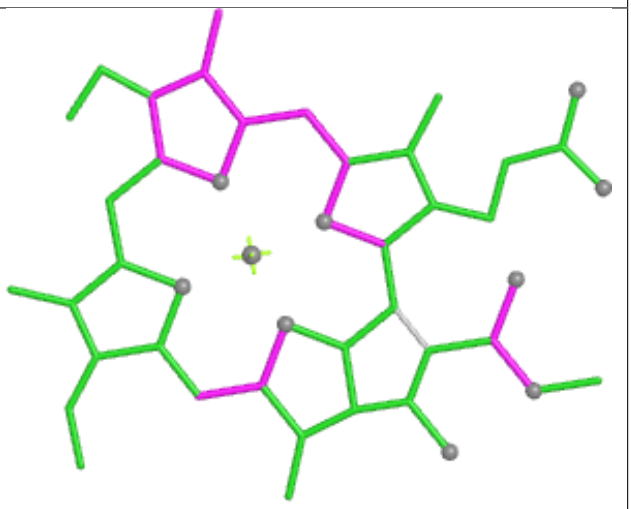
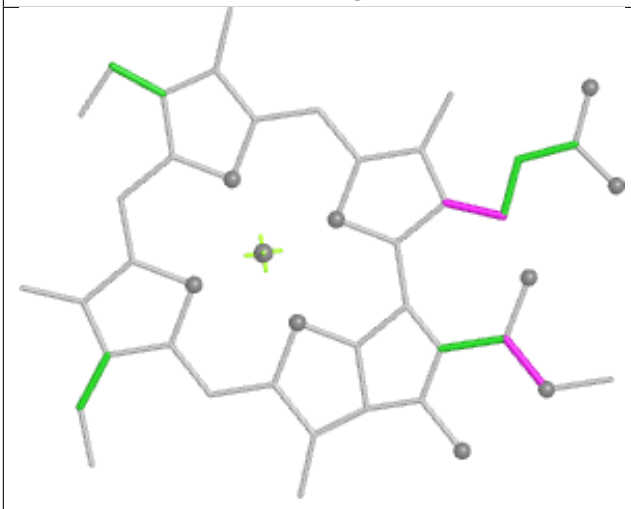


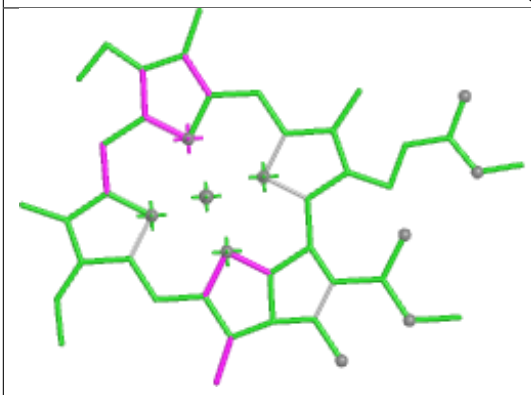
Bond angles



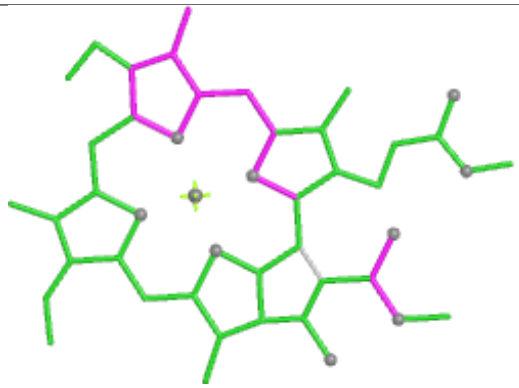
Torsions

Rings

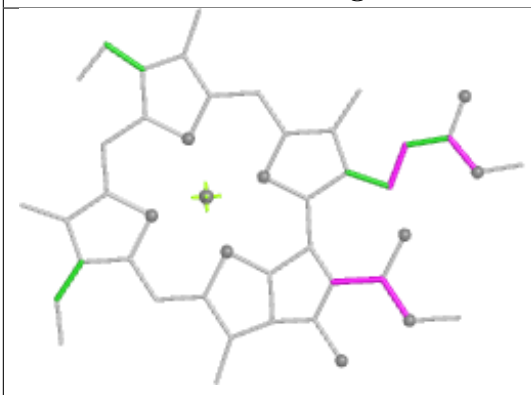
Ligand CLA J 318



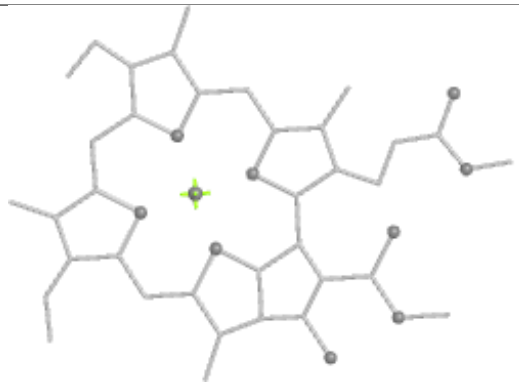
Bond lengths



Bond angles

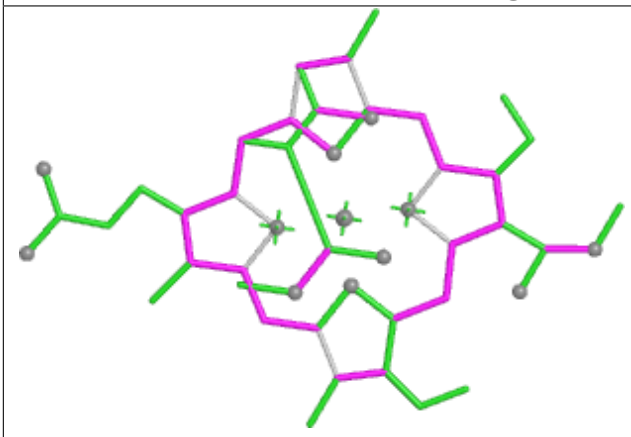


Torsions



Rings

Ligand A1ECV 4 315



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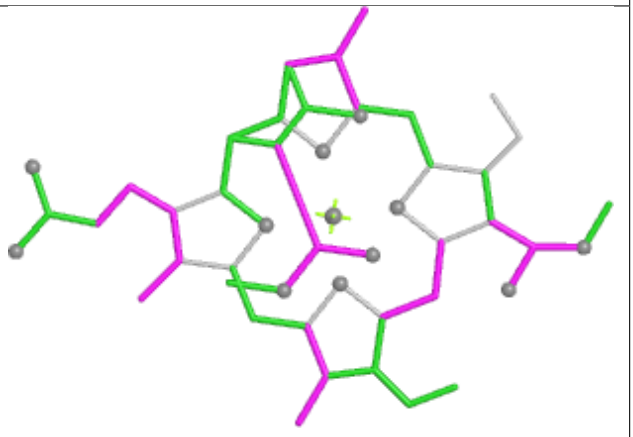
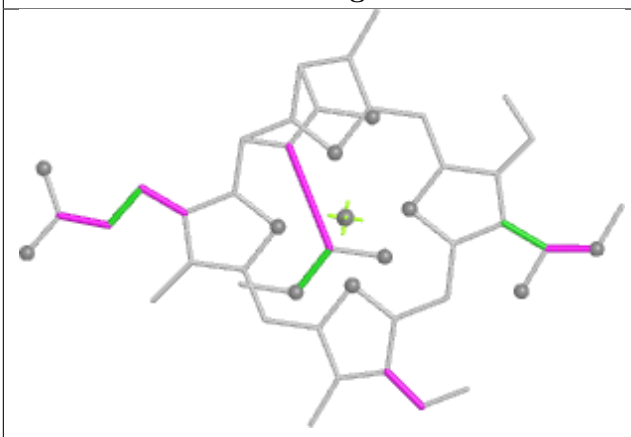
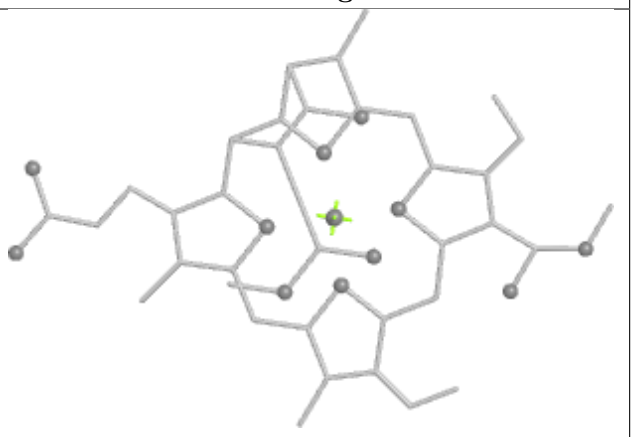


Bond angles

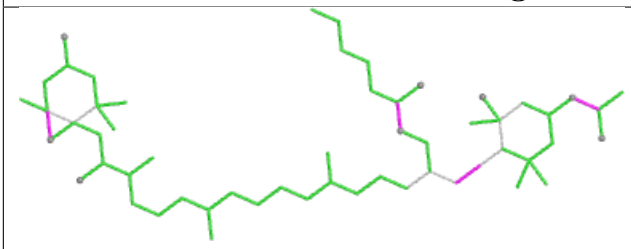


Torsions

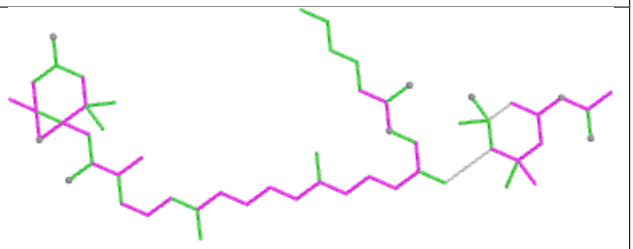


Rings

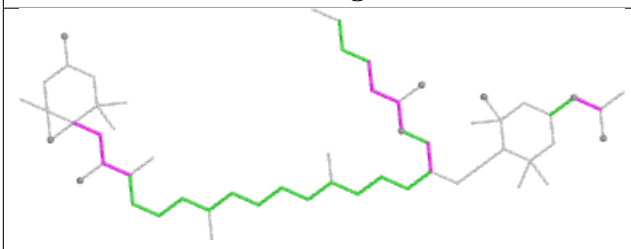
Ligand A1EB1 7 304



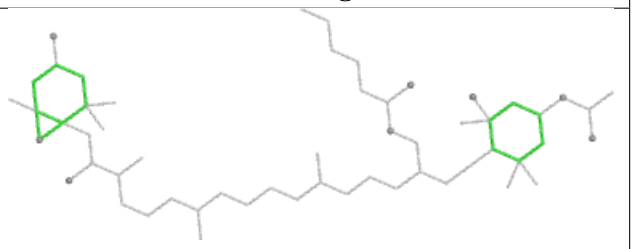
Bond lengths



Bond angles

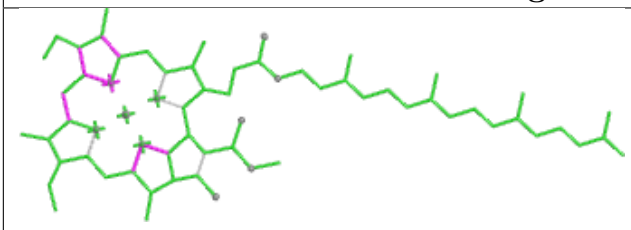


Torsions



Rings

Ligand CLA J 314



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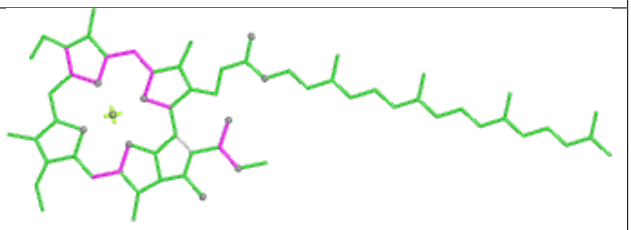

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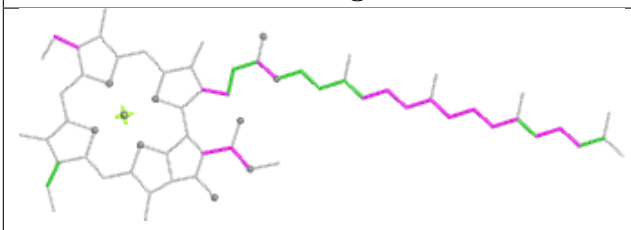

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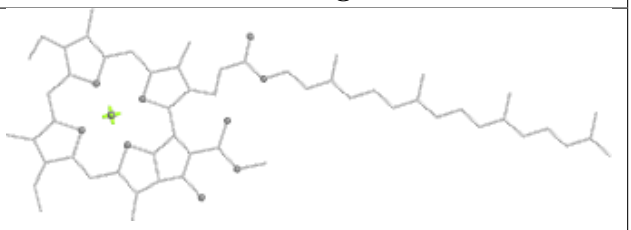
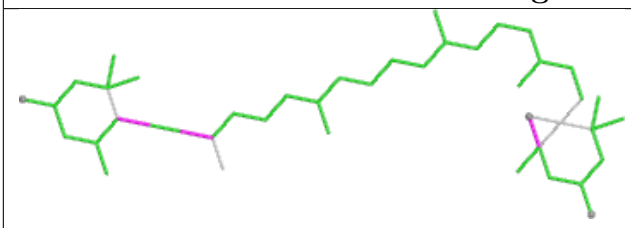


Rings

Ligand DD6 I 305



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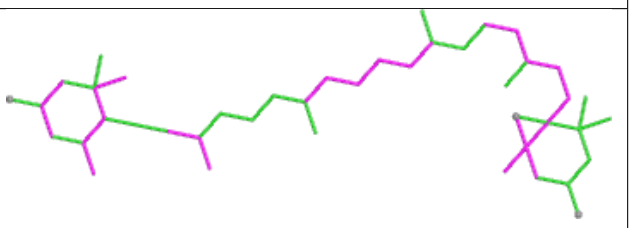

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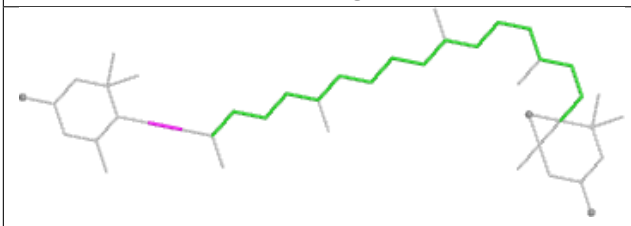

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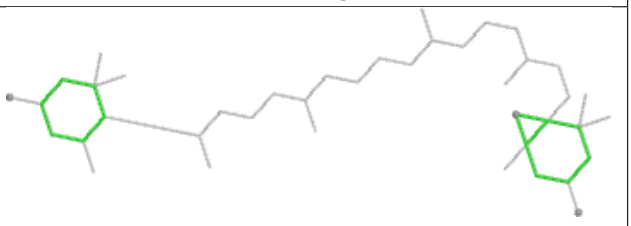
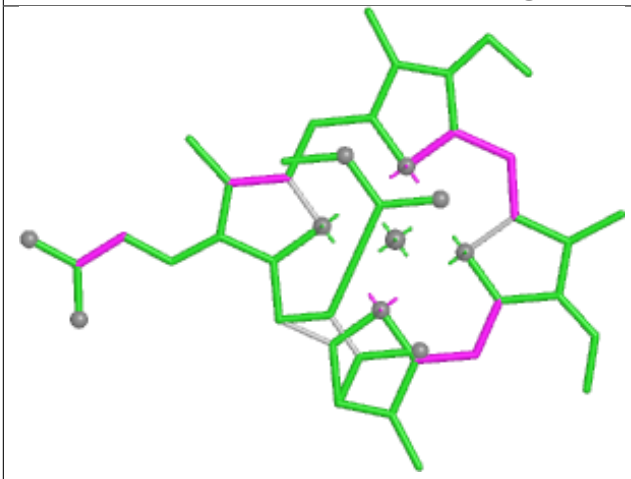


Rings

Ligand KC2 W 315



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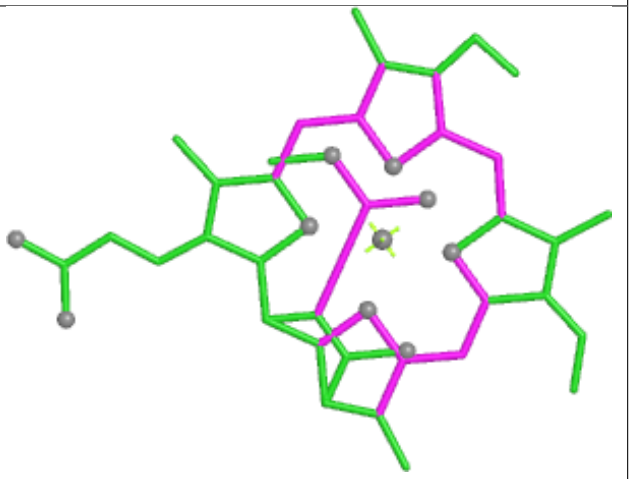
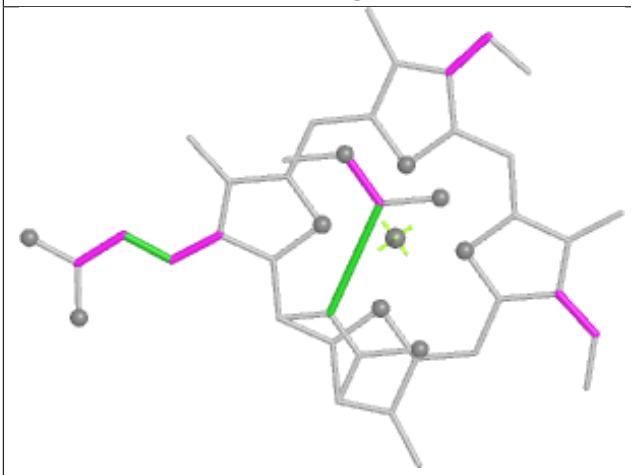


Bond angles



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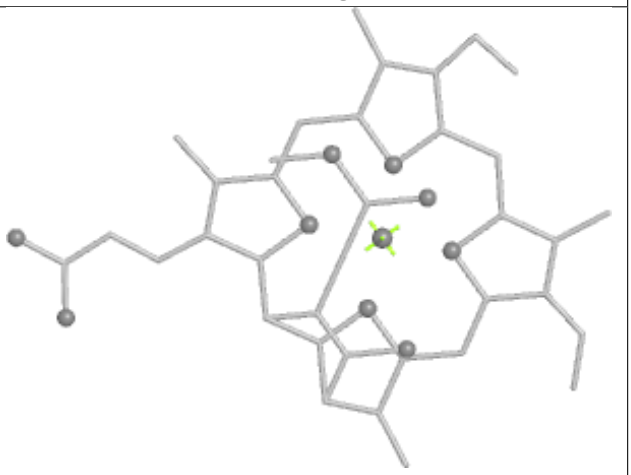
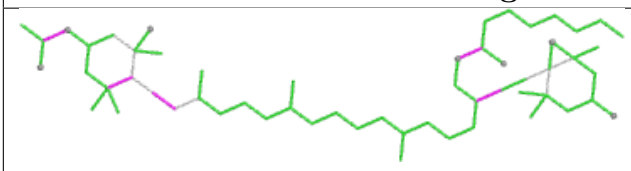


Rings

Ligand A1EB4 W 321



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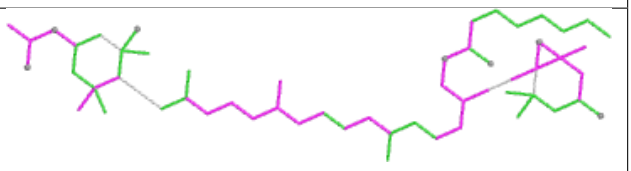
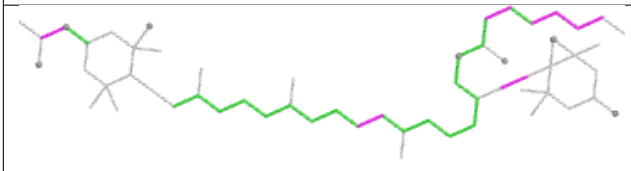


Bond angles



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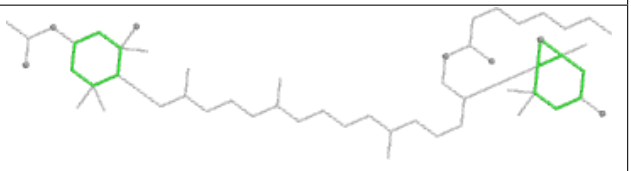
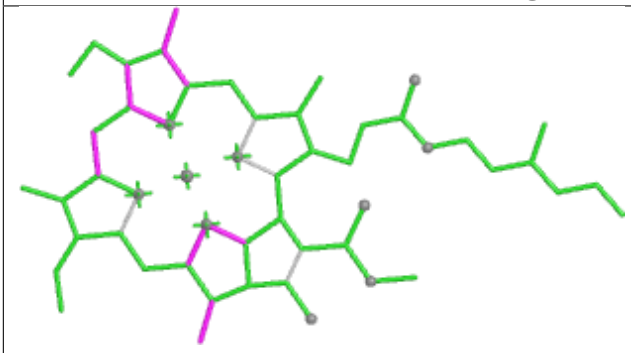
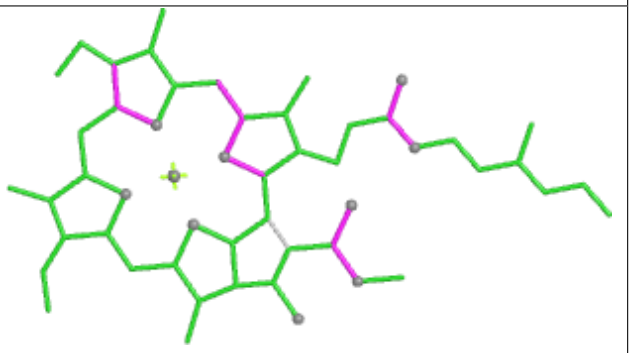
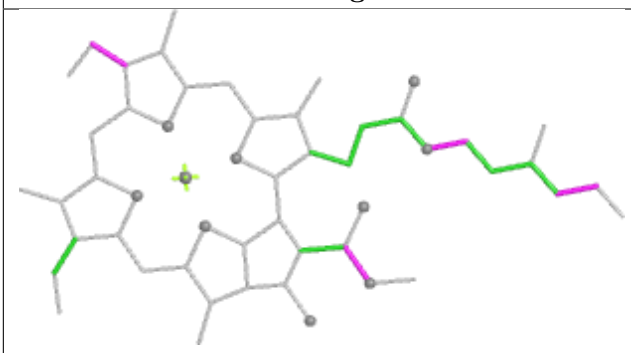
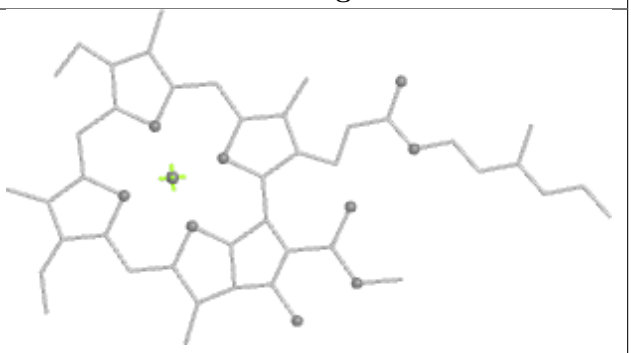
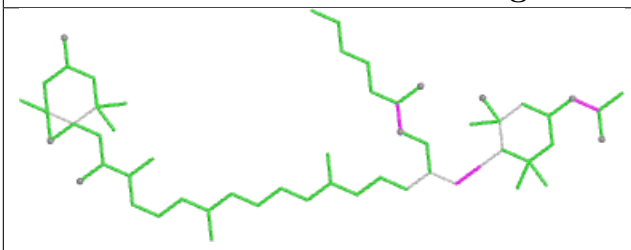
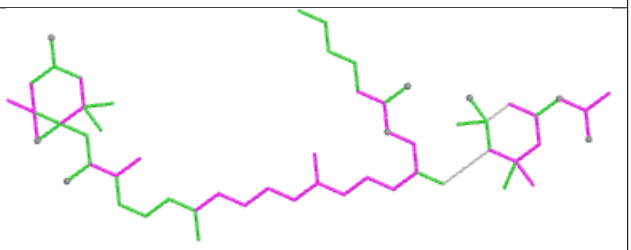
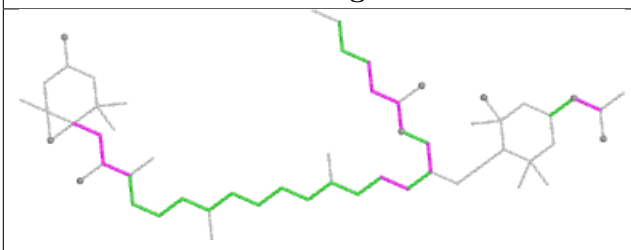
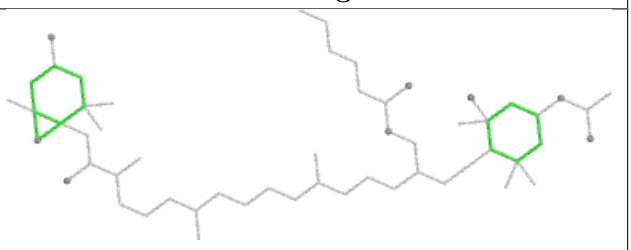
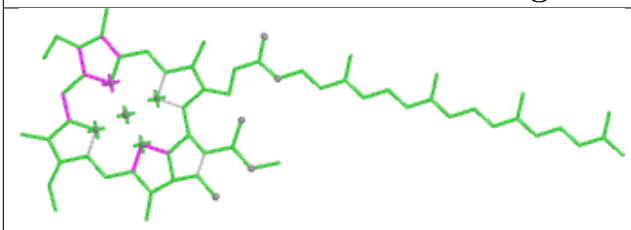


Rings

Ligand CLA V 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A1EB1 8 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA I 313



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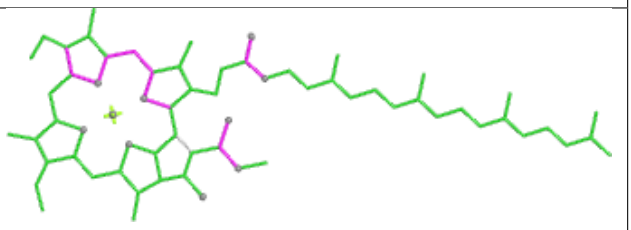
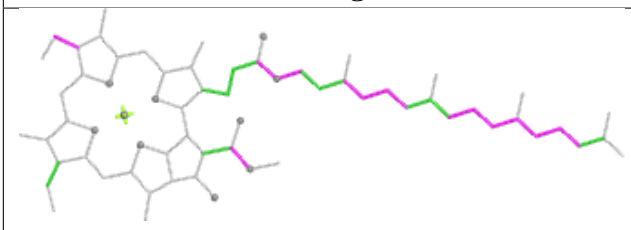
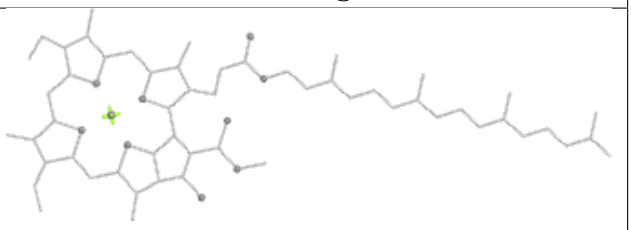


Bond angles

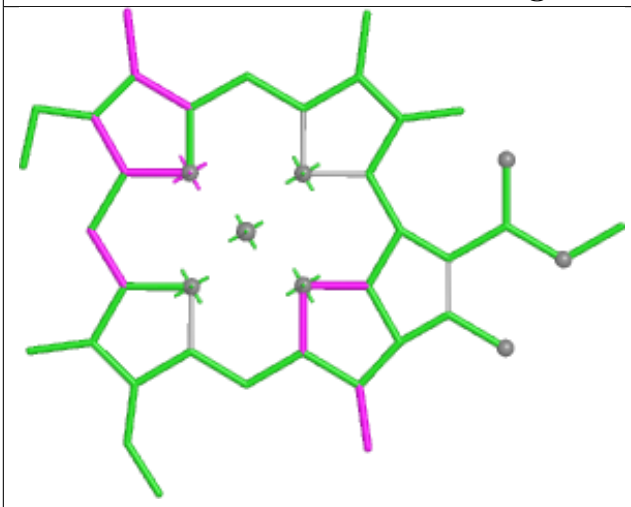


Torsions



Rings

Ligand CLA 2 312



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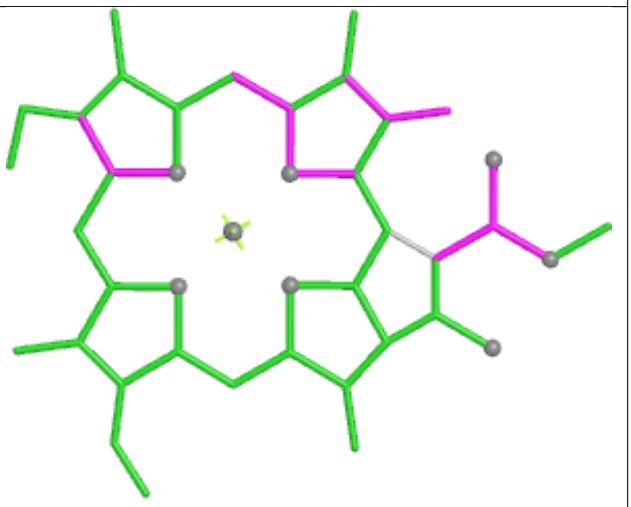
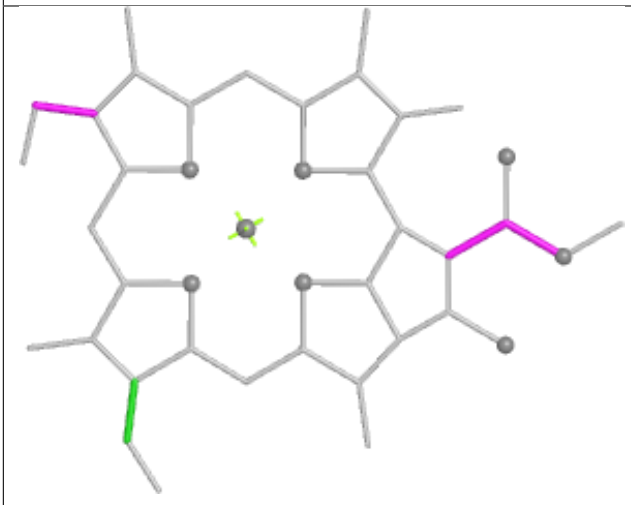
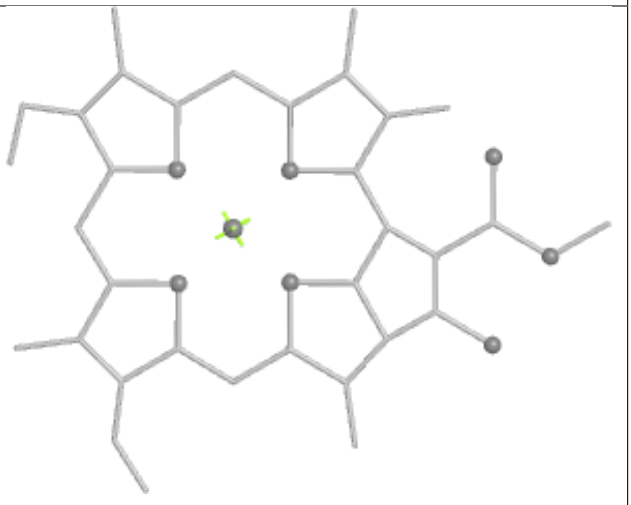


Bond angles

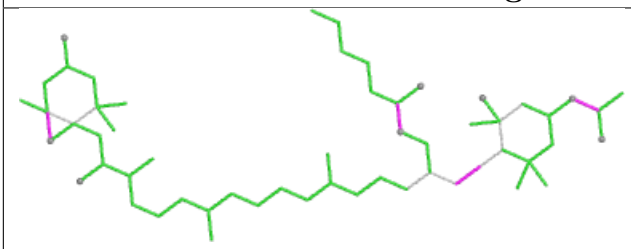


Torsions



Rings

Ligand A1EB1 O 301



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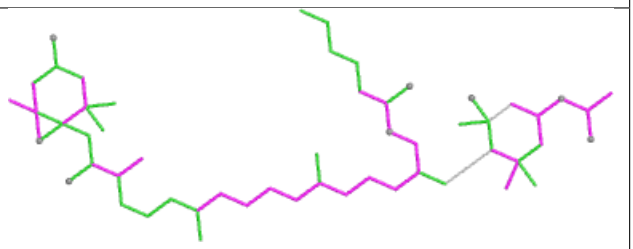
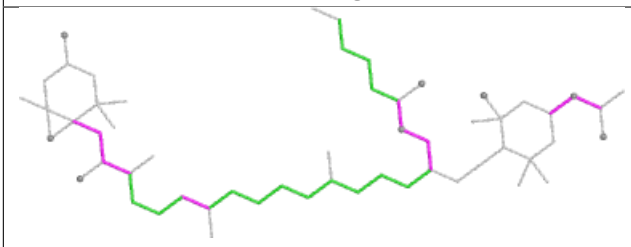


Bond angles



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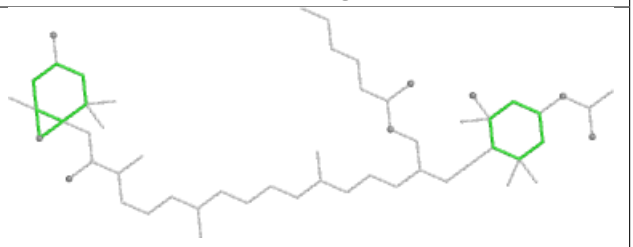
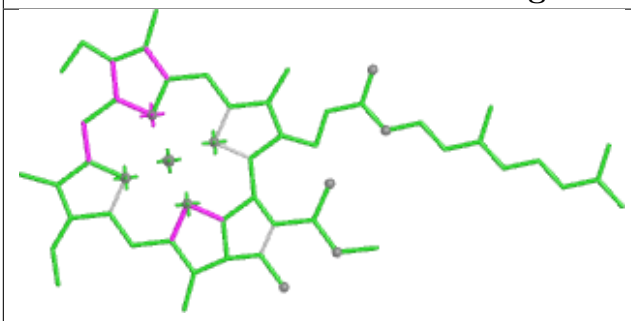


Rings

Ligand CLA 8 311



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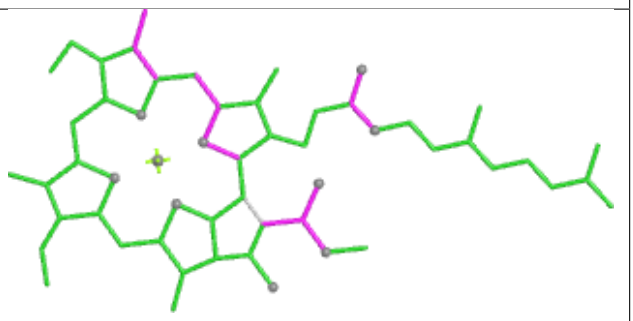
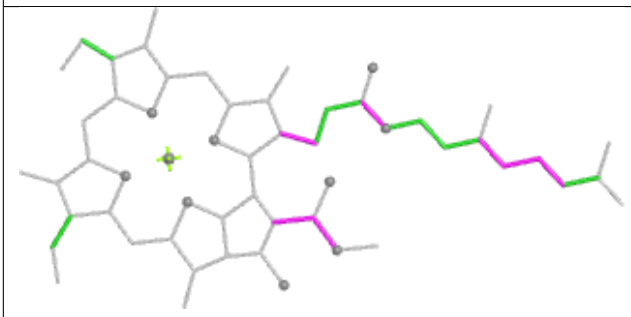
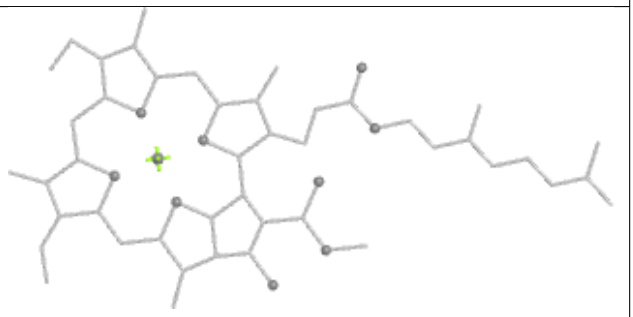


Bond angles

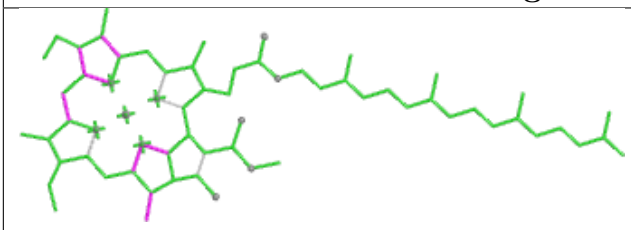


Torsions



Rings

Ligand CLA X 309



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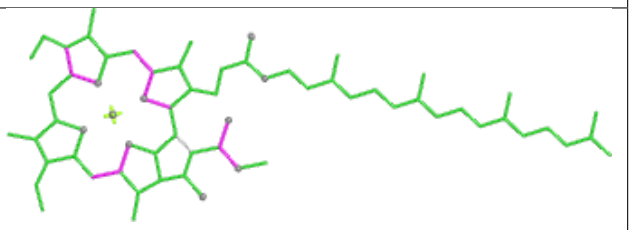
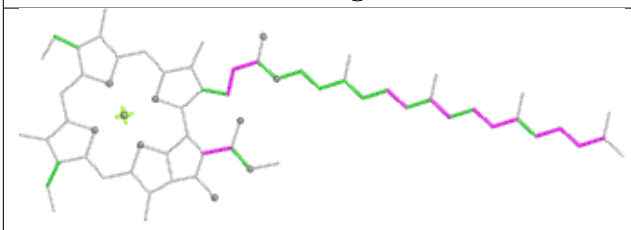
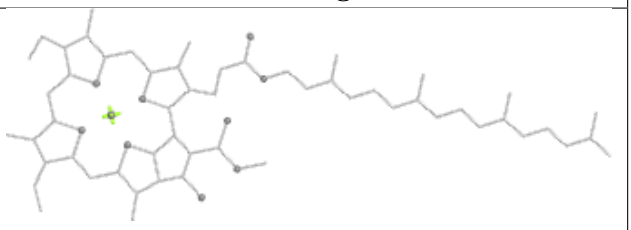


Bond angles

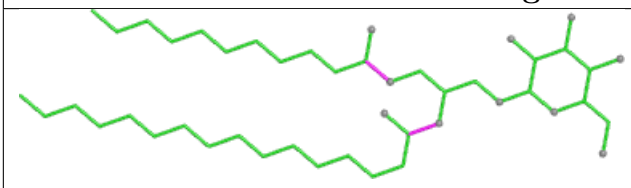


Torsions



Rings

Ligand LMG S 322



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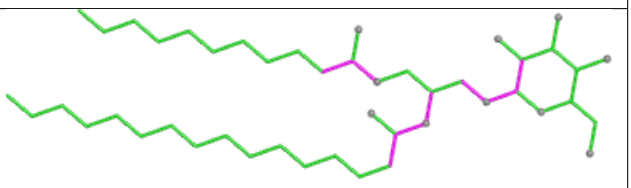
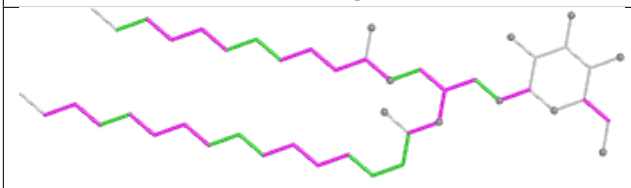


Bond angles



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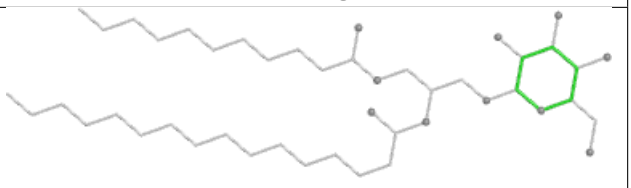
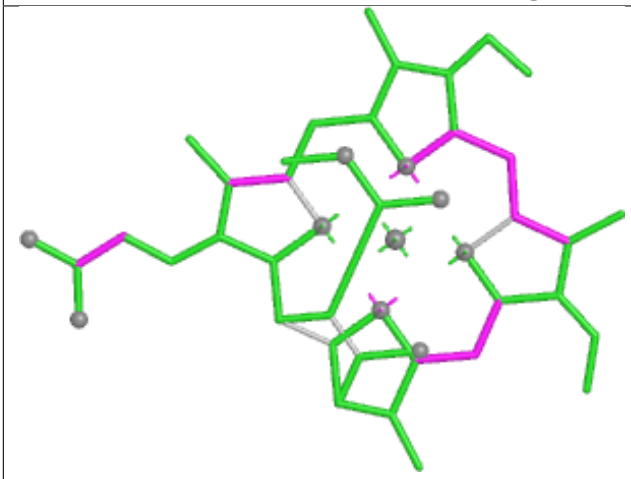
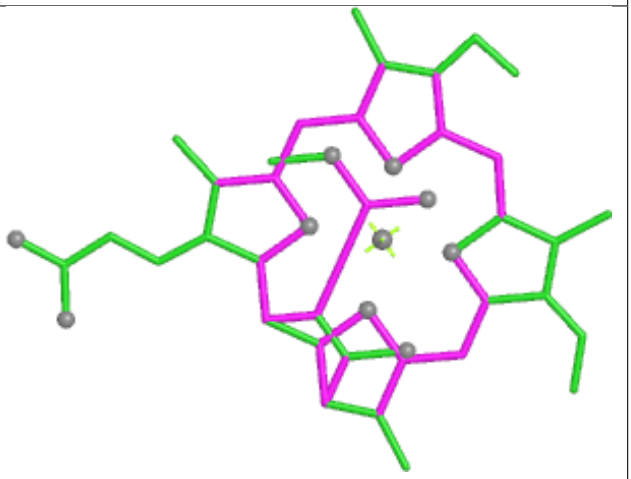


Rings

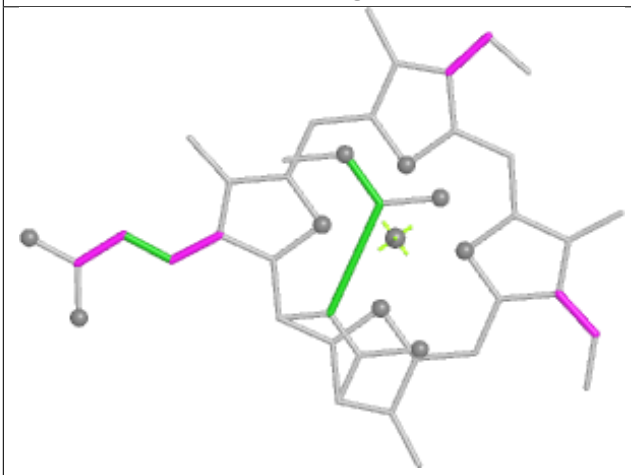
Ligand KC2 G 317



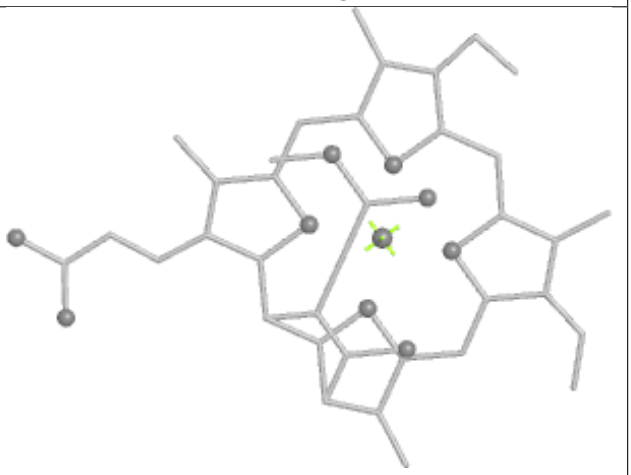
Bond lengths



Bond angles

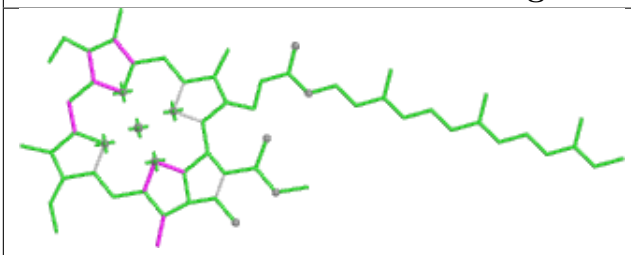


Torsions

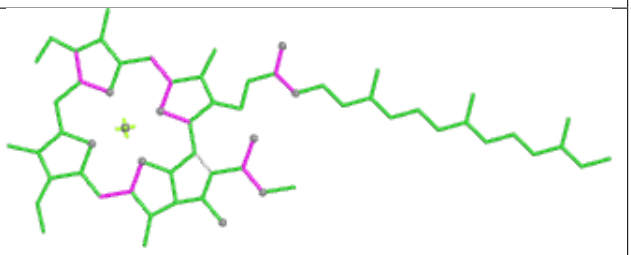


Rings

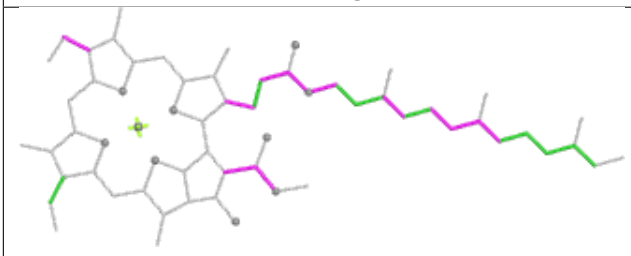
Ligand CLA S 308



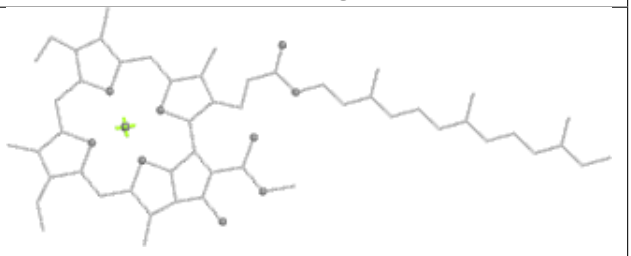
Bond lengths



Bond angles

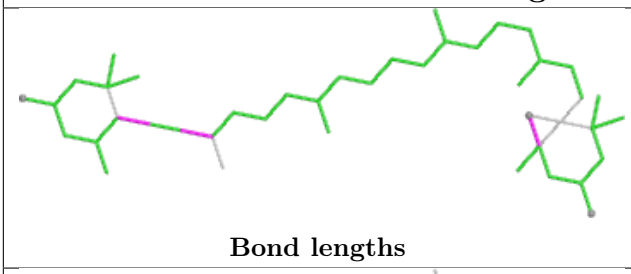


Torsions



Rings

Ligand DD6 x 303



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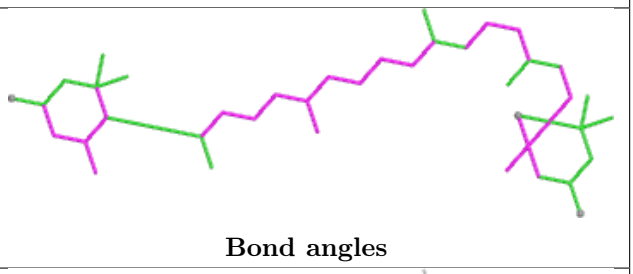
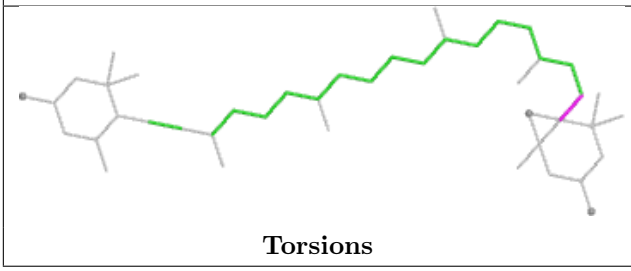


Bond angles



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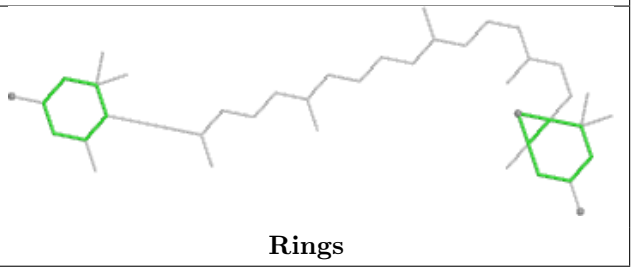
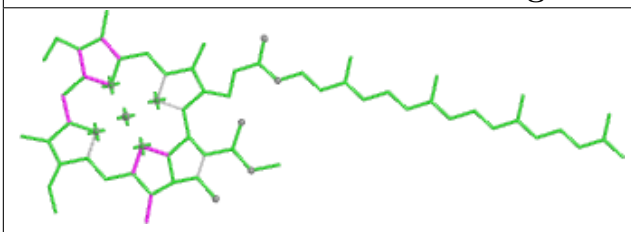


Rings

Ligand CLA b 832



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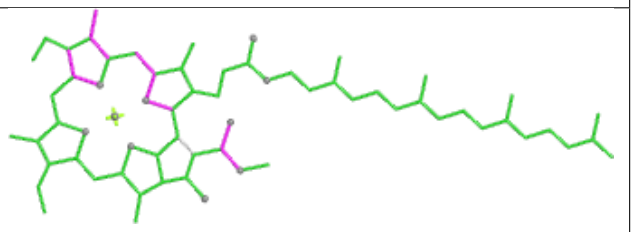
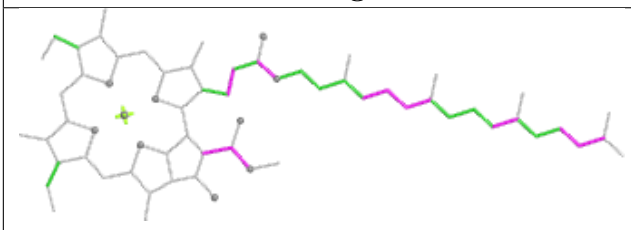


Bond angles



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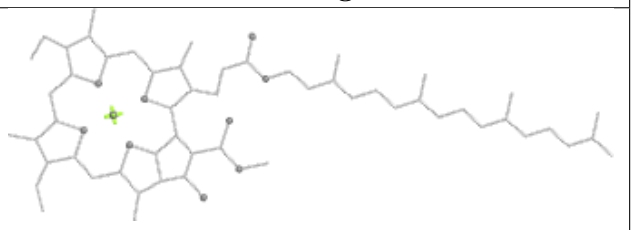
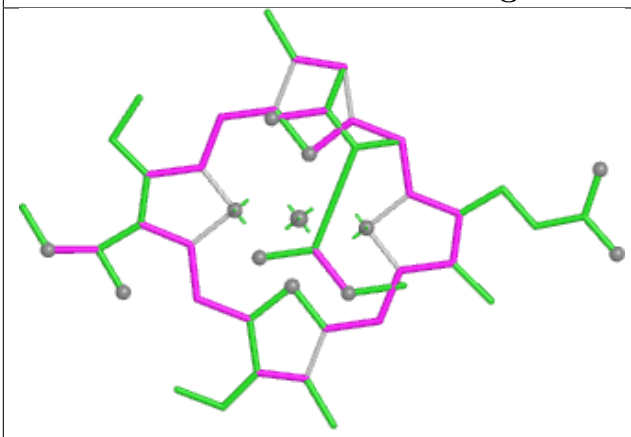


Rings

Ligand A1ECV Y 312



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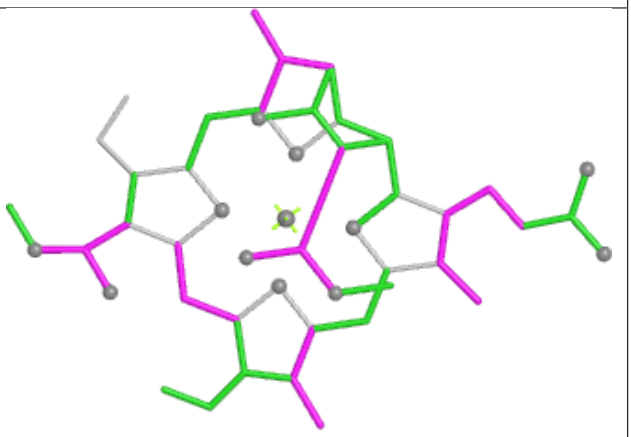
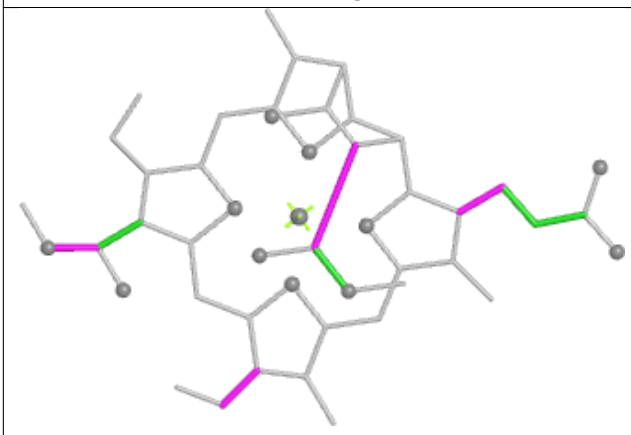


Bond angles



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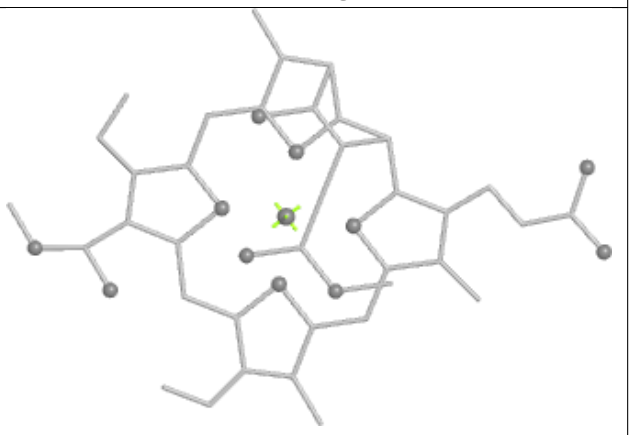
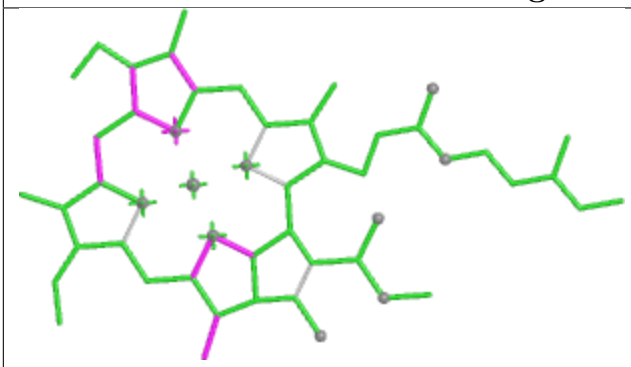


Rings

Ligand CLA 3 322



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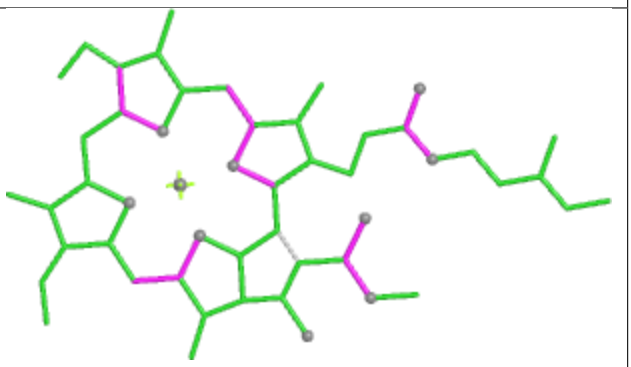
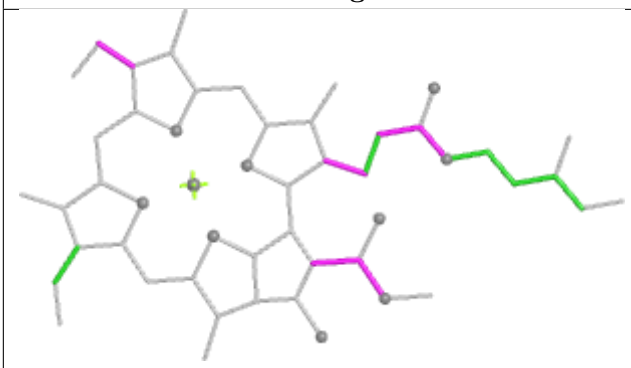


Bond angles



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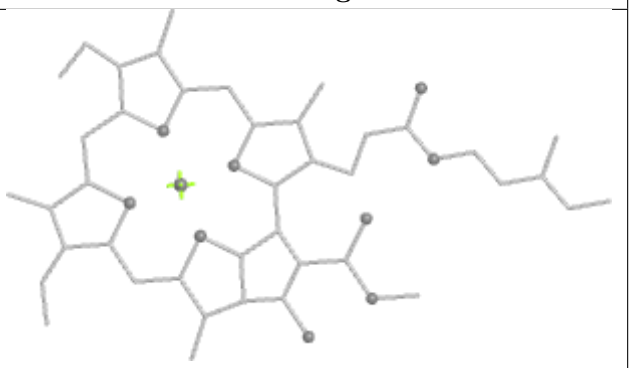
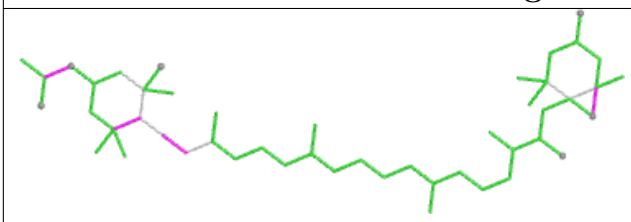


Rings

Ligand A86 W 307



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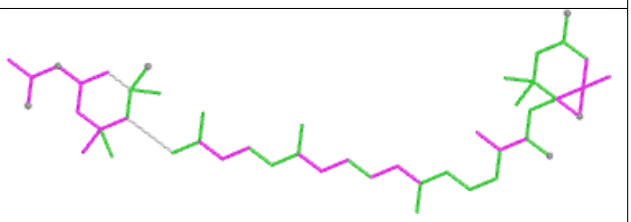
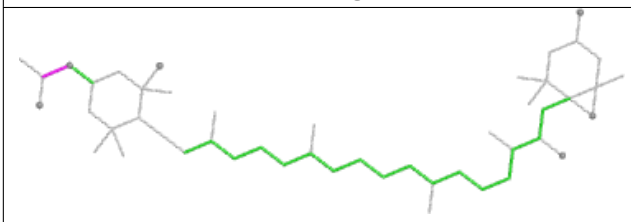


Bond angles



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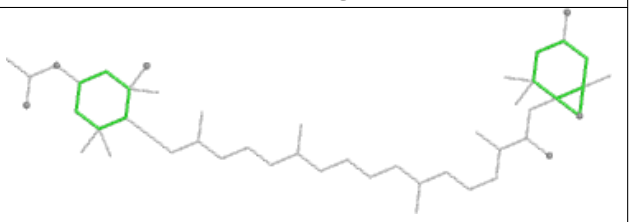
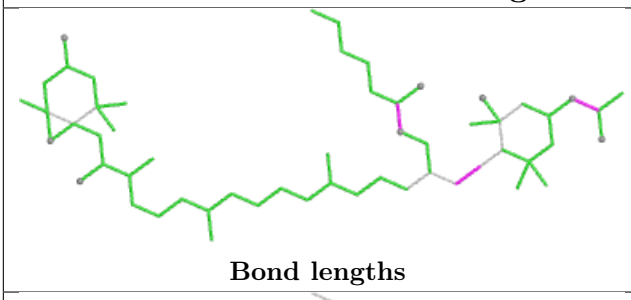


Rings

Ligand A1EB1 1 301



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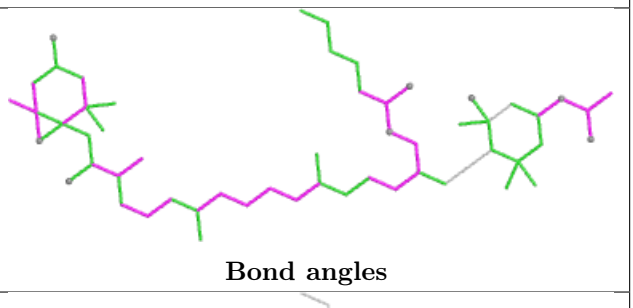
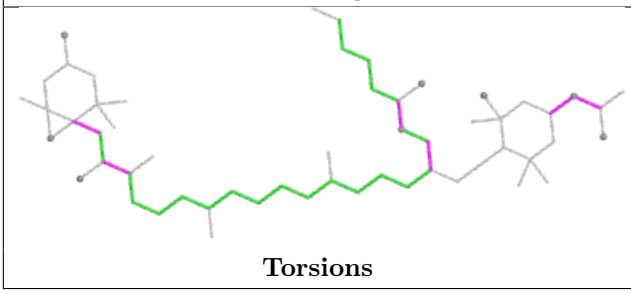


Bond angles



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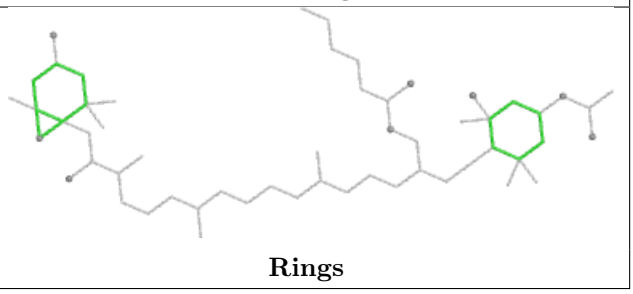
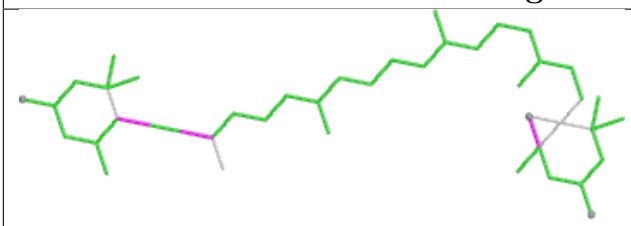


Rings

Ligand DD6 P 304



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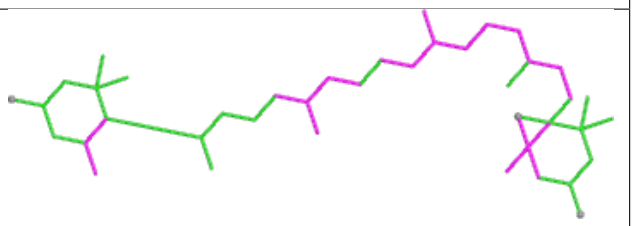
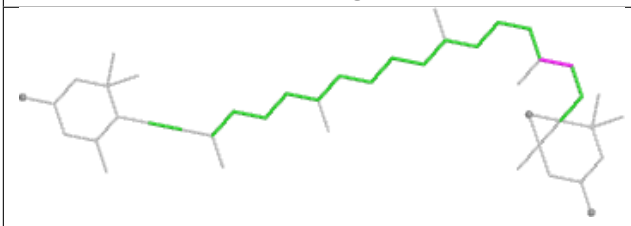


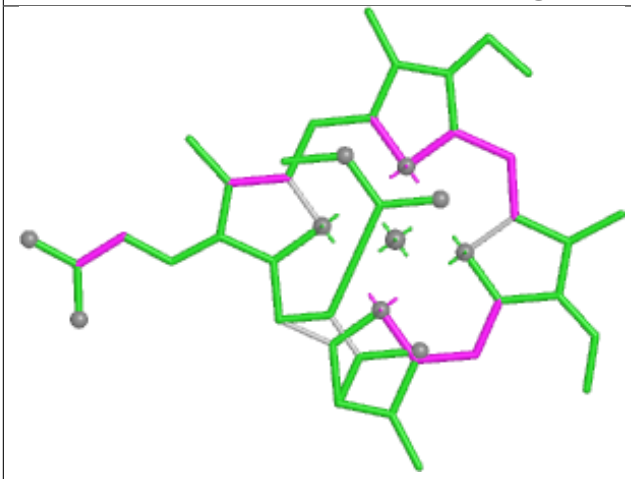
Bond angles



Torsions

Rings

Ligand KC2 0 319



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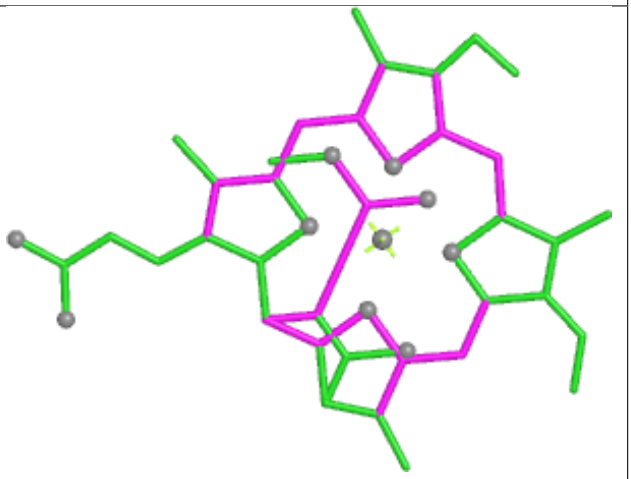
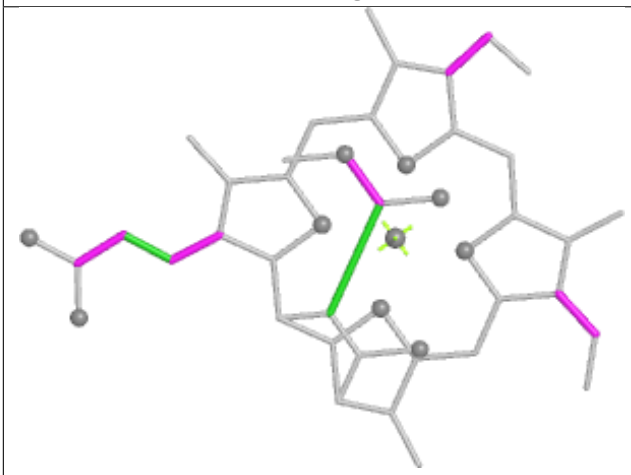


Bond angles



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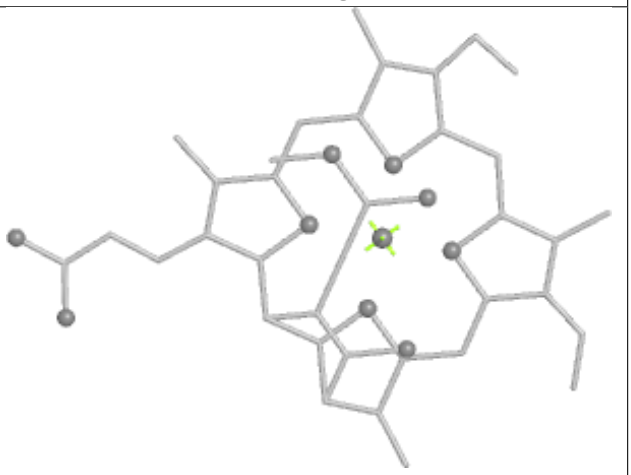
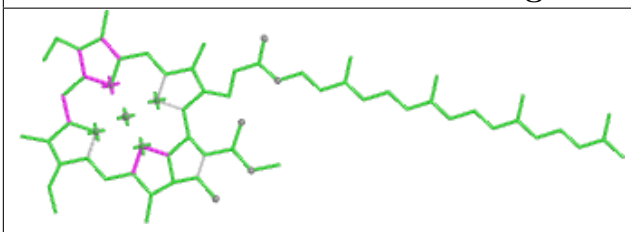


Rings

Ligand CLA E 308



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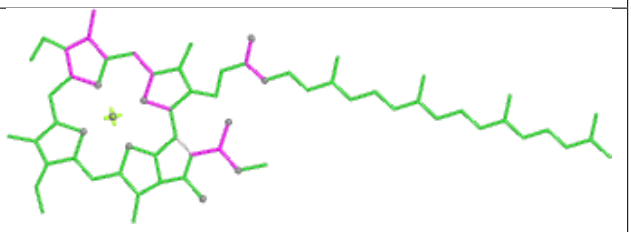
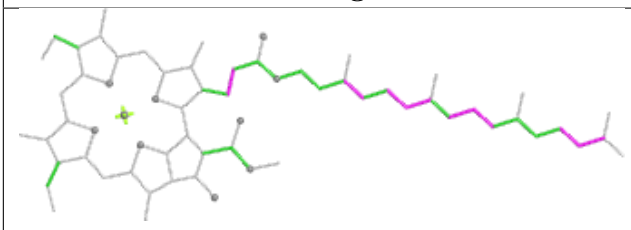
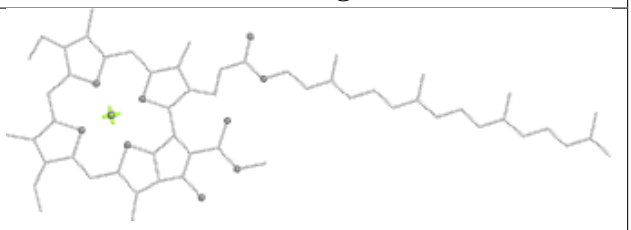


Bond angles

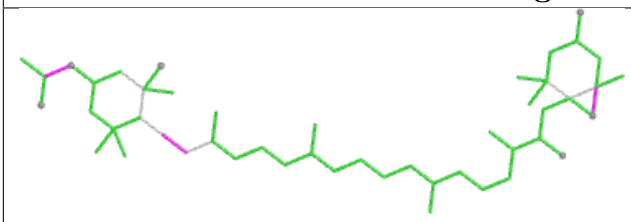


Torsions



Rings

Ligand A86 8 303



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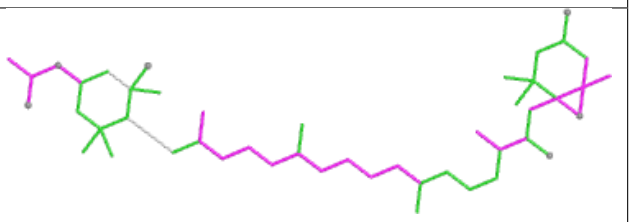
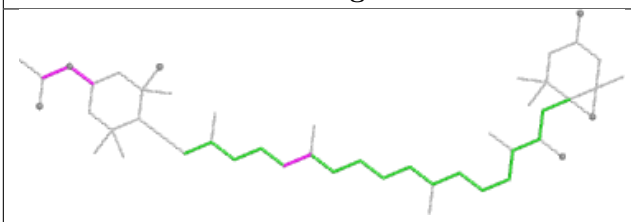
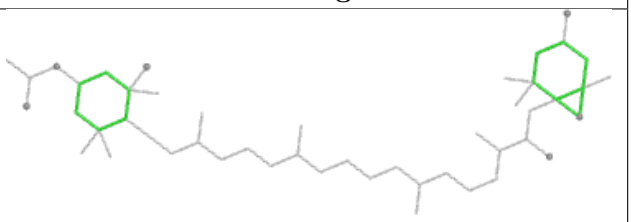


Bond angles

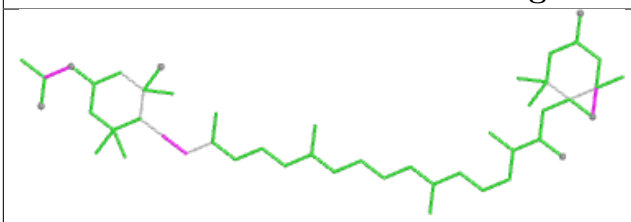


Torsions



Rings

Ligand A86 H 302



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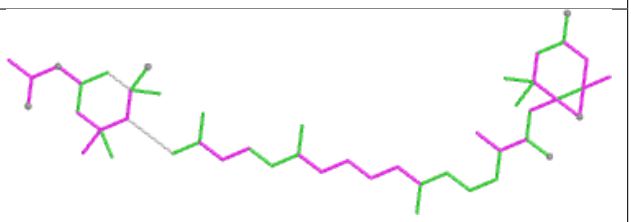
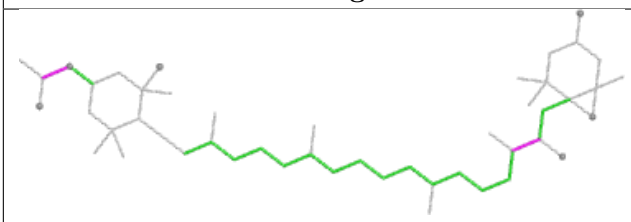


Bond angles



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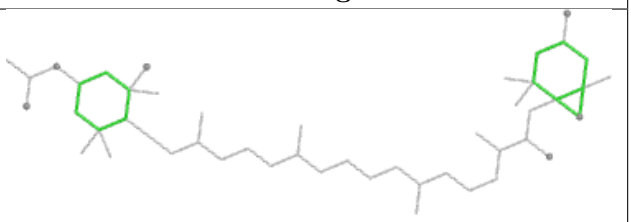
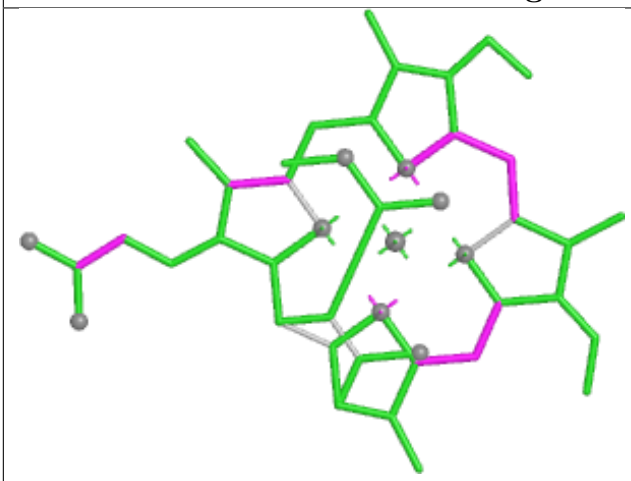


Rings

Ligand KC2 Y 308



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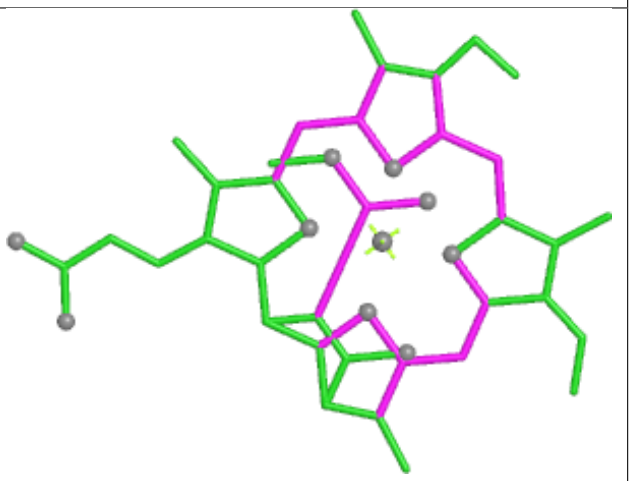
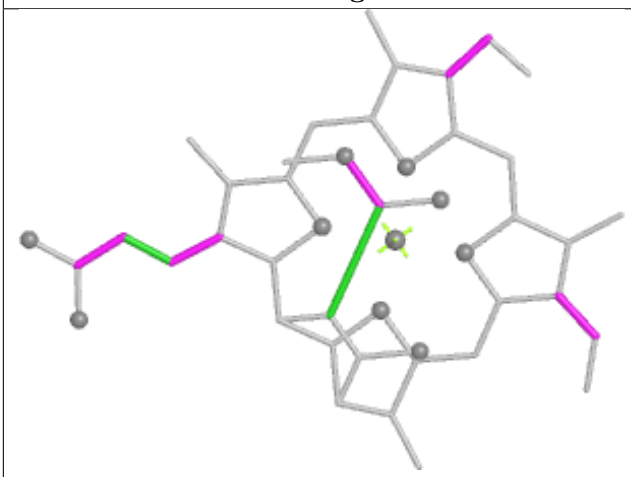


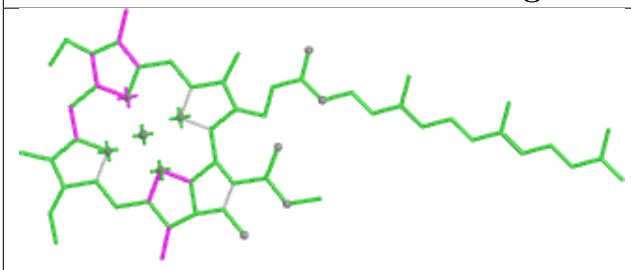
Bond angles



Torsions

Rings

Ligand CLA U 210



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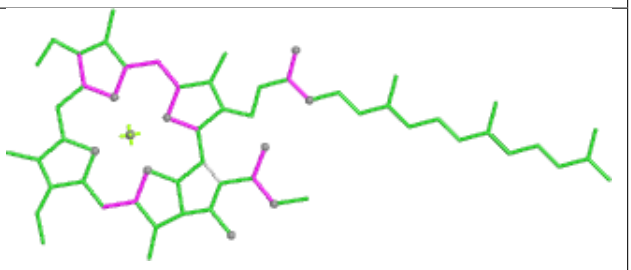
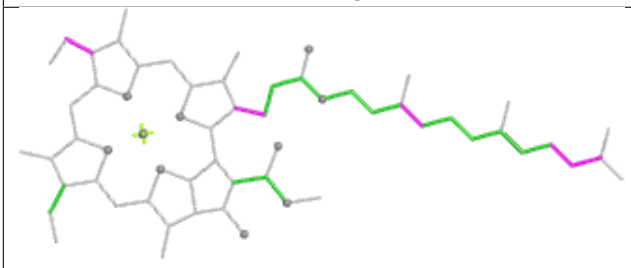
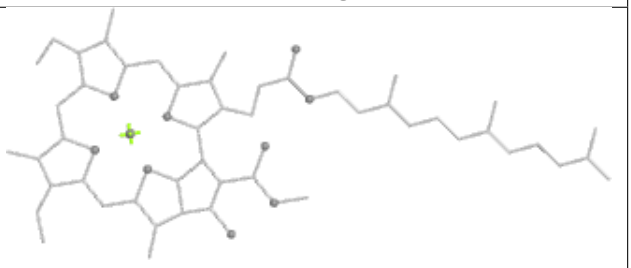


Bond angles

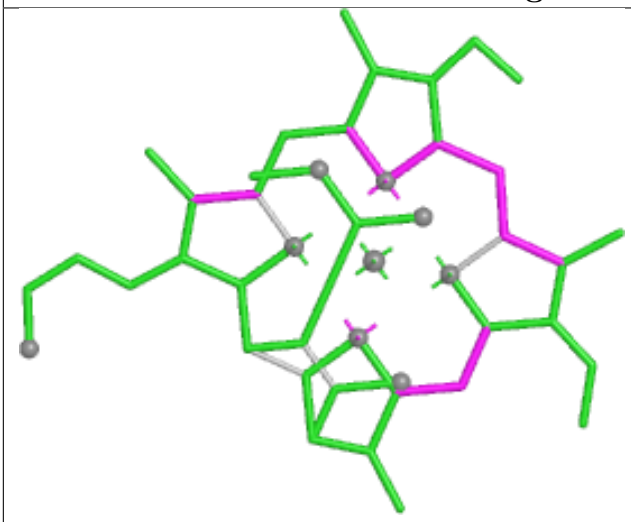


Torsions



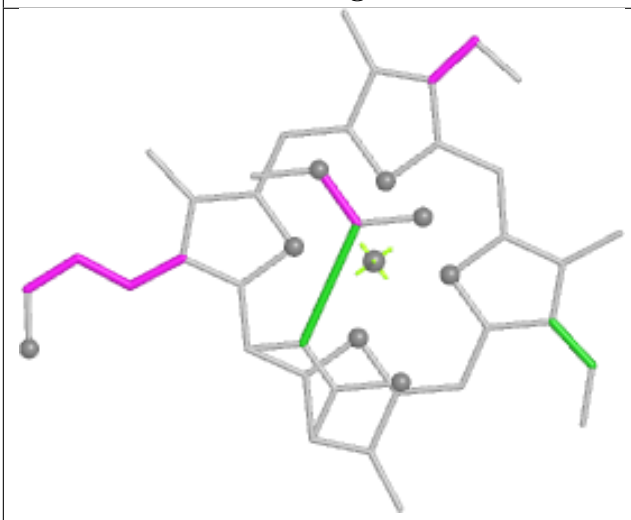
Rings

Ligand KC2 O 317

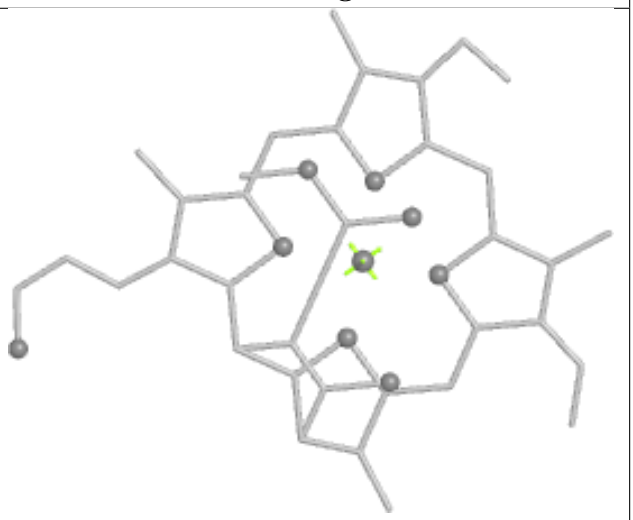


Bond lengths

Bond angles

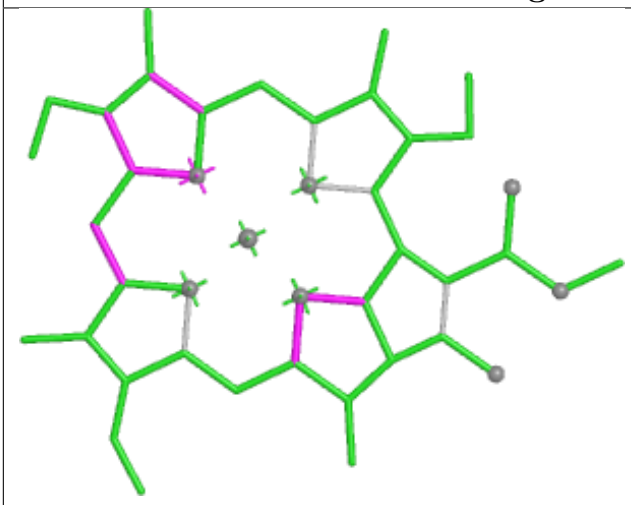


Torsions



Rings

Ligand CLA o 202



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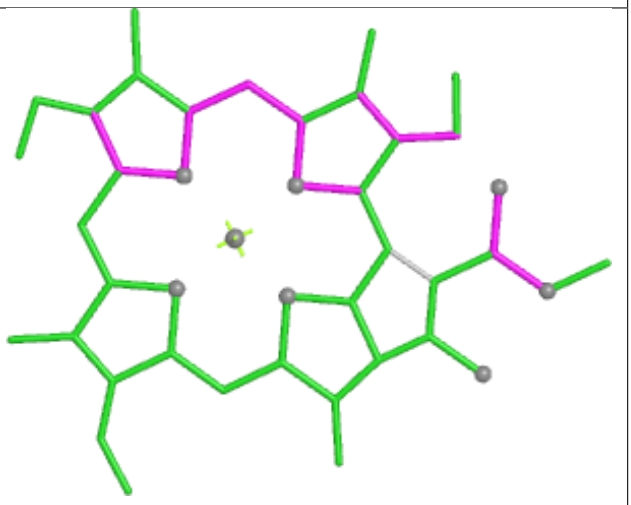

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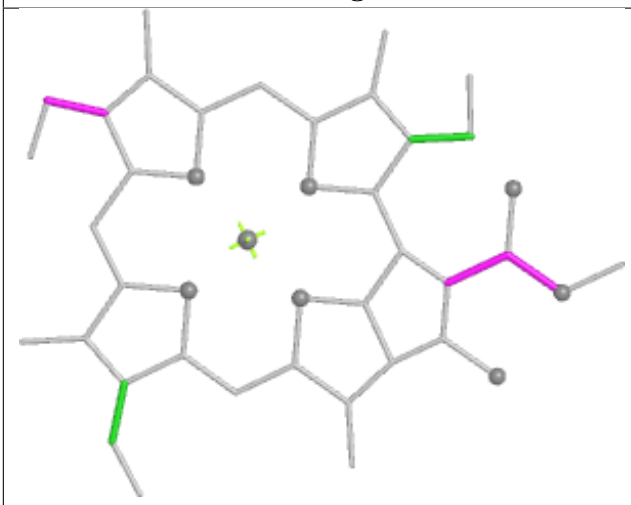
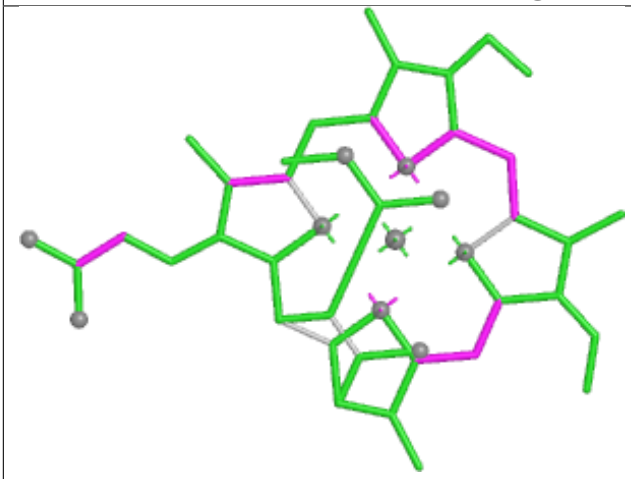


Torsions

Rings

Ligand KC2 S 315



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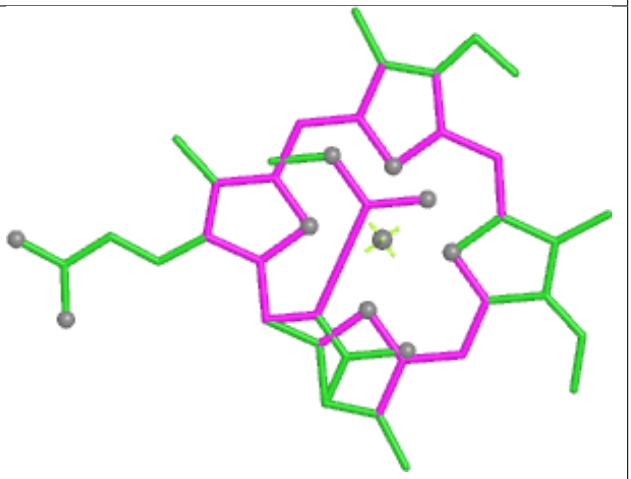

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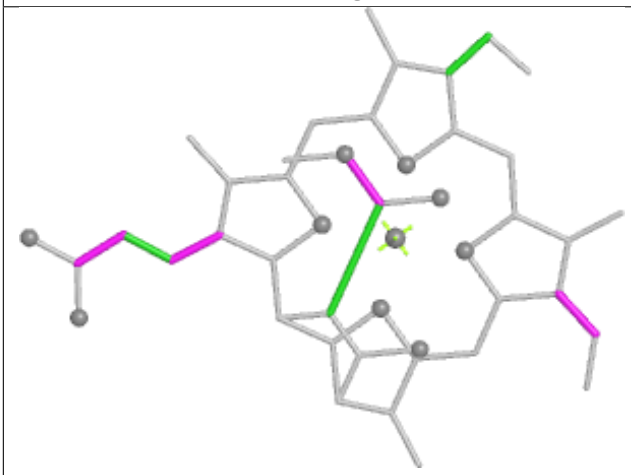

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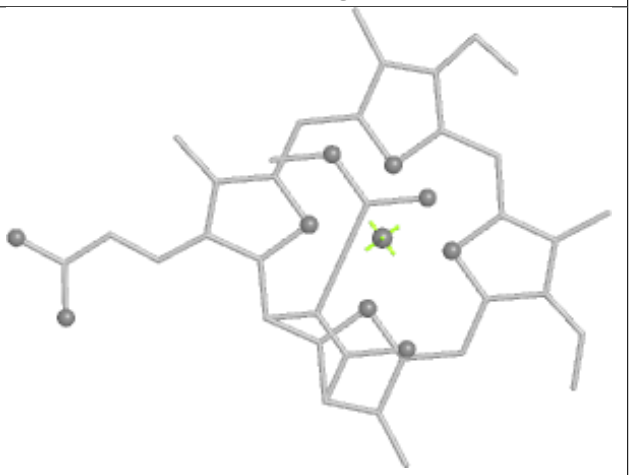
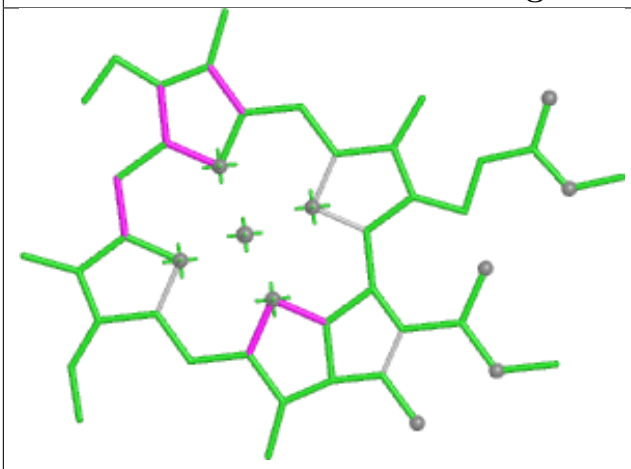


Rings

Ligand CLA L 320



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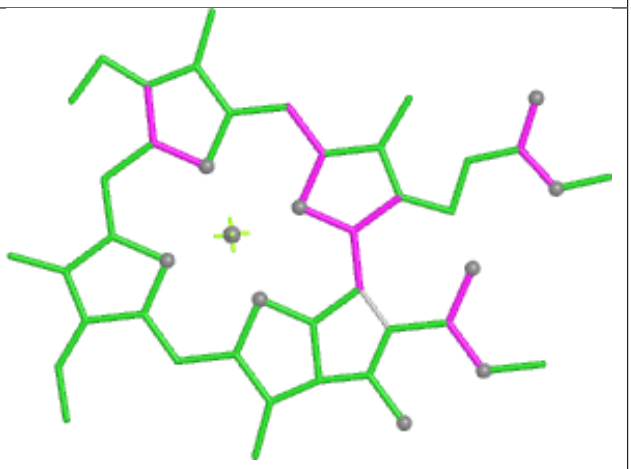
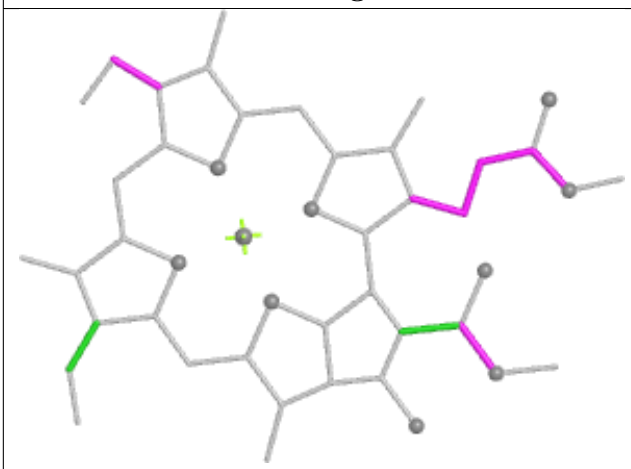


Bond angles



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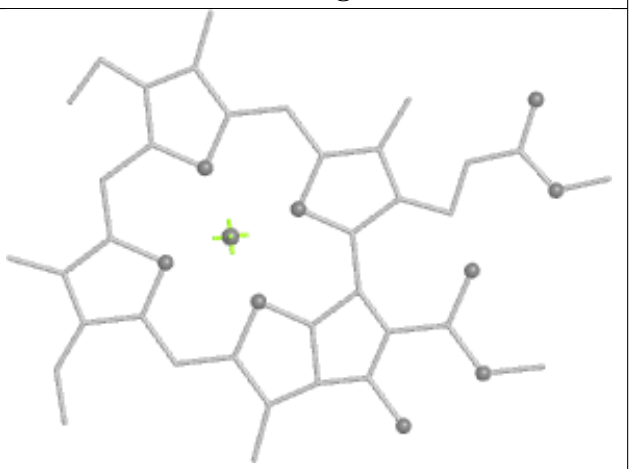
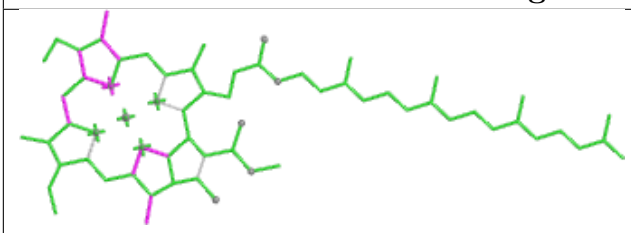


Rings

Ligand CLA a 807



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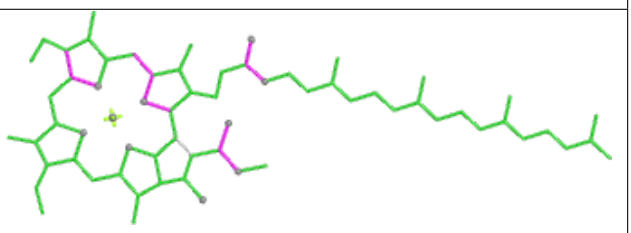

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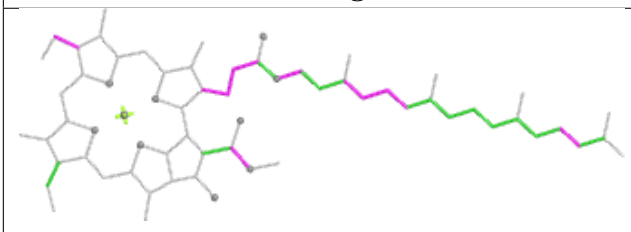

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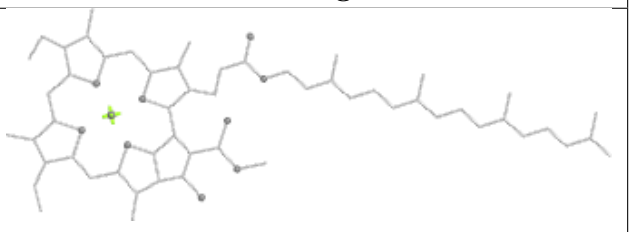
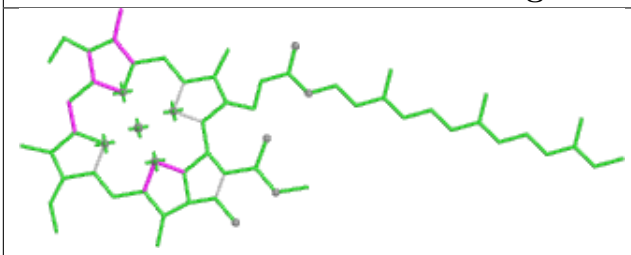


Rings

Ligand CLA L 308



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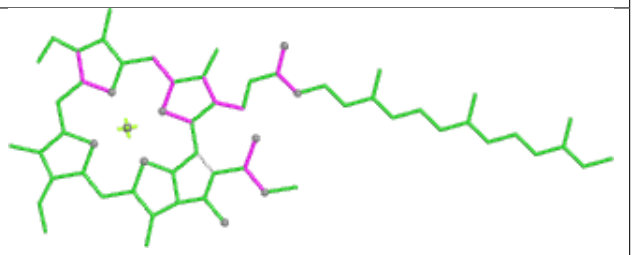
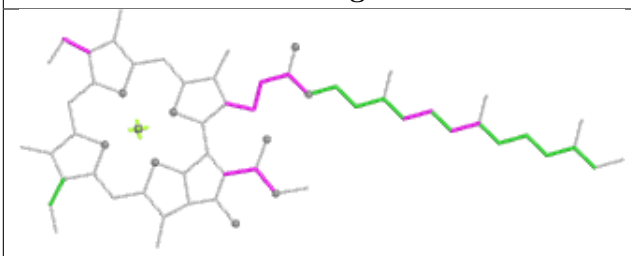


Bond angles



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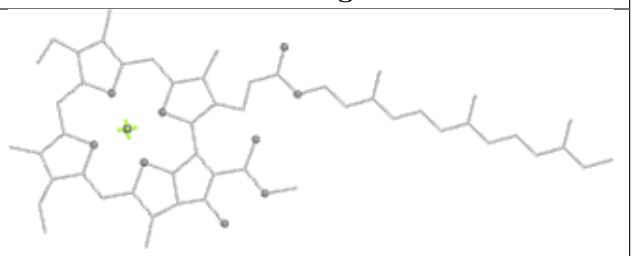
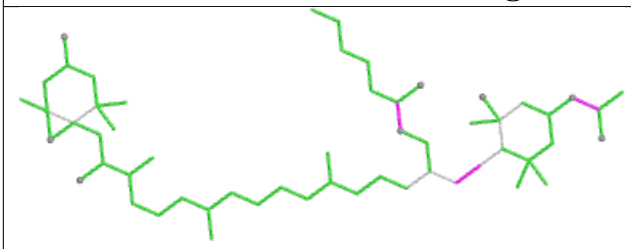


Rings

Ligand A1EB1 H 304



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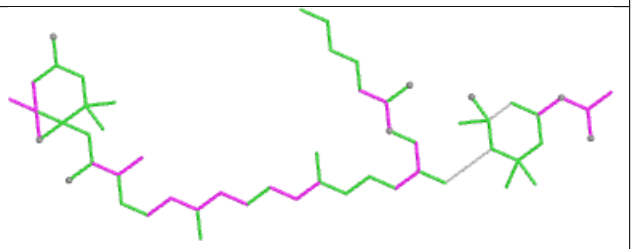

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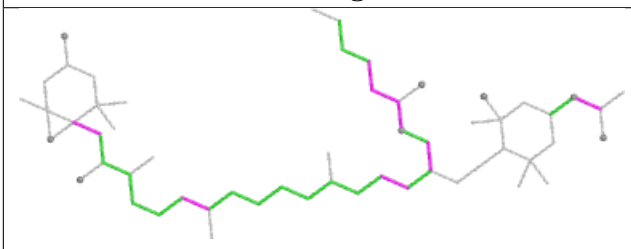

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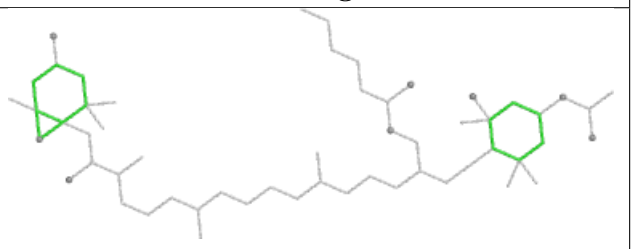
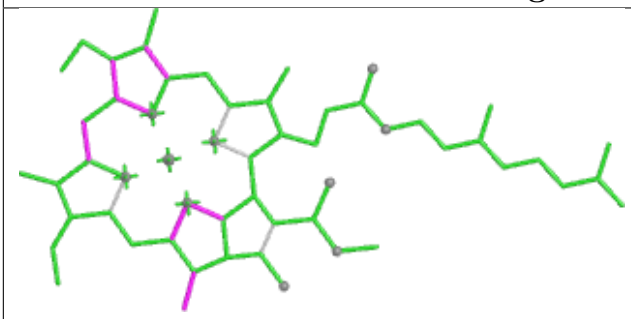


Rings

Ligand CLA o 203



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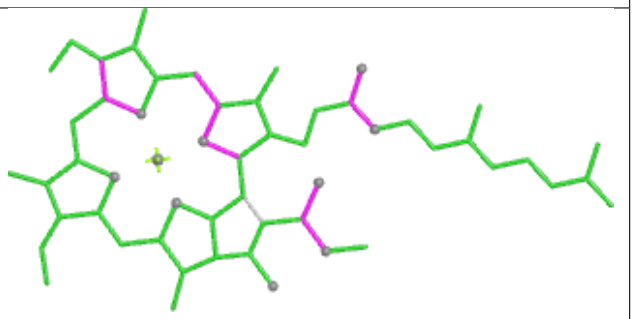
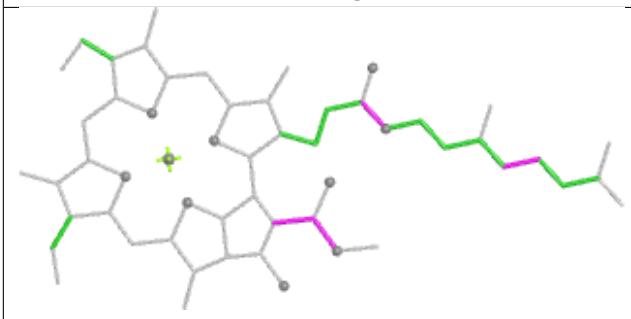


Bond angles



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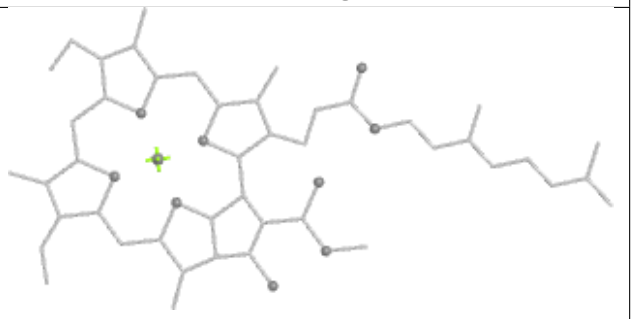
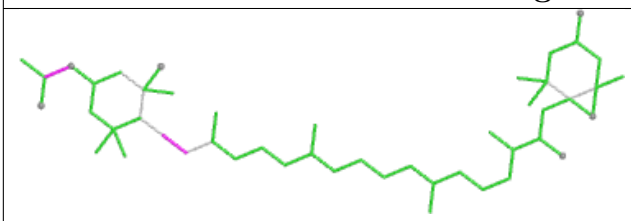


Rings

Ligand A86 3 305



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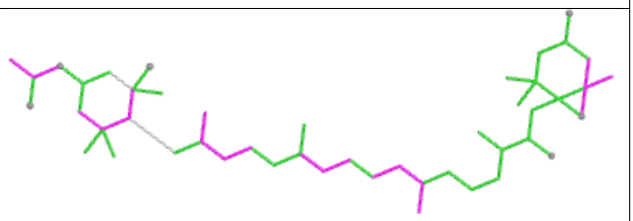

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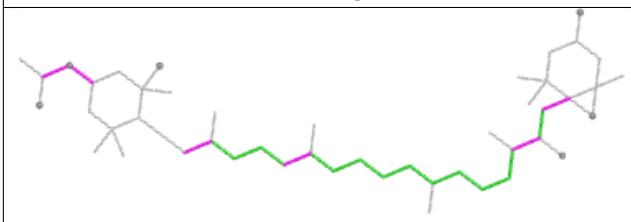

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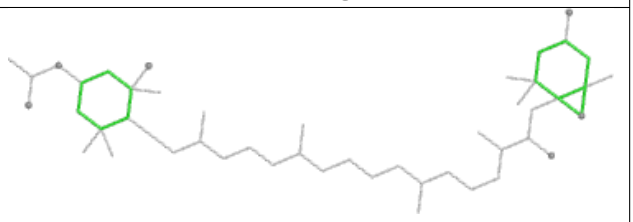
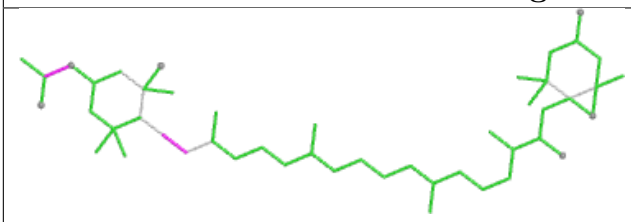


Rings

Ligand A86 Q 308



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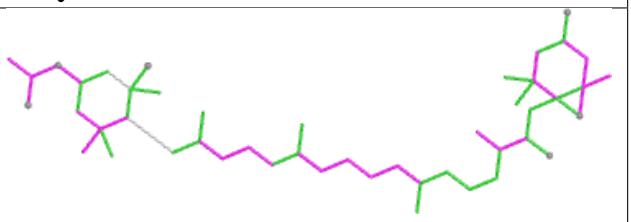

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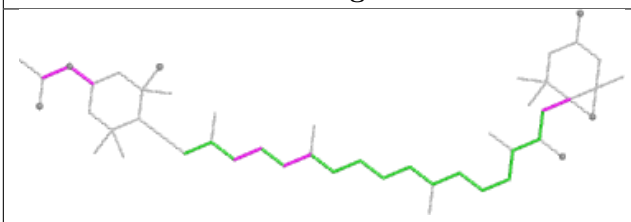

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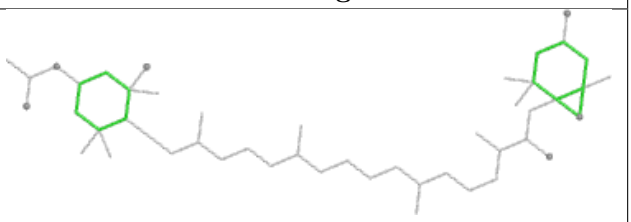
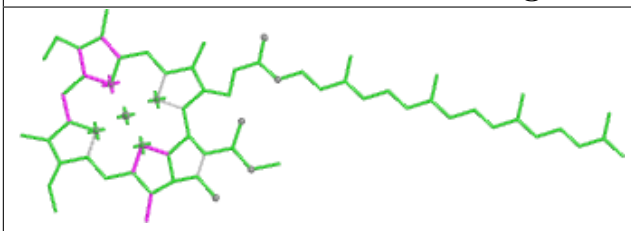


Rings

Ligand CLA K 312



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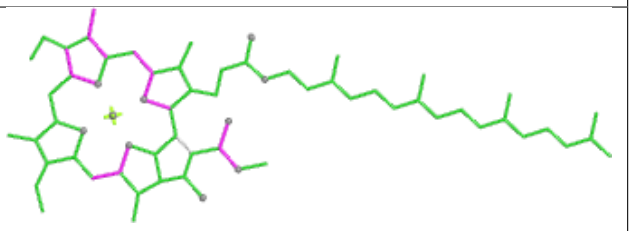

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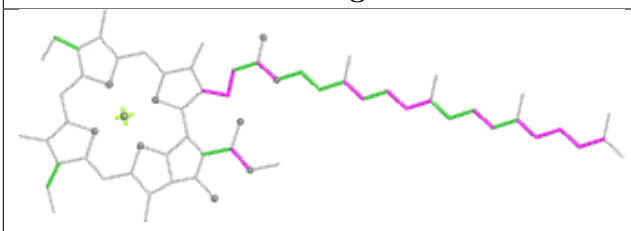

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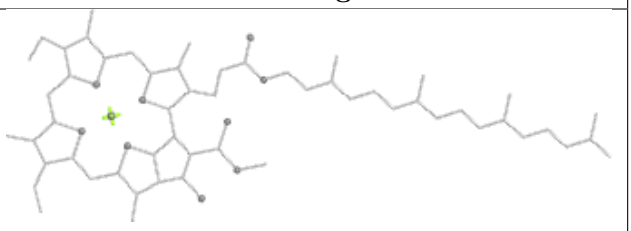
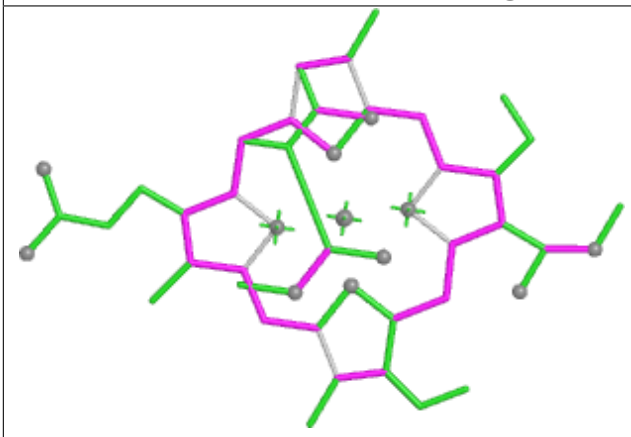


Rings

Ligand A1ECV T 317



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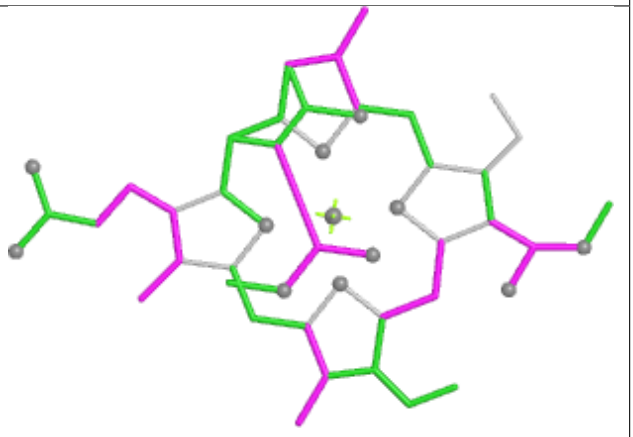
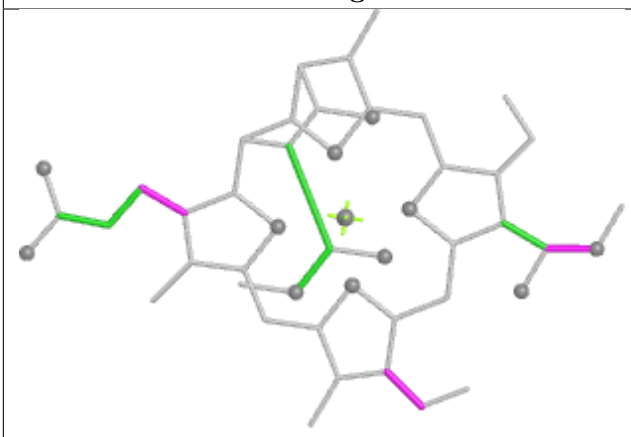


Bond angles



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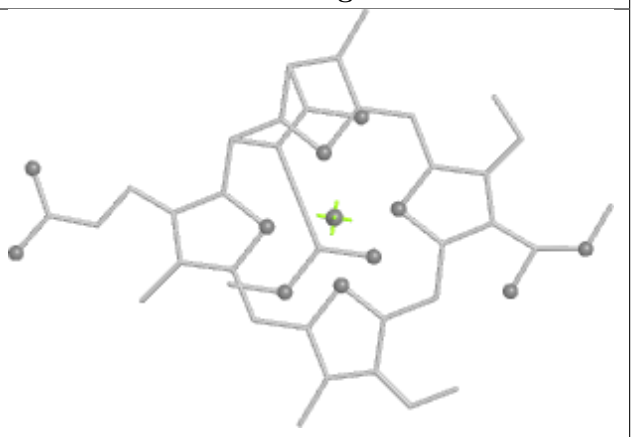
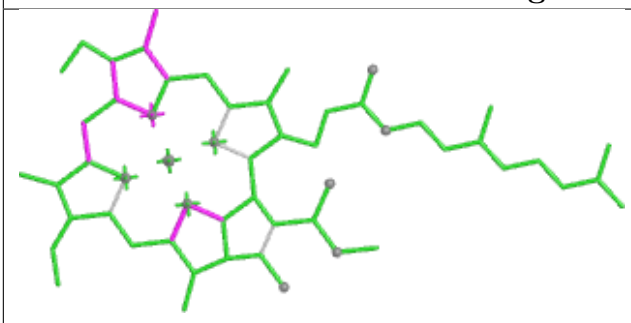


Rings

Ligand CLA J 310



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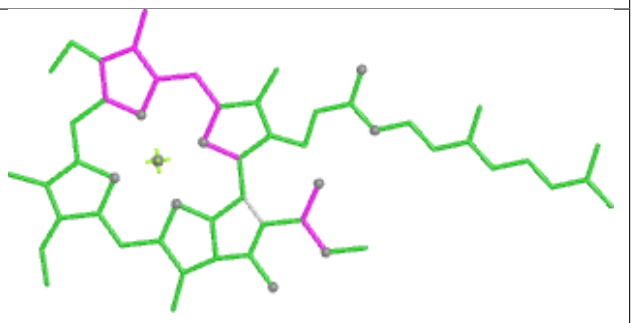
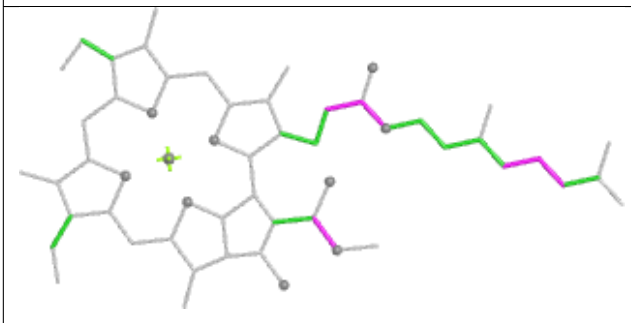


Bond angles



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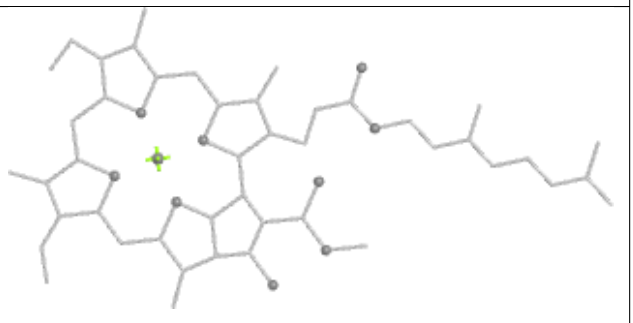
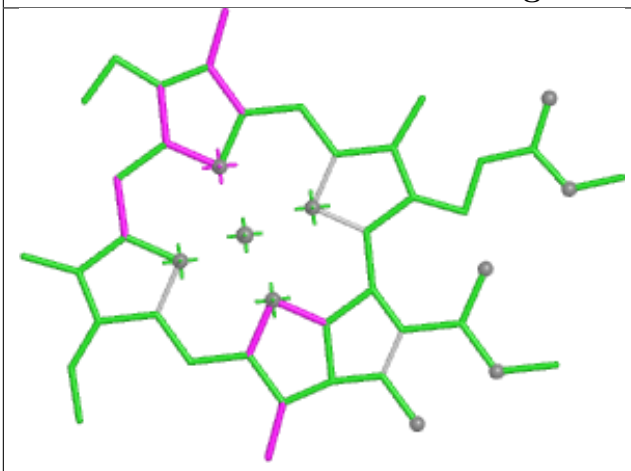


Rings

Ligand CLA U 208



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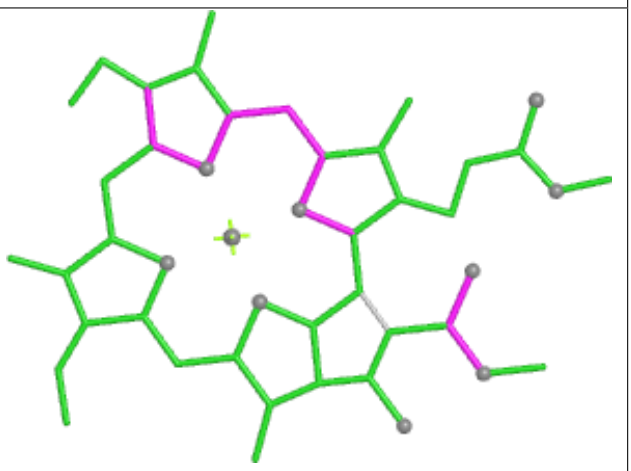
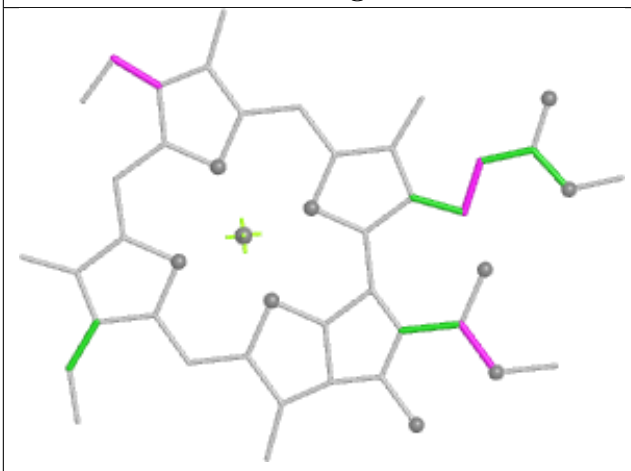
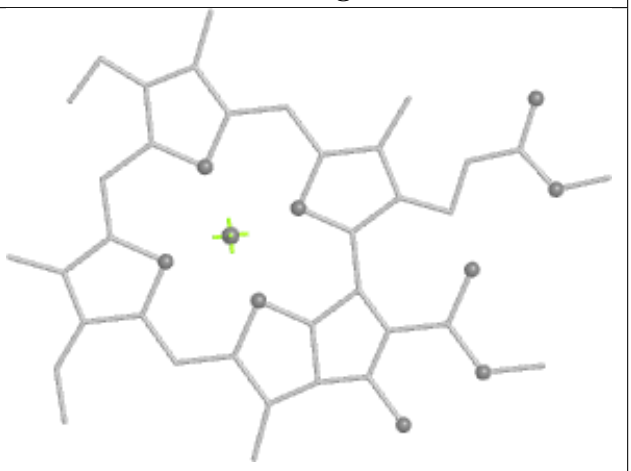


Bond angles

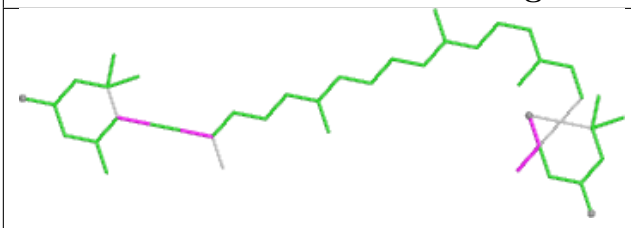


Torsions

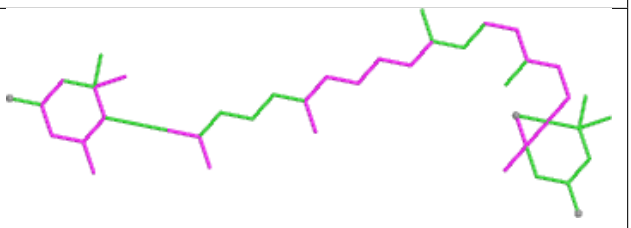


Rings

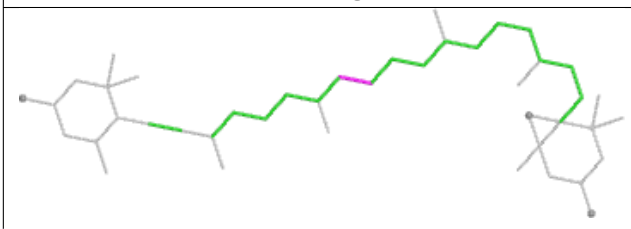
Ligand DD6 O 304



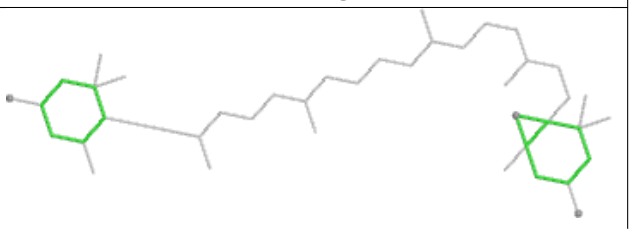
Bond lengths



Bond angles

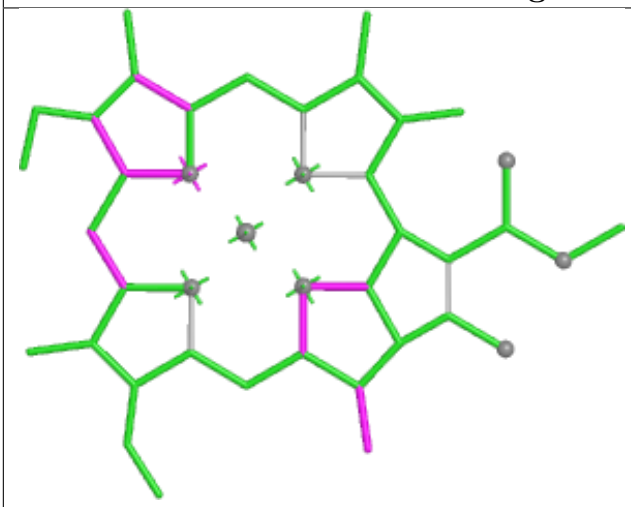


Torsions



Rings

Ligand CLA 9 309



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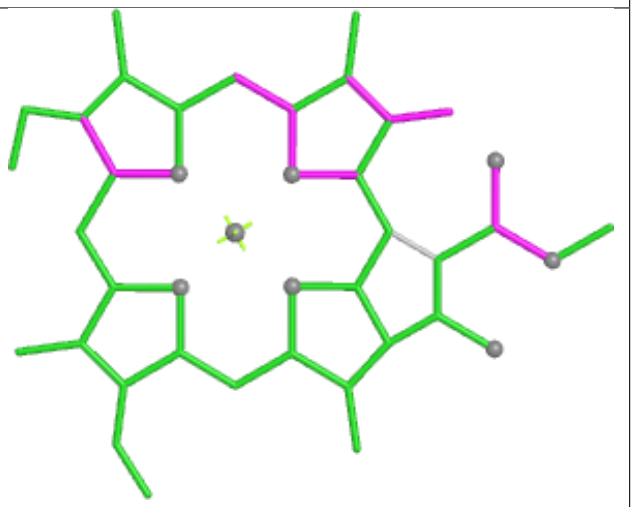
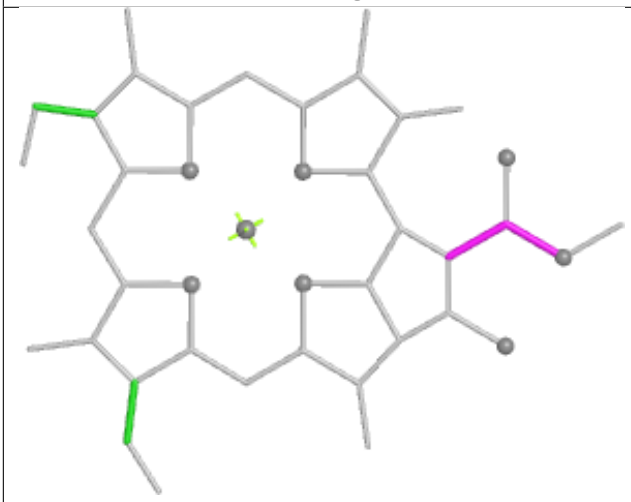
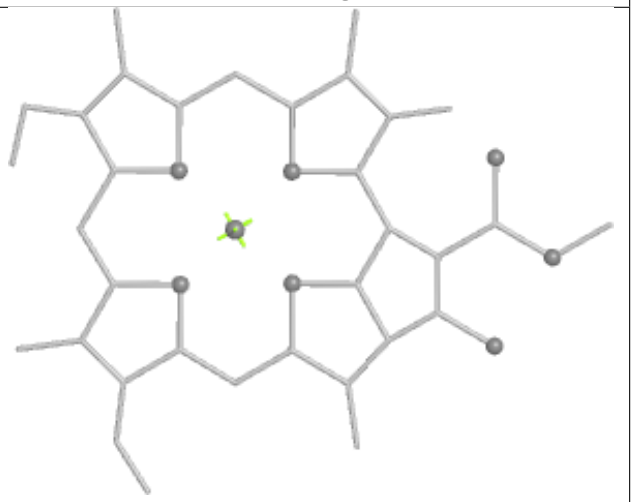


Bond angles

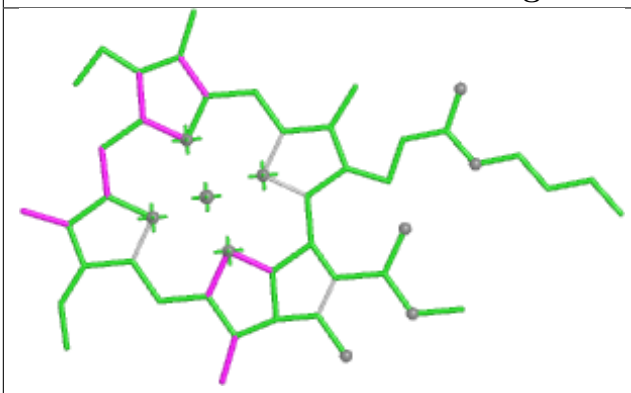


Torsions



Rings

Ligand CLA G 318



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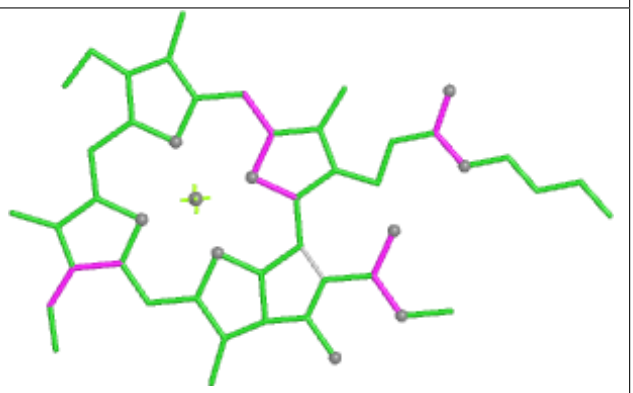
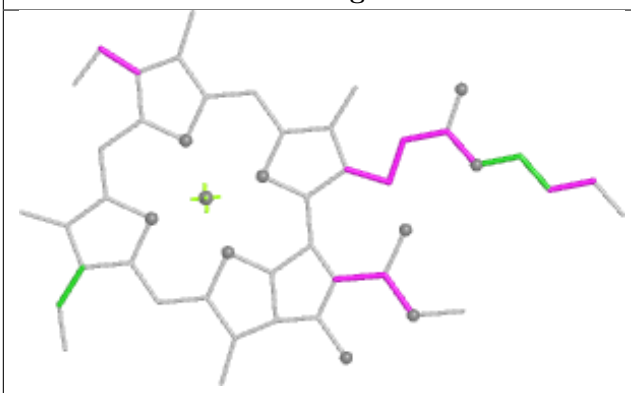


Bond angles



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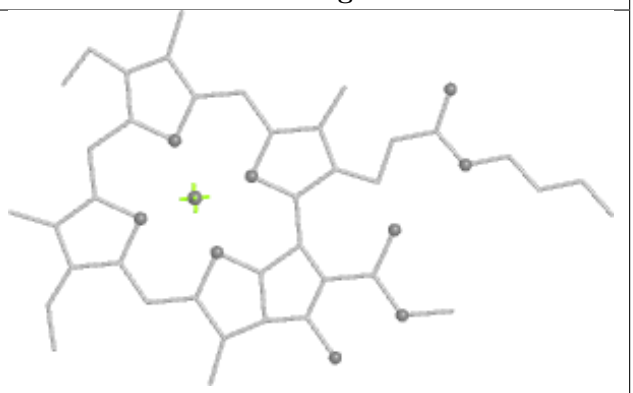
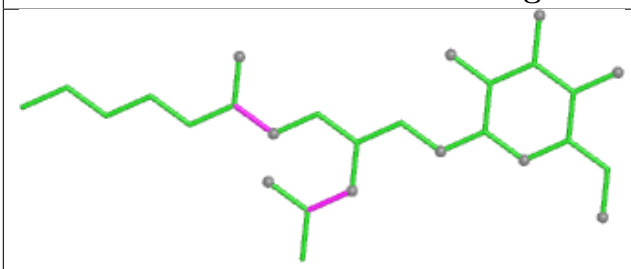


Rings

Ligand LMG 0 324



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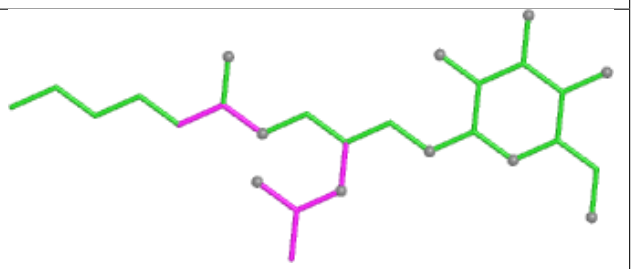
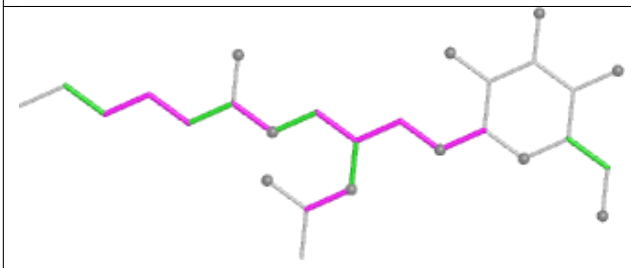


Bond angles



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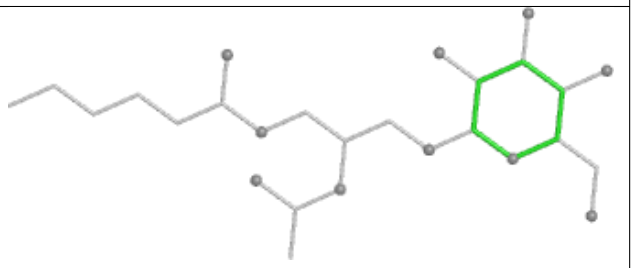
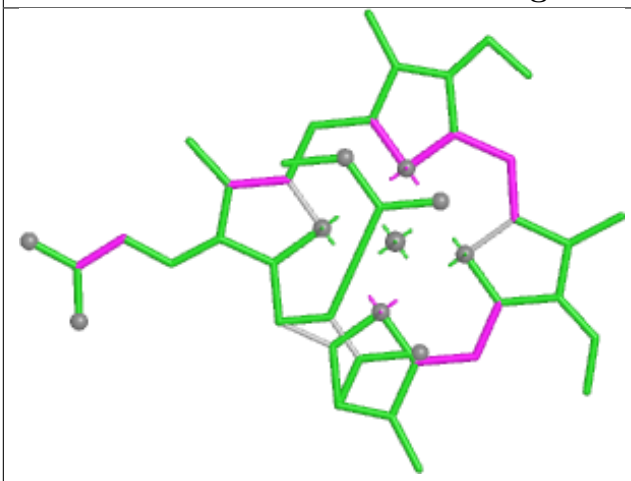


Rings

Ligand KC2 0 317



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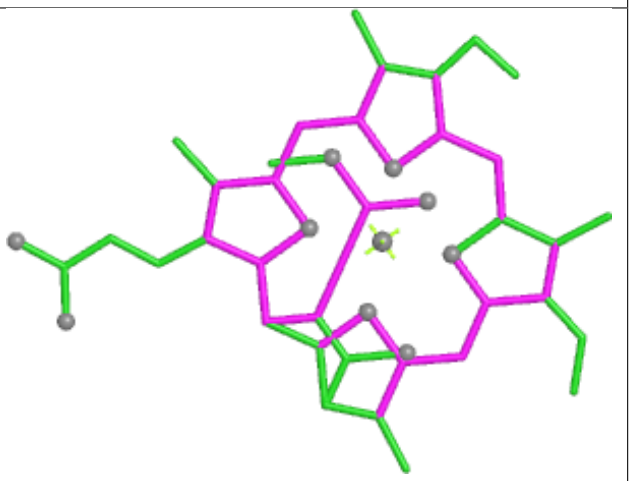
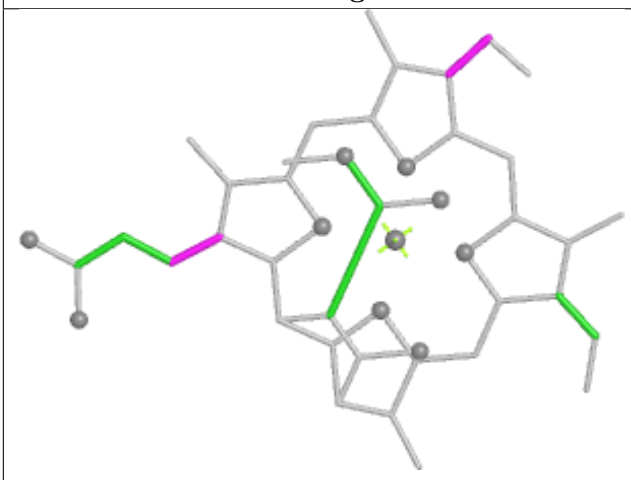


Bond angles



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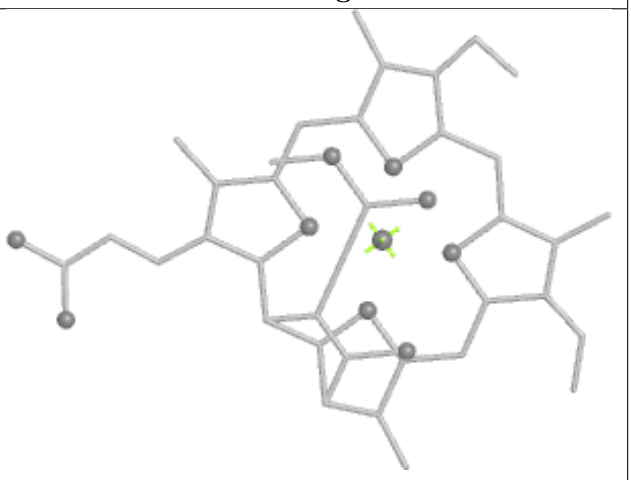
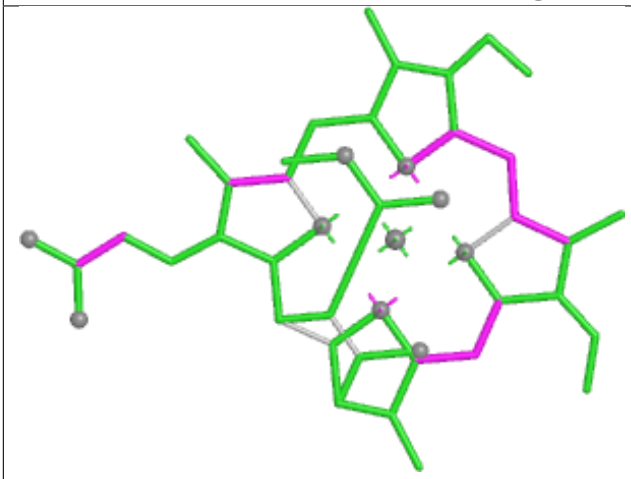


Rings

Ligand KC2 y 313



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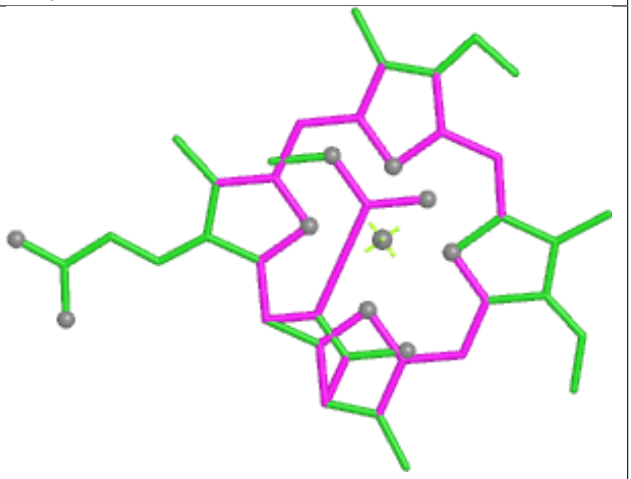
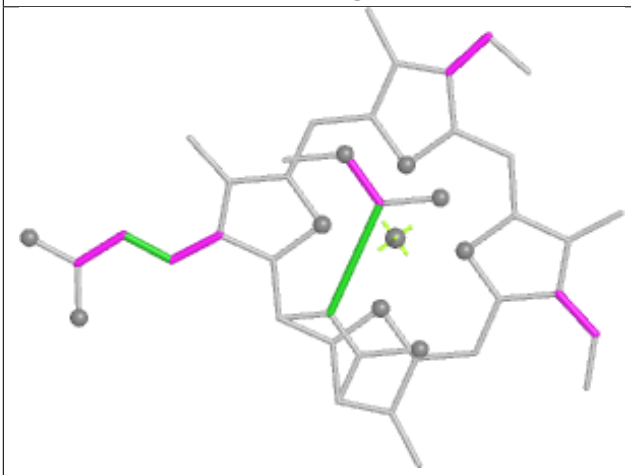


Bond angles



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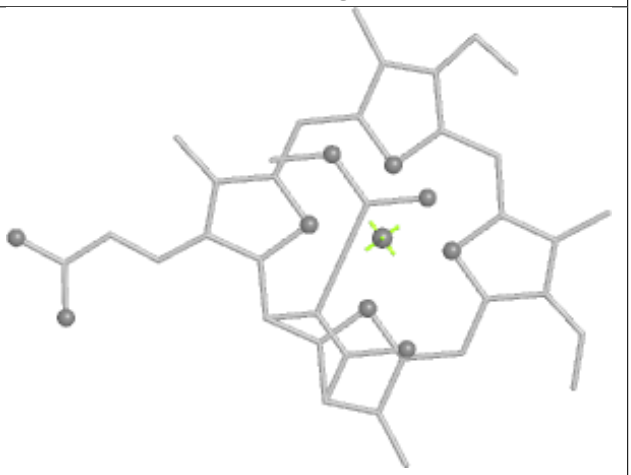
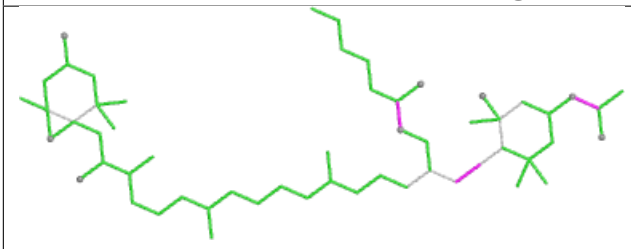


Rings

Ligand A1EB1 7 306



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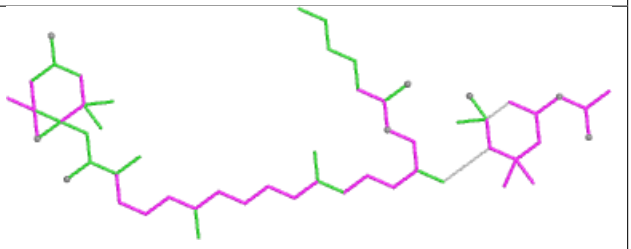

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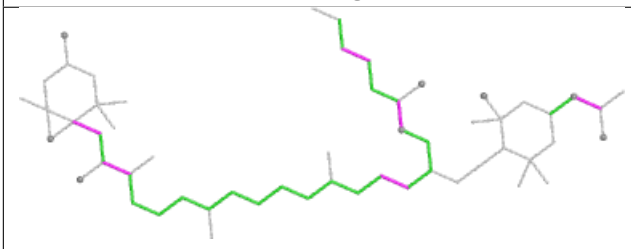

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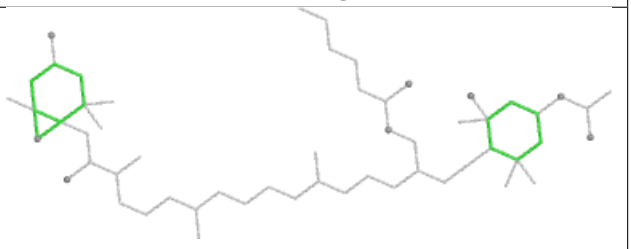
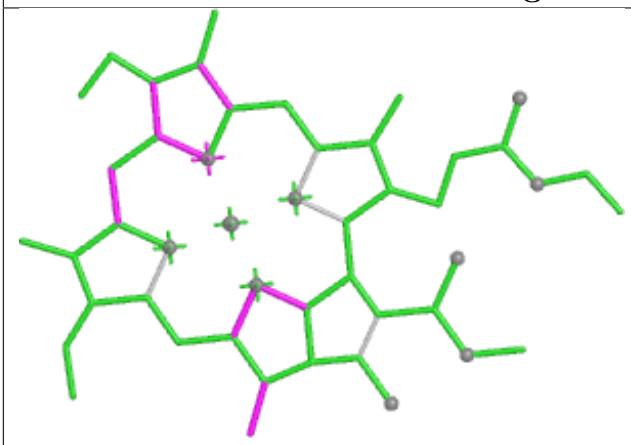


Rings

Ligand CLA R 315



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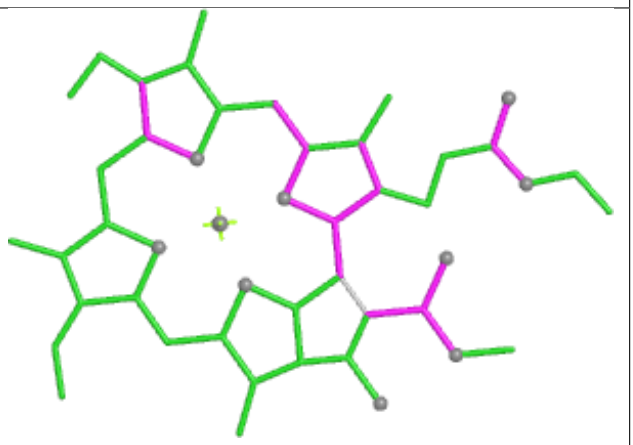
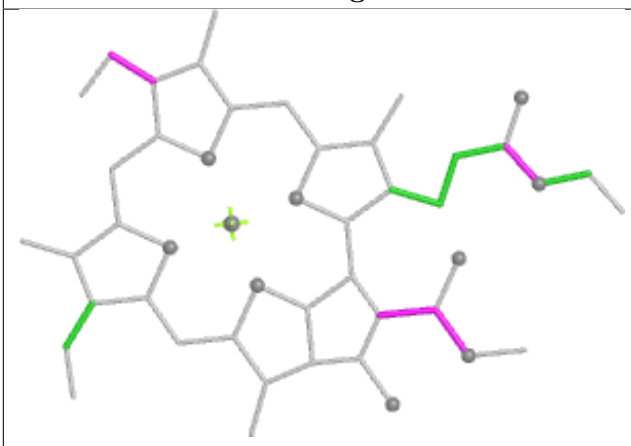
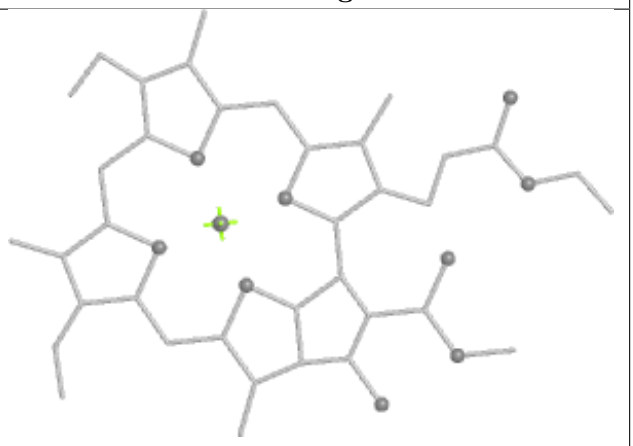


Bond angles

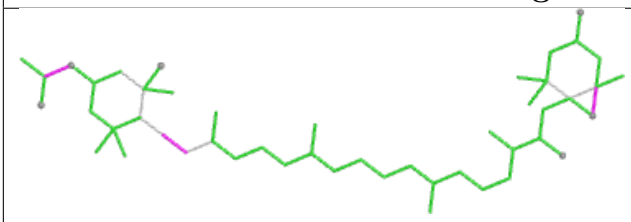


Torsions



Rings

Ligand A86 L 307



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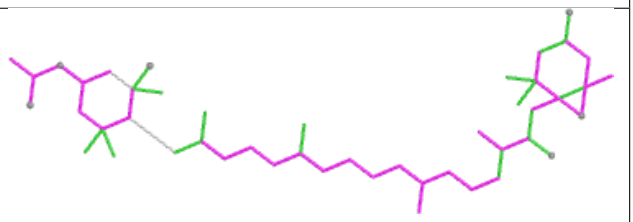
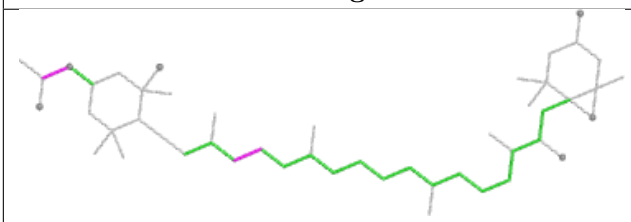
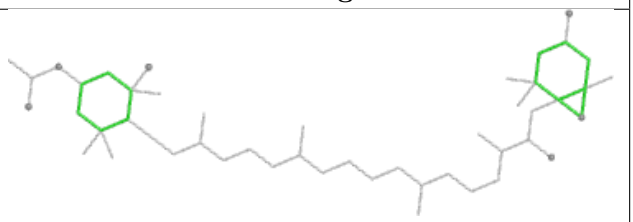


Bond angles

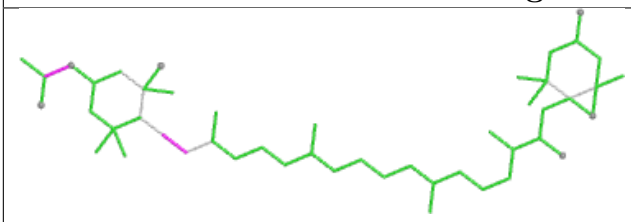


Torsions



Rings

Ligand A86 M 302



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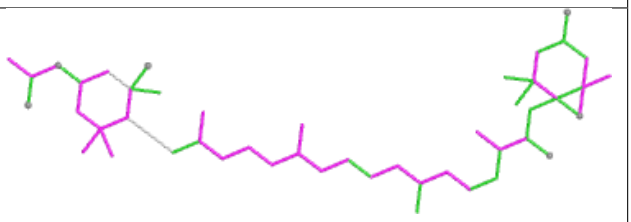
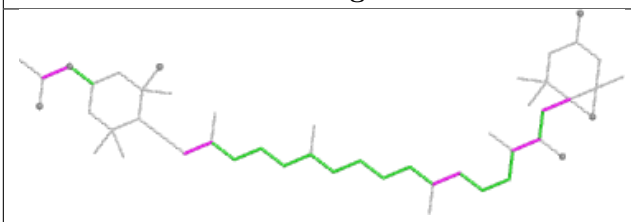


Bond angles



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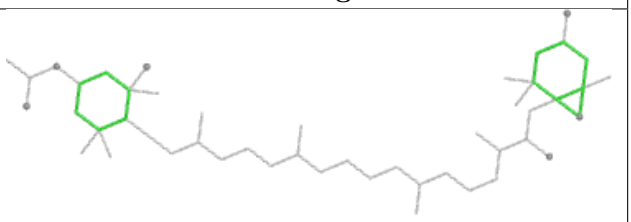
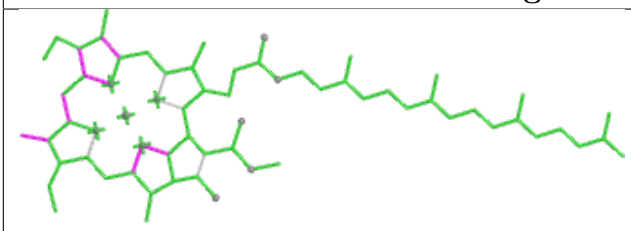


Rings

Ligand CLA Q 312



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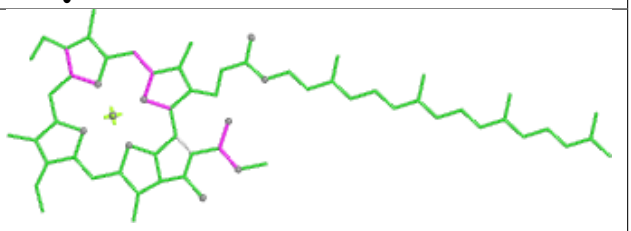
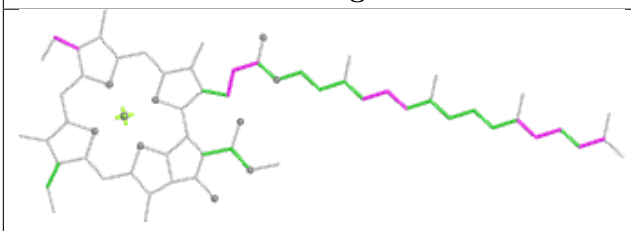


Bond angles



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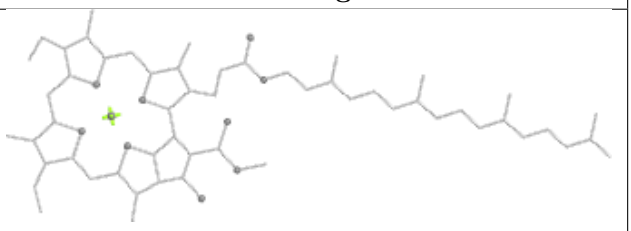
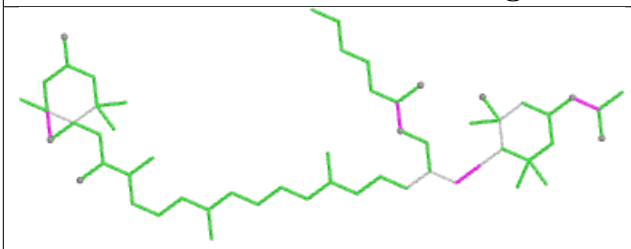


Rings

Ligand A1EB1 G 302



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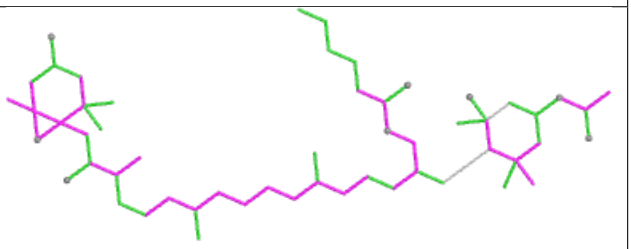
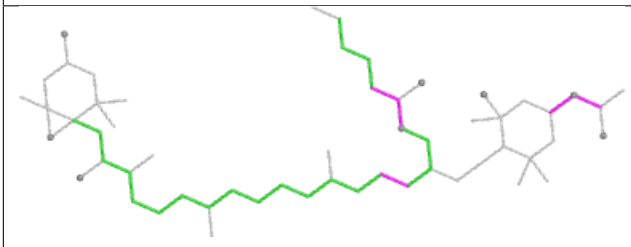
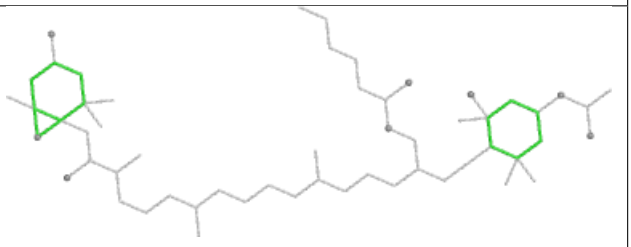


Bond angles

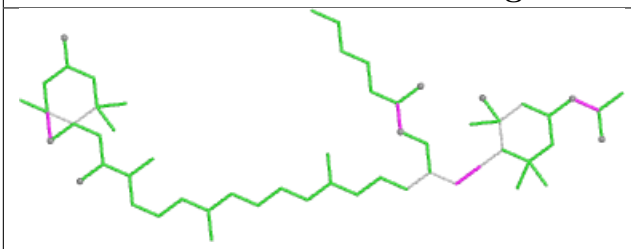


Torsions

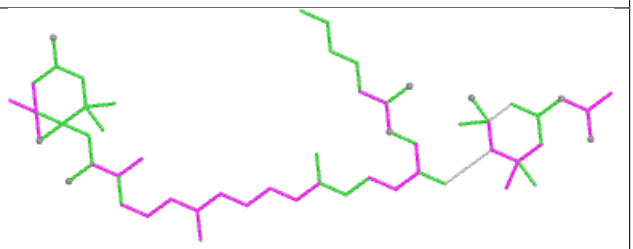


Rings

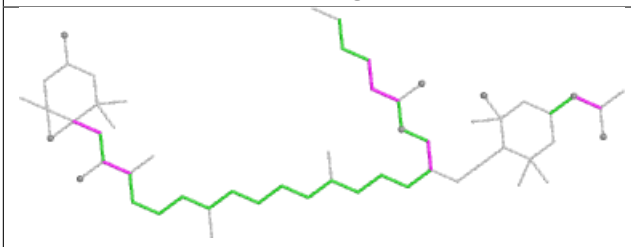
Ligand A1EB1 V 305



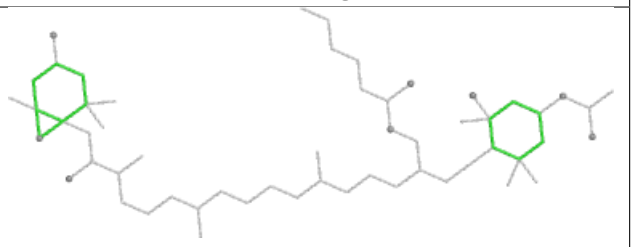
Bond lengths



Bond angles

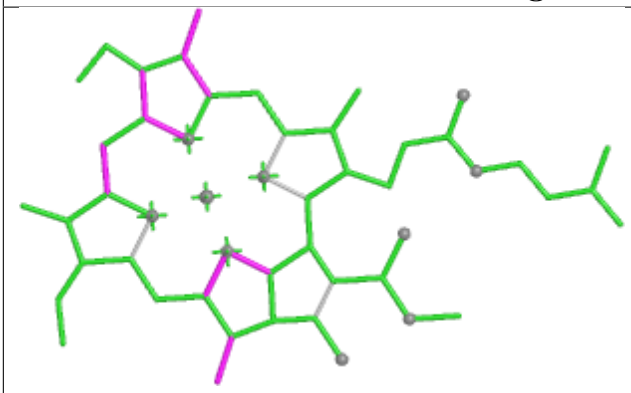


Torsions

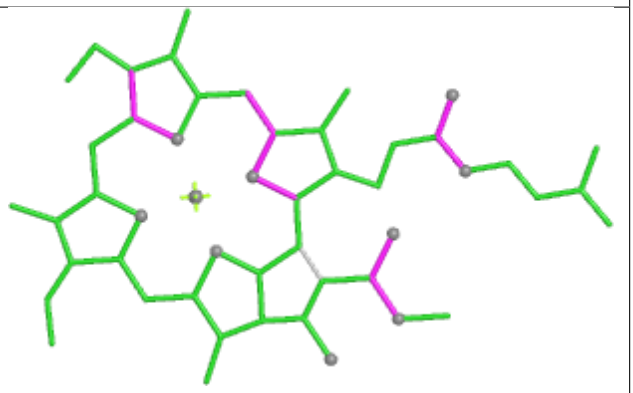


Rings

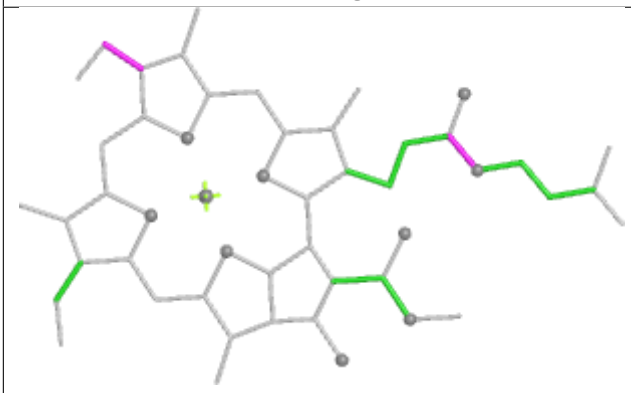
Ligand CLA b 822



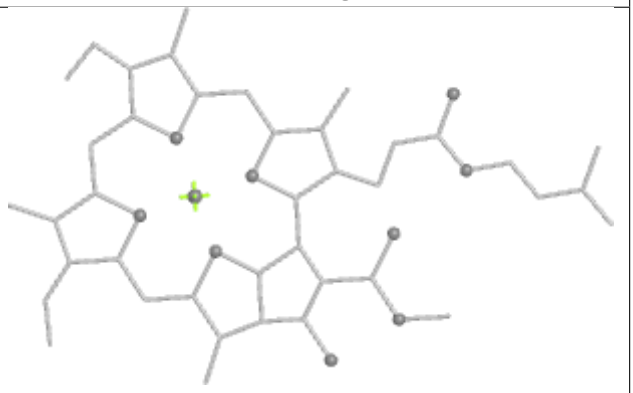
Bond lengths



Bond angles

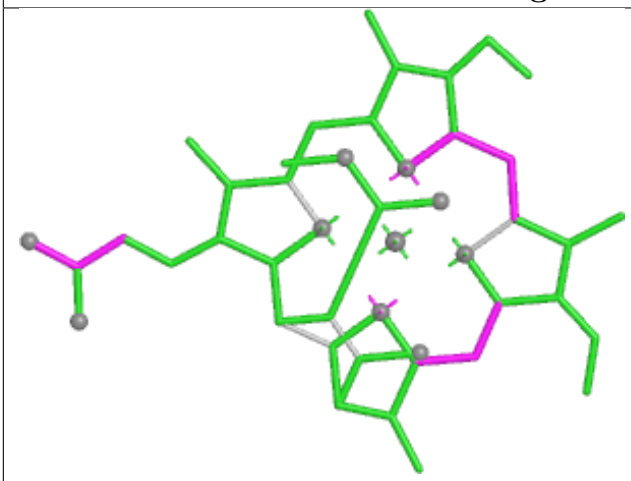


Torsions



Rings

Ligand KC2 3 321



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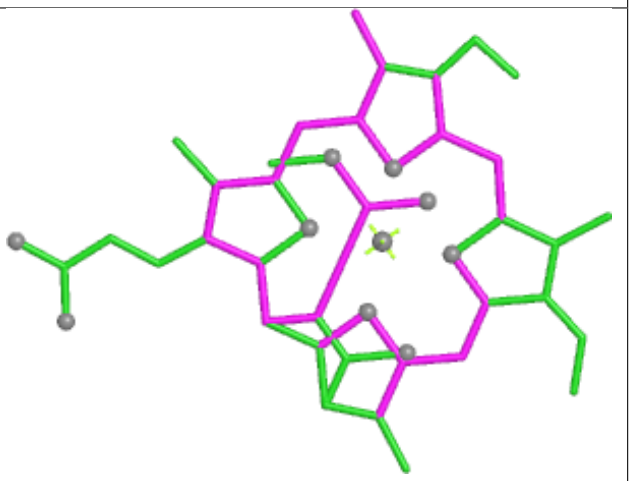
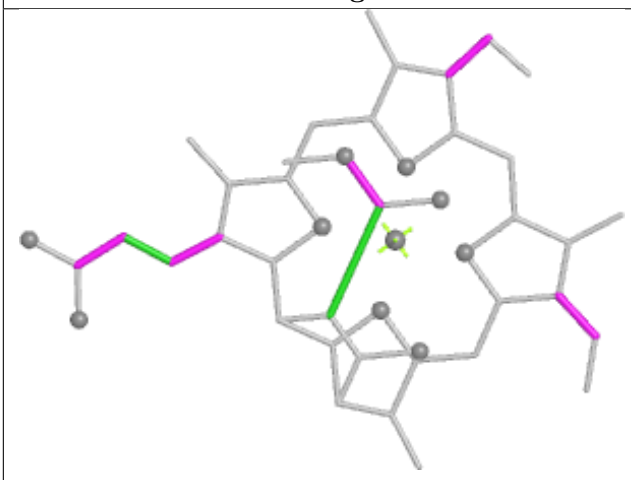


Bond angles



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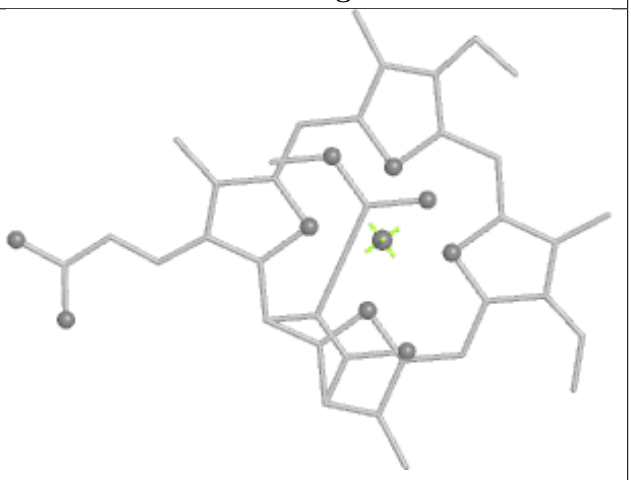
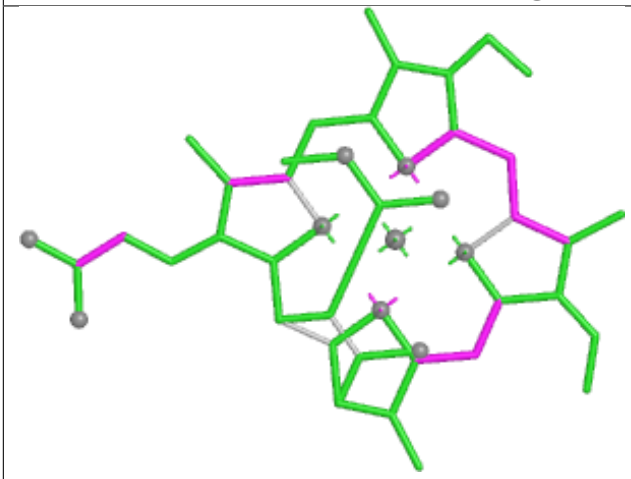


Rings

Ligand KC2 L 317



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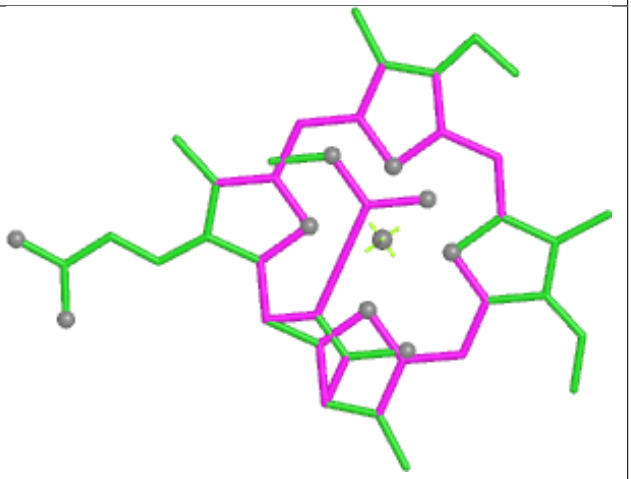
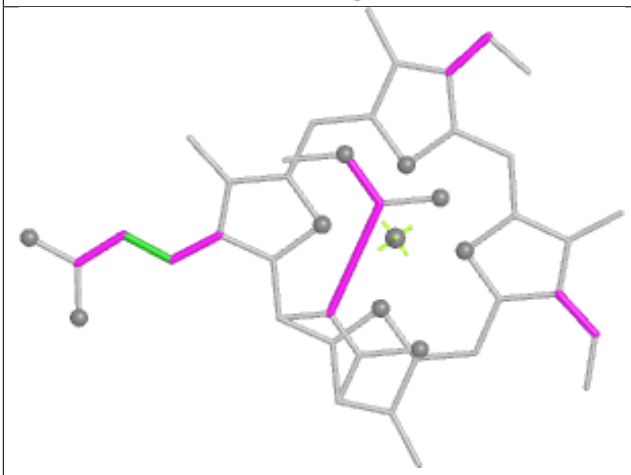
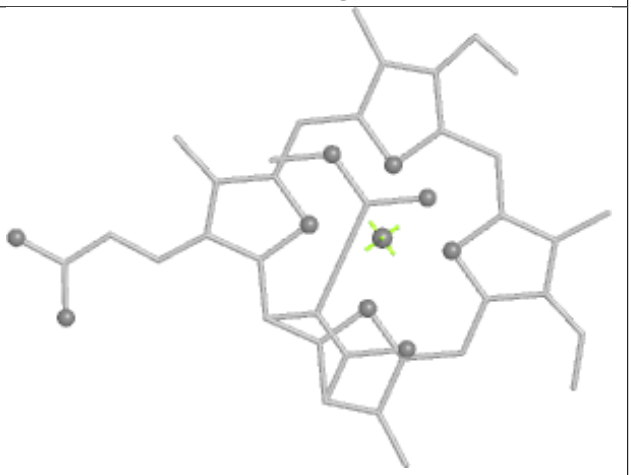


Bond angles

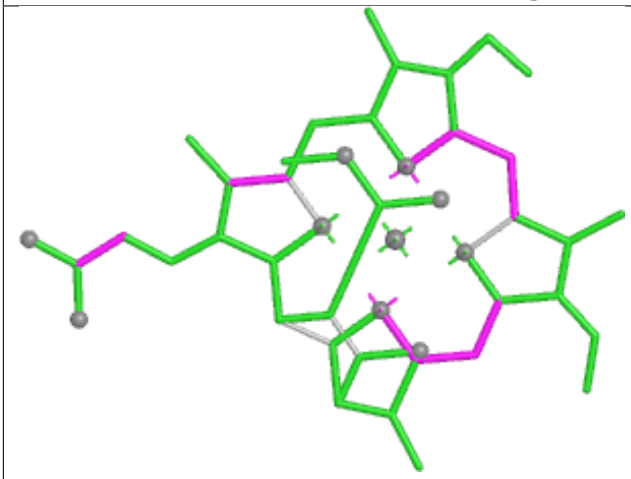


Torsions



Rings

Ligand KC2 G 315



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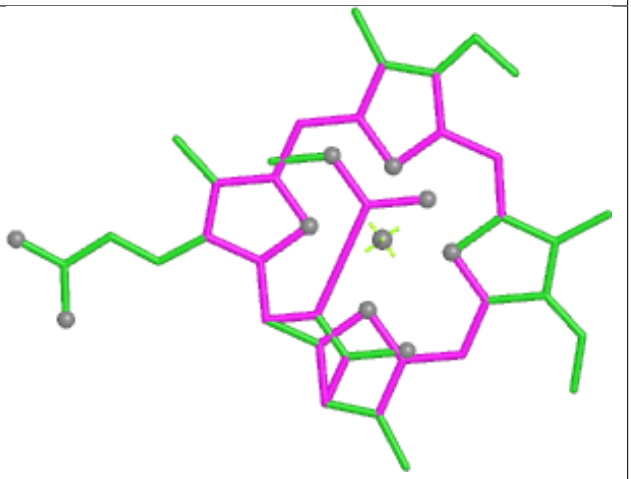
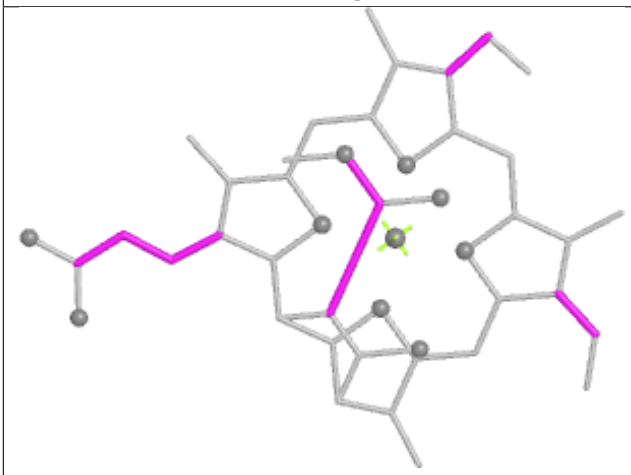


Bond angles



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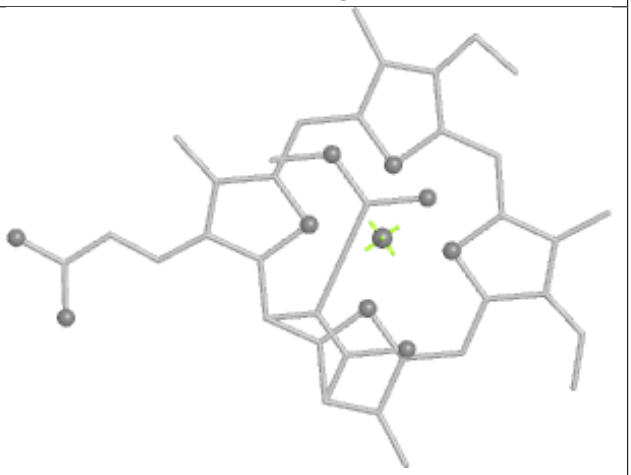
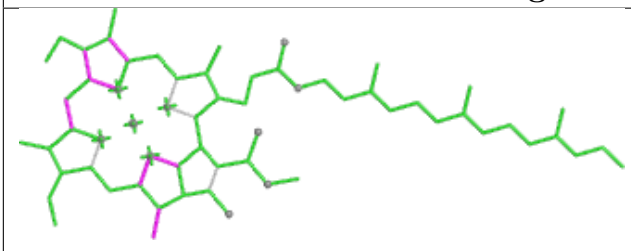


Rings

Ligand CLA a 809



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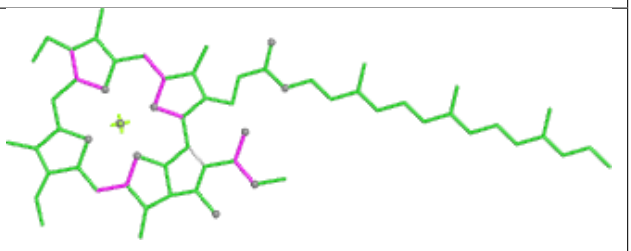
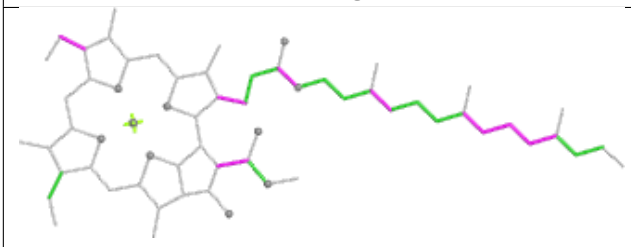


Bond angles



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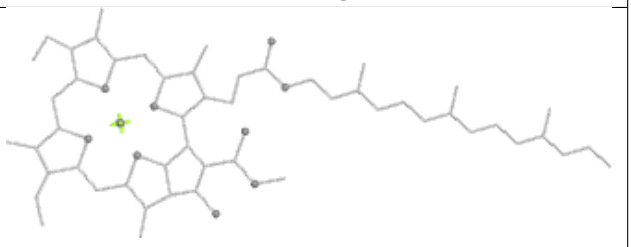
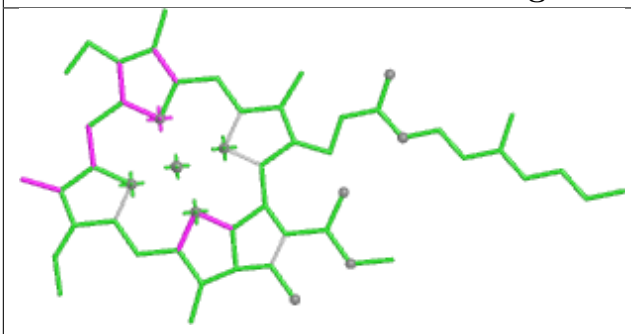


Rings

Ligand CLA 3 313



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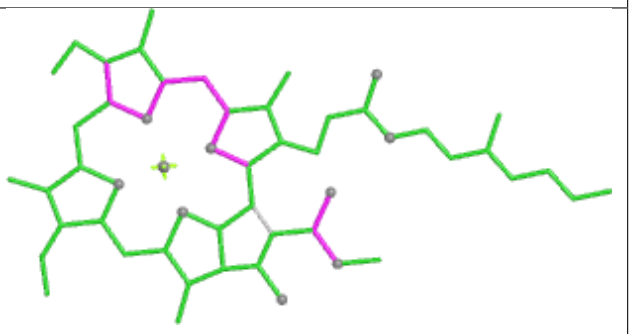
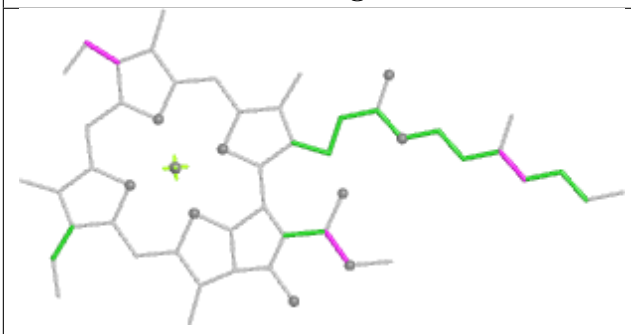


Bond angles



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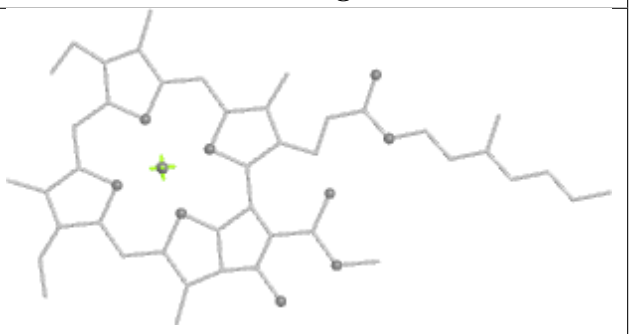
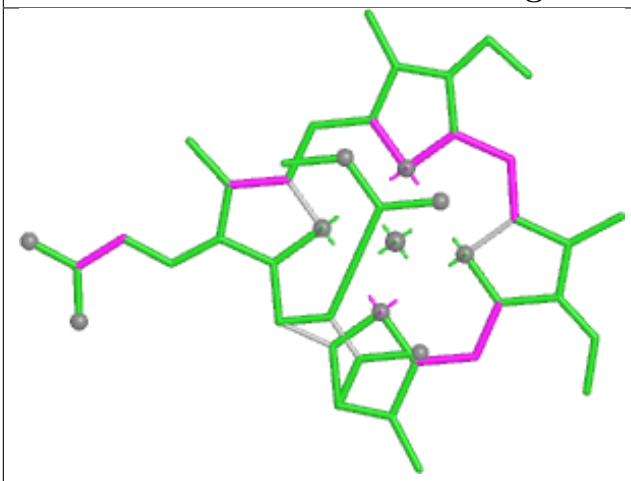
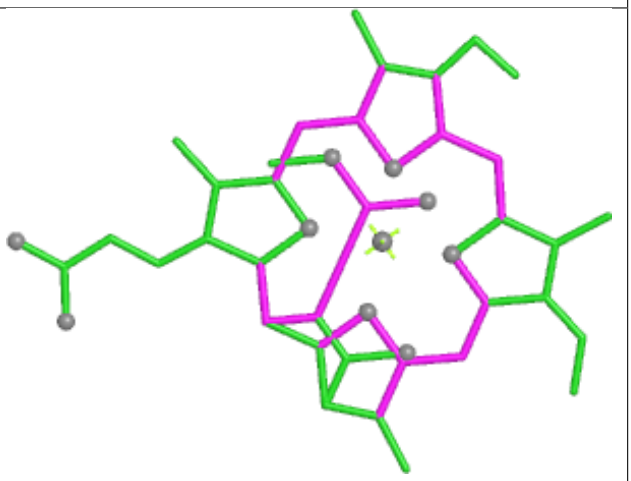


Rings

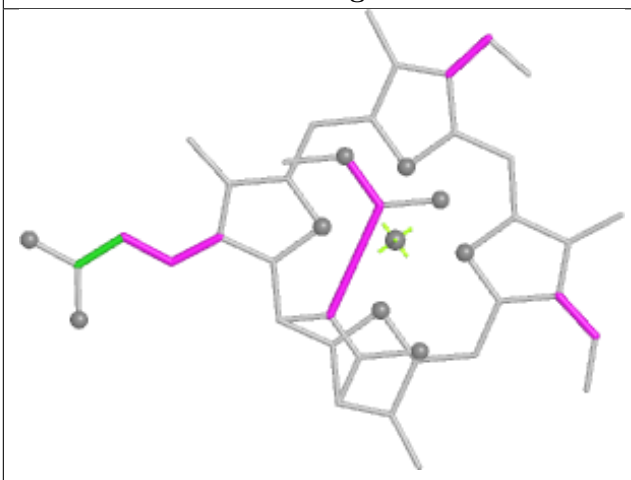
Ligand KC2 X 306



Bond lengths



Bond angles



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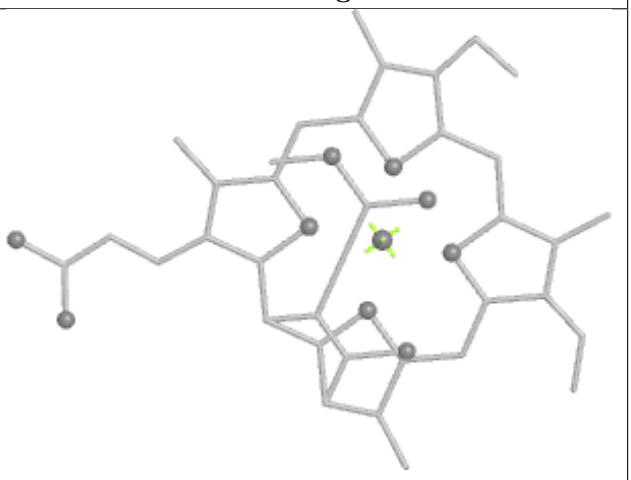
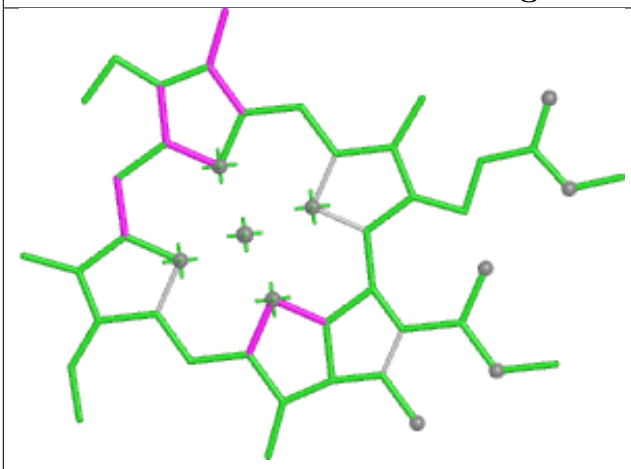


Rings

Ligand CLA M 321



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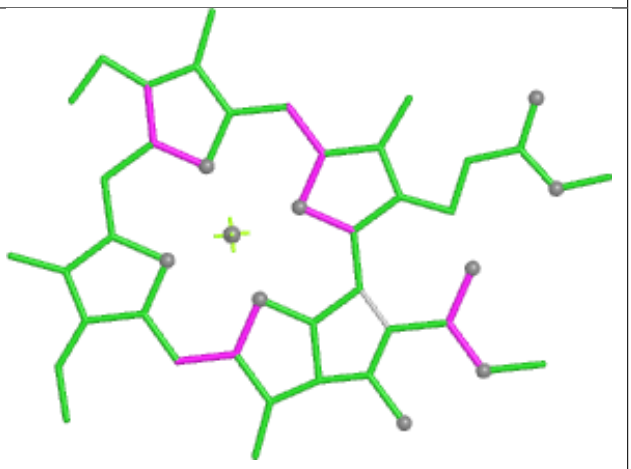
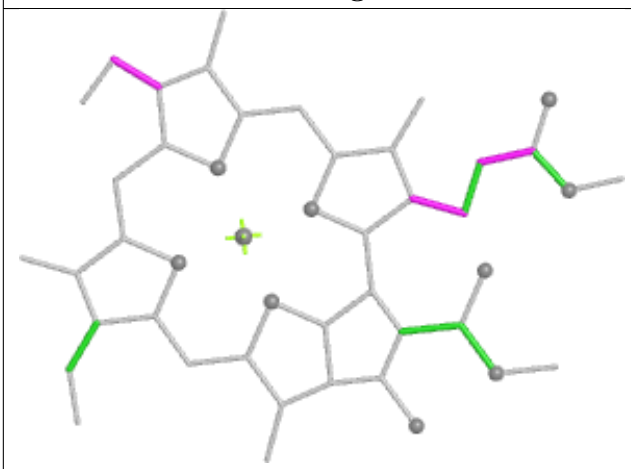


Bond angles



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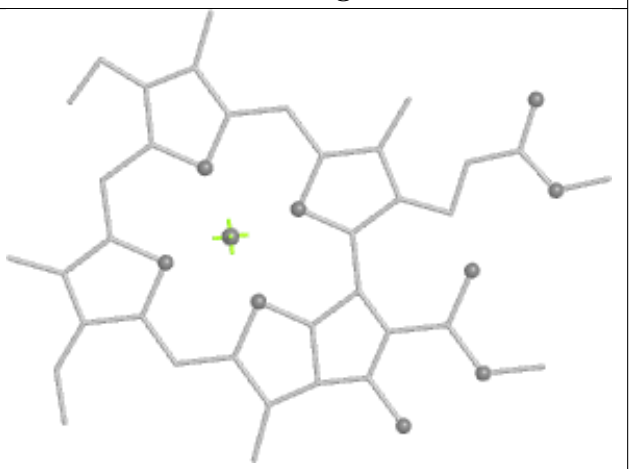
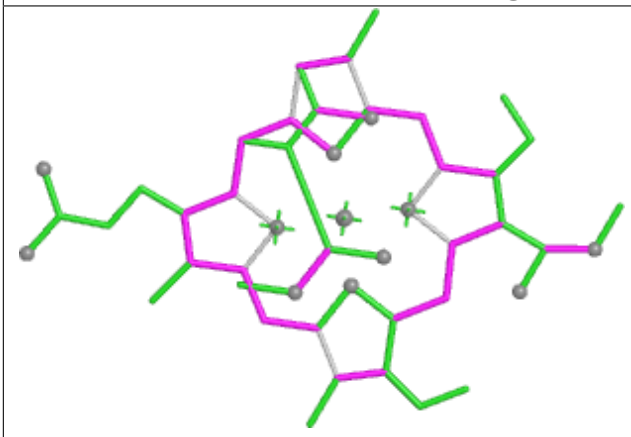
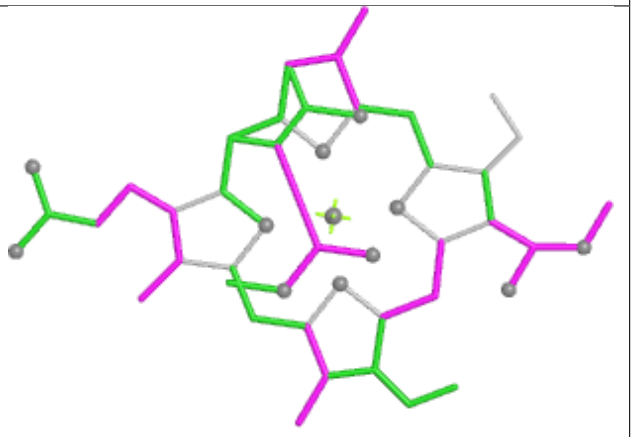
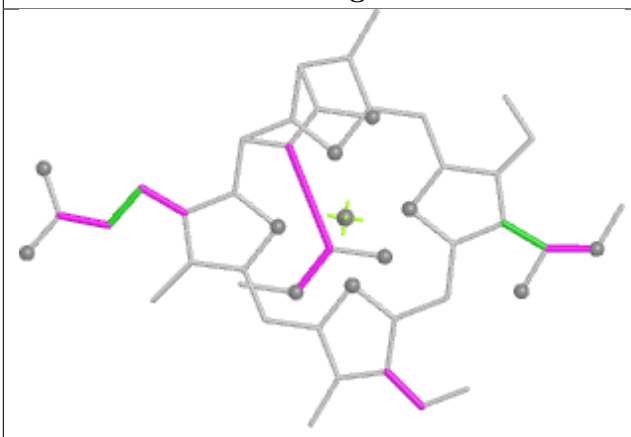
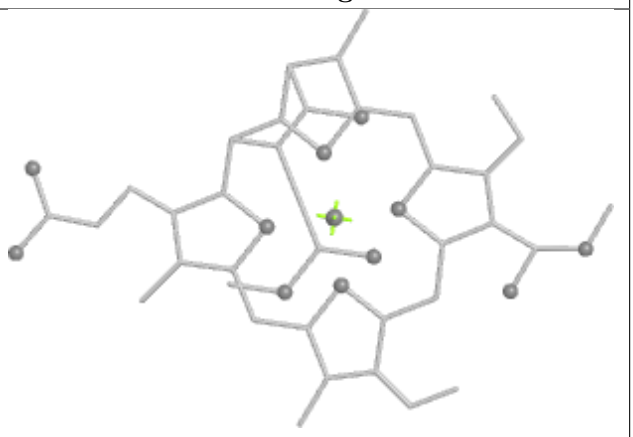
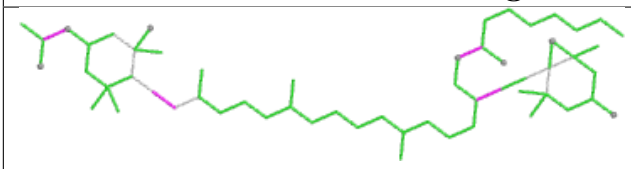
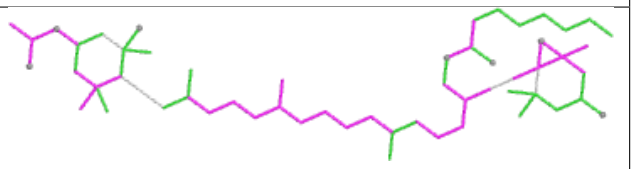
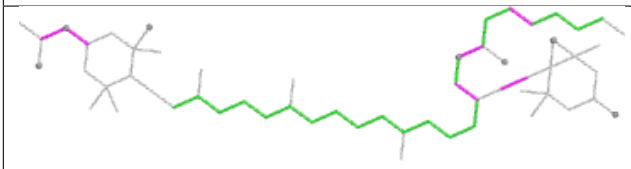
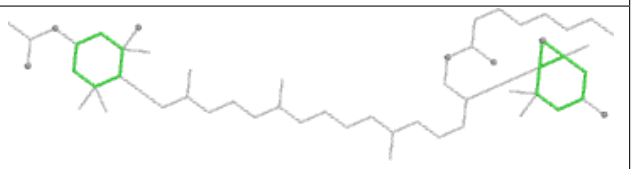
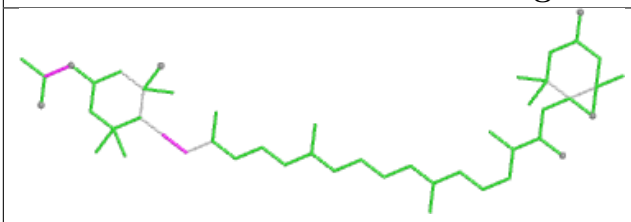


Rings

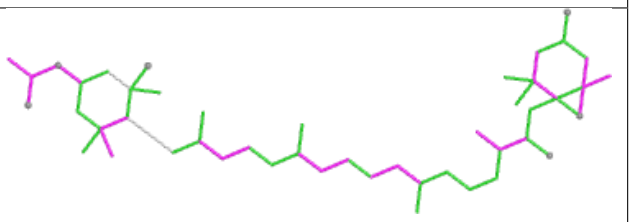
Ligand A1ECV 5 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1EB4 R 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

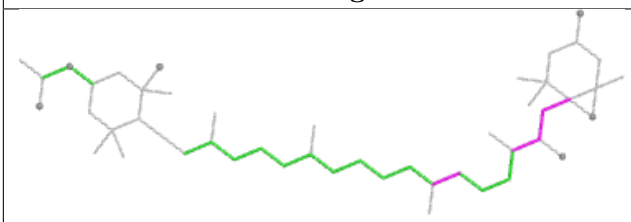
Ligand A86 4 305



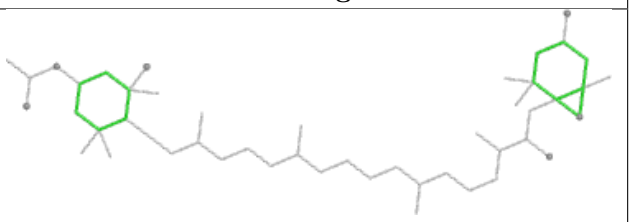
Bond lengths



Bond angles

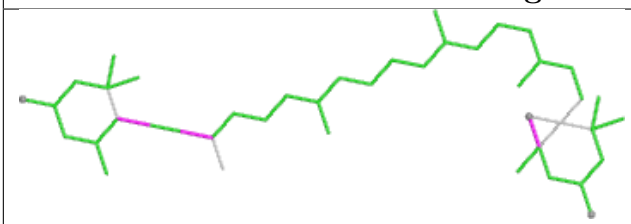


Torsions



Rings

Ligand DD6 D 307



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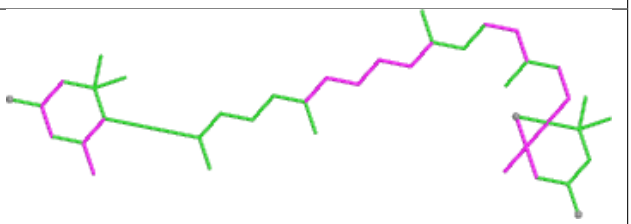
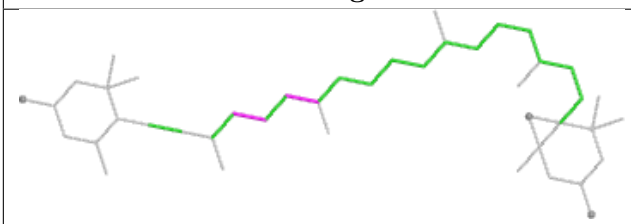


Bond angles



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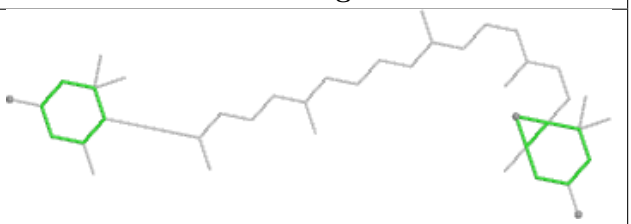
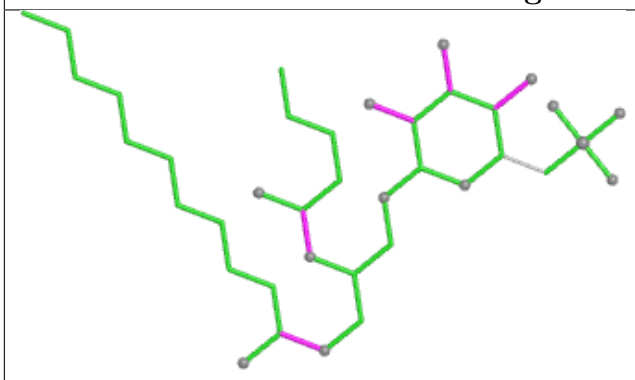


Rings

Ligand SQD H 318



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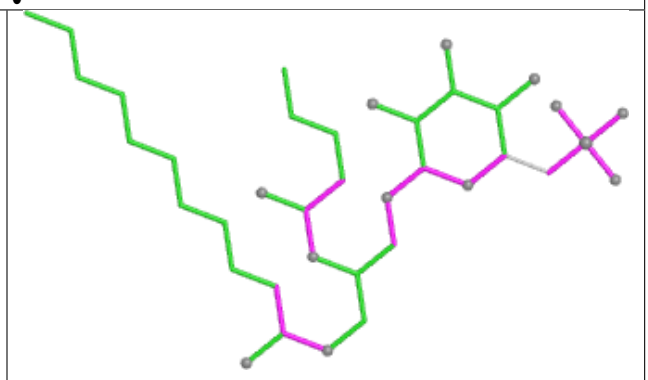
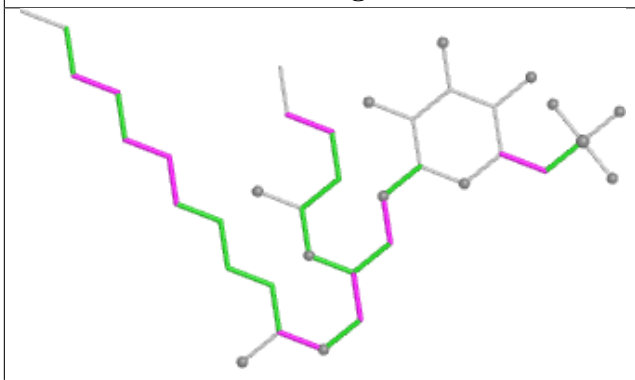
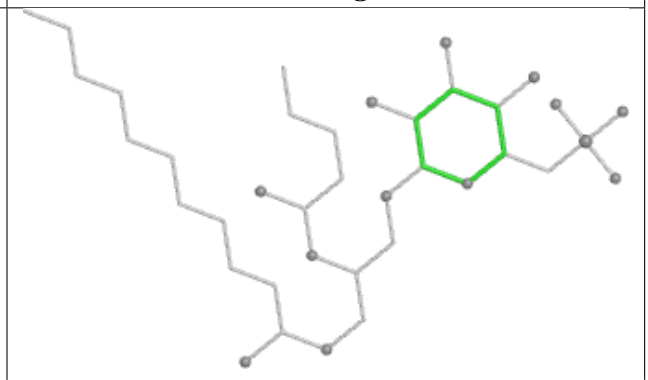


Bond angles

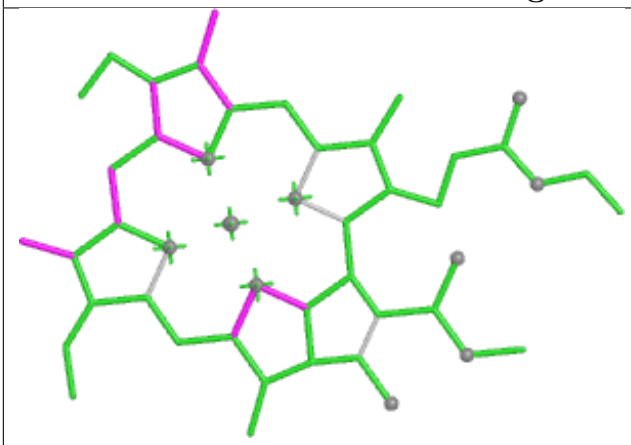


Torsions

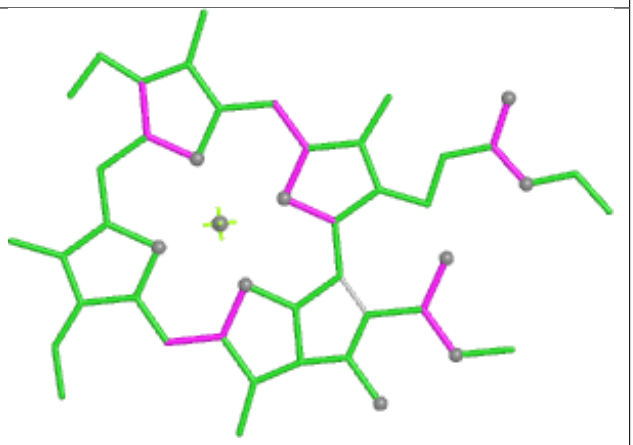


Rings

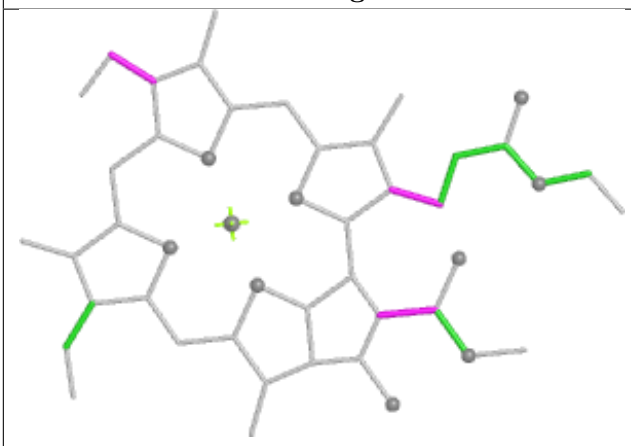
Ligand CLA b 839



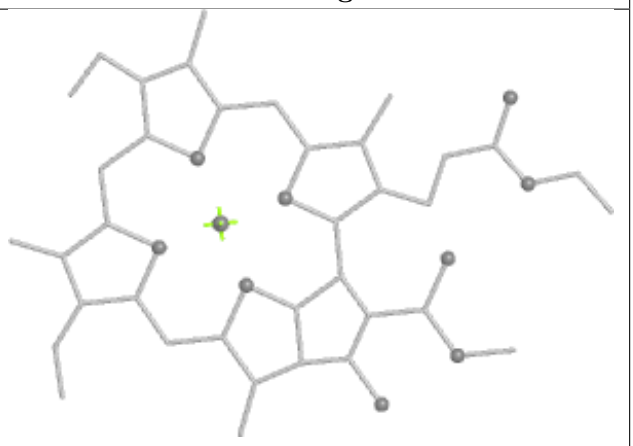
Bond lengths



Bond angles



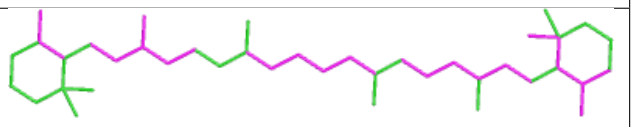
Torsions



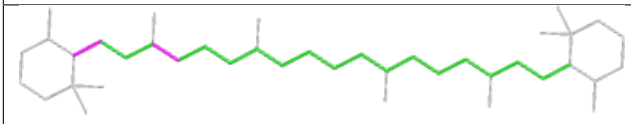
Rings

Ligand BCR l 202

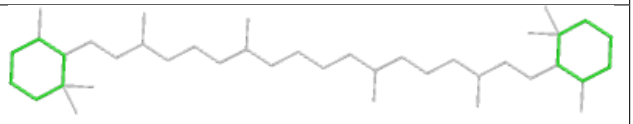
Bond lengths



Bond angles

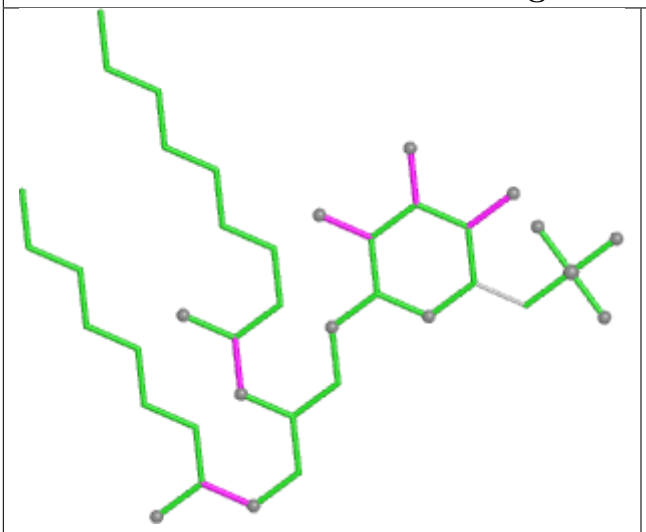


Torsions



Rings

Ligand SQD 7 302



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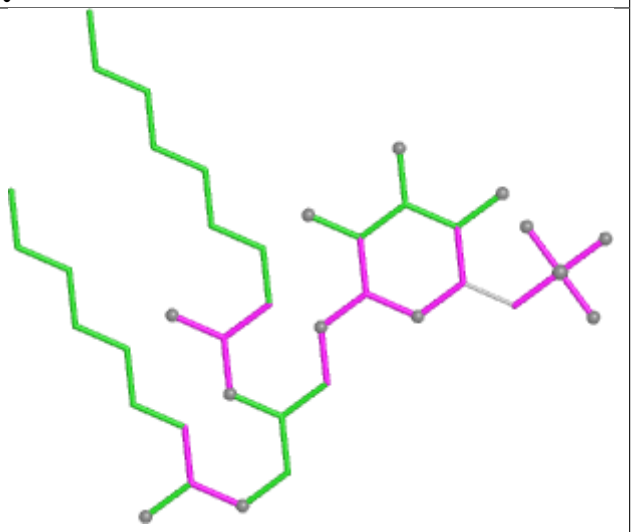
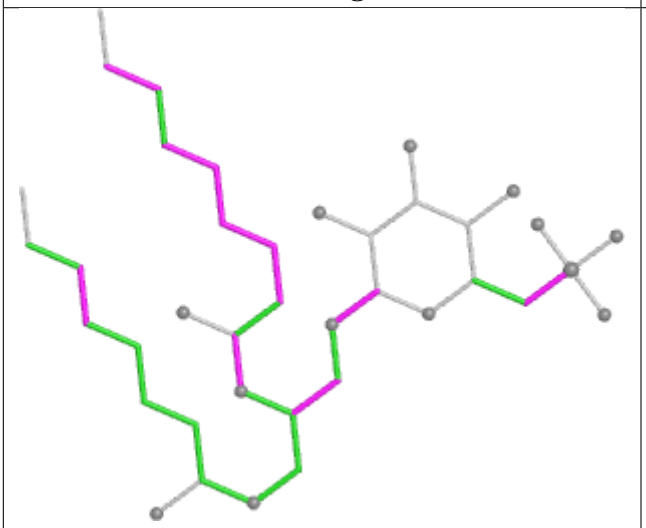


Bond angles



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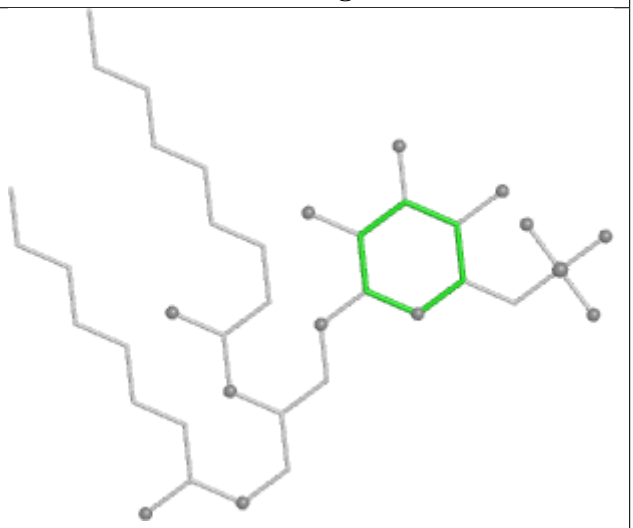
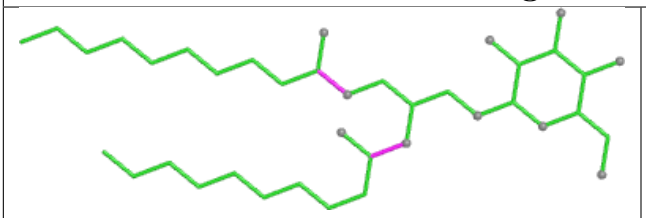


Rings

Ligand LMG F 317



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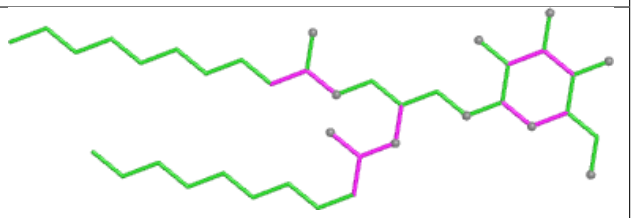
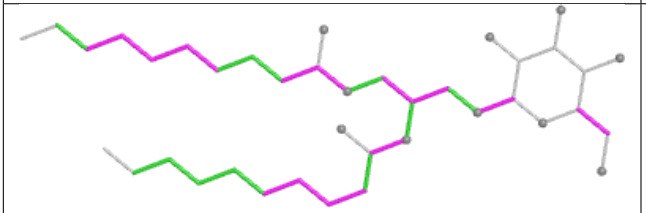


Bond angles



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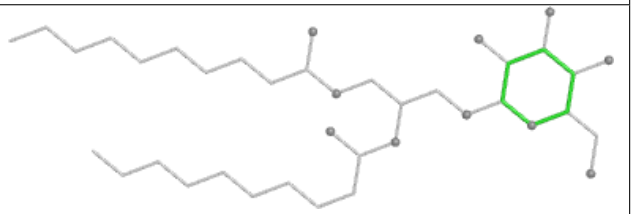
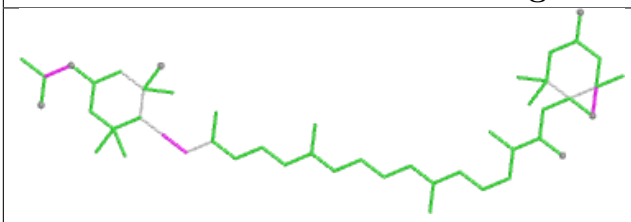


Rings

Ligand A86 K 301



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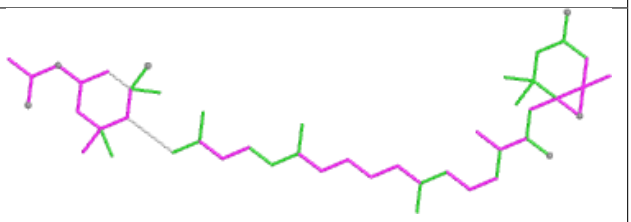
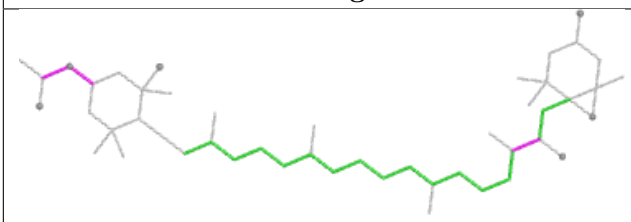


Bond angles



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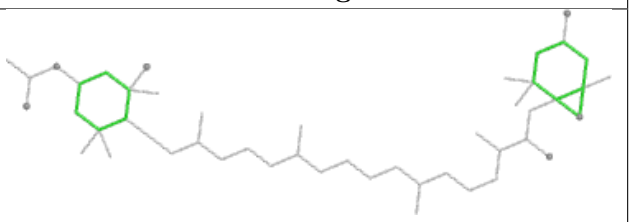
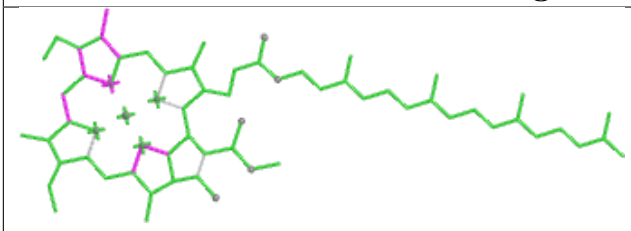


Rings

Ligand CLA l 204



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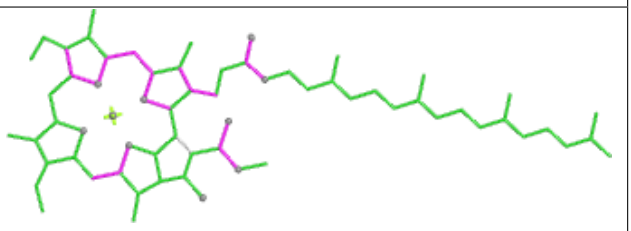
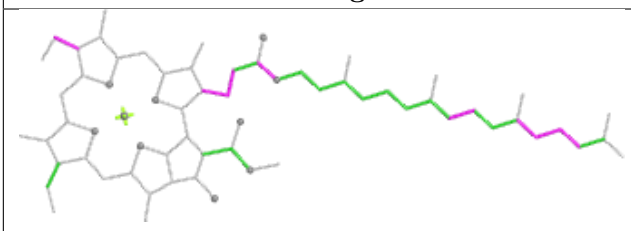


Bond angles



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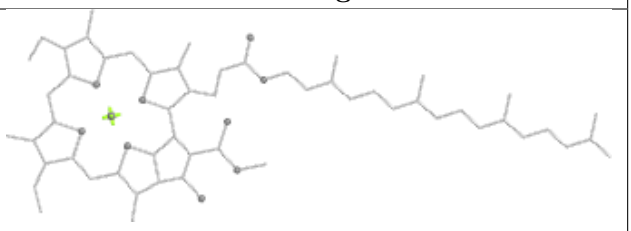
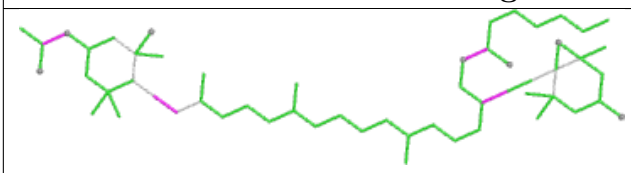


Rings

Ligand A1EB4 W 306



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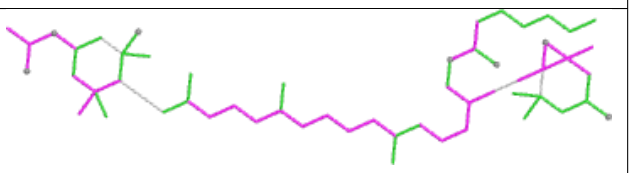
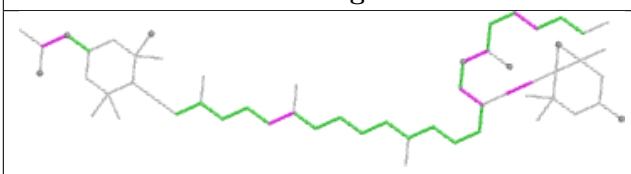


Bond angles



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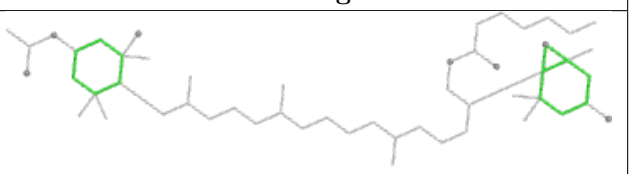
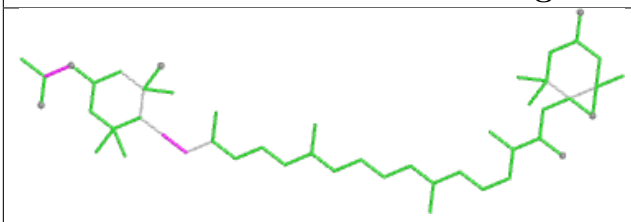


Rings

Ligand A86 z 303



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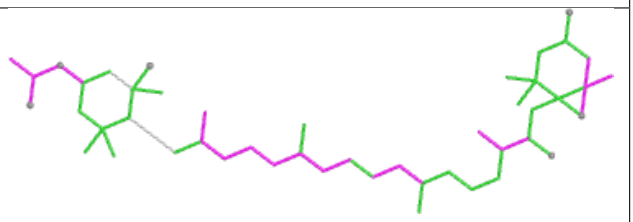
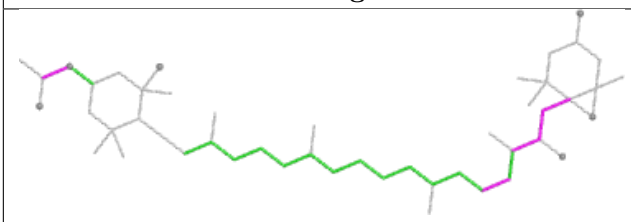
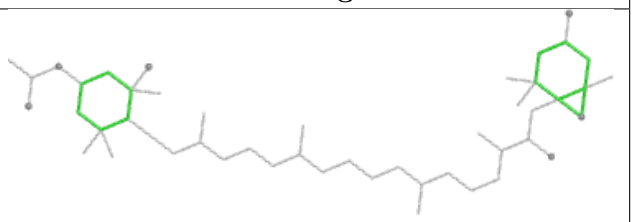


Bond angles

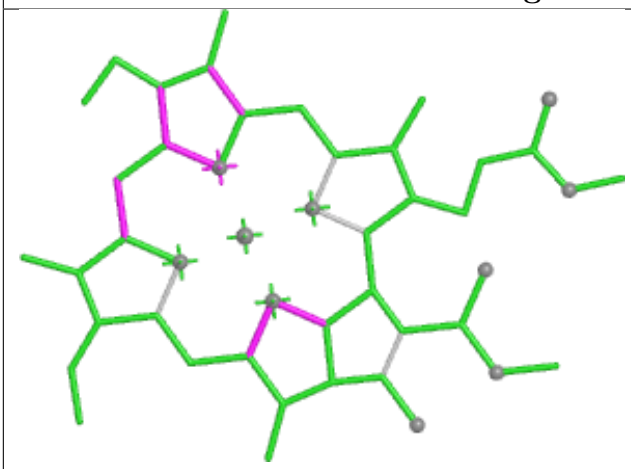


Torsions



Rings

Ligand CLA O 318



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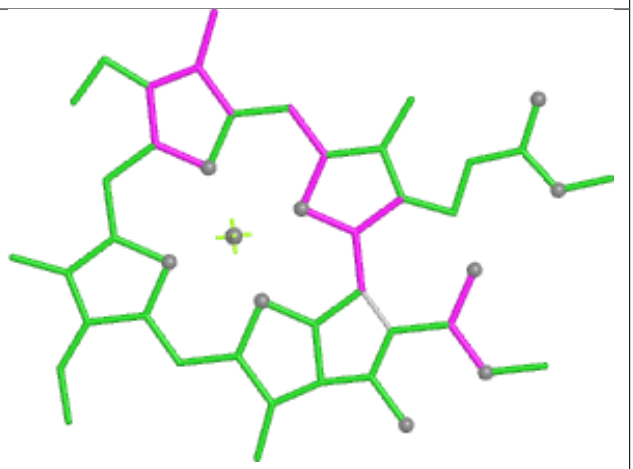
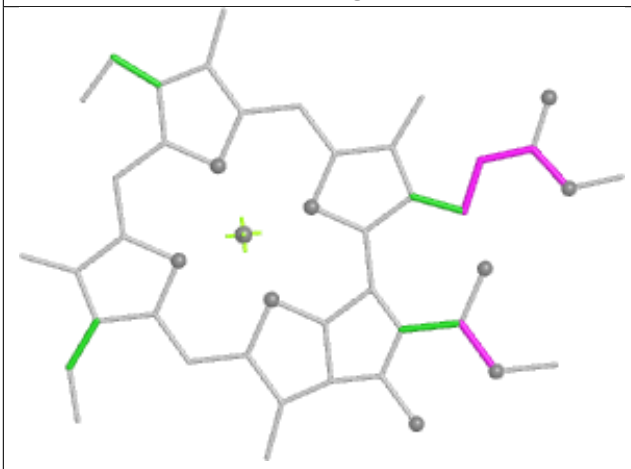
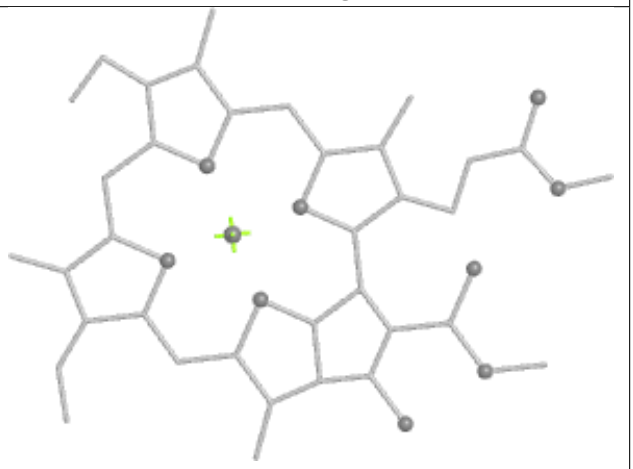


Bond angles

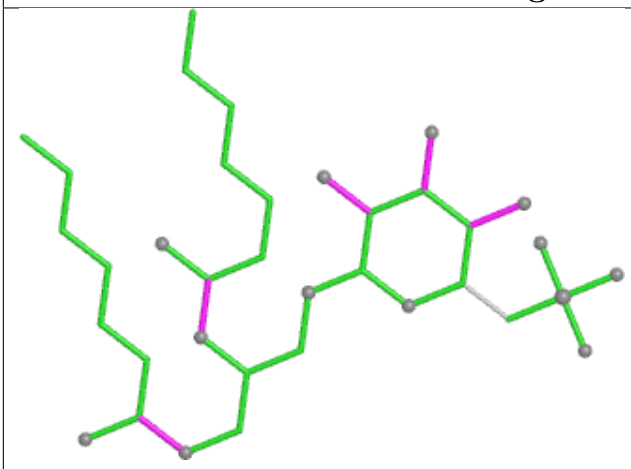


Torsions



Rings

Ligand SQD 9 322



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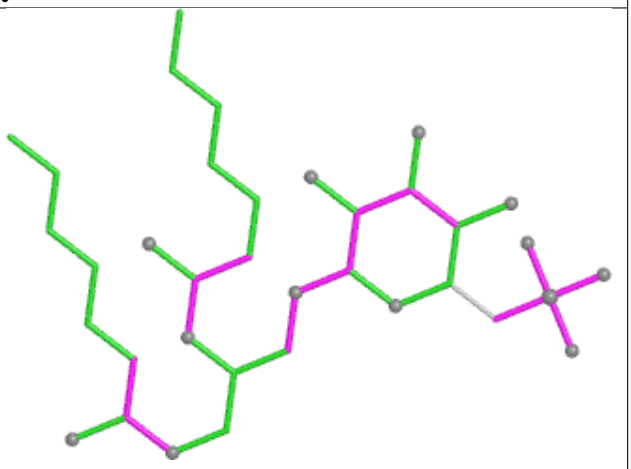
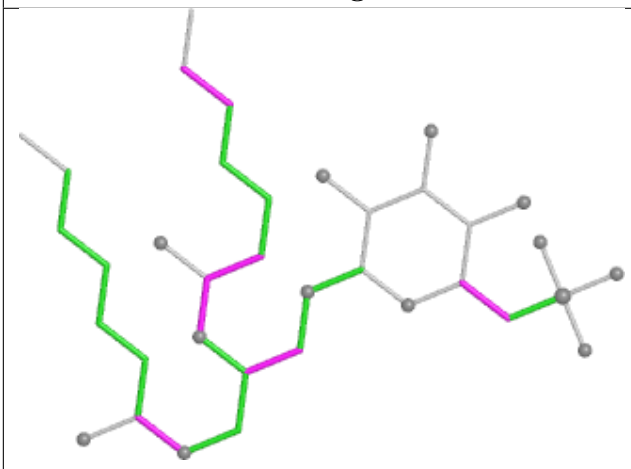


Bond angles



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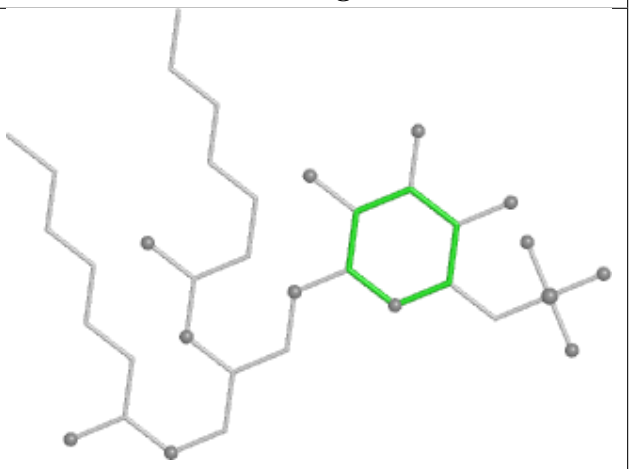
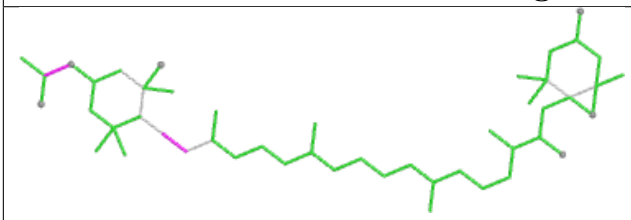


Rings

Ligand A86 S 305



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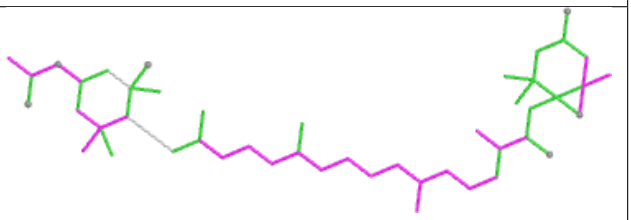
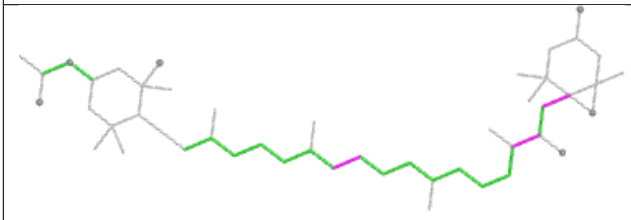


Bond angles



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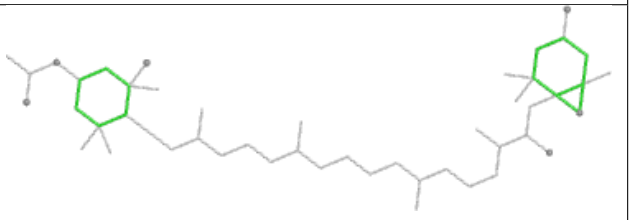
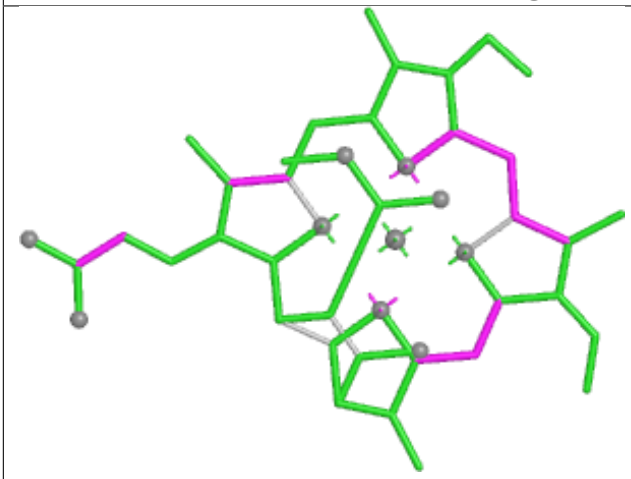


Rings

Ligand KC2 V 320



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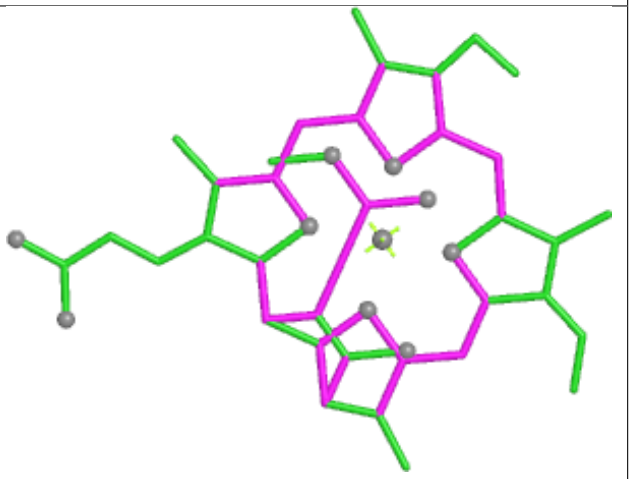
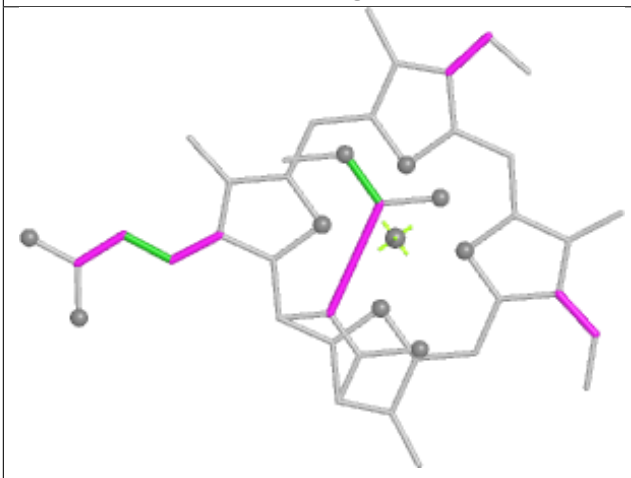


Bond angles



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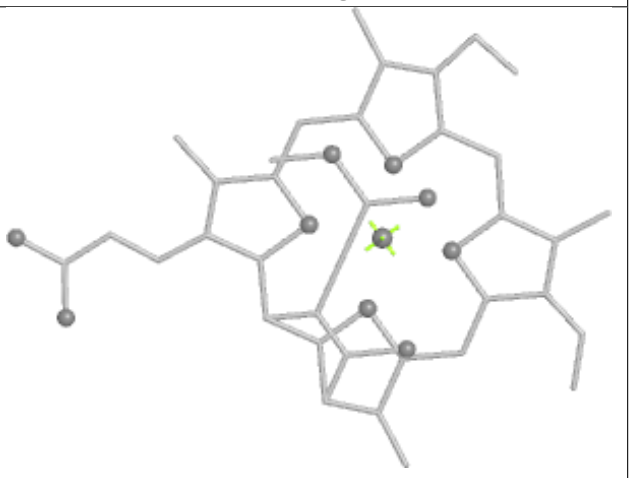
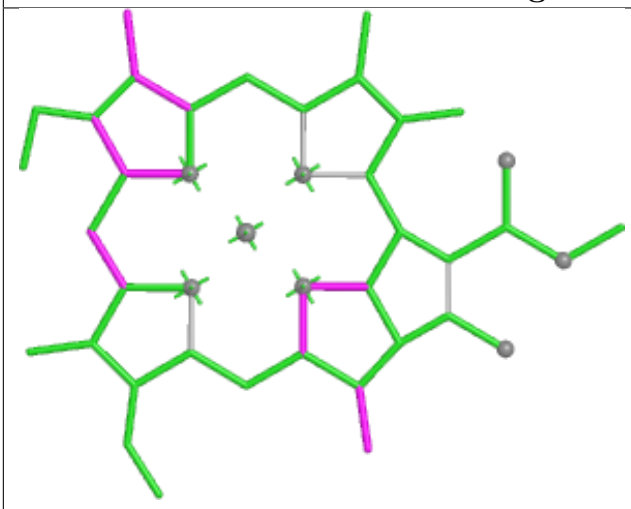


Rings

Ligand CLA 1 313



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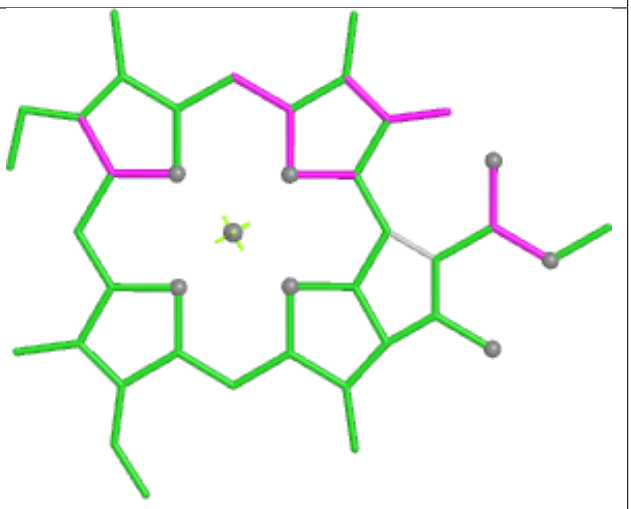
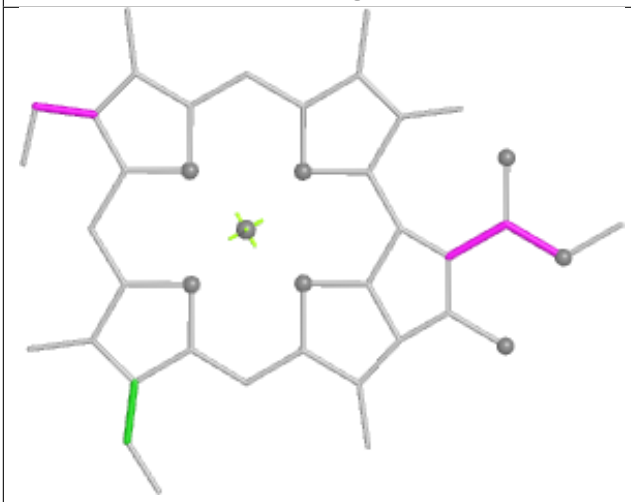
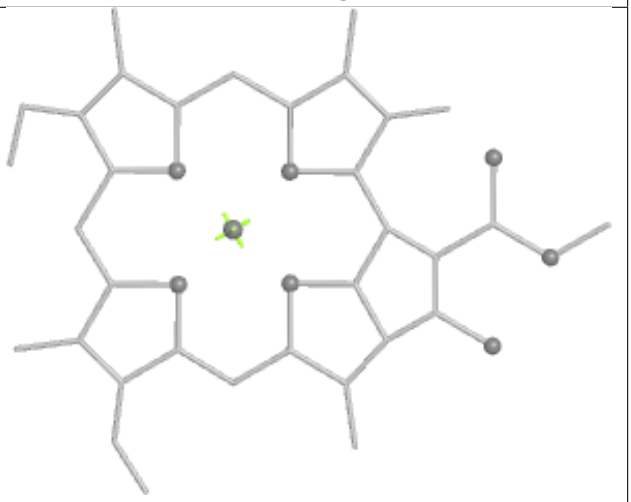


Bond angles

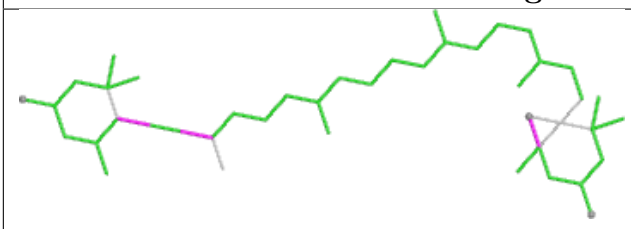


Torsions



Rings

Ligand DD6 O 303



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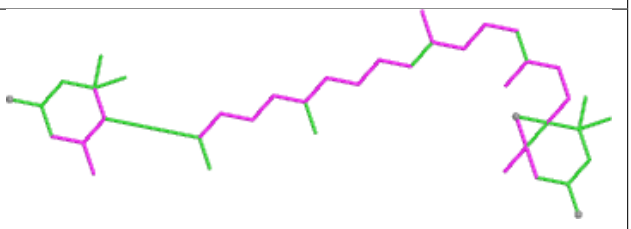
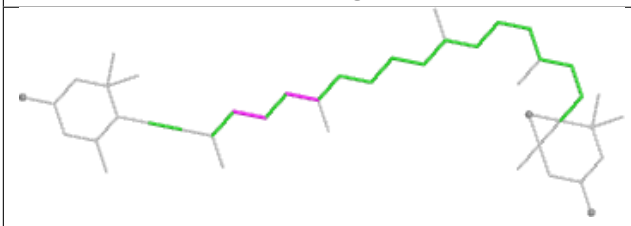


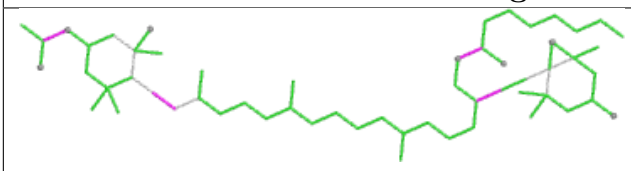
Bond angles



Torsions

Rings

Ligand A1EB4 5 304



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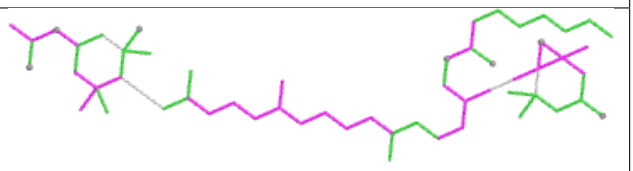
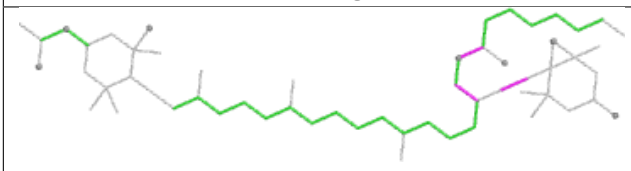
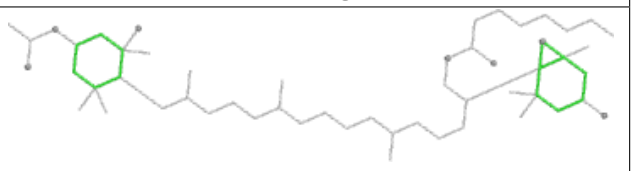


Bond angles

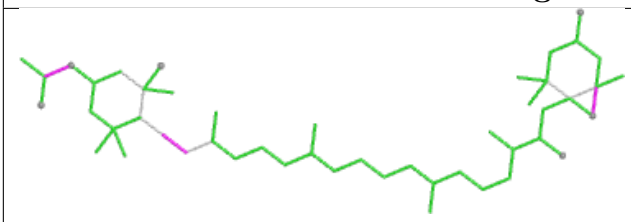


Torsions

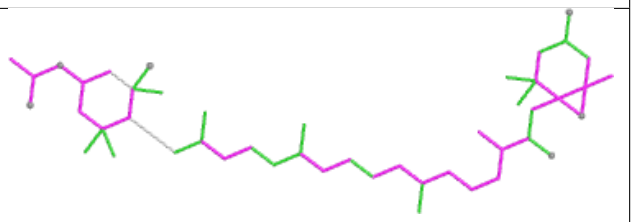


Rings

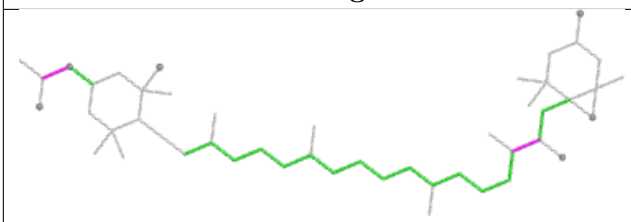
Ligand A86 J 303



Bond lengths



Bond angles



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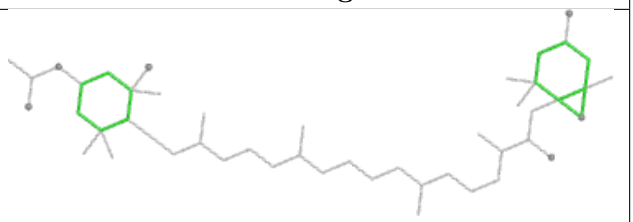
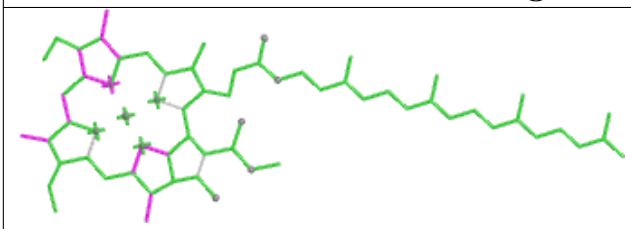


Rings

Ligand CLA b 840



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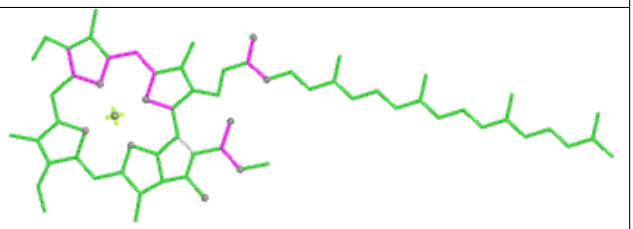

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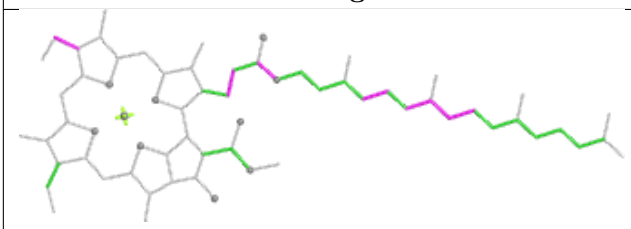

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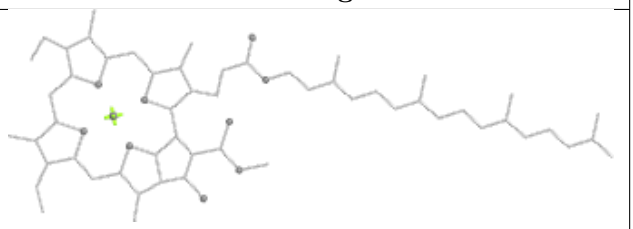
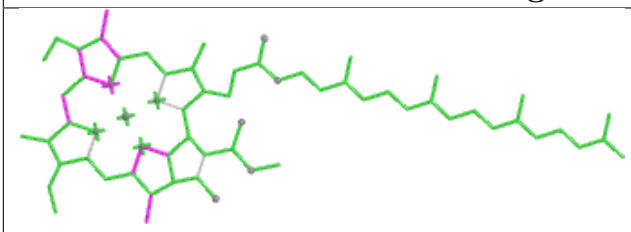


Rings

Ligand CLA S 320



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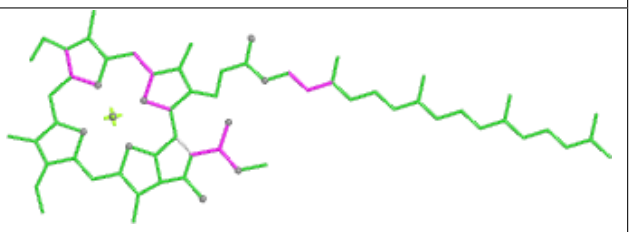
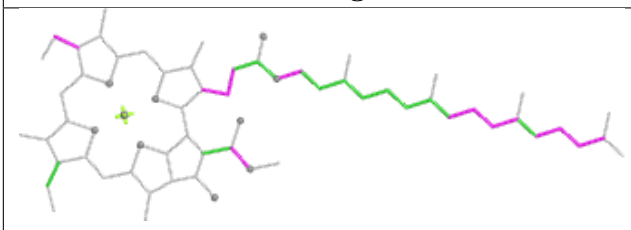


Bond angles



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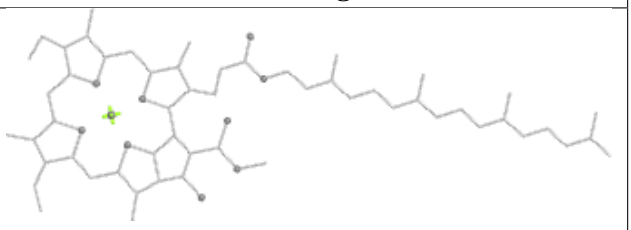
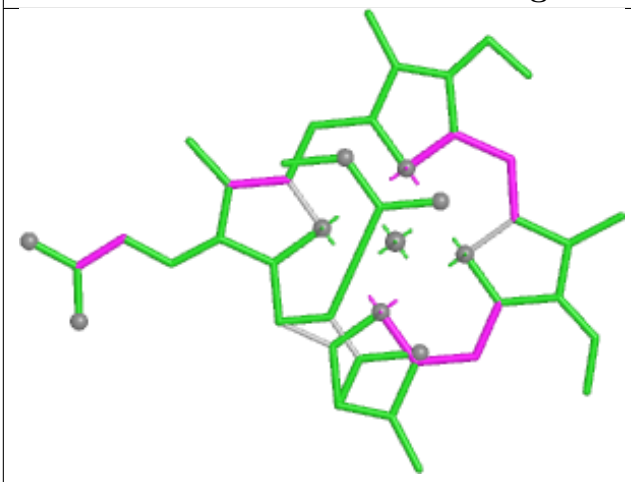


Rings

Ligand KC2 8 314



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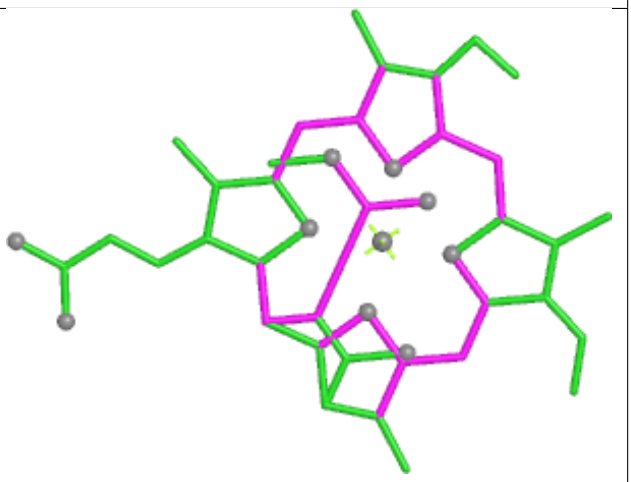

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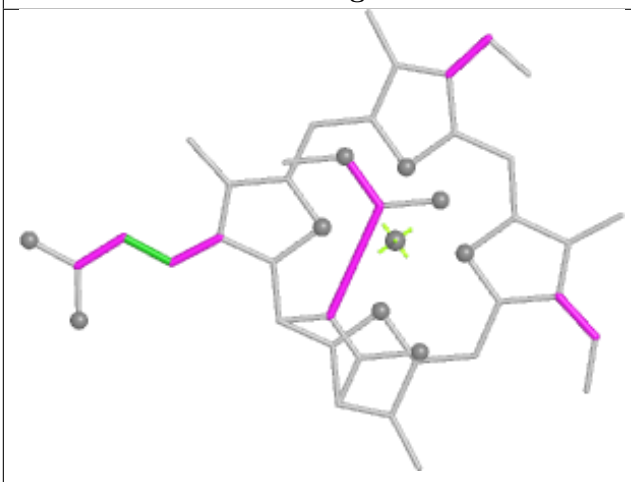

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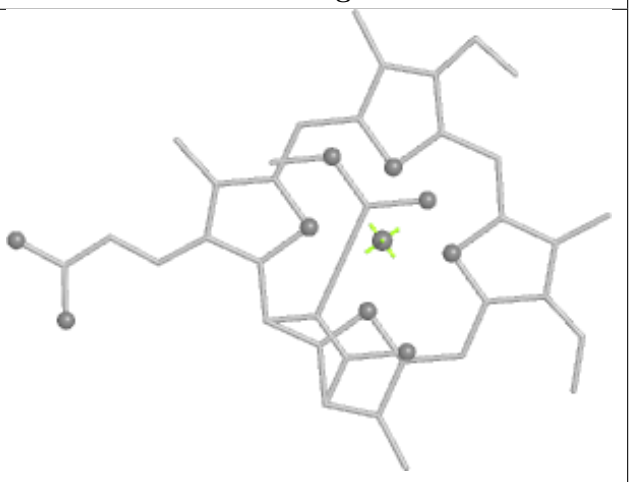
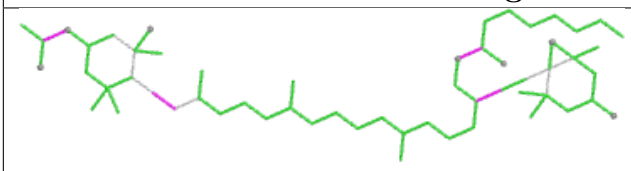


Rings

Ligand A1EB4 X 305



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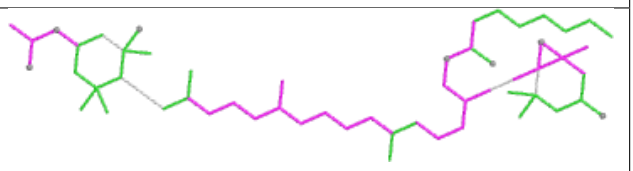

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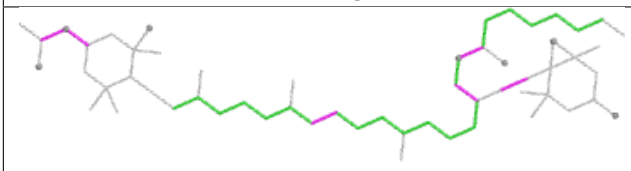

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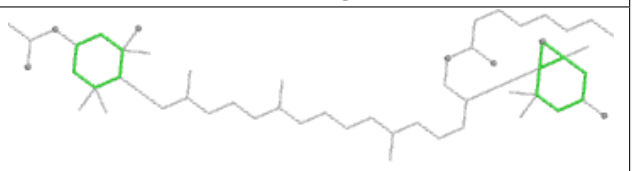
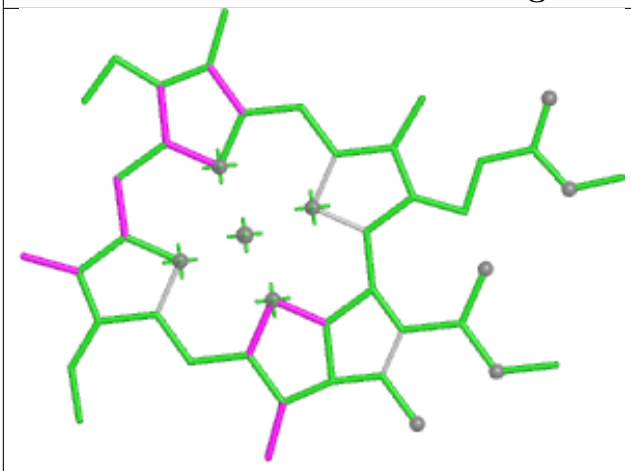


Rings

Ligand CLA 7 318



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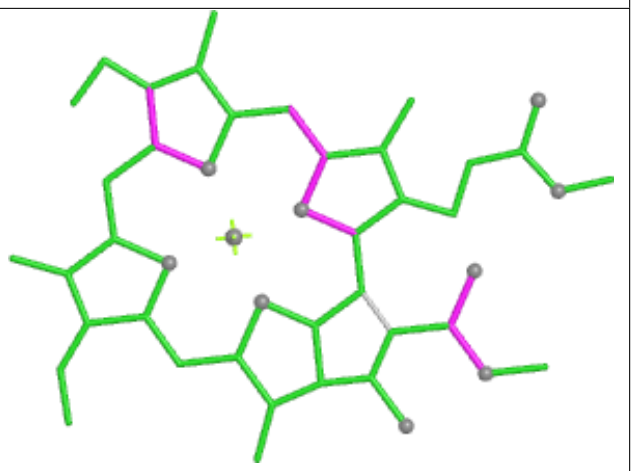

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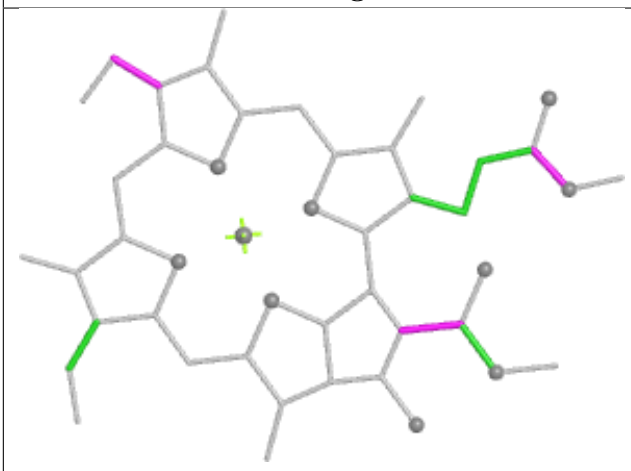
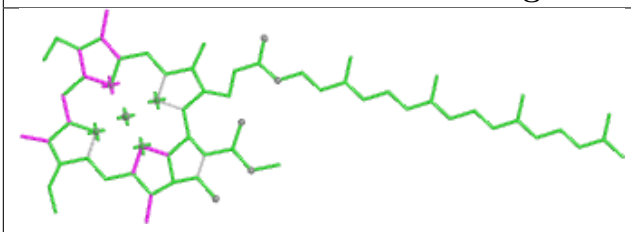


Torsions

Rings

Ligand CLA G 310



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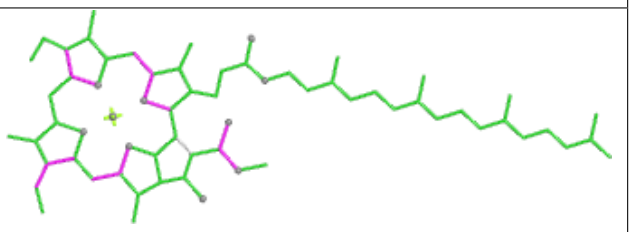
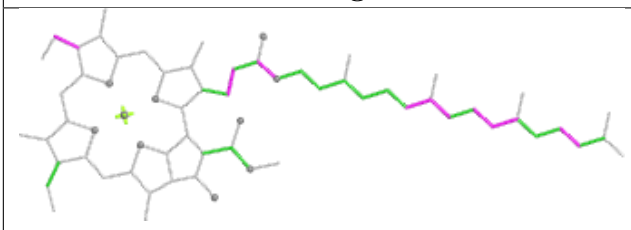


Bond angles



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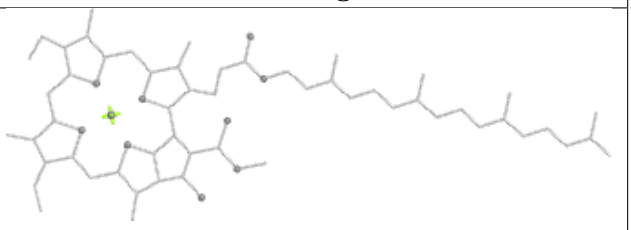
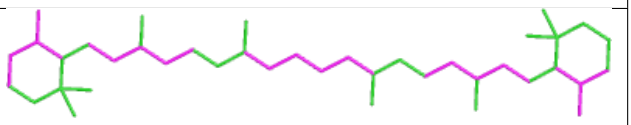


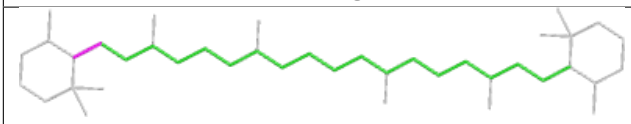
Rings

Ligand BCR l 207

Bond lengths



Bond angles



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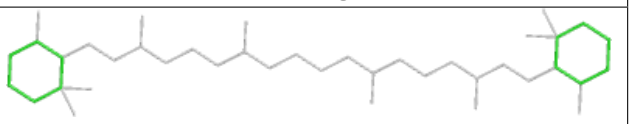
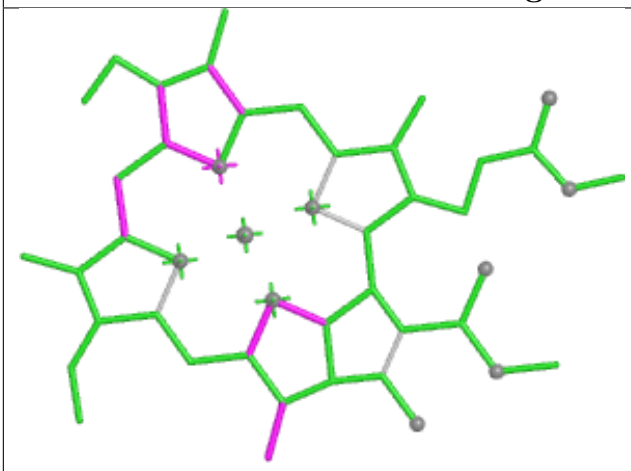
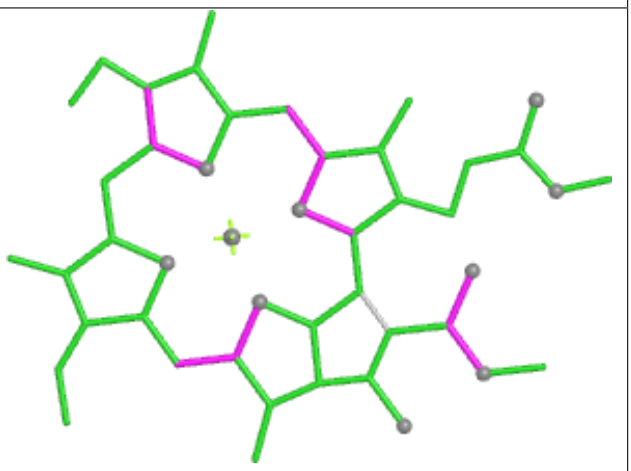


Rings

Ligand CLA E 318	
	
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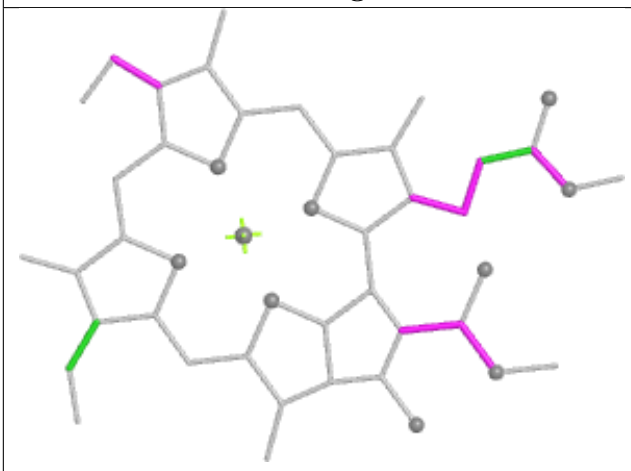
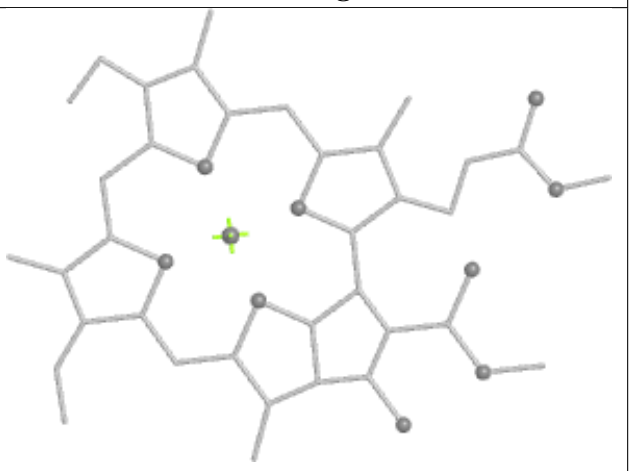
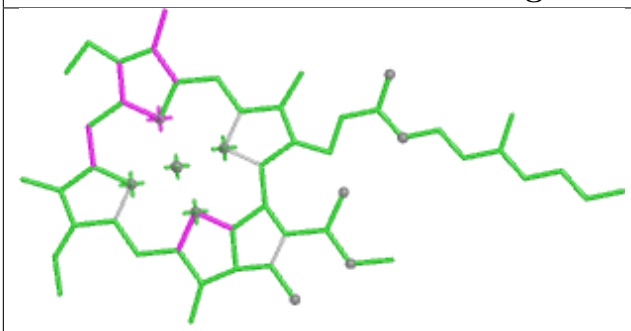
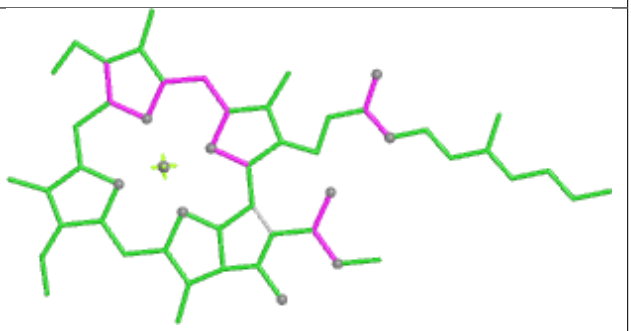
	
Torsions	**Rings**

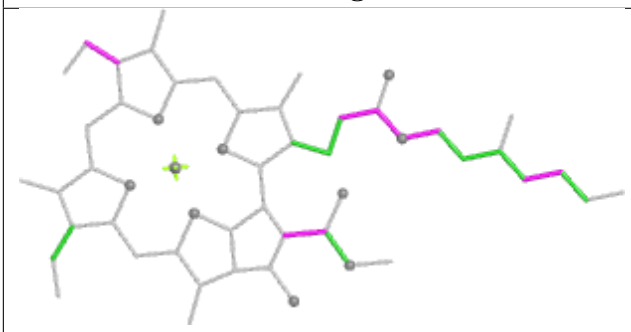
Ligand CLA E 309



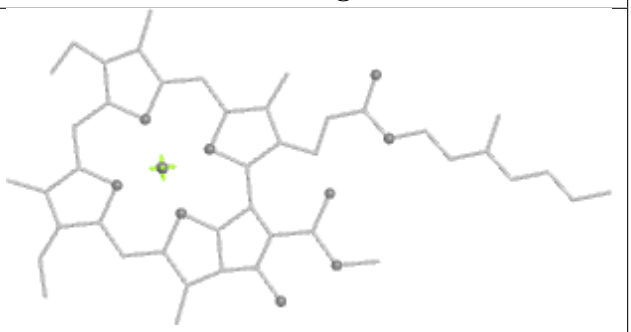
Bond lengths



Bond angles

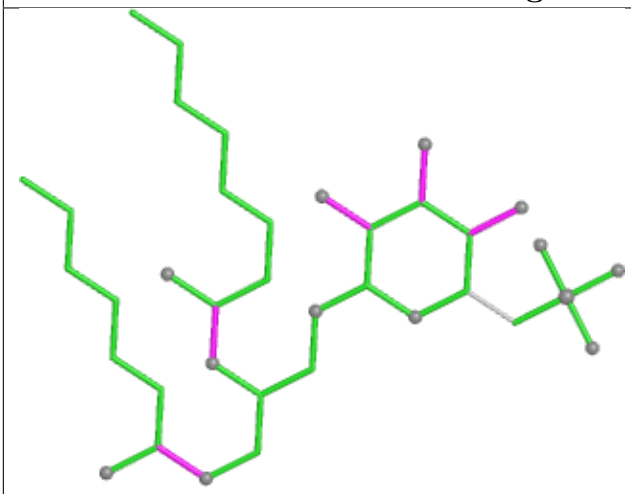


Torsions



Rings

Ligand SQD F 319



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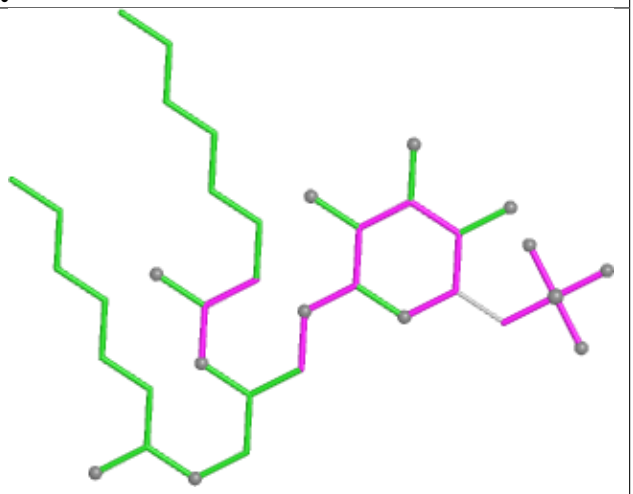
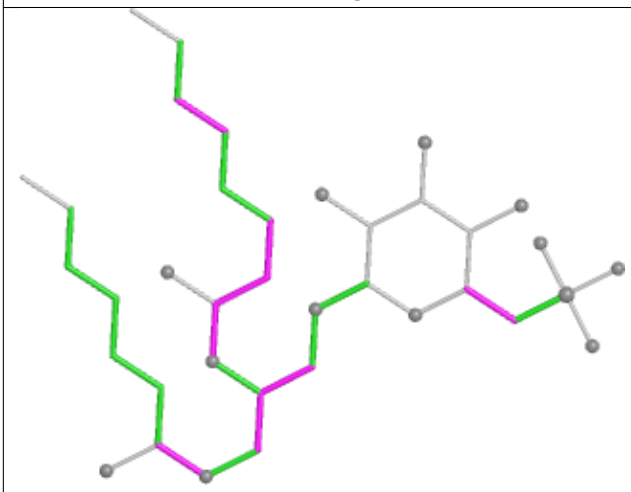


Bond angles



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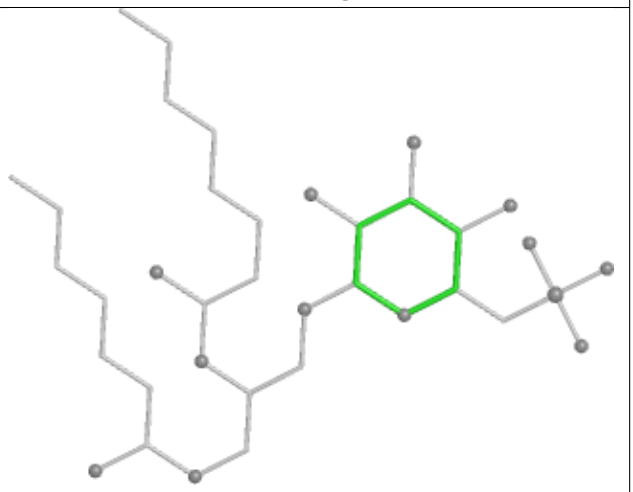
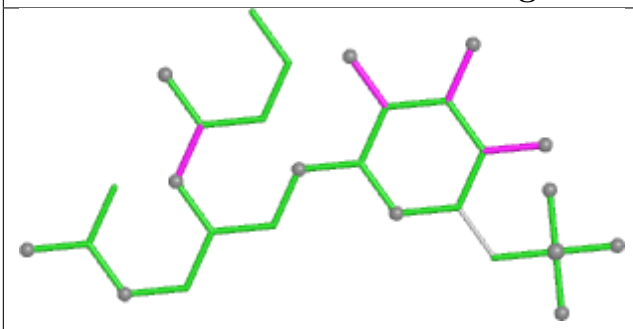


Rings

Ligand SQD W 301



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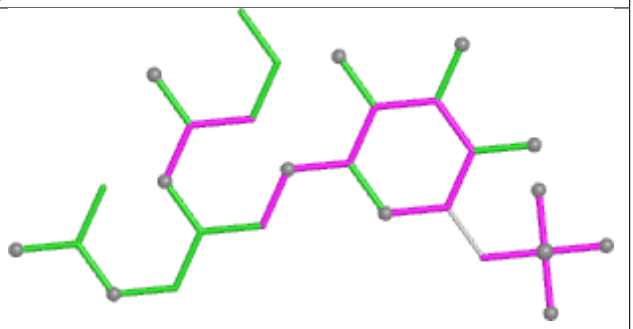
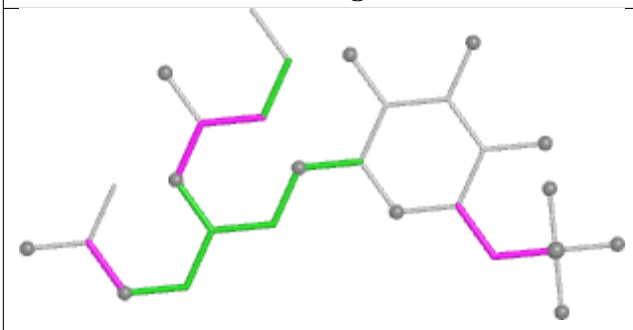


Bond angles



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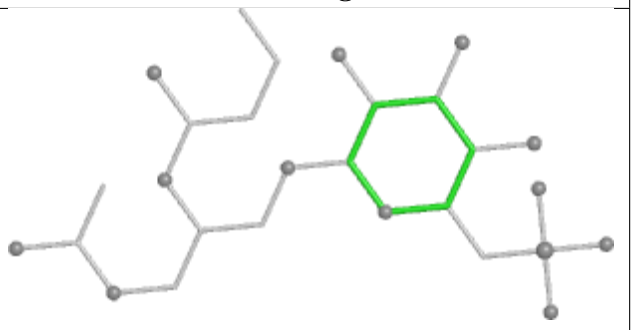
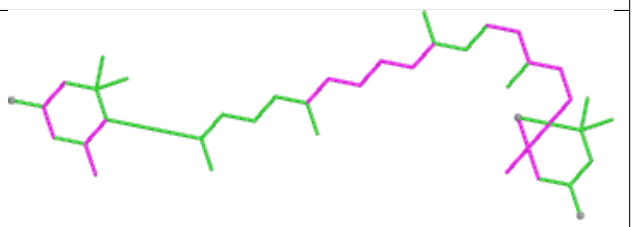


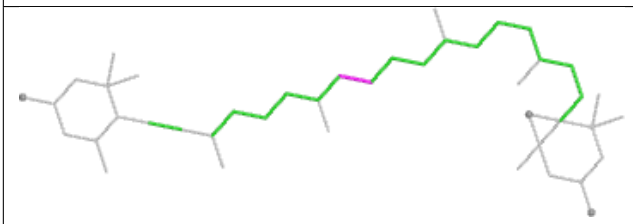
Rings

Ligand DD6 E 303

Bond lengths



Bond angles



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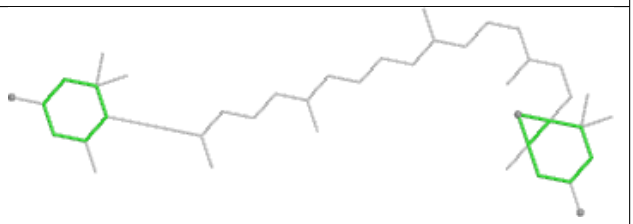
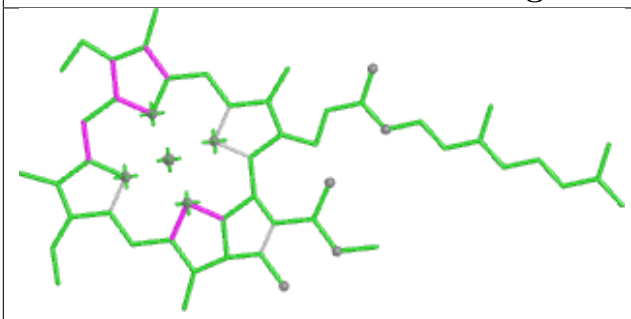
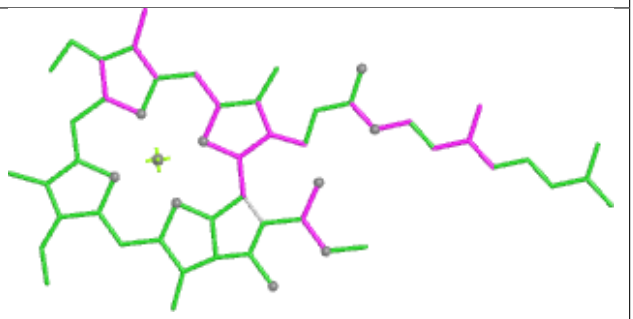


Rings

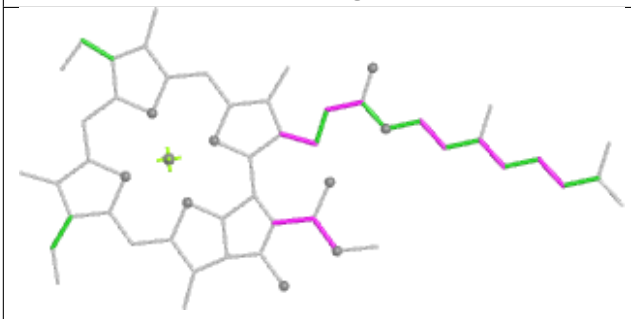
Ligand CLA F 314



Bond lengths



Bond angles



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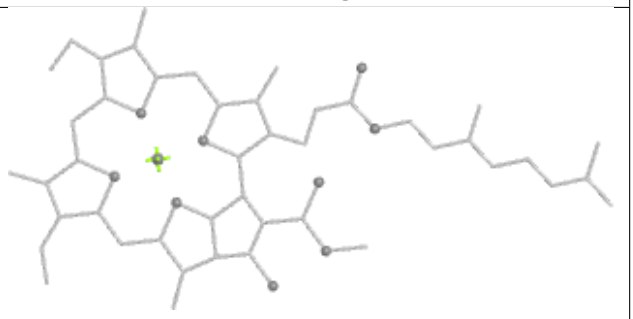
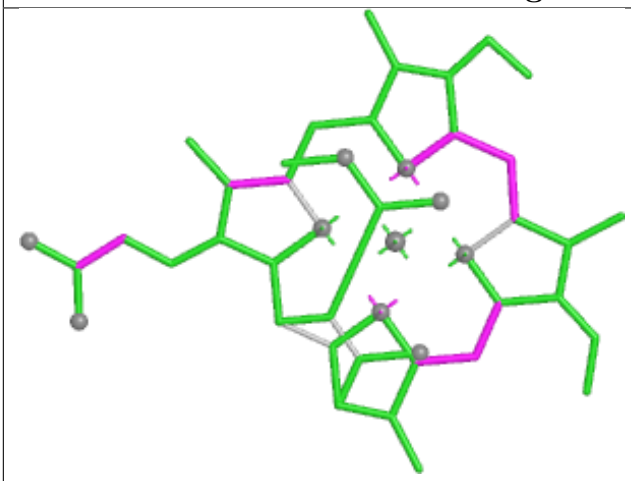
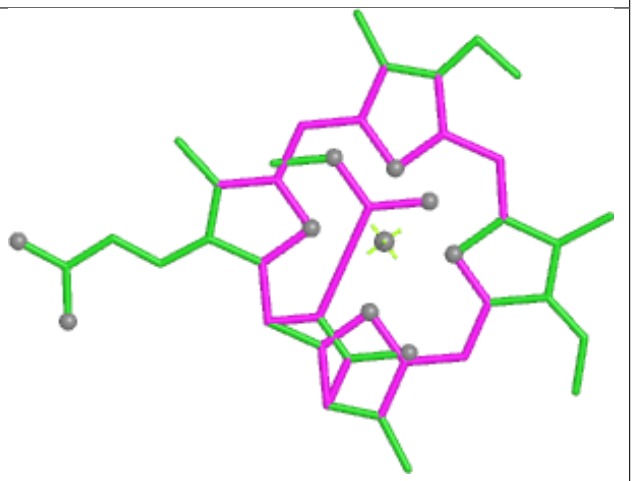


Rings

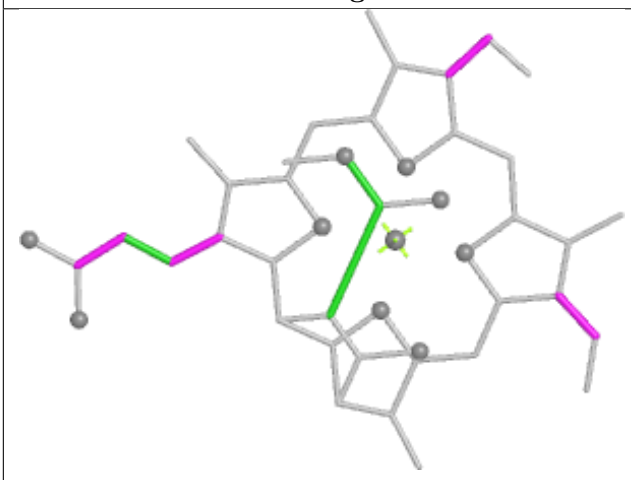
Ligand KC2 Y 309



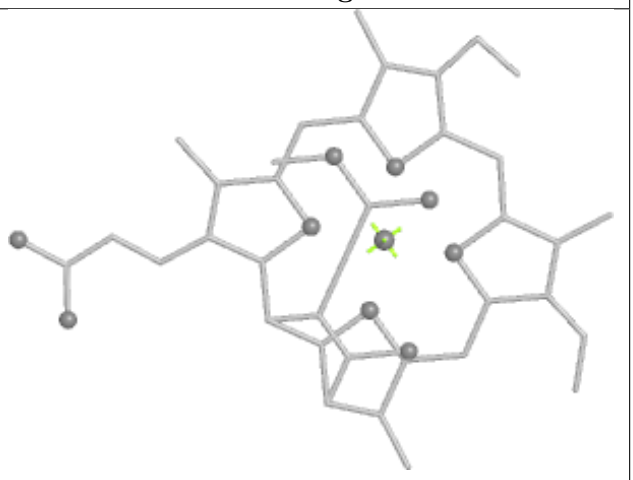
Bond lengths



Bond angles

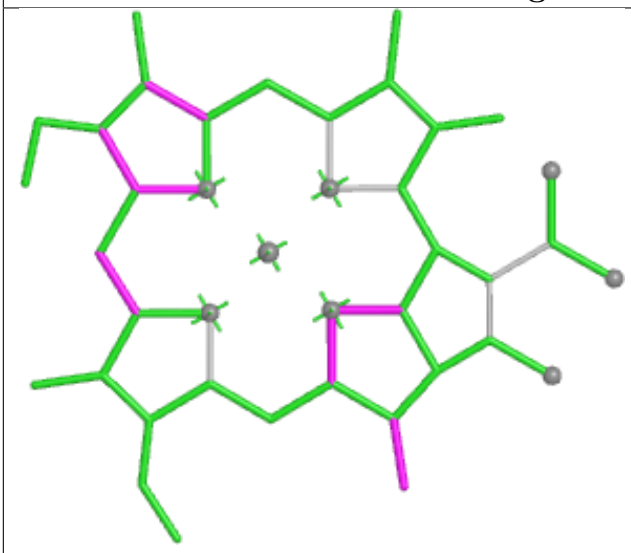


Torsions



Rings

Ligand CLA 6 311



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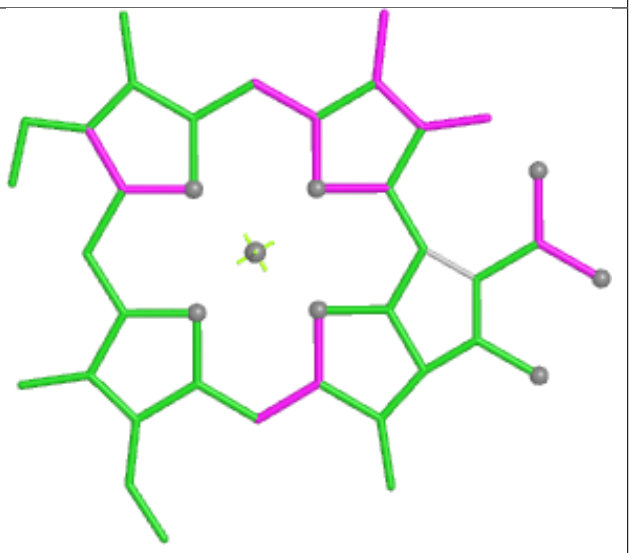
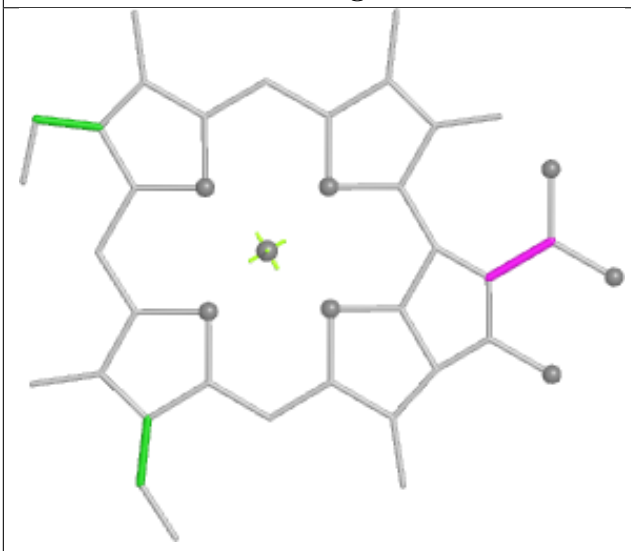


Bond angles



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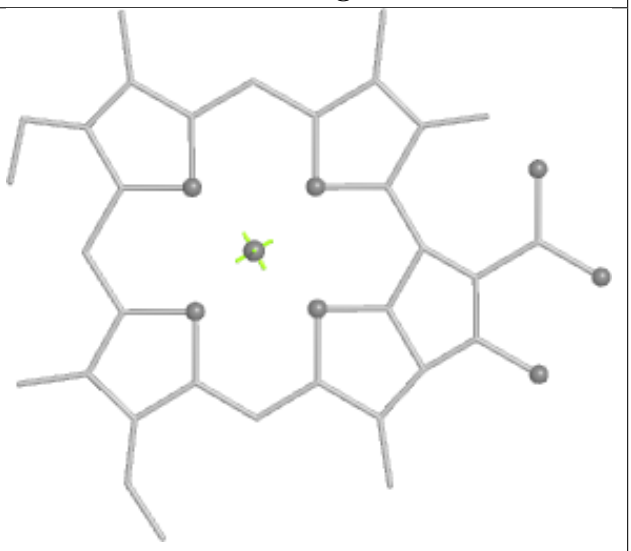
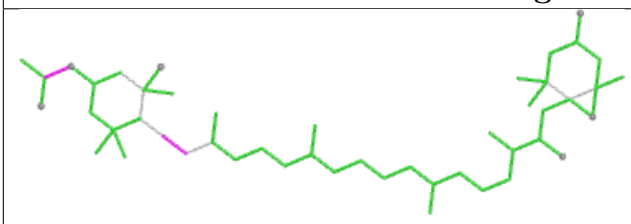


Rings

Ligand A86 7 312



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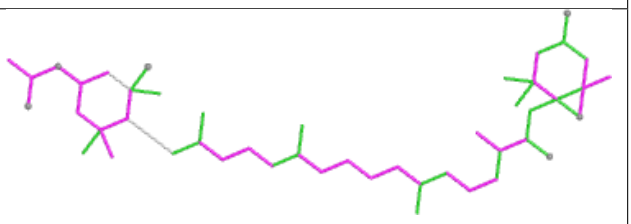

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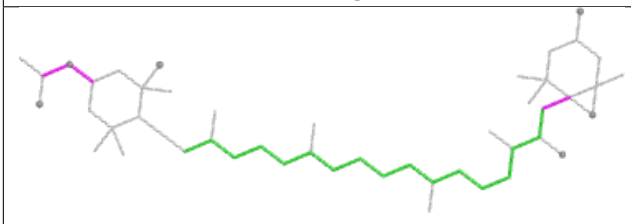

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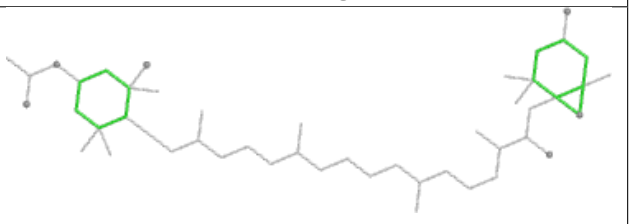
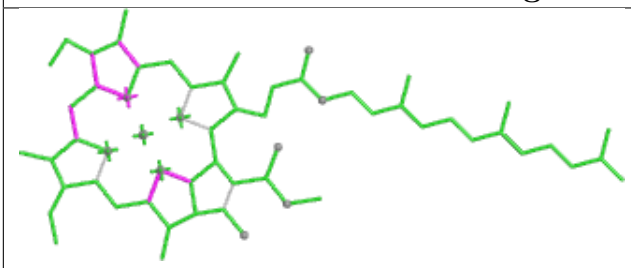


Rings

Ligand CLA U 211



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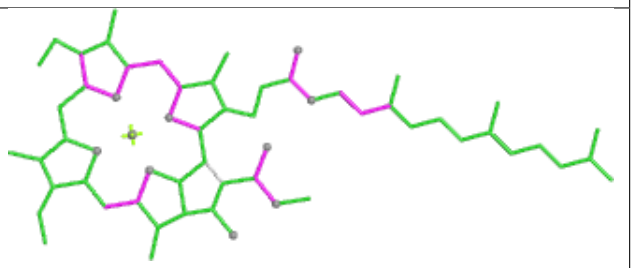

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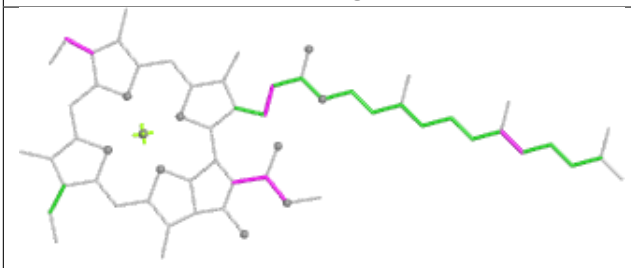

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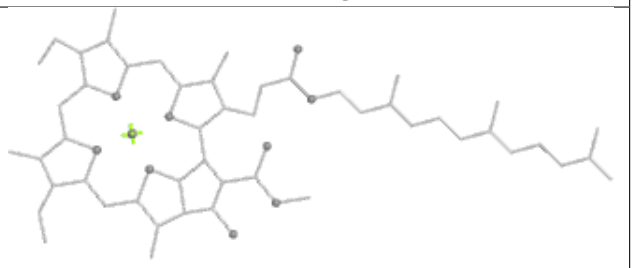
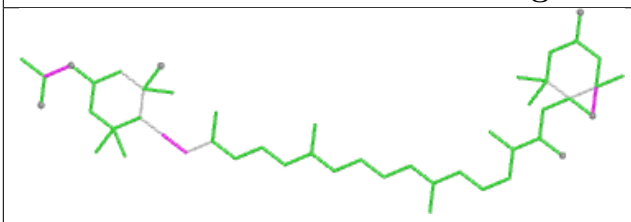


Rings

Ligand A86 E 304



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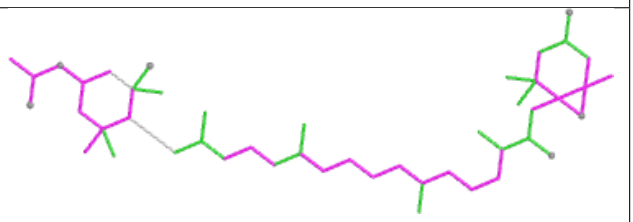

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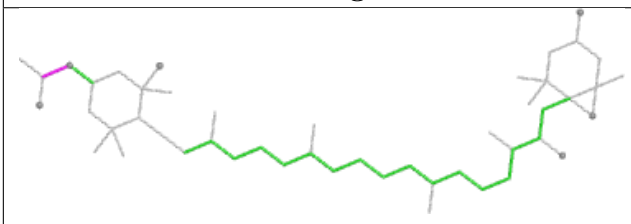

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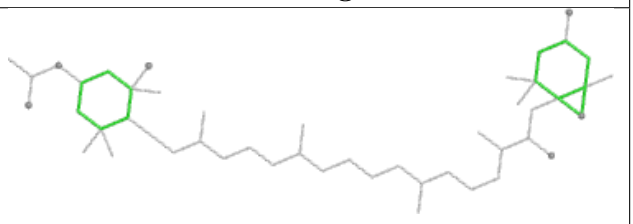
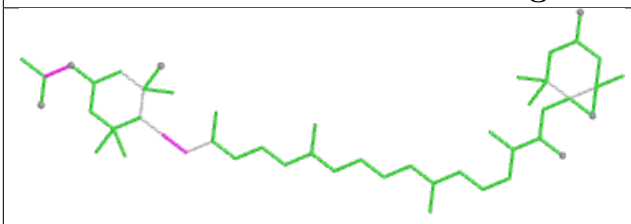


Rings

Ligand A86 R 317



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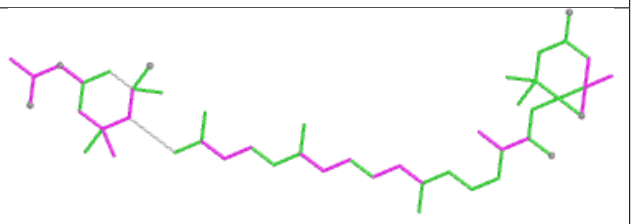
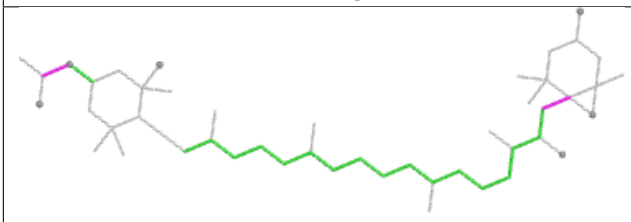


Bond angles



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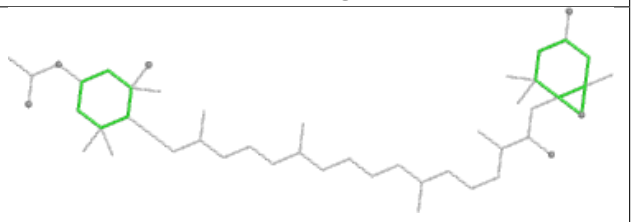
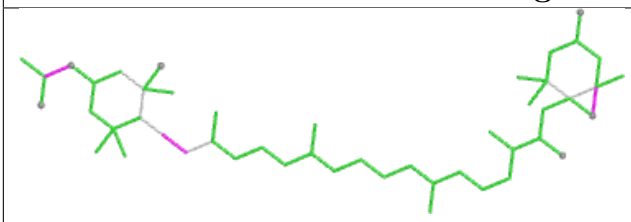


Rings

Ligand A86 9 301



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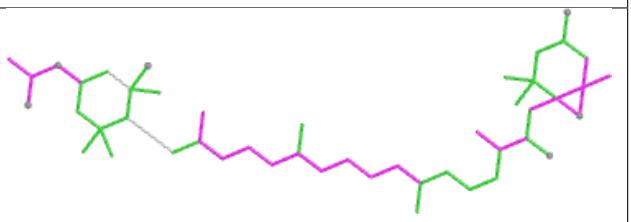
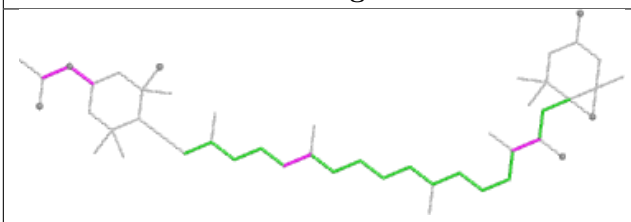


Bond angles



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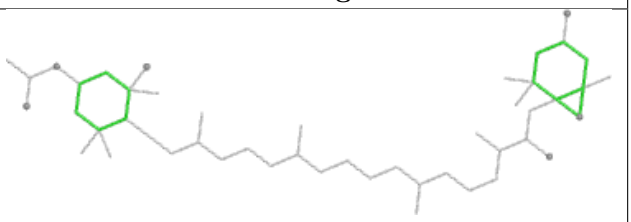
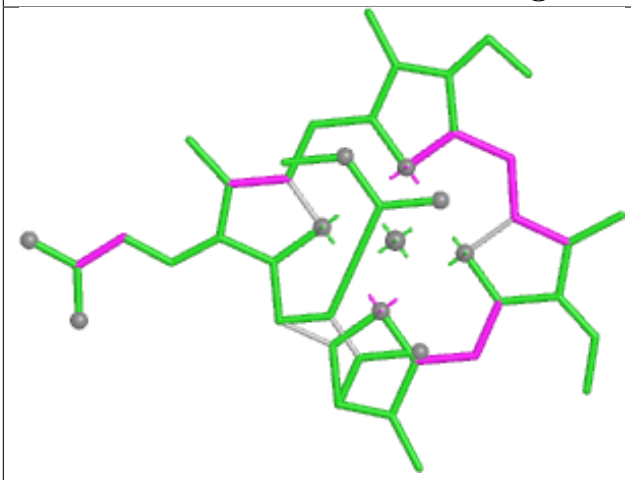


Rings

Ligand KC2 3 315



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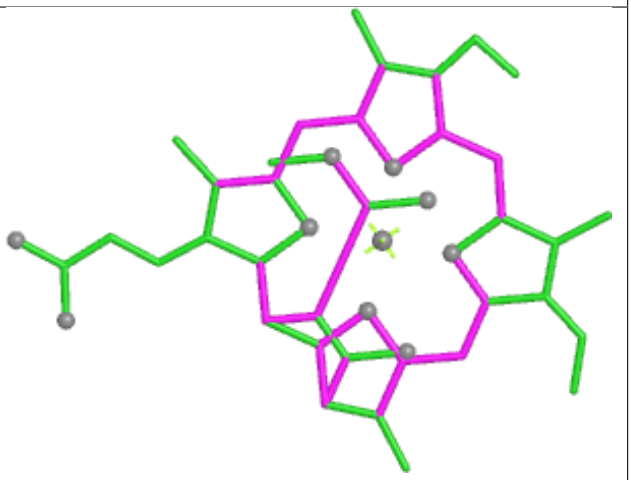

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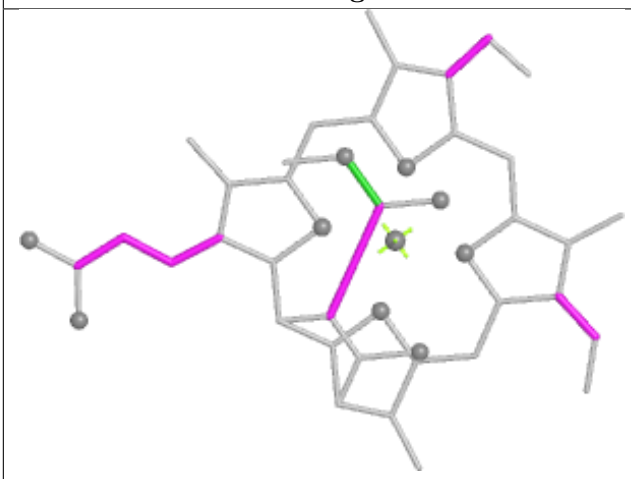

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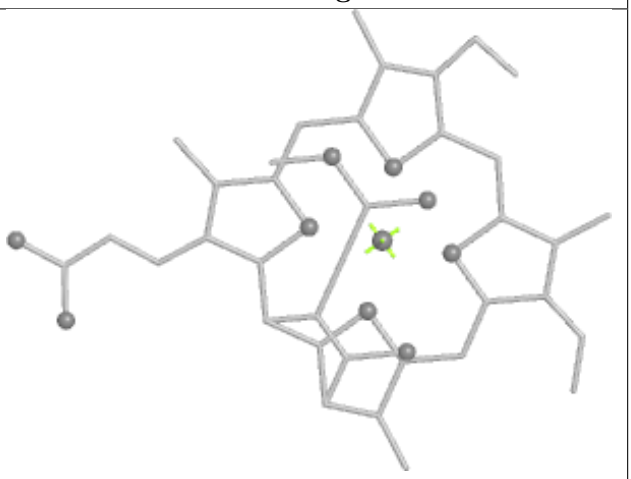
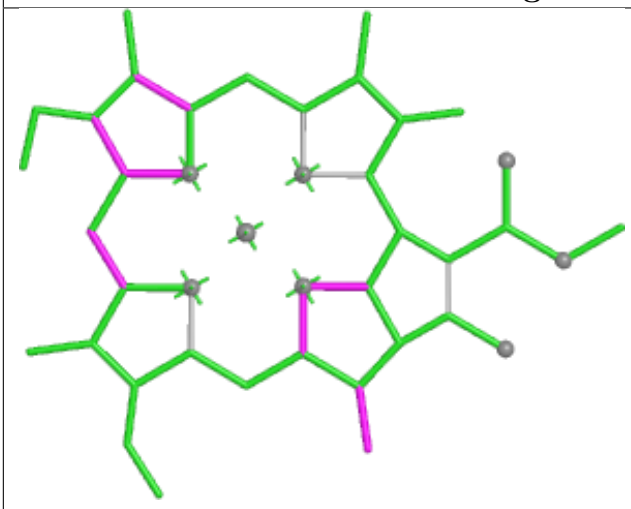


Rings

Ligand CLA U 213



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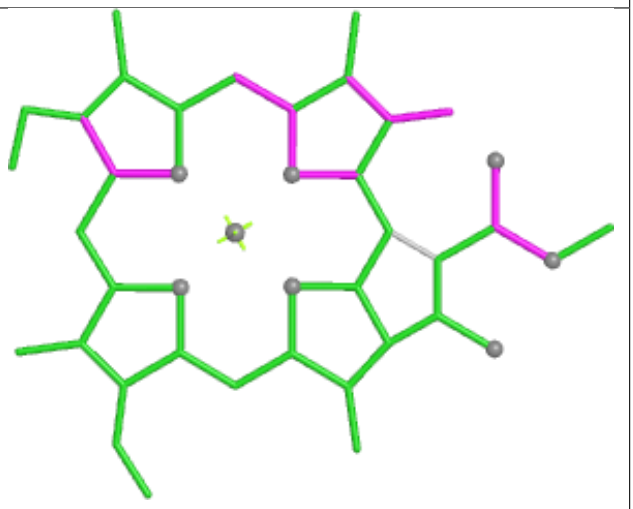
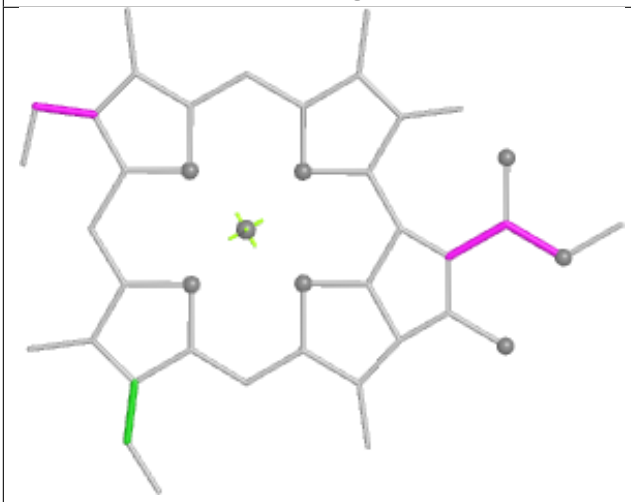


Bond angles



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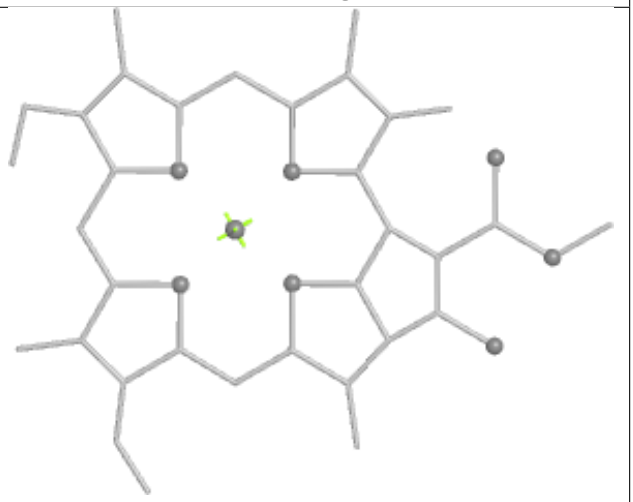
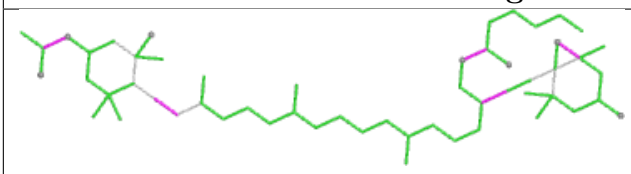


Rings

Ligand A1EB4 T 304



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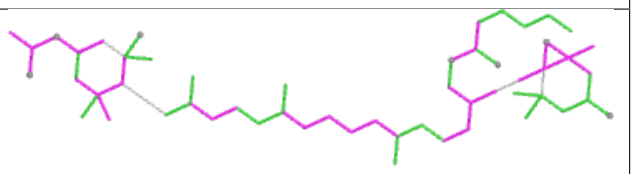

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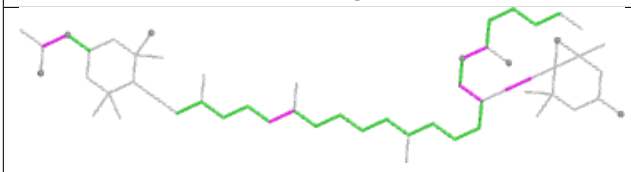

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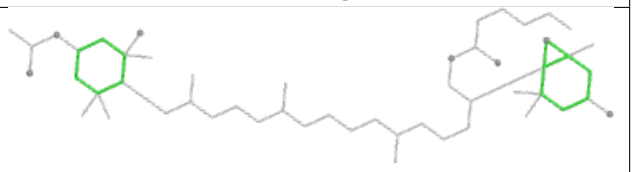
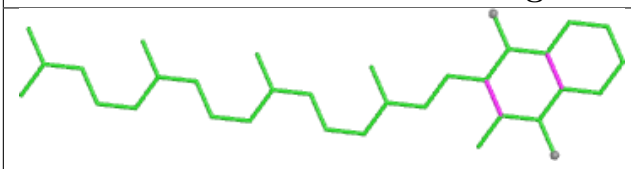


Rings

Ligand PQN a 839



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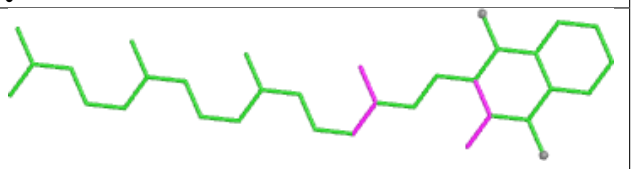
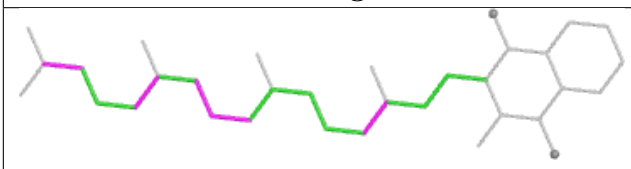


Bond angles



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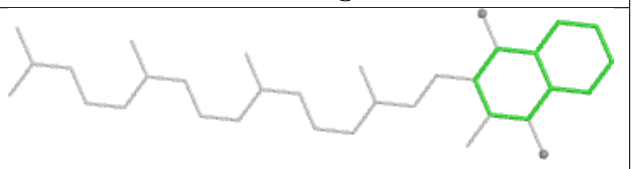
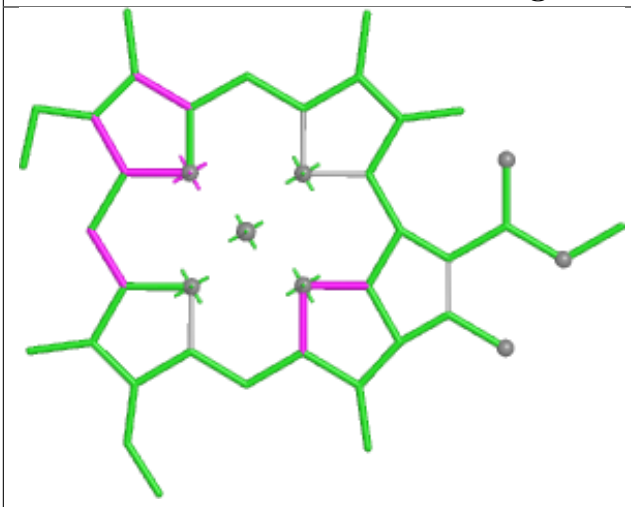


Rings

Ligand CLA z 306



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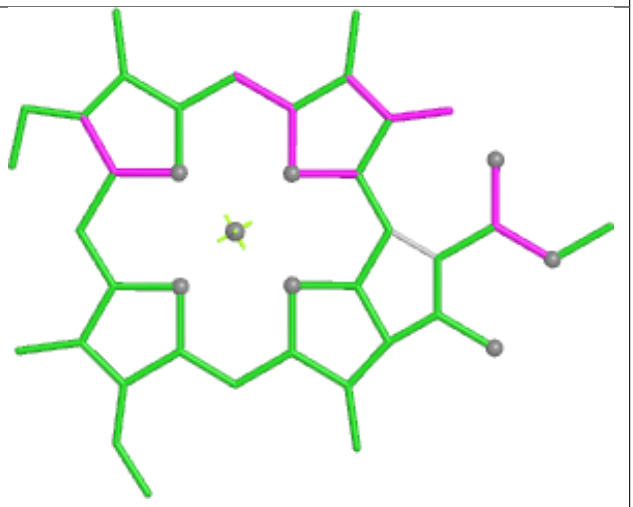
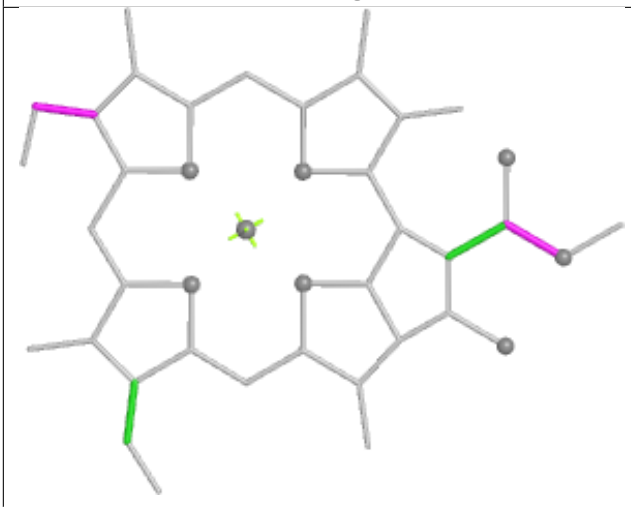
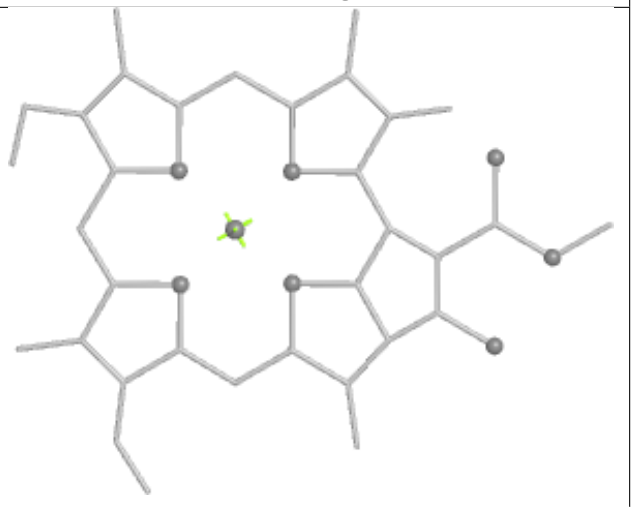


Bond angles

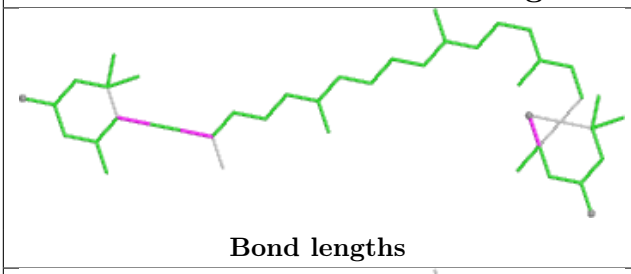


Torsions



Rings

Ligand DD6 B 202



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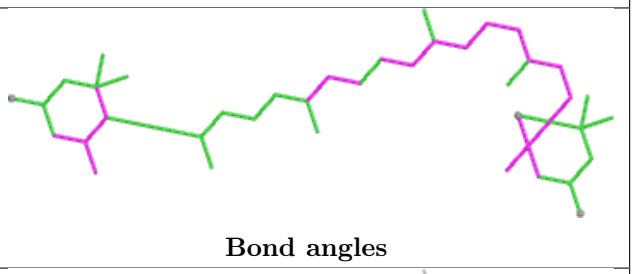
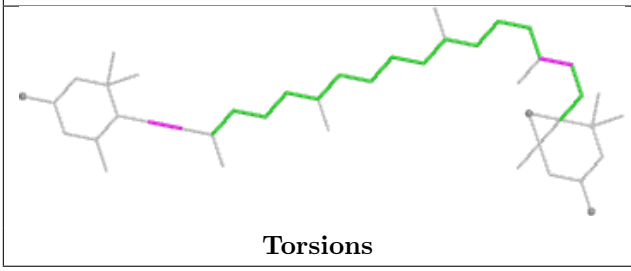
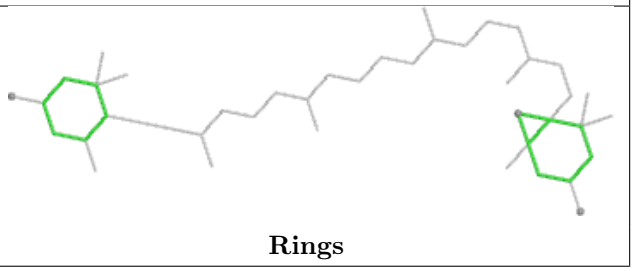


Bond angles

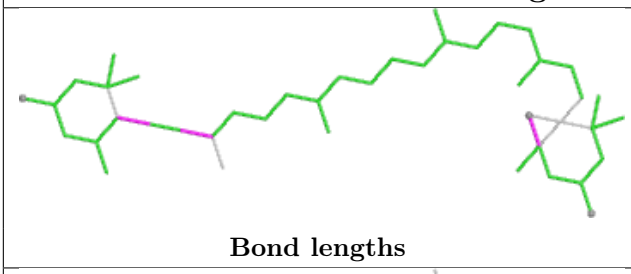


Torsions



Rings

Ligand DD6 3 304



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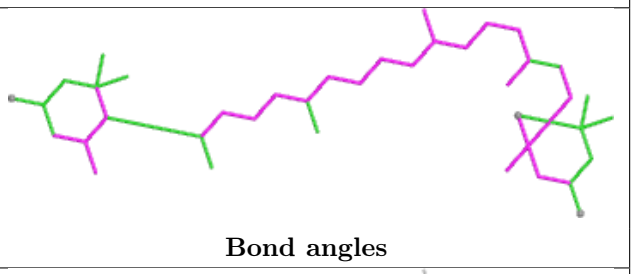
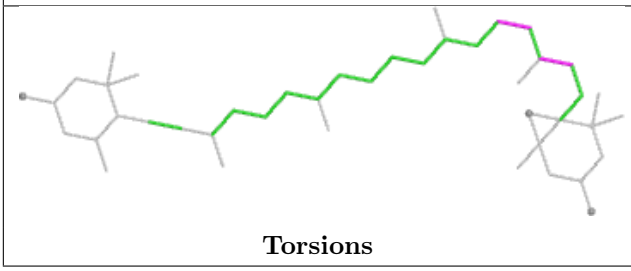
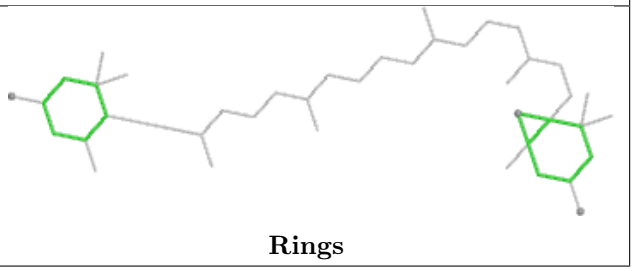


Bond angles

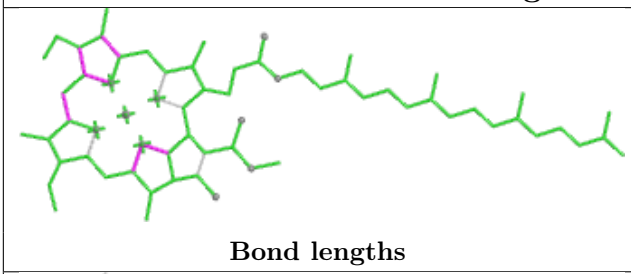


Torsions

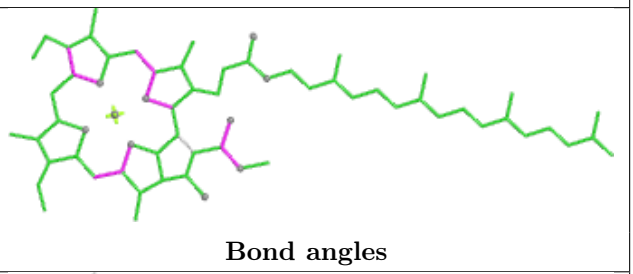


Rings

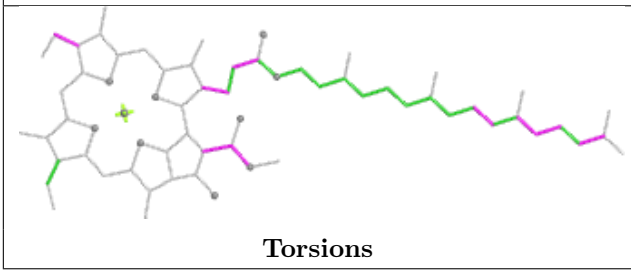
Ligand CLA D 318



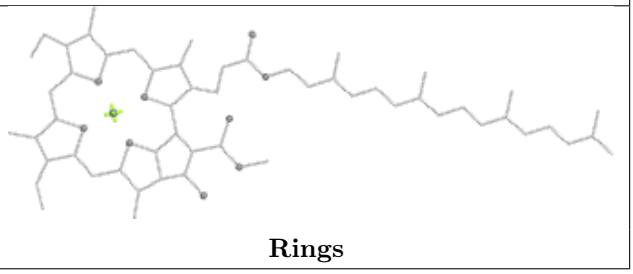
Bond lengths



Bond angles

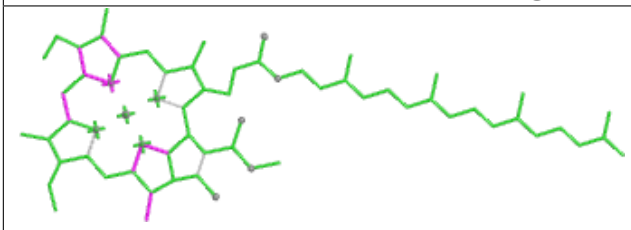


Torsions



Rings

Ligand CLA a 805



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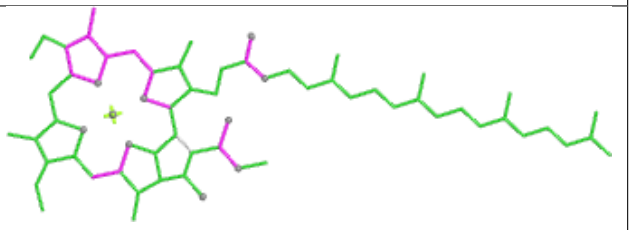
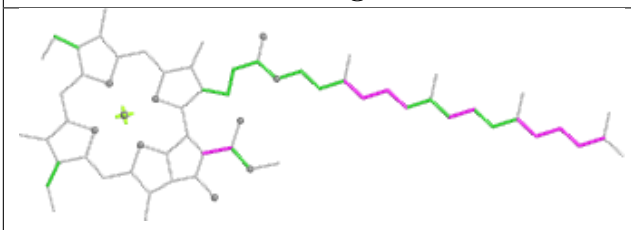
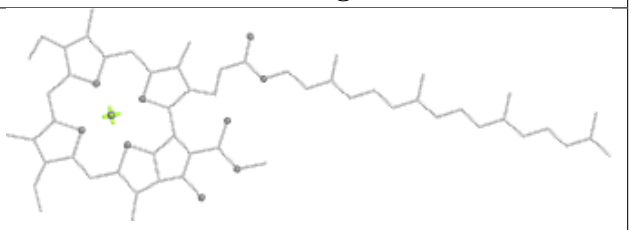


Bond angles



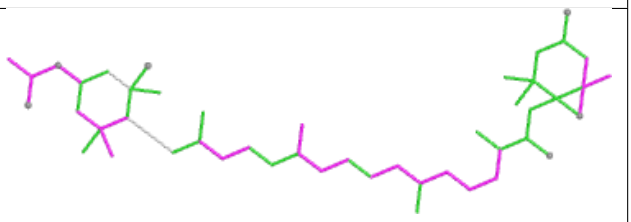
Torsions



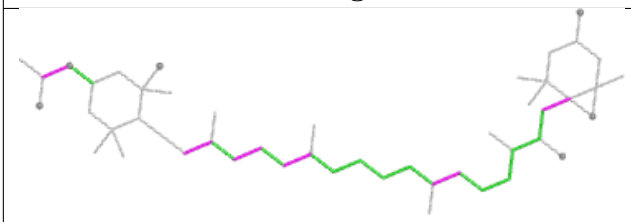
Rings

Ligand A86 R 302

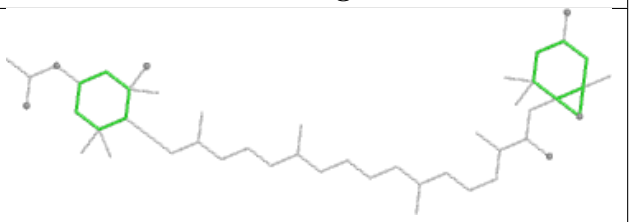
Bond lengths



Bond angles

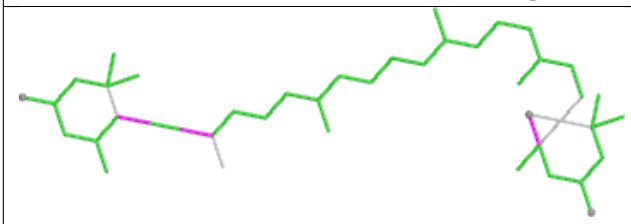


Torsions



Rings

Ligand DD6 G 306



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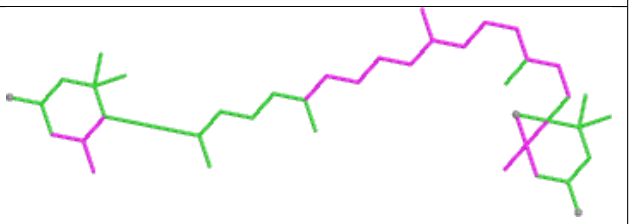
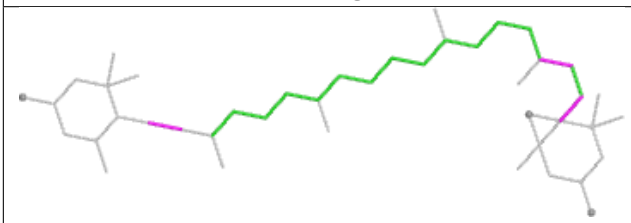
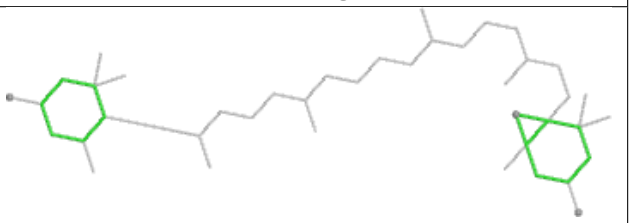


Bond angles

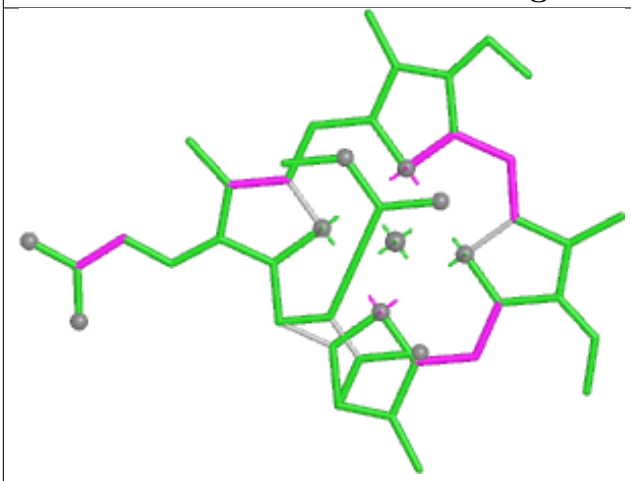


Torsions



Rings

Ligand KC2 8 317



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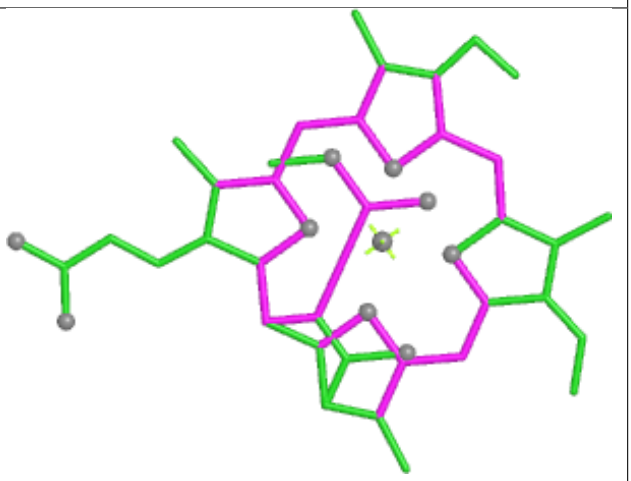
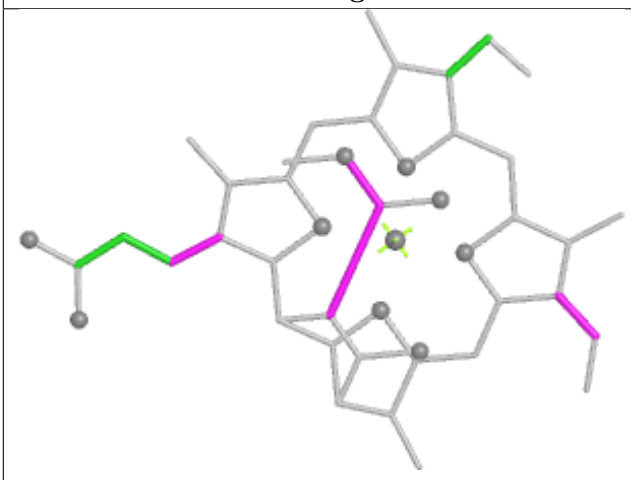


Bond angles



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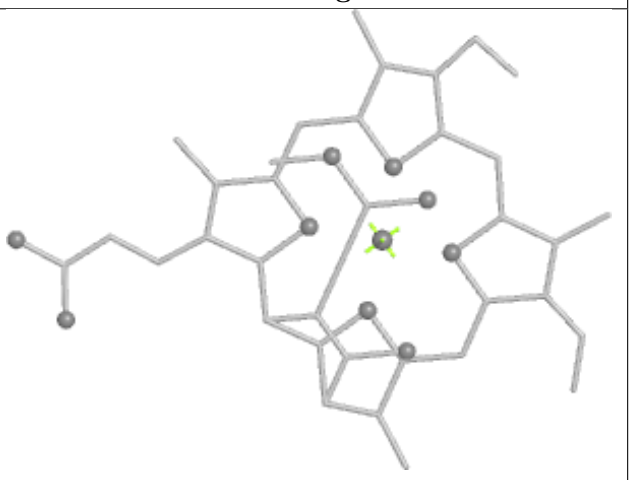
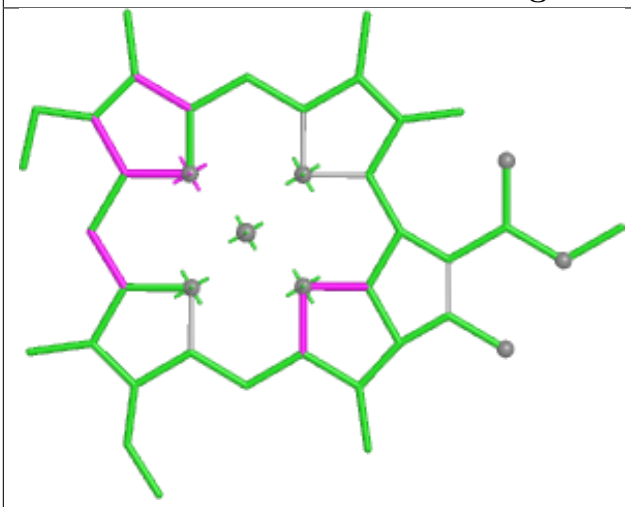
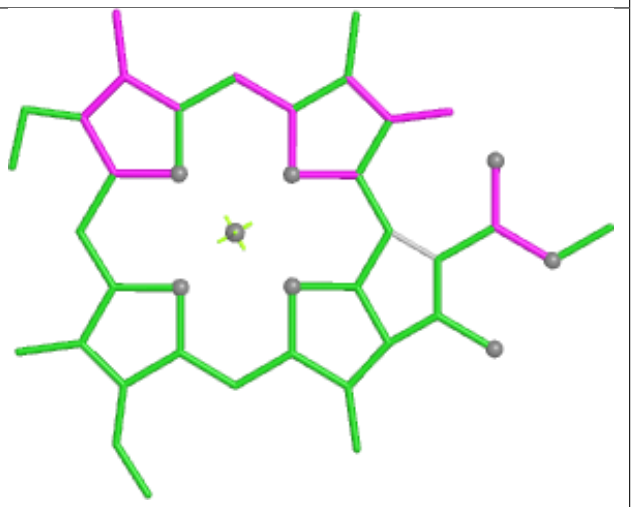


Rings

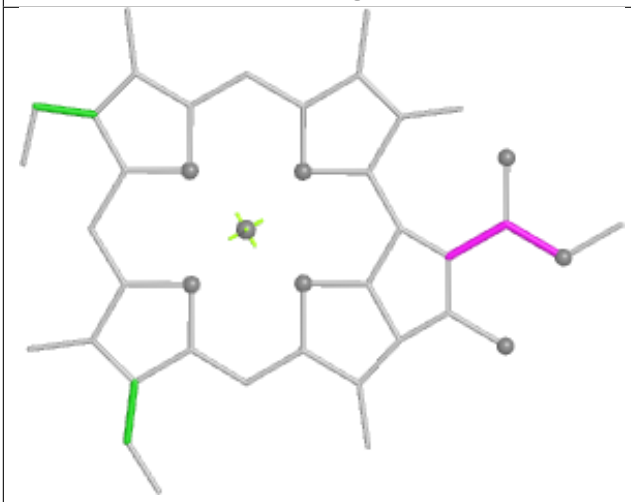
Ligand CLA z 318



Bond lengths



Bond angles



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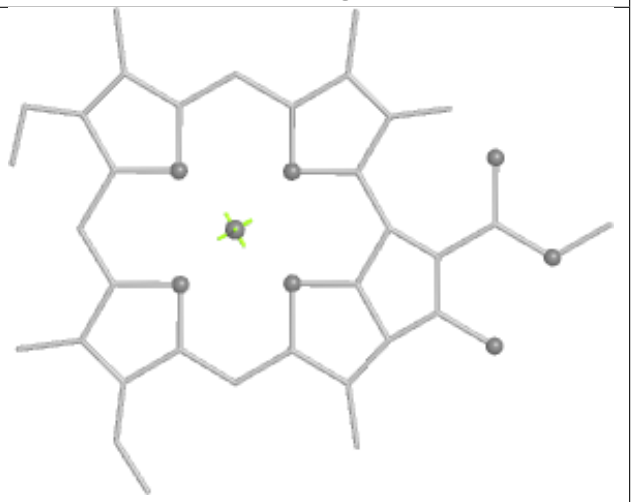
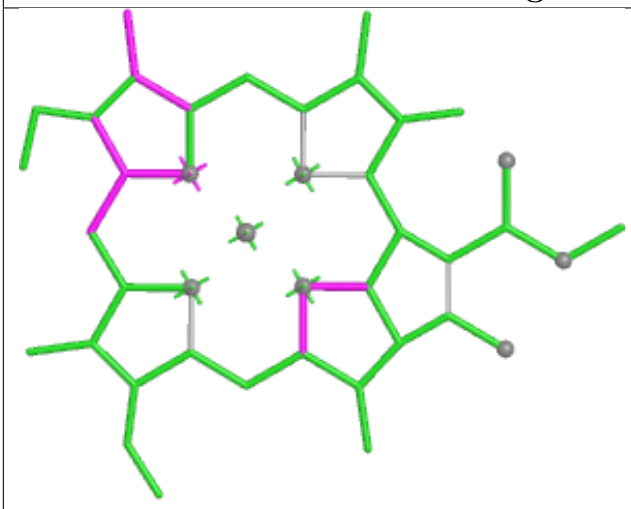
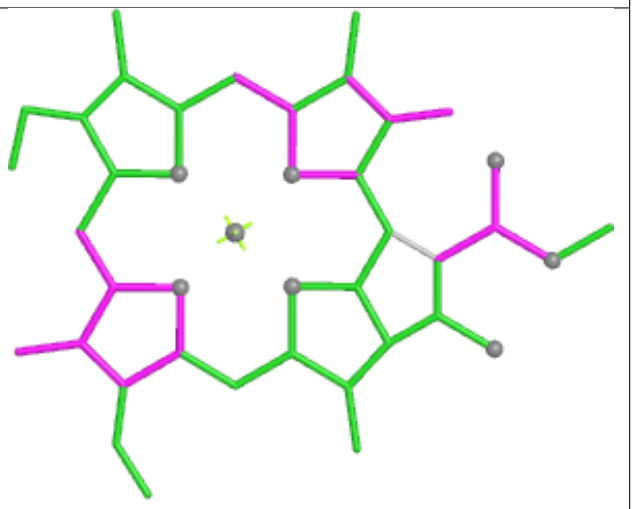


Rings

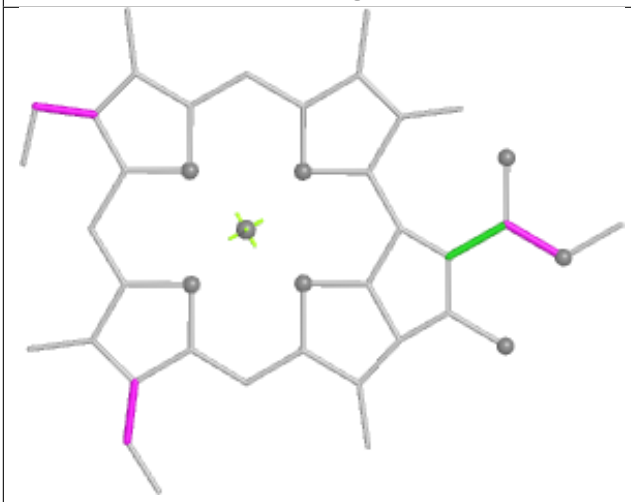
Ligand CLA Z 313



Bond lengths



Bond angles



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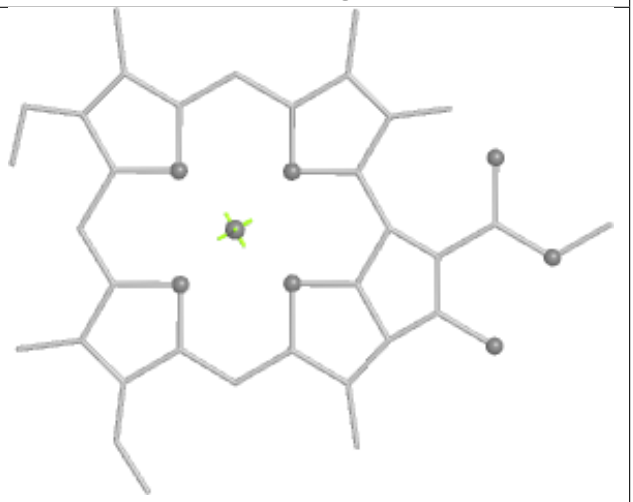
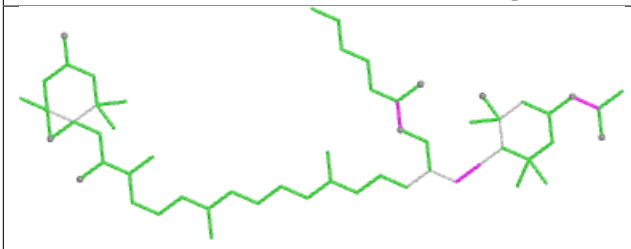


Rings

Ligand A1EB1 T 302



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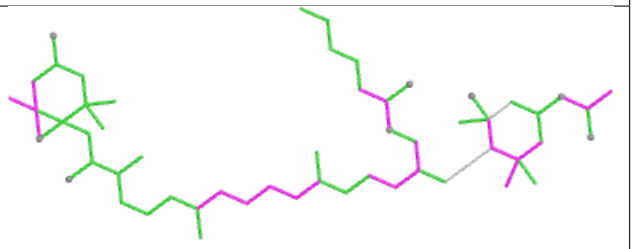
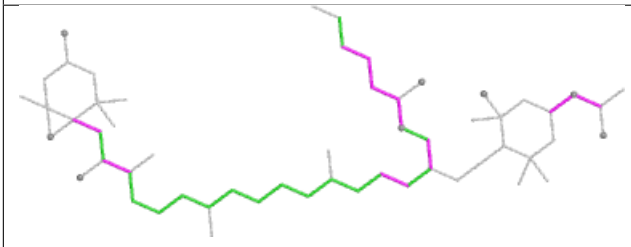


Bond angles



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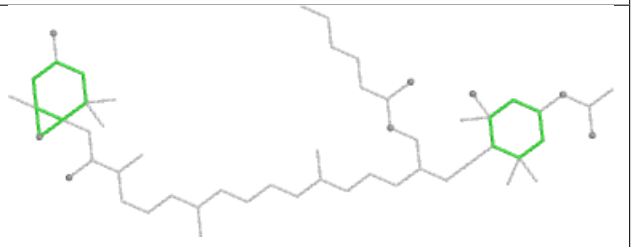
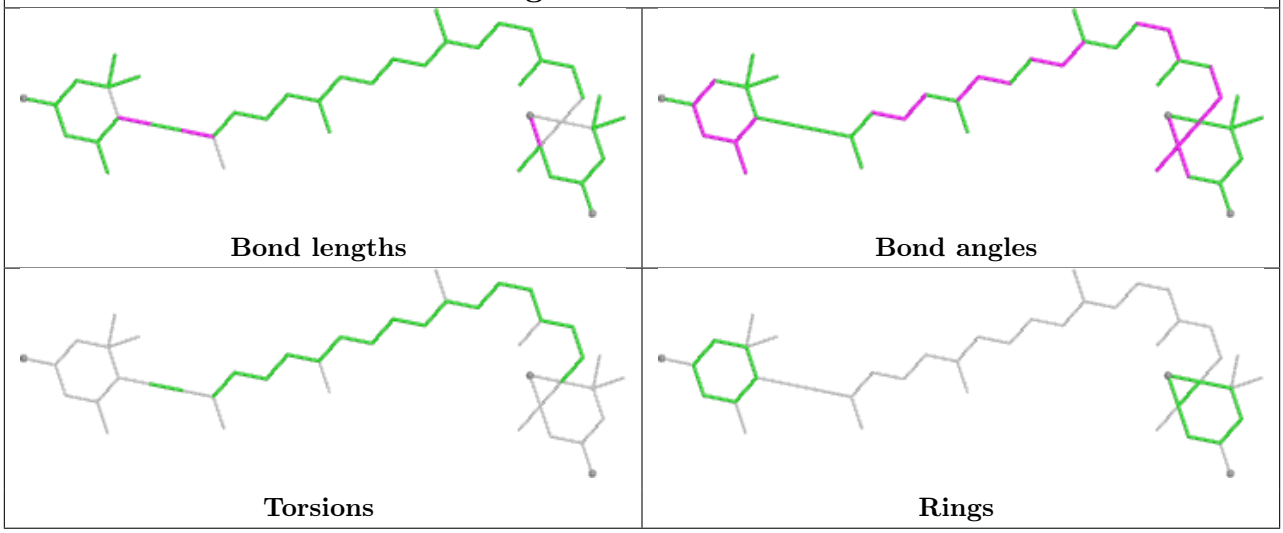
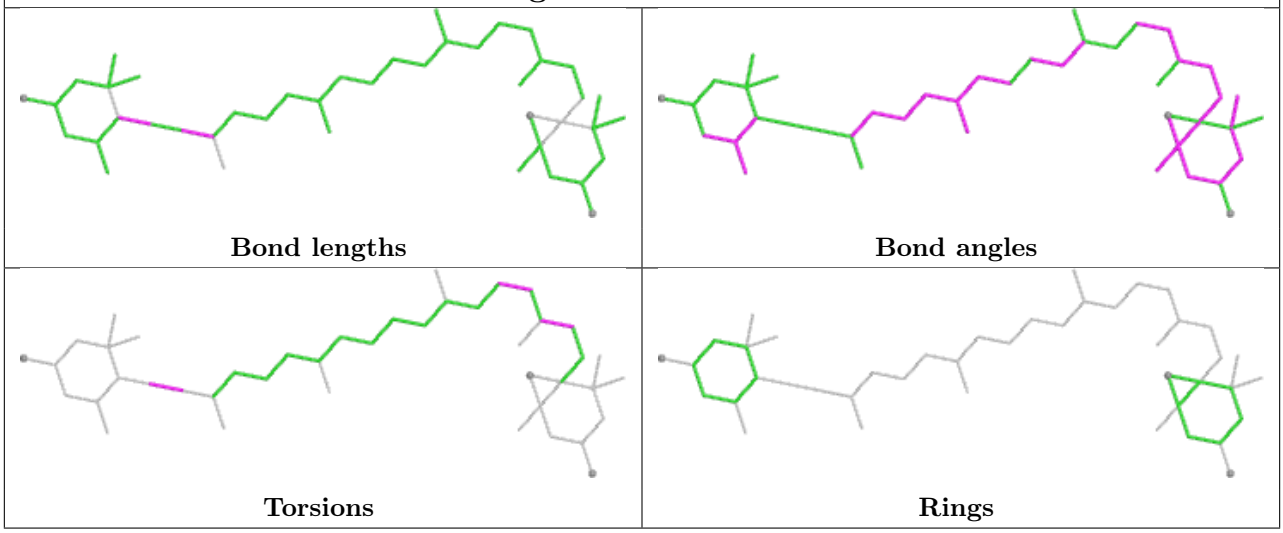


Rings

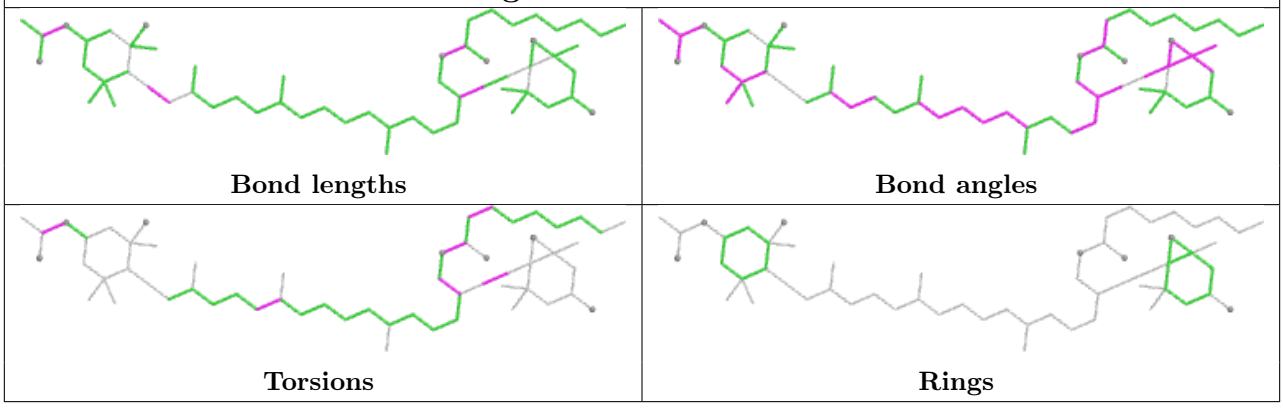
Ligand DD6 A 302



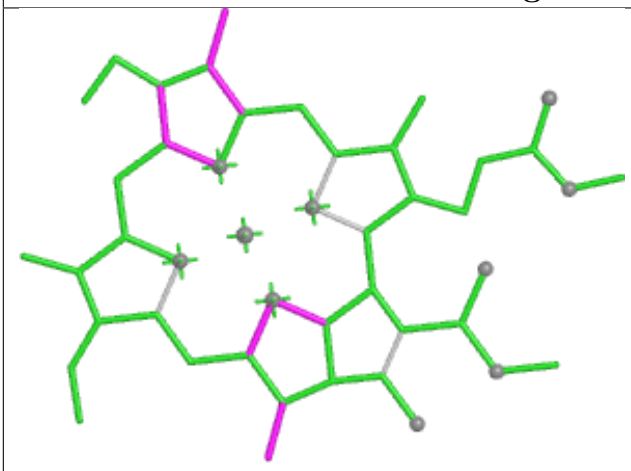
Ligand DD6 S 306



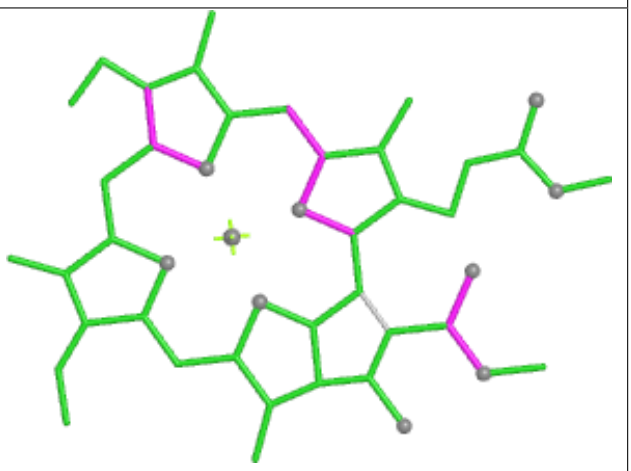
Ligand A1EB4 M 305



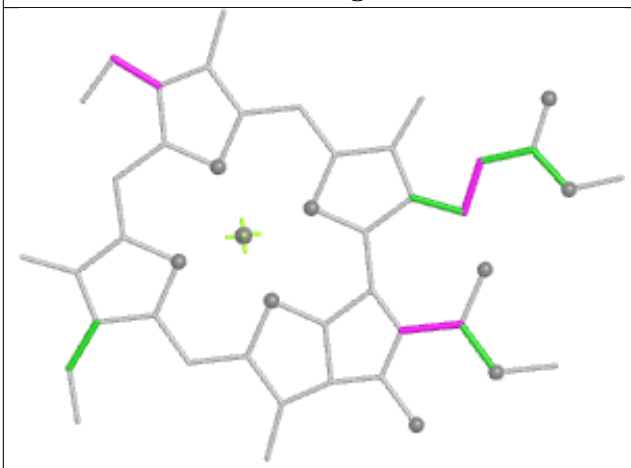
Ligand CLA U 214



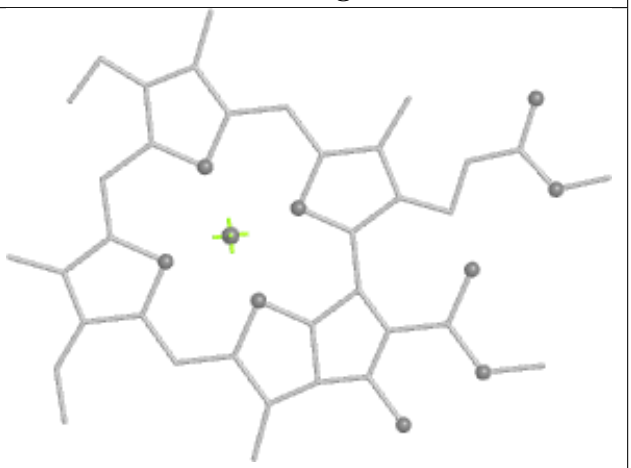
Bond lengths



Bond angles

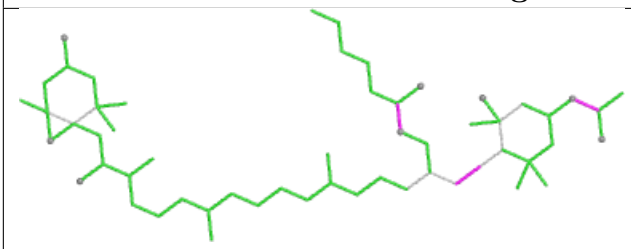


Torsions



Rings

Ligand A1EB1 z 302



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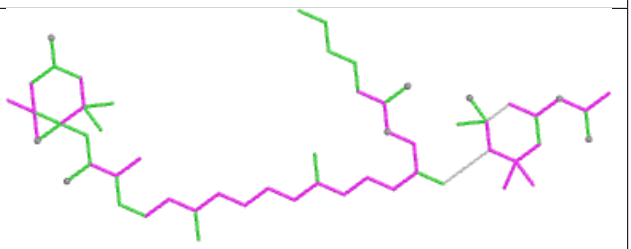
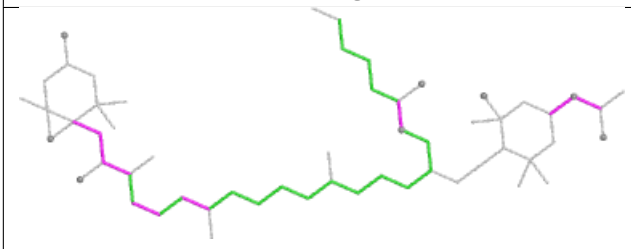
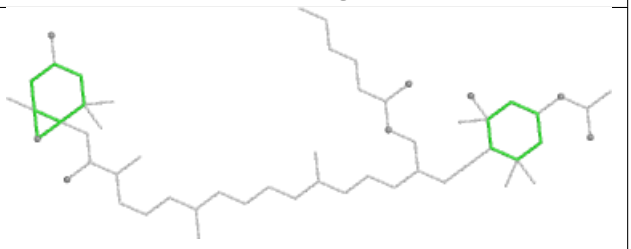


Bond angles

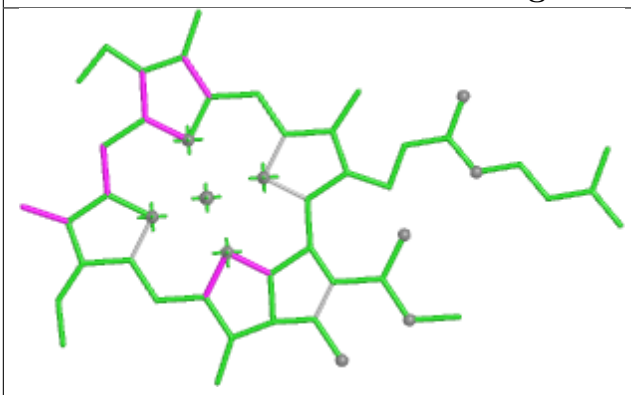


Torsions

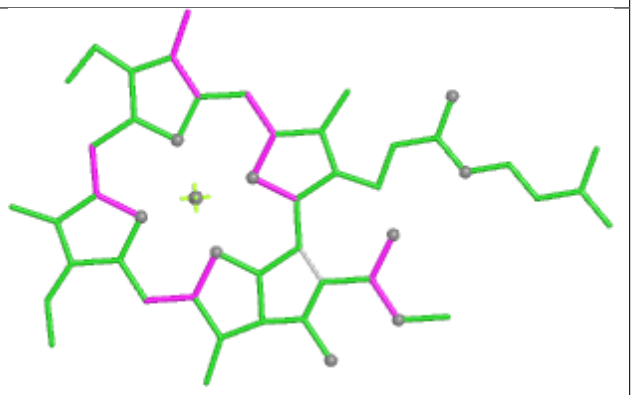


Rings

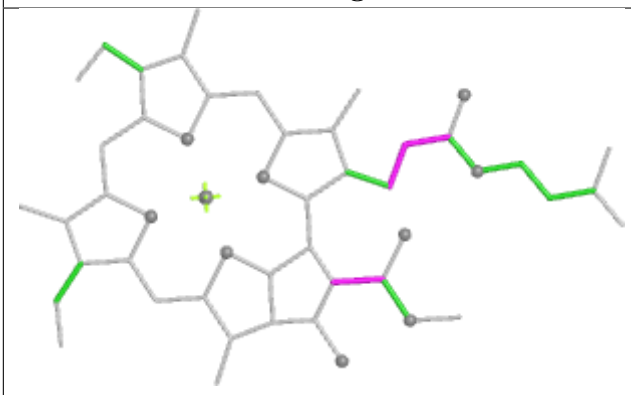
Ligand CLA a 813



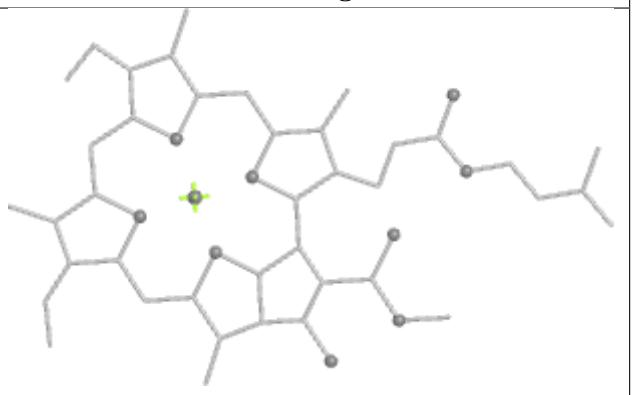
Bond lengths



Bond angles

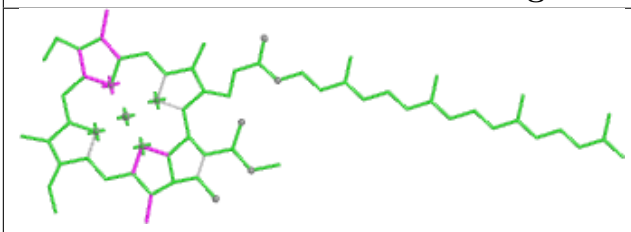


Torsions

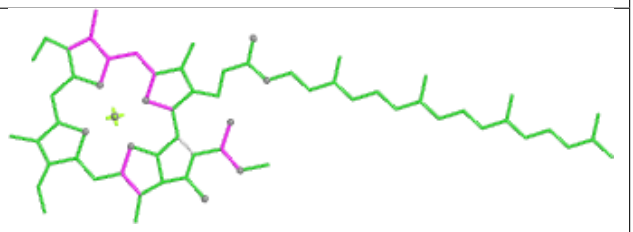


Rings

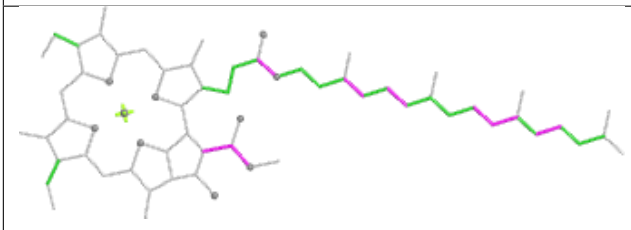
Ligand CLA b 830



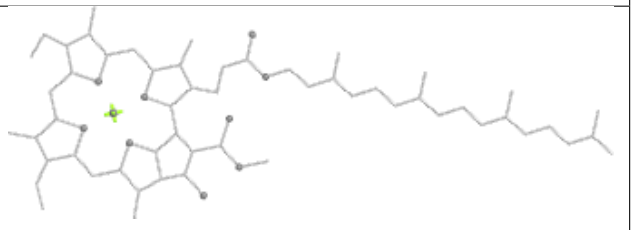
Bond lengths



Bond angles

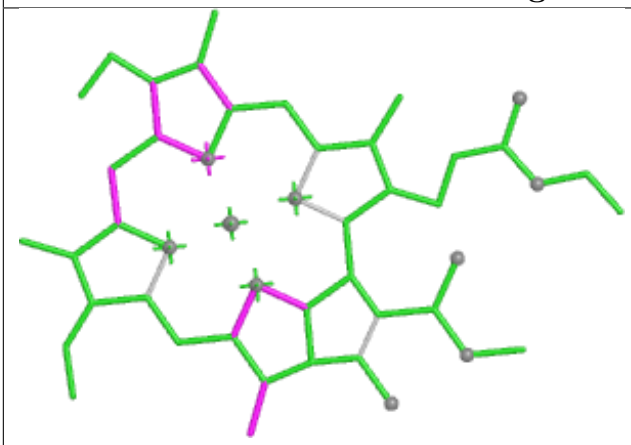


Torsions

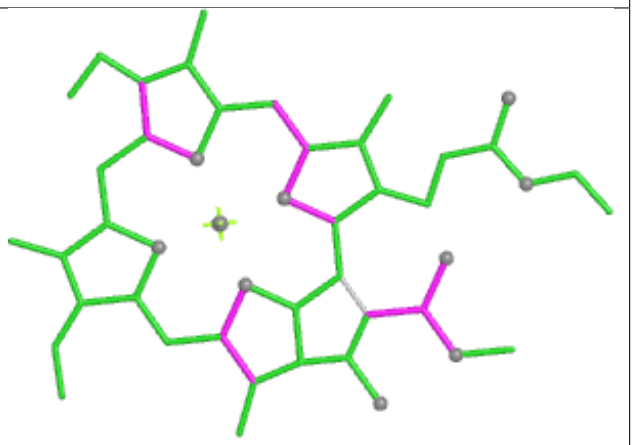


Rings

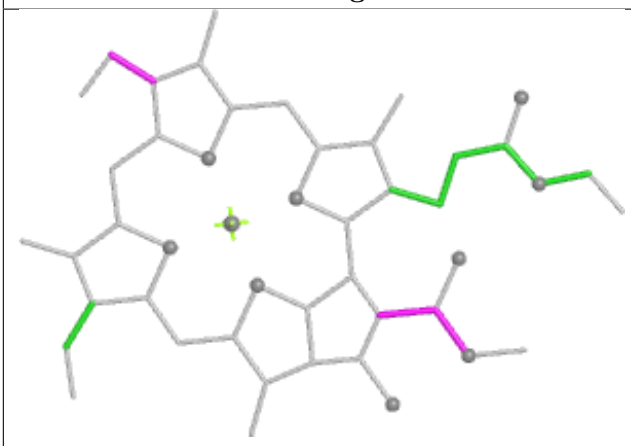
Ligand CLA 5 315



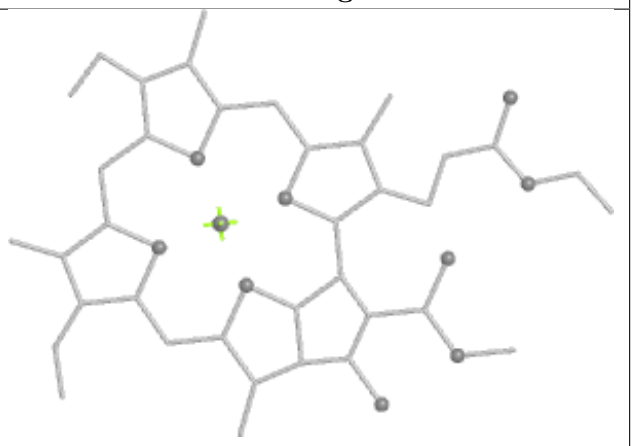
Bond lengths



Bond angles

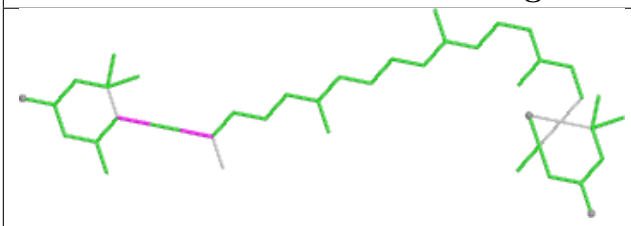


Torsions

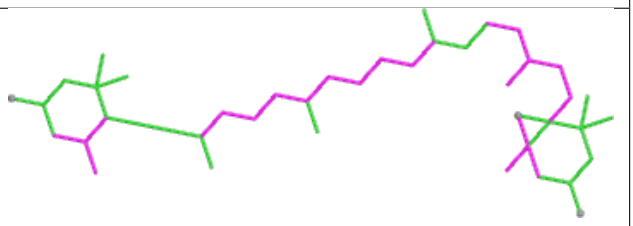


Rings

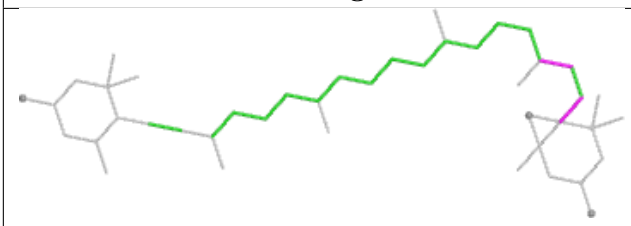
Ligand DD6 A 304



Bond lengths



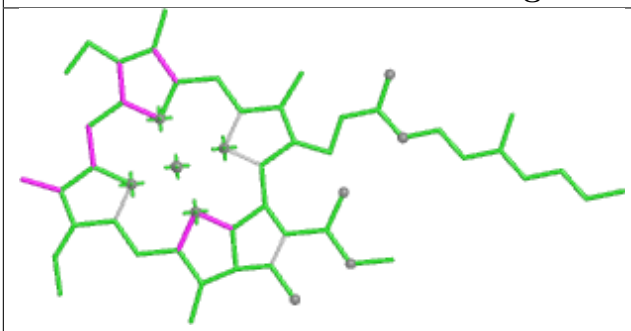
Bond angles



Torsions

Rings

Ligand CLA Q 321



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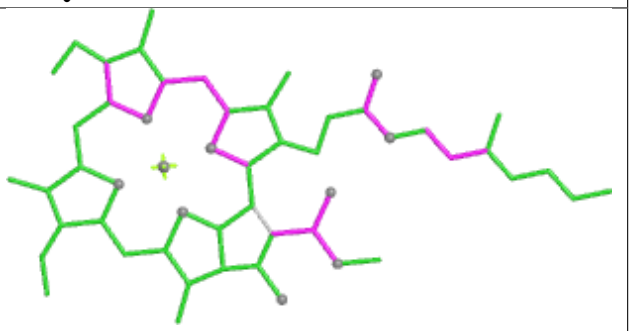

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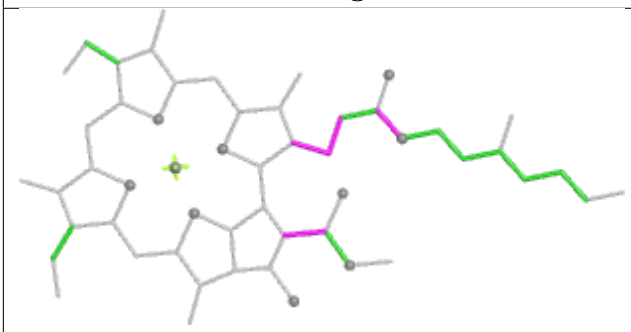

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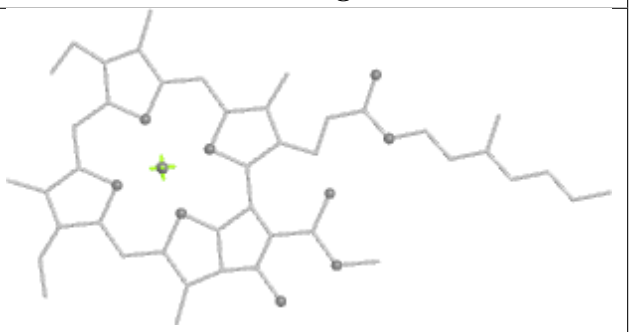
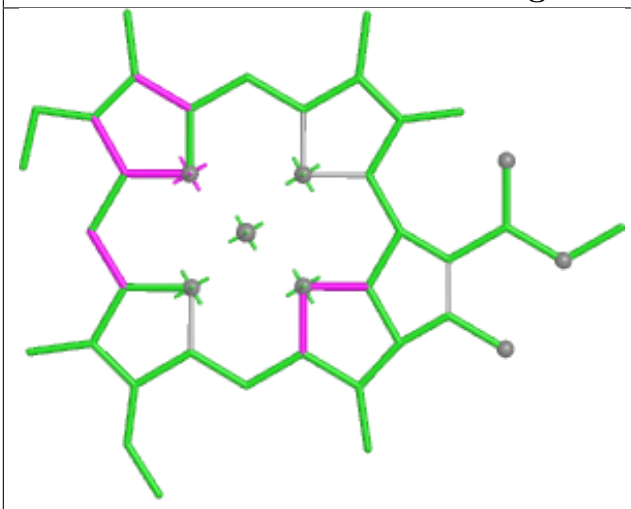


Rings

Ligand CLA 8 313



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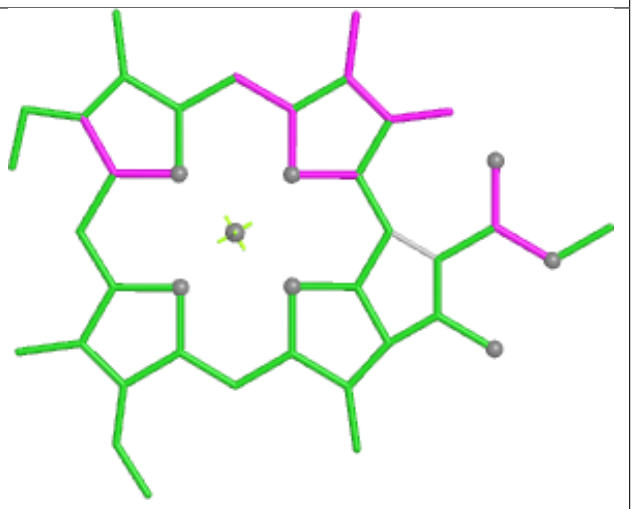

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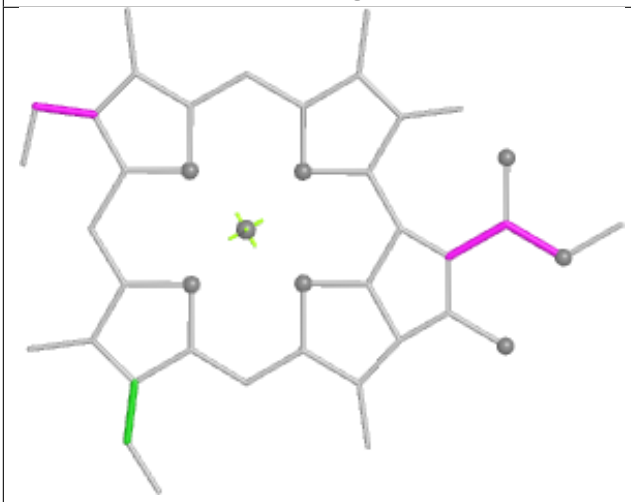

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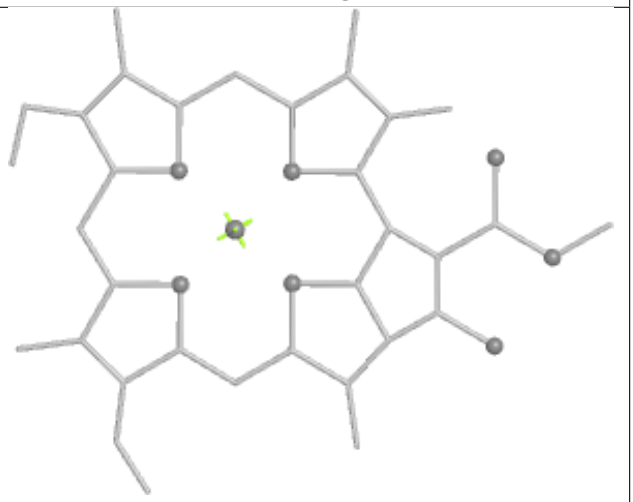
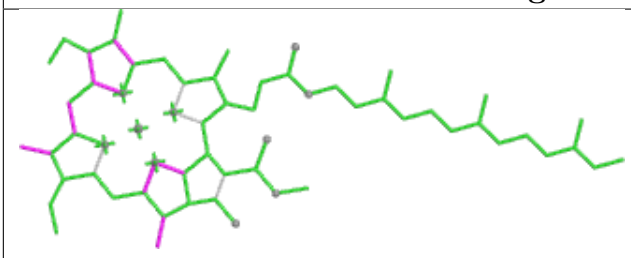


Rings

Ligand CLA a 814



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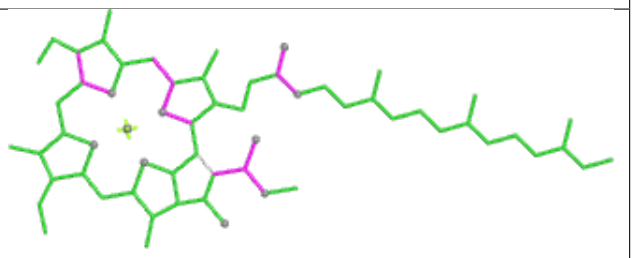
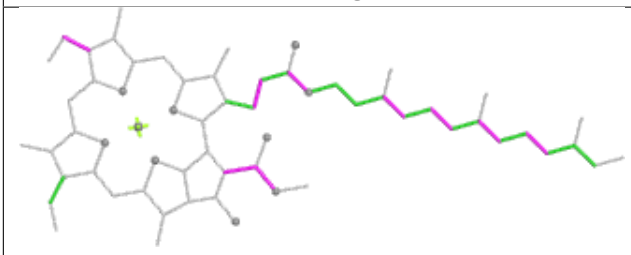


Bond angles



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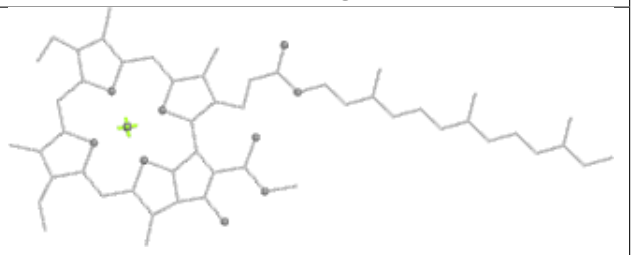
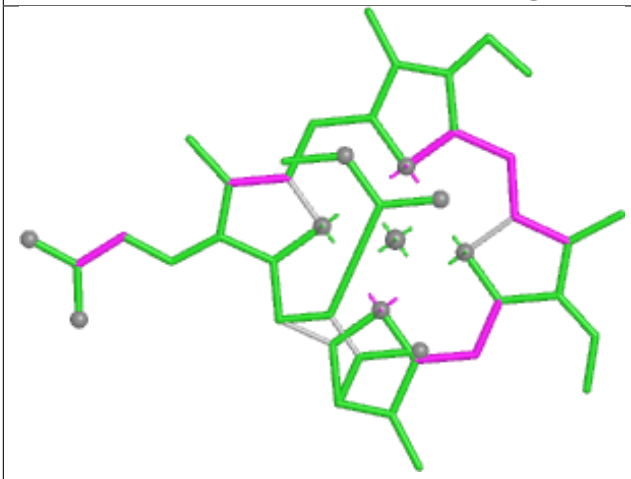


Rings

Ligand KC2 K 313



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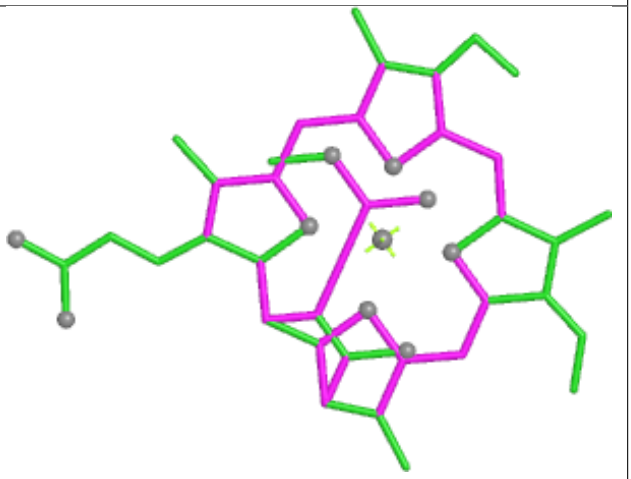

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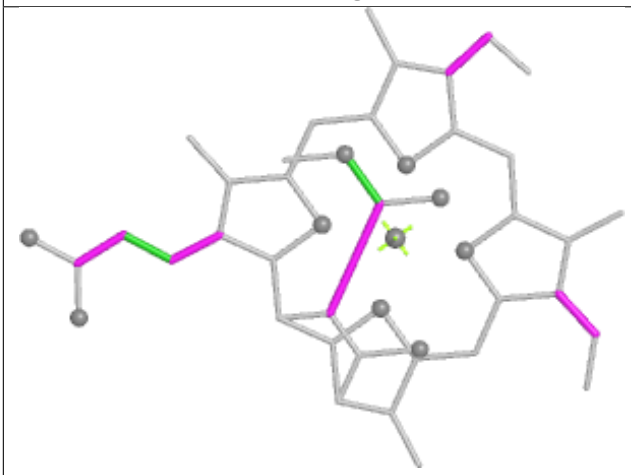

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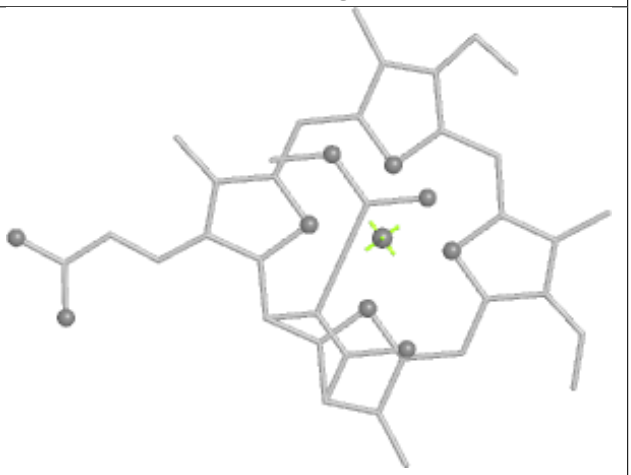
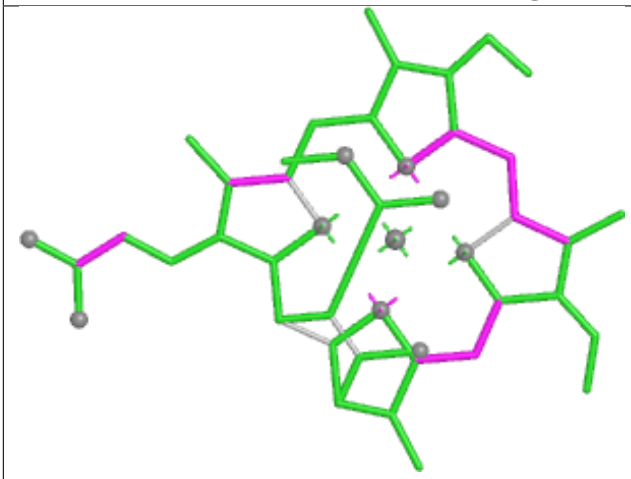


Rings

Ligand KC2 C 312



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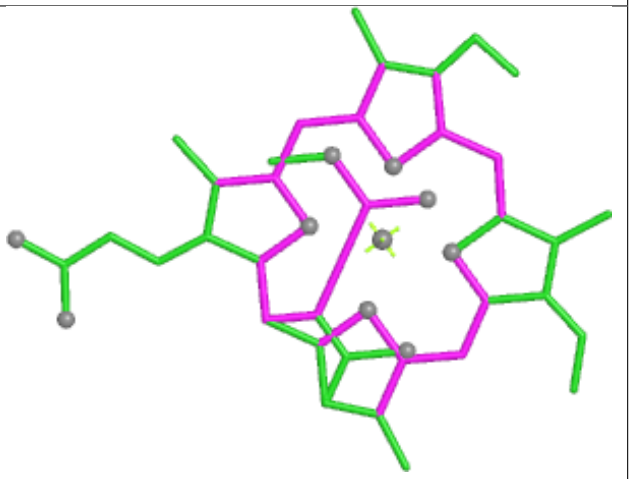
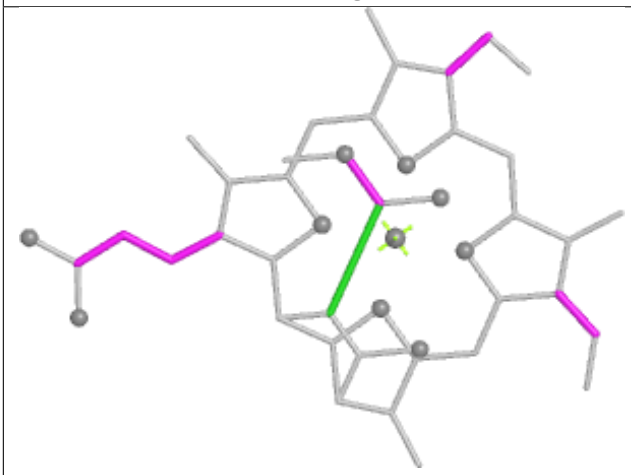


Bond angles



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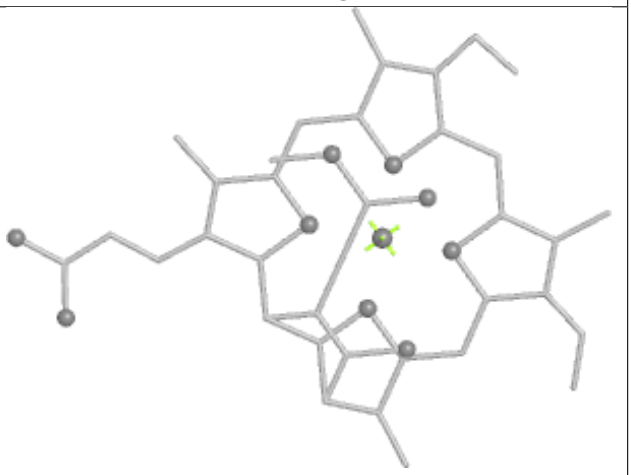
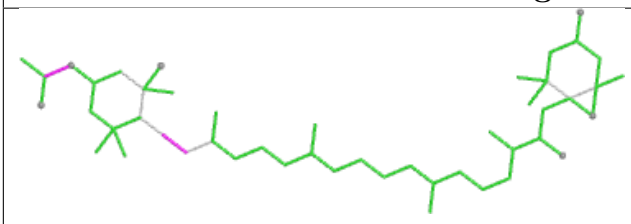


Rings

Ligand A86 9 306



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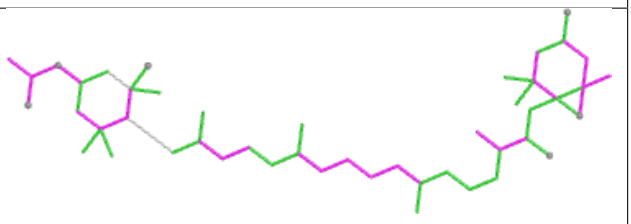

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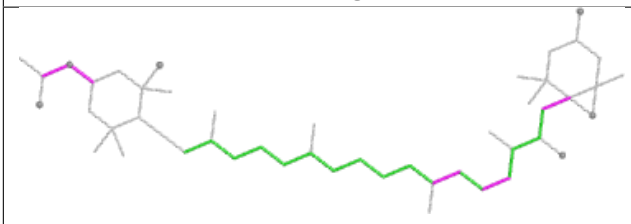

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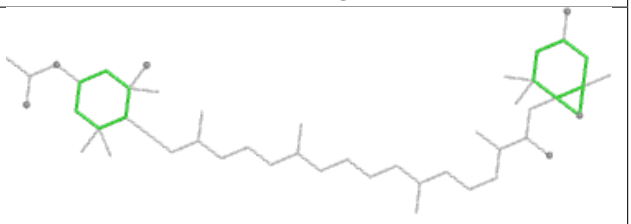
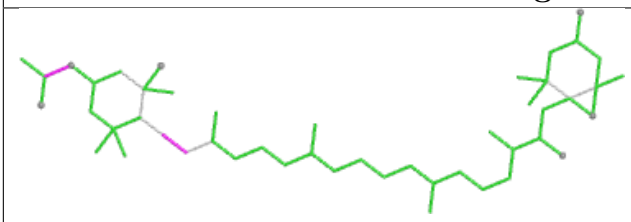


Rings

Ligand A86 6 309



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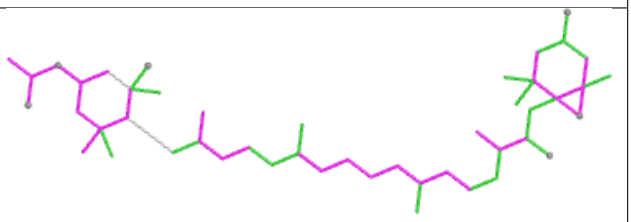
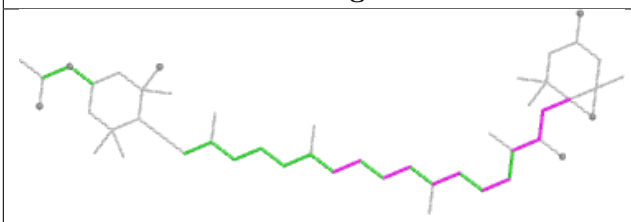


Bond angles



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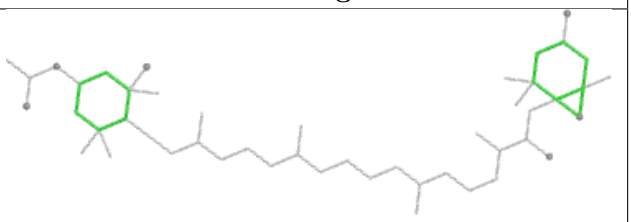
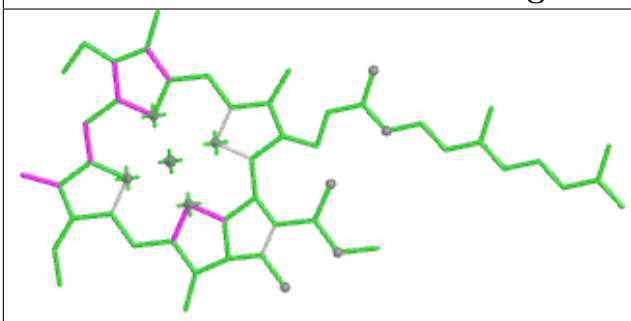


Rings

Ligand CLA b 818



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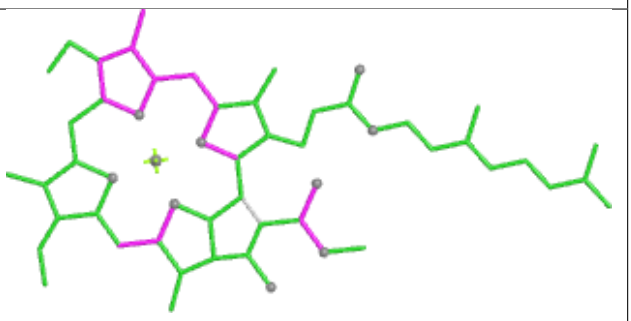

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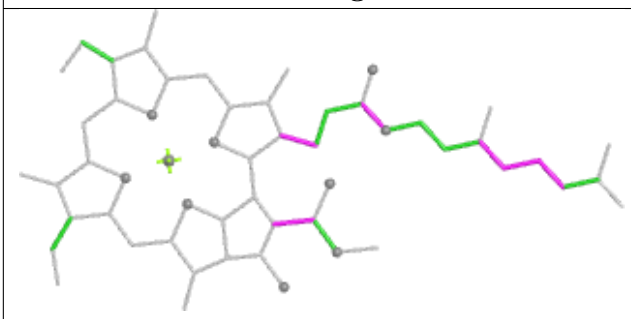

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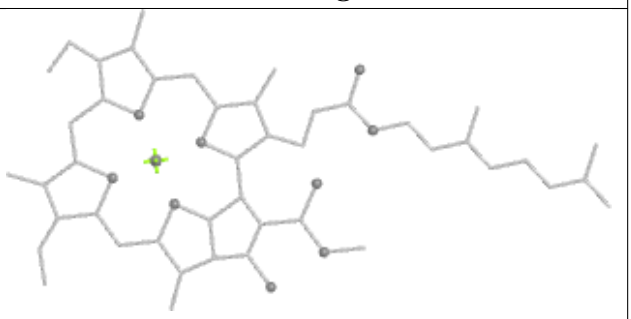
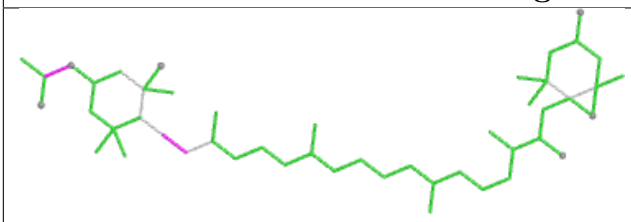


Rings

Ligand A86 y 306



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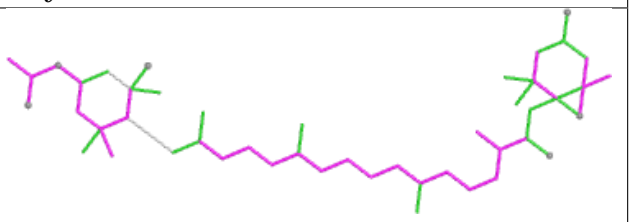

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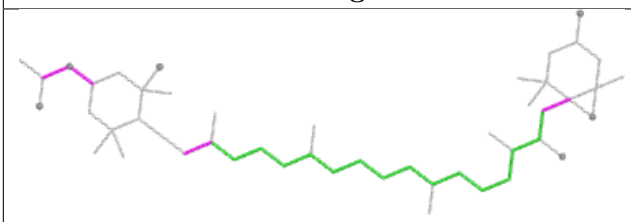

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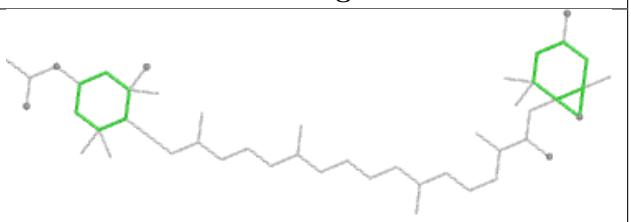
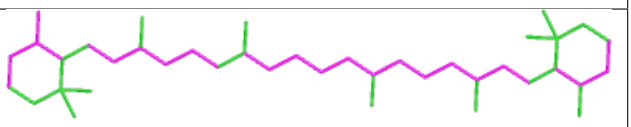


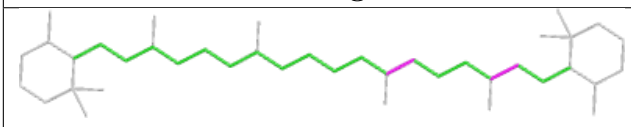
Rings

Ligand BCR f 801

Bond lengths



Bond angles



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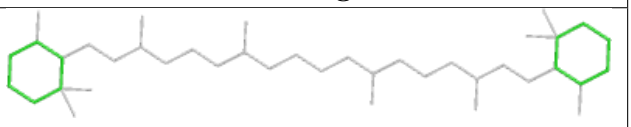
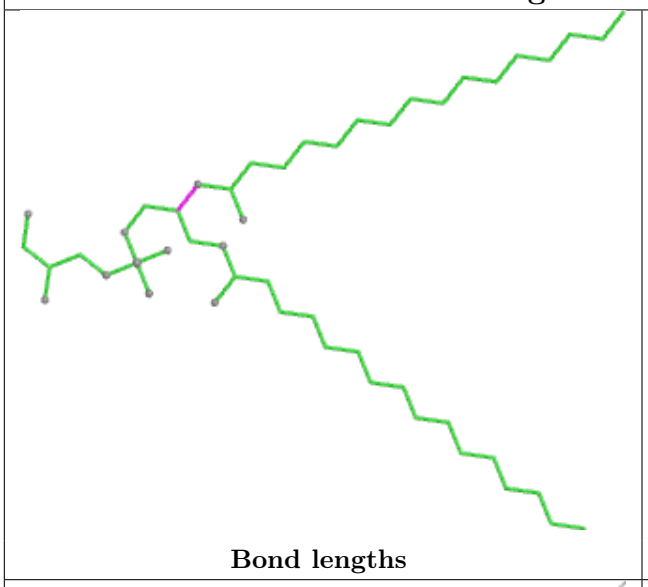


Rings

Ligand LHG a 840



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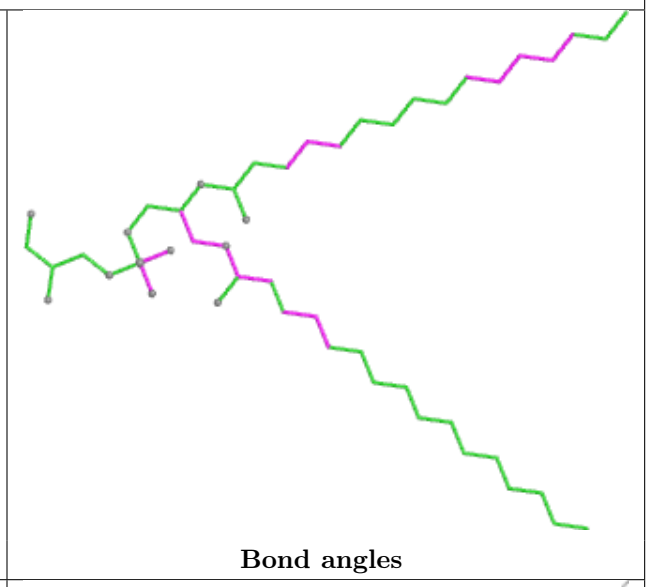
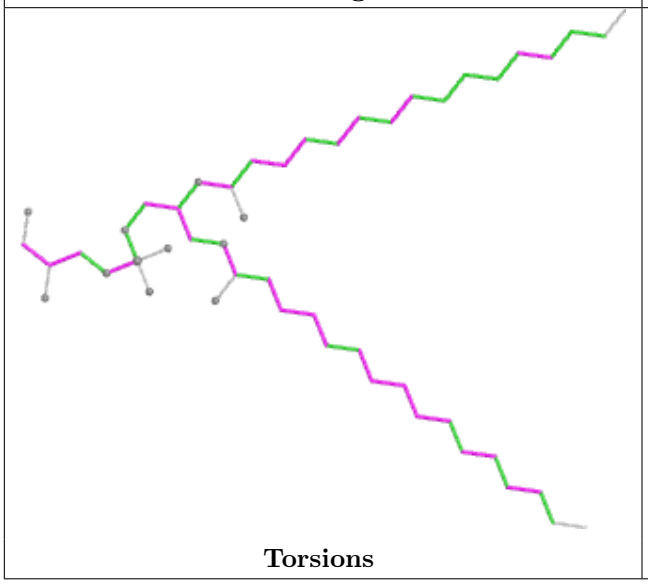


Bond angles



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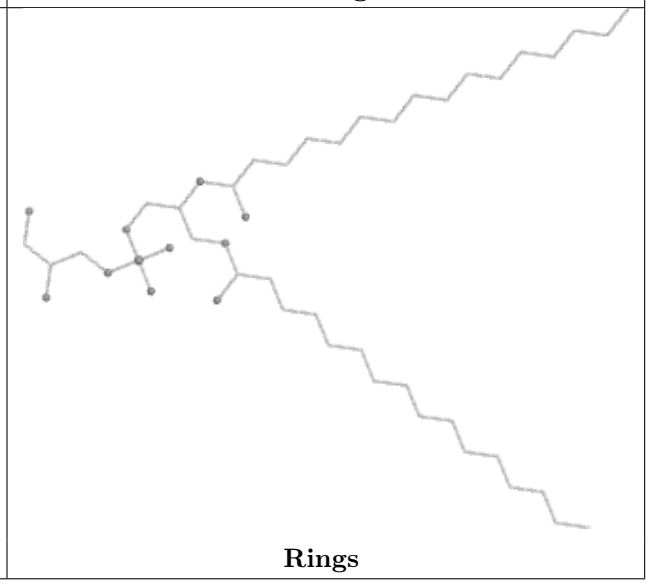
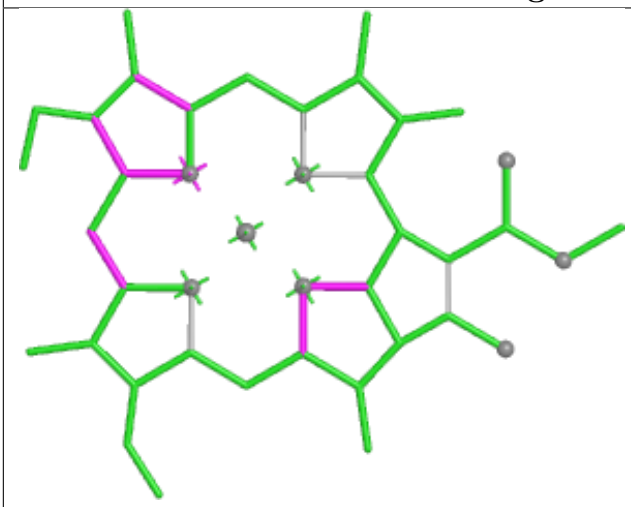


Rings

Ligand CLA x 314



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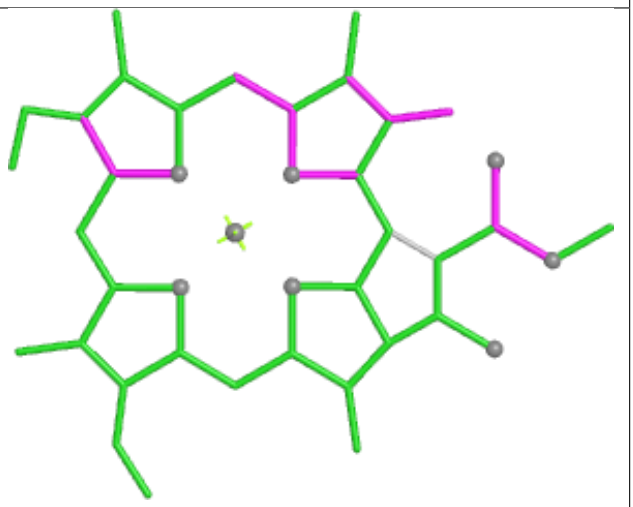
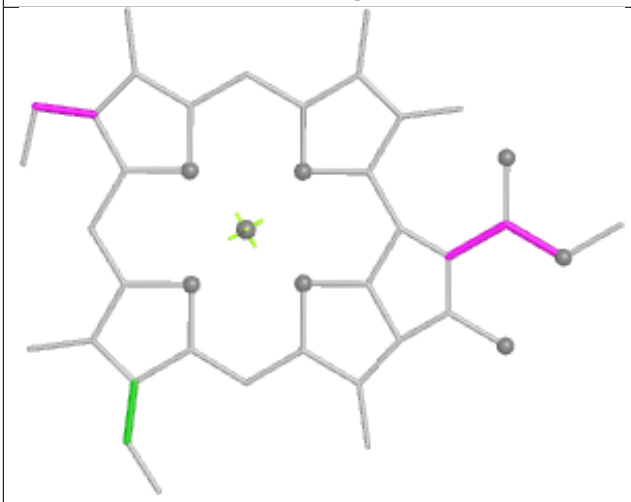
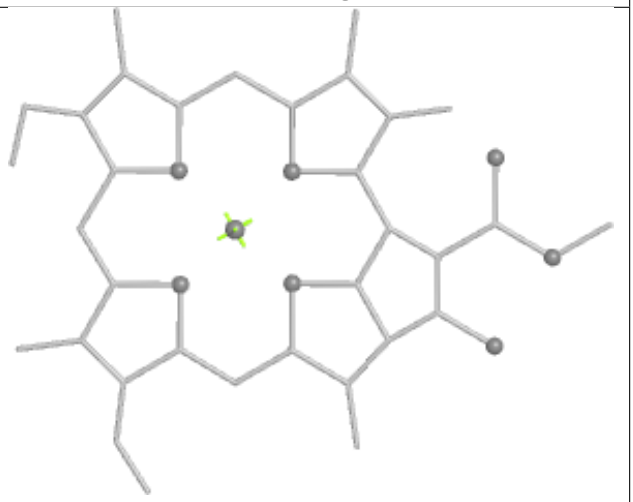


Bond angles

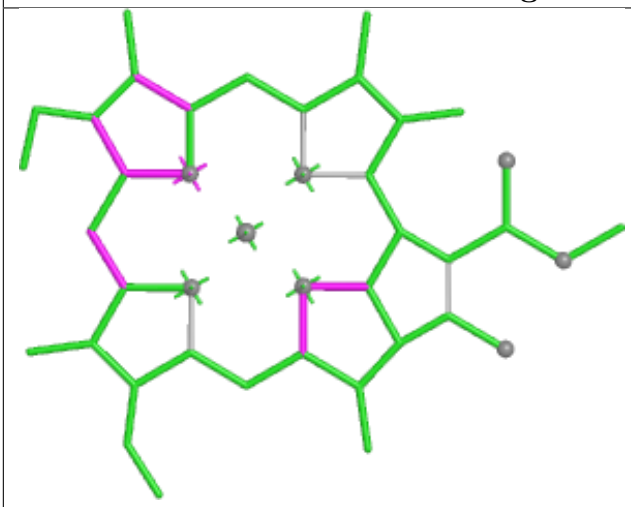


Torsions



Rings

Ligand CLA M 315



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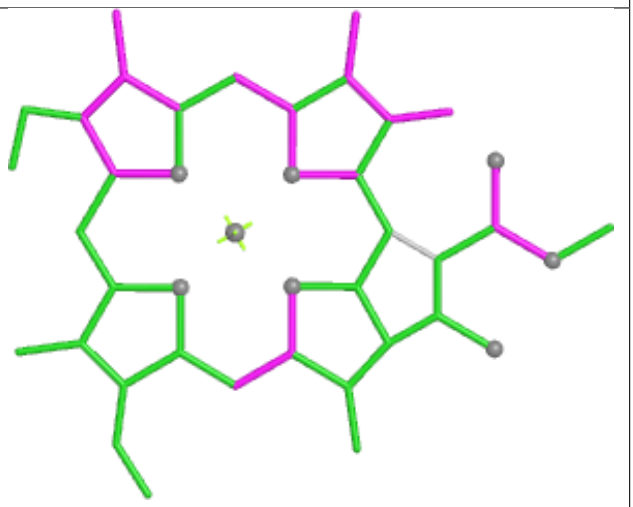
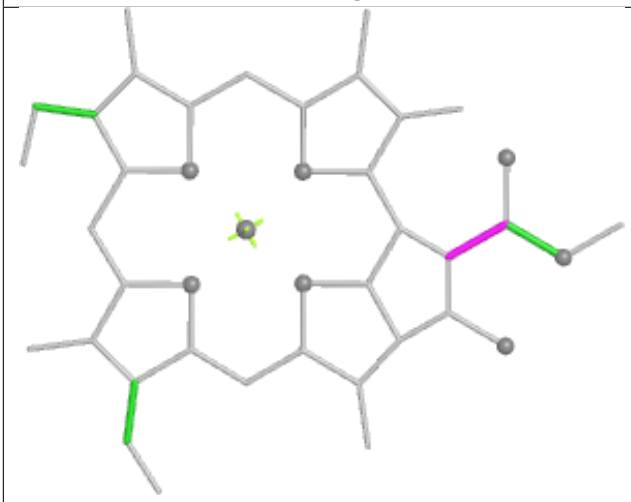
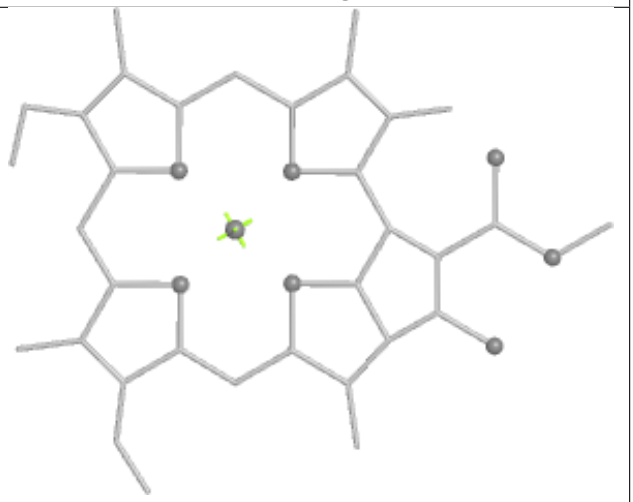


Bond angles

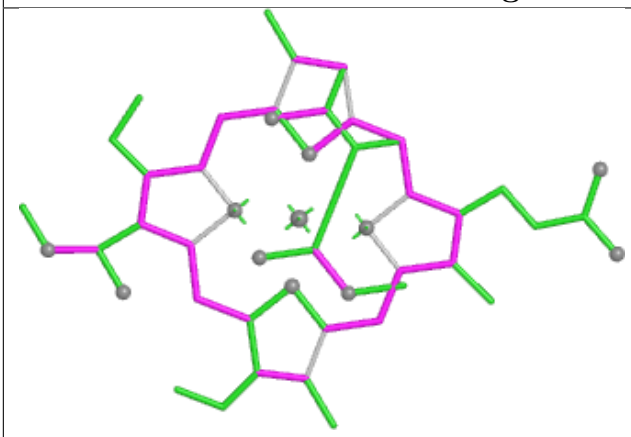


Torsions

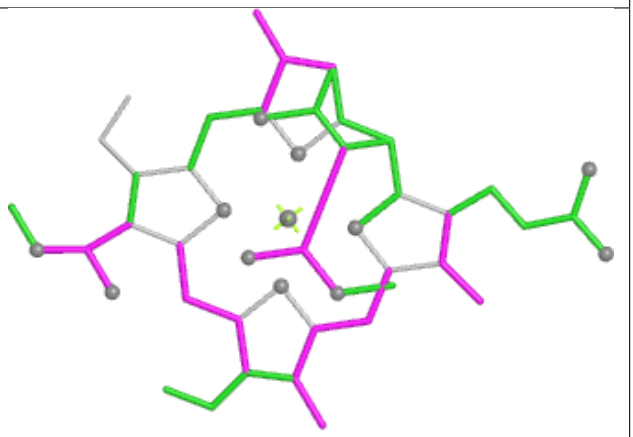


Rings

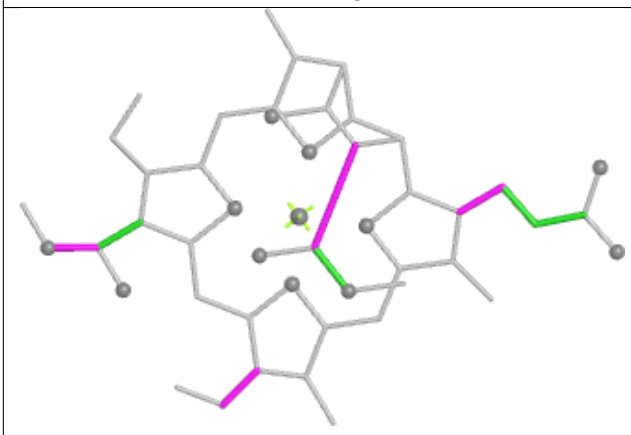
Ligand A1ECV E 311



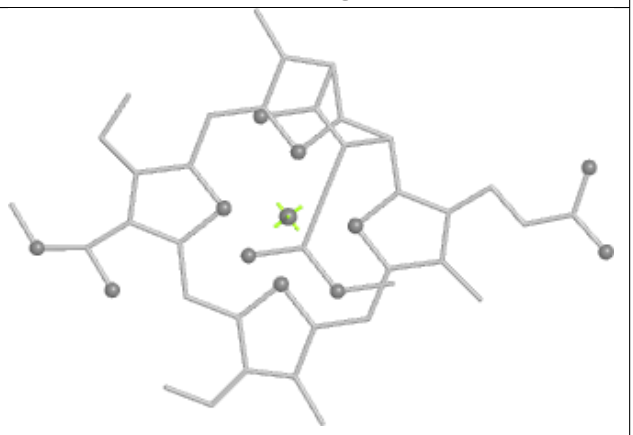
Bond lengths



Bond angles

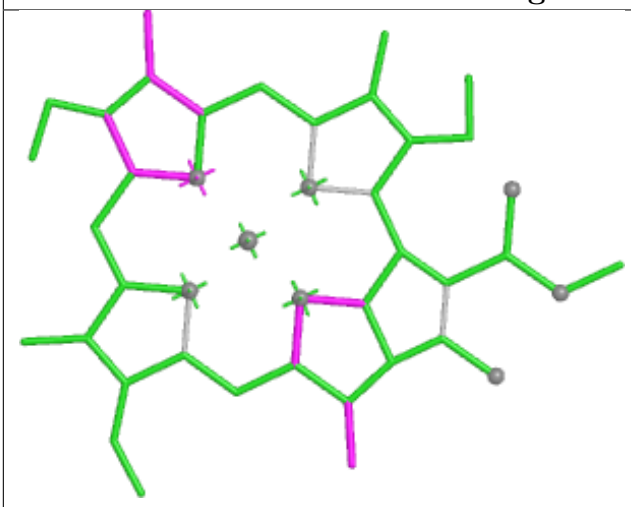


Torsions

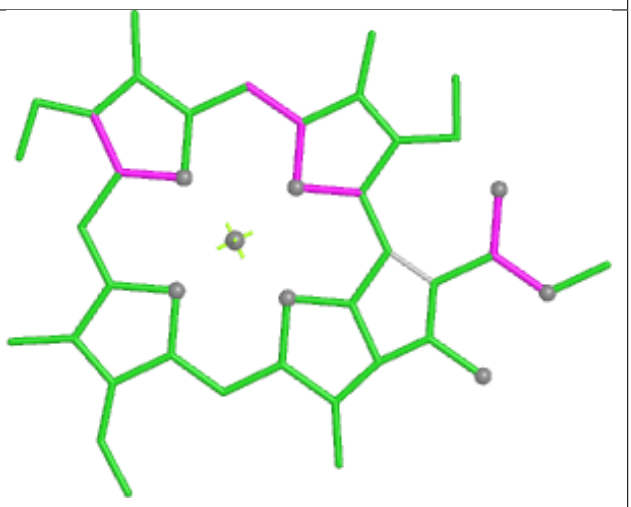


Rings

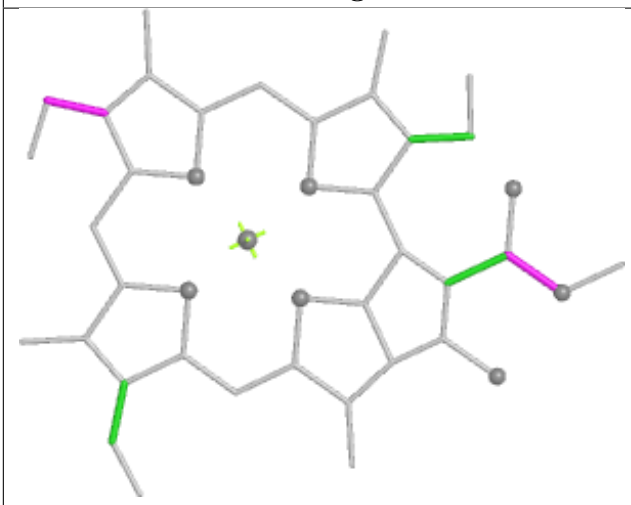
Ligand CLA J 317



Bond lengths



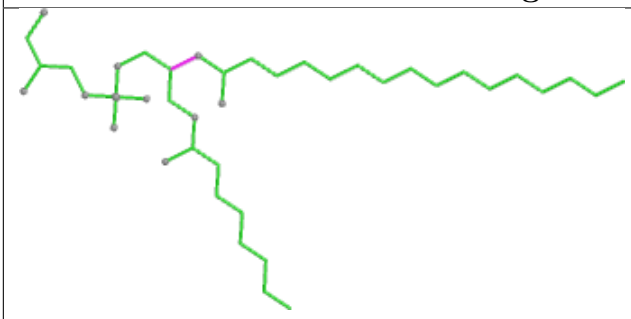
Bond angles



Torsions

Rings

Ligand LHG X 301



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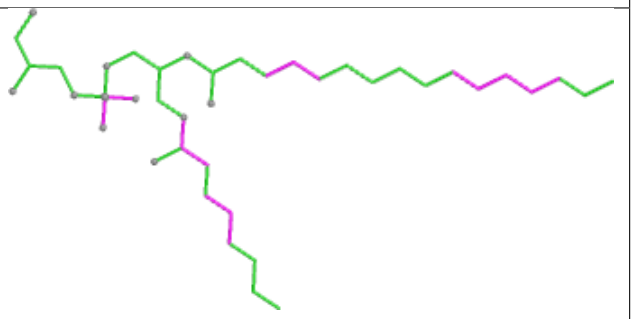
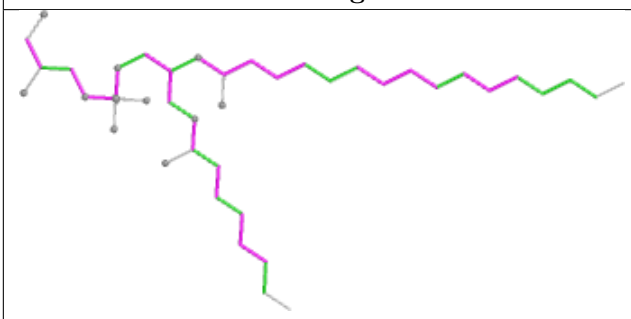
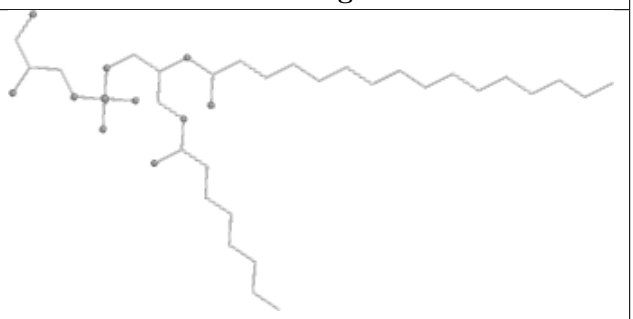


Bond angles

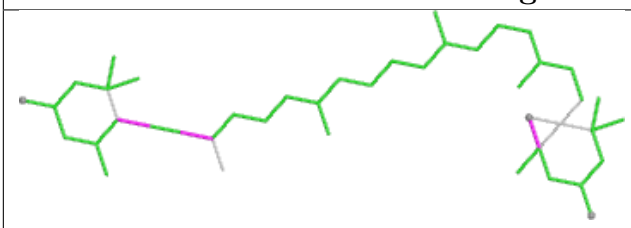


Torsions



Rings

Ligand DD6 W 305



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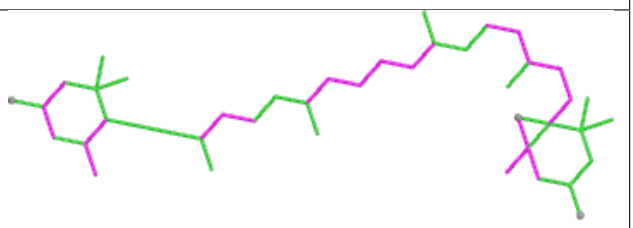
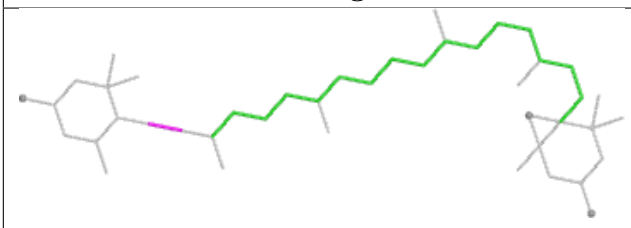
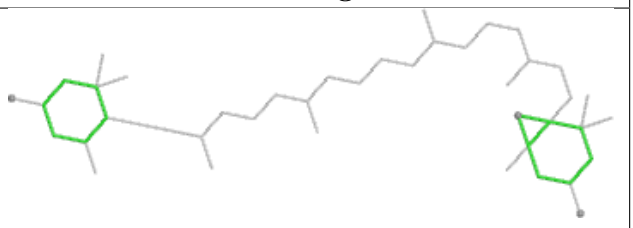


Bond angles

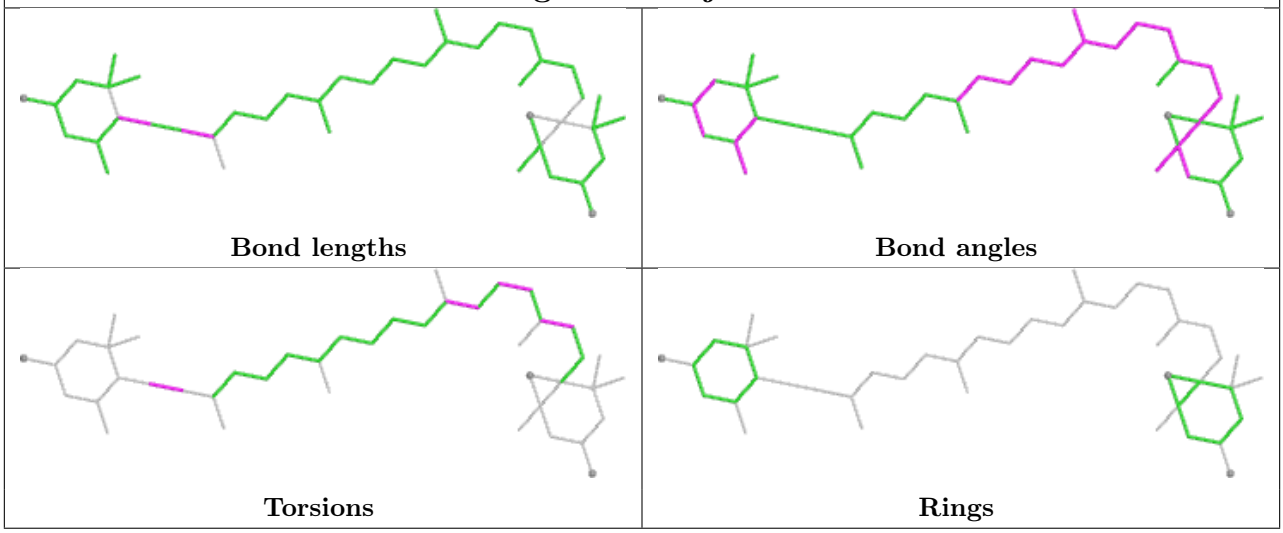


Torsions

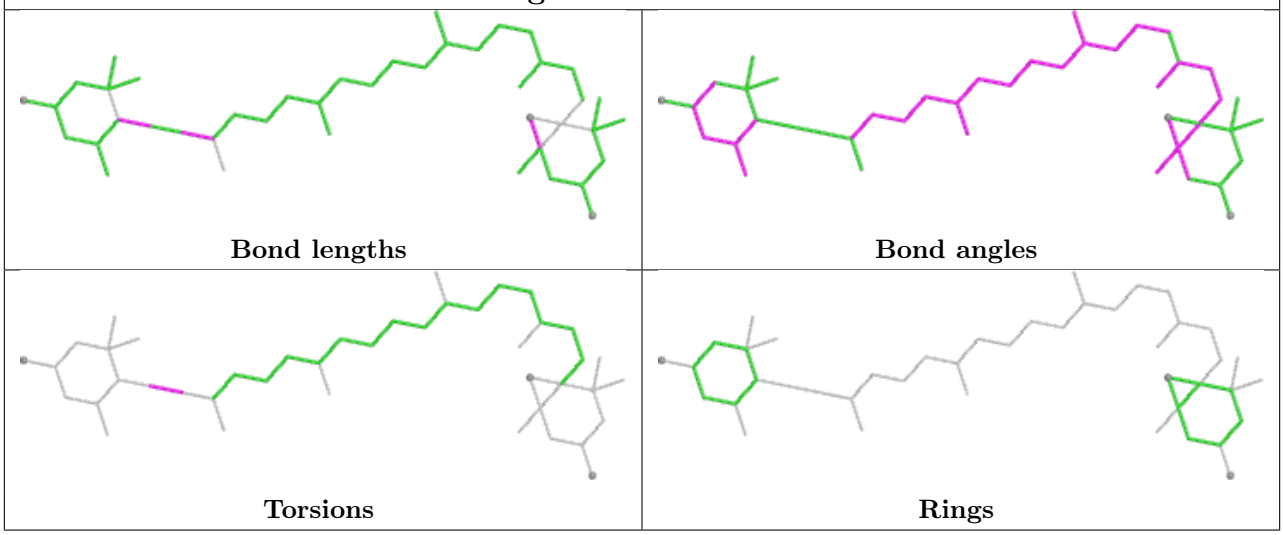


Rings

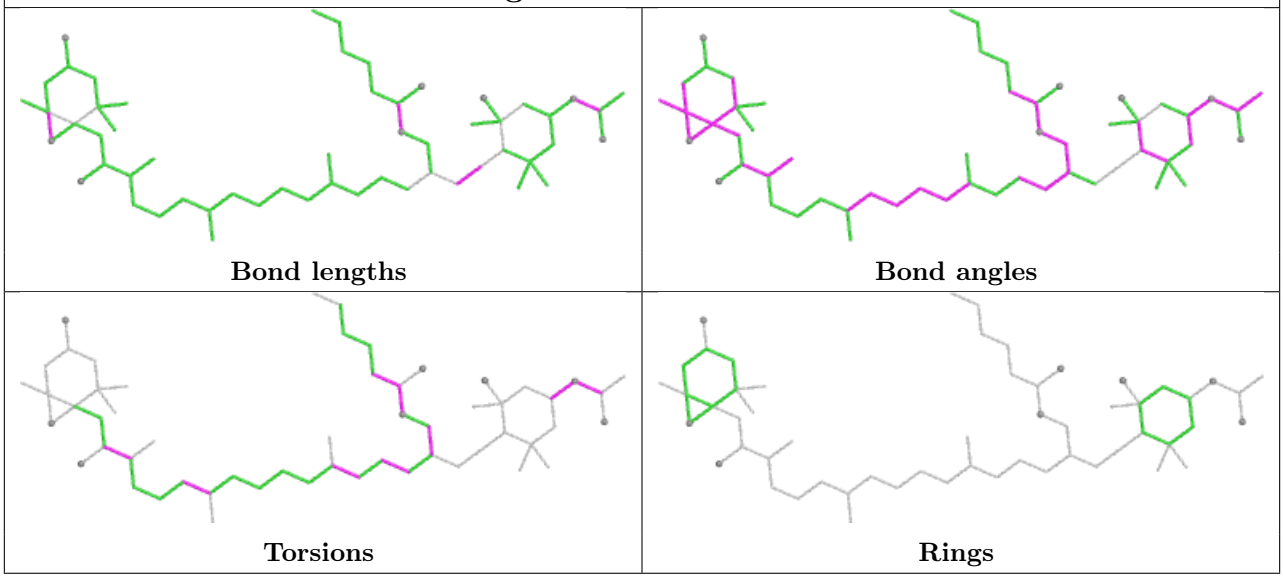
Ligand DD6 j 102



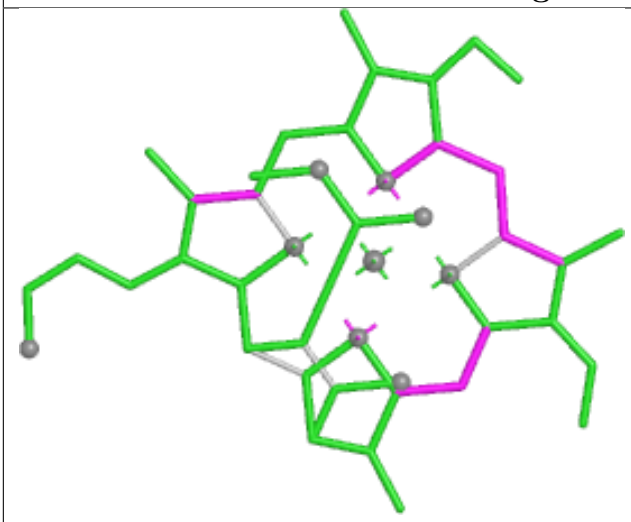
Ligand DD6 F 305



Ligand A1EB1 G 307

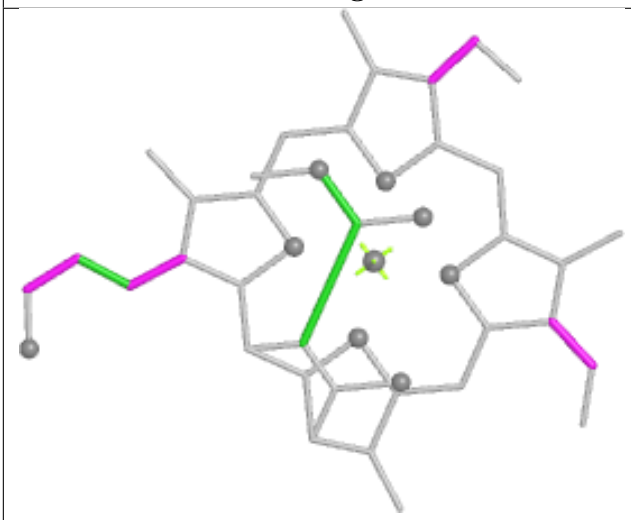


Ligand KC2 I 312

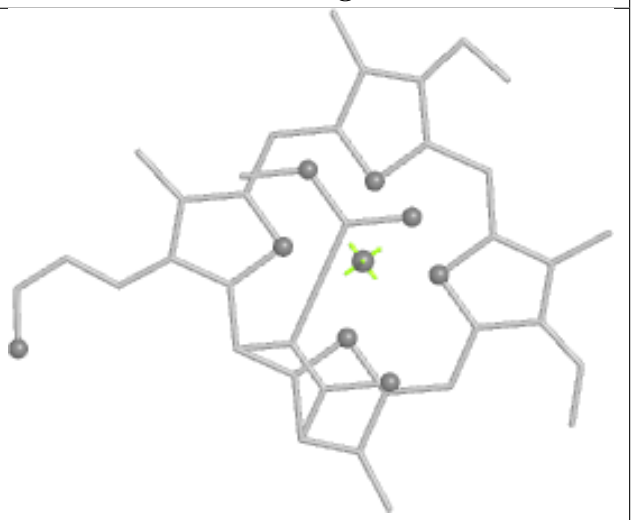


Bond lengths

Bond angles

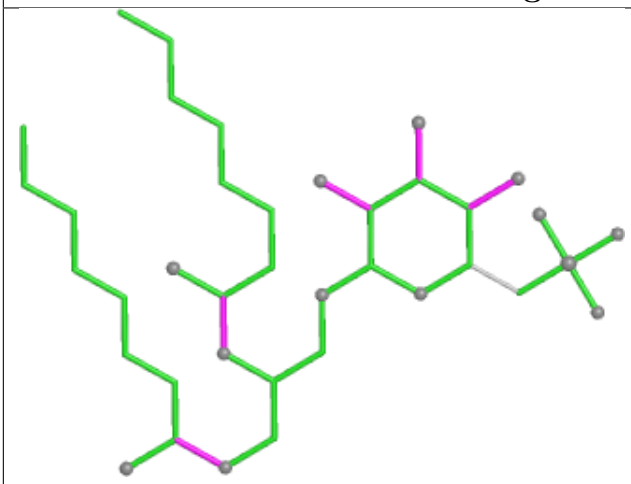


Torsions



Rings

Ligand SQD D 304



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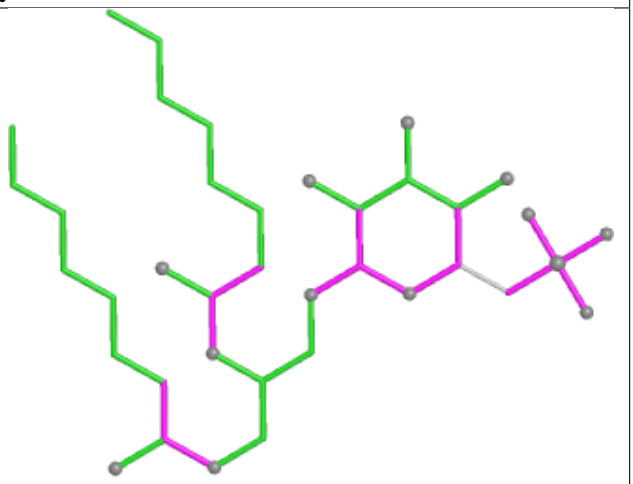
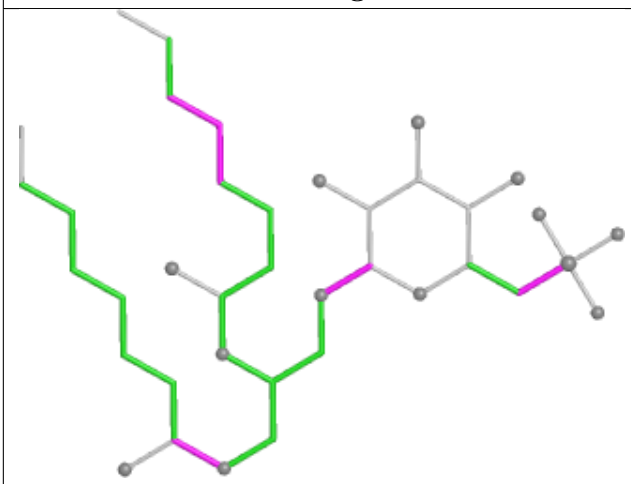


Bond angles



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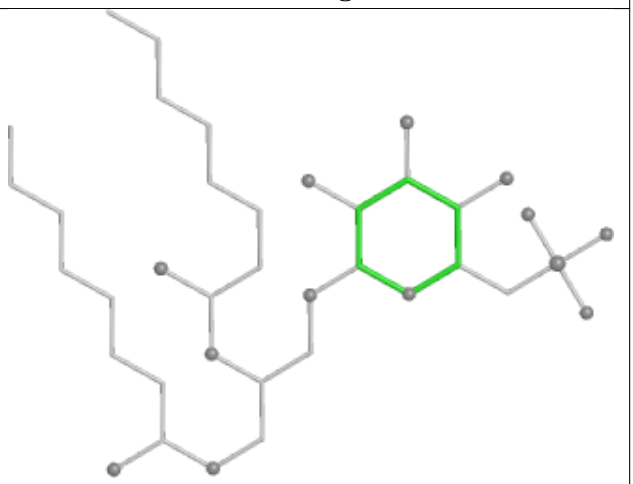
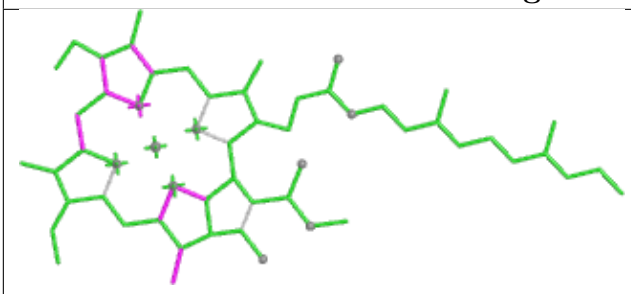


Rings

Ligand CLA H 310



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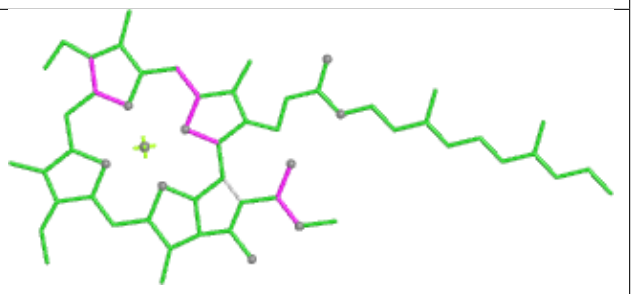
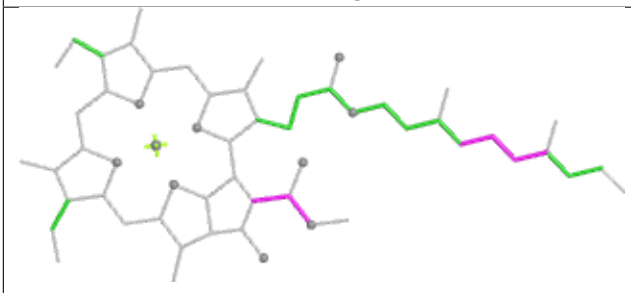


Bond angles



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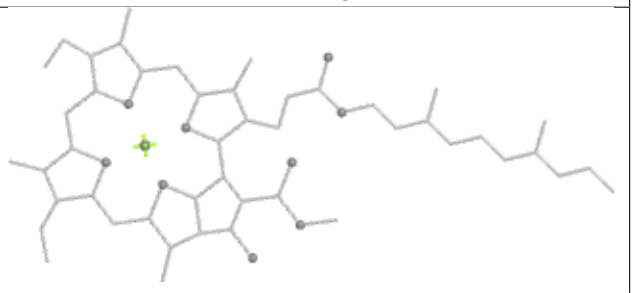
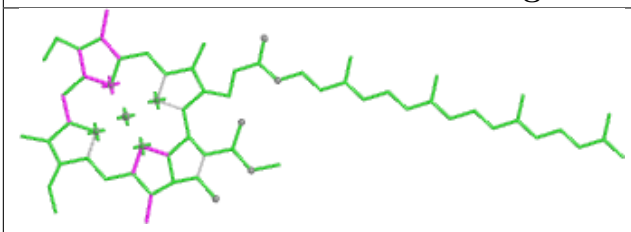


Rings

Ligand CLA H 312



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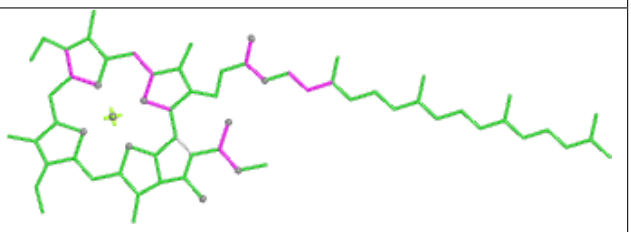
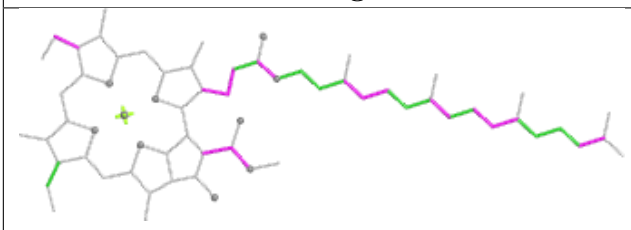


Bond angles



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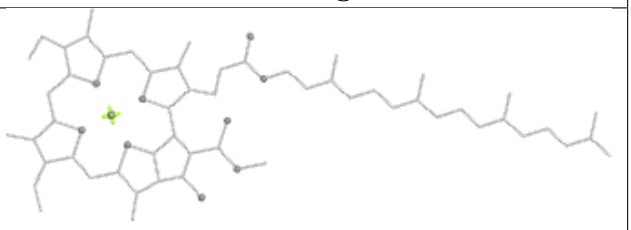
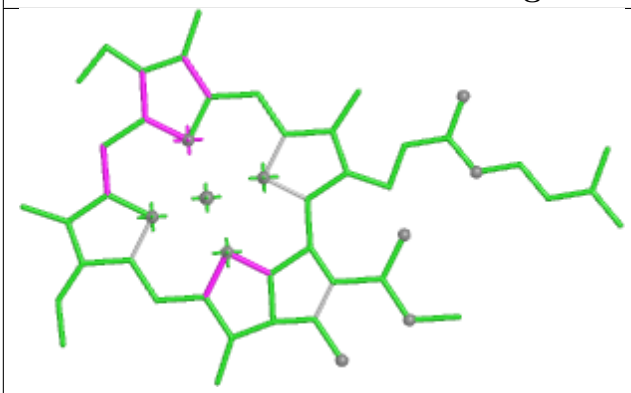


Rings

Ligand CLA V 316



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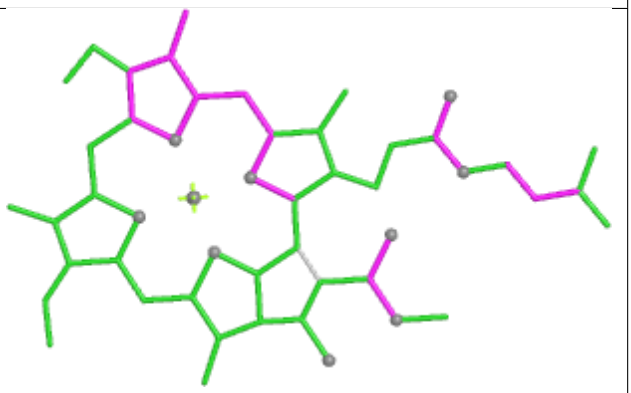
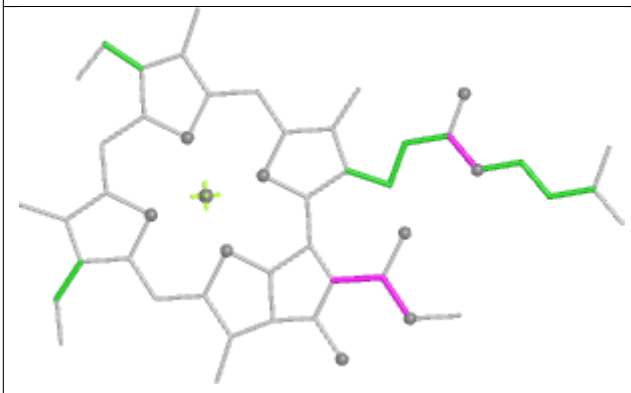


Bond angles



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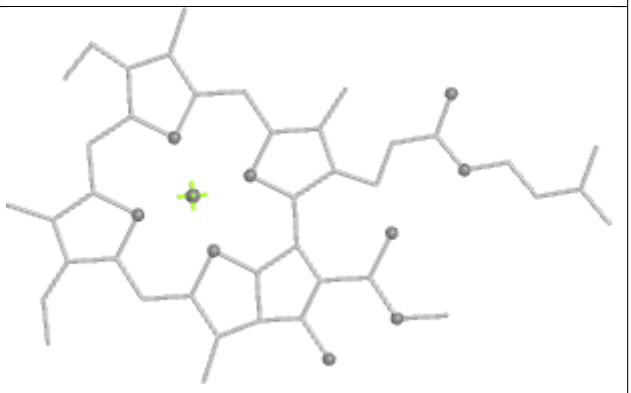
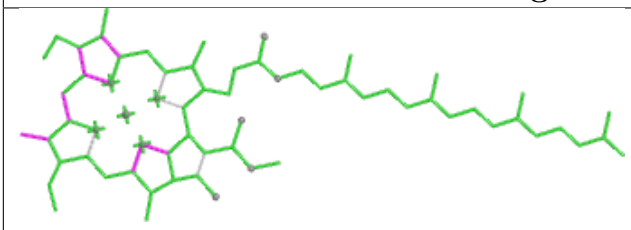


Rings

Ligand CLA I 311



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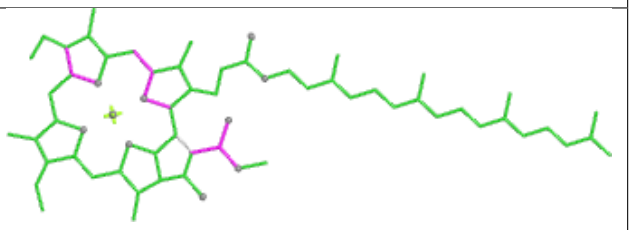
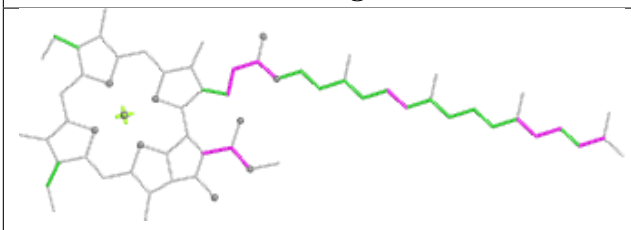


Bond angles



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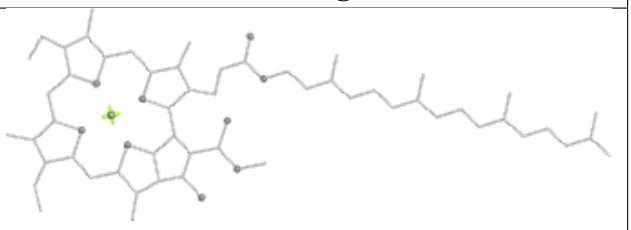
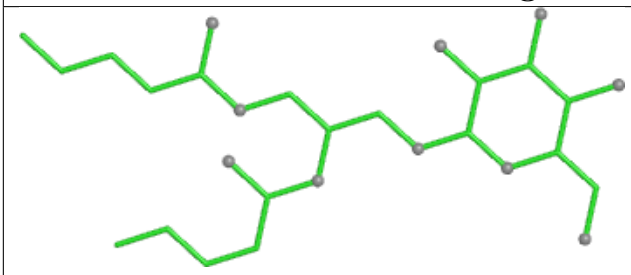


Rings

Ligand LMG A 316



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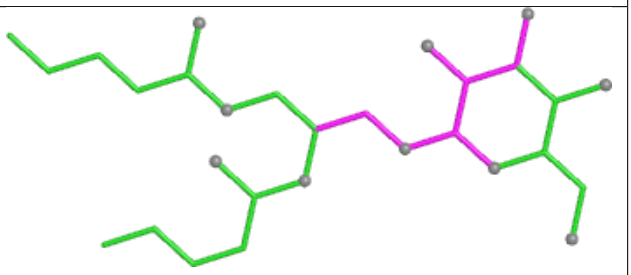
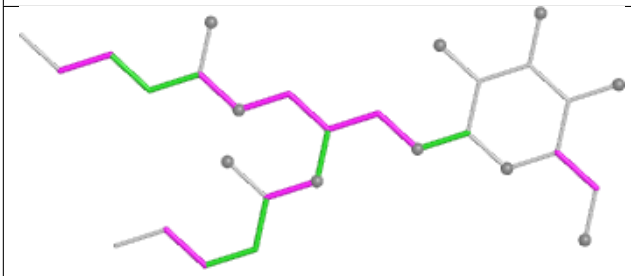


Bond angles



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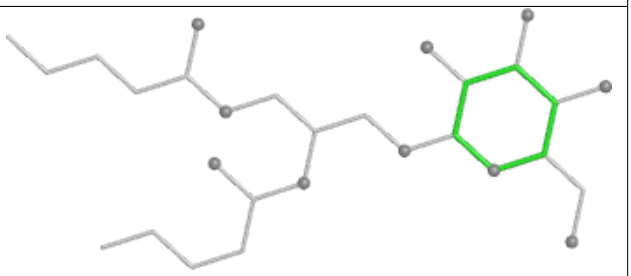
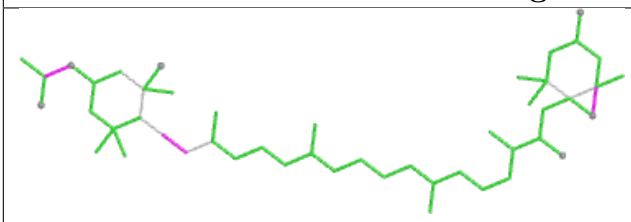


Rings

Ligand A86 Q 305



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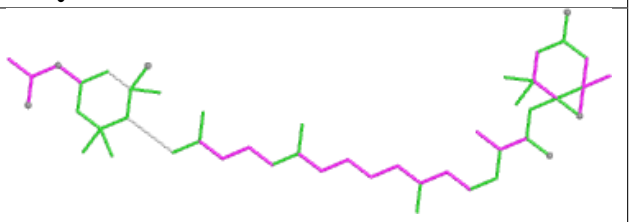
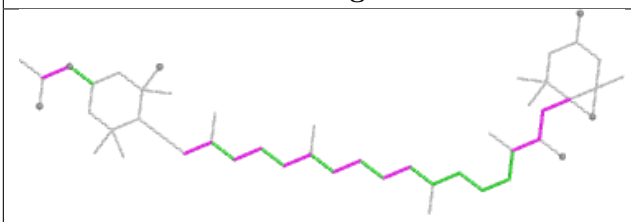


Bond angles



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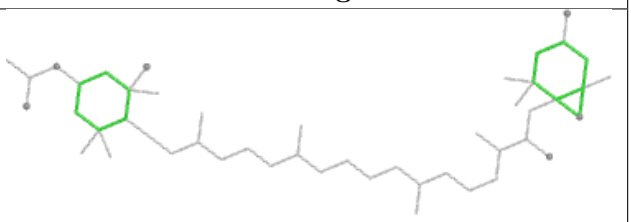
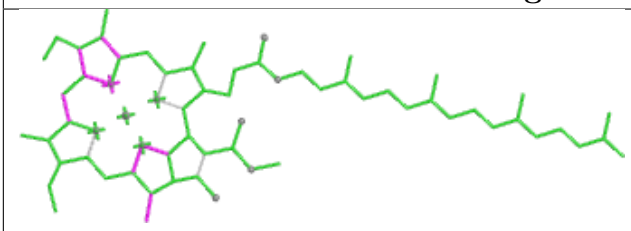
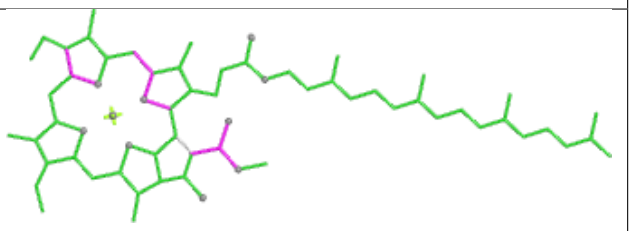


Rings

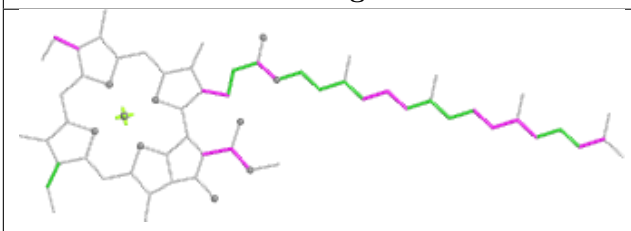
Ligand CLA C 310



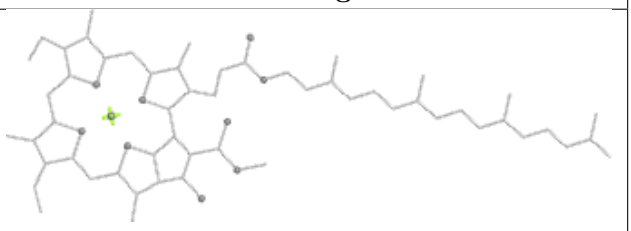
Bond lengths



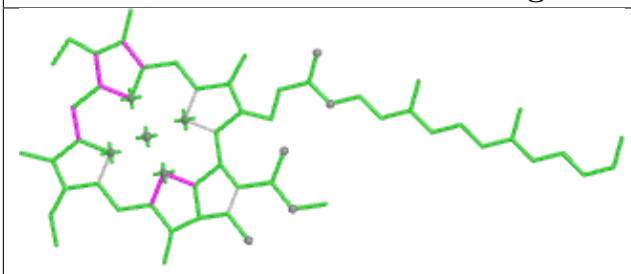
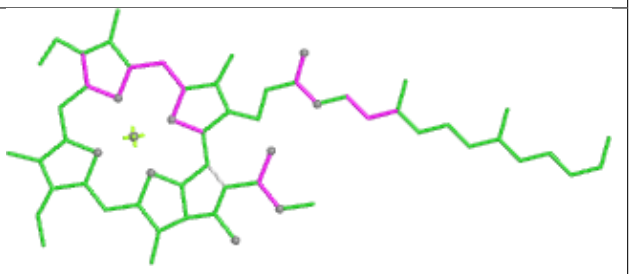
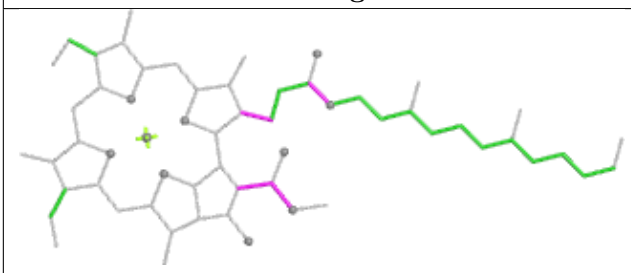
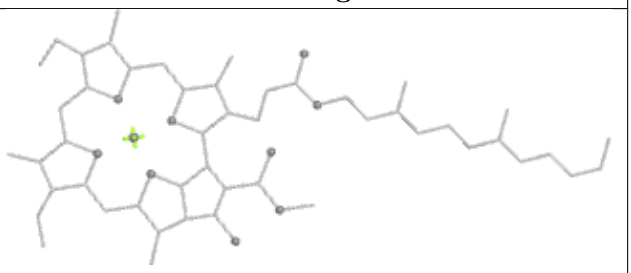
Bond angles

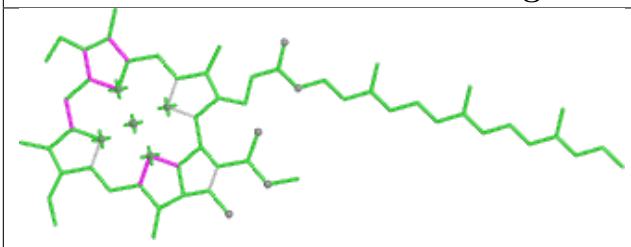
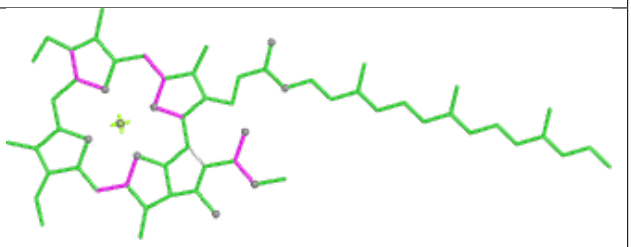
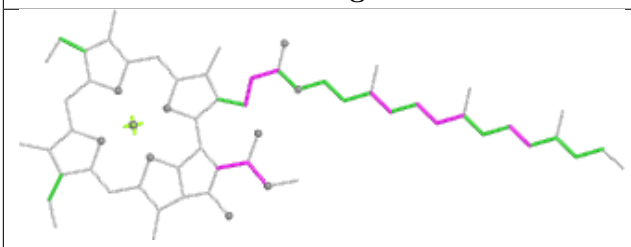
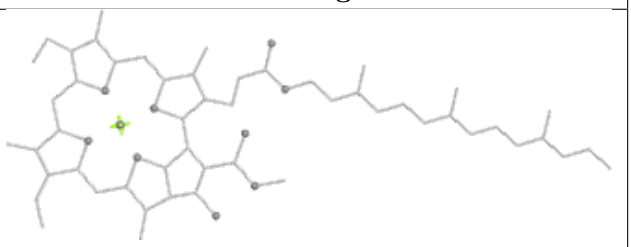


Torsions

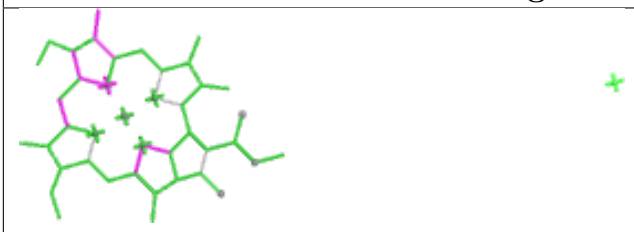


Rings

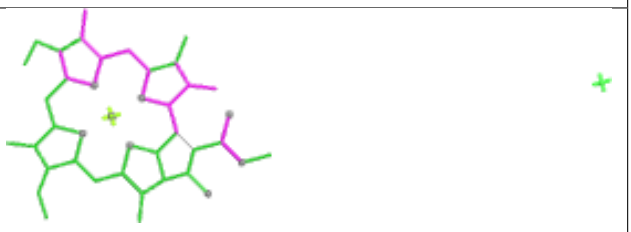
Ligand CLA b 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA K 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

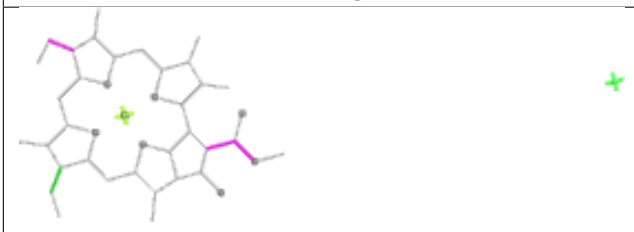
Ligand CLA x 318



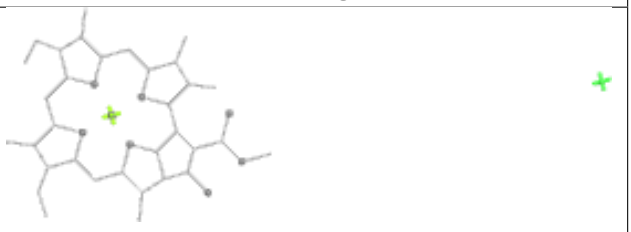
Bond lengths



Bond angles

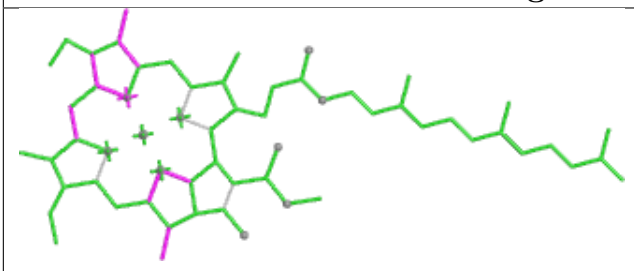


Torsions



Rings

Ligand CLA b 820



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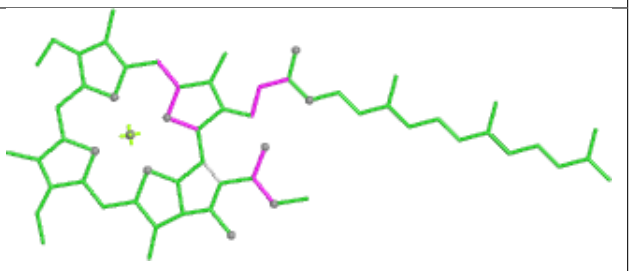
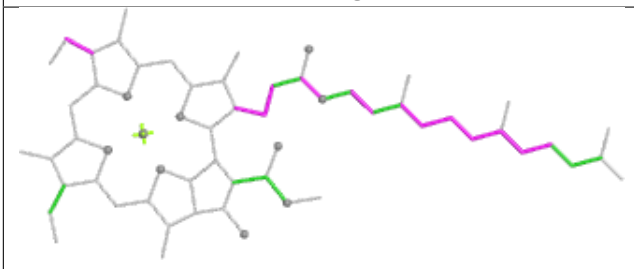


Bond angles



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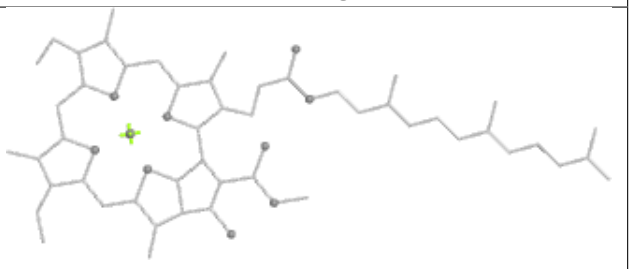
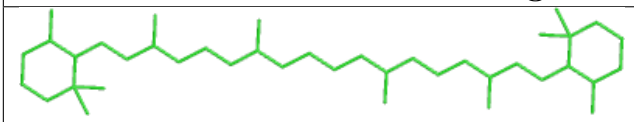
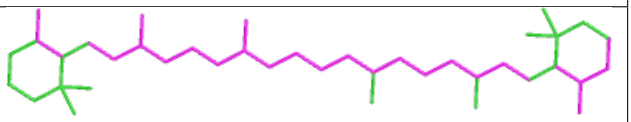


Rings

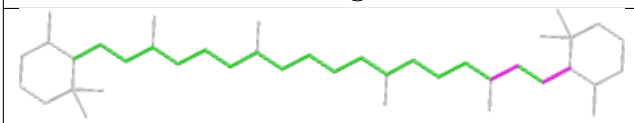
Ligand BCR a 845



Bond lengths



Bond angles



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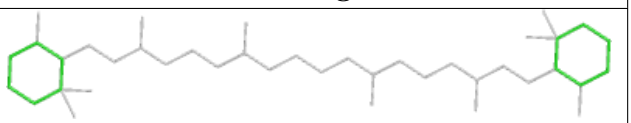
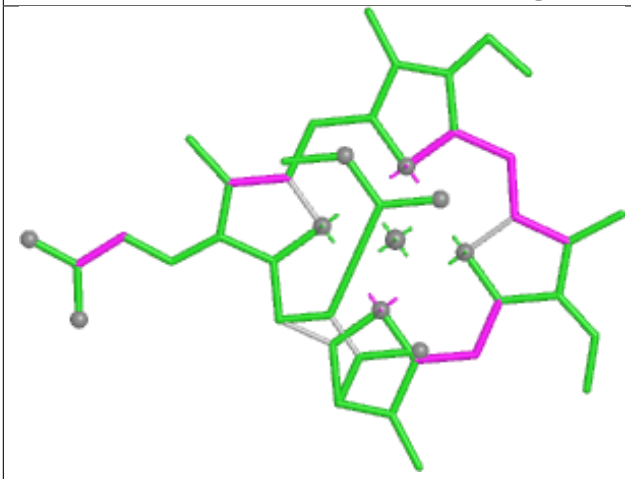


Rings

Ligand KC2 4 318



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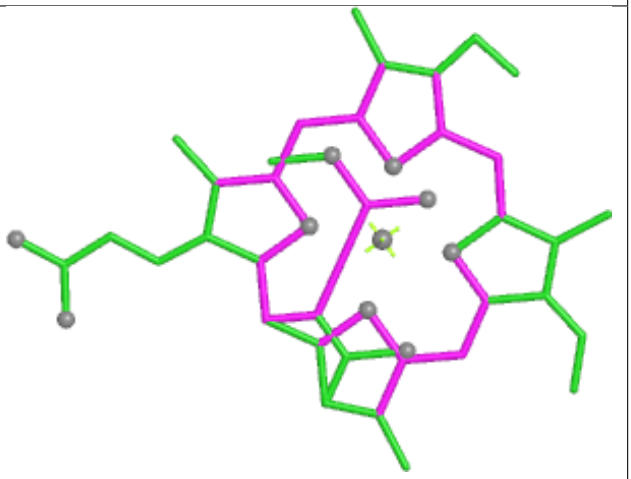
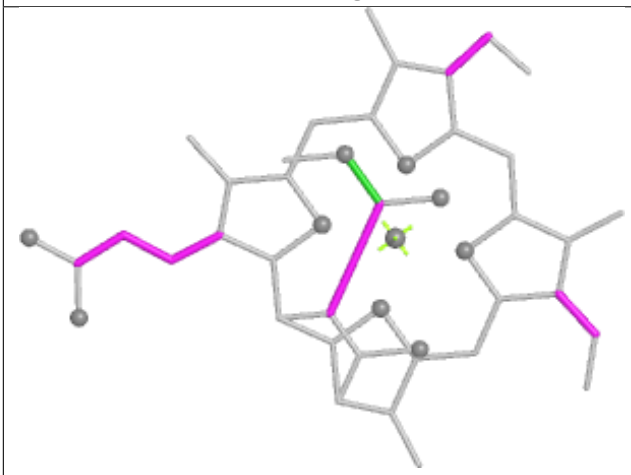


Bond angles



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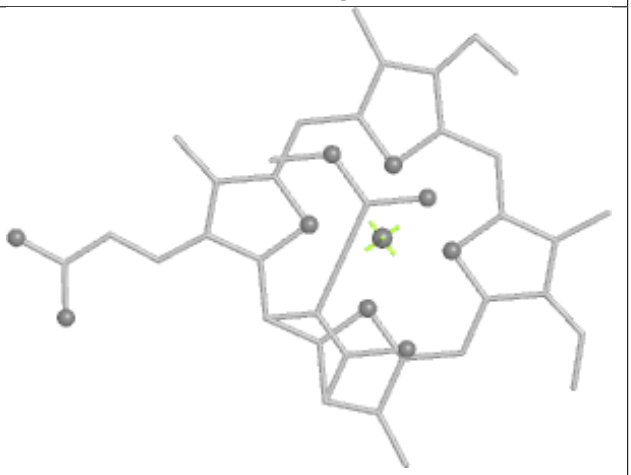
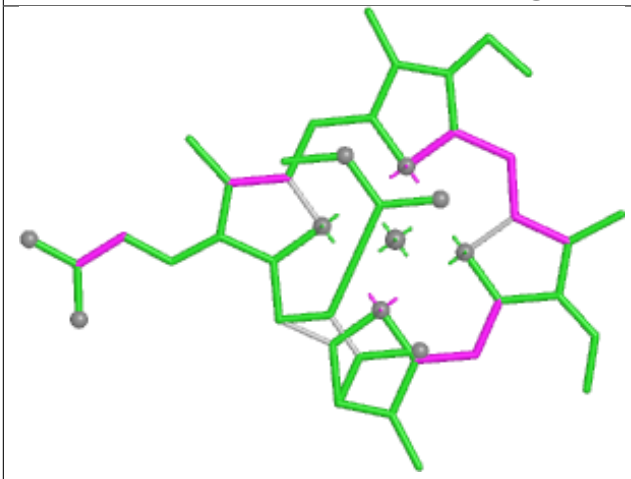


Rings

Ligand KC2 F 307



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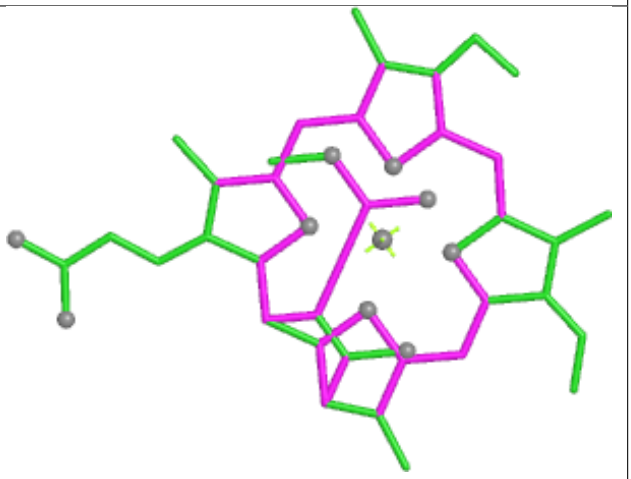
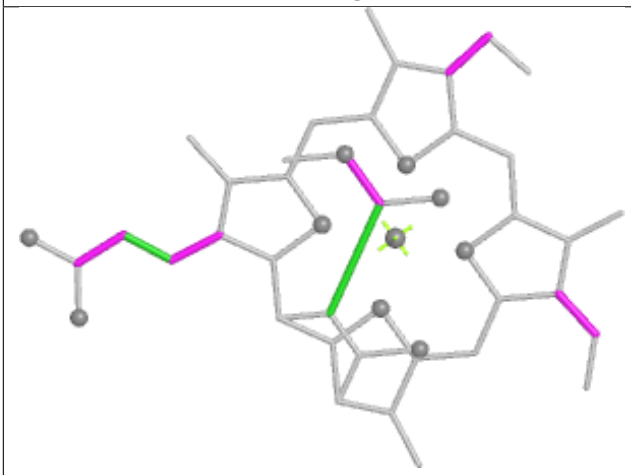


Bond angles



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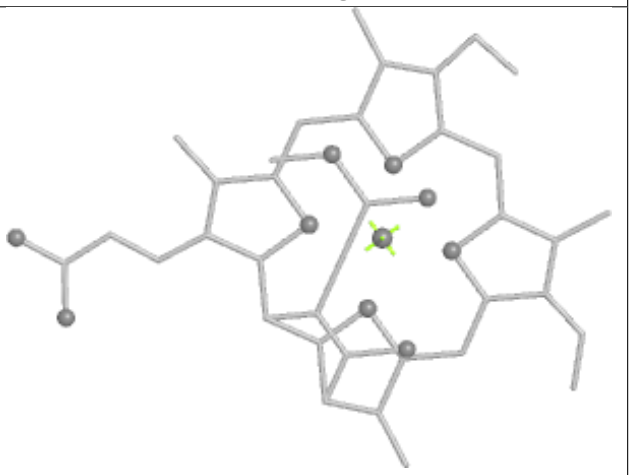
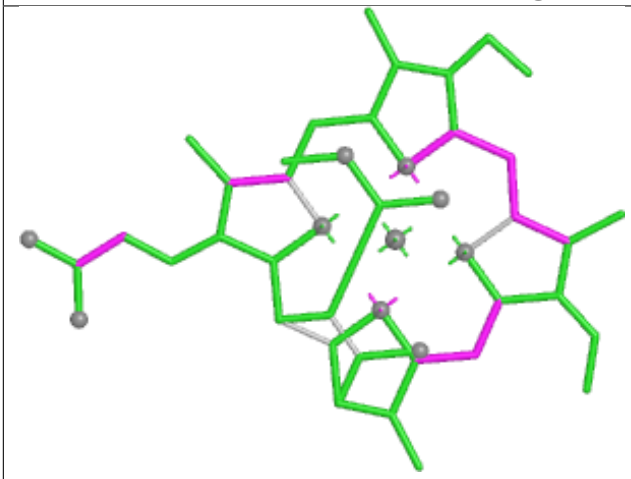
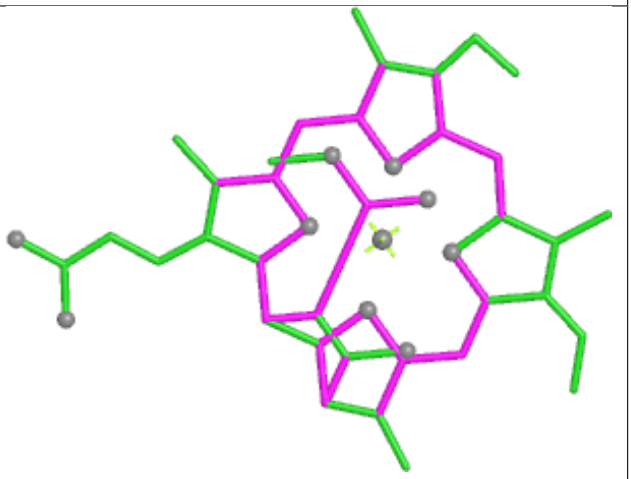


Rings

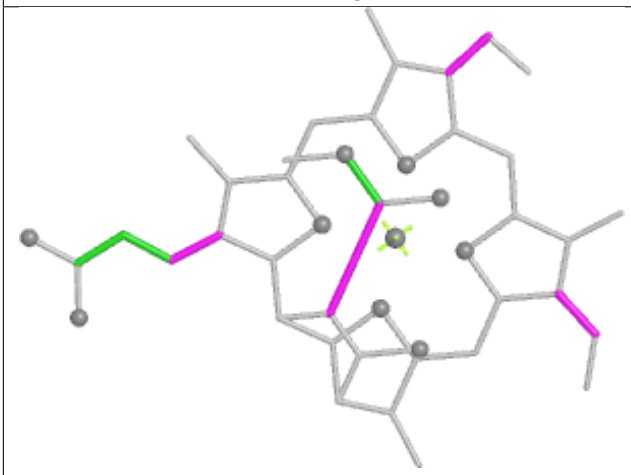
Ligand KC2 x 312



Bond lengths



Bond angles



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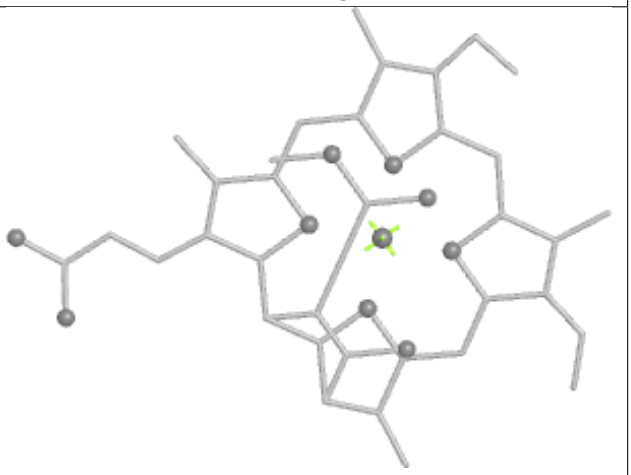
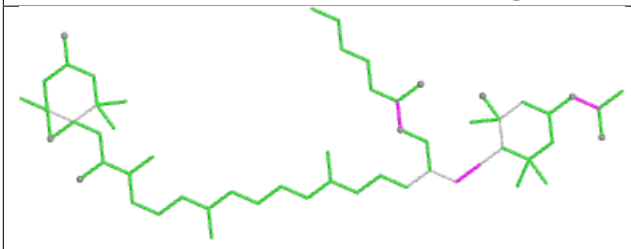


Rings

Ligand A1EB1 L 303



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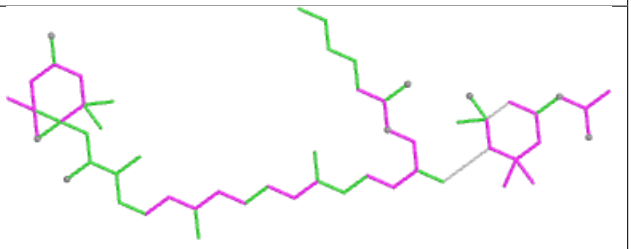
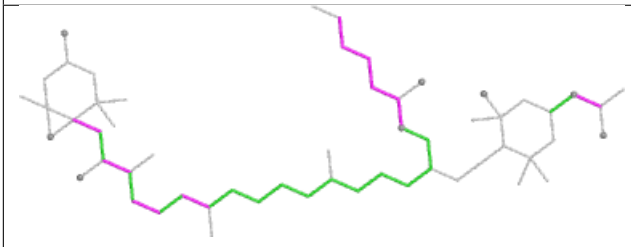


Bond angles



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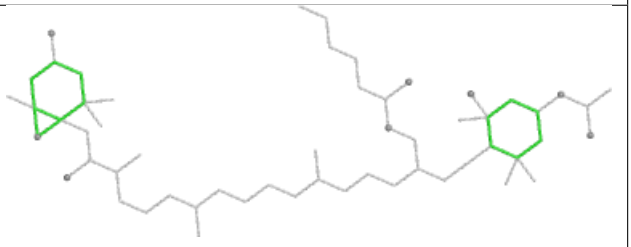
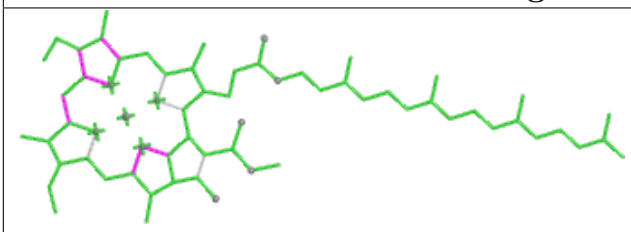


Rings

Ligand CLA b 809



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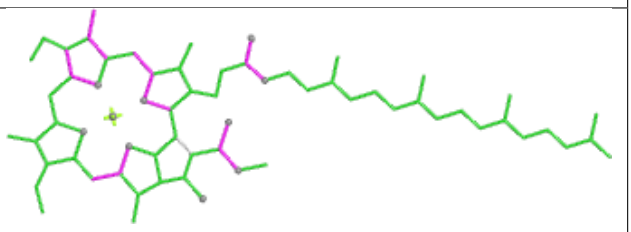
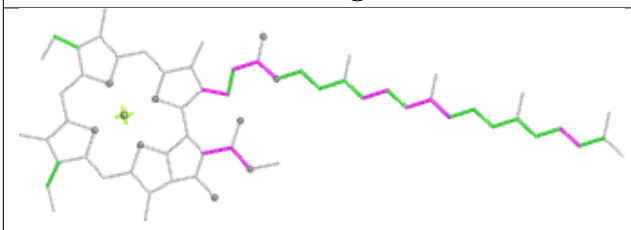


Bond angles



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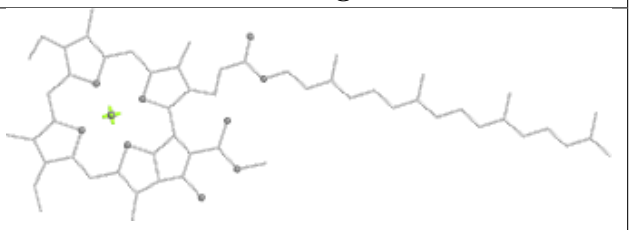
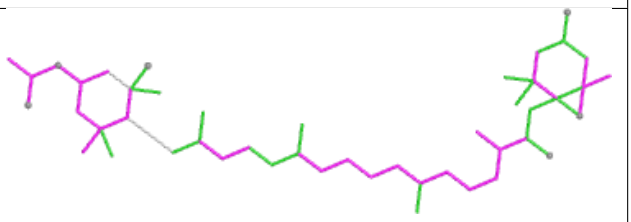


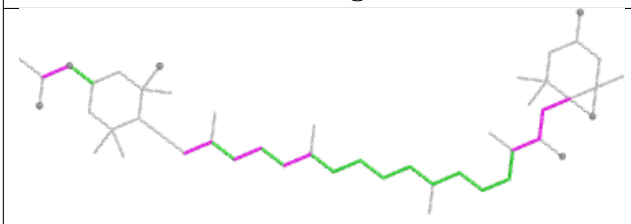
Rings

Ligand A86 P 302

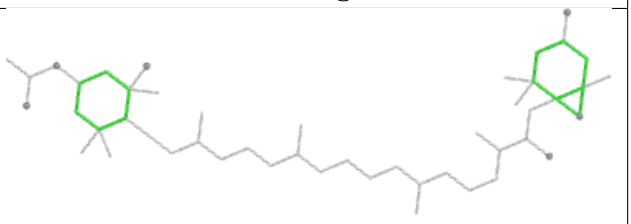
Bond lengths



Bond angles

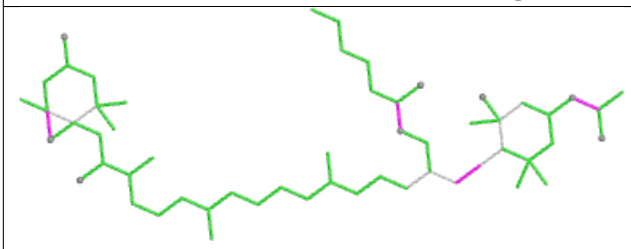


Torsions

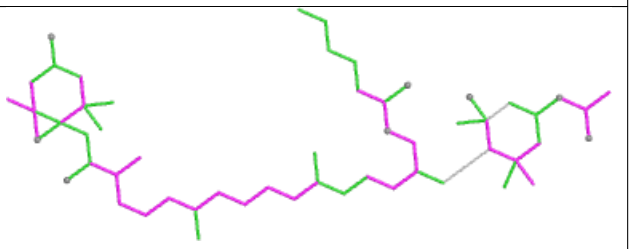


Rings

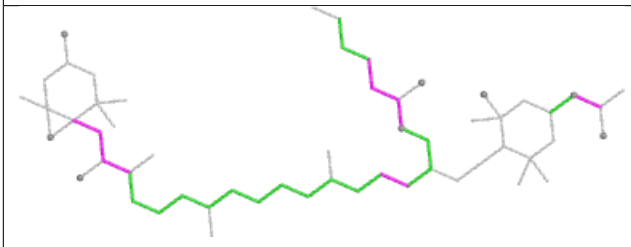
Ligand A1EB1 6 308



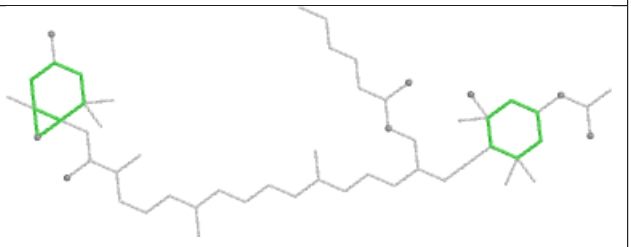
Bond lengths



Bond angles

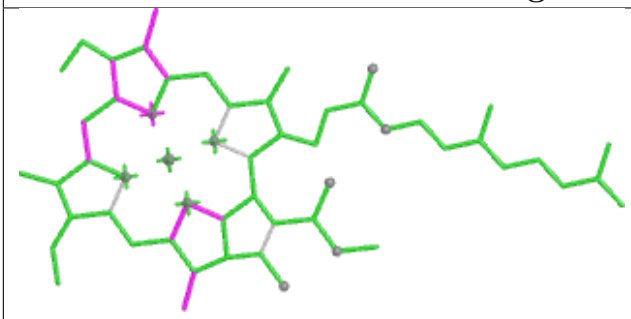


Torsions



Rings

Ligand CLA k 202



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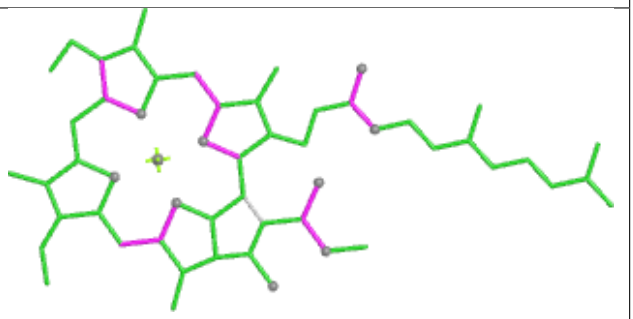
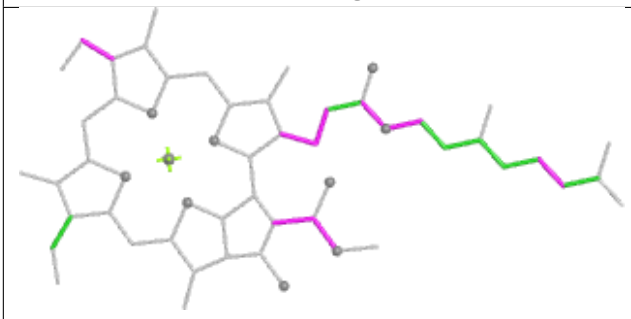
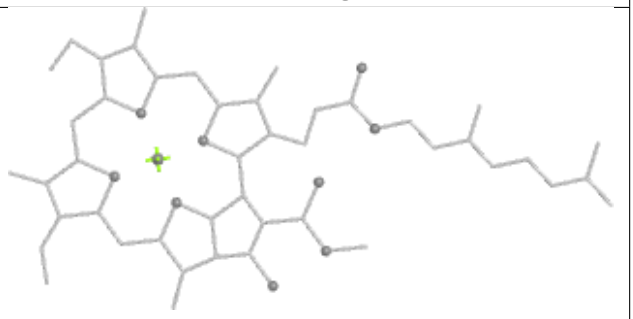


Bond angles

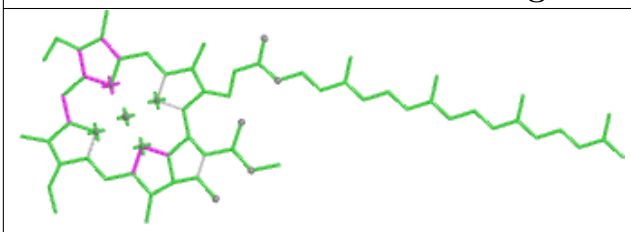


Torsions

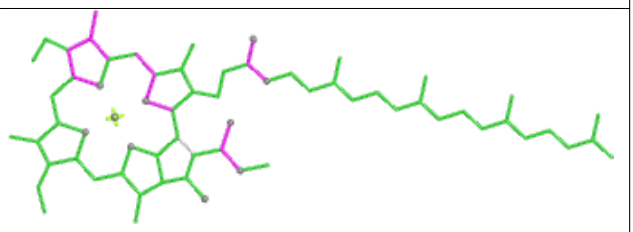


Rings

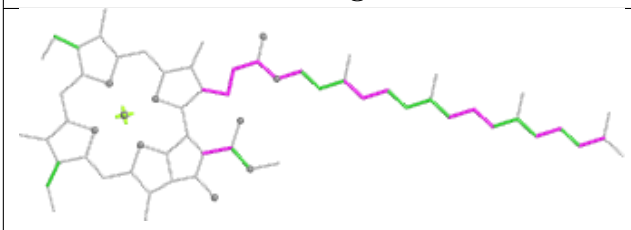
Ligand CLA J 309



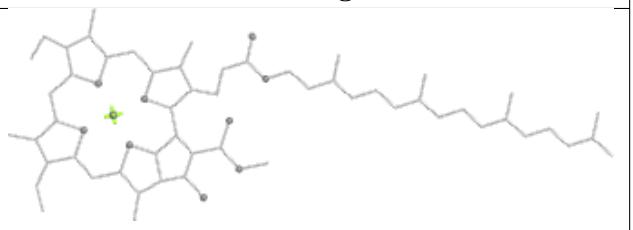
Bond lengths



Bond angles

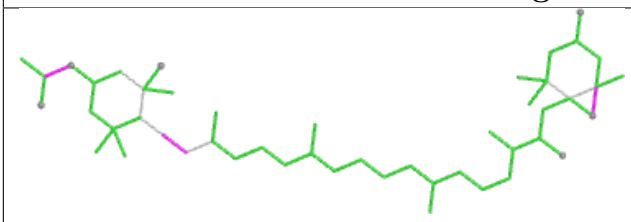


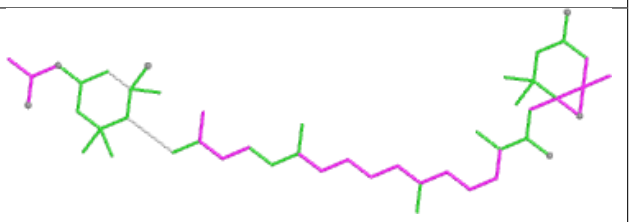
Torsions

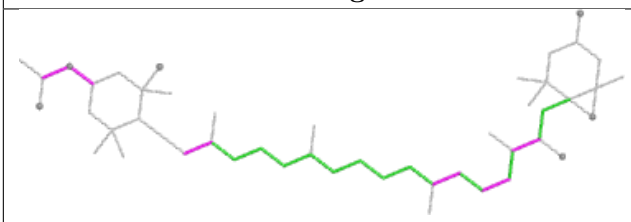


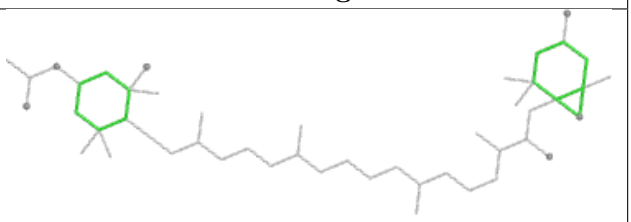
Rings

Ligand A86 L 306

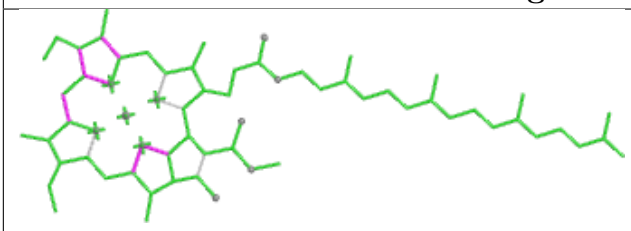

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA b 810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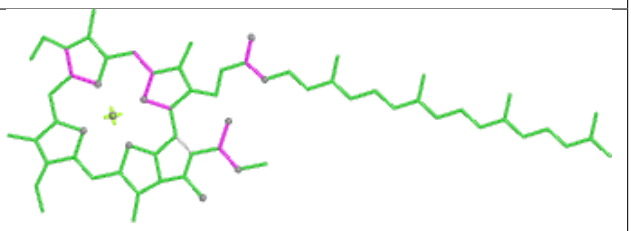
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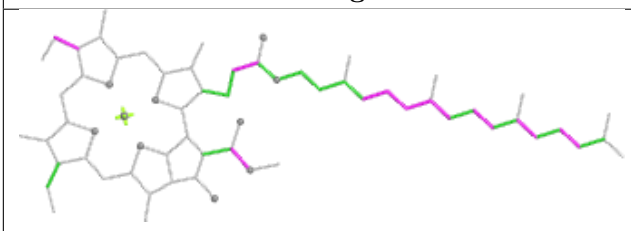
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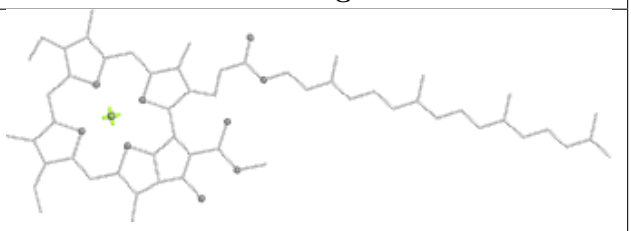
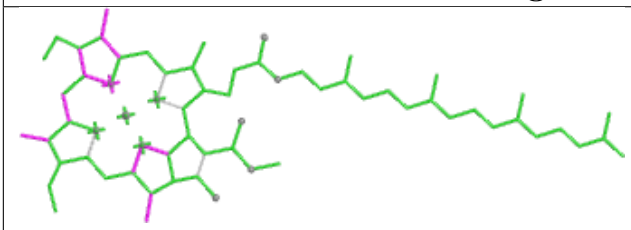

Rings

Ligand CLA b 811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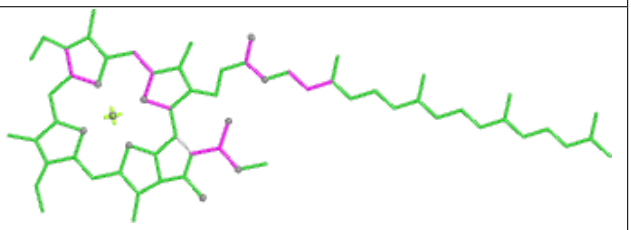
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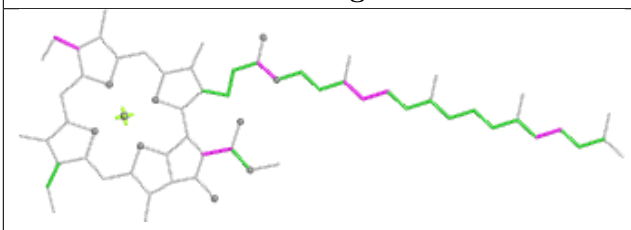
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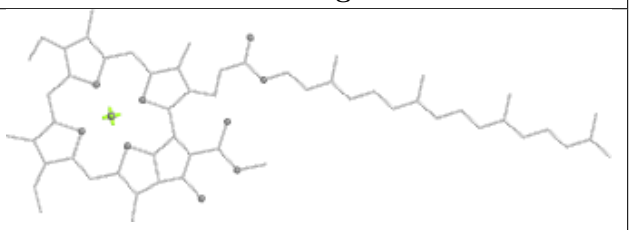
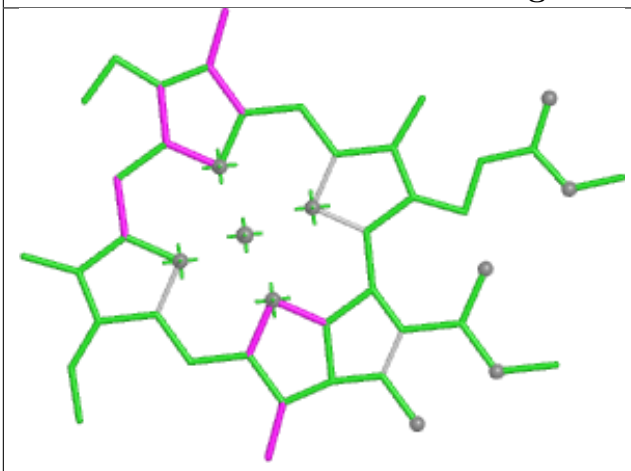

Rings

Ligand CLA 2 308



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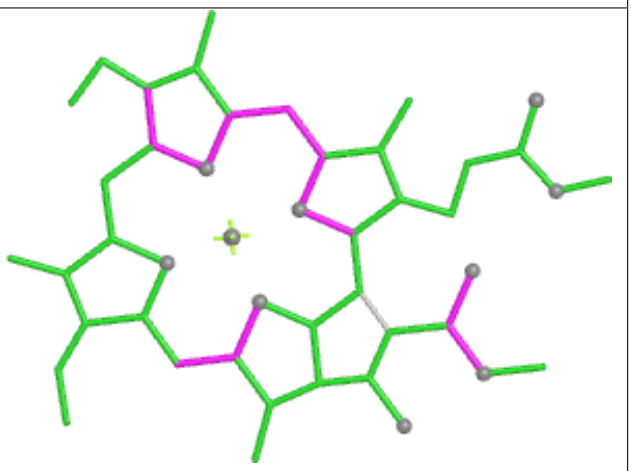

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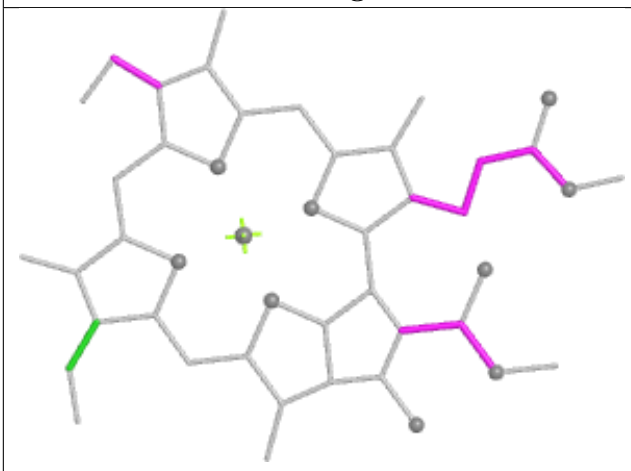

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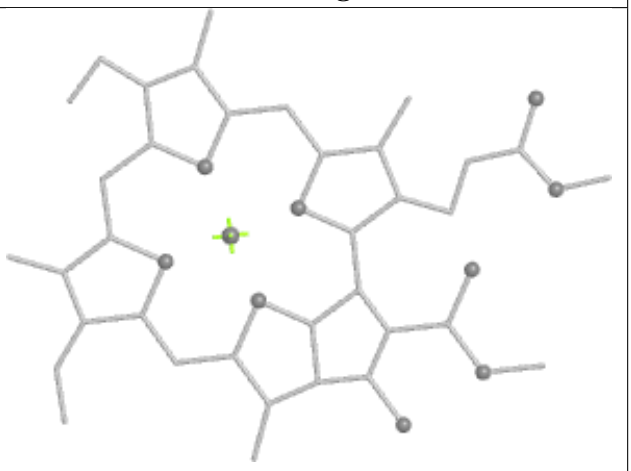
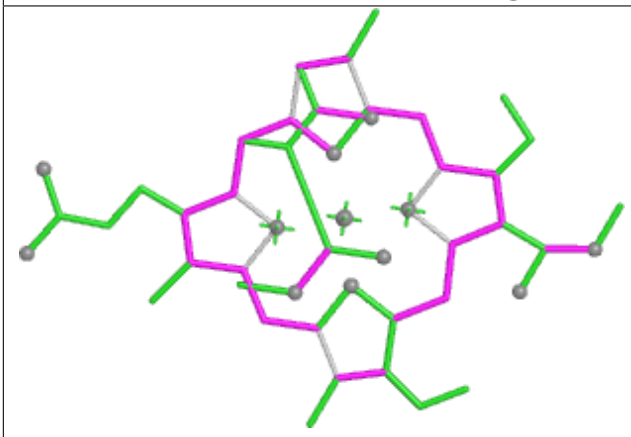


Rings

Ligand A1ECV 9 314



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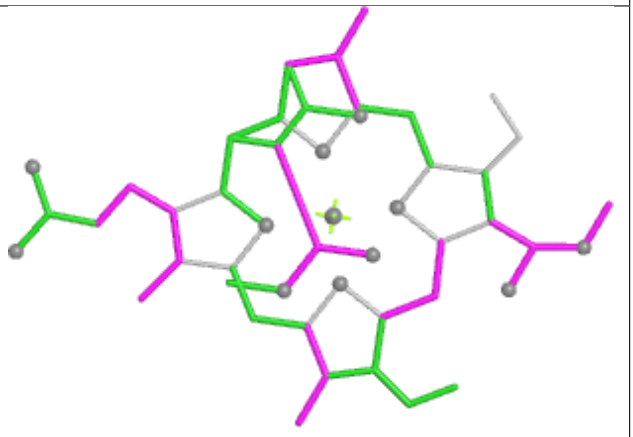

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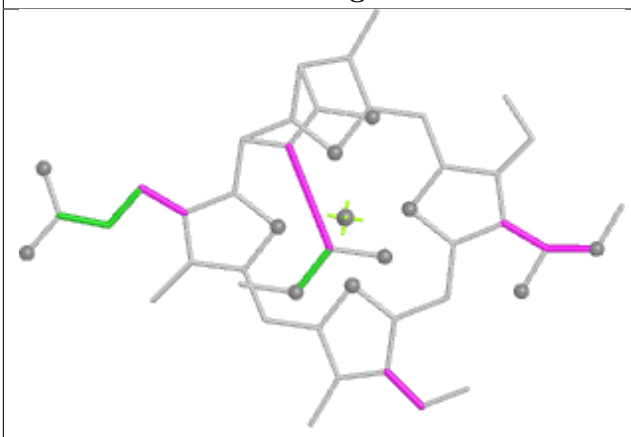

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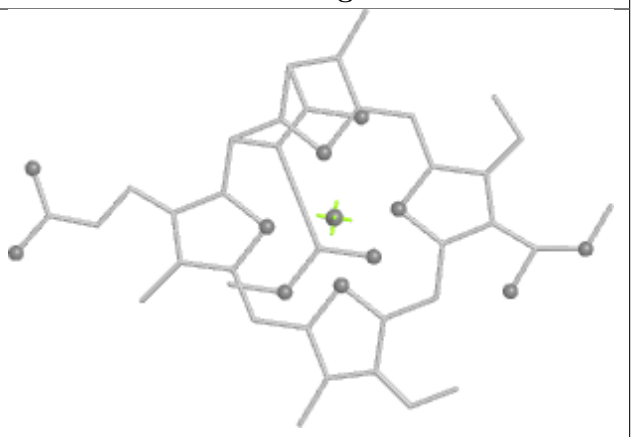
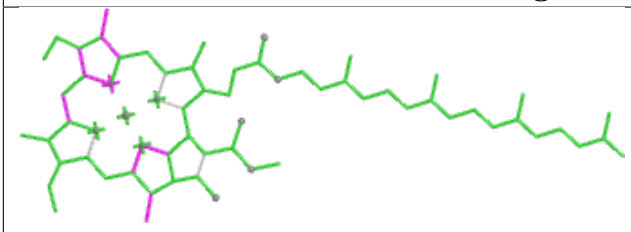


Rings

Ligand CLA i 103



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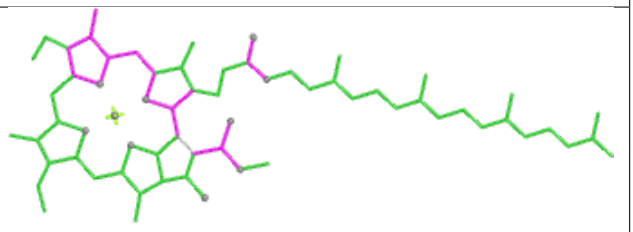

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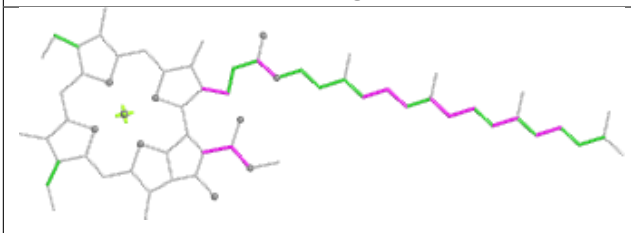

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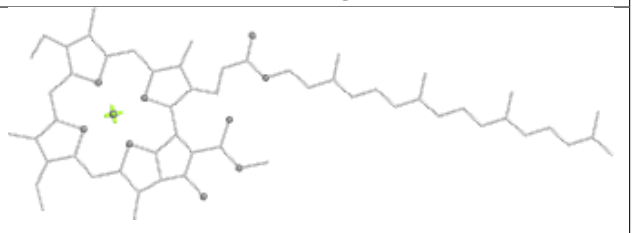
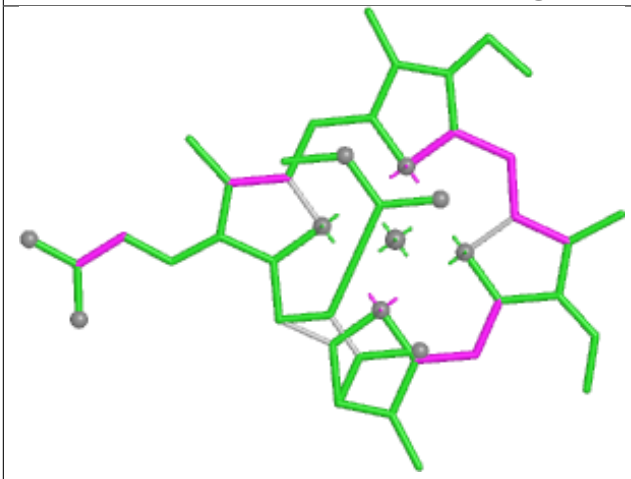


Rings

Ligand KC2 4 320



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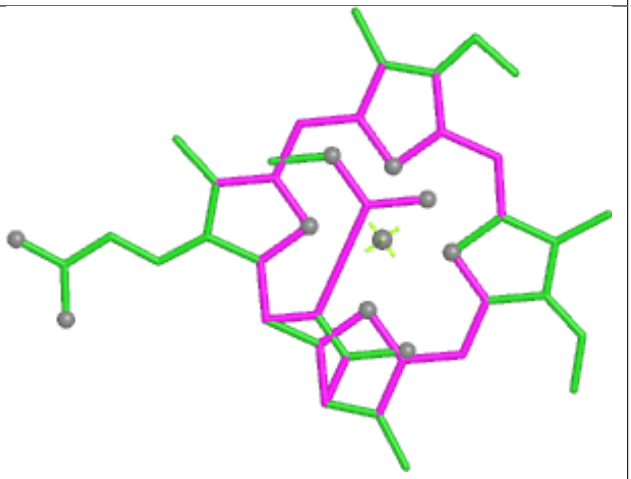

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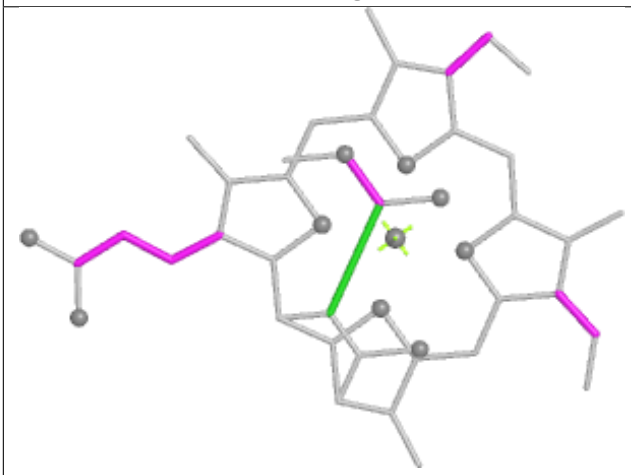

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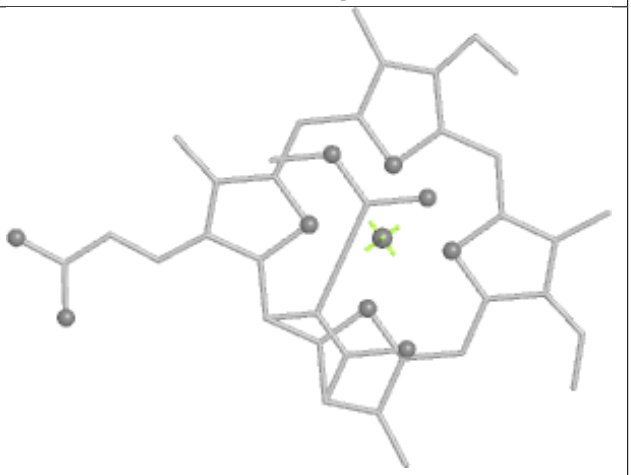
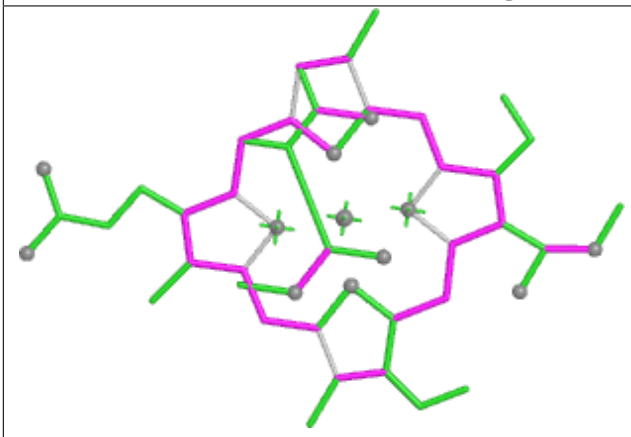


Rings

Ligand A1ECV R 313



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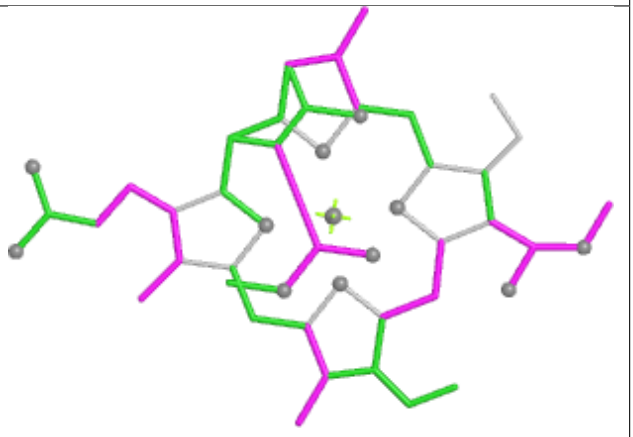
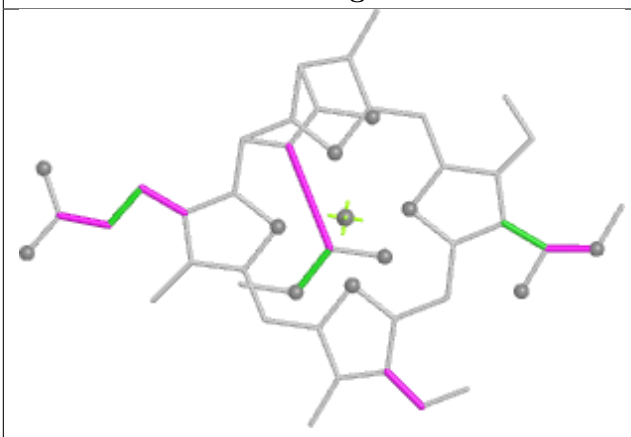


Bond angles



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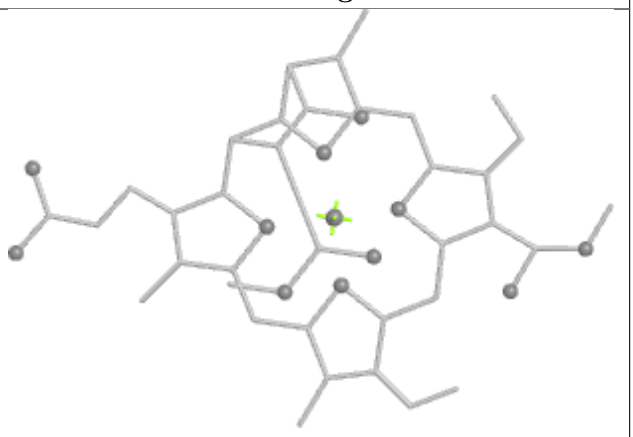
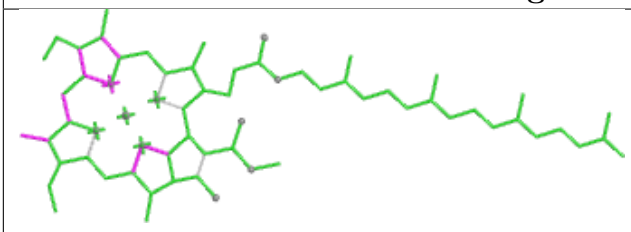


Rings

Ligand CLA b 815



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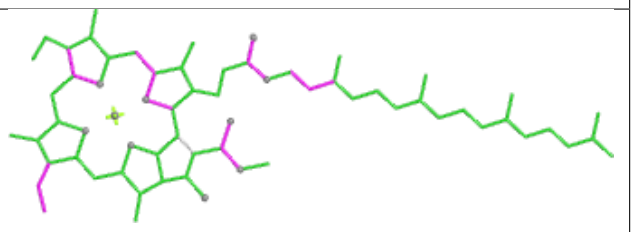
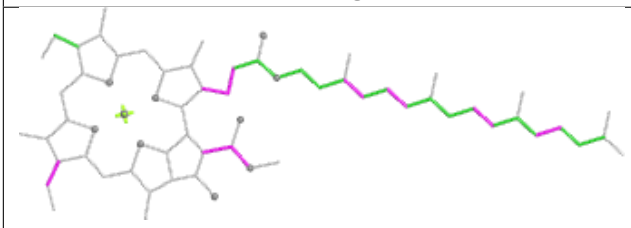


Bond angles



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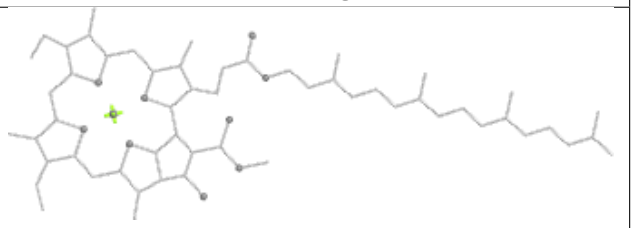
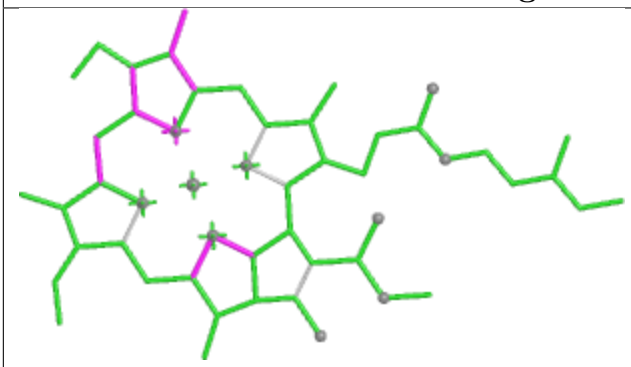


Rings

Ligand CLA W 318



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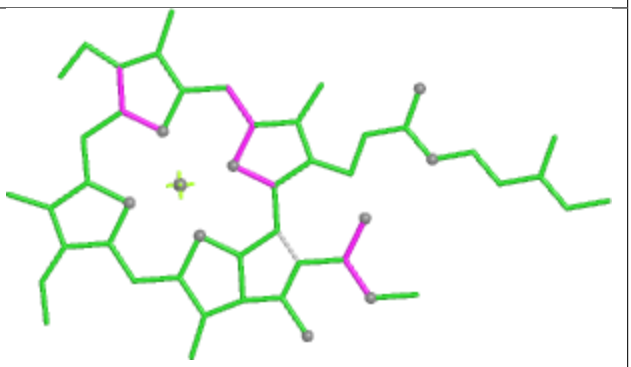

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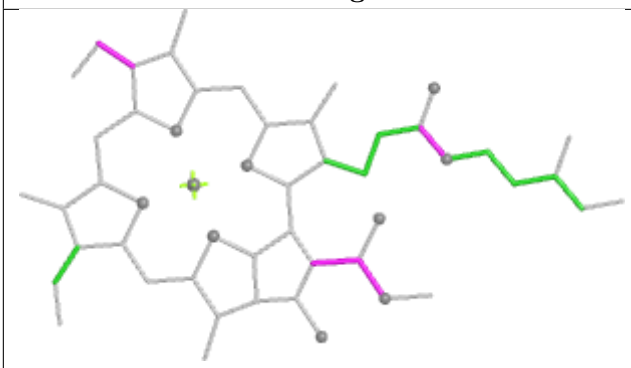

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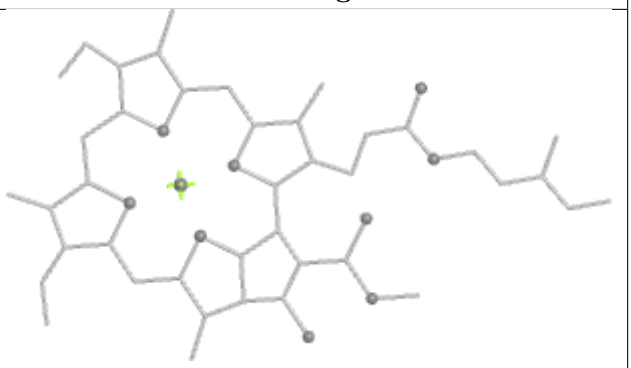
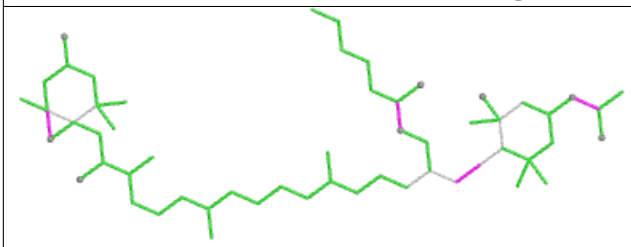


Rings

Ligand A1EB1 2 304



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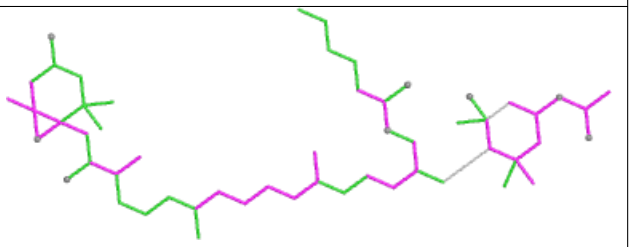
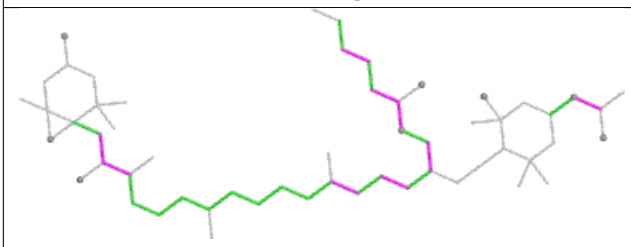


Bond angles



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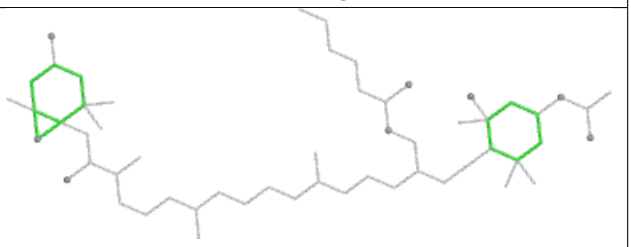
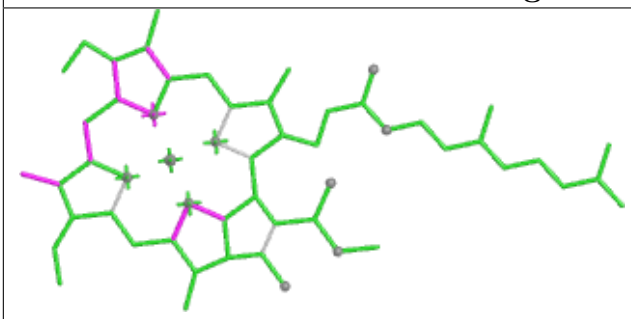
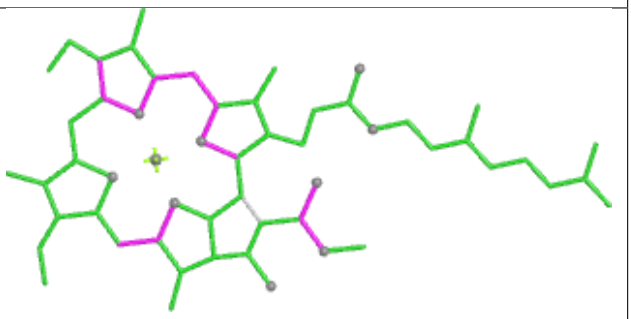
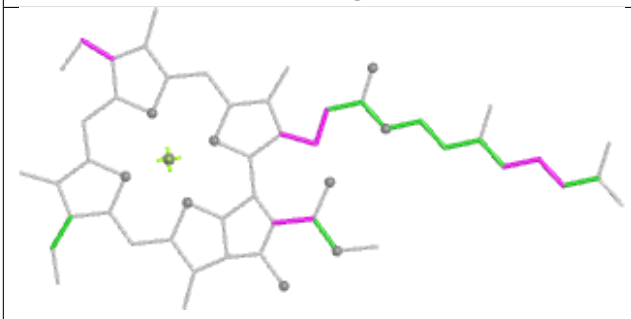
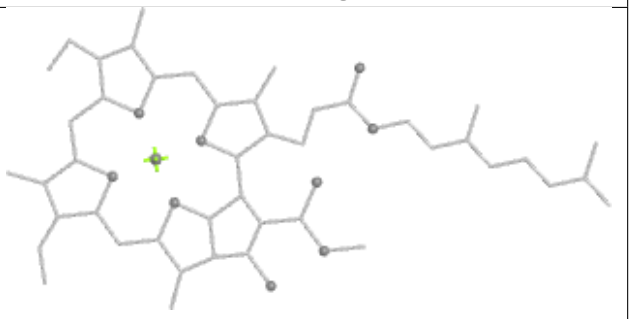
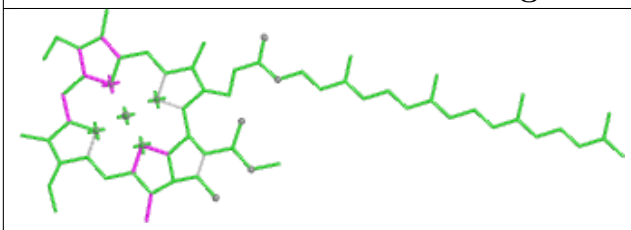
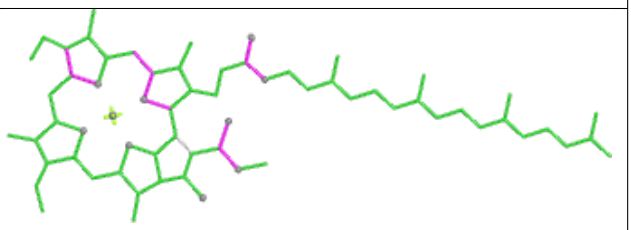
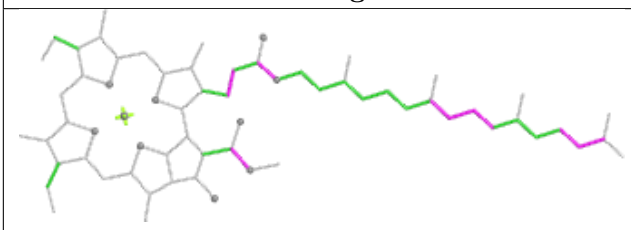
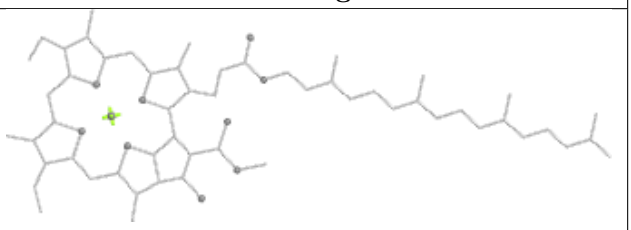
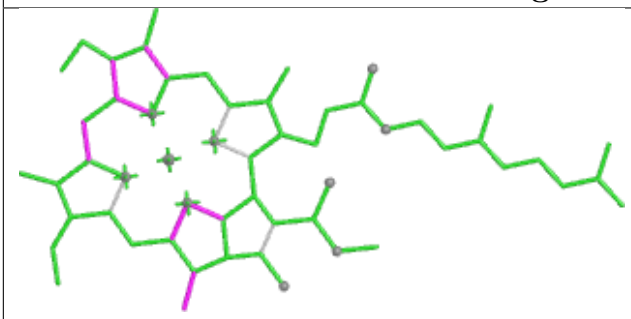


Rings

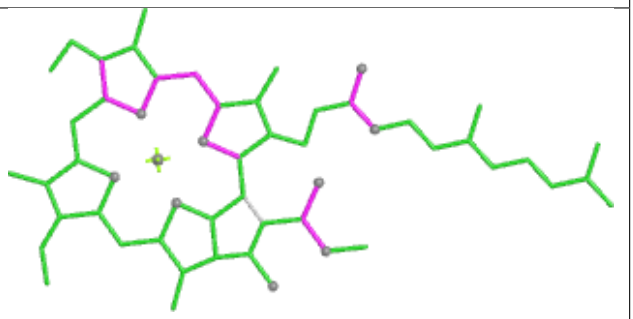
Ligand CLA O 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA M 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

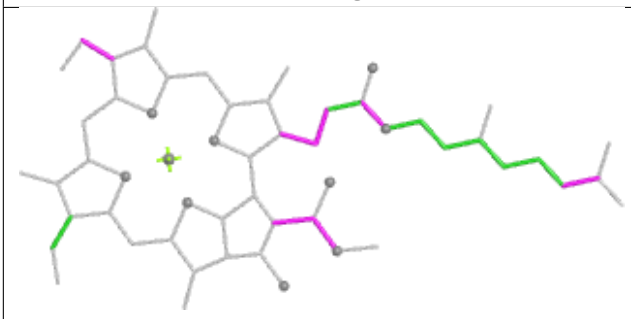
Ligand CLA f 803



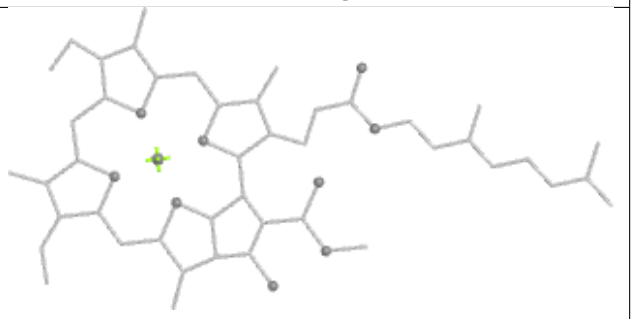
Bond lengths



Bond angles

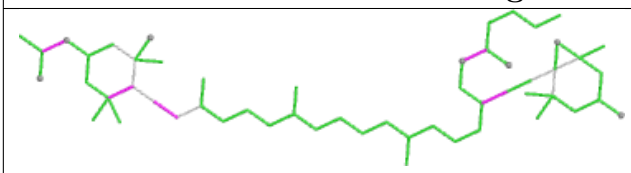


Torsions



Rings

Ligand A1EB4 P 318



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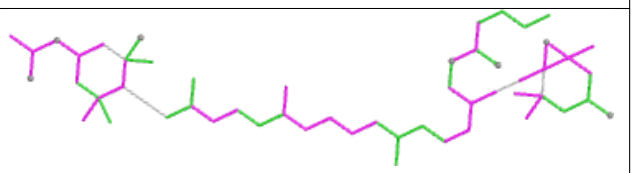

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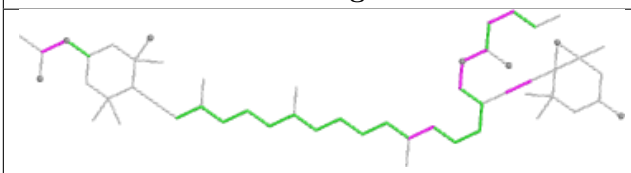

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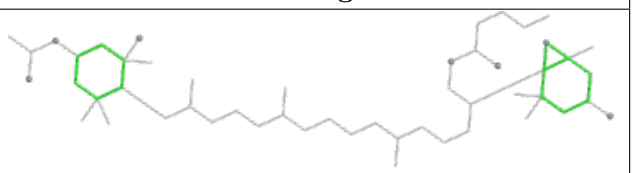
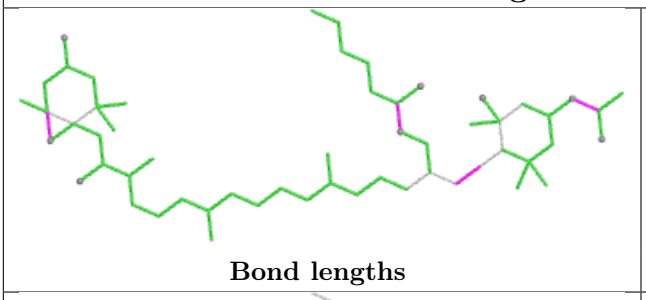


Rings

Ligand A1EB1 3 310



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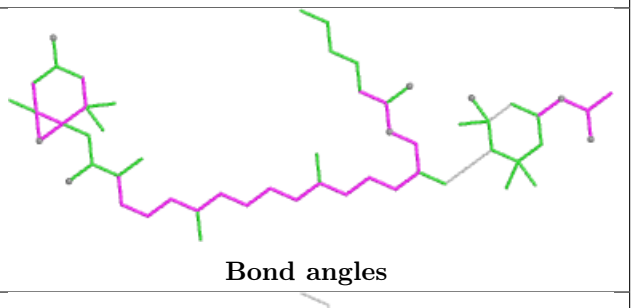

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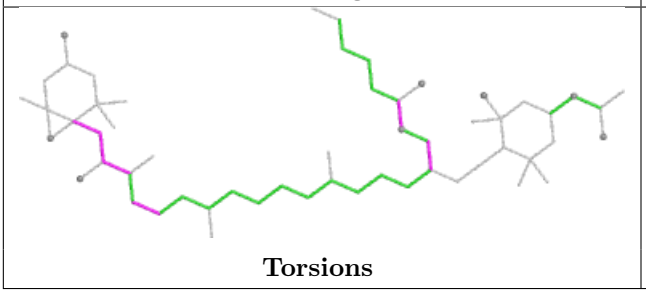

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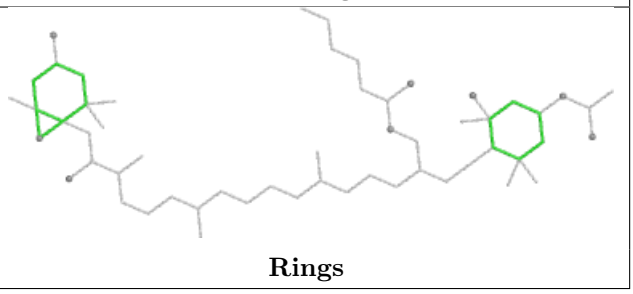
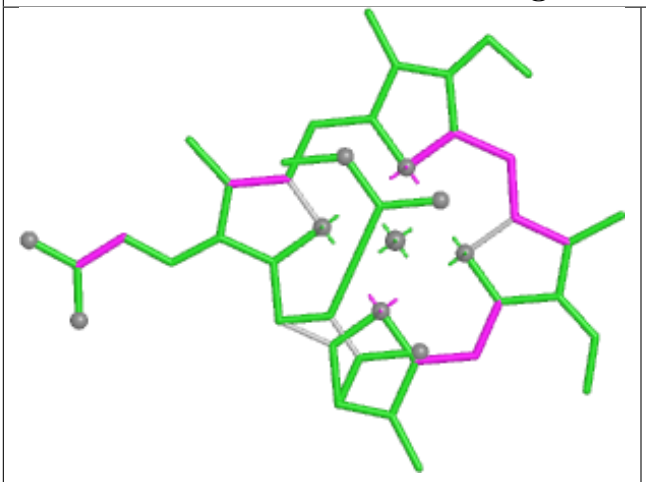


Rings

Ligand KC2 9 311



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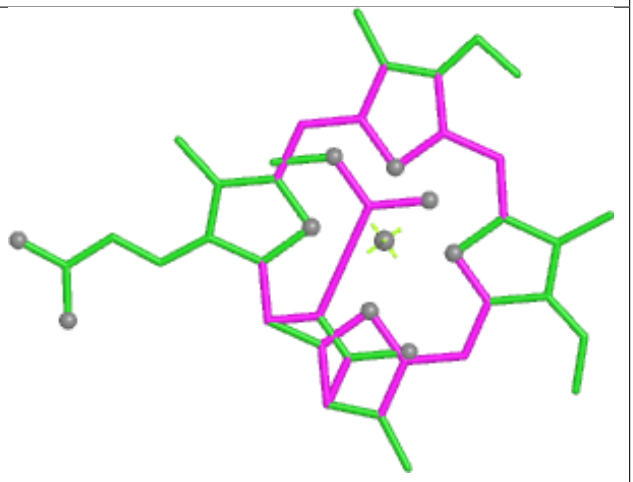

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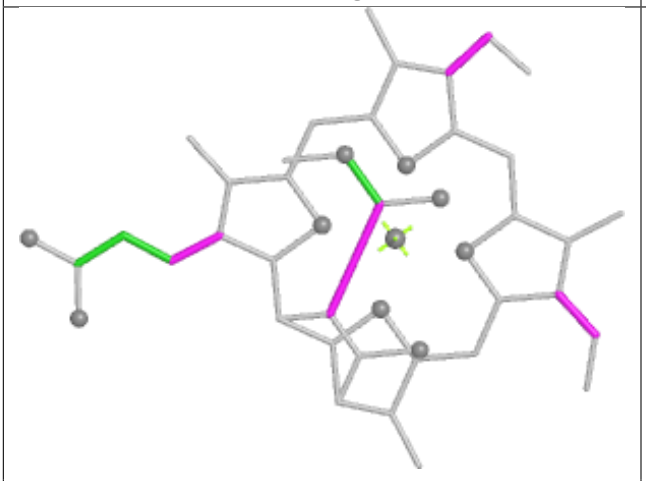

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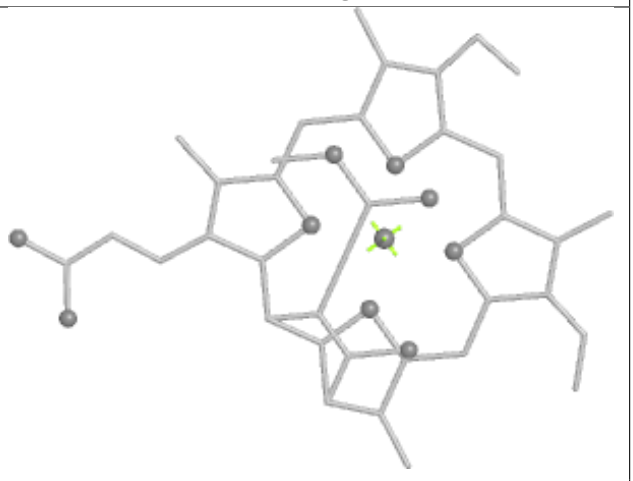
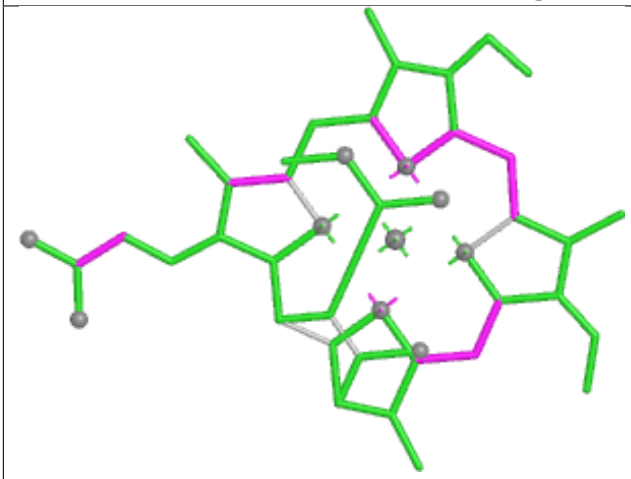


Rings

Ligand KC2 3 318



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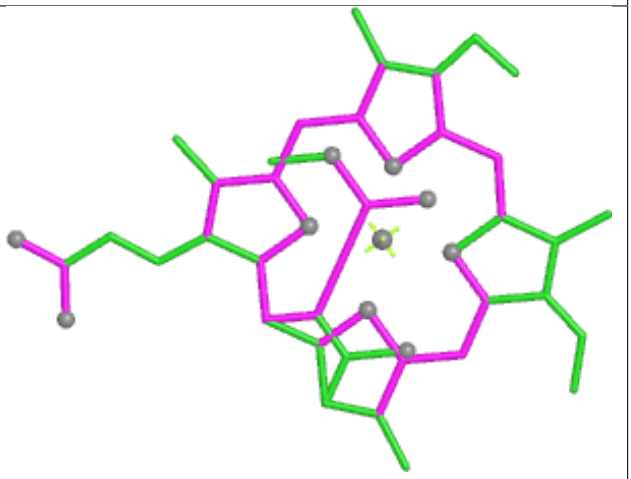

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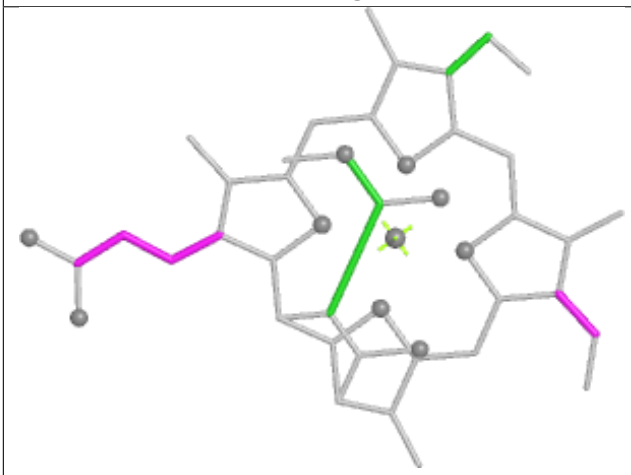

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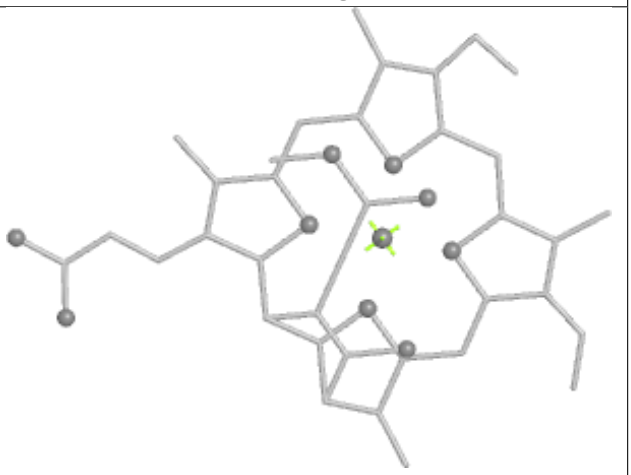
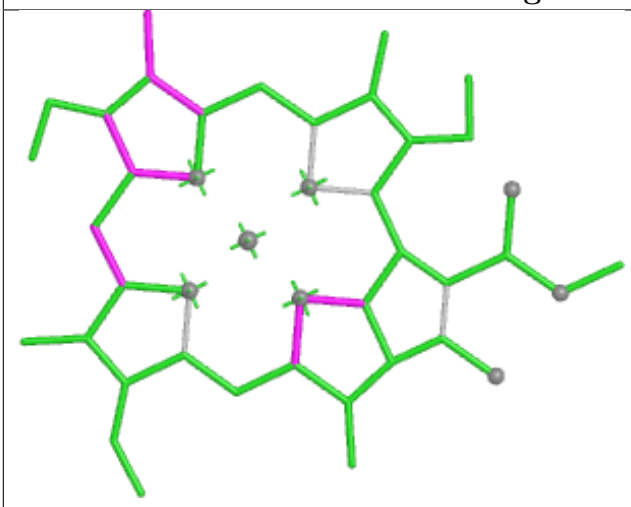


Rings

Ligand CLA O 311



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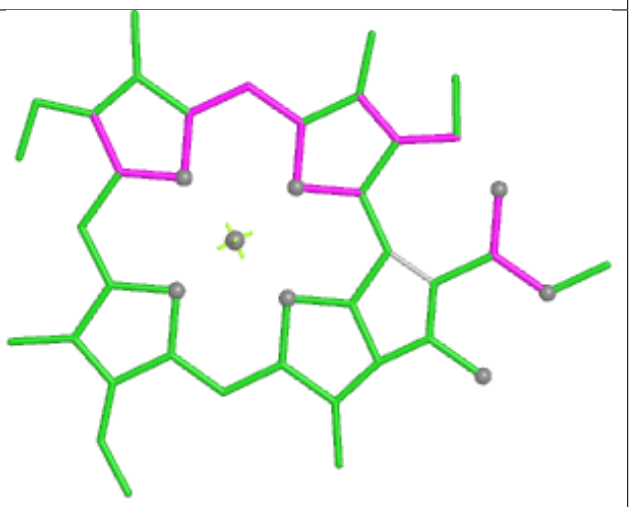

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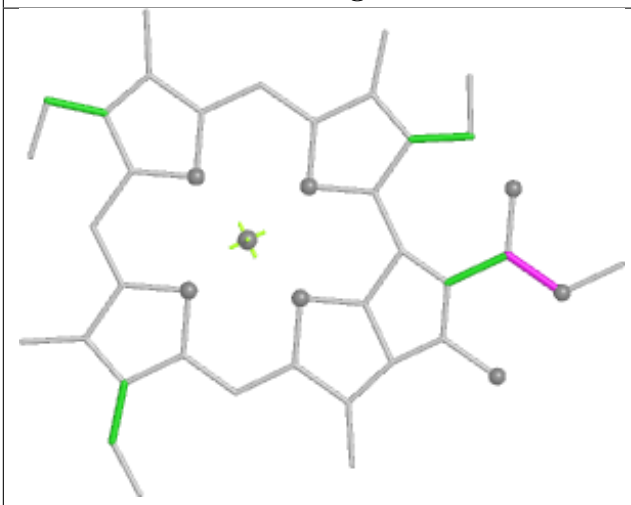

Torsions

Rings

Ligand BCR a 844

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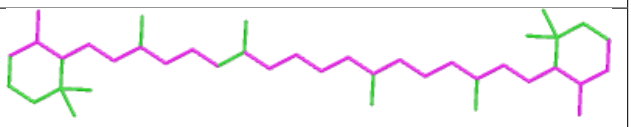

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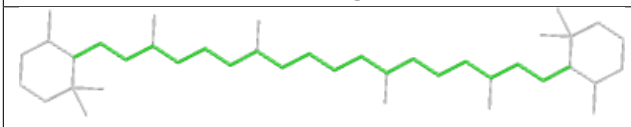

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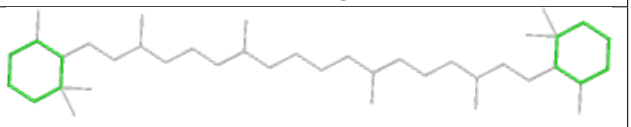
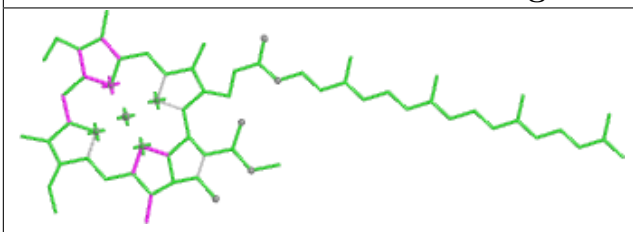


Rings

Ligand CLA 7 316



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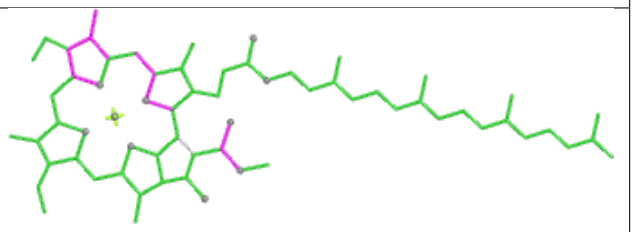

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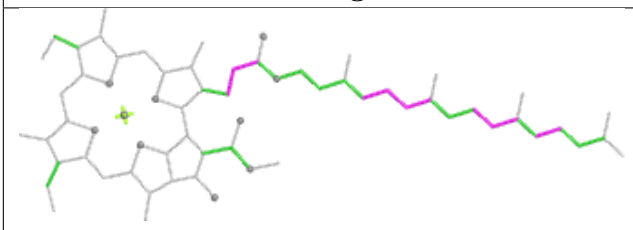

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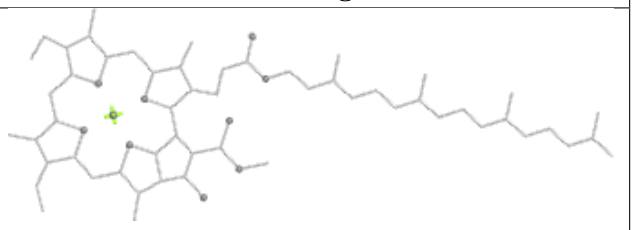
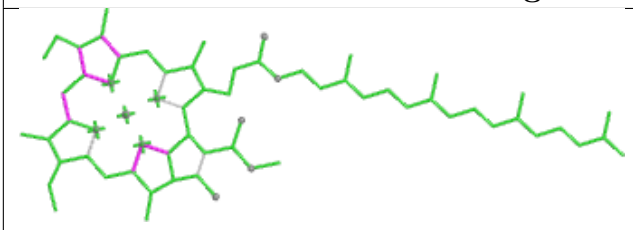


Rings

Ligand CLA A 314



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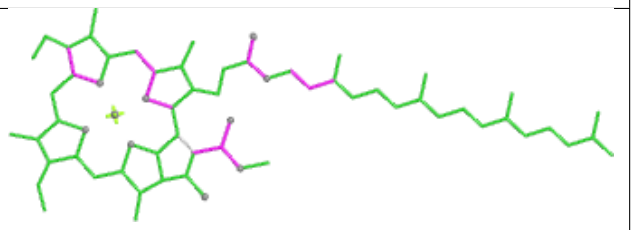

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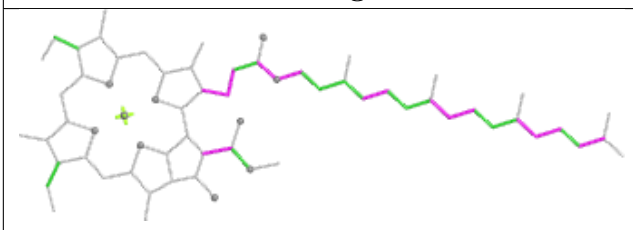

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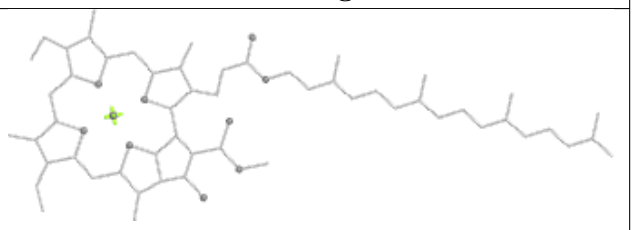
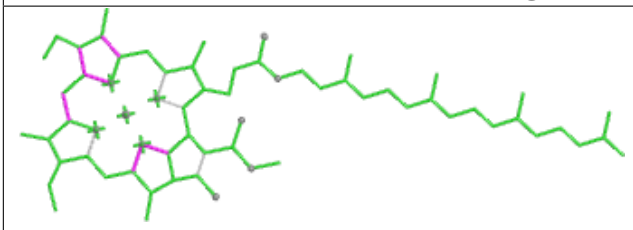


Rings

Ligand CLA K 311



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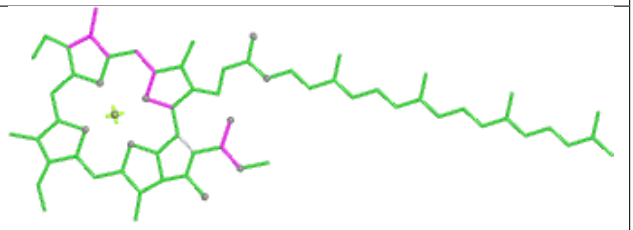
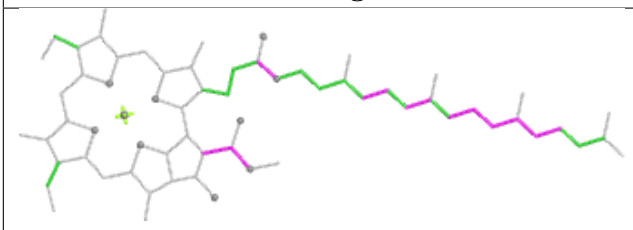


Bond angles



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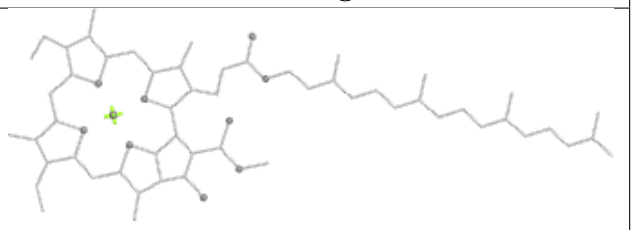
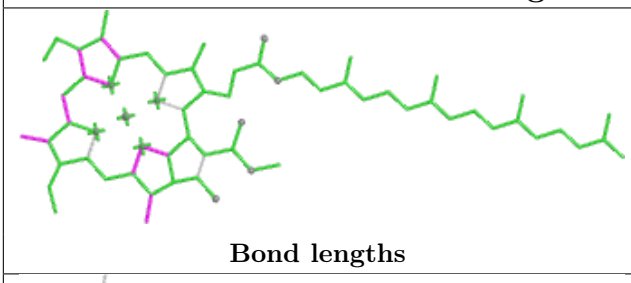


Rings

Ligand CLA b 807



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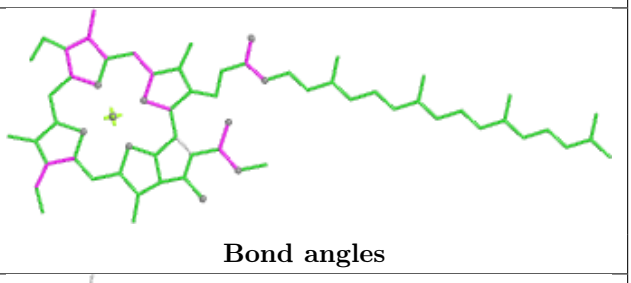

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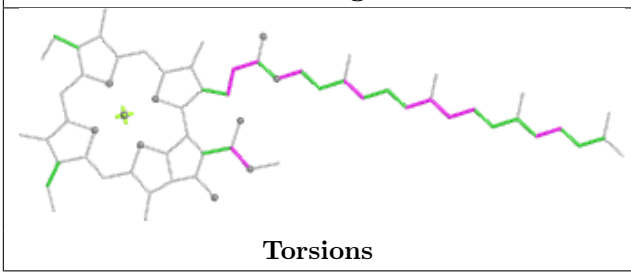

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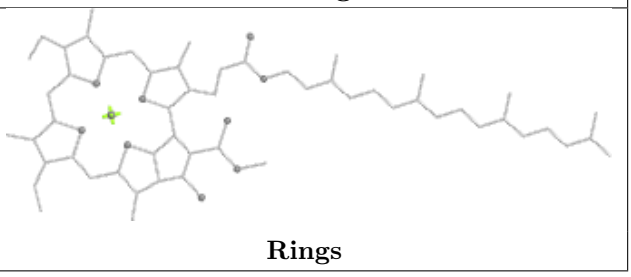
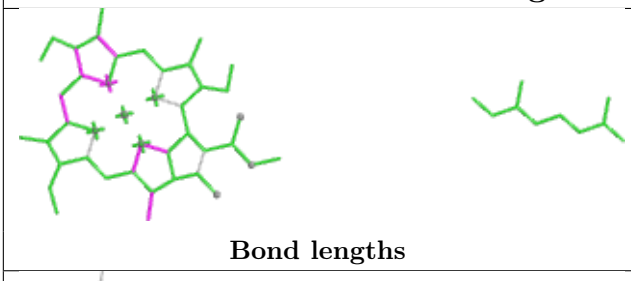


Rings

Ligand CLA 6 312



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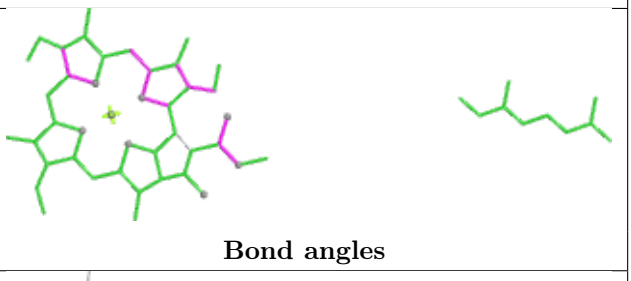

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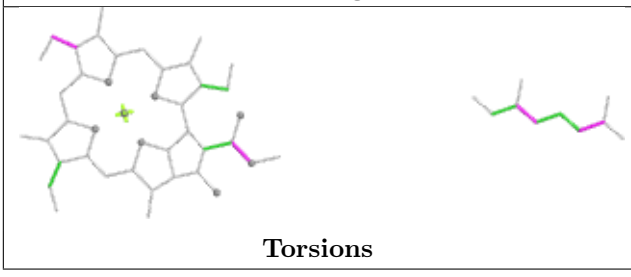

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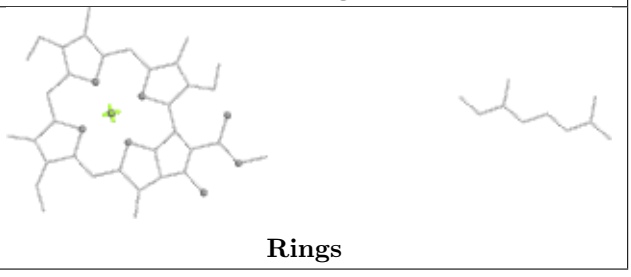
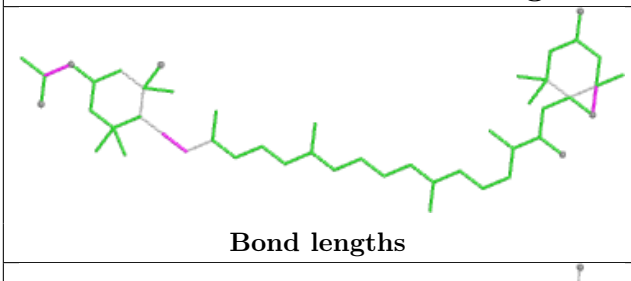


Rings

Ligand A86 M 306



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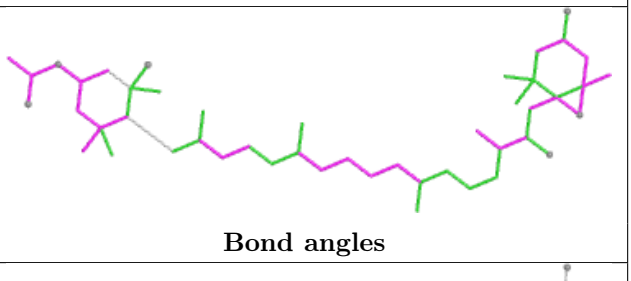

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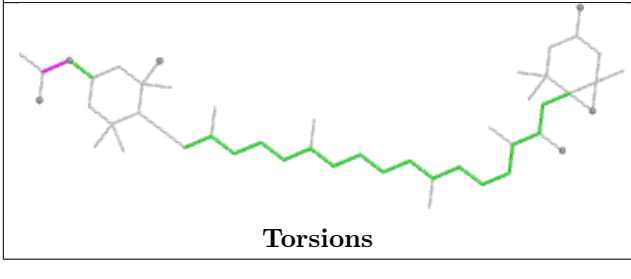
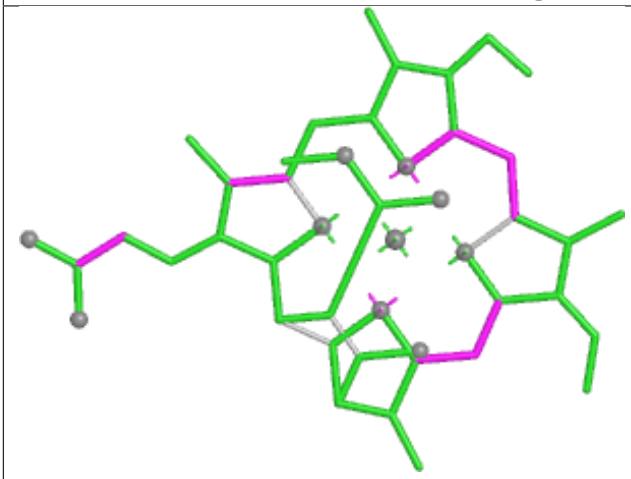


Torsions

Rings

Ligand KC2 8 320



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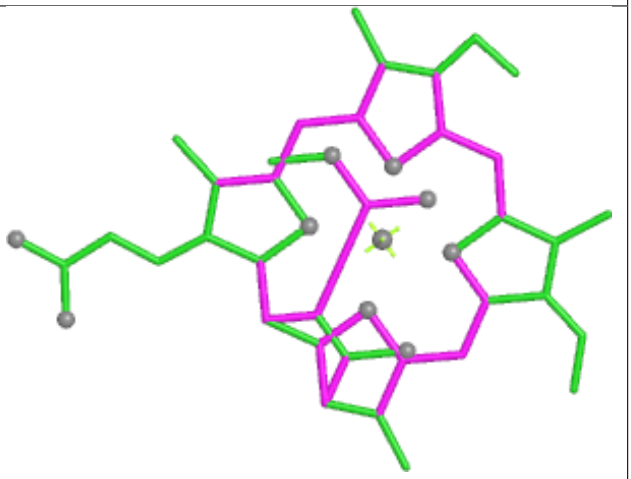
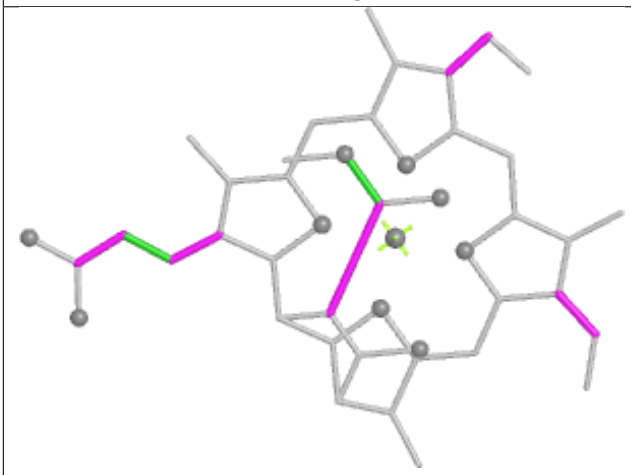


Bond angles



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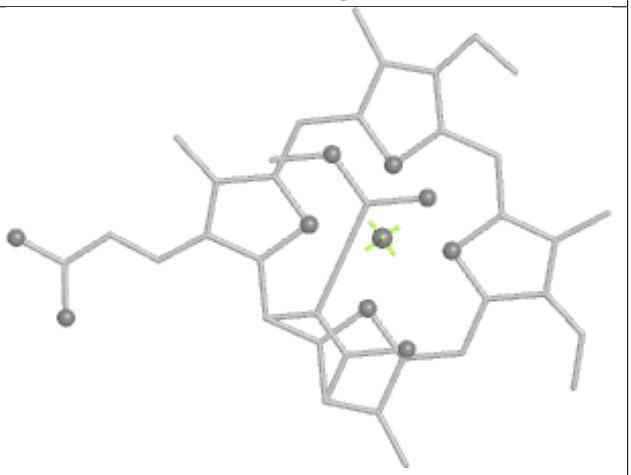
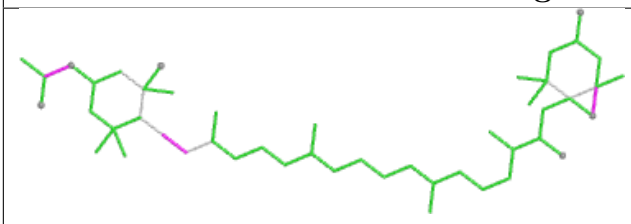


Rings

Ligand A86 0 301



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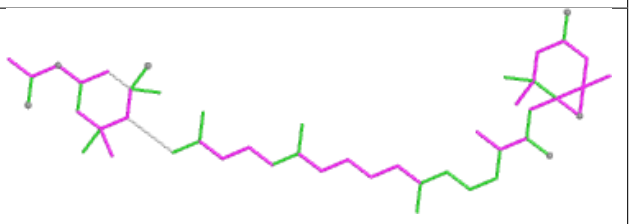
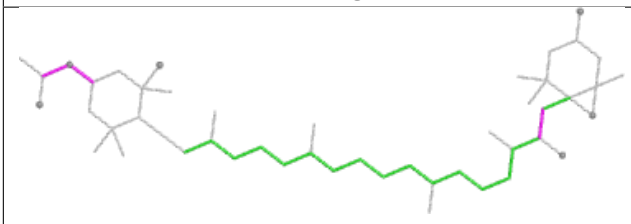


Bond angles



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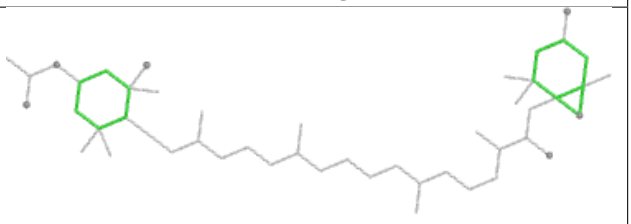
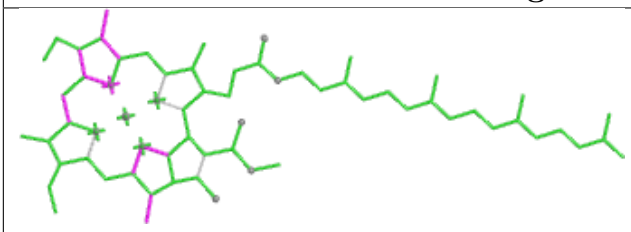
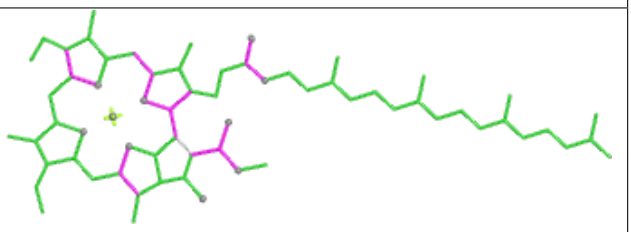


Rings

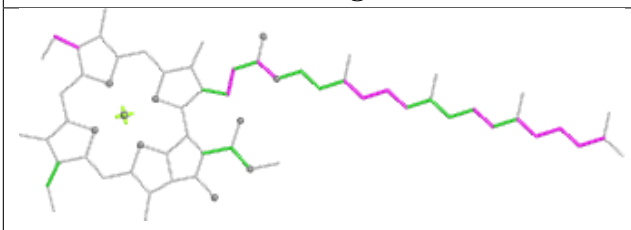
Ligand CLA b 825



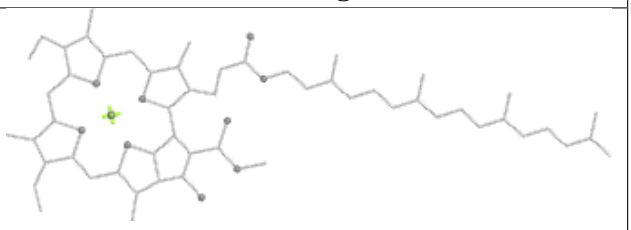
Bond lengths



Bond angles

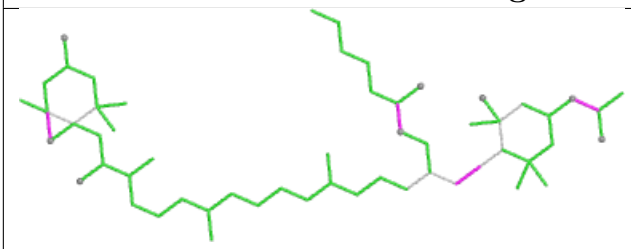


Torsions



Rings

Ligand A1EB1 y 301



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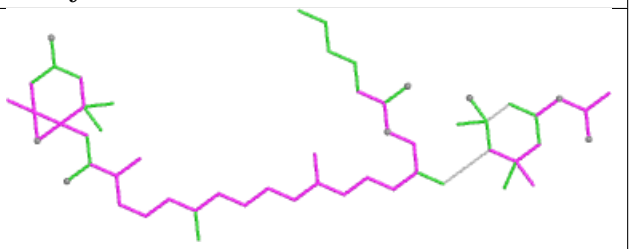
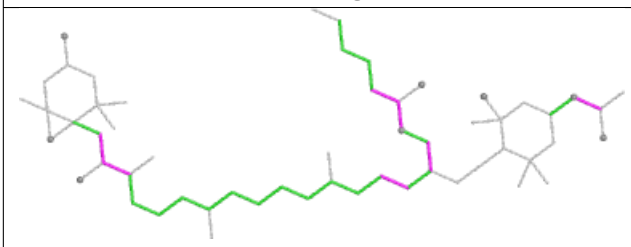
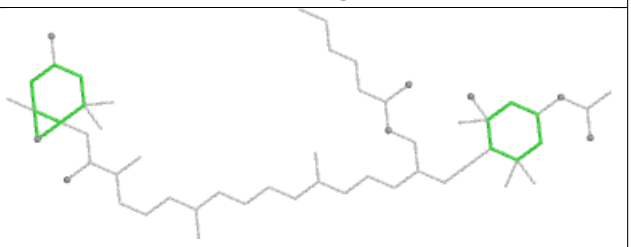


Bond angles

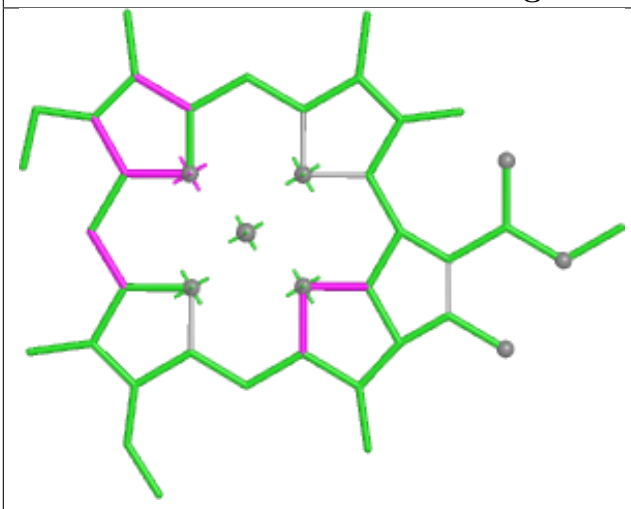


Torsions



Rings

Ligand CLA Y 303



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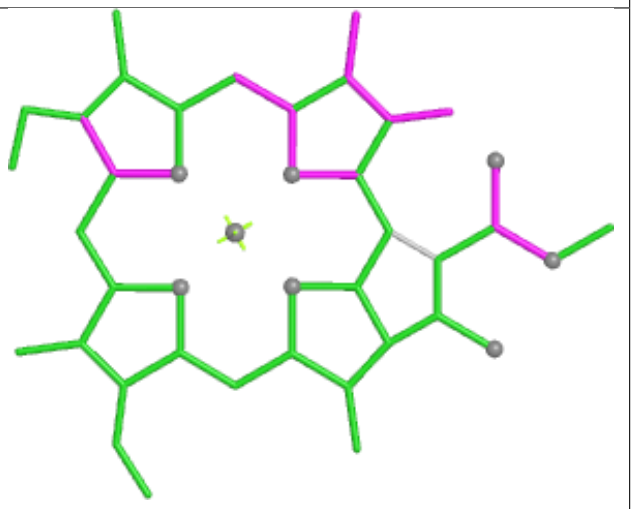
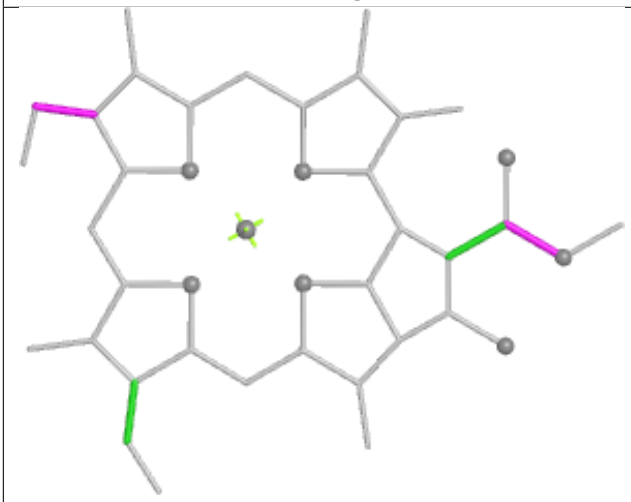
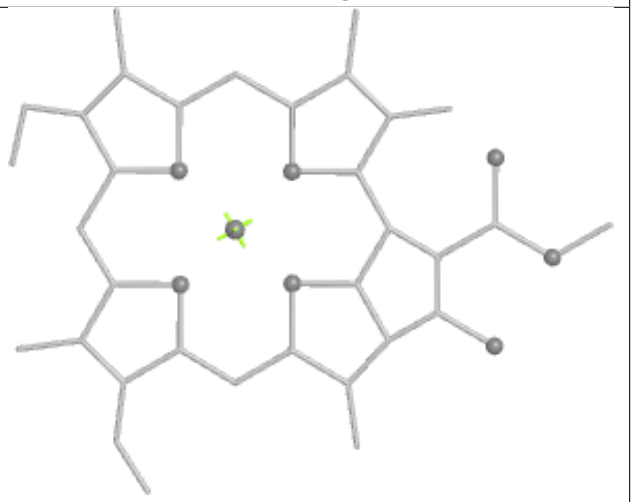


Bond angles

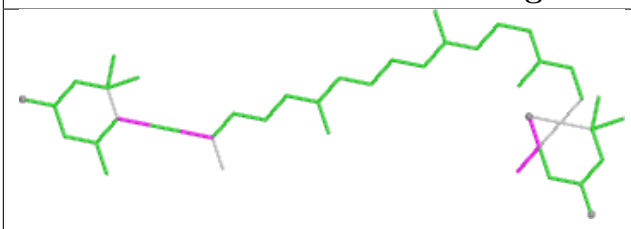


Torsions



Rings

Ligand DD6 C 301



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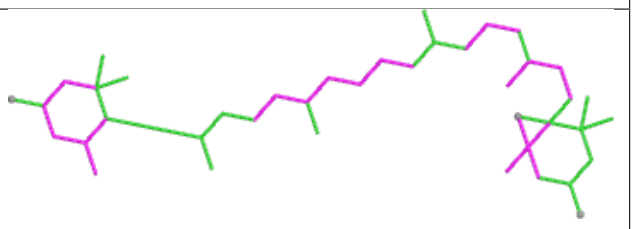
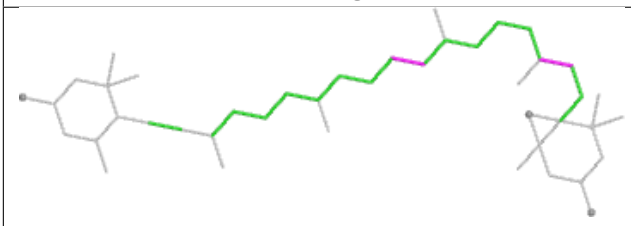


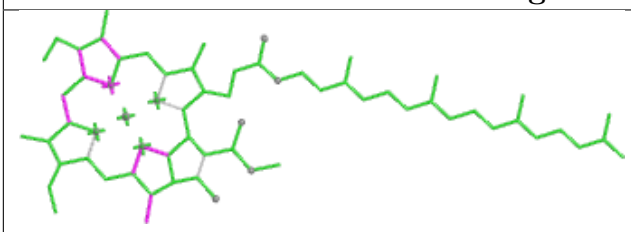
Bond angles



Torsions

Rings

Ligand CLA a 823



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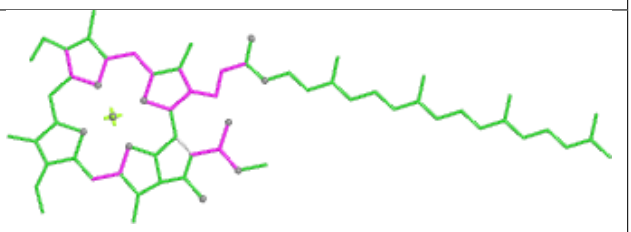
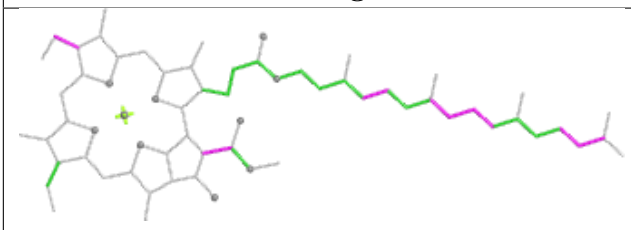


Bond angles



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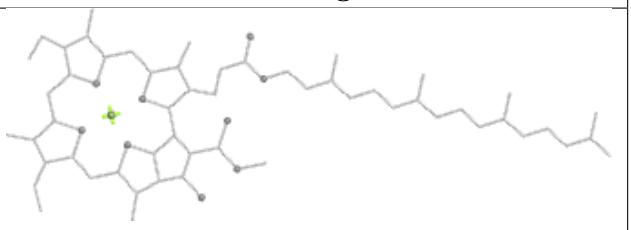
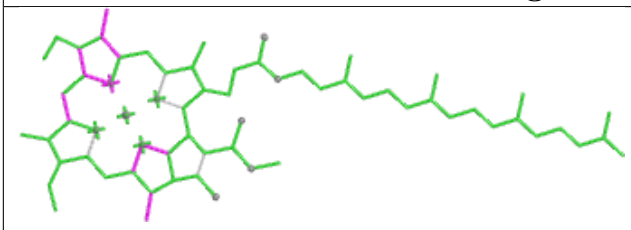


Rings

Ligand CLA F 308



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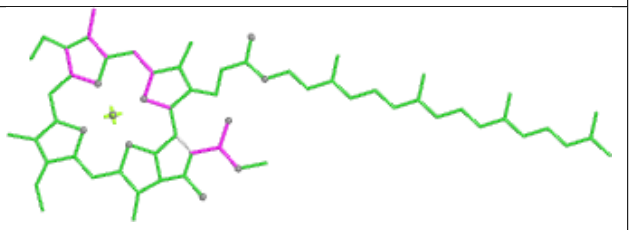

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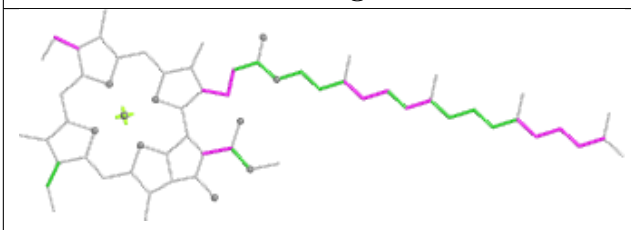

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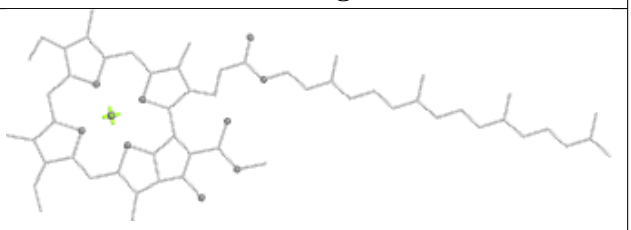
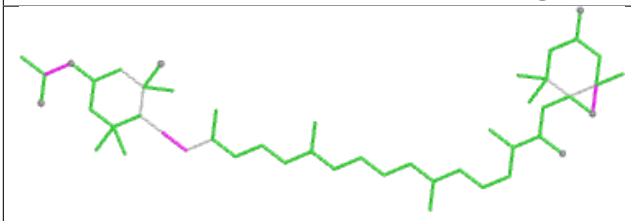


Rings

Ligand A86 k 206



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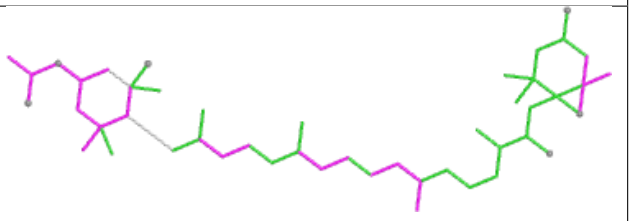

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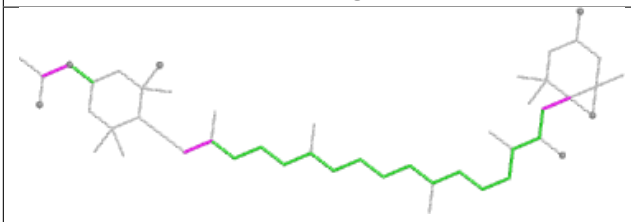

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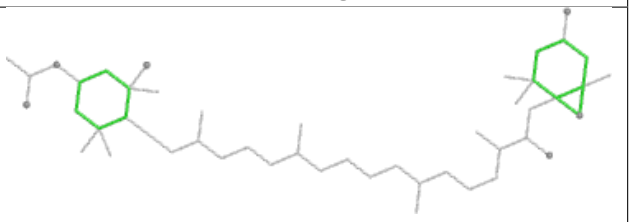
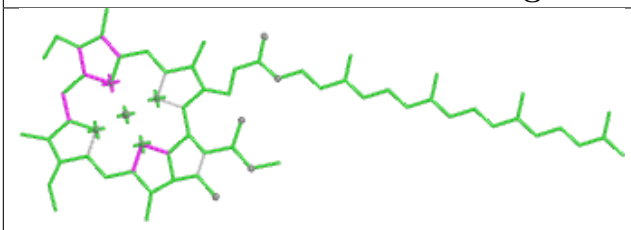


Rings

Ligand CLA A 311



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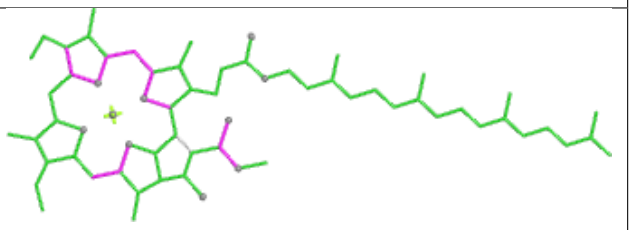

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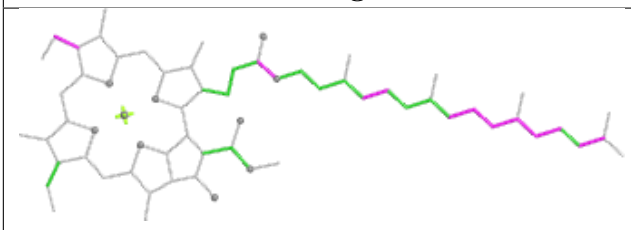

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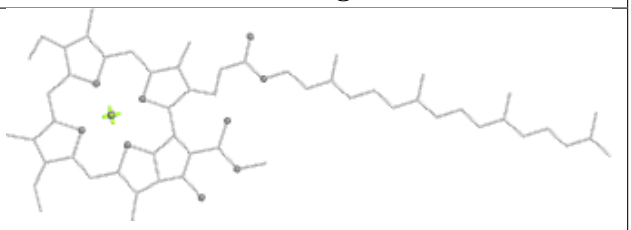
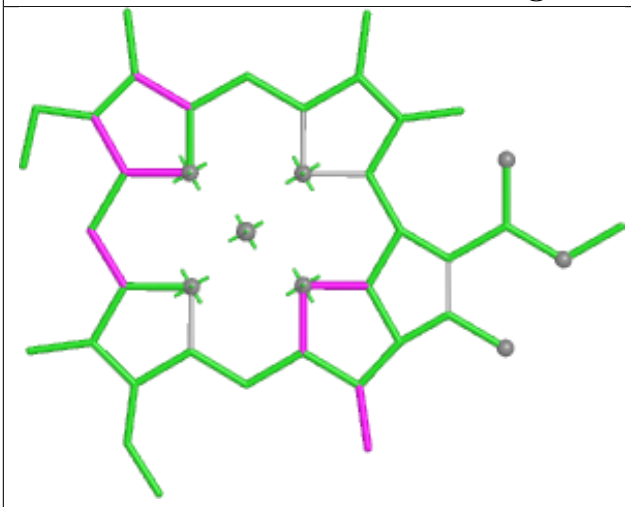


Rings

Ligand CLA y 315



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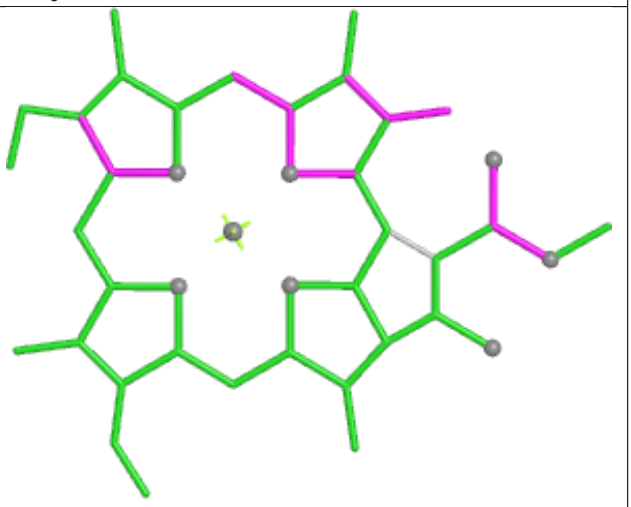

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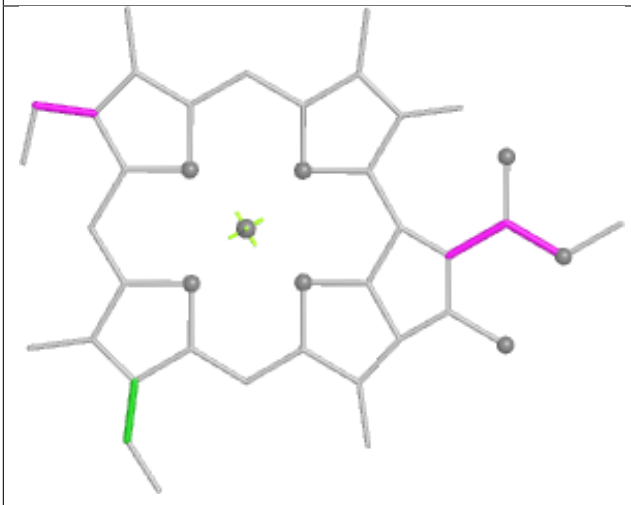

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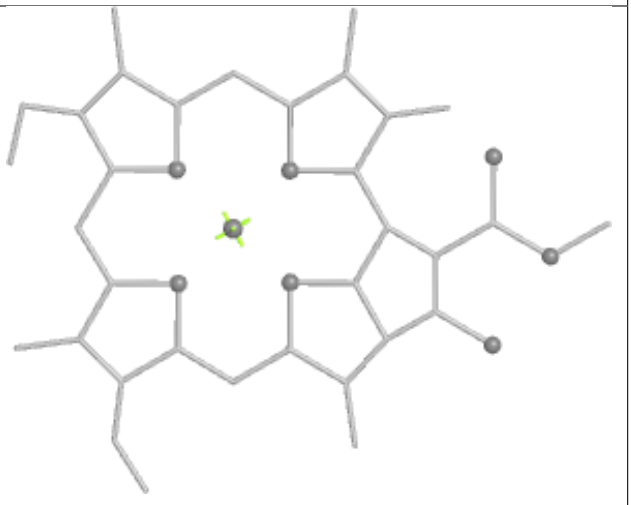
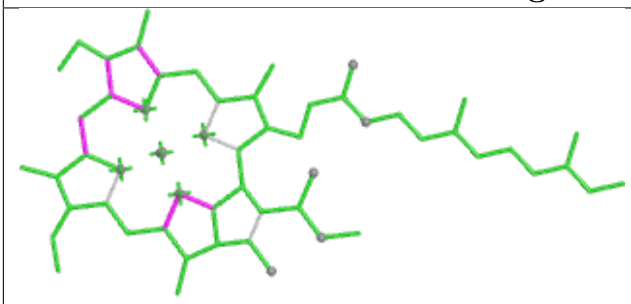


Rings

Ligand CLA a 829



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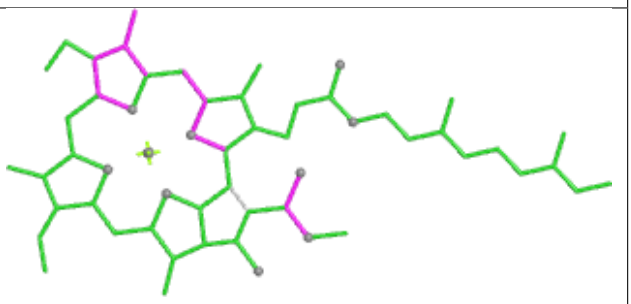

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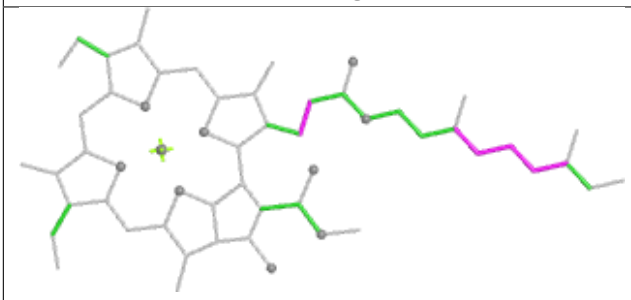

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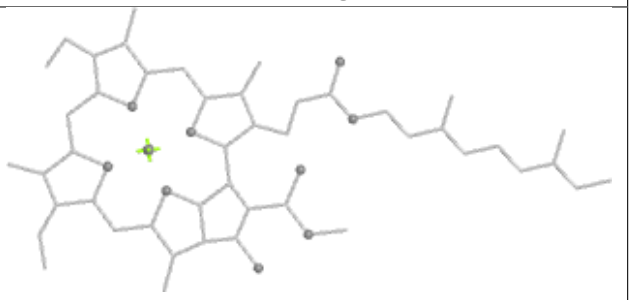
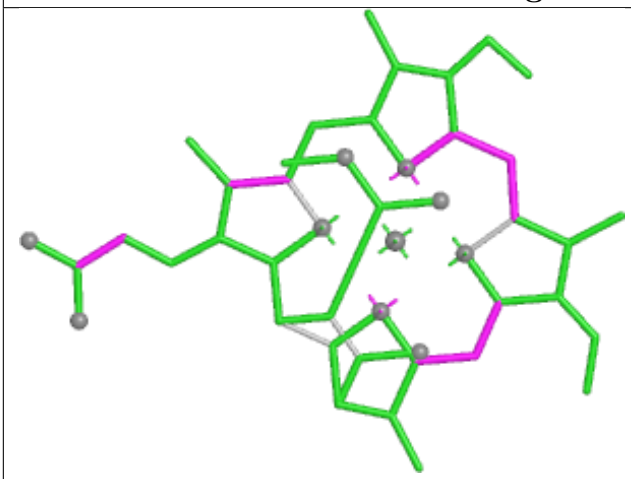


Rings

Ligand KC2 V 314



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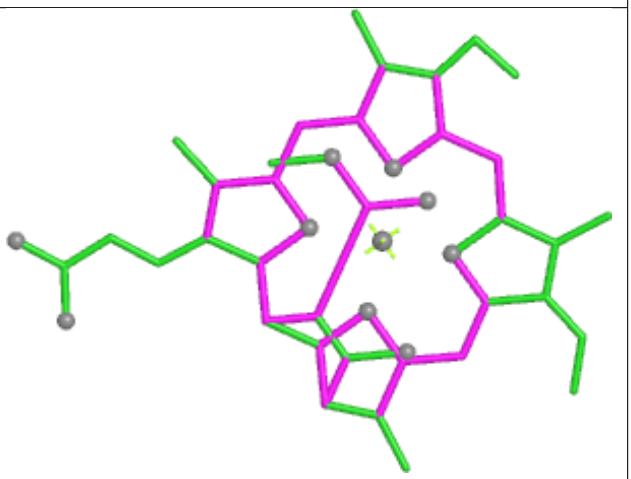
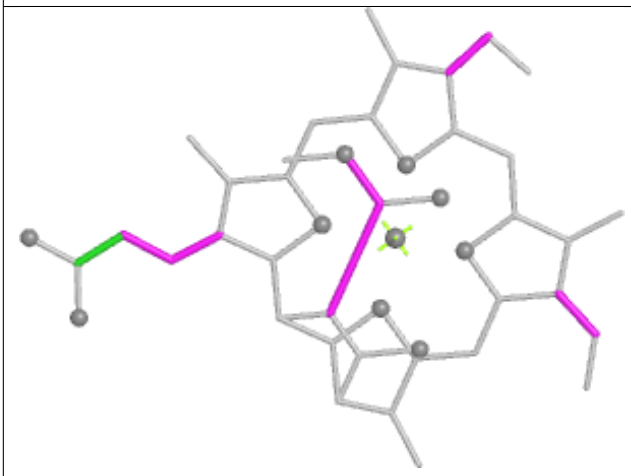


Bond angles



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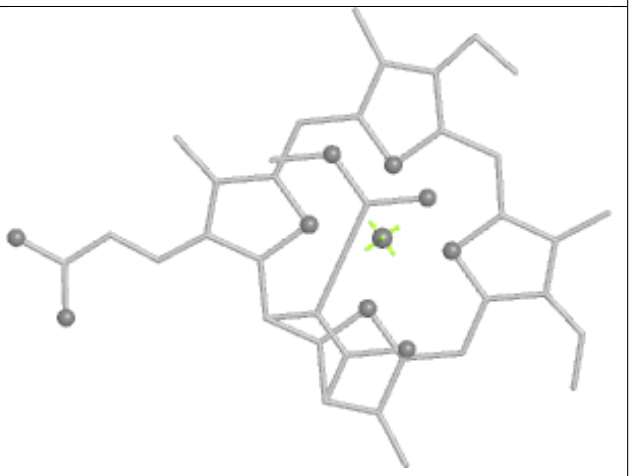
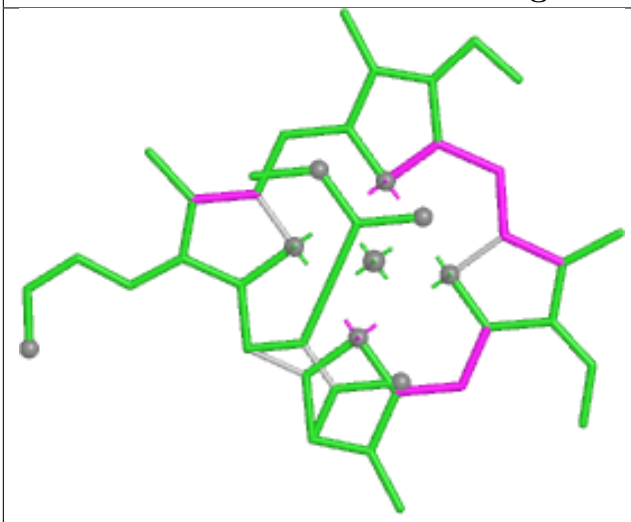


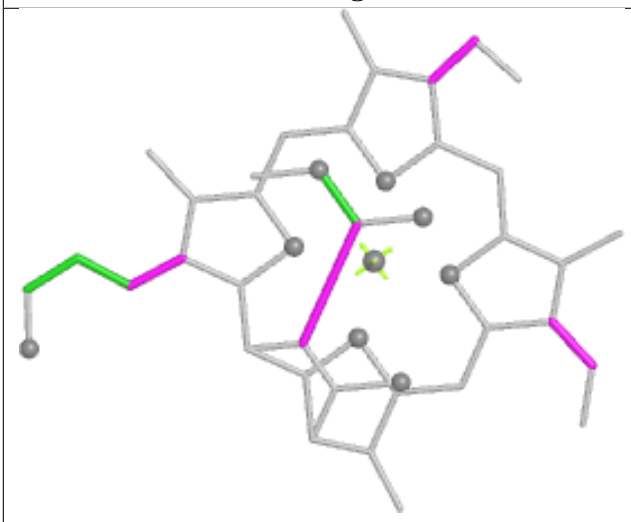
Rings

Ligand KC2 5 313



Bond lengths

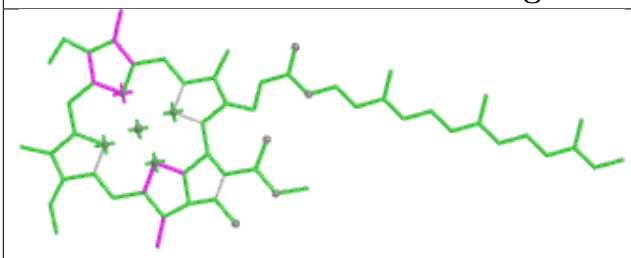
Bond angles



Torsions

Rings

Ligand CLA Q 309



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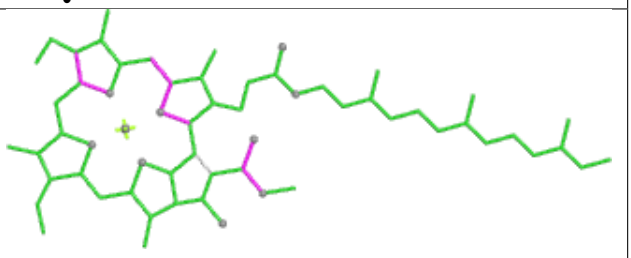
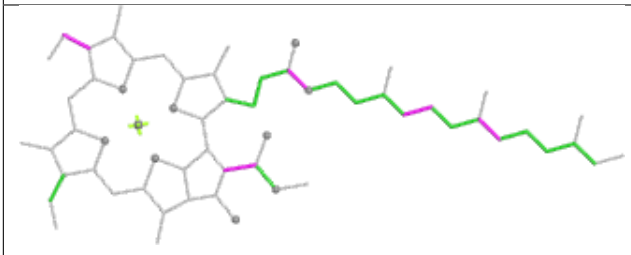
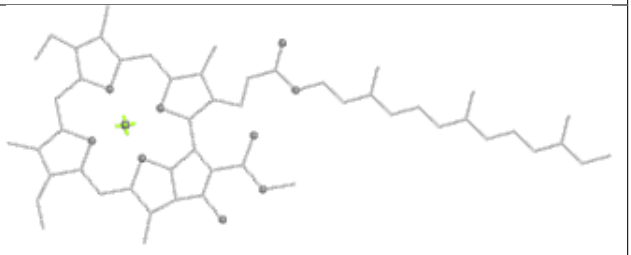


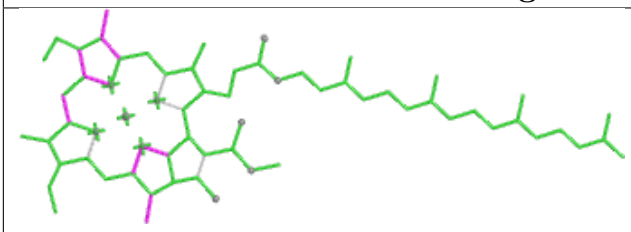
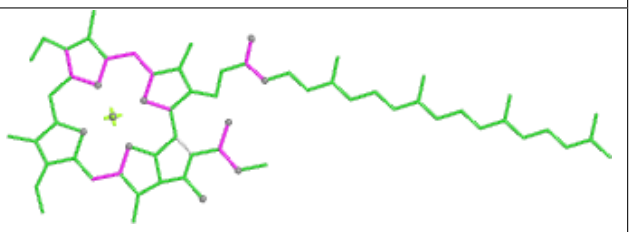
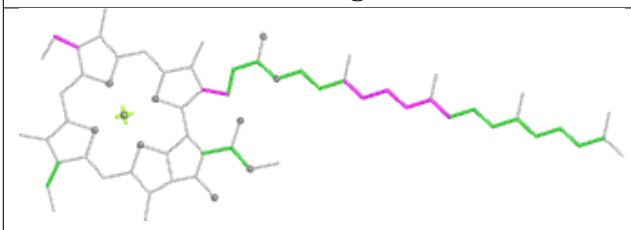
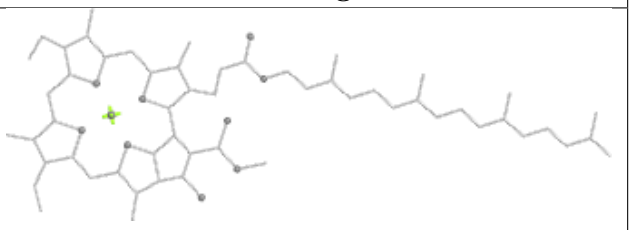
Bond angles



Torsions



Rings

Ligand CLA W 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

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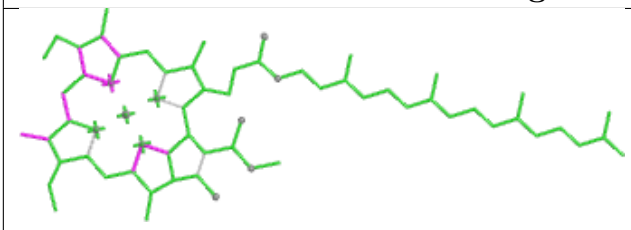
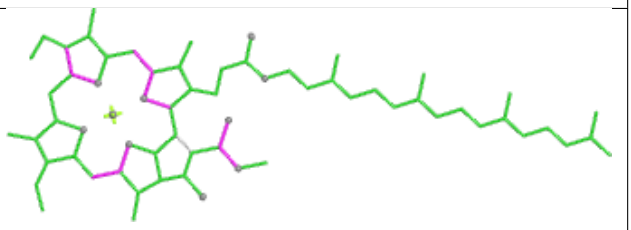
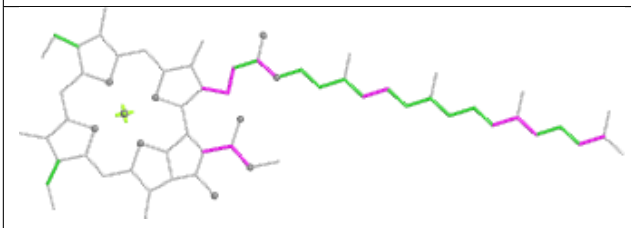
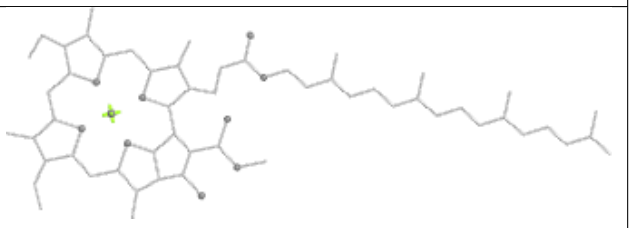
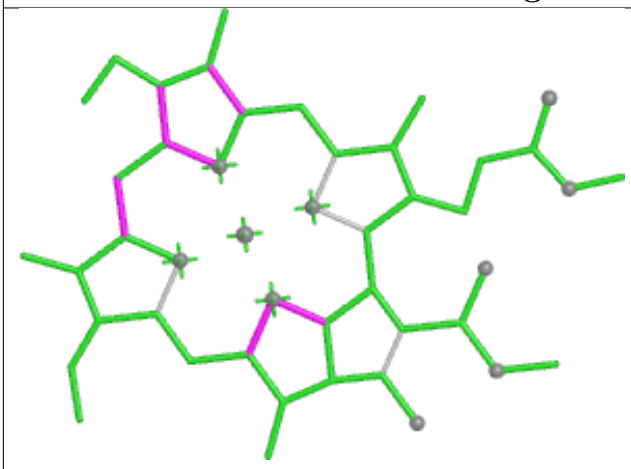
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 304



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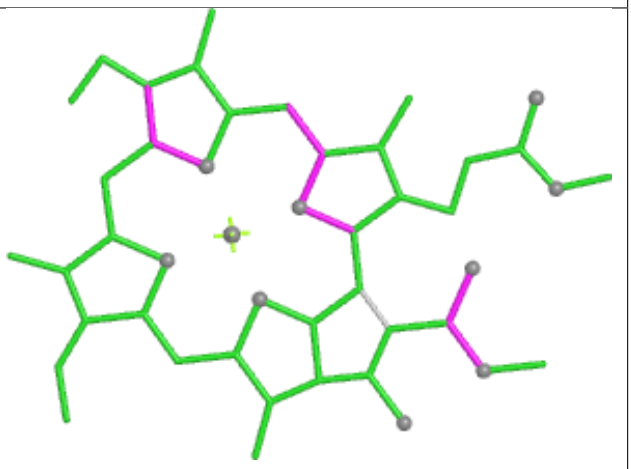

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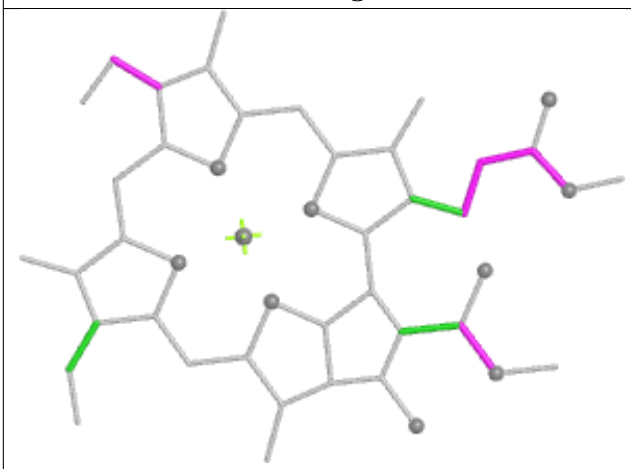

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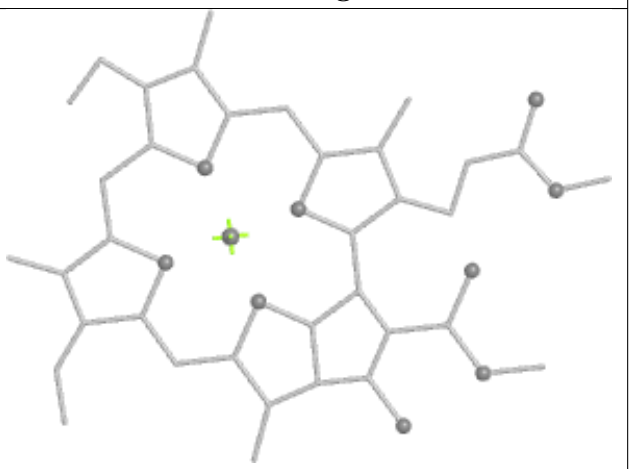
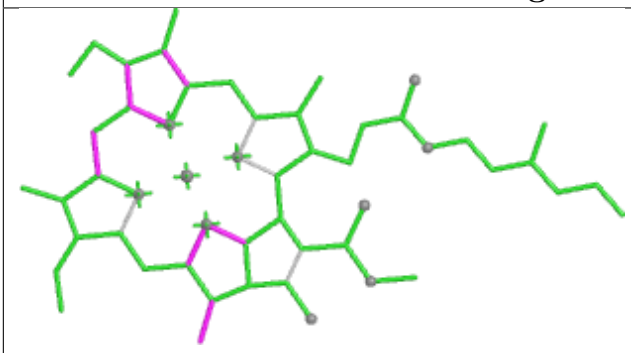


Rings

Ligand CLA o 205



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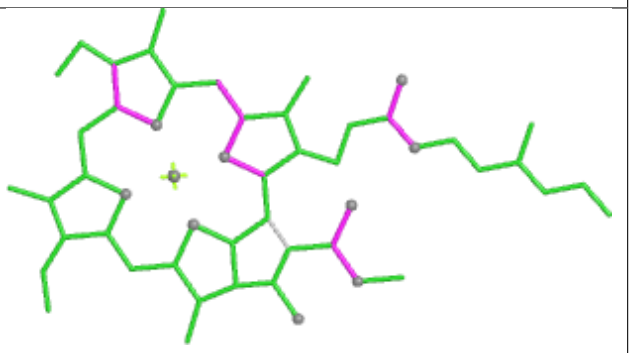

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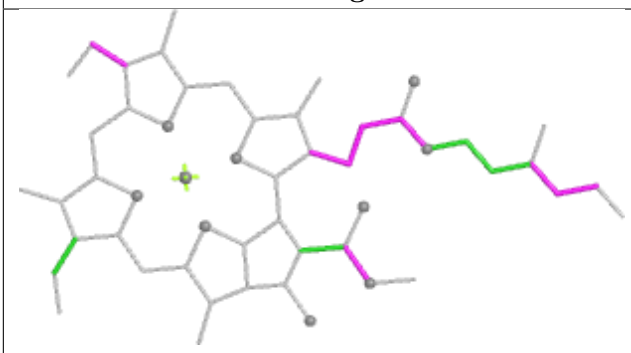

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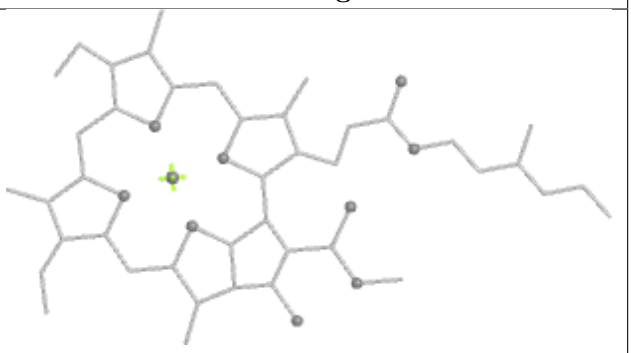
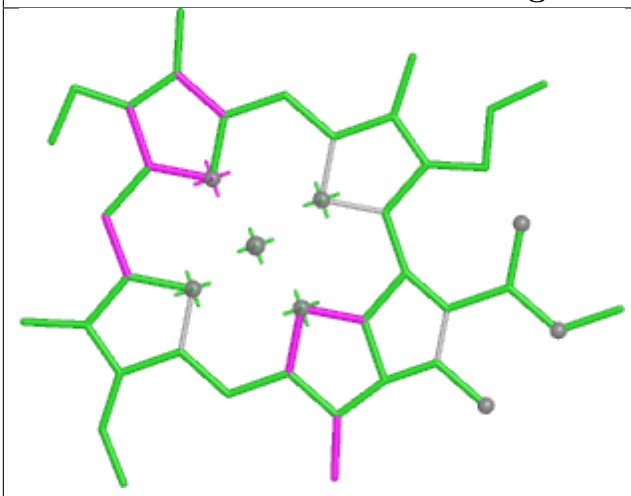


Rings

Ligand CLA 8 315



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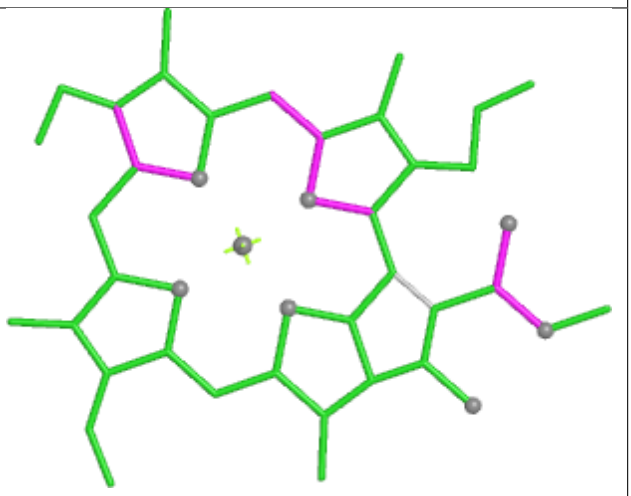

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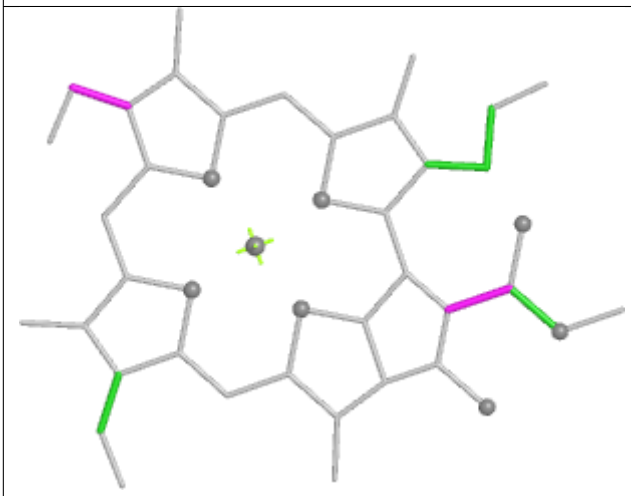

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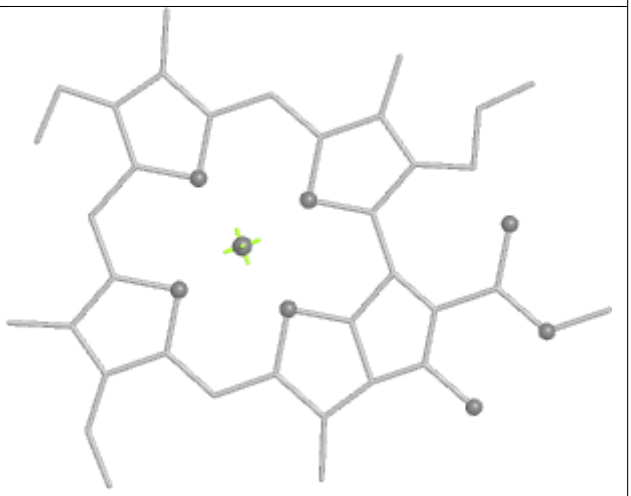
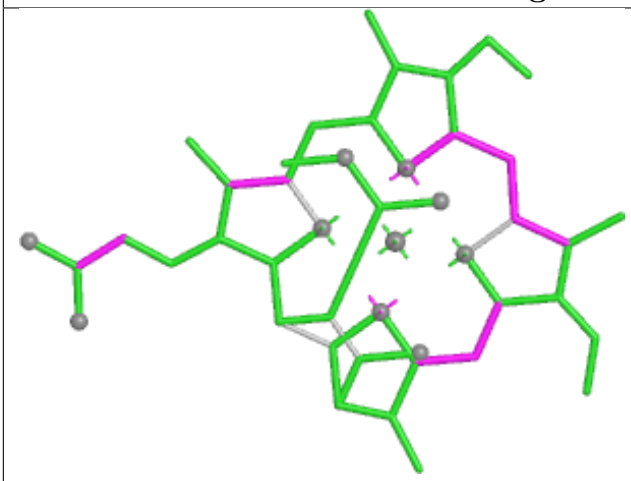


Rings

Ligand KC2 S 317



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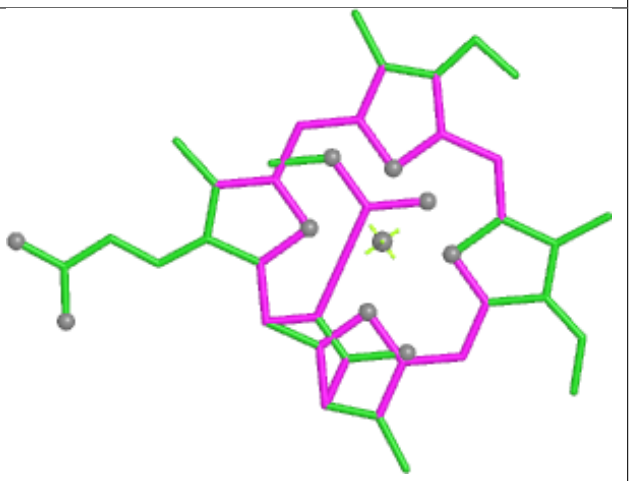

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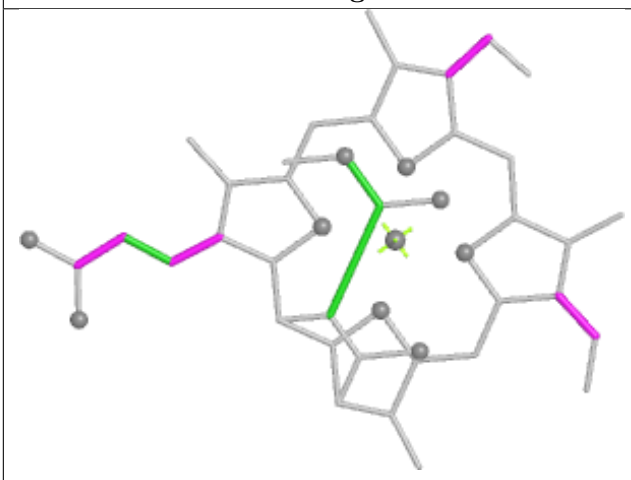

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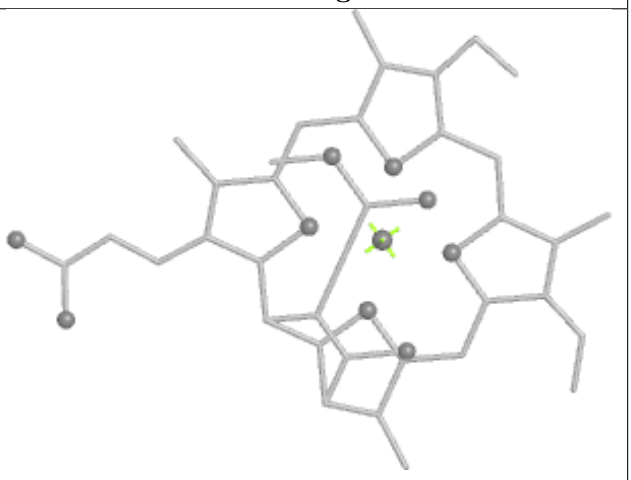
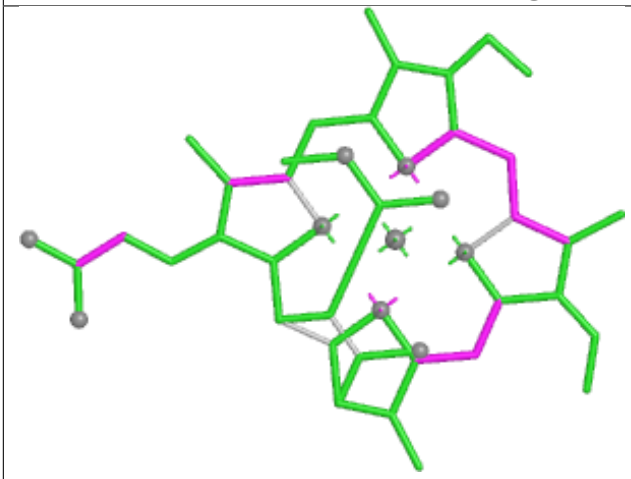


Rings

Ligand KC2 X 315



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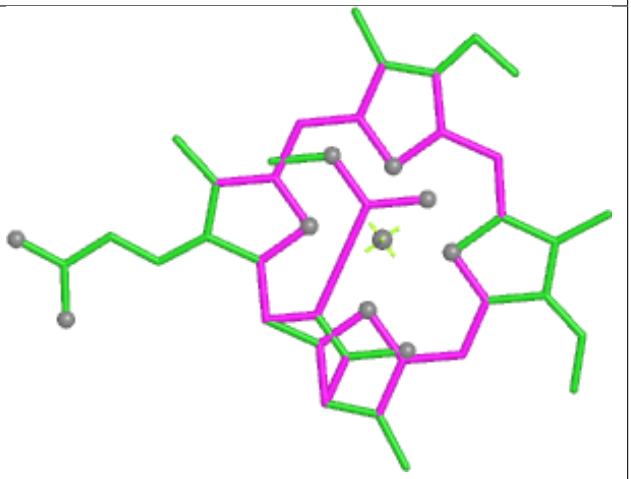

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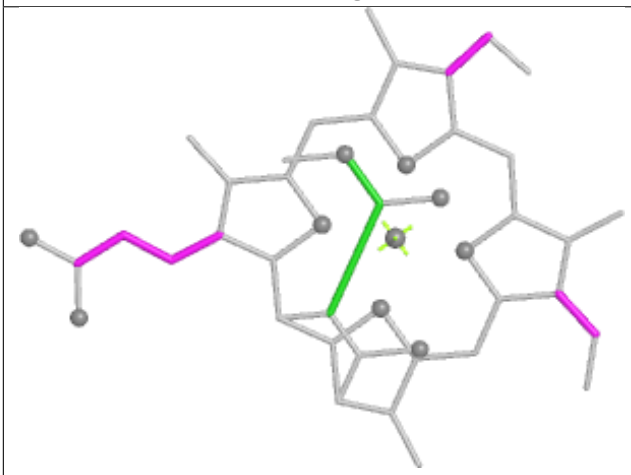

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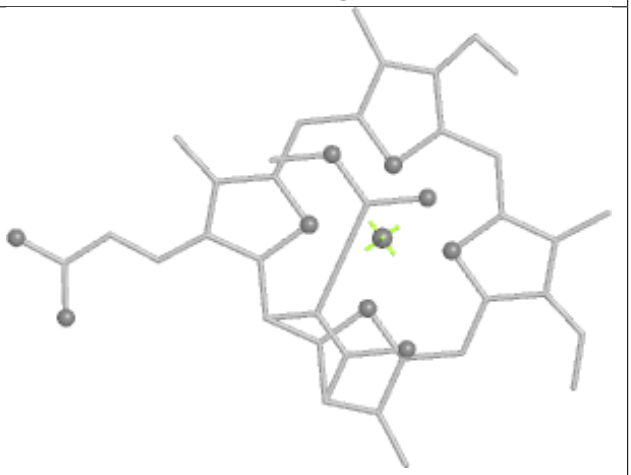
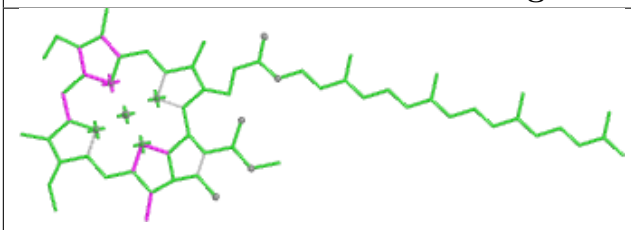


Rings

Ligand CLA S 311



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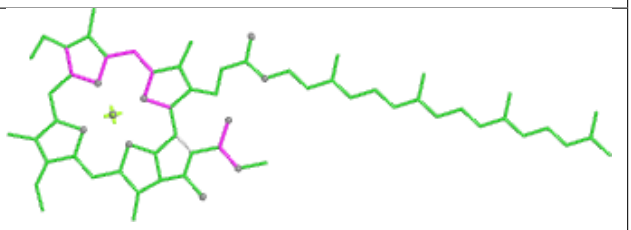

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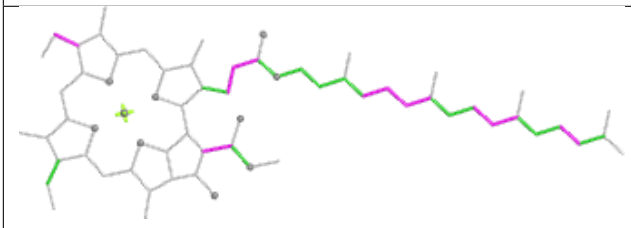

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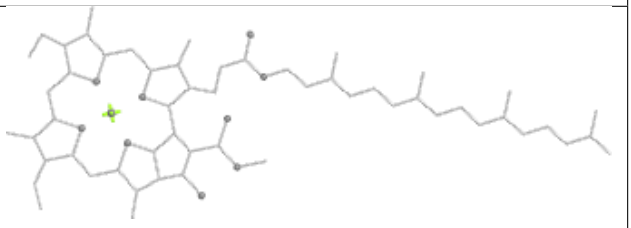
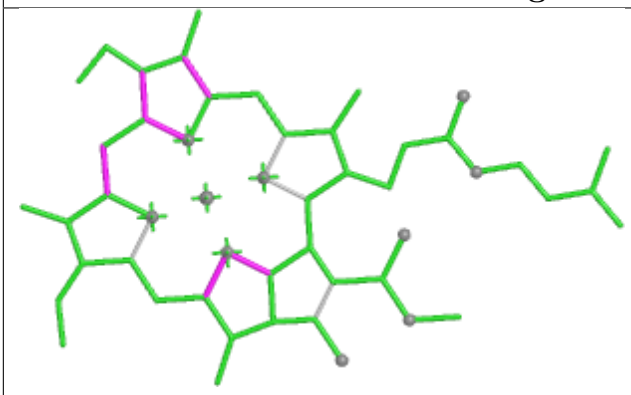


Rings

Ligand CLA 5 310



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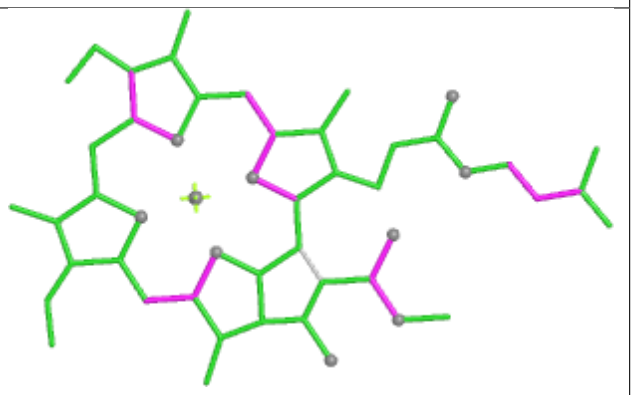

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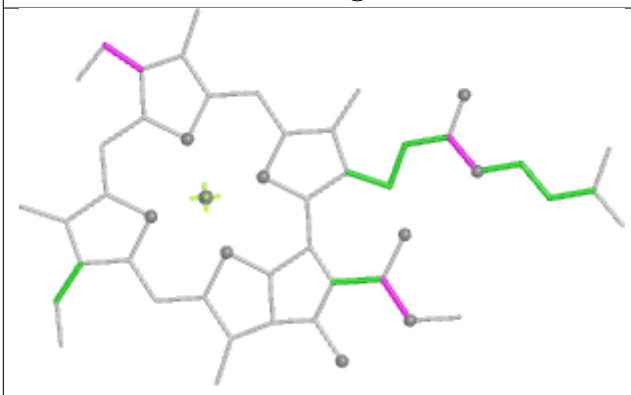

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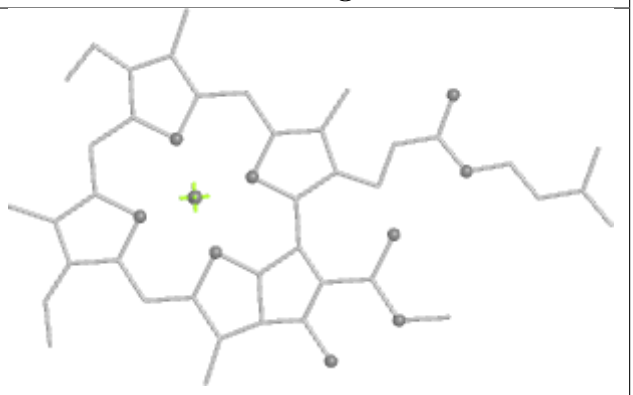
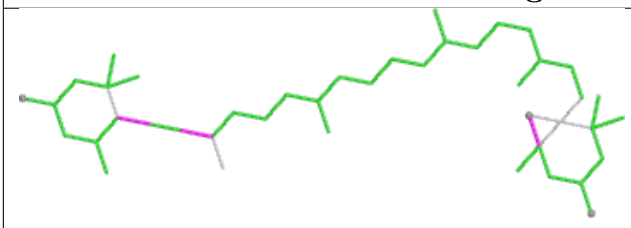


Rings

Ligand DD6 T 303



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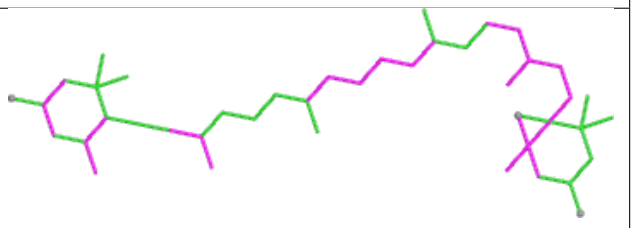
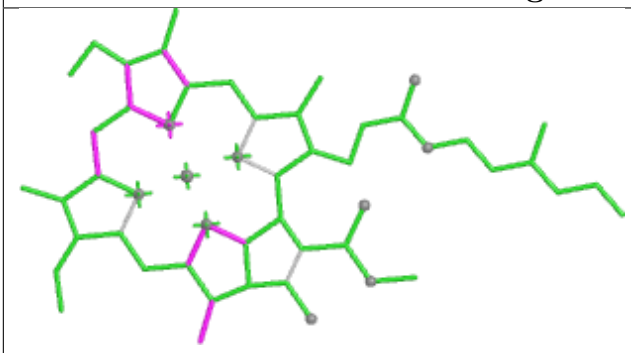


Bond angles

Torsions

Rings

Ligand CLA L 311



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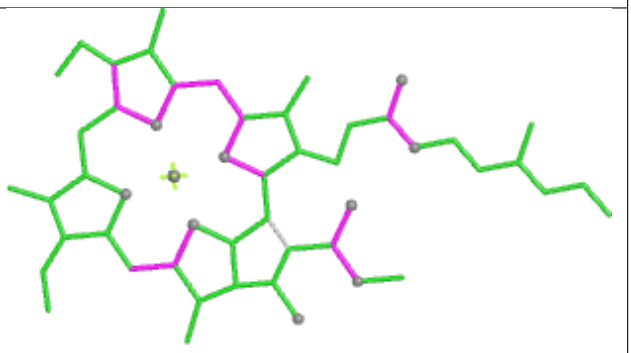

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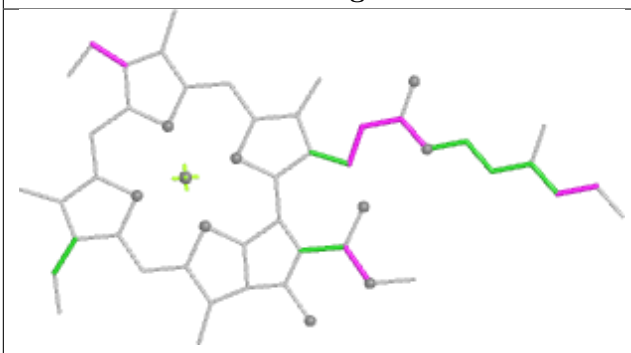

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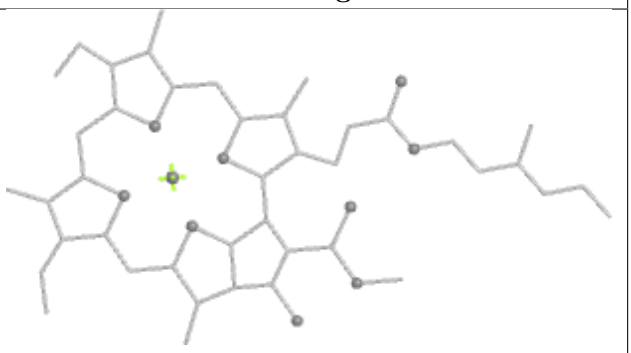
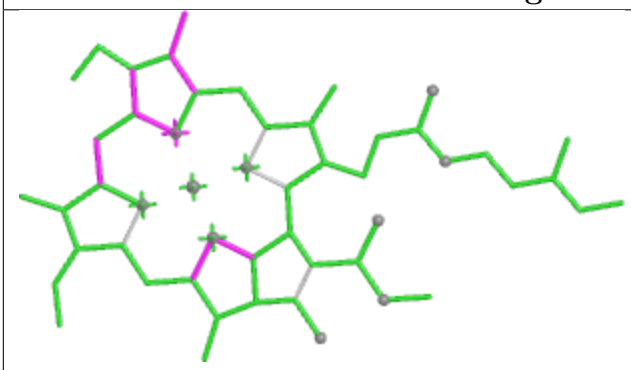


Rings

Ligand CLA P 316



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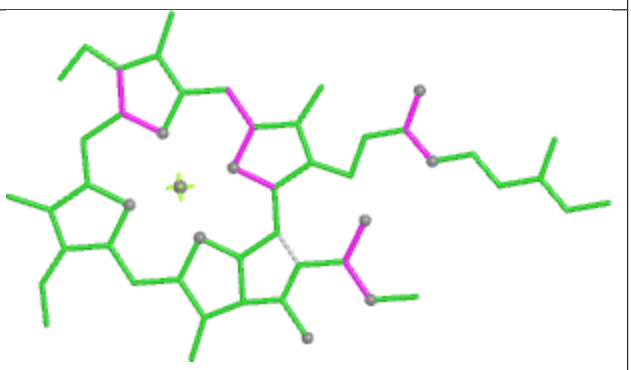

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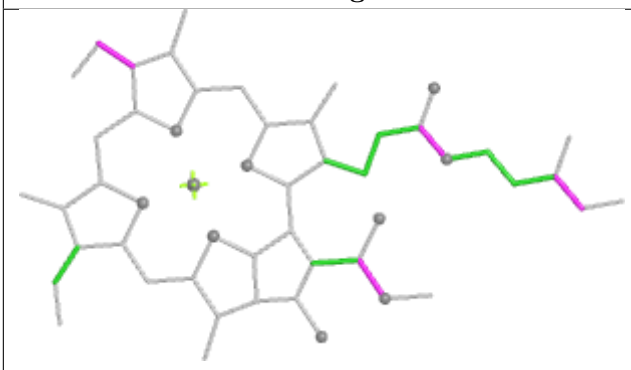

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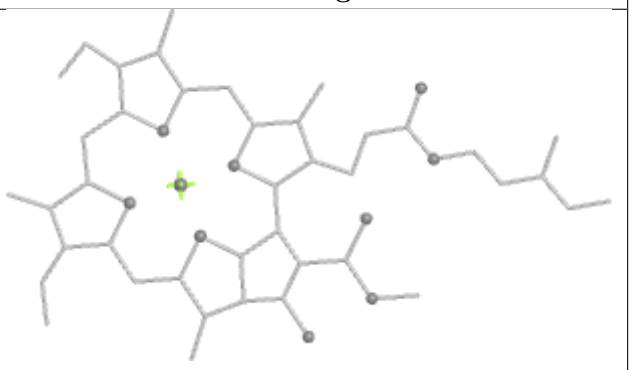
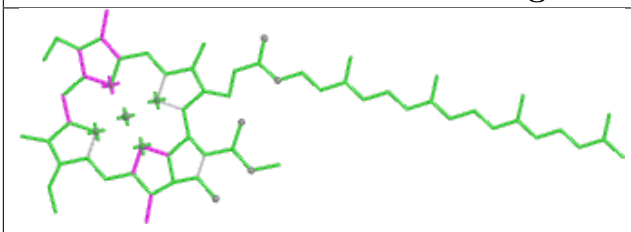


Rings

Ligand CLA a 838



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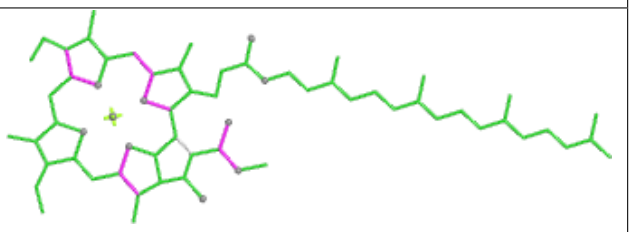
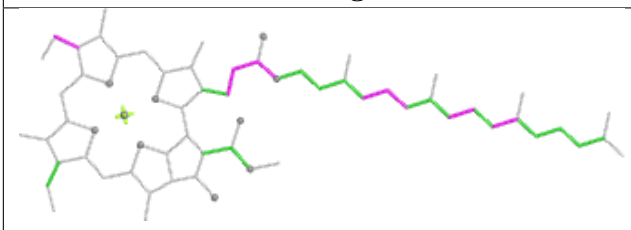


Bond angles



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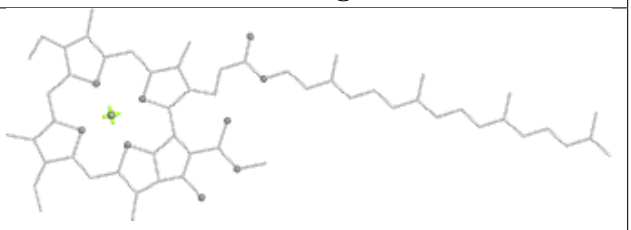
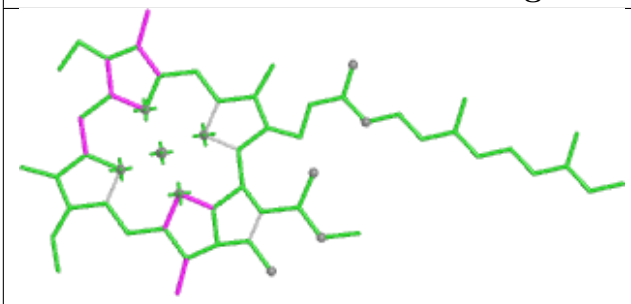


Rings

Ligand CLA B 209



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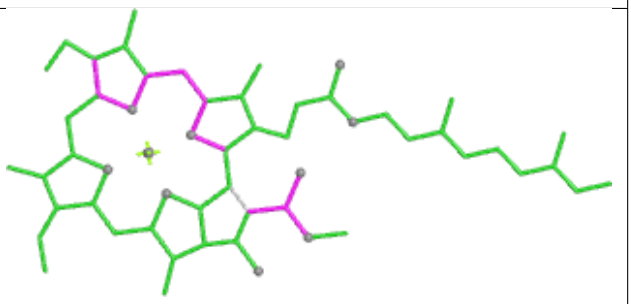

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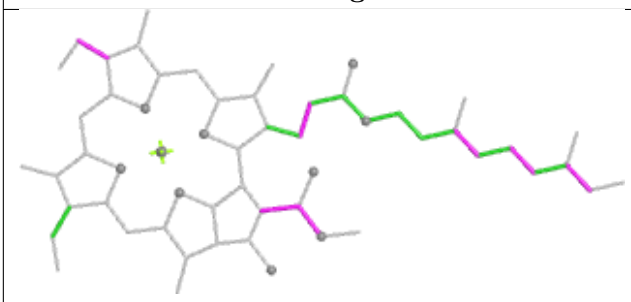

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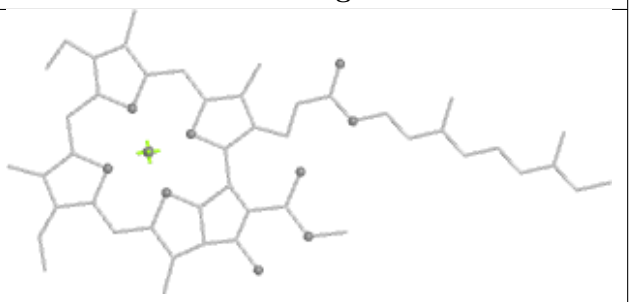
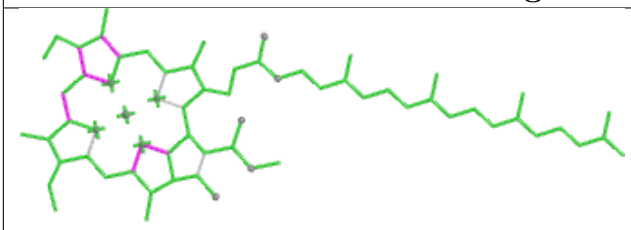


Rings

Ligand CLA C 311



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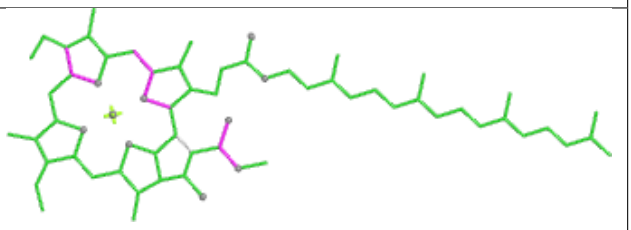
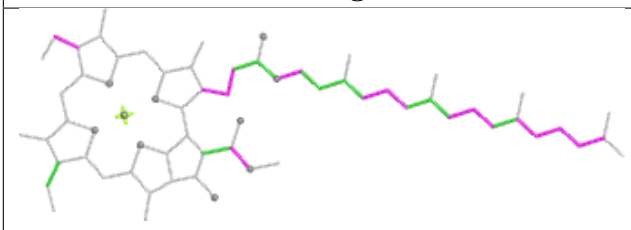


Bond angles



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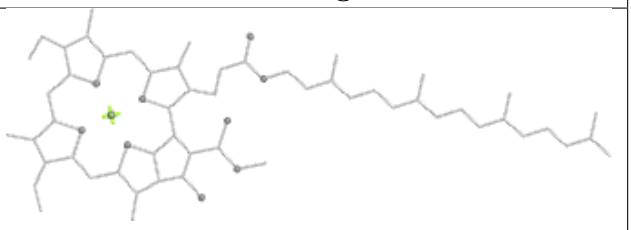
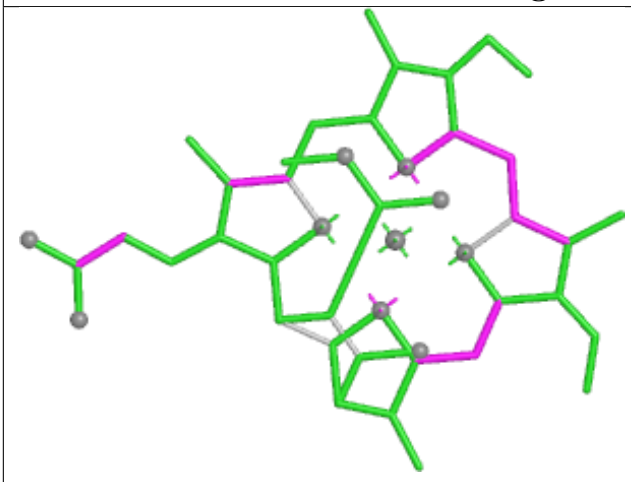


Rings

Ligand KC2 0 316



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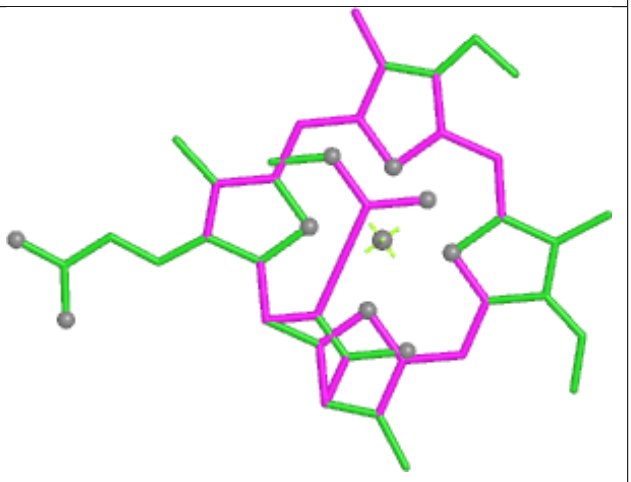
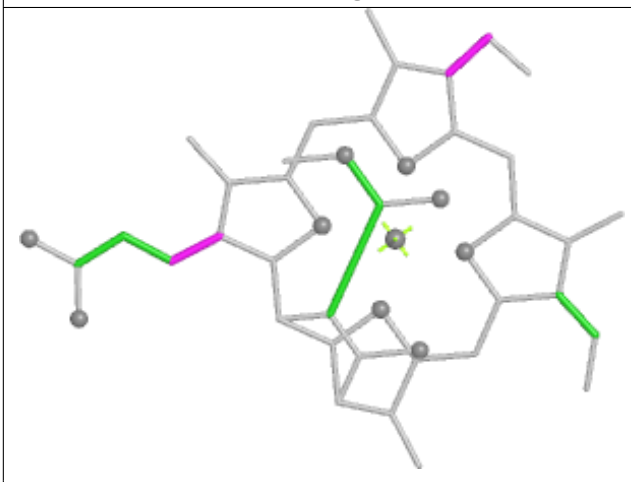
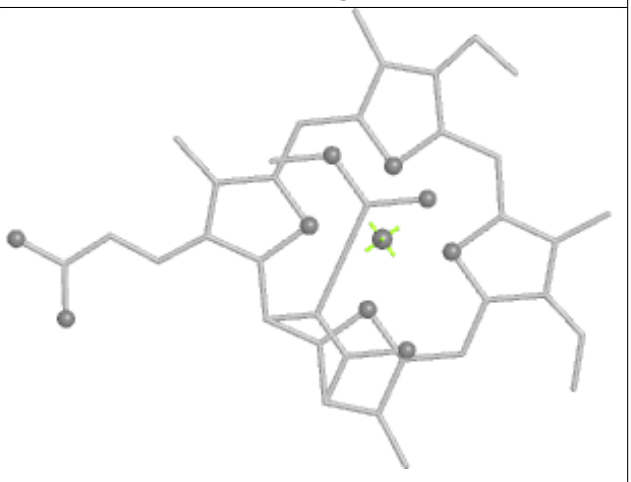


Bond angles

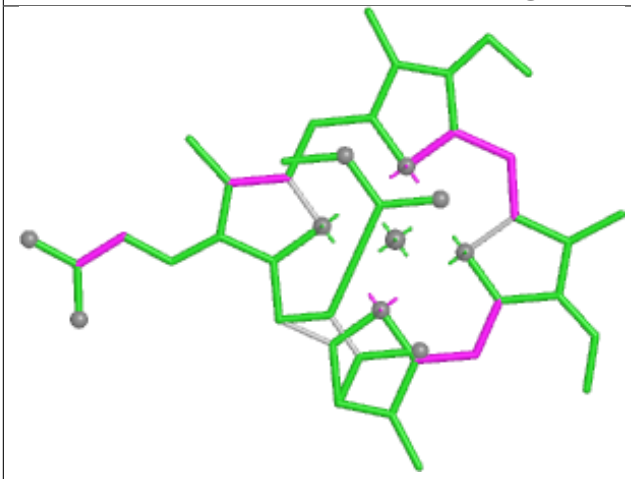


Torsions



Rings

Ligand KC2 M 313



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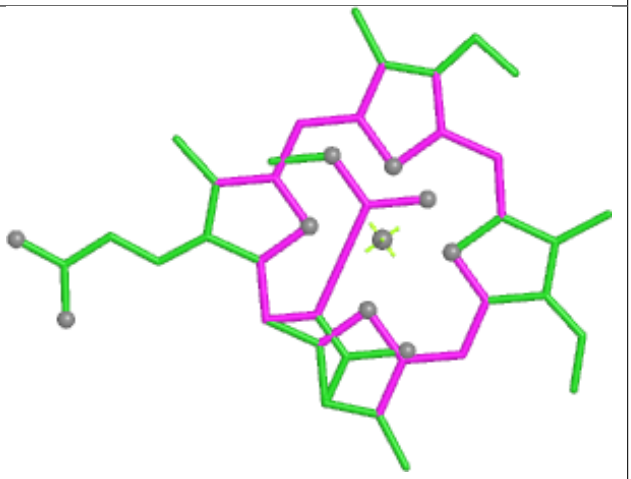

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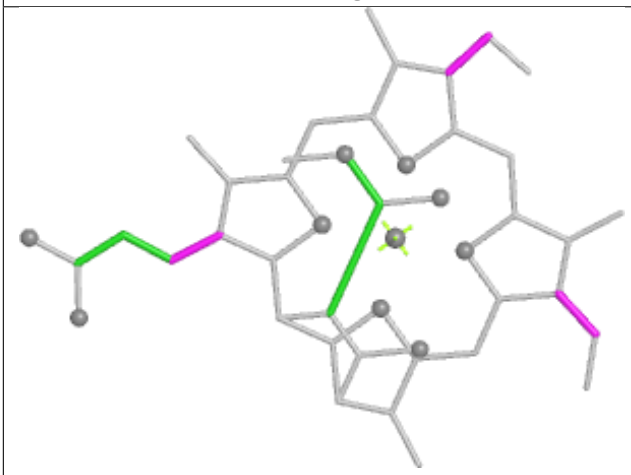

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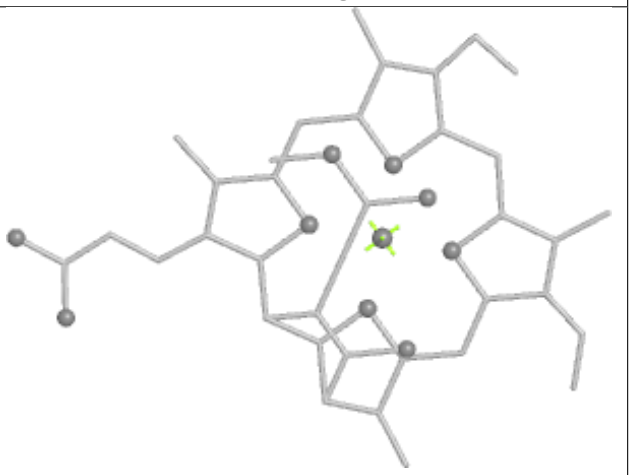
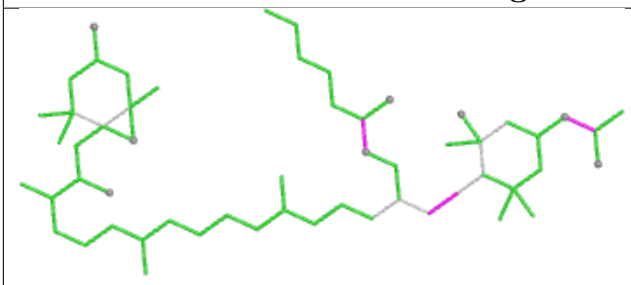


Rings

Ligand A1EB1 2 306



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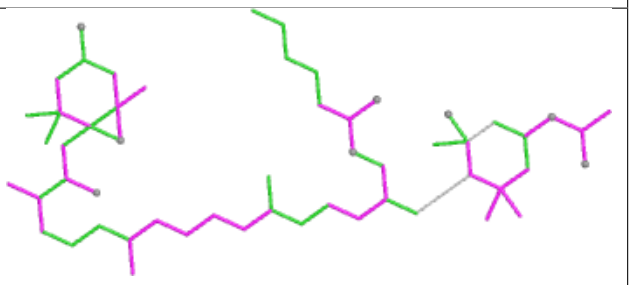

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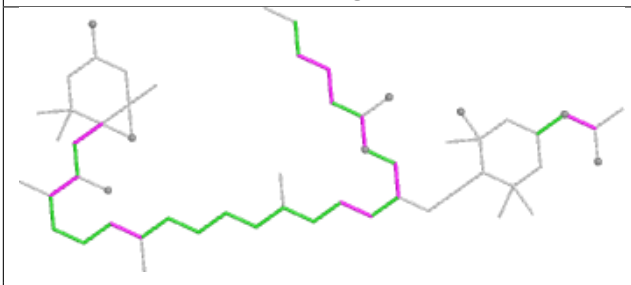

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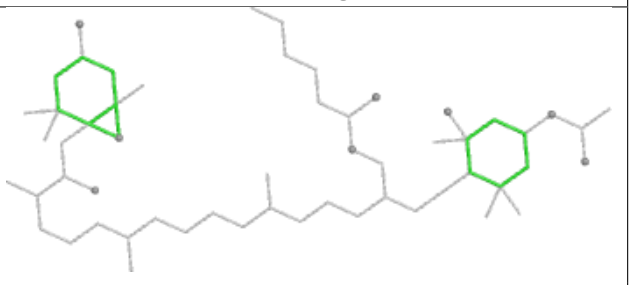
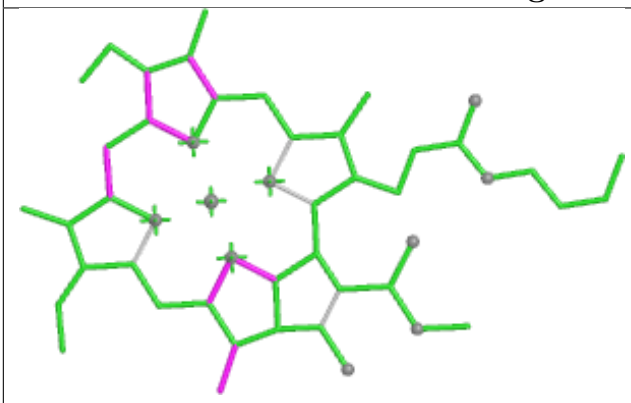


Rings

Ligand CLA J 307



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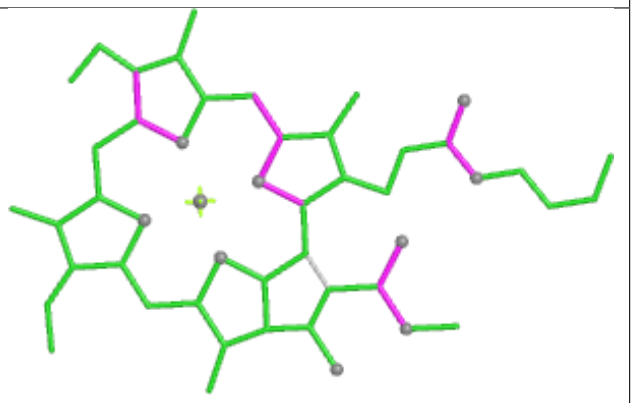
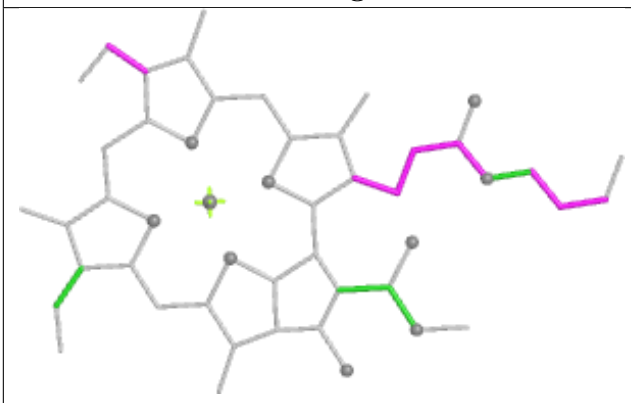


Bond angles



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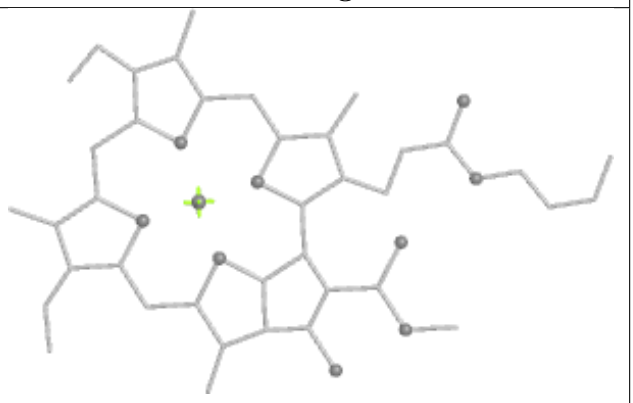
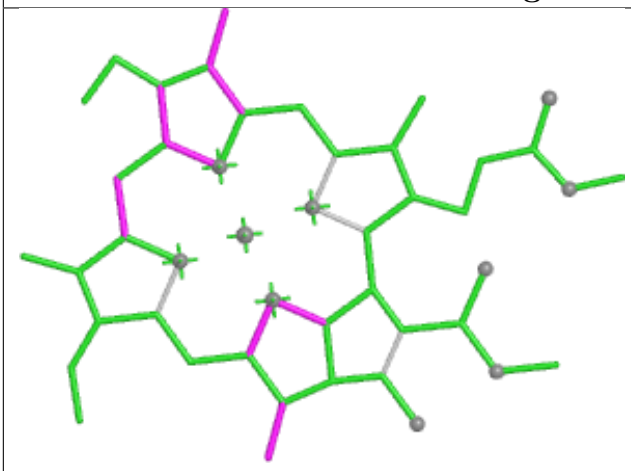


Rings

Ligand CLA H 316



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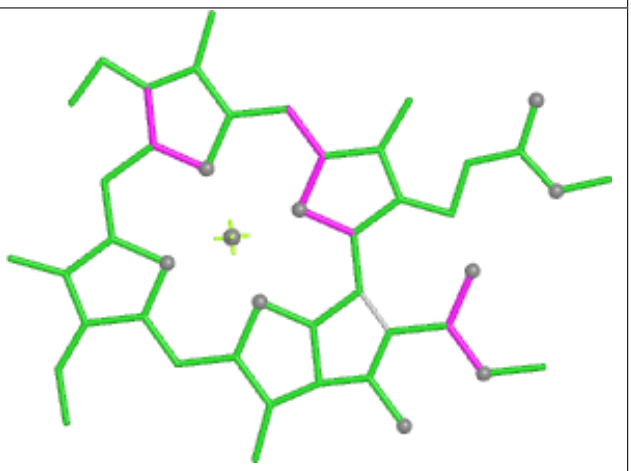
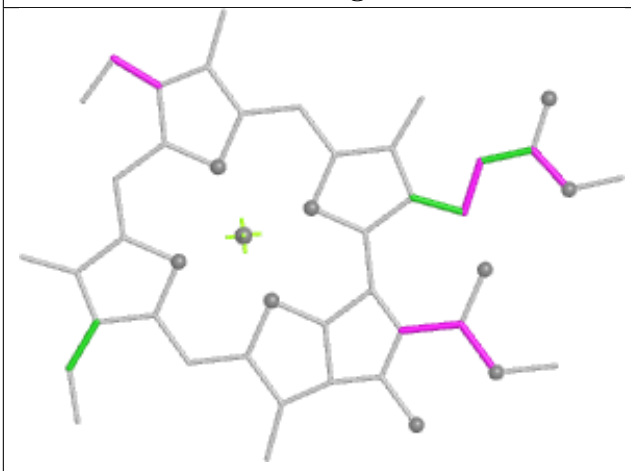


Bond angles



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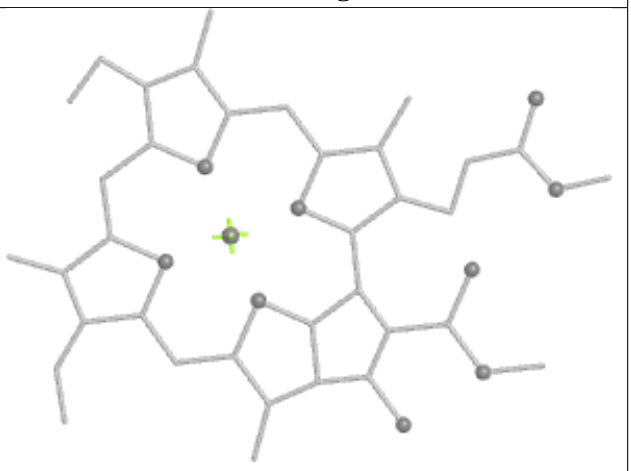
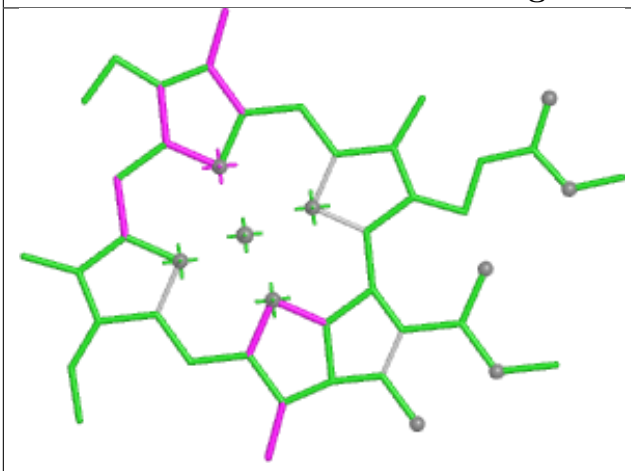


Rings

Ligand CLA 2 309



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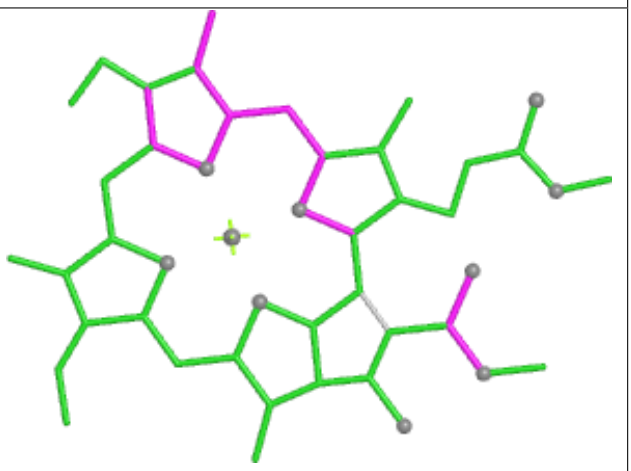
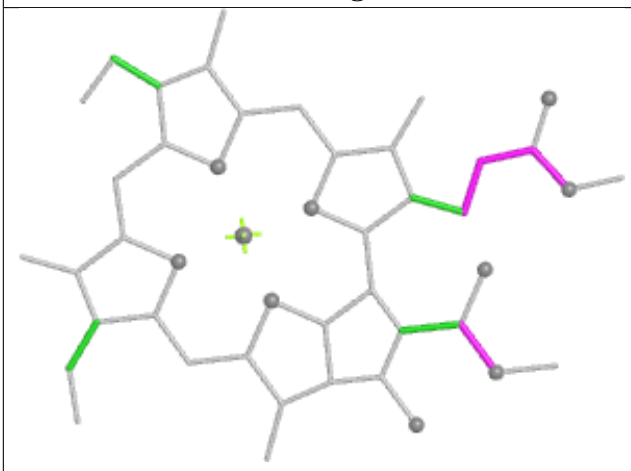


Bond angles



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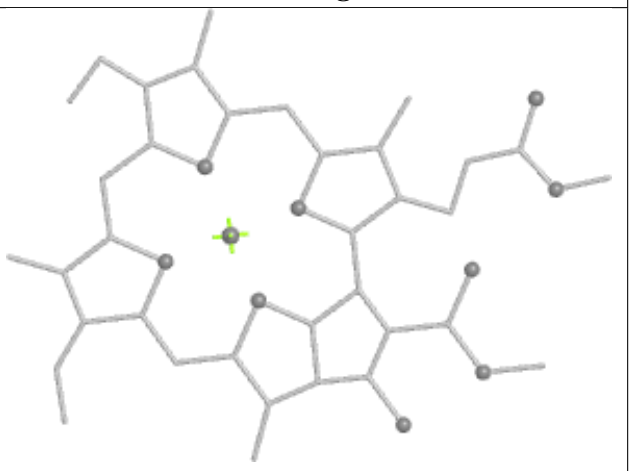
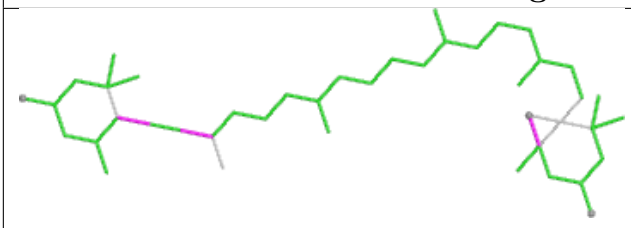


Rings

Ligand DD6 a 846



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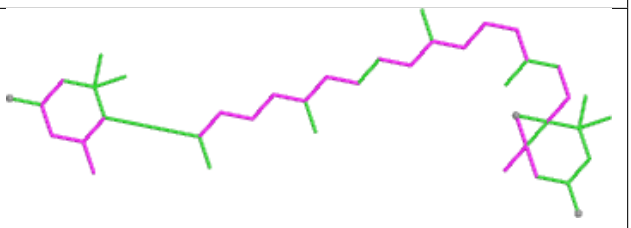
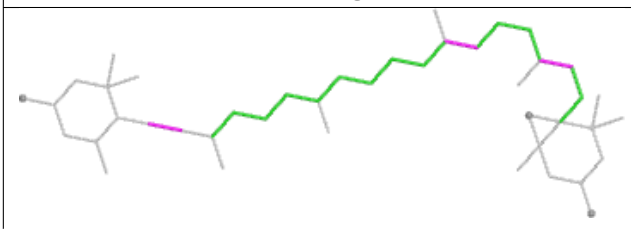
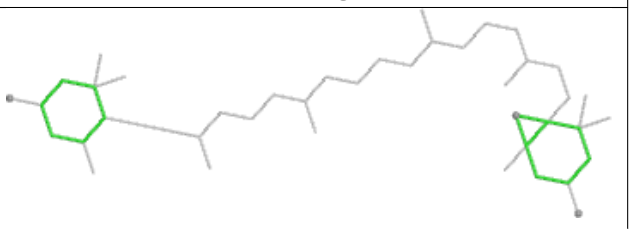


Bond angles

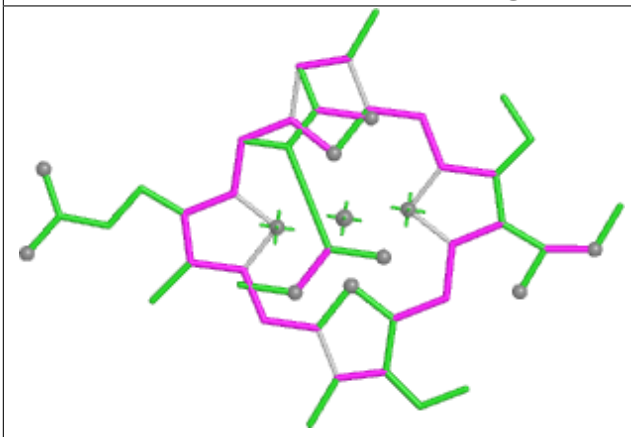


Torsions



Rings

Ligand A1ECV 0 321



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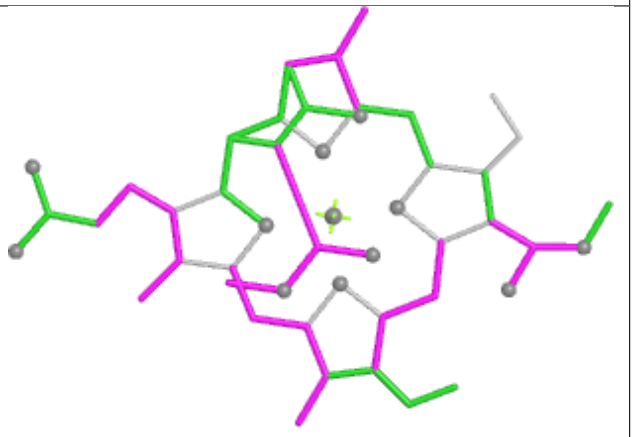
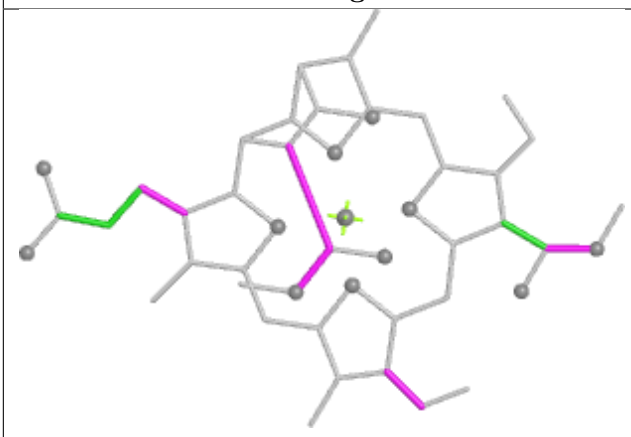


Bond angles



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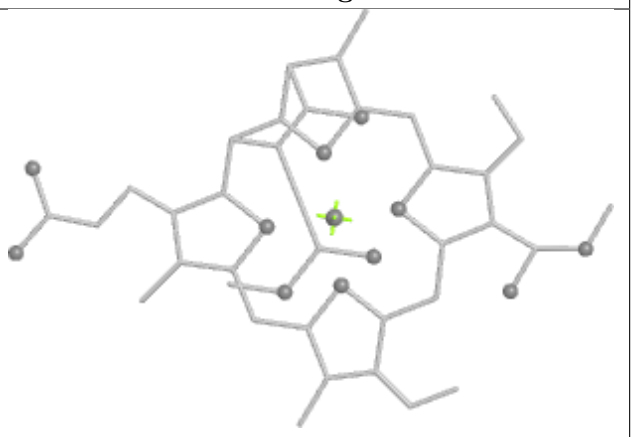
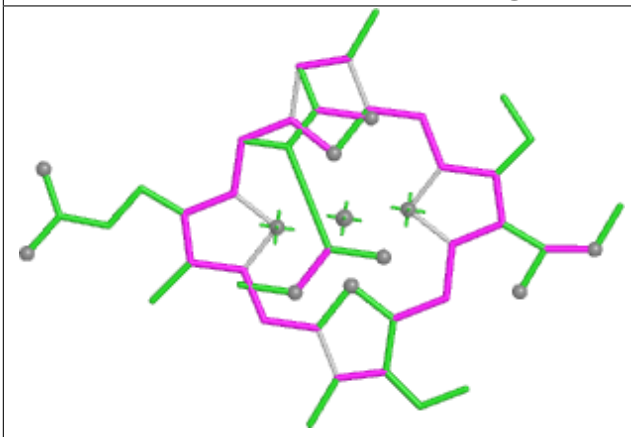


Rings

Ligand A1ECV z 316



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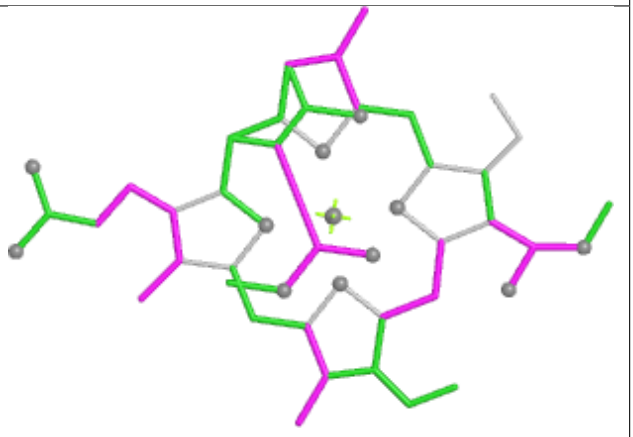
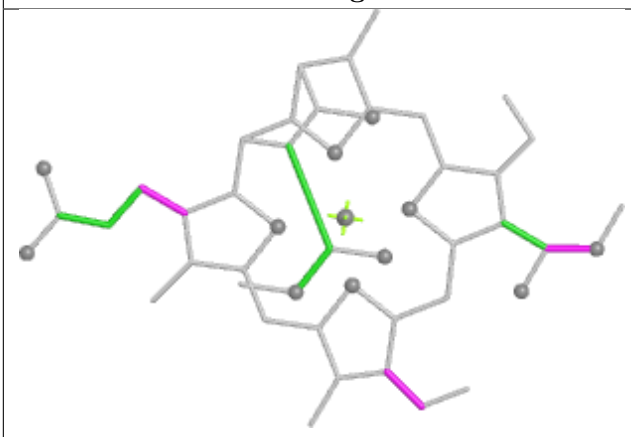
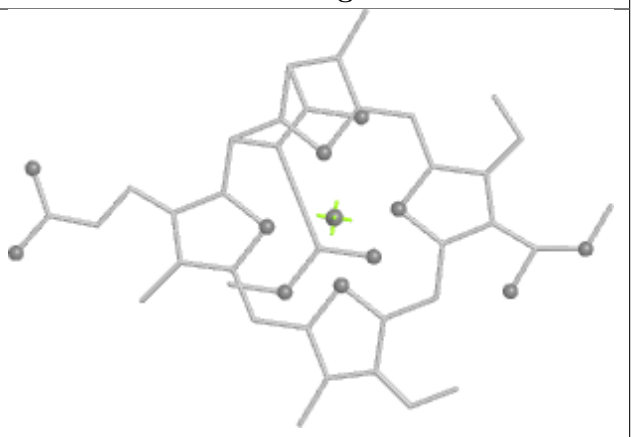


Bond angles

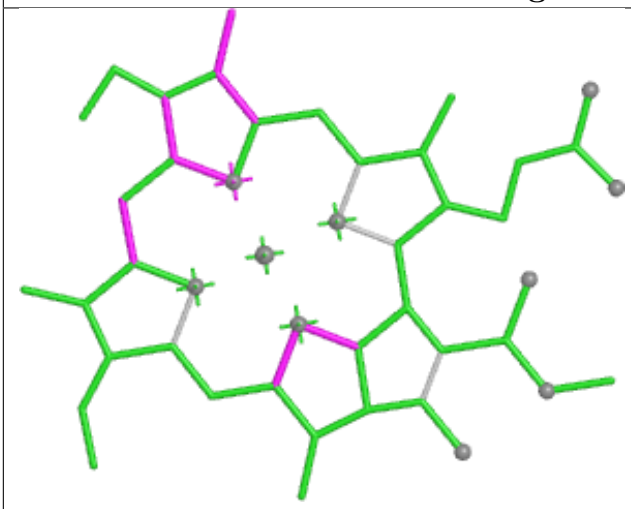


Torsions



Rings

Ligand CLA a 812



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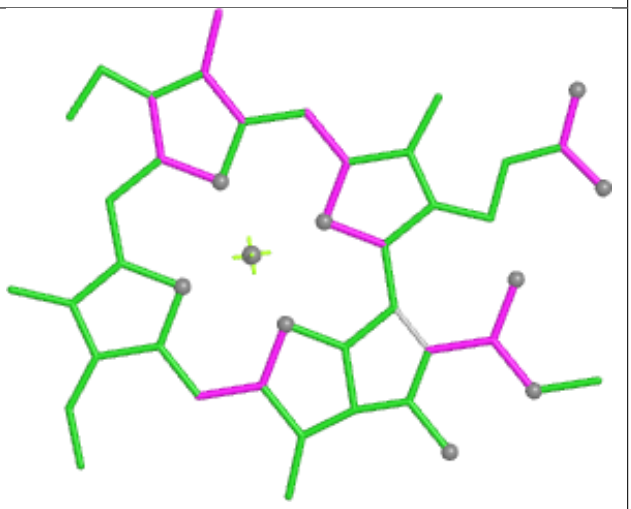
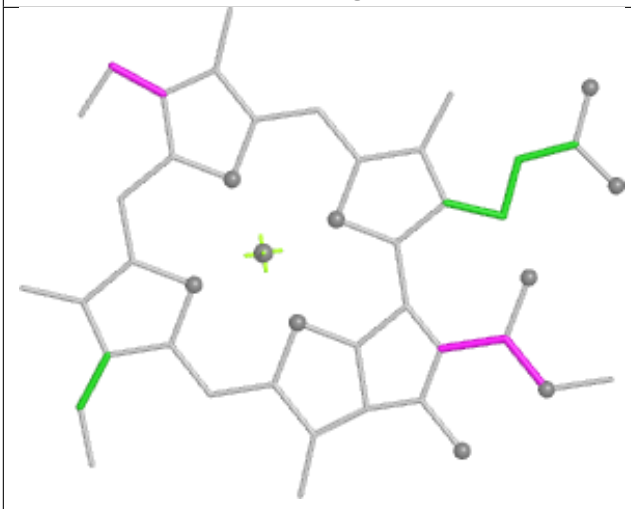


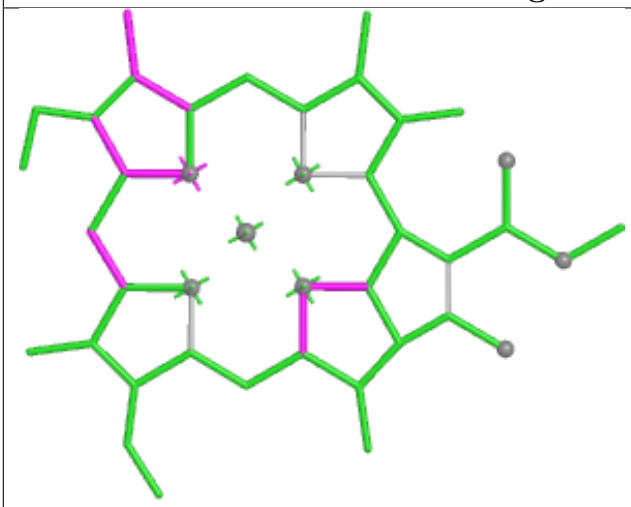
Bond angles



Torsions

Rings

Ligand CLA 9 320



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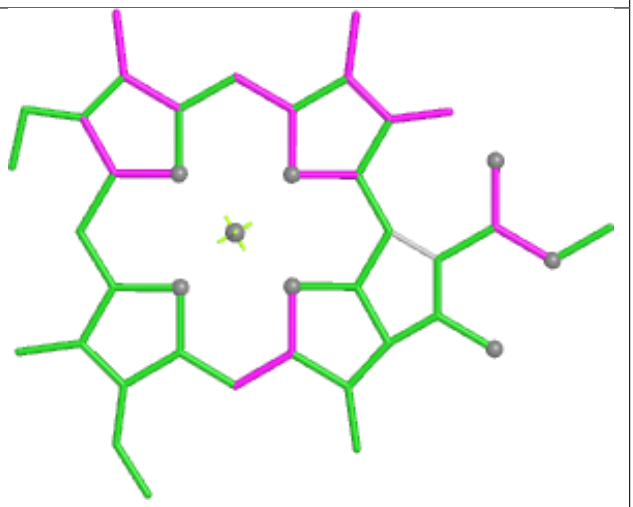
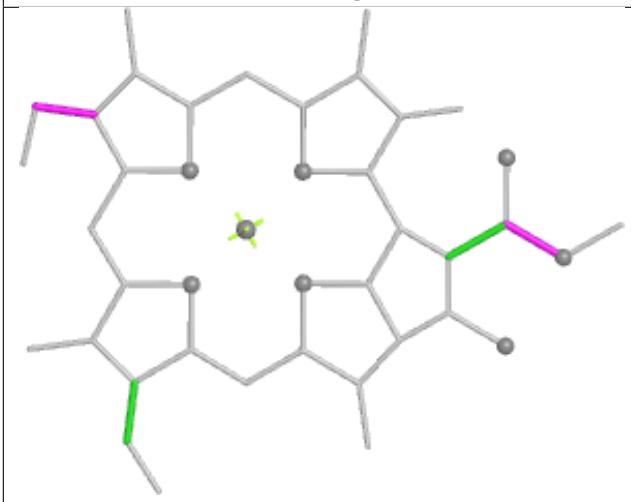
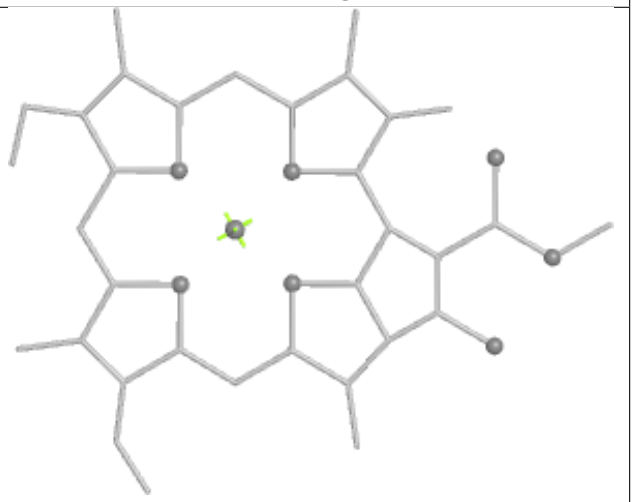


Bond angles

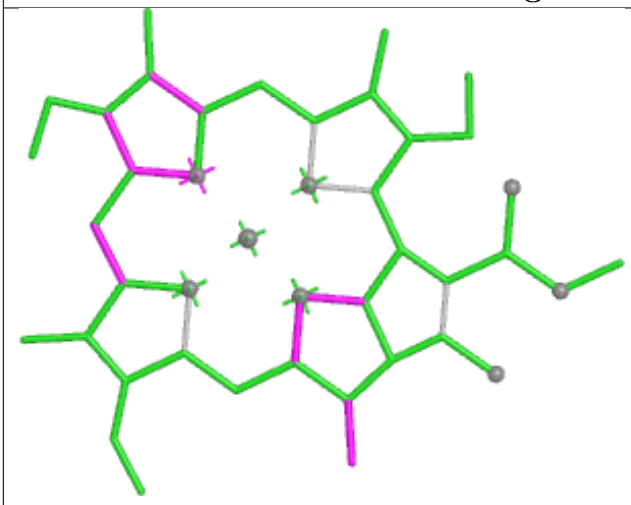


Torsions



Rings

Ligand CLA B 206



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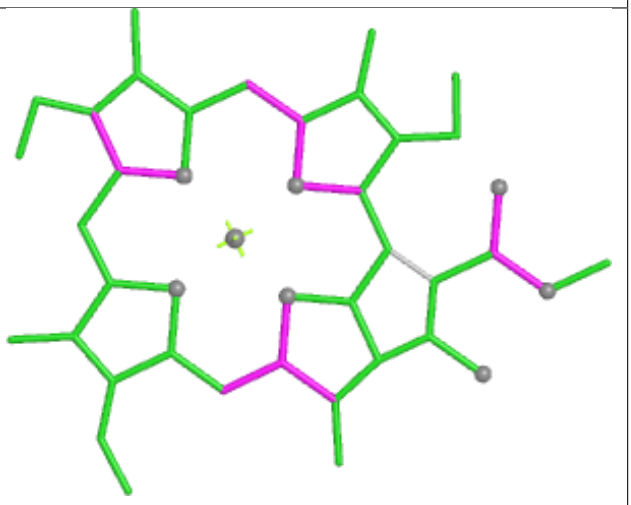
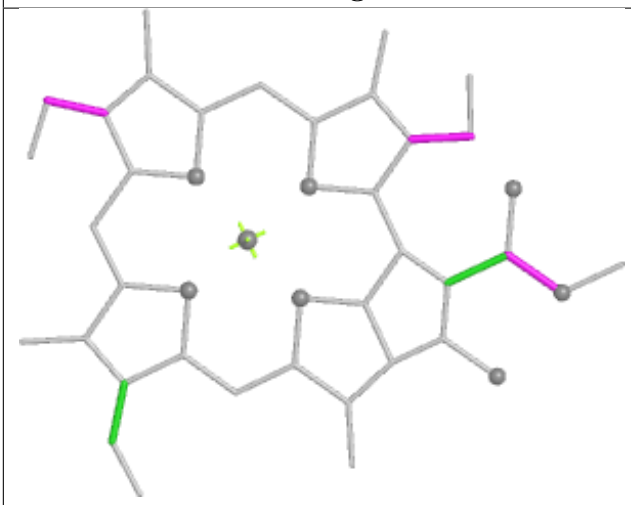


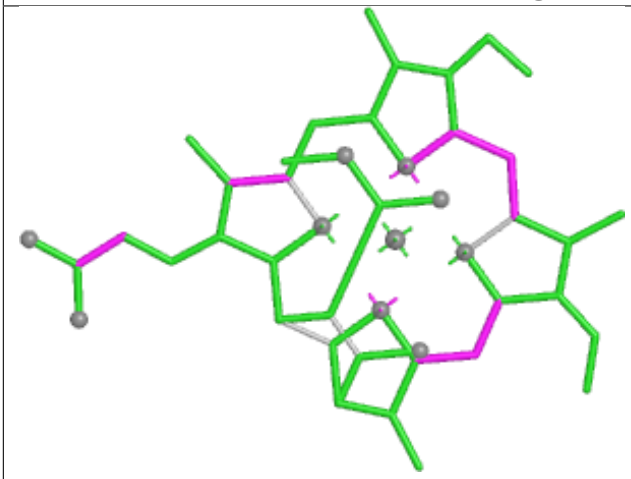
Bond angles



Torsions

Rings

Ligand KC2 3 317



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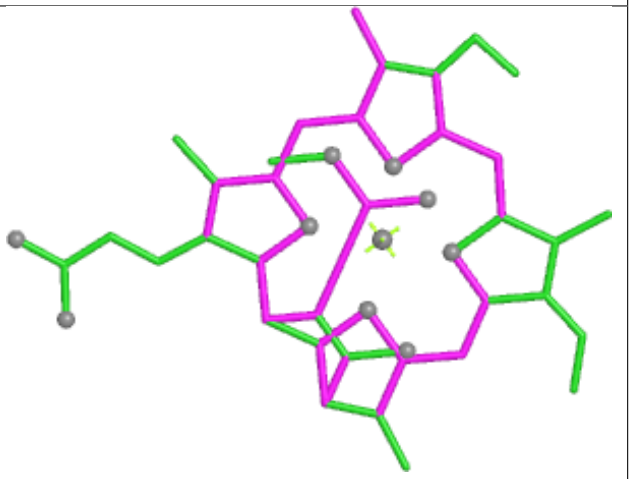
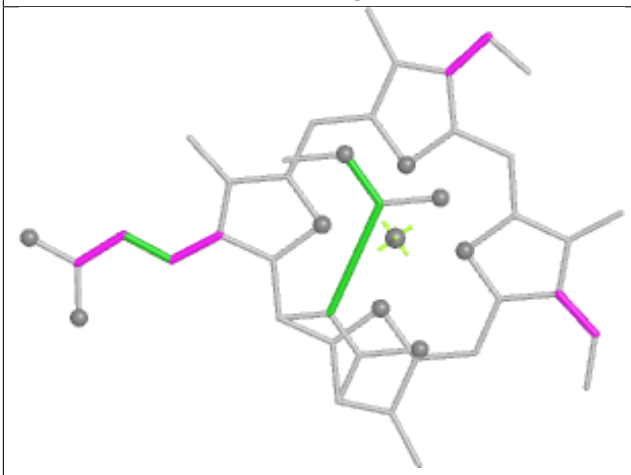
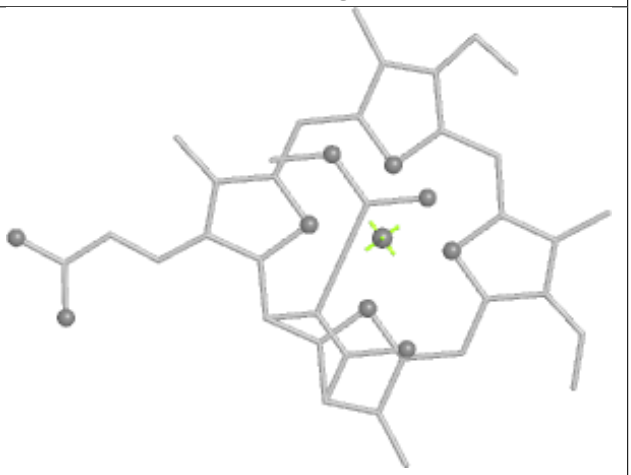


Bond angles

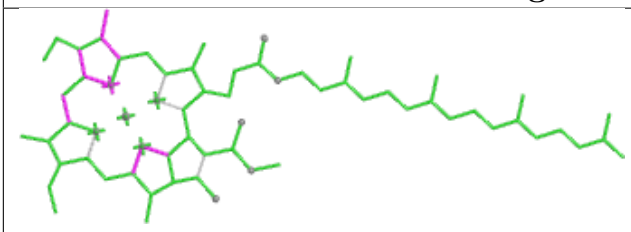


Torsions

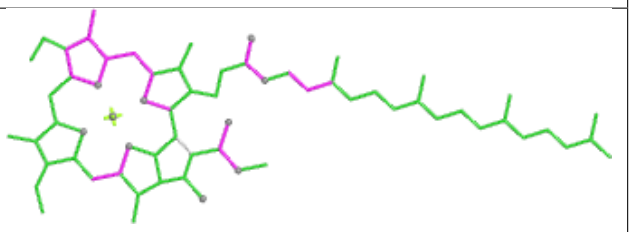


Rings

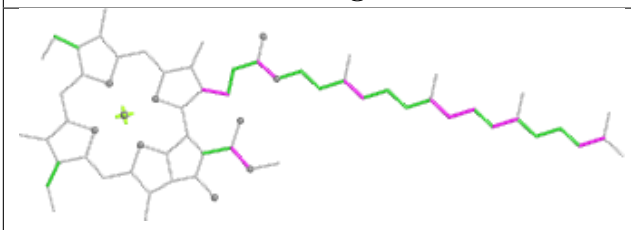
Ligand CLA a 816



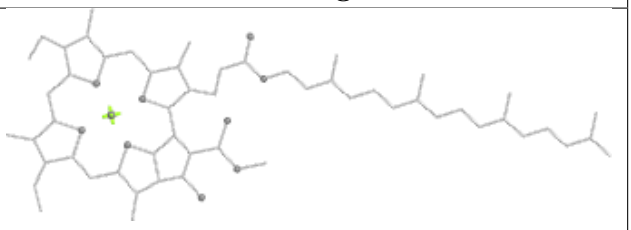
Bond lengths



Bond angles

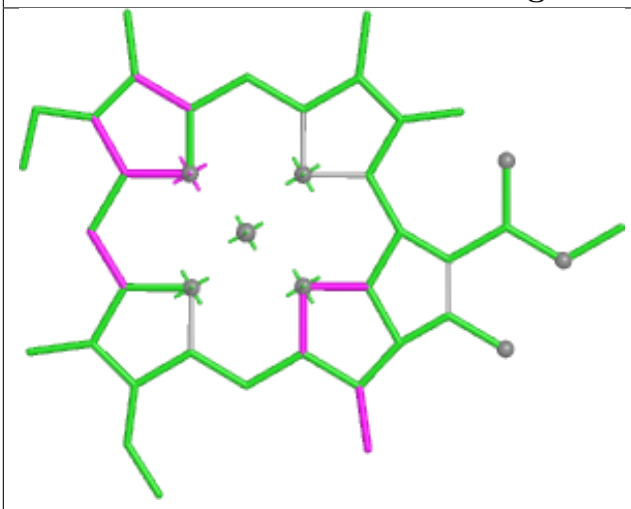


Torsions



Rings

Ligand CLA y 307



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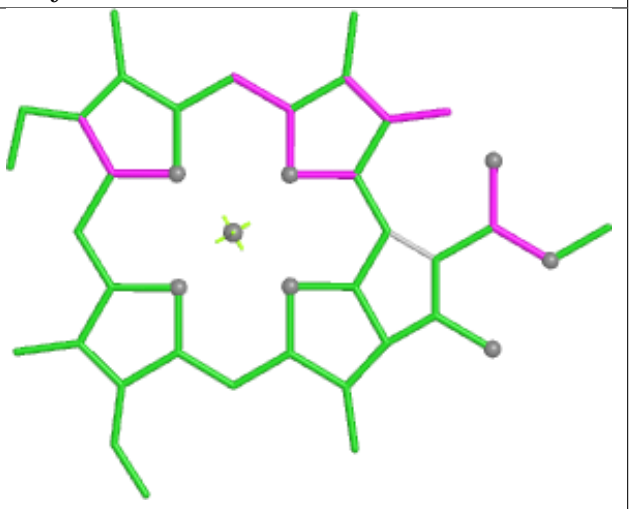
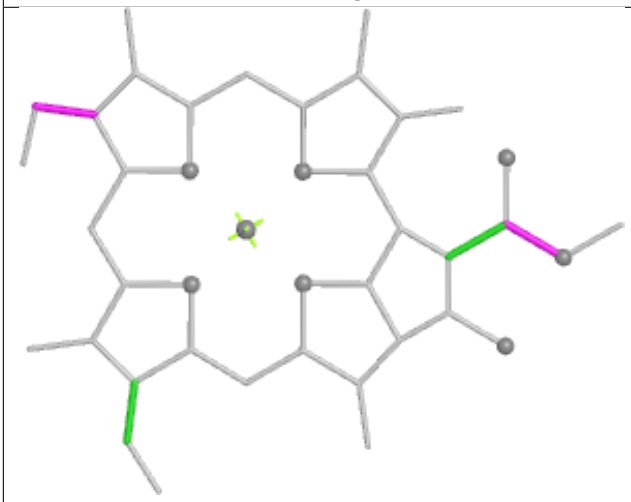
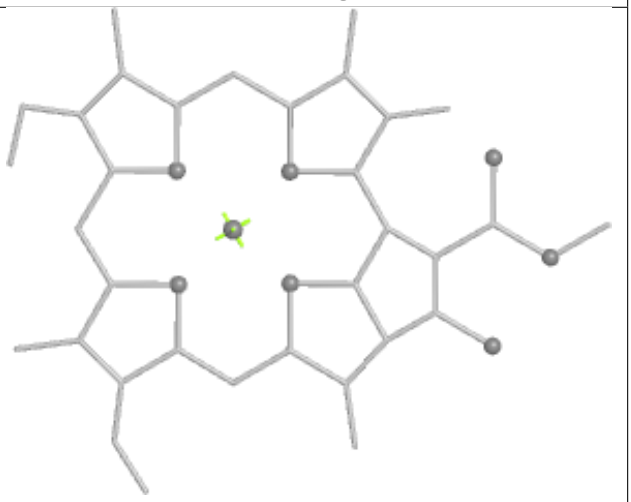


Bond angles

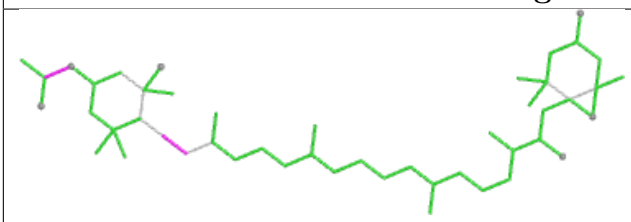


Torsions

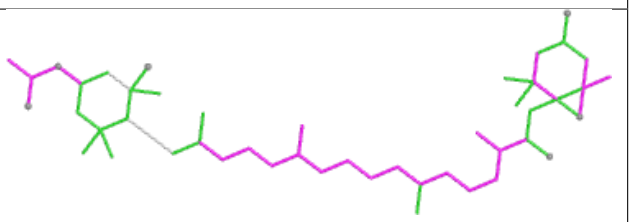


Rings

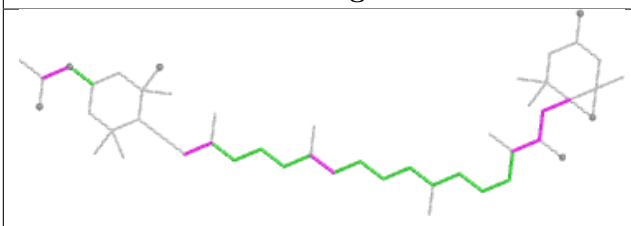
Ligand A86 2 305



Bond lengths



Bond angles



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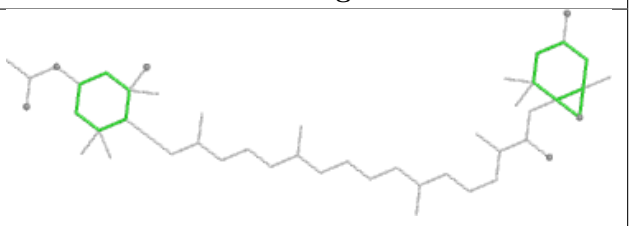
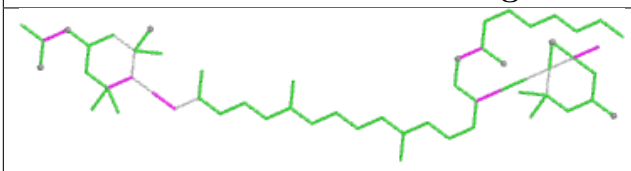


Rings

Ligand A1EB4 M 322



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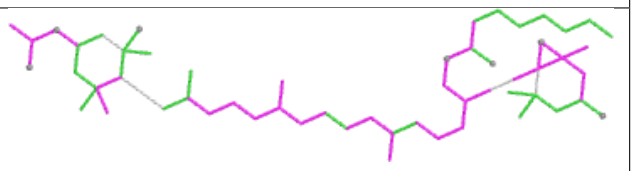
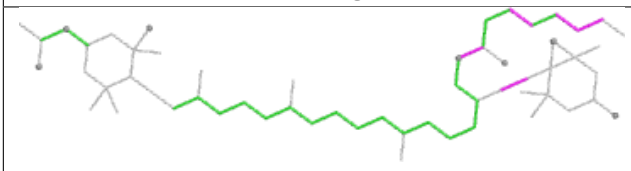
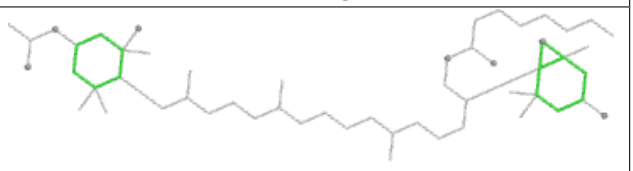


Bond angles

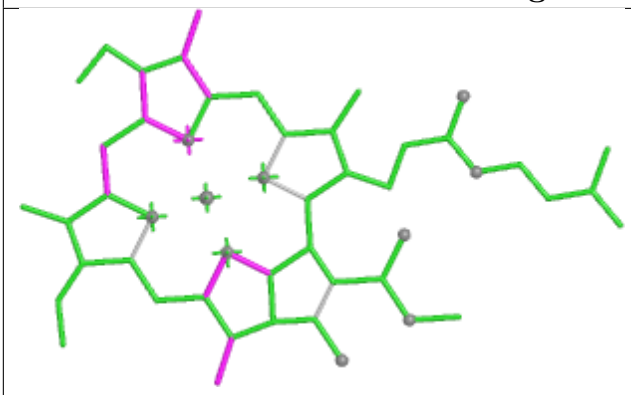


Torsions



Rings

Ligand CLA a 828



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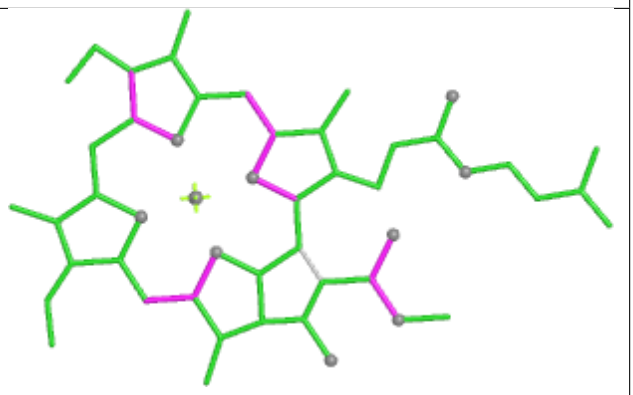
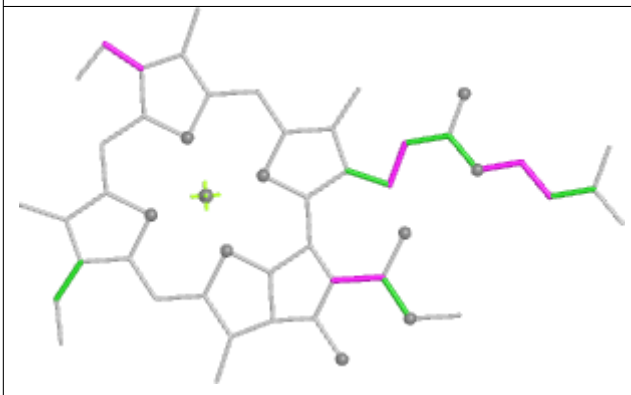


Bond angles



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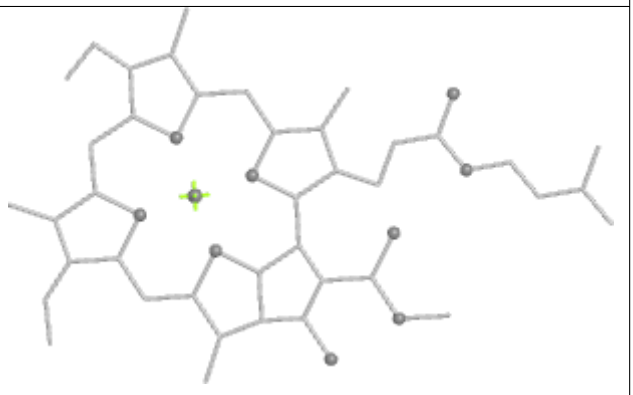
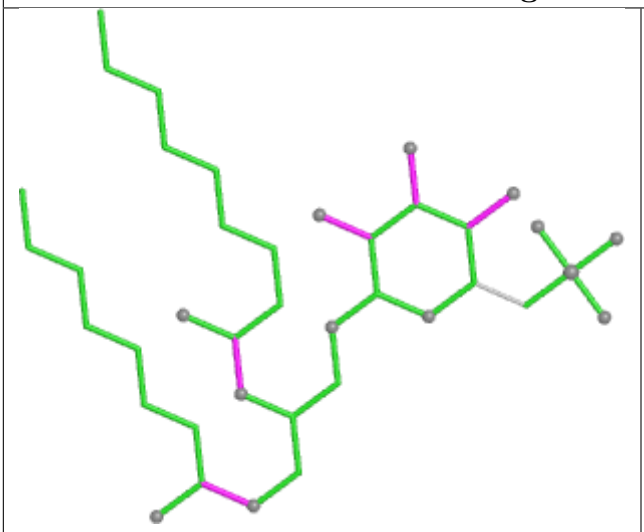
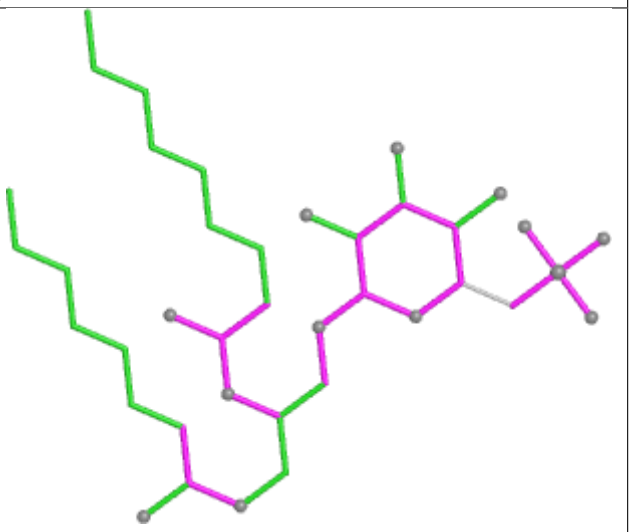


Rings

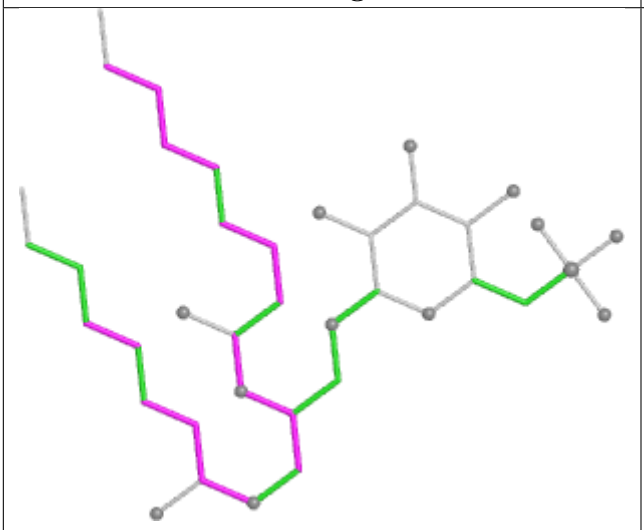
Ligand SQD M 301



Bond lengths



Bond angles



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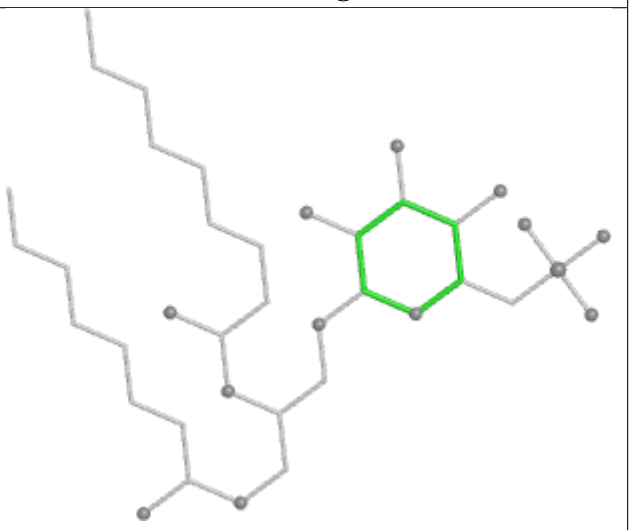
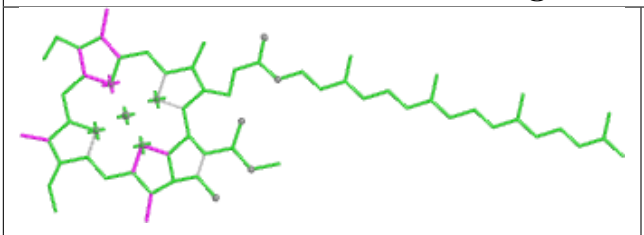


Rings

Ligand CLA a 801



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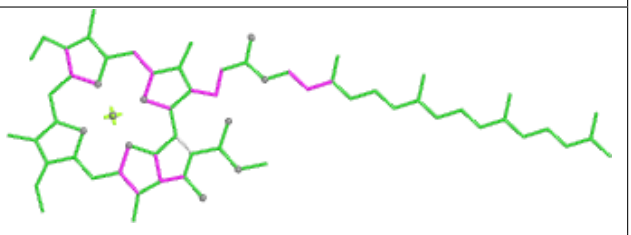
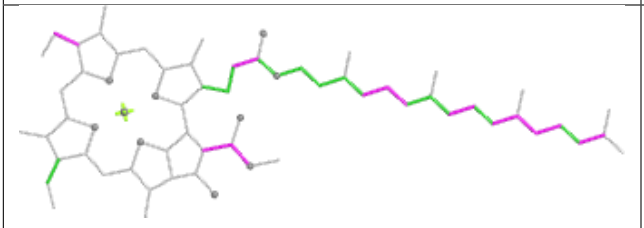


Bond angles



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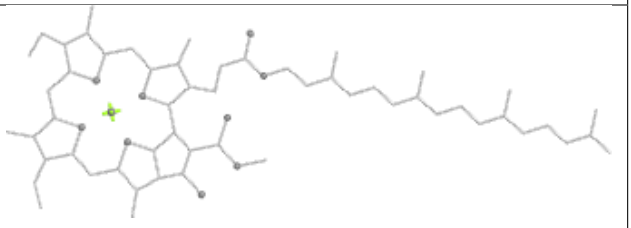
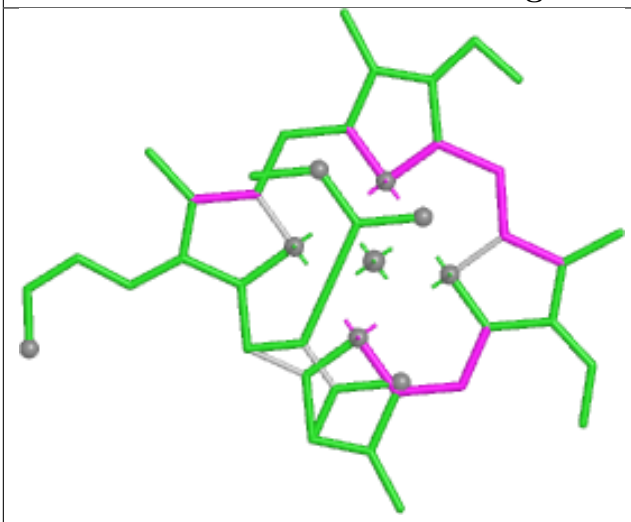
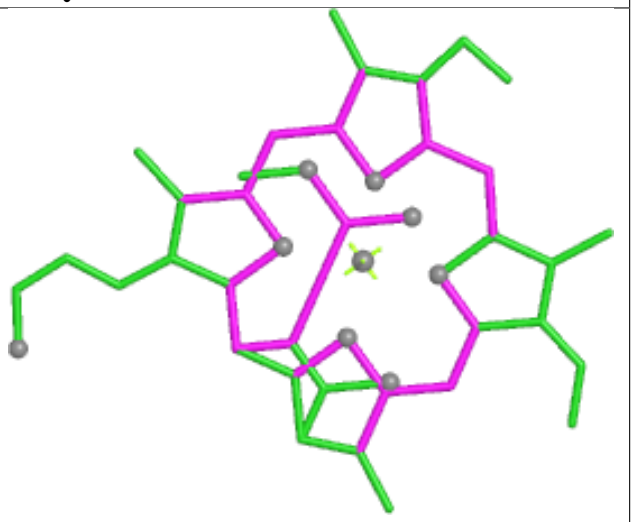


Rings

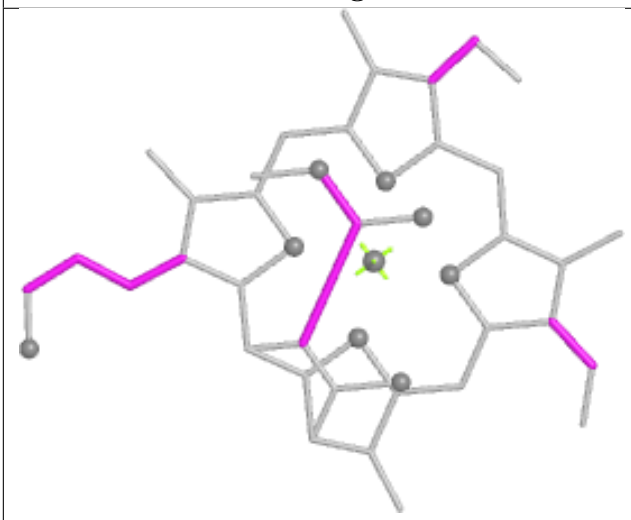
Ligand KC2 Q 313



Bond lengths



Bond angles



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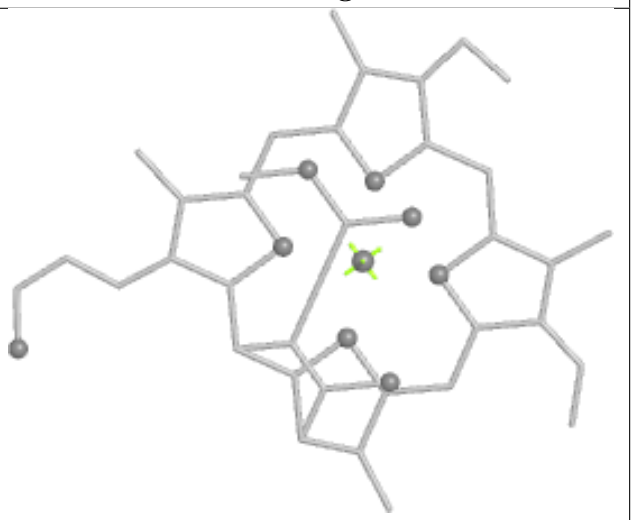
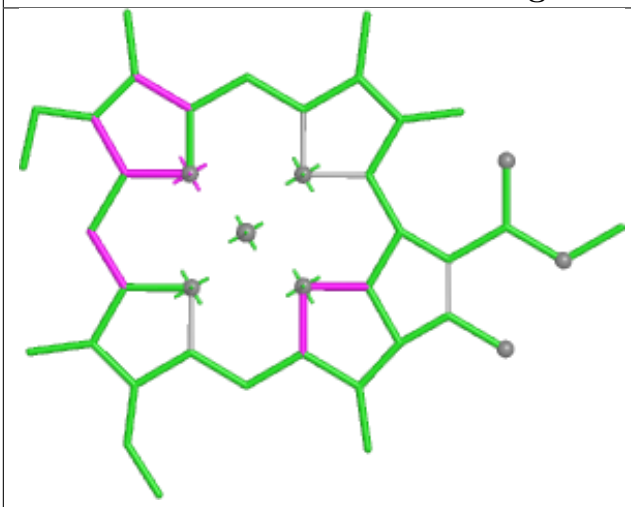


Rings

Ligand CLA 7 321



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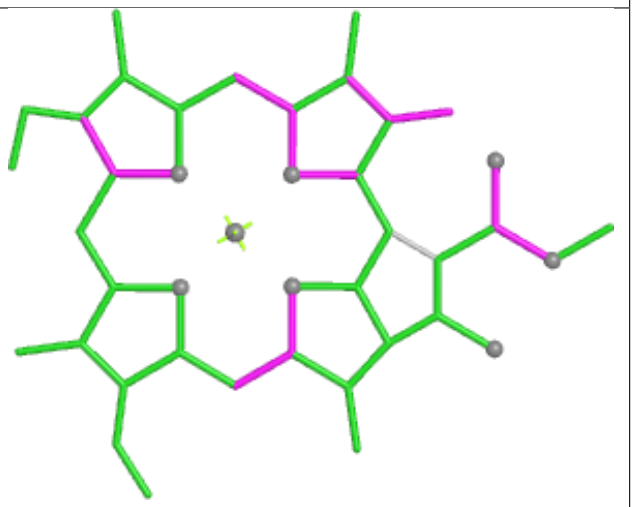
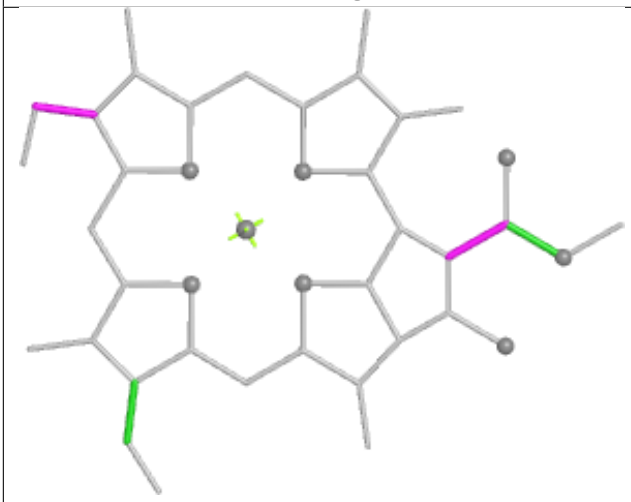


Bond angles



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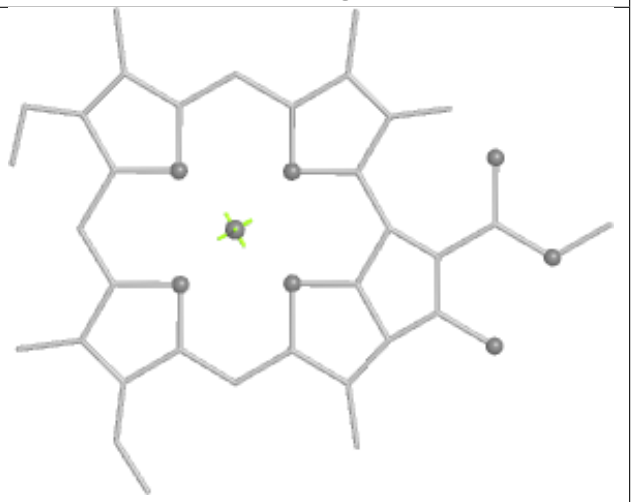
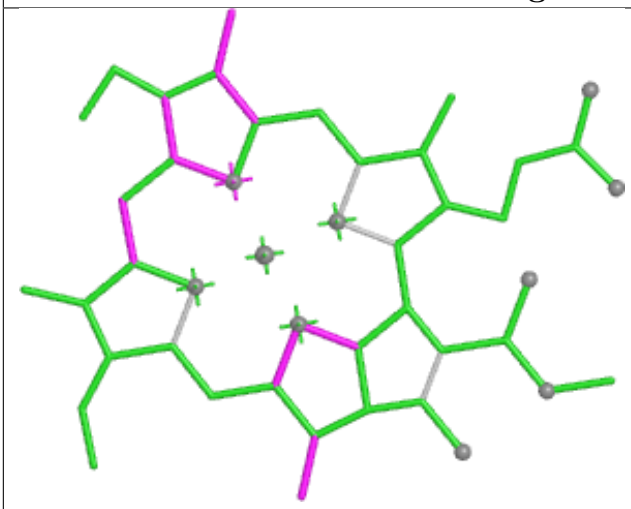


Rings

Ligand CLA a 817



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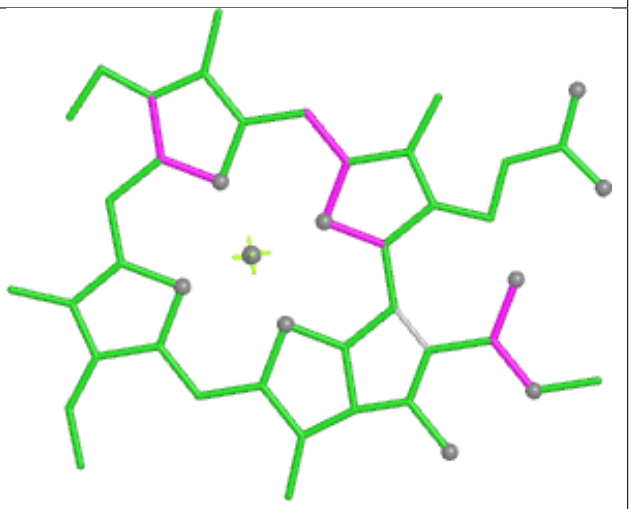
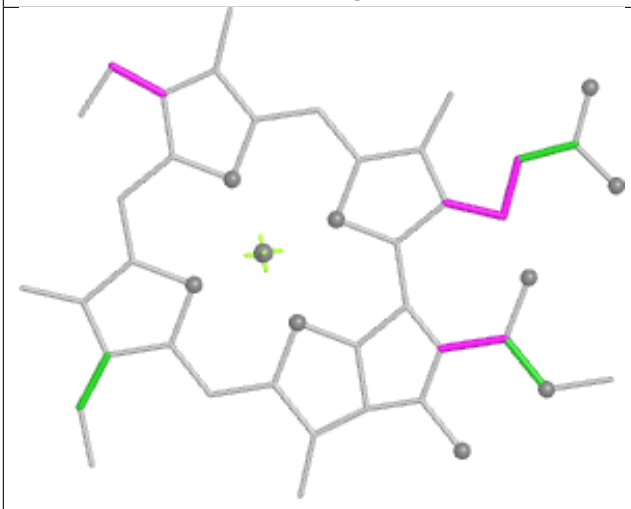


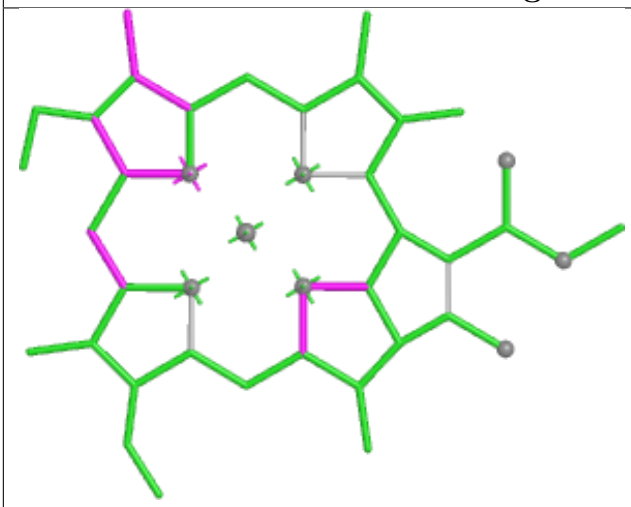
Bond angles



Torsions

Rings

Ligand CLA Y 313



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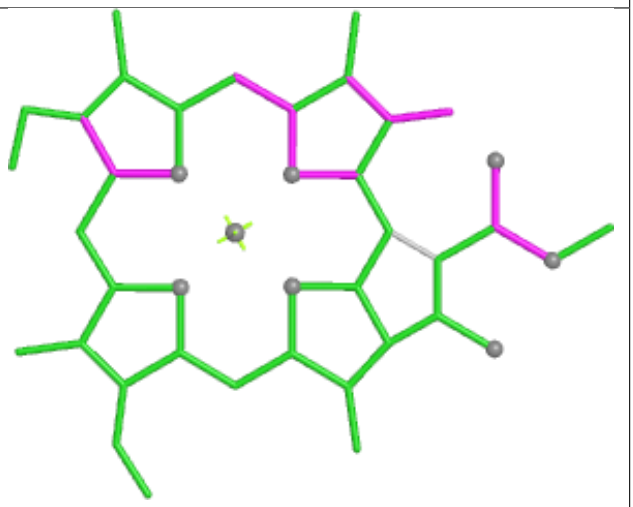
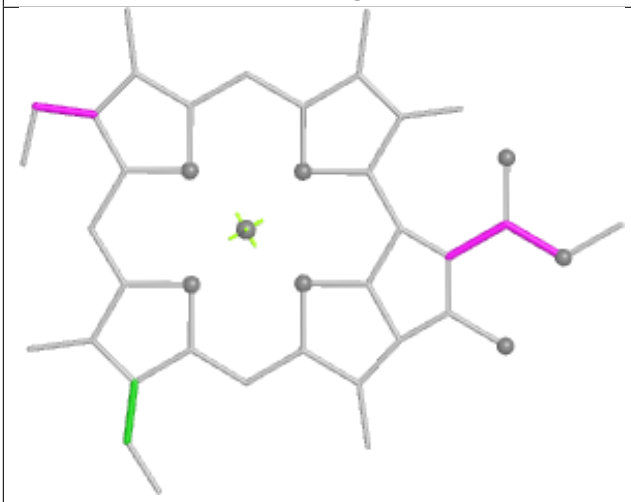
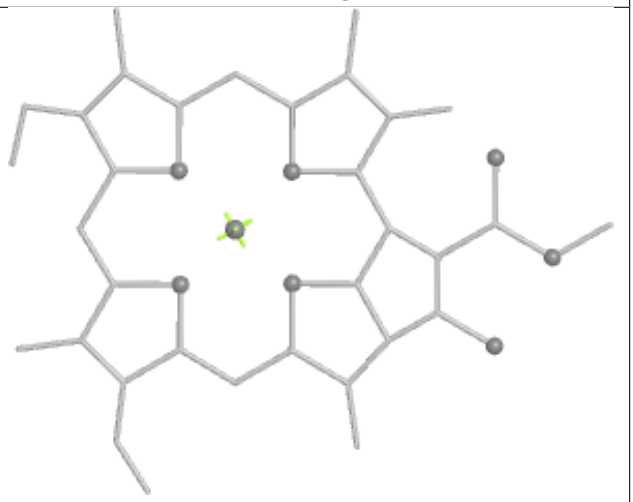


Bond angles

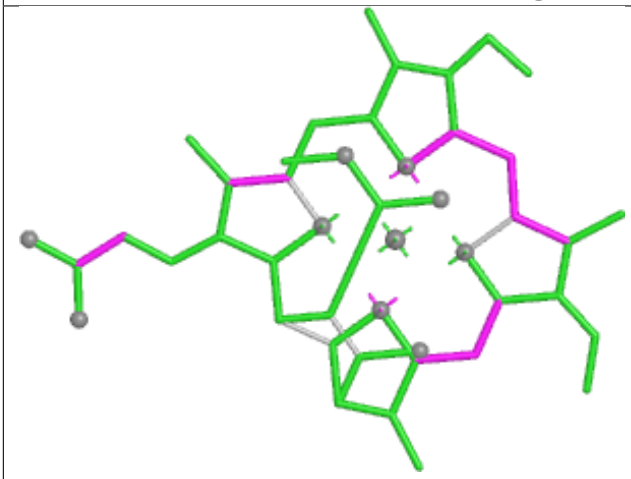


Torsions



Rings

Ligand KC2 7 322



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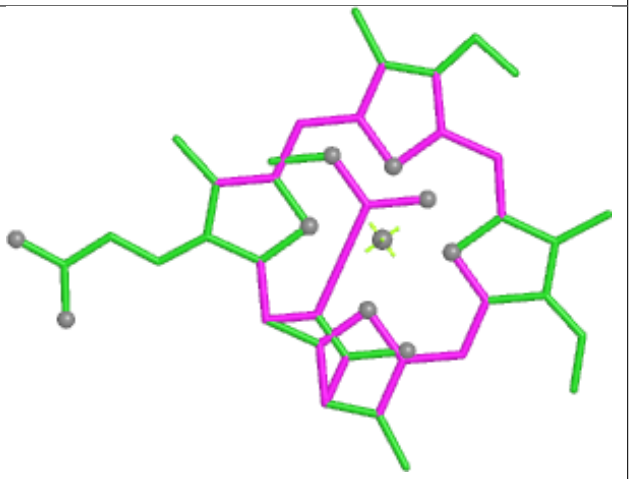
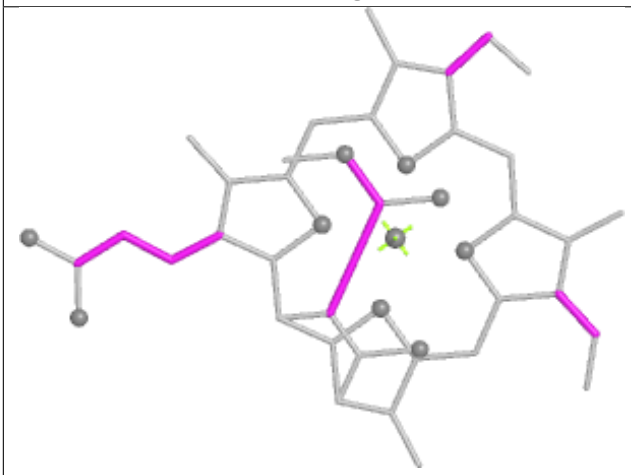


Bond angles



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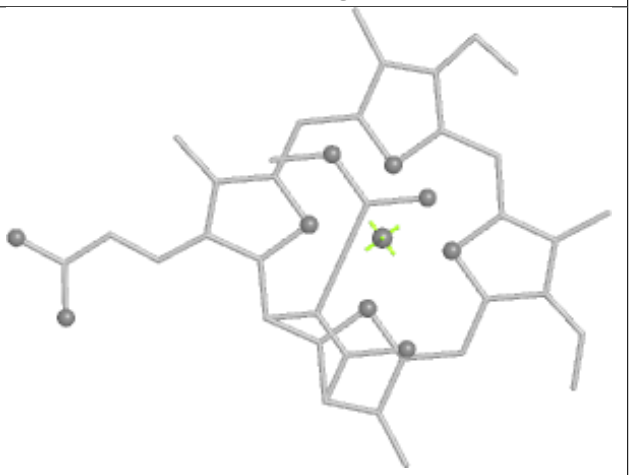
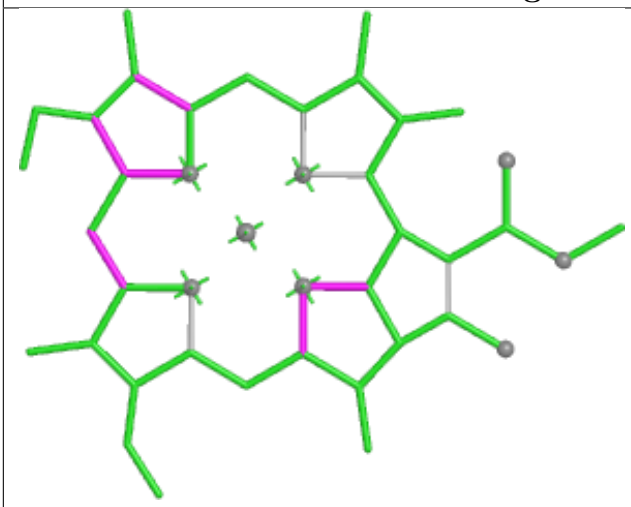


Rings

Ligand CLA O 316



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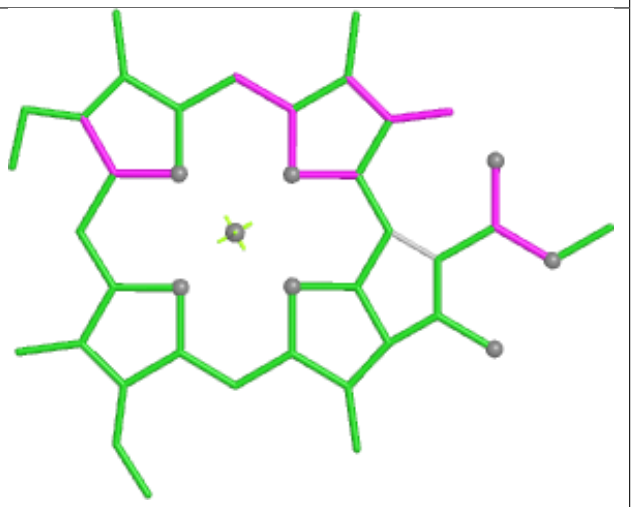
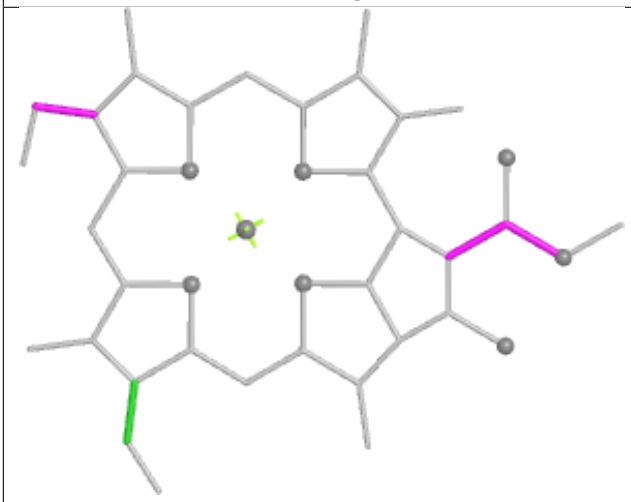
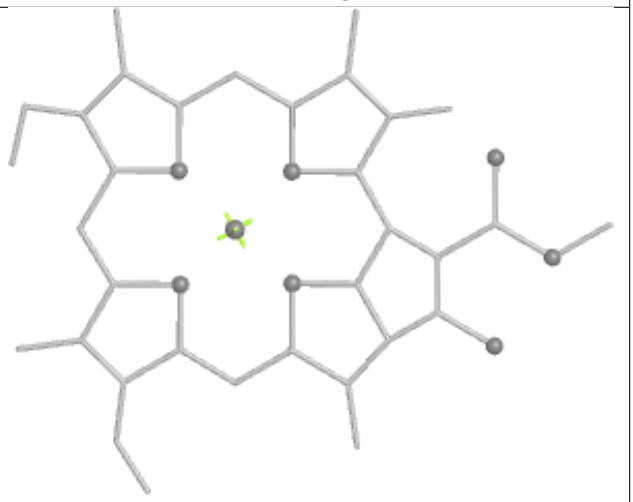


Bond angles

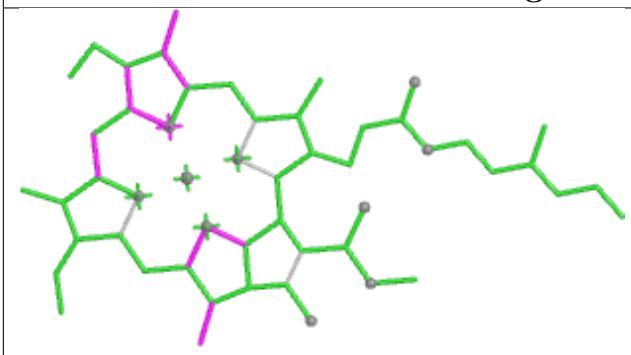


Torsions



Rings

Ligand CLA E 316



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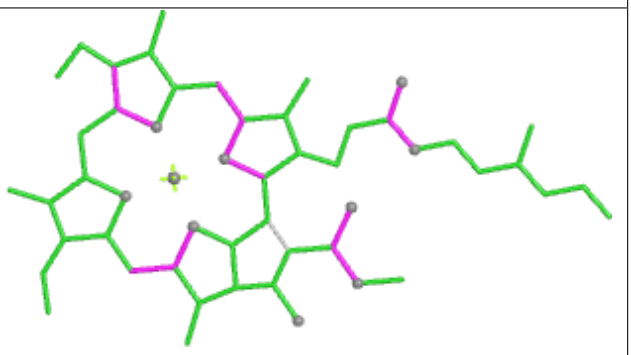
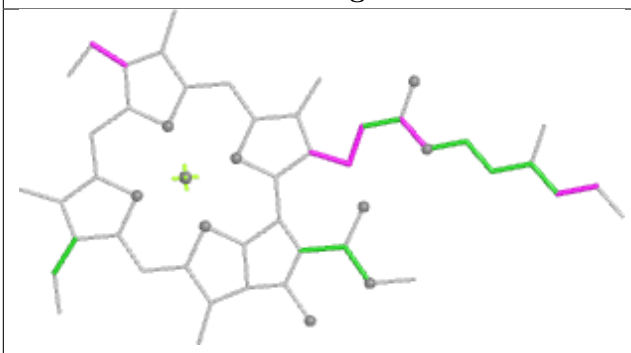
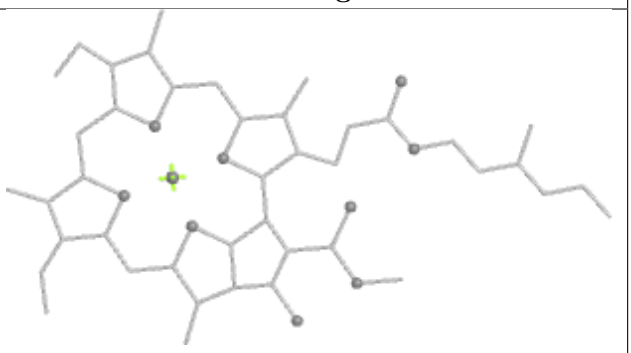


Bond angles

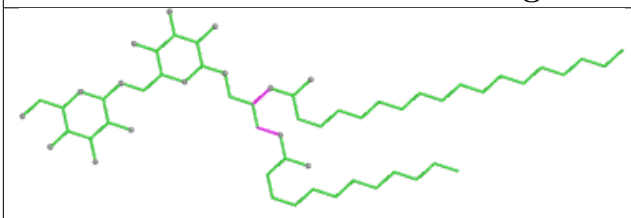


Torsions

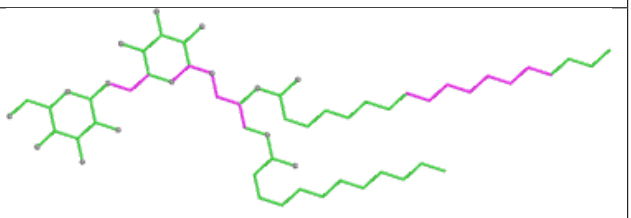


Rings

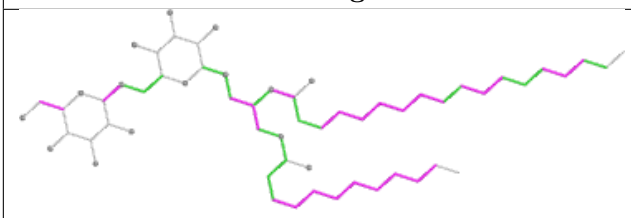
Ligand DGD b 849



Bond lengths



Bond angles



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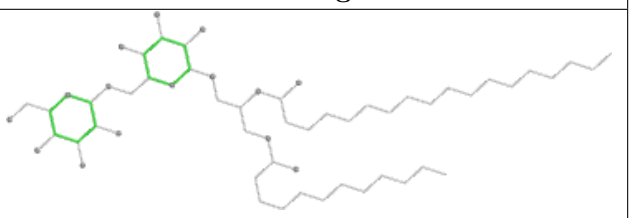
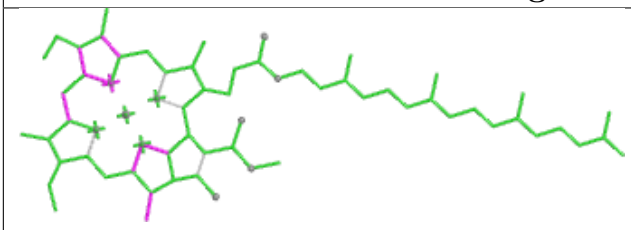
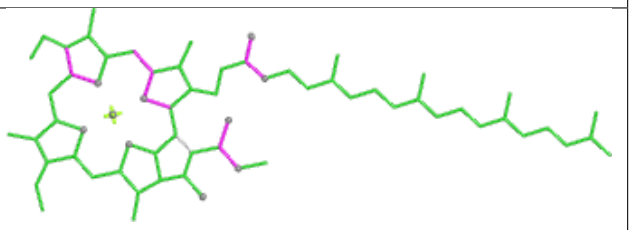


Rings

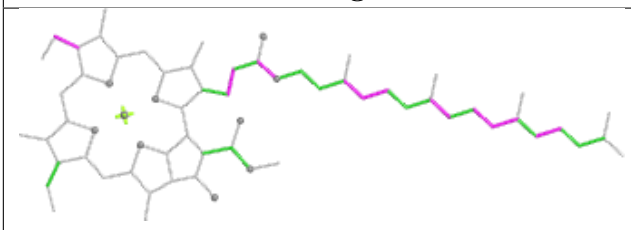
Ligand CLA 5 306



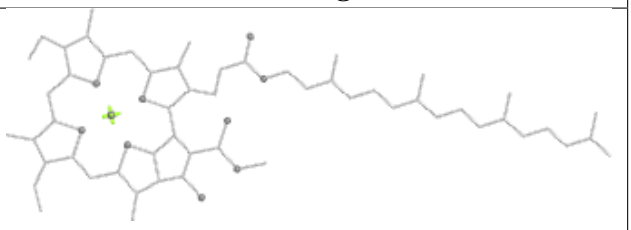
Bond lengths



Bond angles

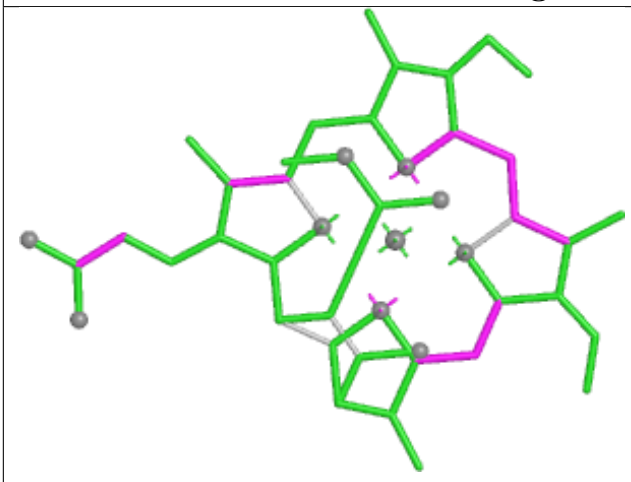


Torsions



Rings

Ligand KC2 7 319



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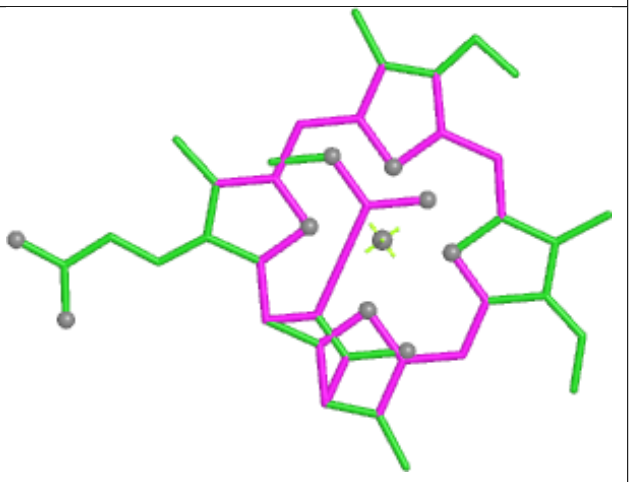

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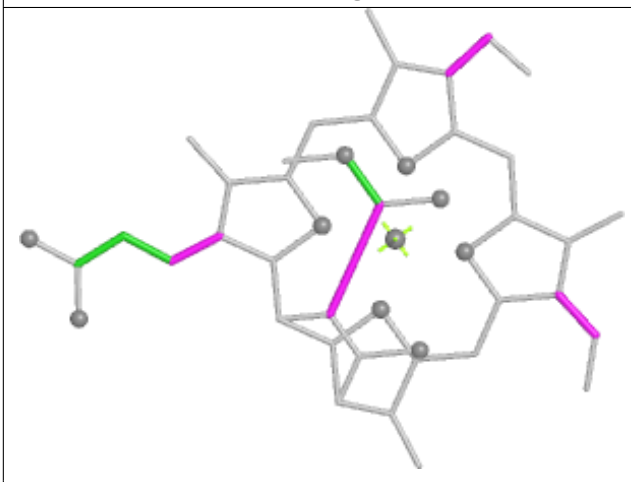

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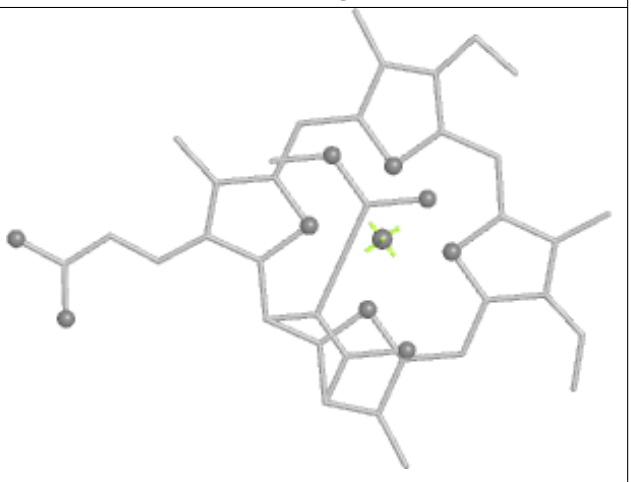
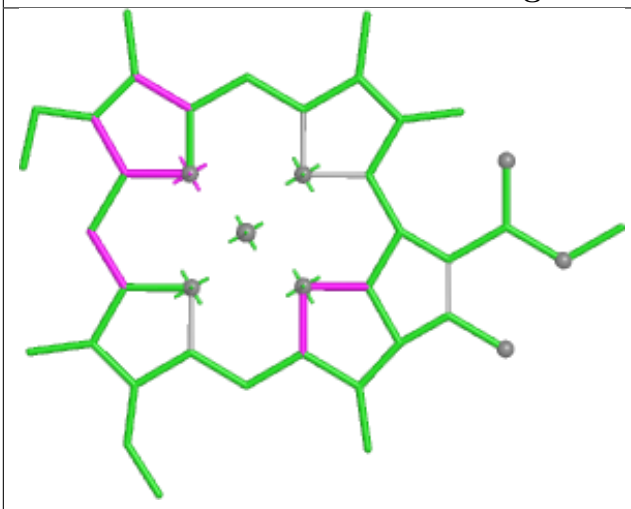


Rings

Ligand CLA Y 302



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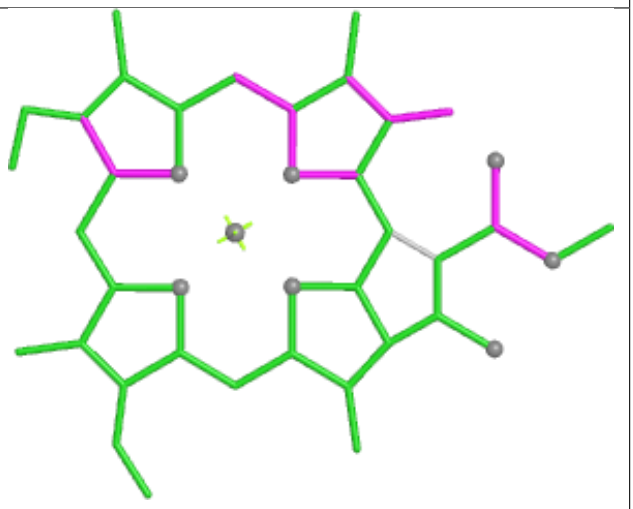

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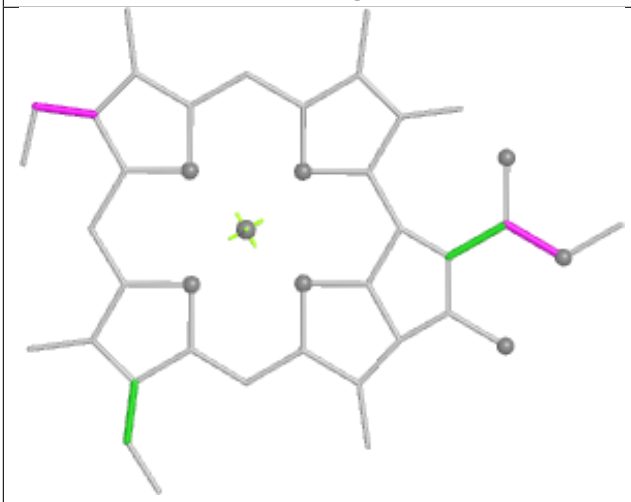

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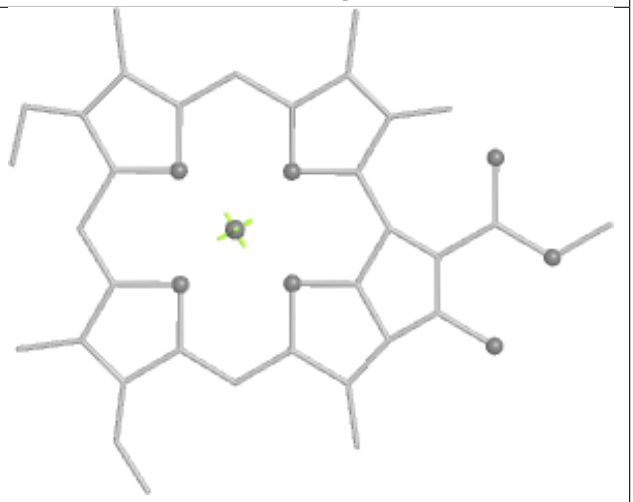
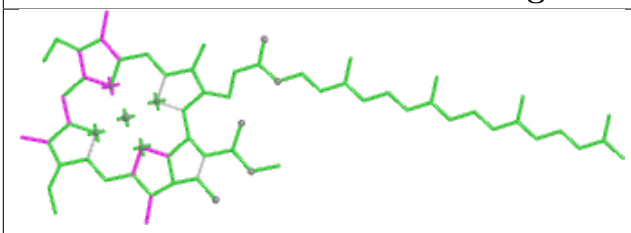


Rings

Ligand CLA b 826



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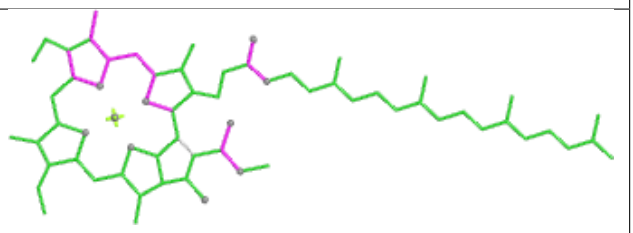

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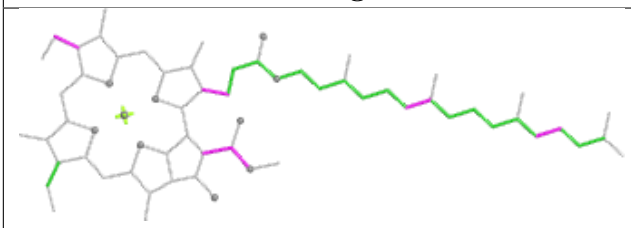

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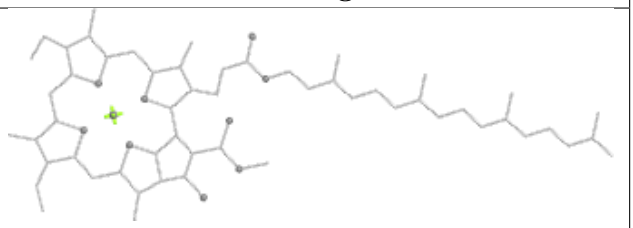
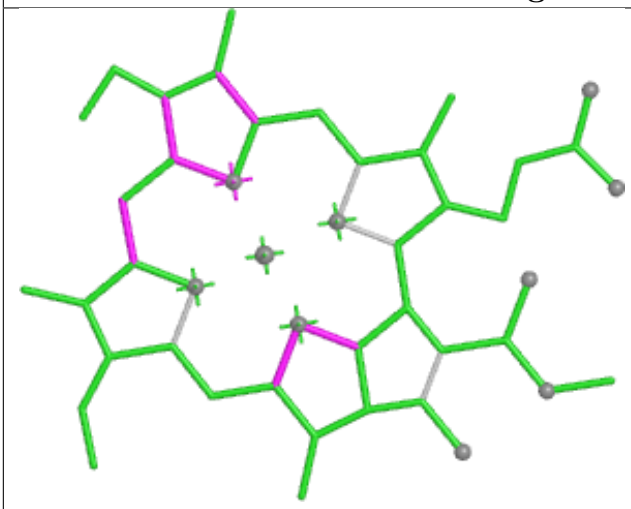


Rings

Ligand CLA x 306



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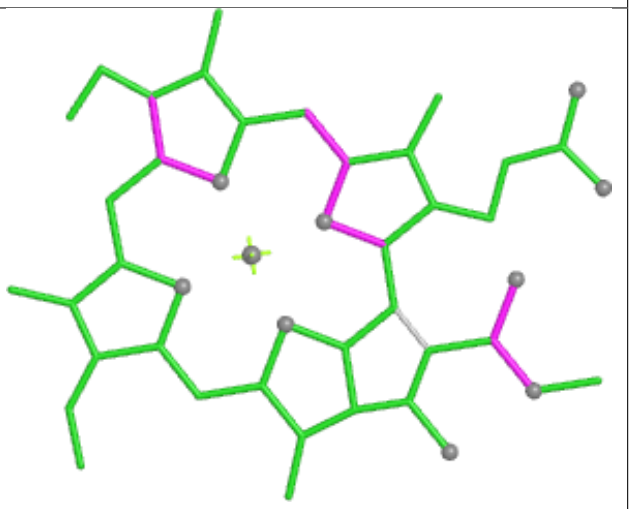
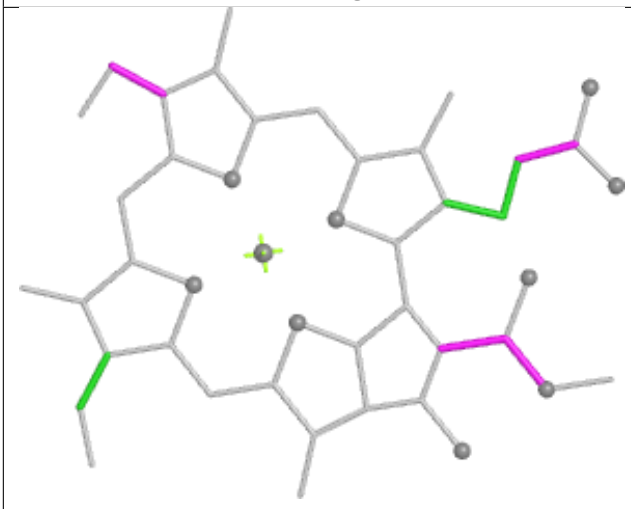


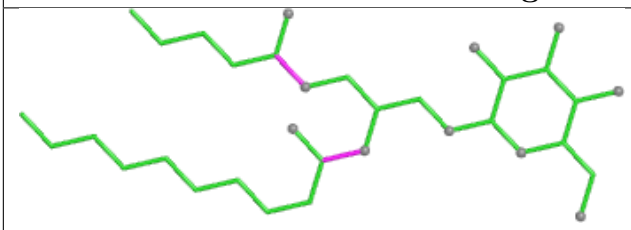
Bond angles



Torsions

Rings

Ligand LMG F 320



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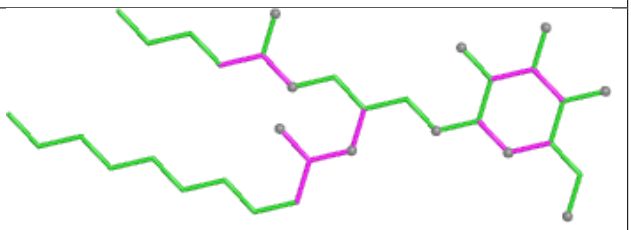
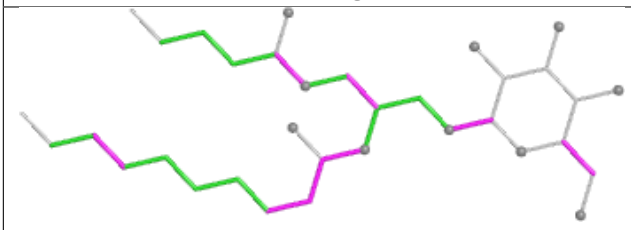


Bond angles



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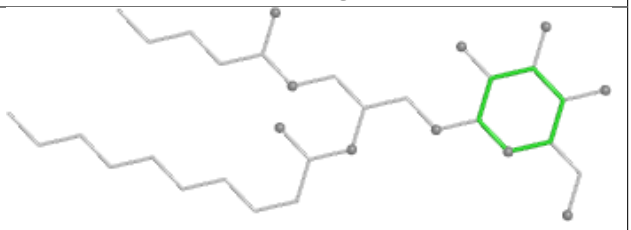
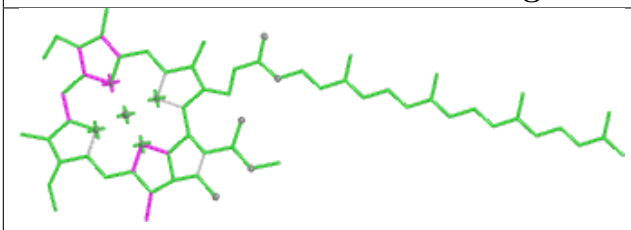


Rings

Ligand CLA K 307



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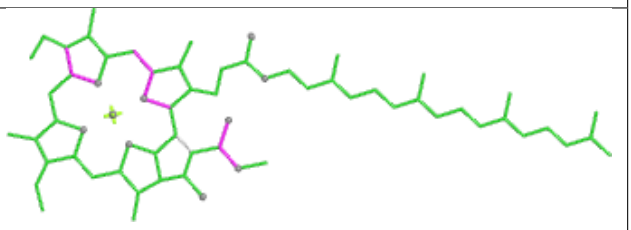
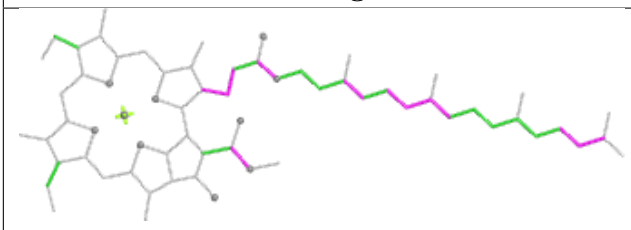


Bond angles



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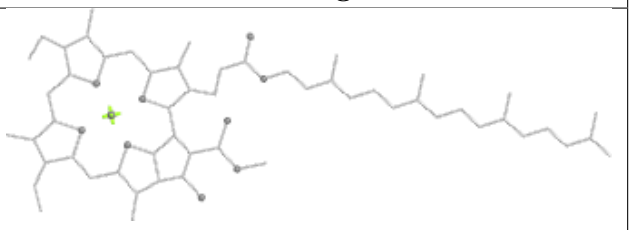
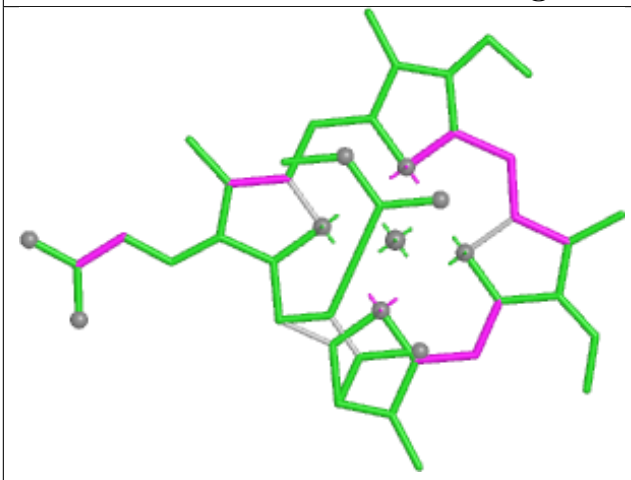


Rings

Ligand KC2 4 324



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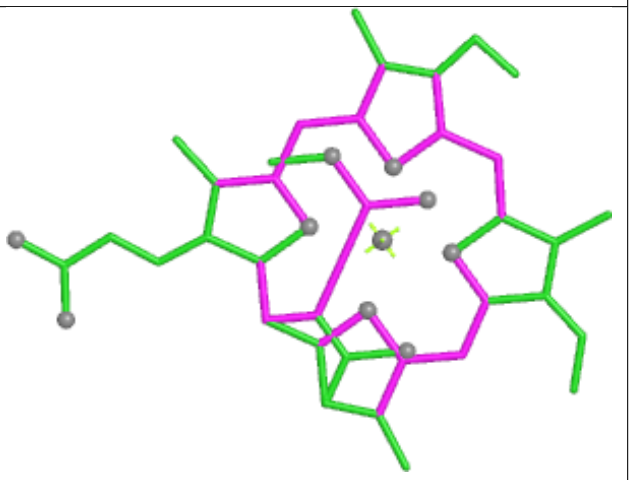

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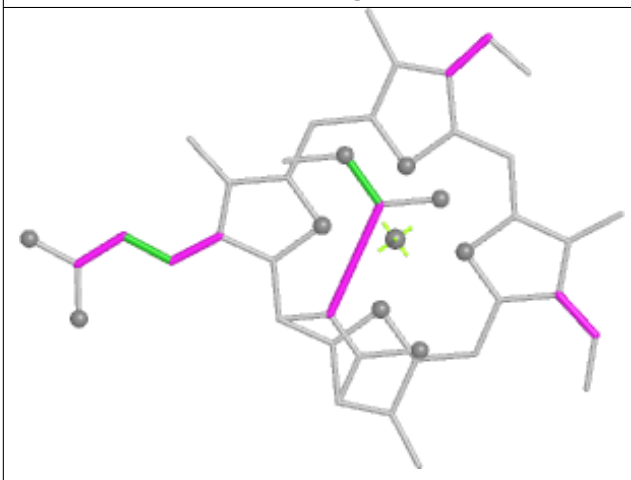

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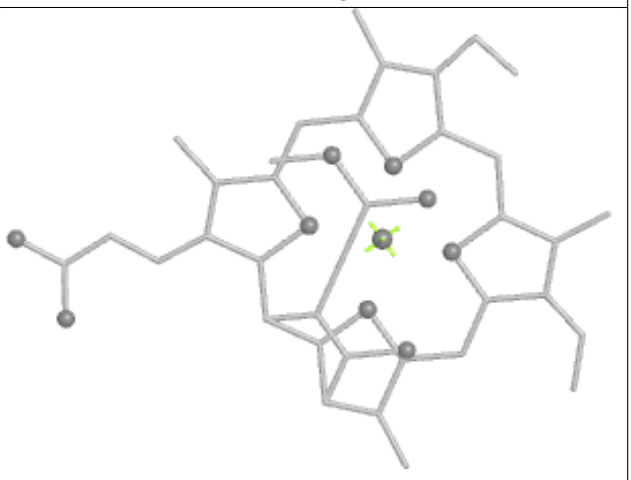
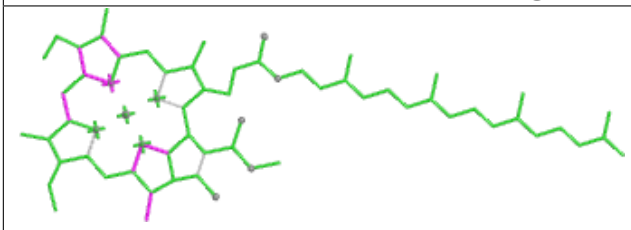


Rings

Ligand CLA 4 314



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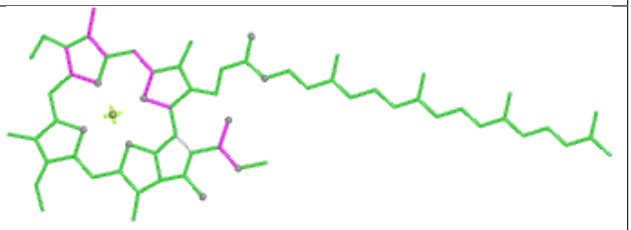
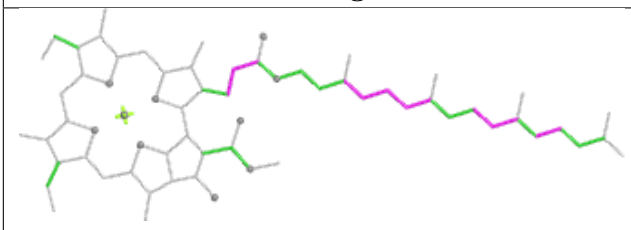
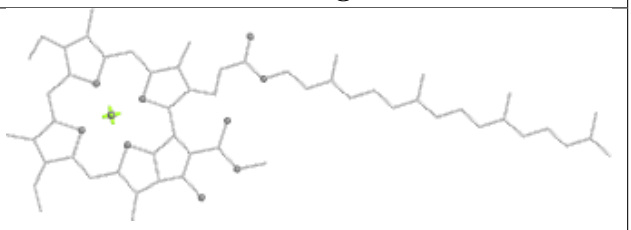


Bond angles

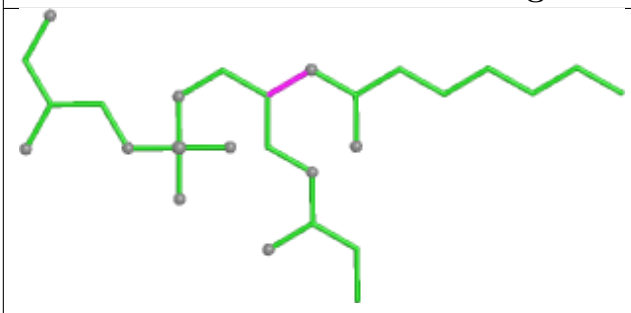


Torsions



Rings

Ligand LHG a 841



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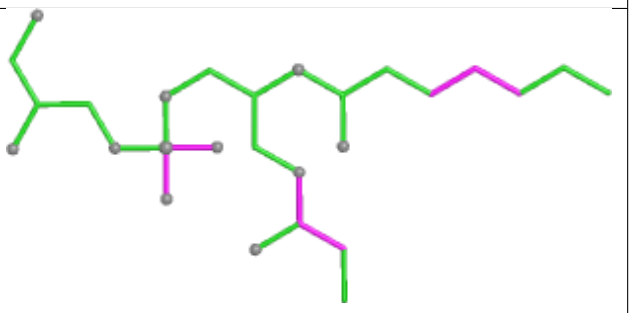
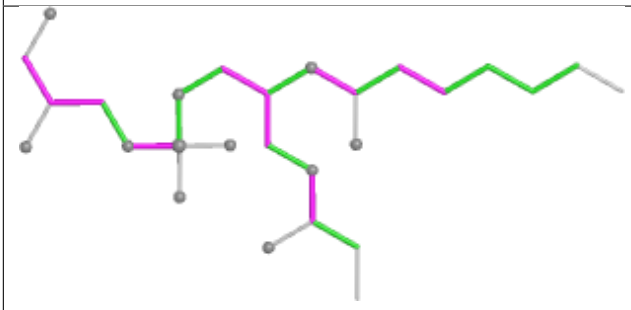


Bond angles



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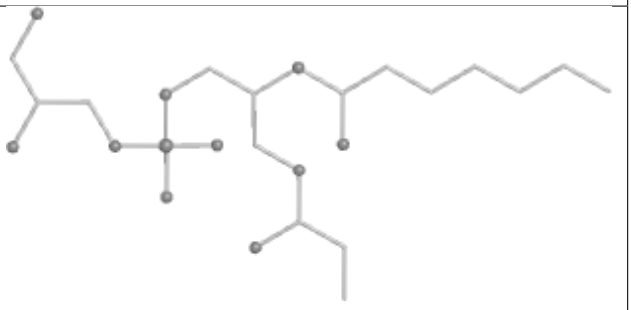
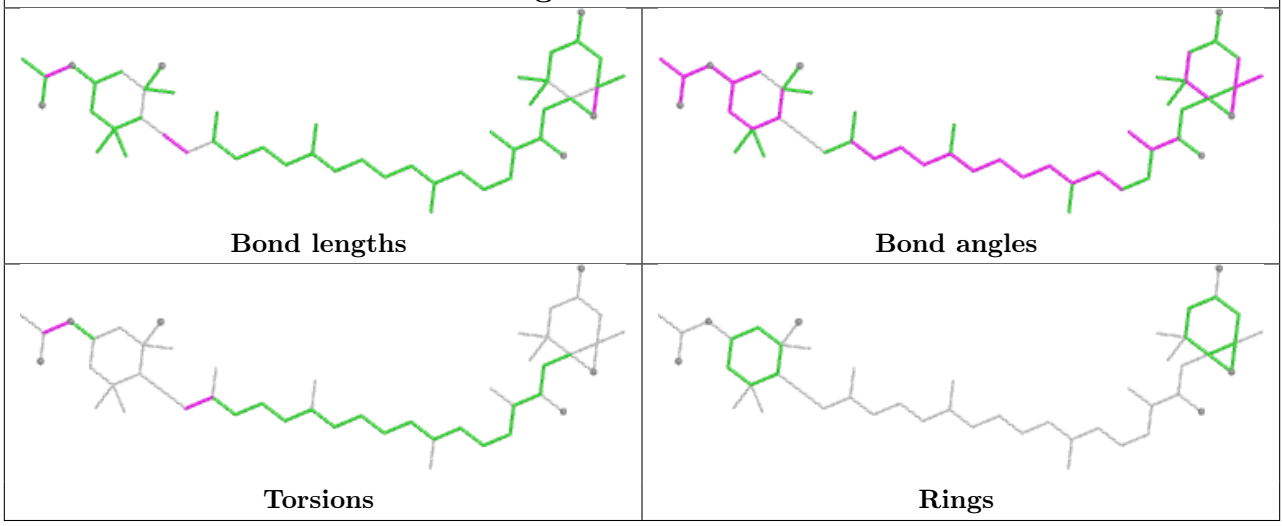
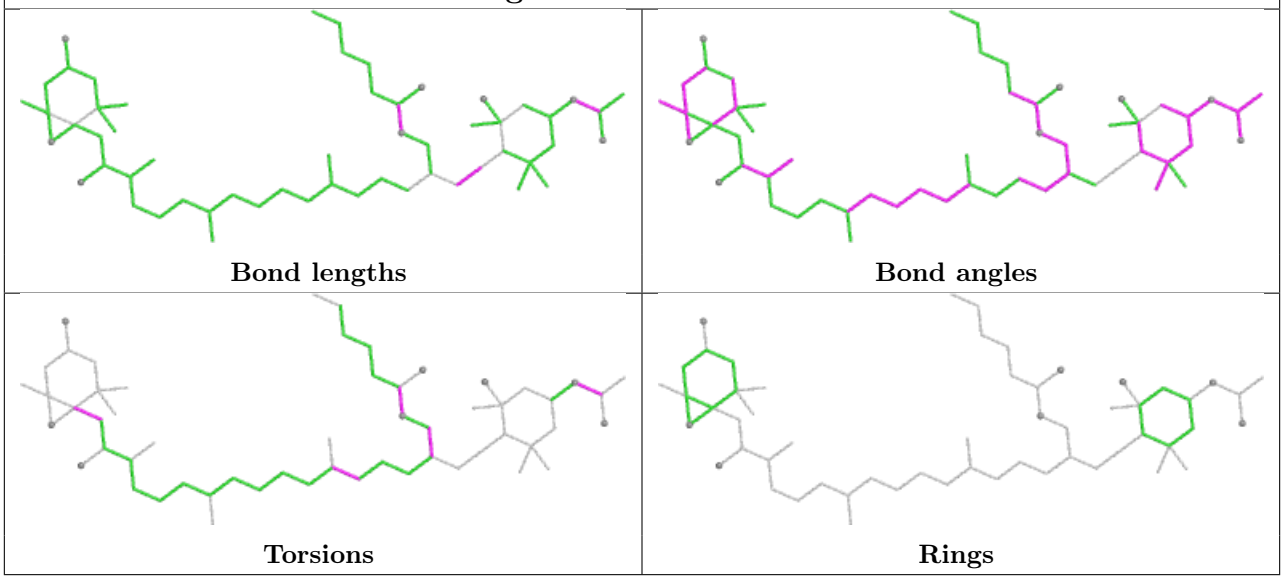


Rings

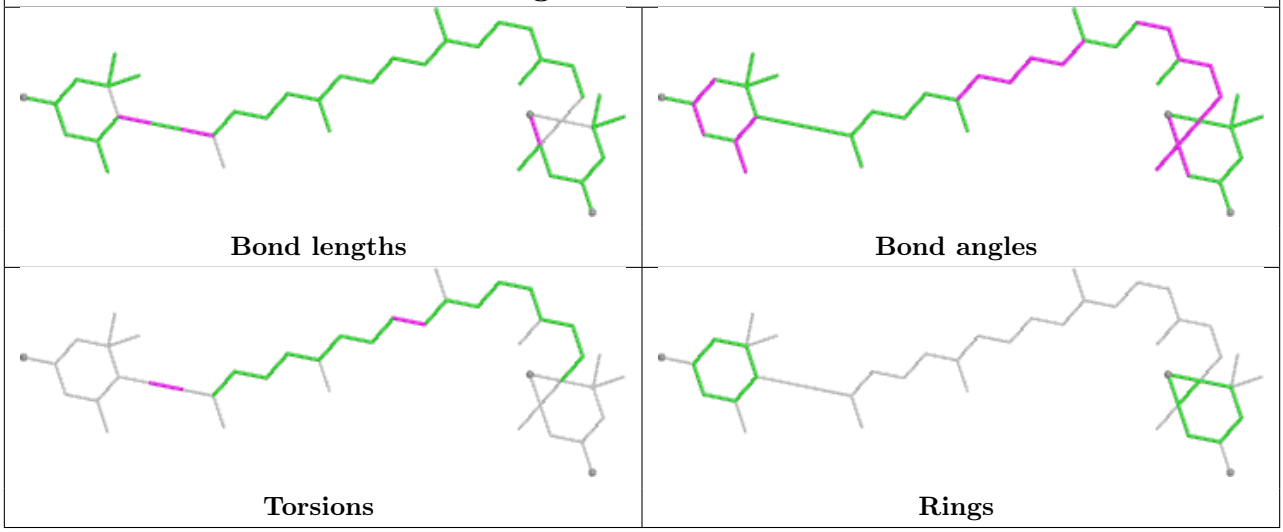
Ligand A86 8 323



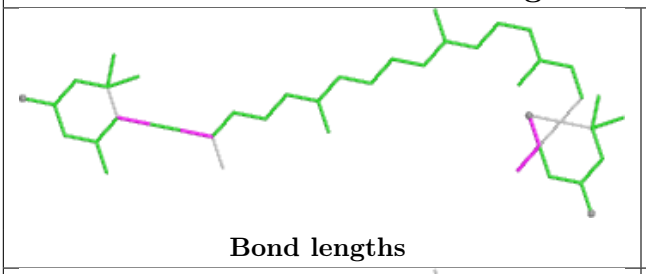
Ligand A1EB1 U 203



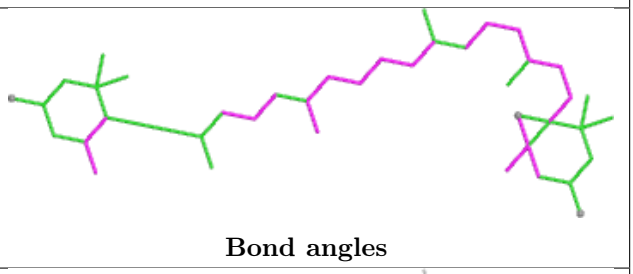
Ligand DD6 I 306



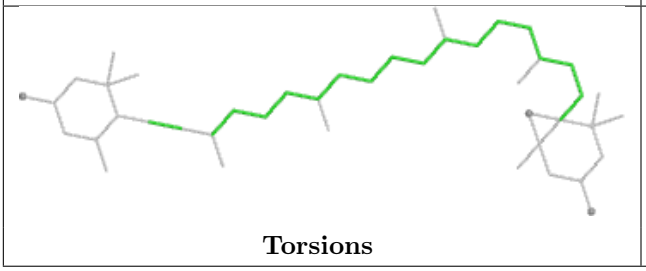
Ligand DD6 D 306



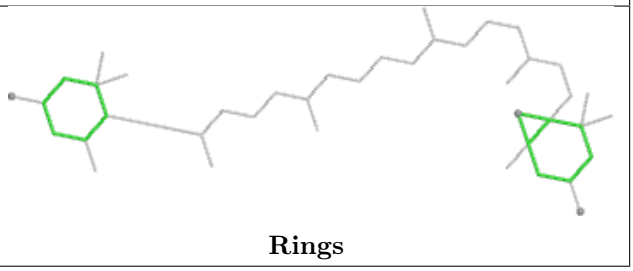
Bond lengths



Bond angles

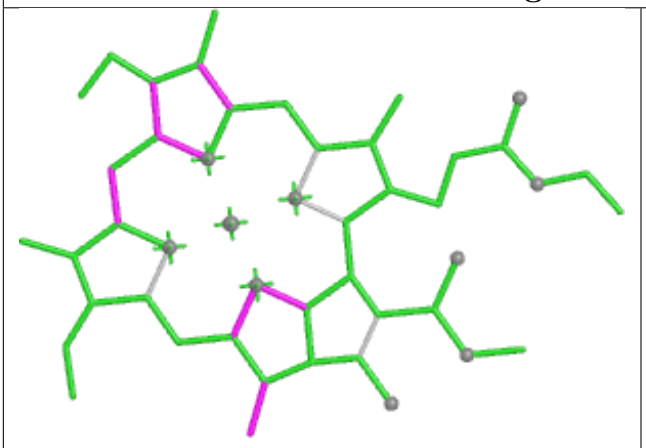


Torsions



Rings

Ligand CLA T 318



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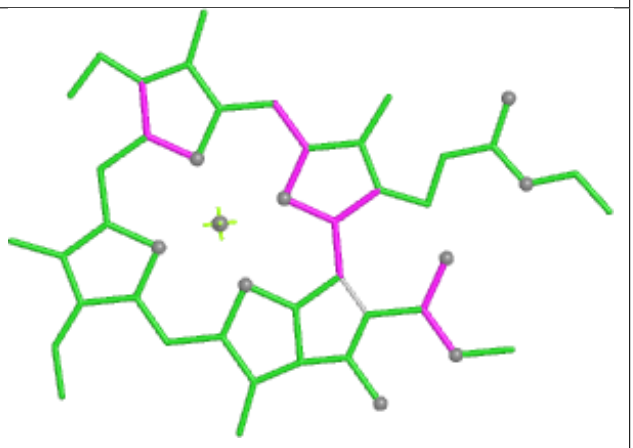
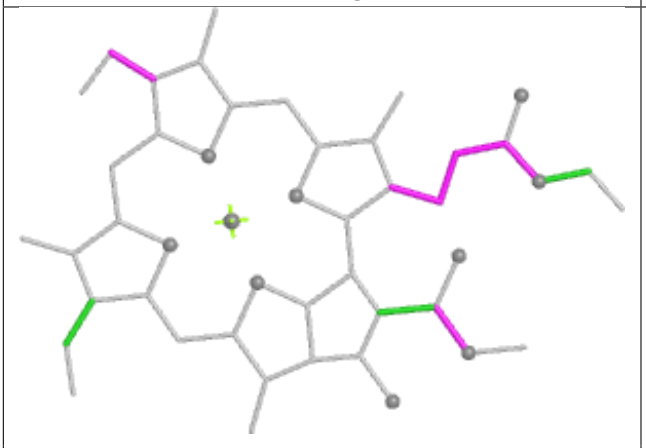


Bond angles



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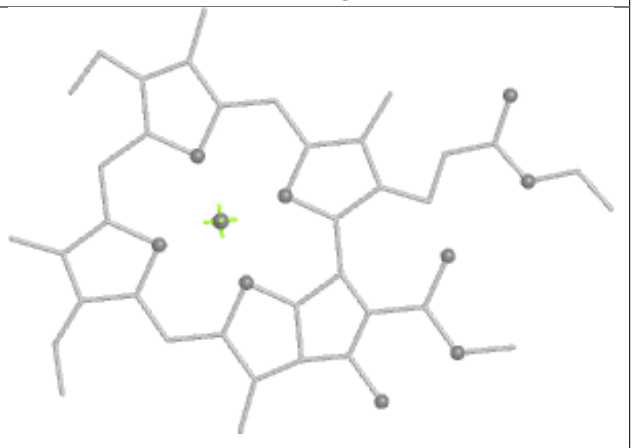
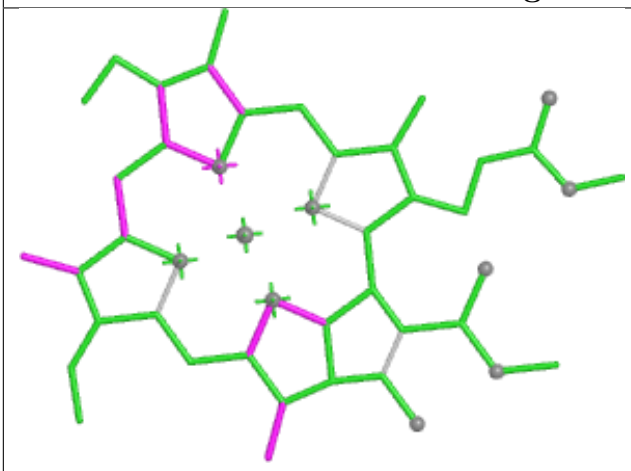
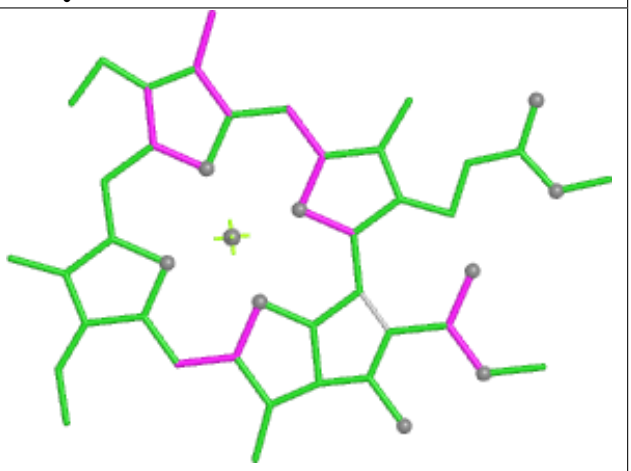


Rings

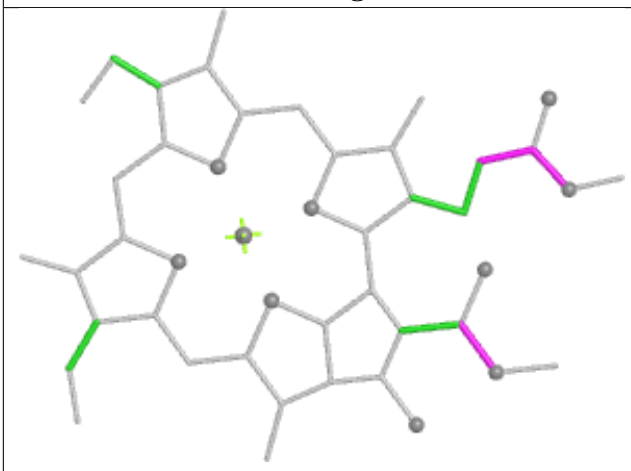
Ligand CLA Q 311



Bond lengths



Bond angles



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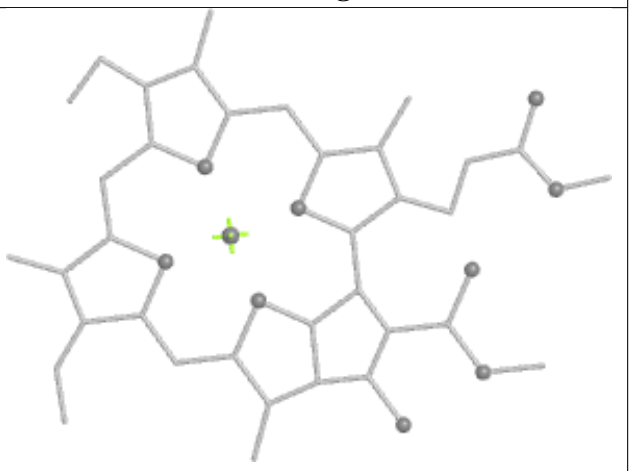
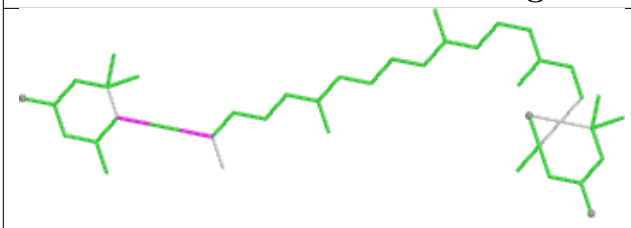
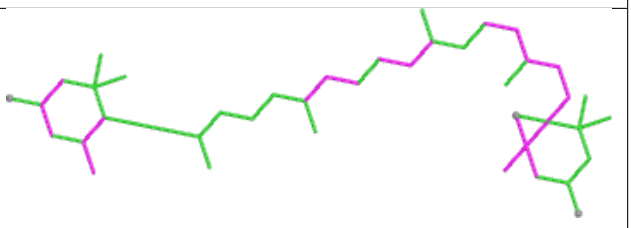


Rings

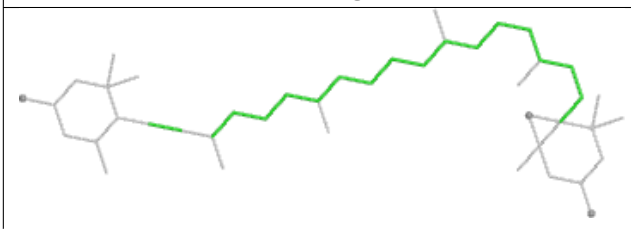
Ligand DD6 F 303



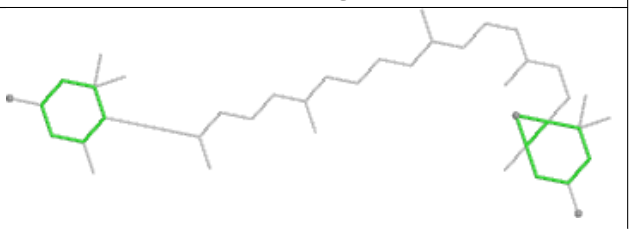
Bond lengths



Bond angles

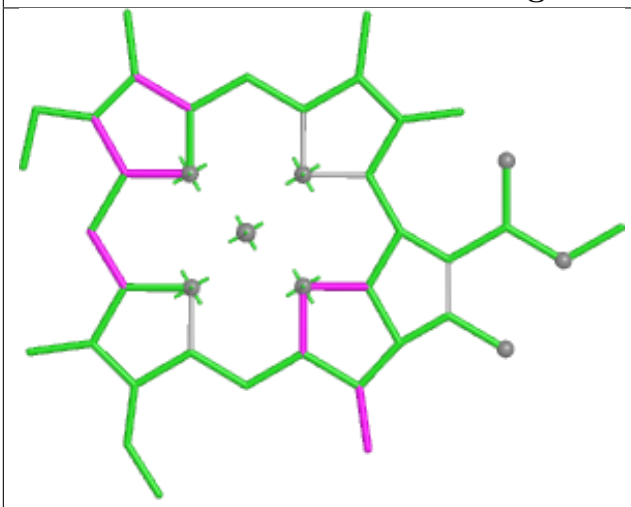


Torsions



Rings

Ligand CLA x 308



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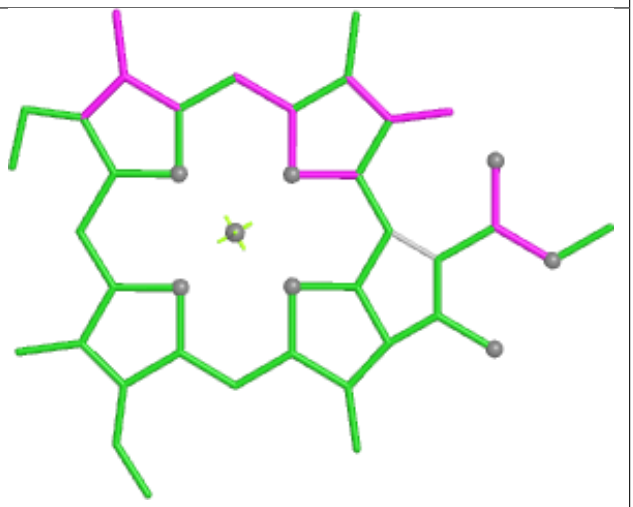
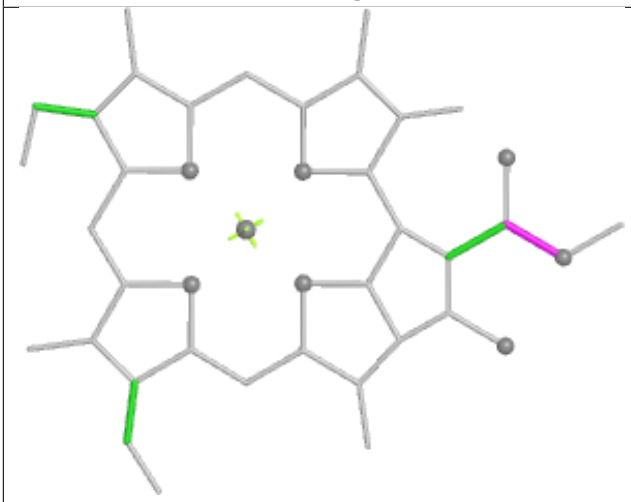
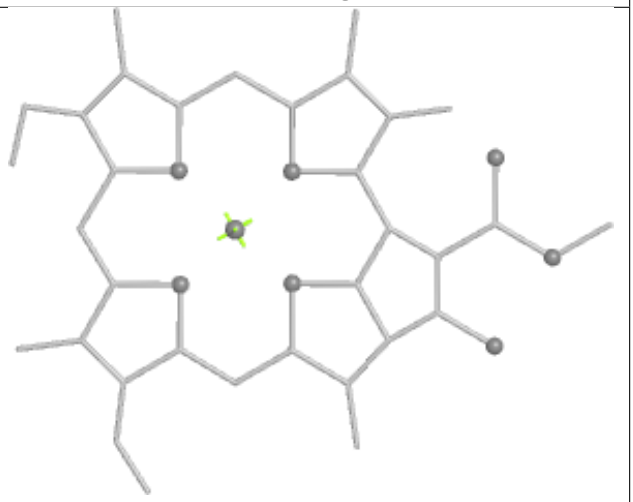


Bond angles

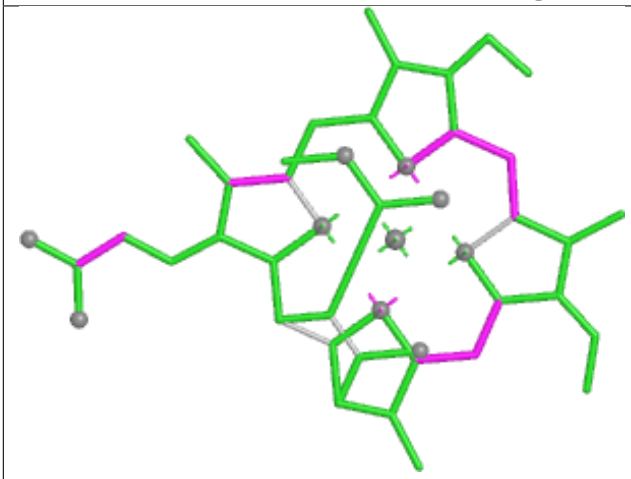


Torsions

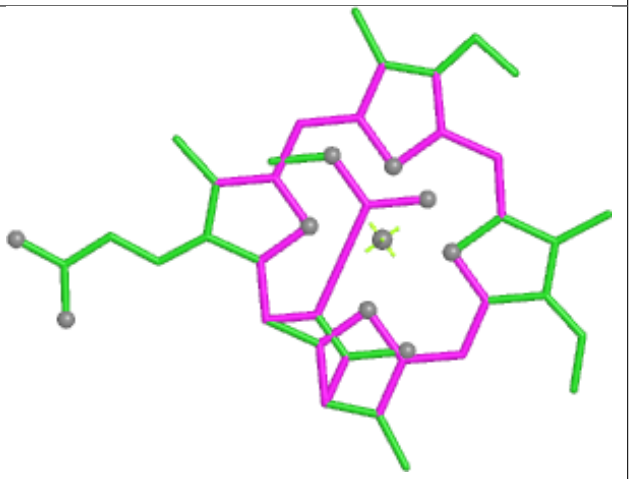


Rings

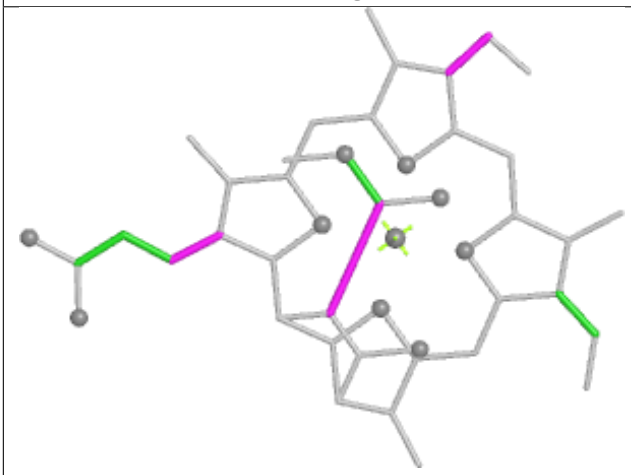
Ligand KC2 4 317



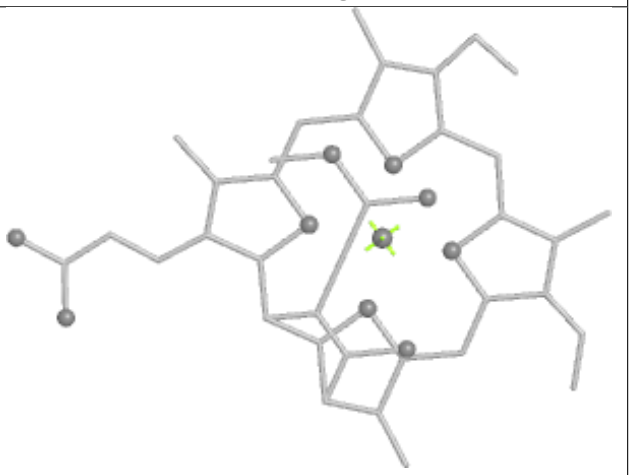
Bond lengths



Bond angles

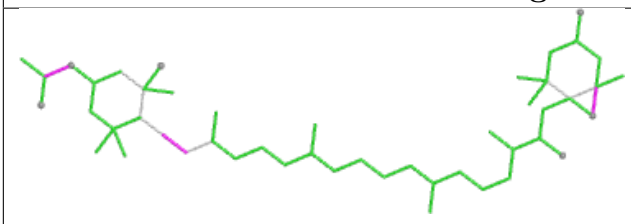


Torsions

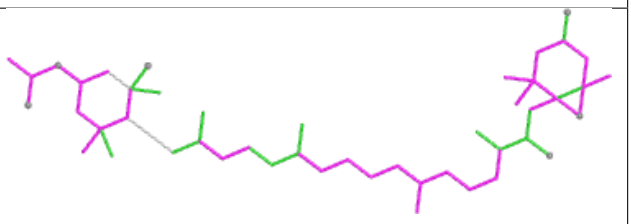


Rings

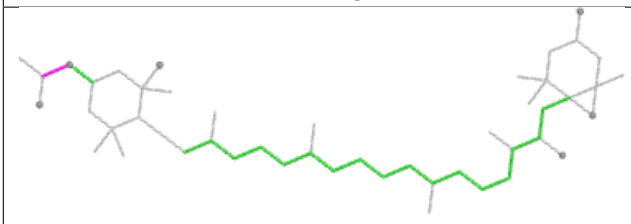
Ligand A86 O 302



Bond lengths



Bond angles



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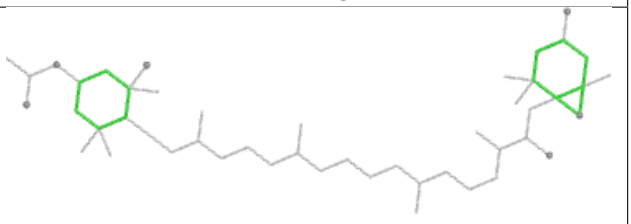
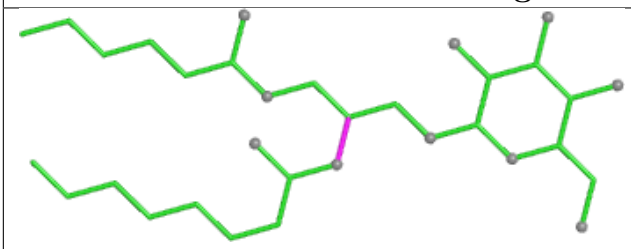
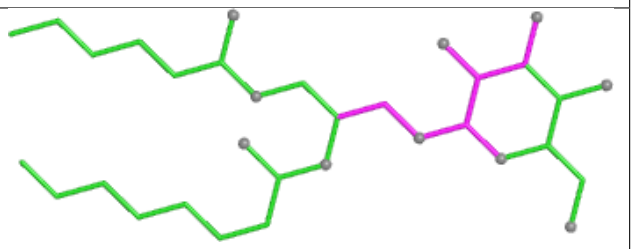


Rings

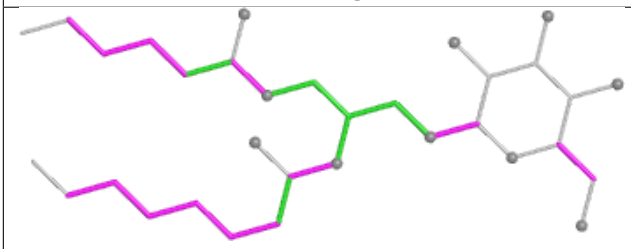
Ligand LMG W 320



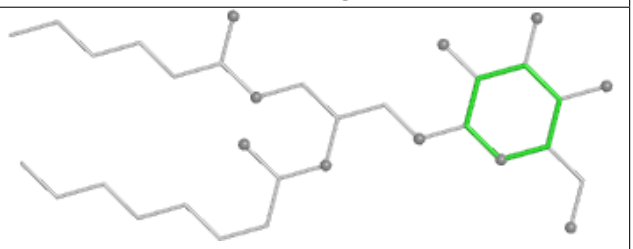
Bond lengths



Bond angles

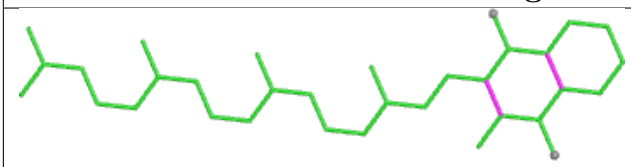


Torsions



Rings

Ligand PQN b 843



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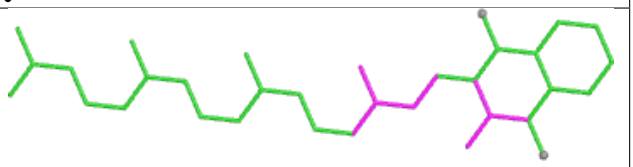
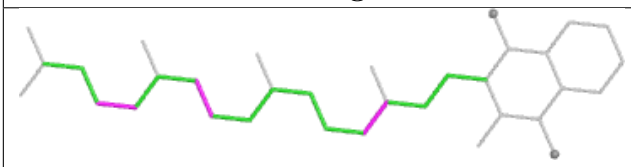


Bond angles



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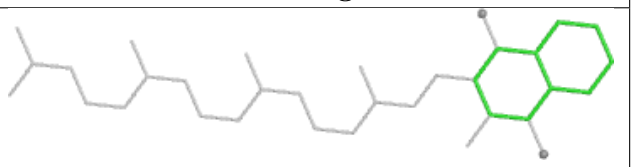
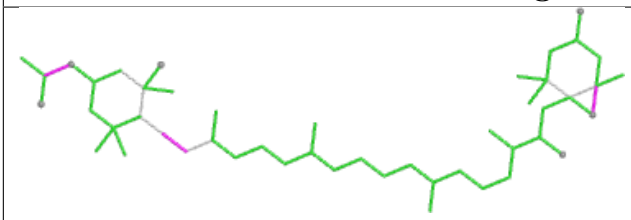
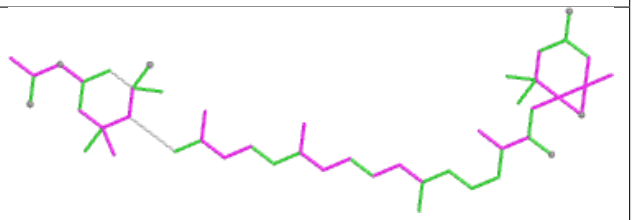


Rings

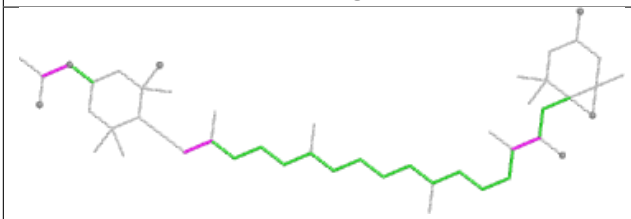
Ligand A86 x 305



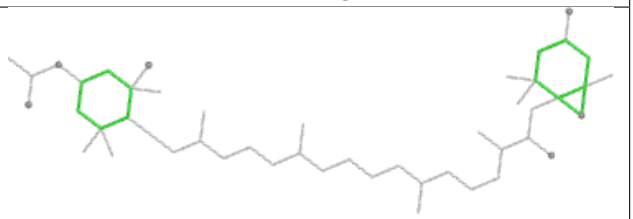
Bond lengths



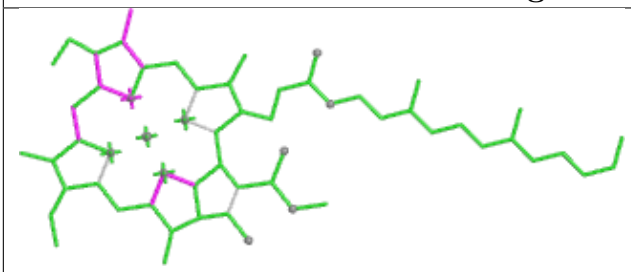
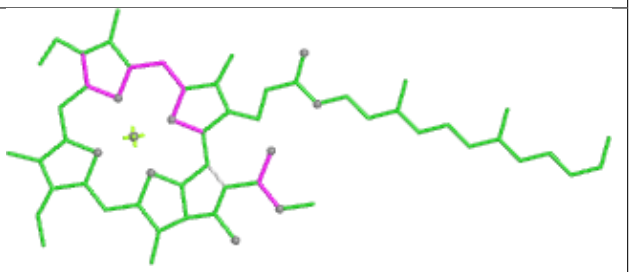
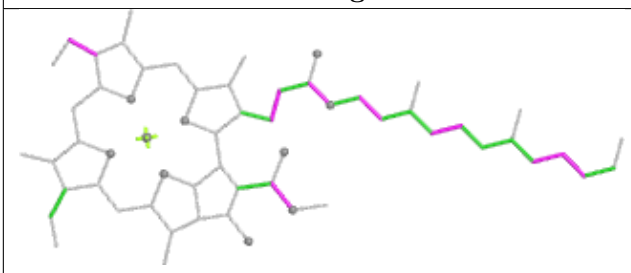
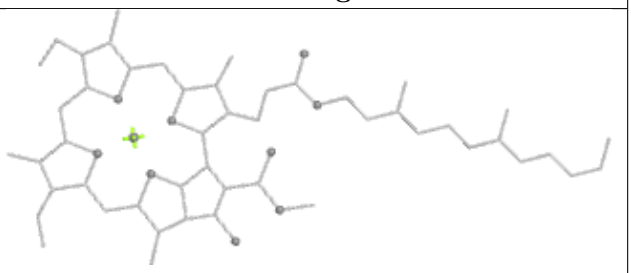
Bond angles

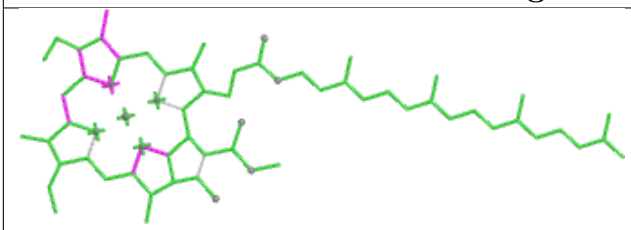
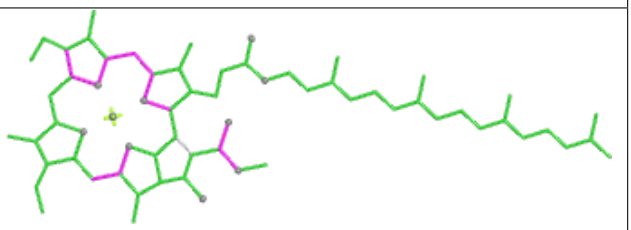
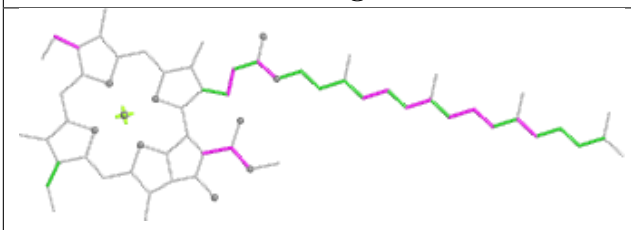
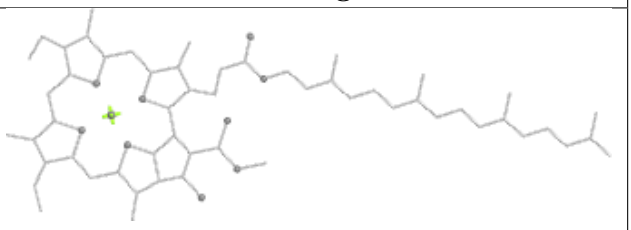


Torsions

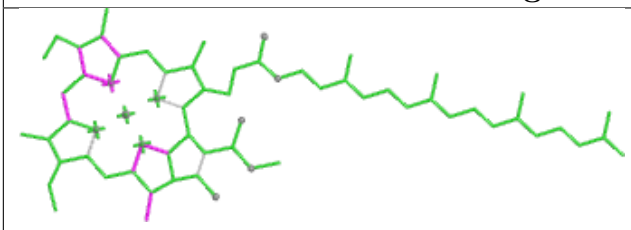


Rings

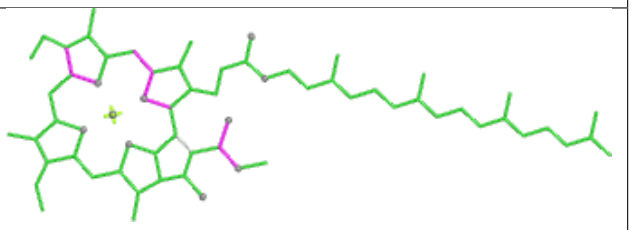
Ligand CLA b 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 833	
	
Bond lengths	Bond angles
	
Torsions	Rings

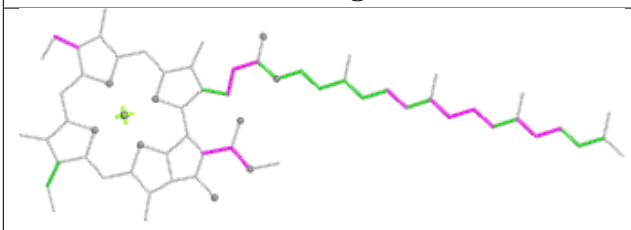
Ligand CLA V 311



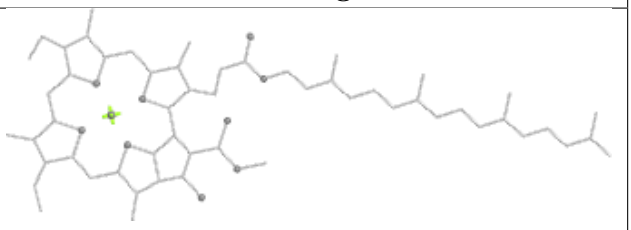
Bond lengths



Bond angles

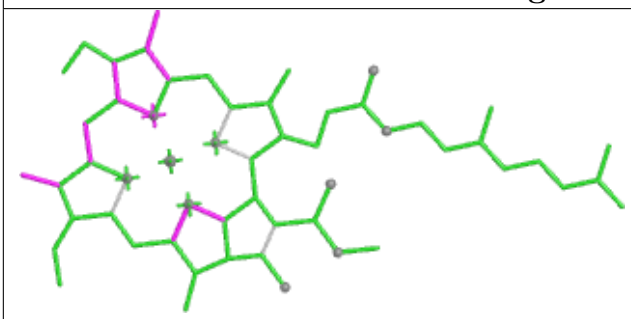


Torsions



Rings

Ligand CLA 0 311



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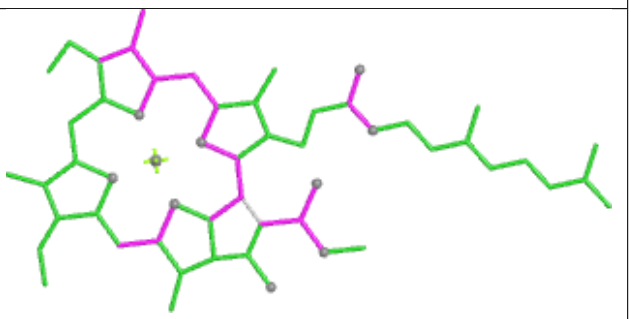
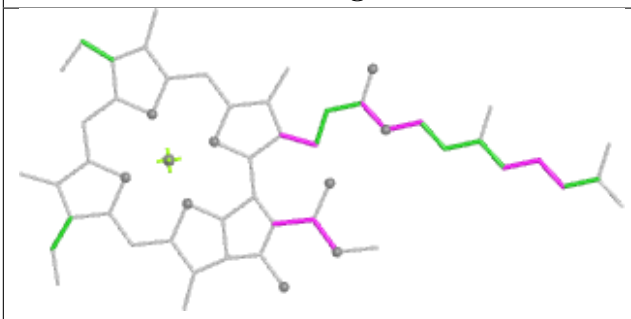


Bond angles



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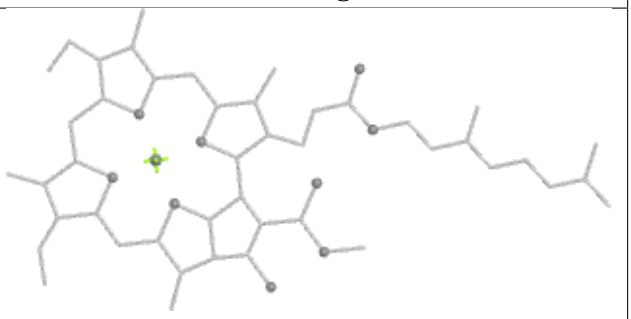
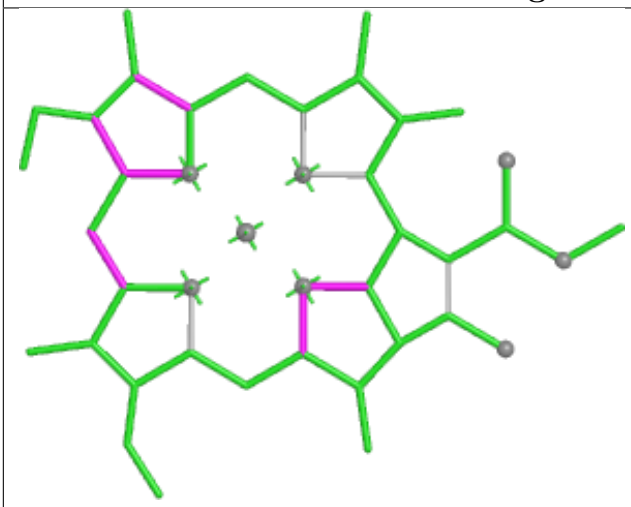
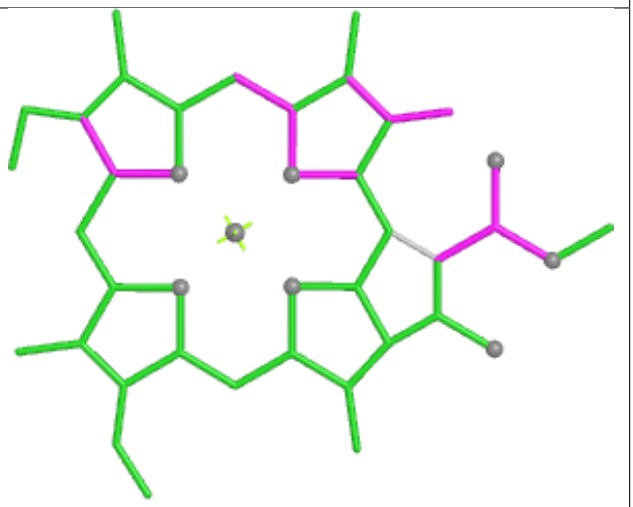


Rings

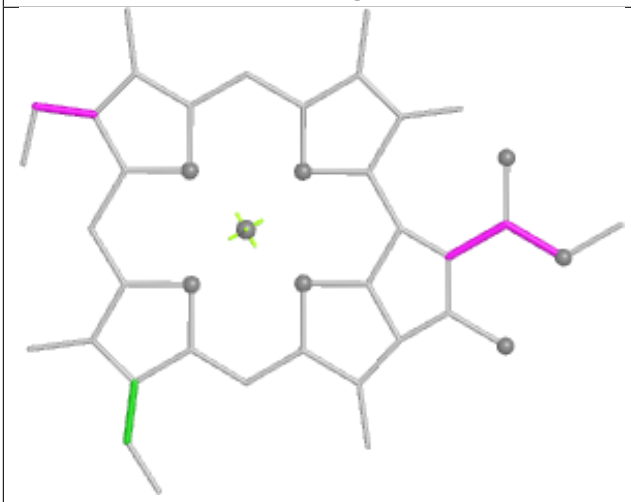
Ligand CLA 8 318



Bond lengths



Bond angles



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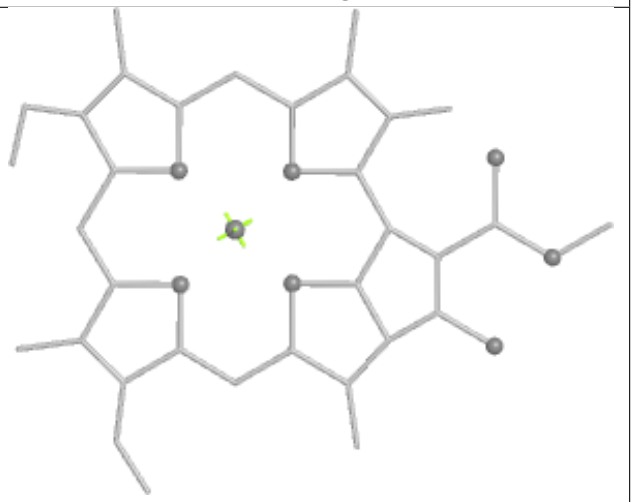
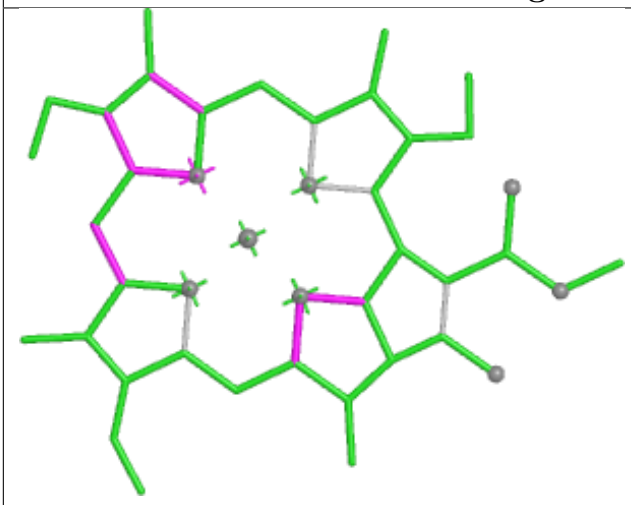
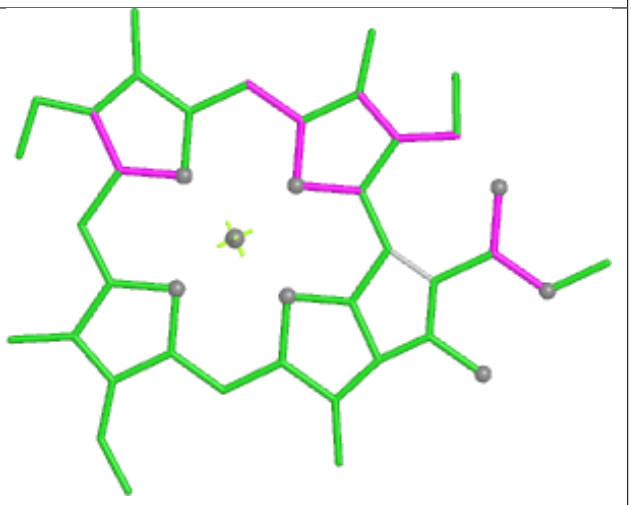


Rings

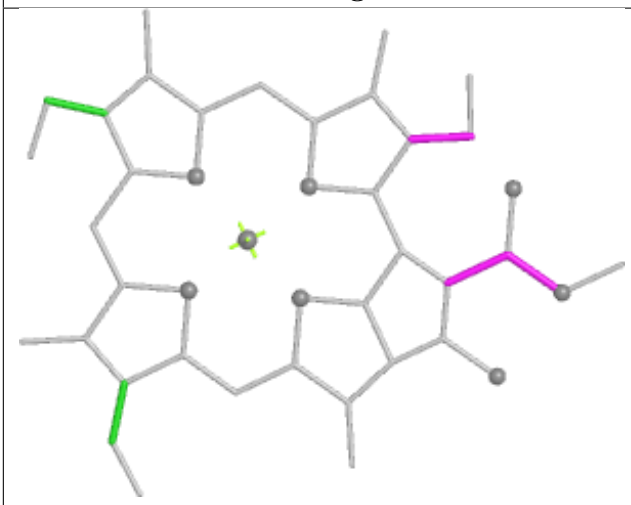
Ligand CLA 2 310



Bond lengths



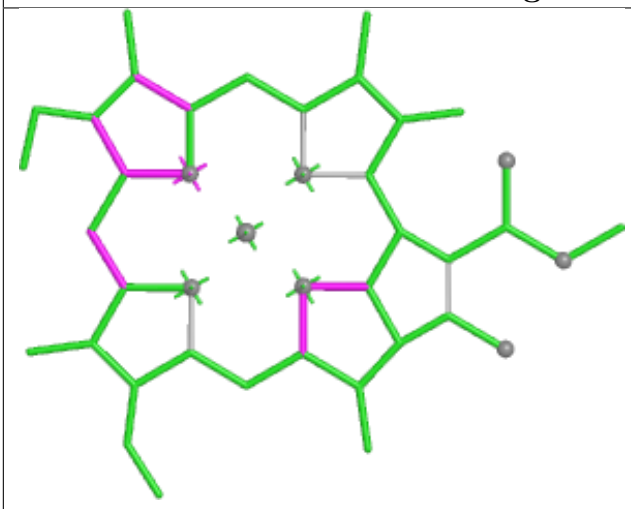
Bond angles



Torsions

Rings

Ligand CLA U 215



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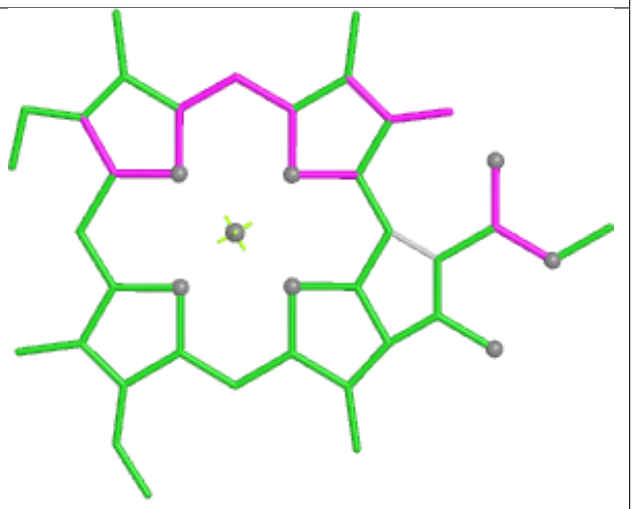
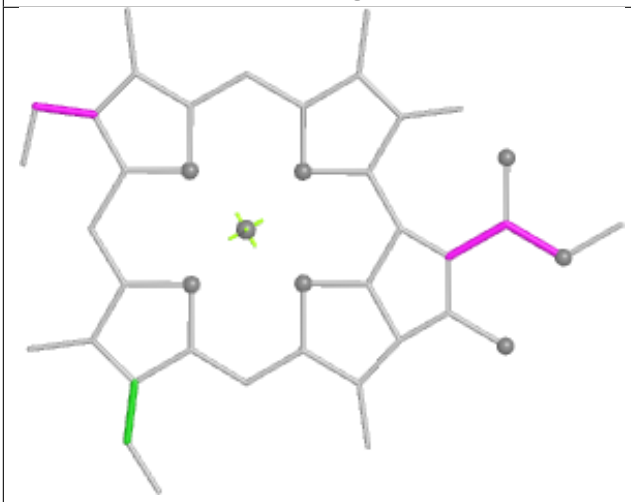
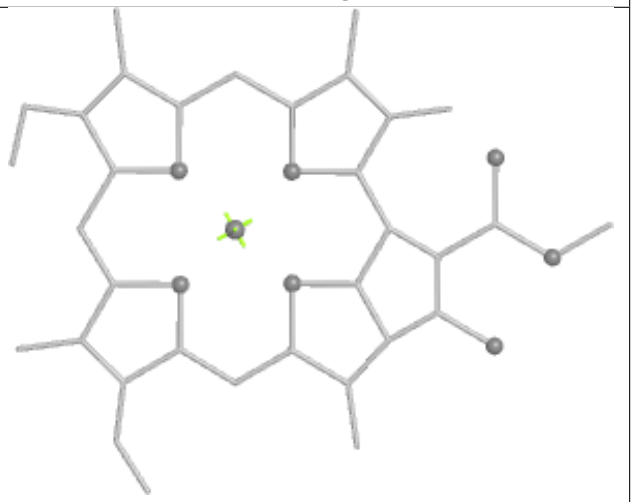


Bond angles

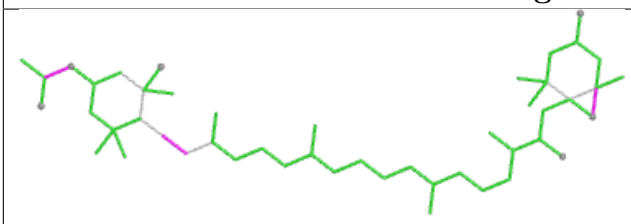


Torsions

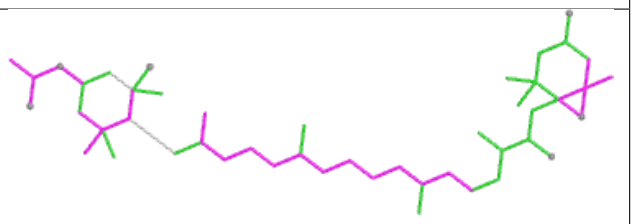


Rings

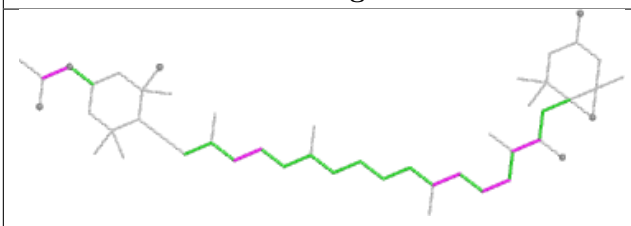
Ligand A86 9 304



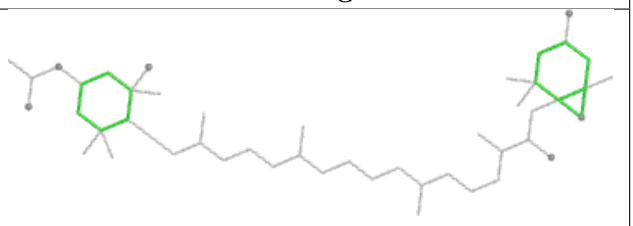
Bond lengths



Bond angles

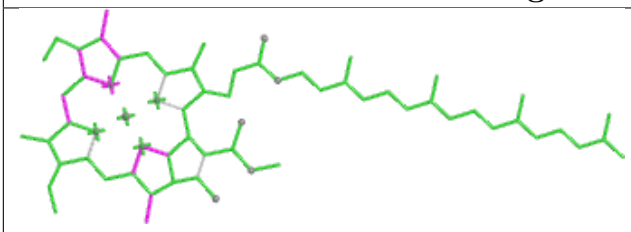


Torsions



Rings

Ligand CLA b 829



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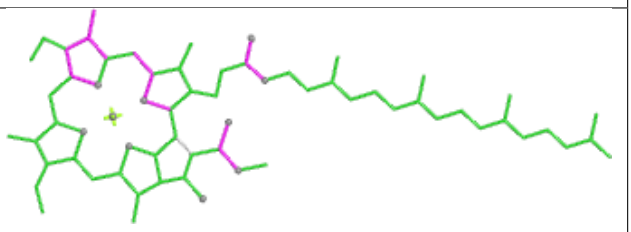

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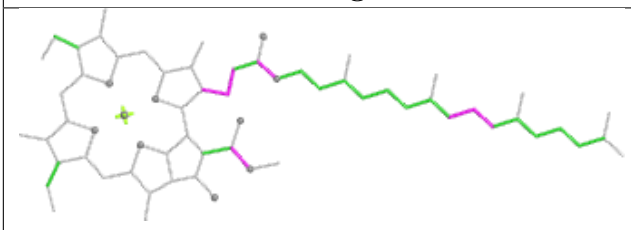

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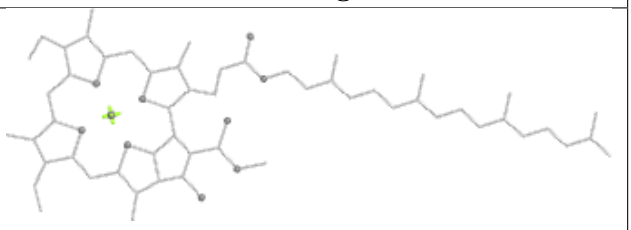
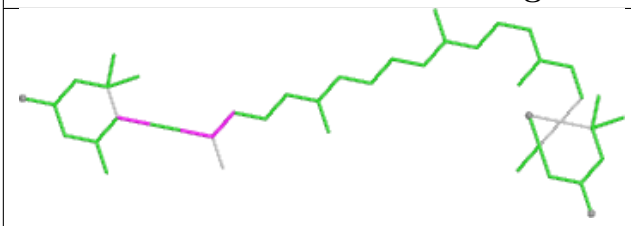


Rings

Ligand DD6 H 305



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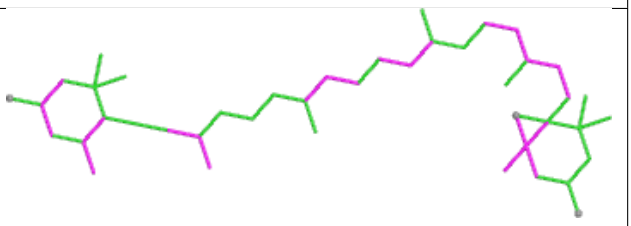

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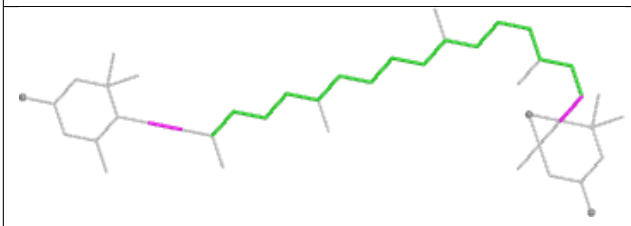

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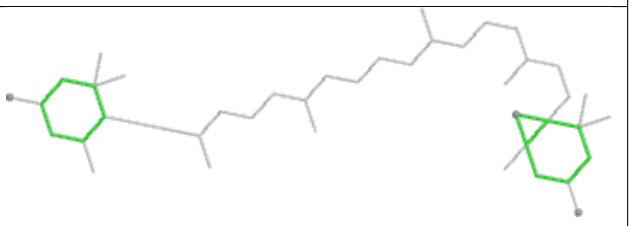
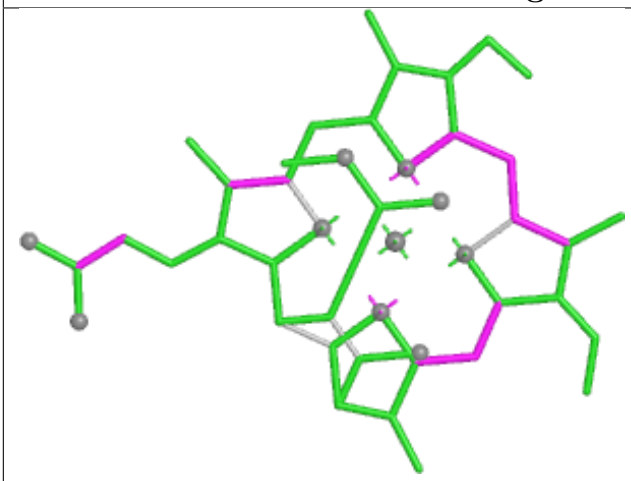


Rings

Ligand KC2 T 315



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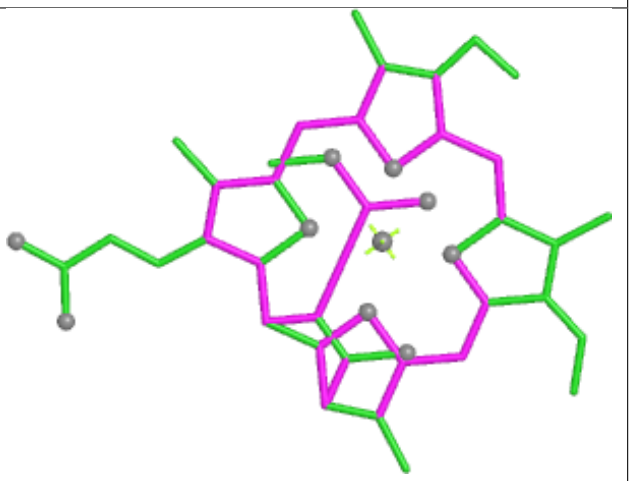

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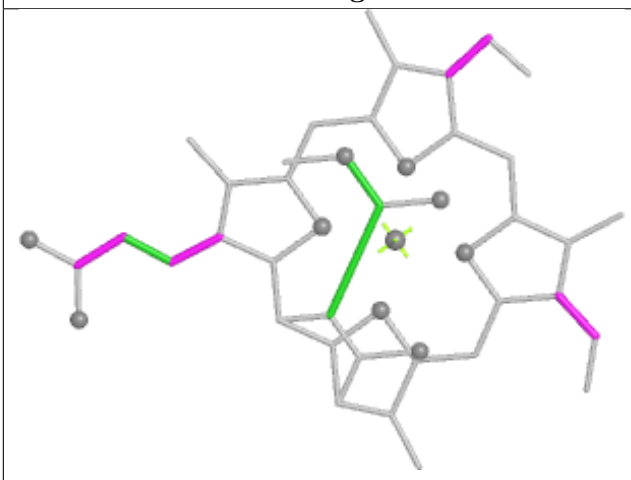

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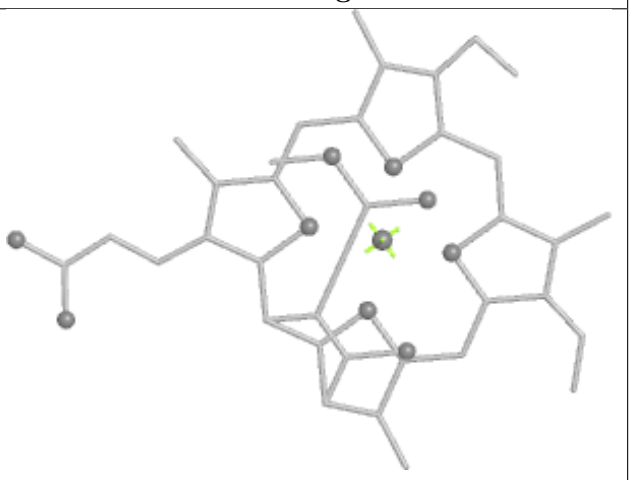
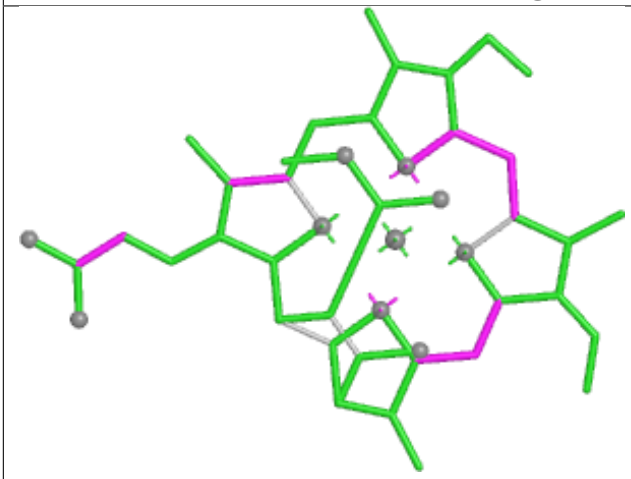


Rings

Ligand KC2 S 314



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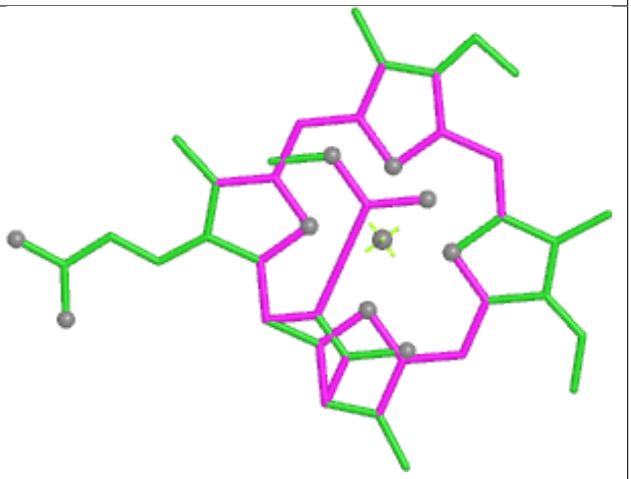
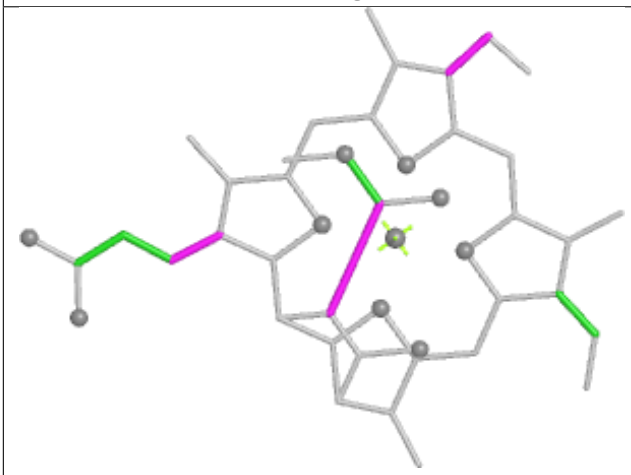


Bond angles



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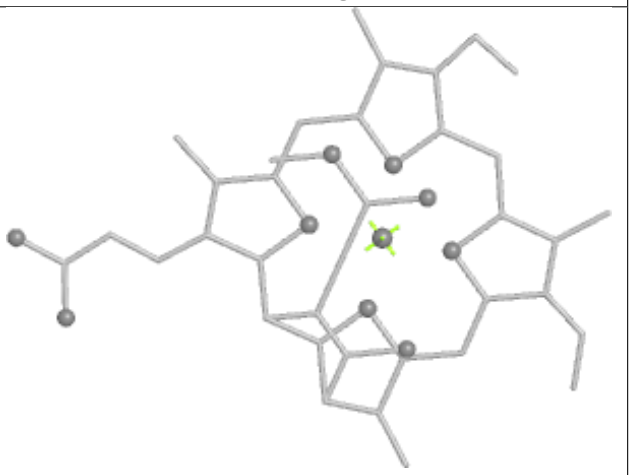
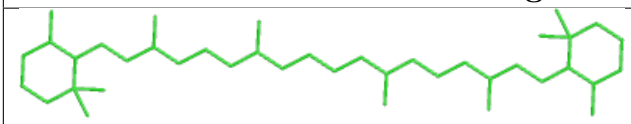


Rings

Ligand BCR b 846



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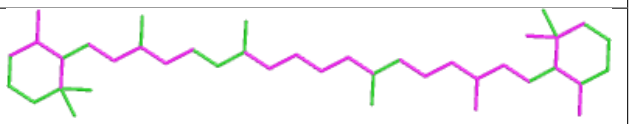
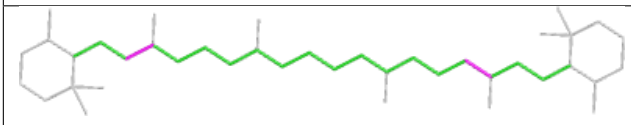


Bond angles



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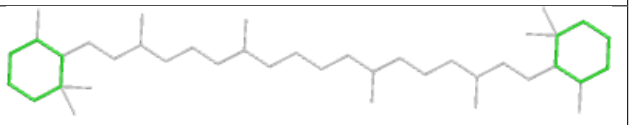
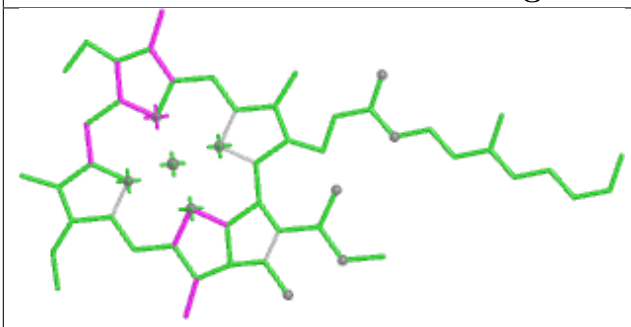


Rings

Ligand CLA Q 314



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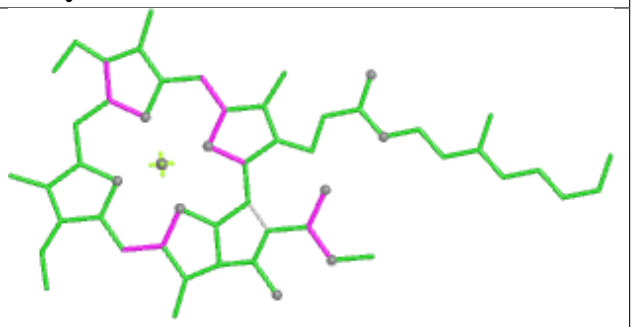
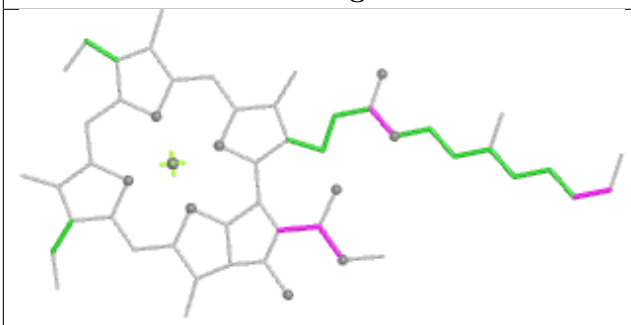


Bond angles



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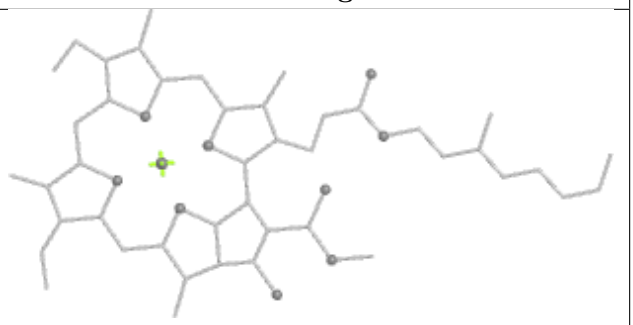
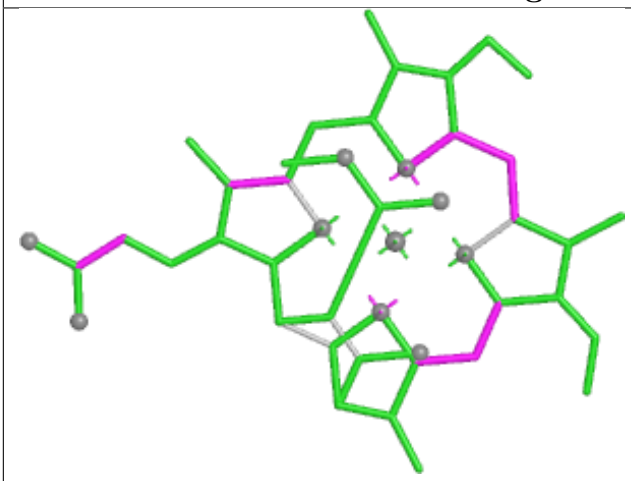


Rings

Ligand KC2 X 318



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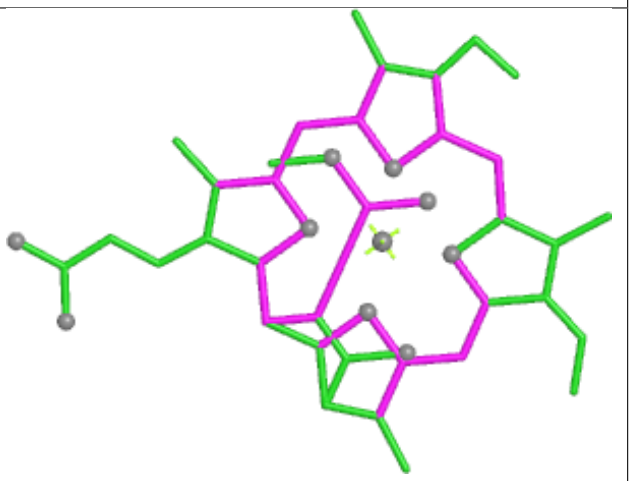
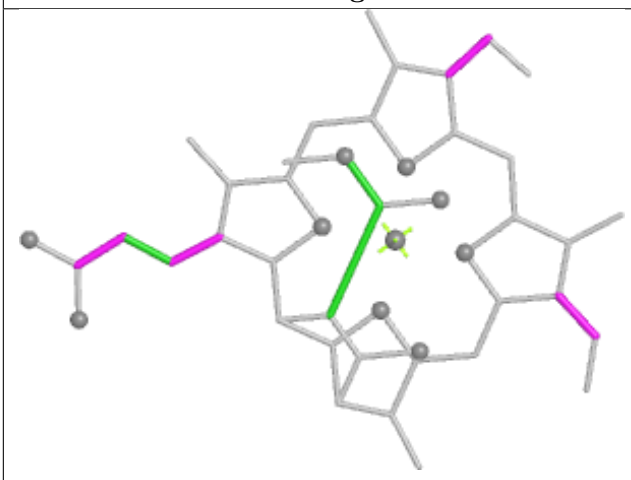


Bond angles



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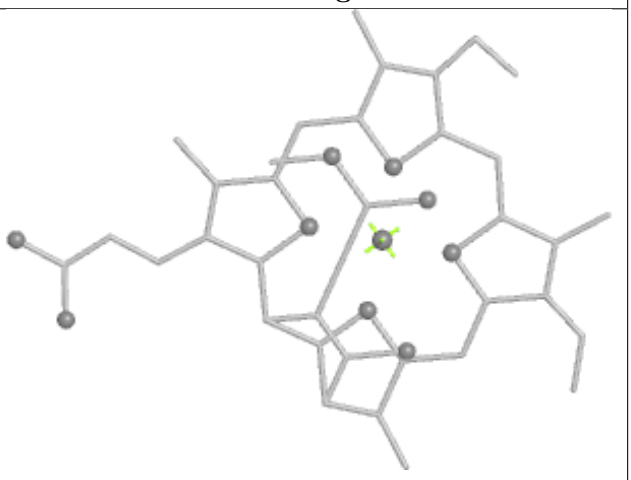
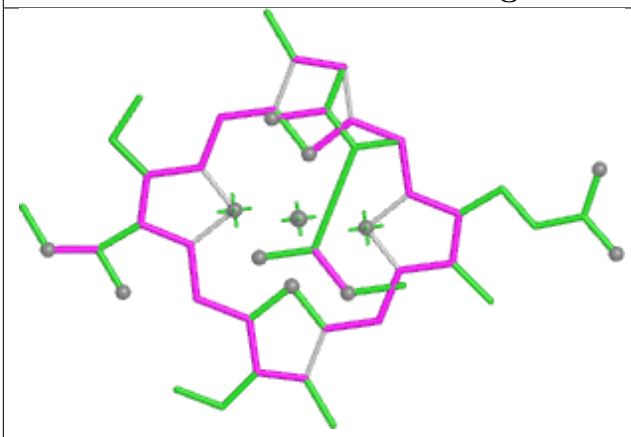


Rings

Ligand A1ECV Q 316



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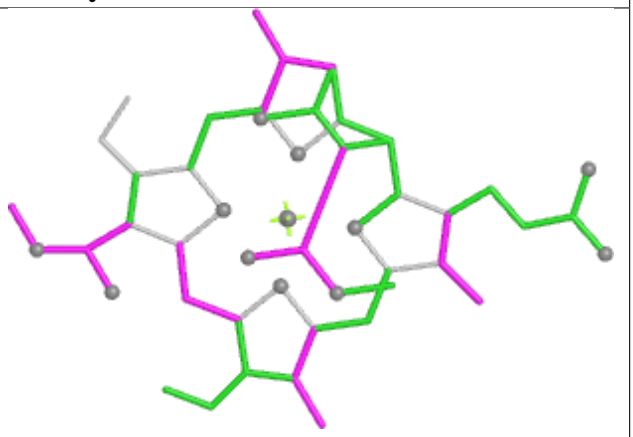
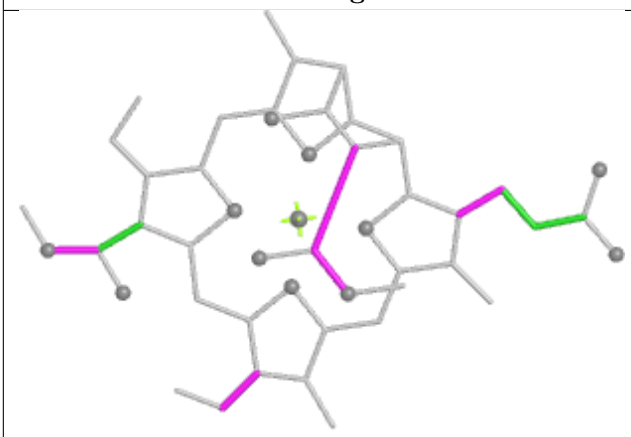


Bond angles



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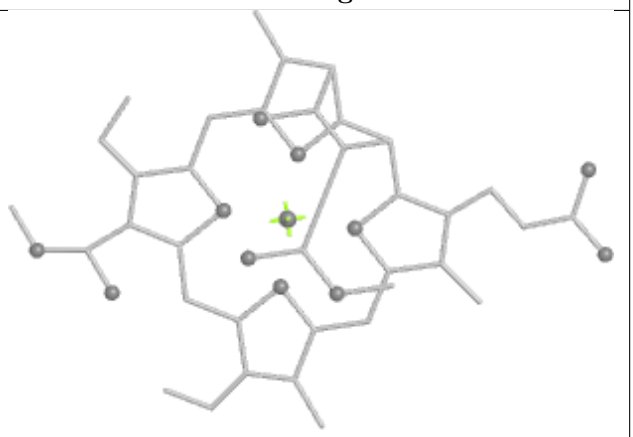
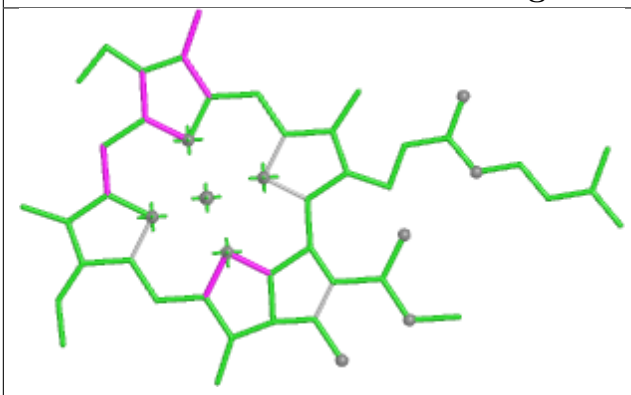


Rings

Ligand CLA 7 325



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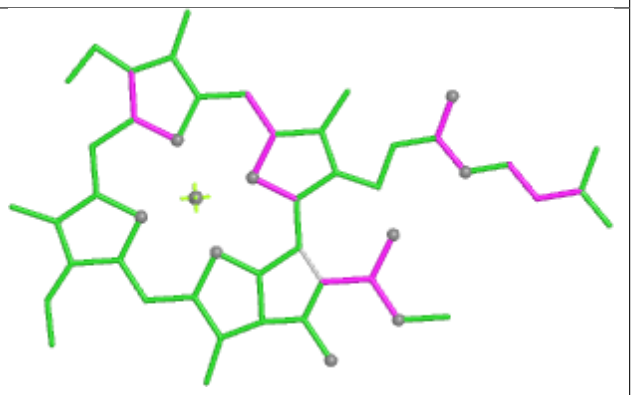
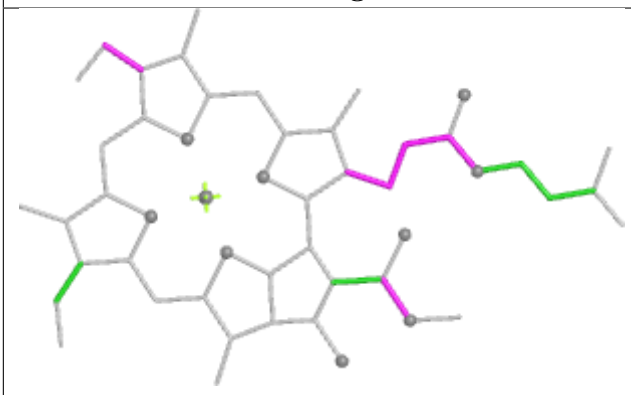


Bond angles



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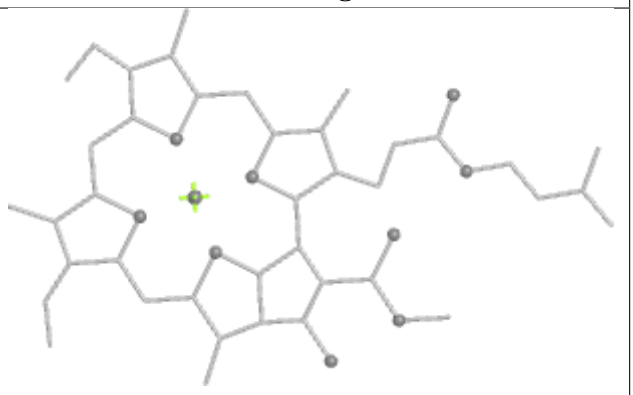
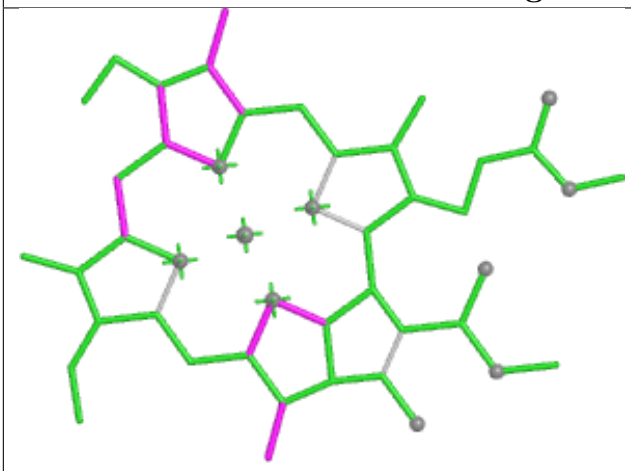


Rings

Ligand CLA E 315



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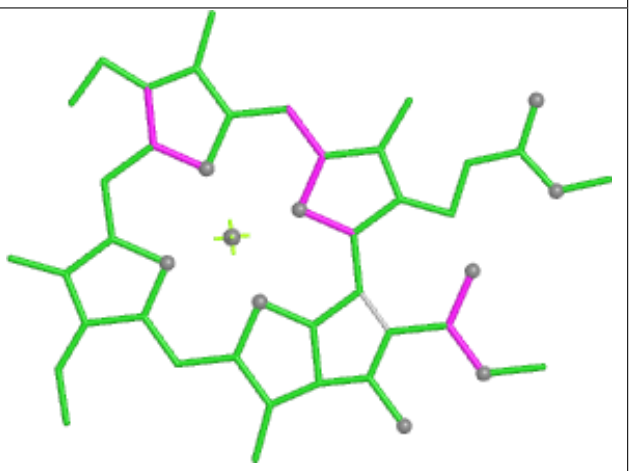
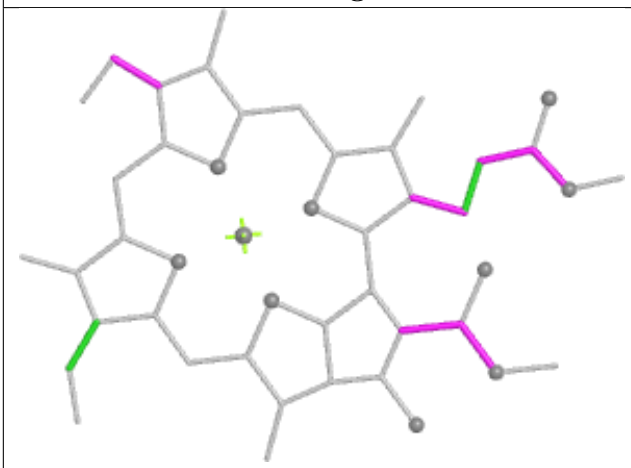


Bond angles



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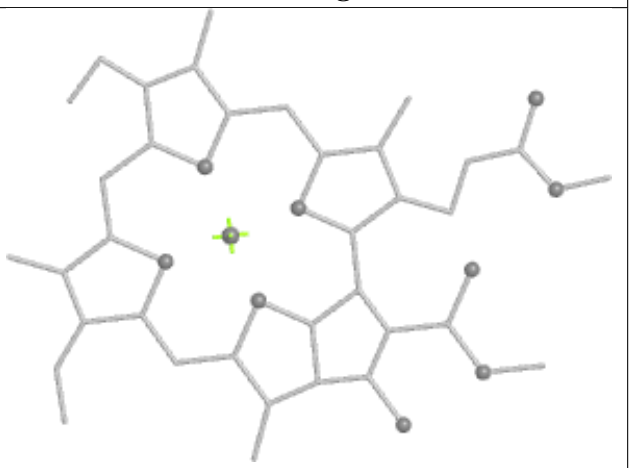
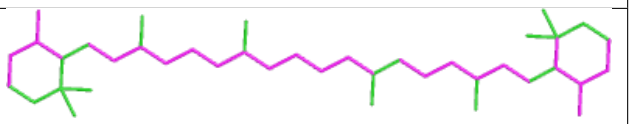


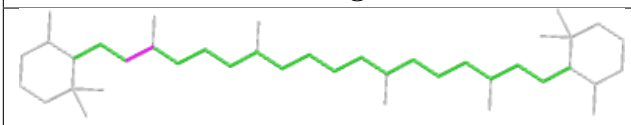
Rings

Ligand BCR b 845

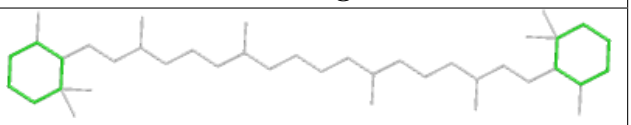
Bond lengths



Bond angles

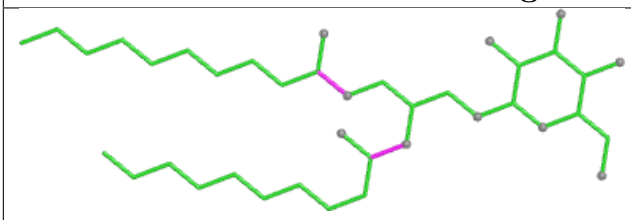


Torsions



Rings

Ligand LMG P 317



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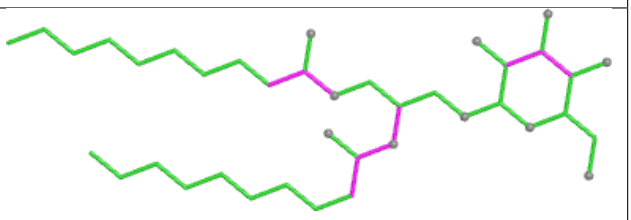
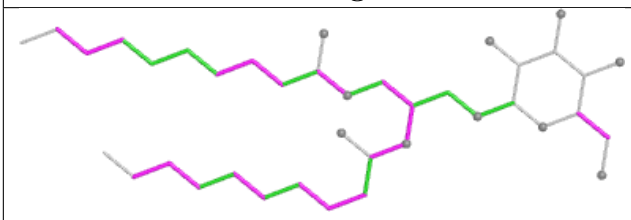


Bond angles



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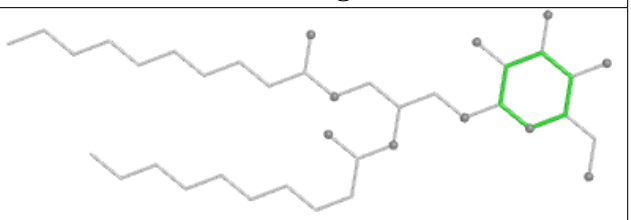
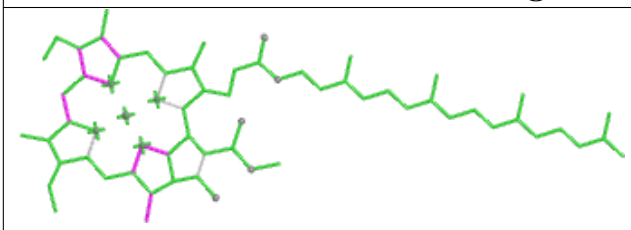


Rings

Ligand CLA b 805



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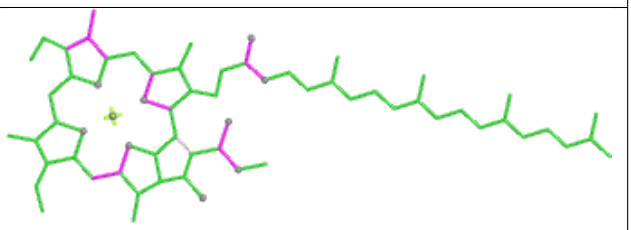
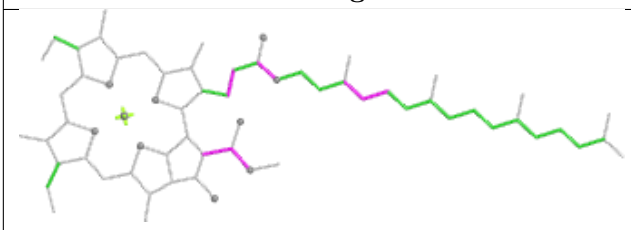
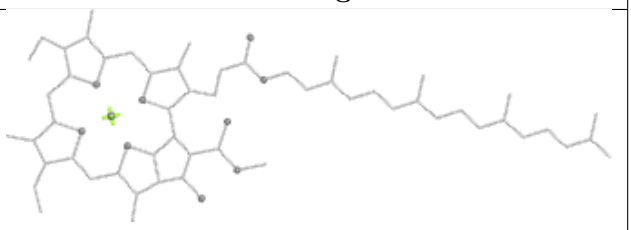


Bond angles

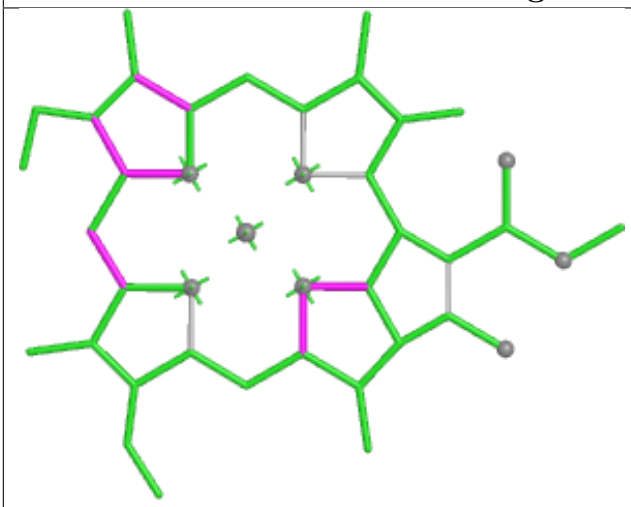


Torsions

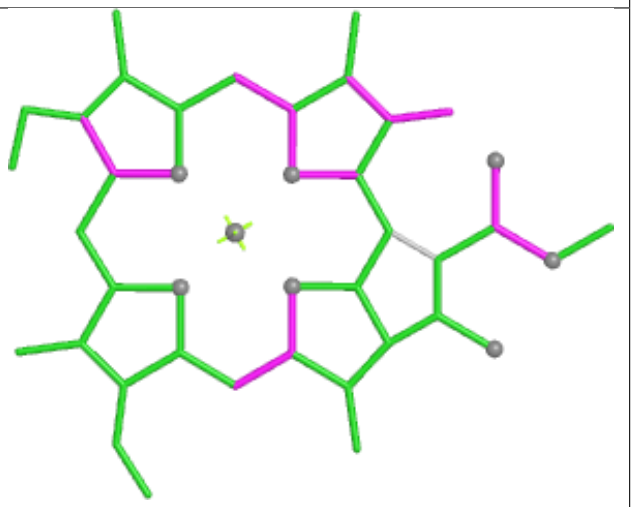


Rings

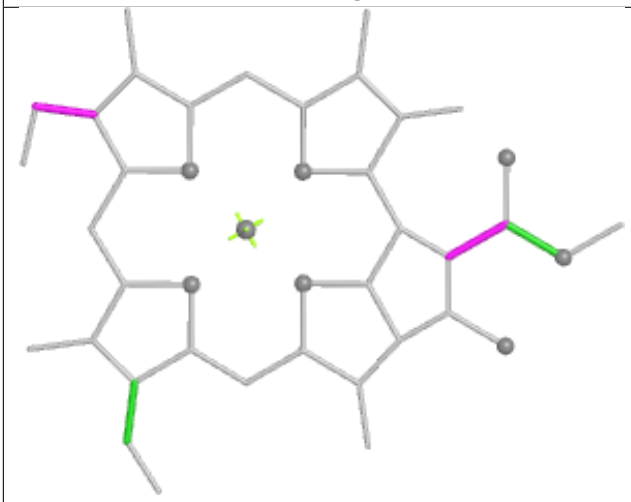
Ligand CLA S 316



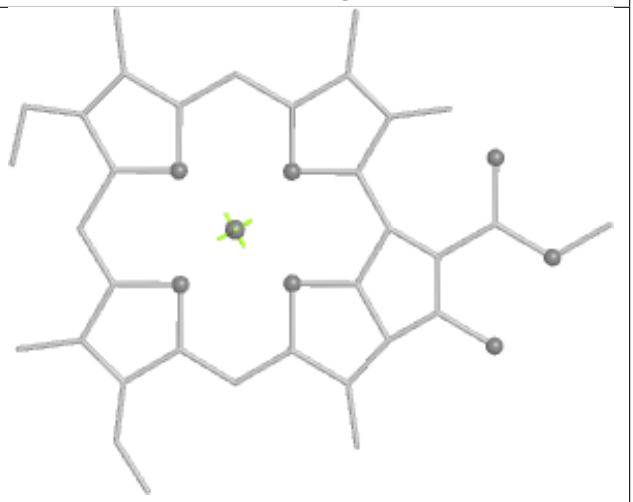
Bond lengths



Bond angles

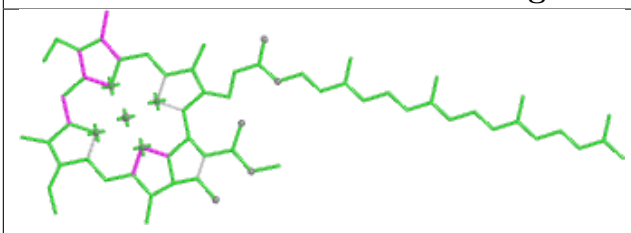


Torsions



Rings

Ligand CLA a 830



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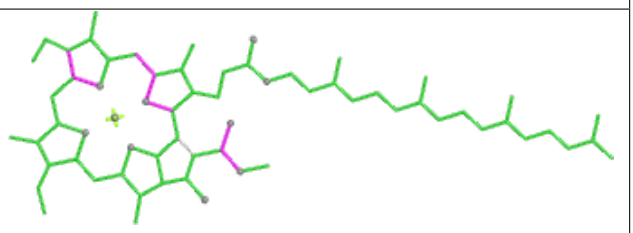

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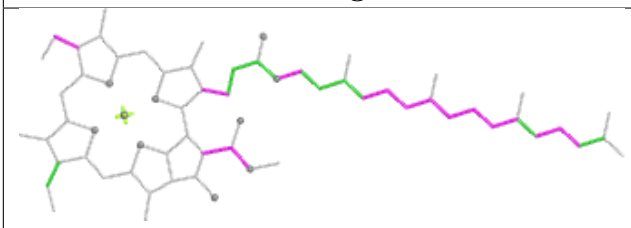

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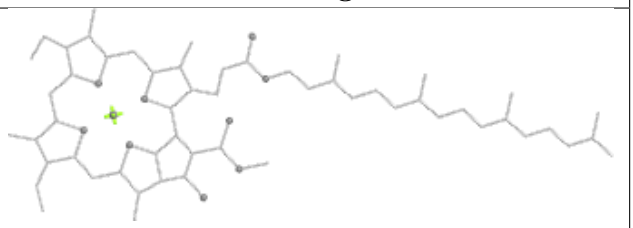
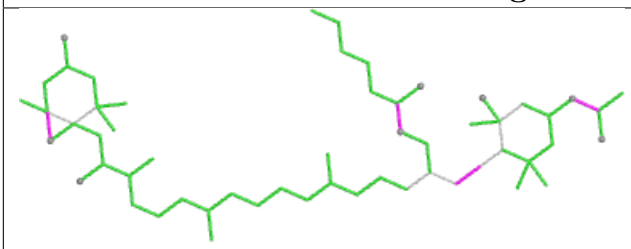


Rings

Ligand A1EB1 7 305



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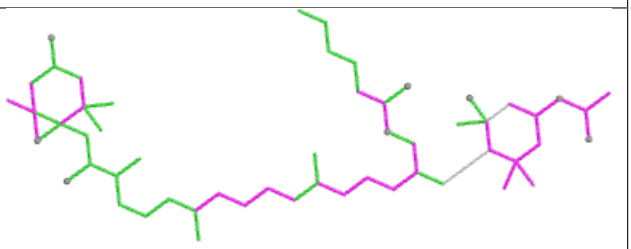
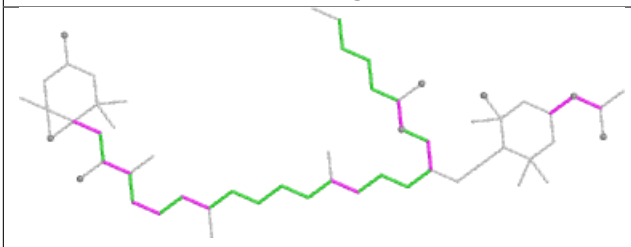
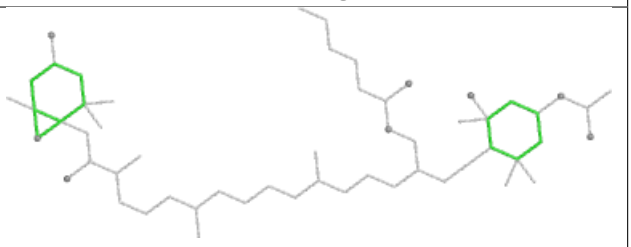


Bond angles

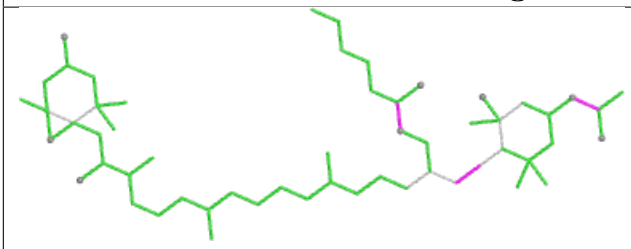


Torsions



Rings

Ligand A1EB1 y 302



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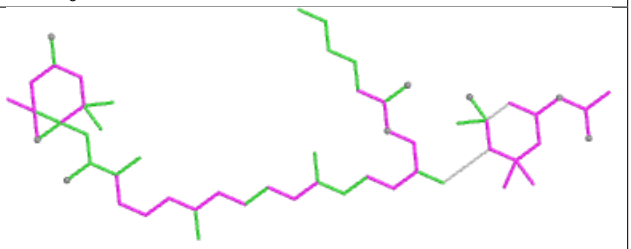
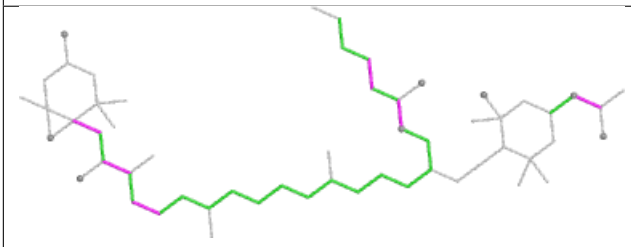
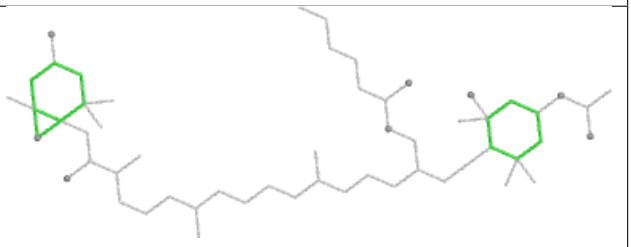


Bond angles

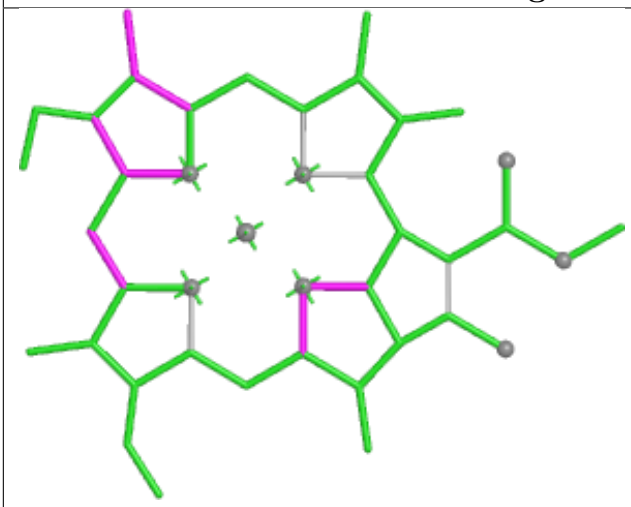


Torsions

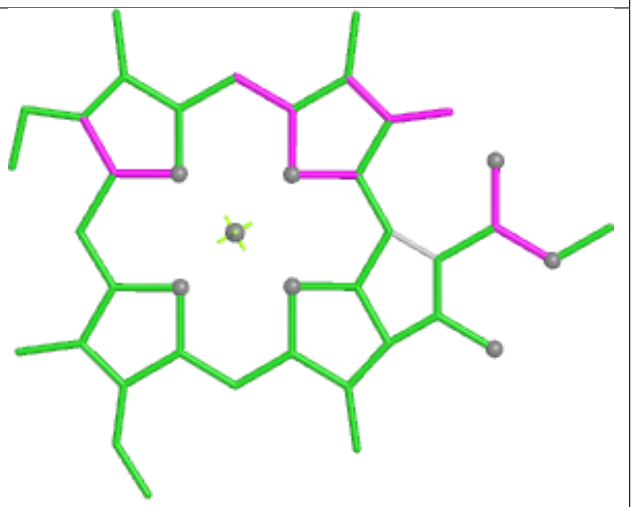


Rings

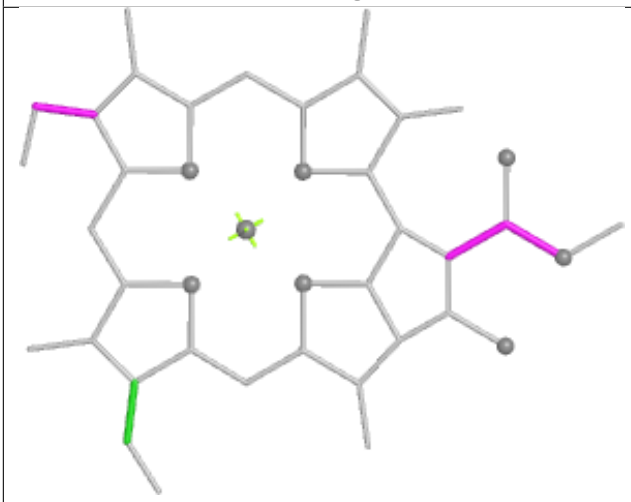
Ligand CLA 2 318



Bond lengths



Bond angles



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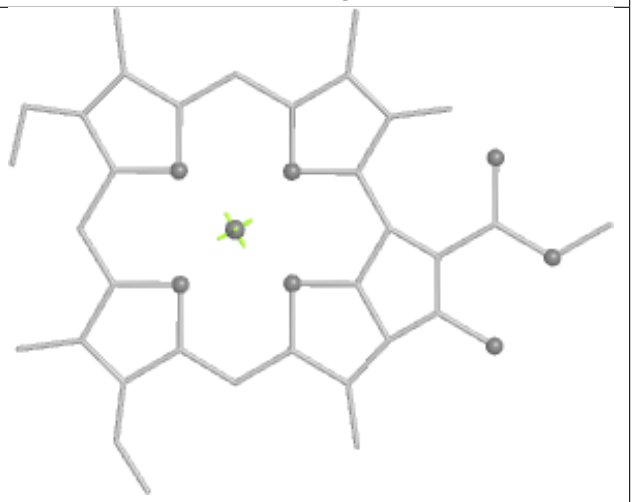
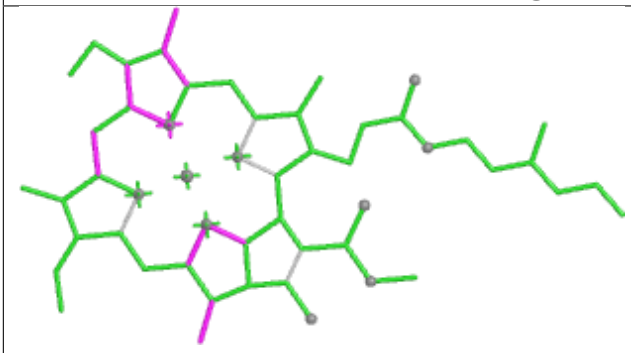
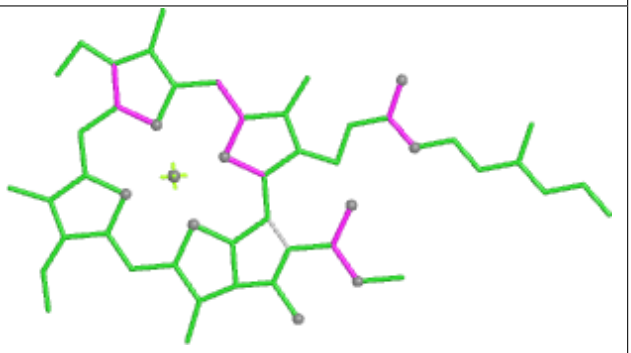
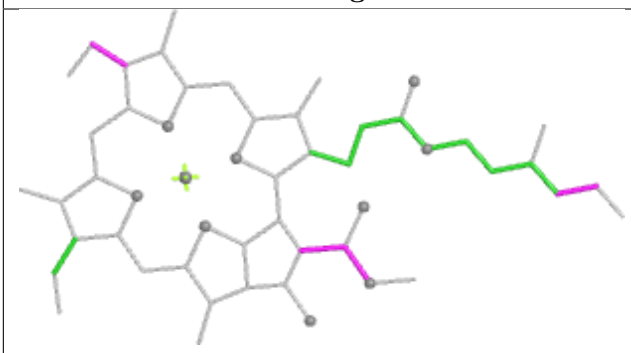
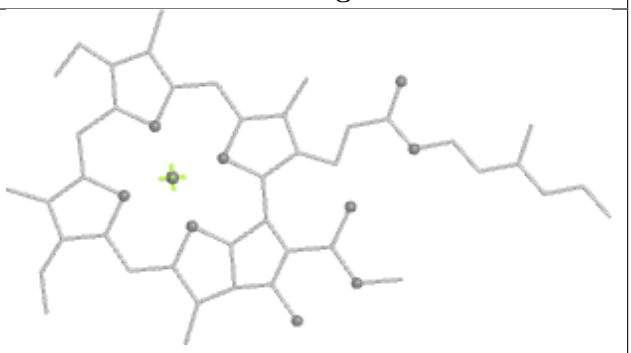
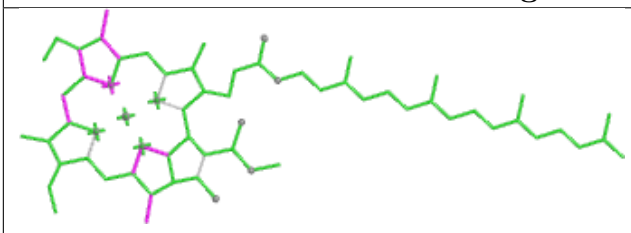
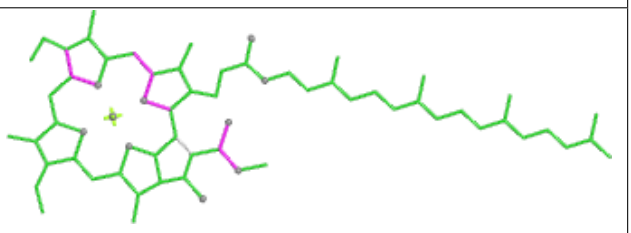
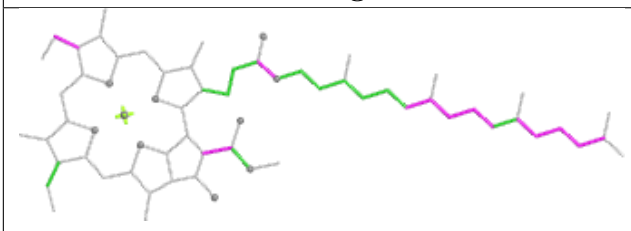
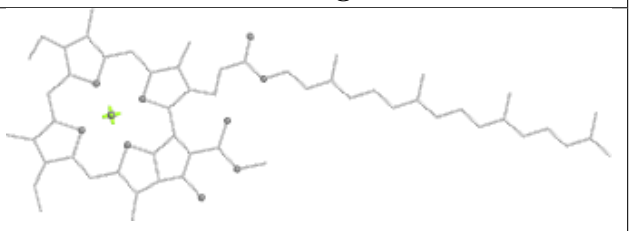
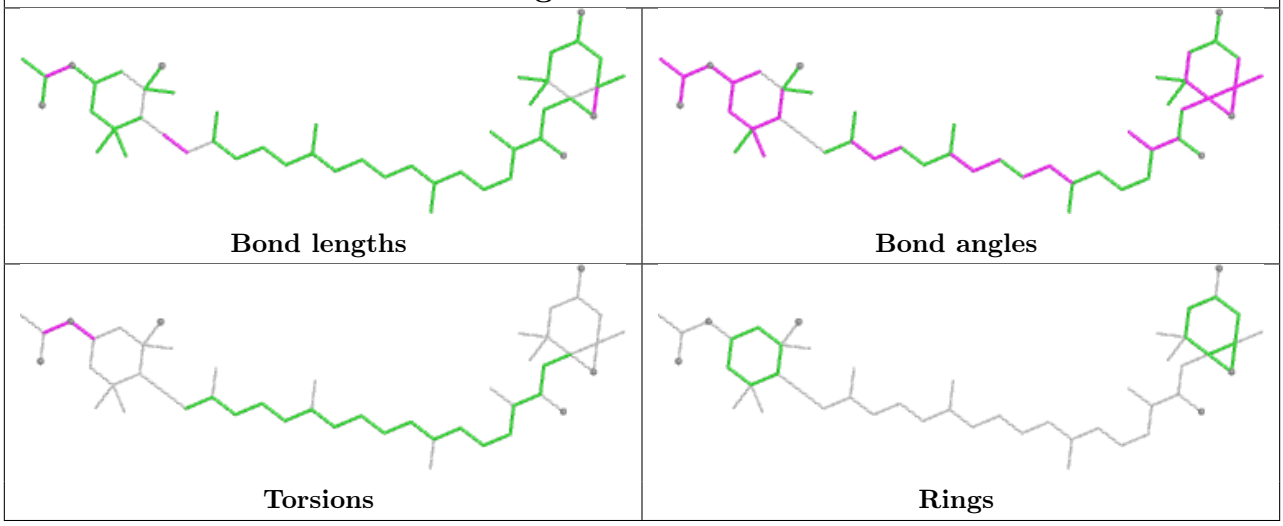


Rings

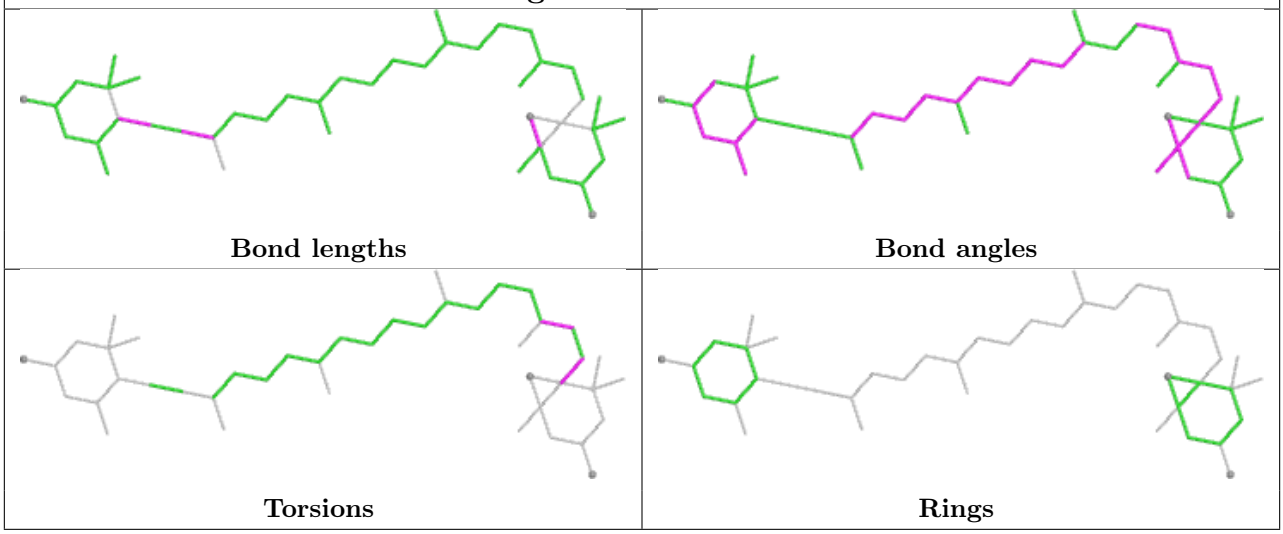
Ligand CLA k 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA M 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

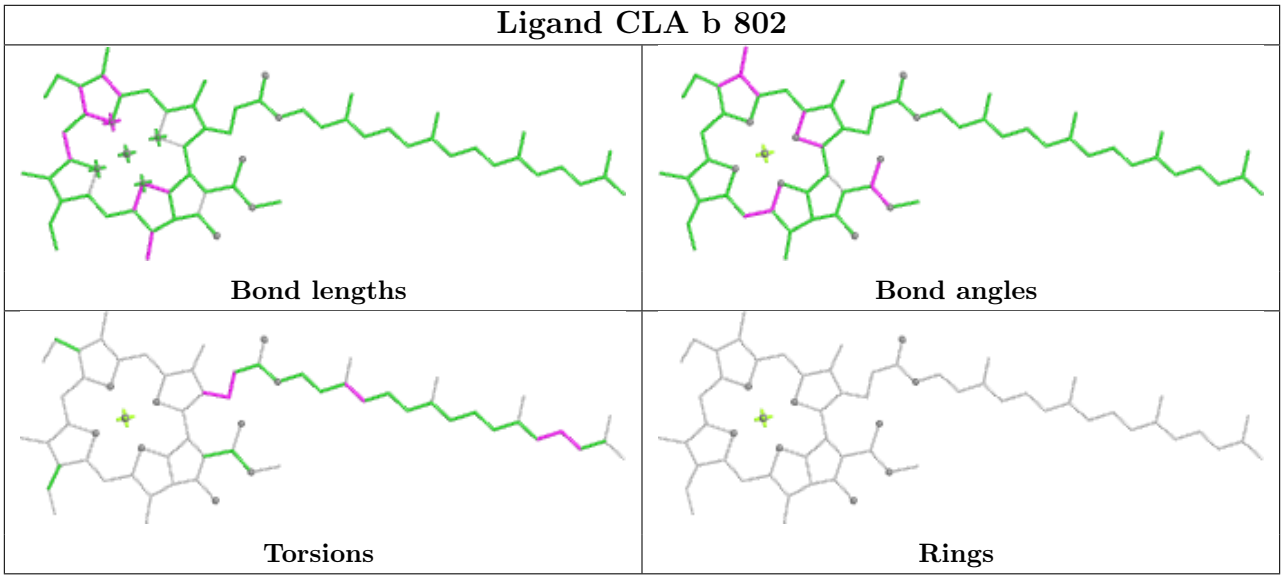
Ligand A86 2 301



Ligand DD6 E 305



Ligand CLA b 802



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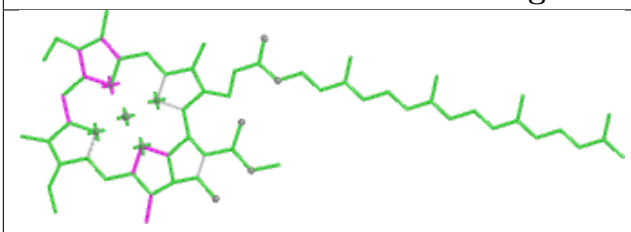
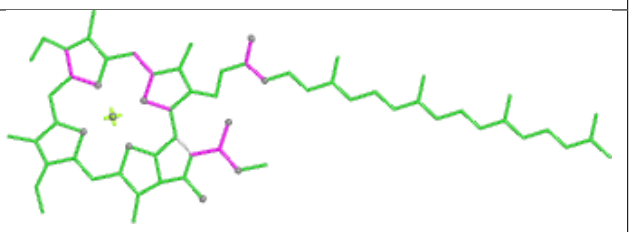
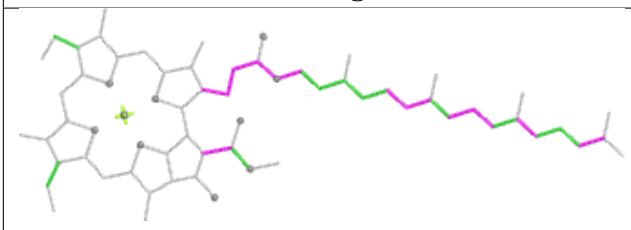


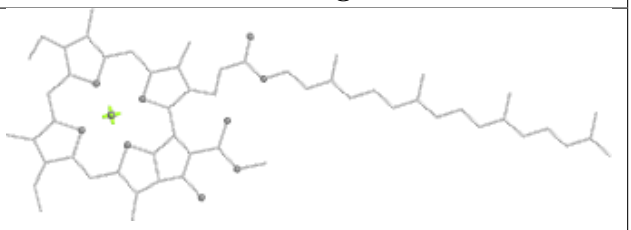
Bond lengths



Bond angles

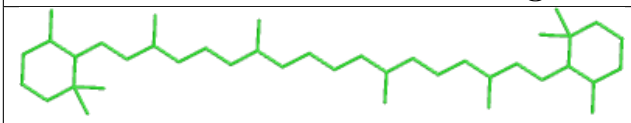


Torsions



Rings

Ligand BCR a 843



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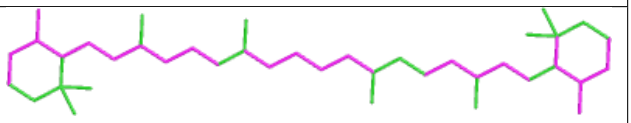
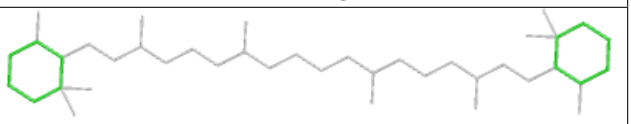


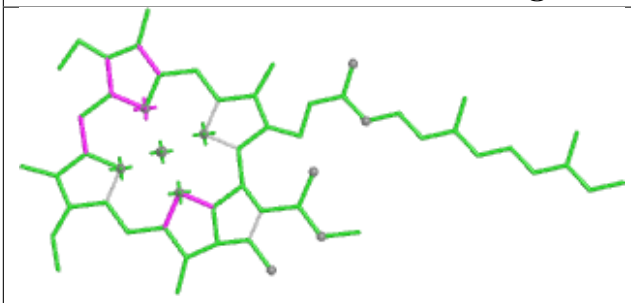
Bond angles

Torsions



Rings

Ligand CLA 7 314



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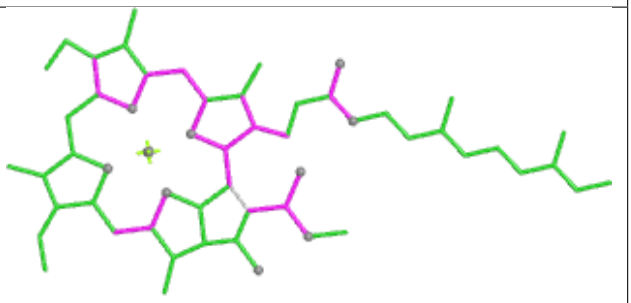
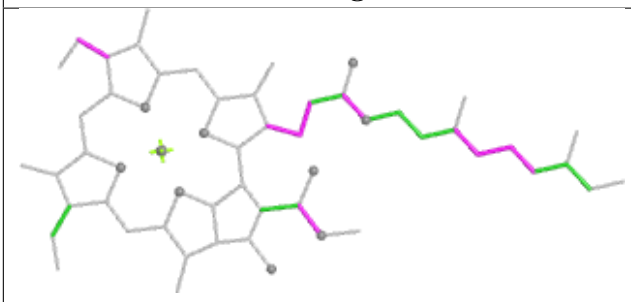


Bond angles



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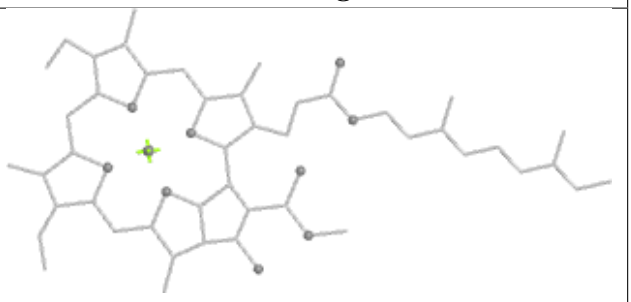
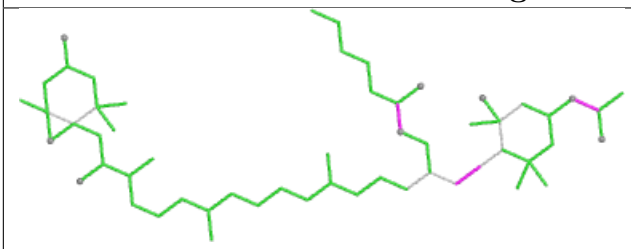


Rings

Ligand A1EB1 9 302



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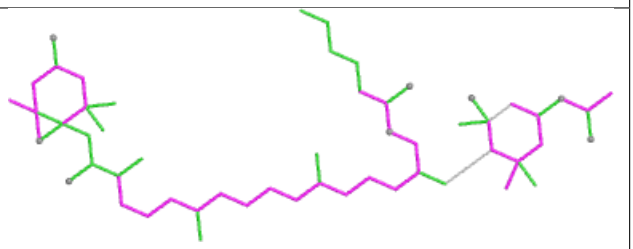
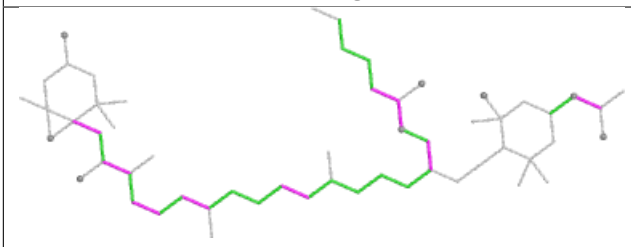
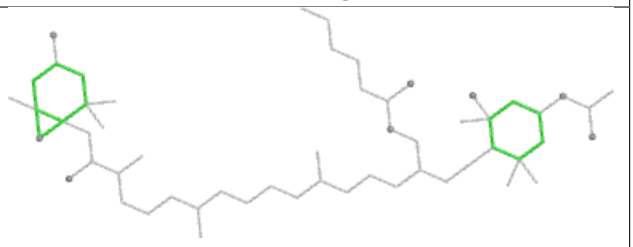


Bond angles

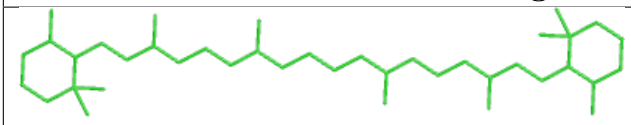


Torsions

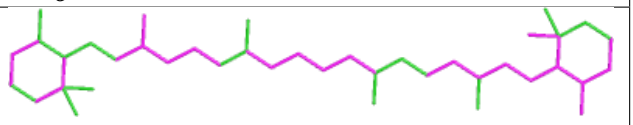


Rings

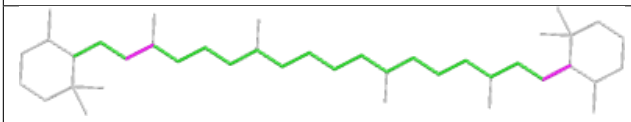
Ligand BCR j 103



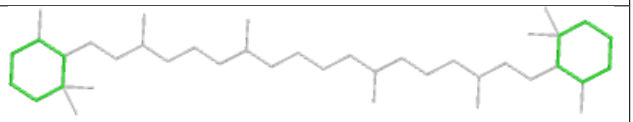
Bond lengths



Bond angles

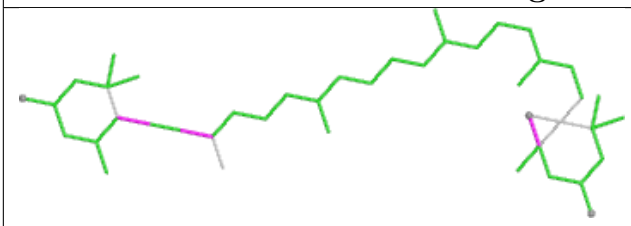


Torsions

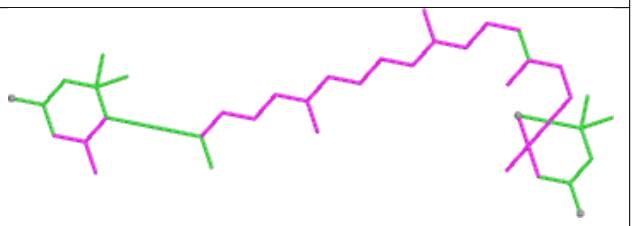


Rings

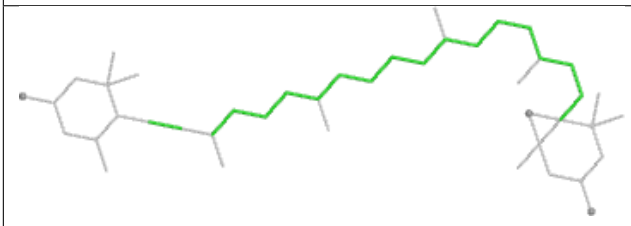
Ligand DD6 x 304



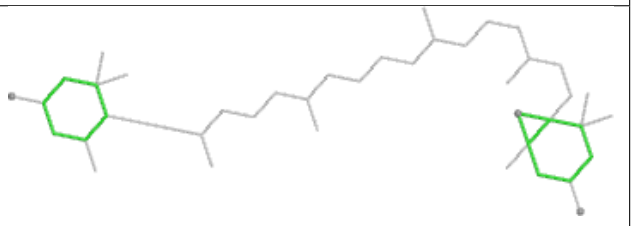
Bond lengths



Bond angles

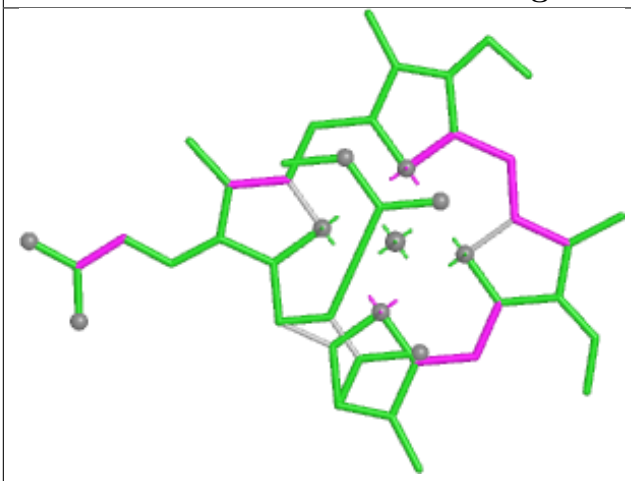


Torsions

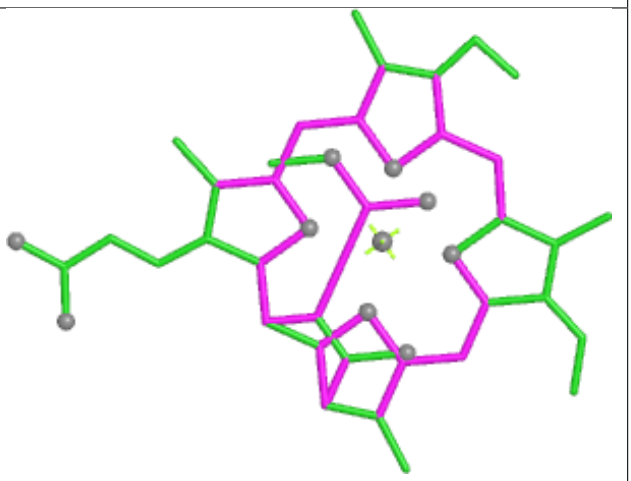


Rings

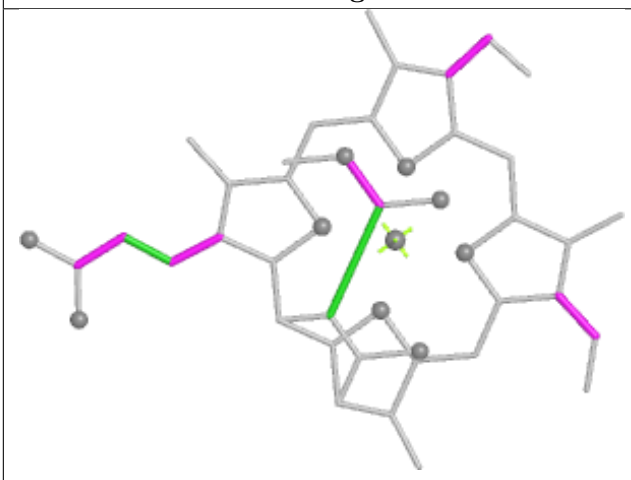
Ligand KC2 z 315



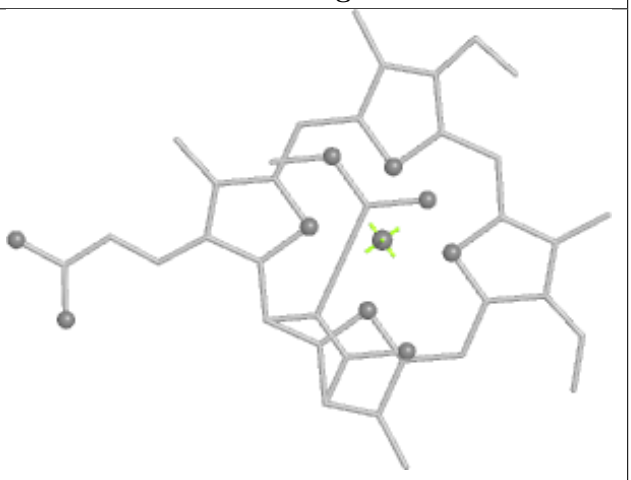
Bond lengths



Bond angles

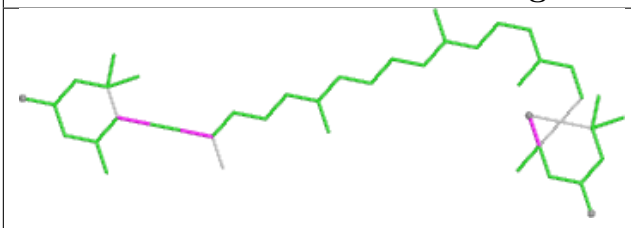


Torsions



Rings

Ligand DD6 4 307



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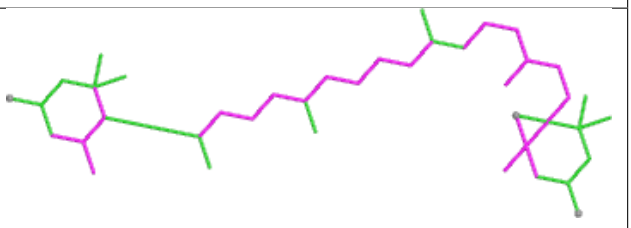

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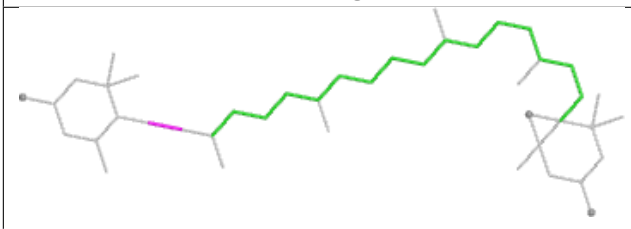
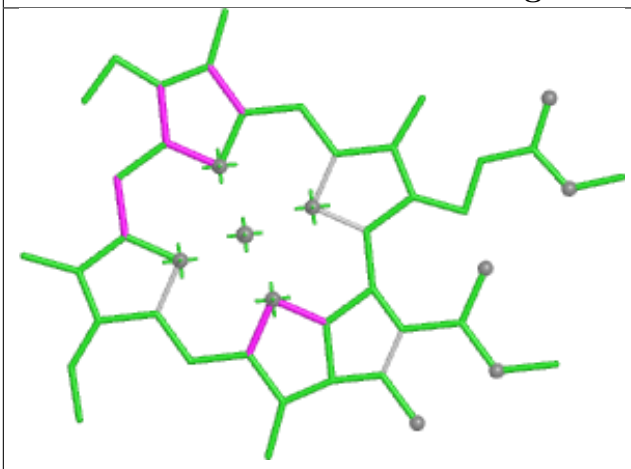


Torsions

Rings

Ligand CLA C 309



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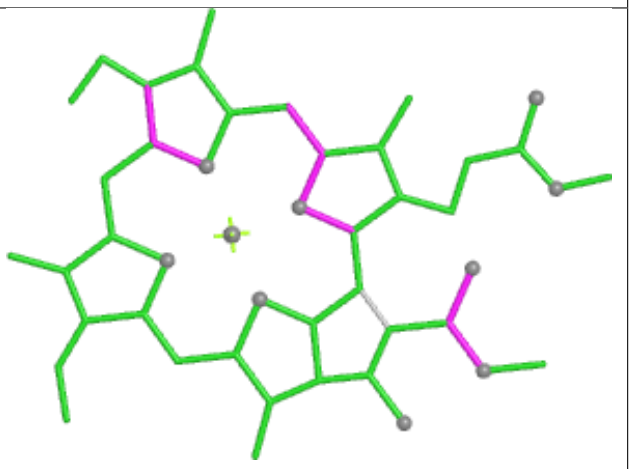

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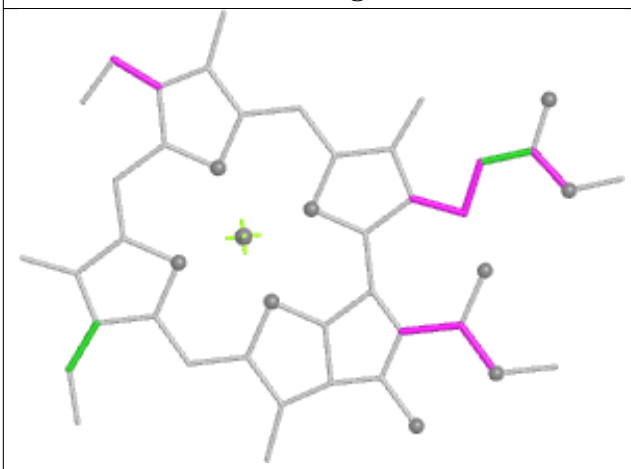

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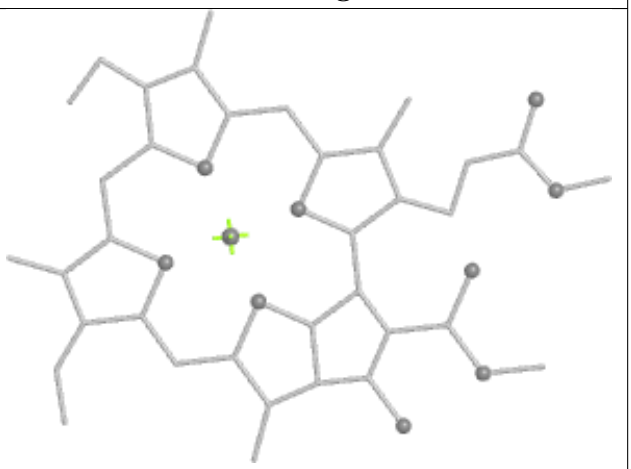
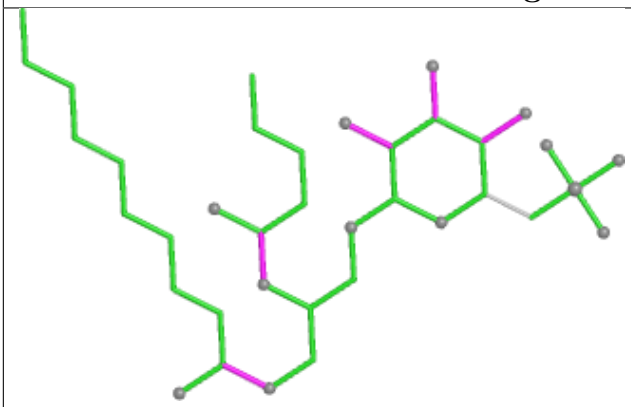


Rings

Ligand SQD D 320



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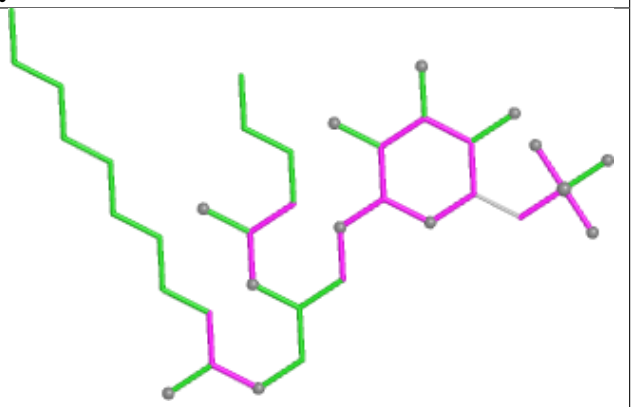
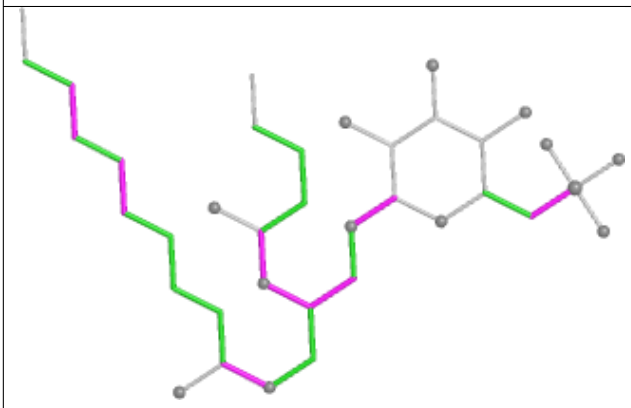


Bond angles



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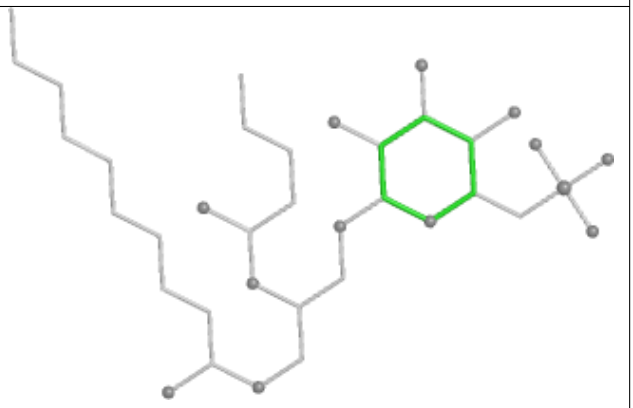
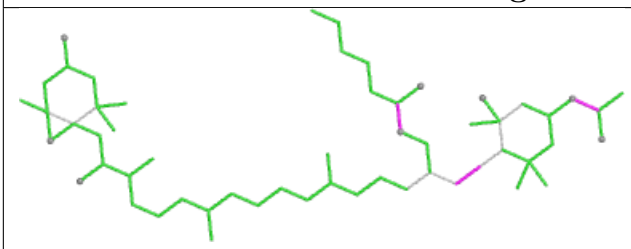


Rings

Ligand A1EB1 7 303



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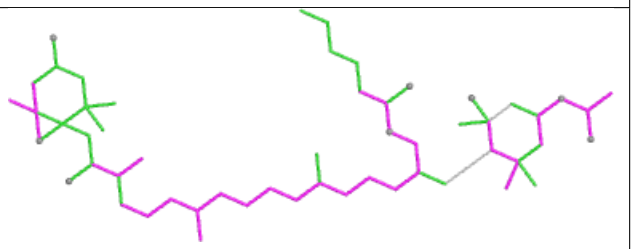

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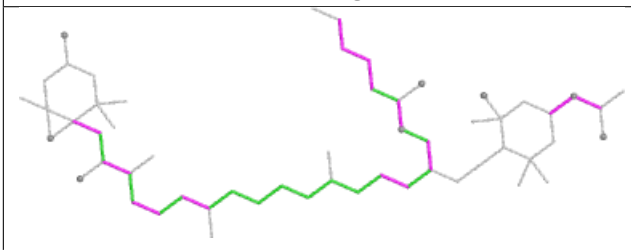

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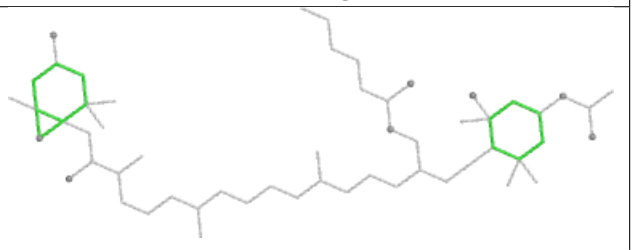
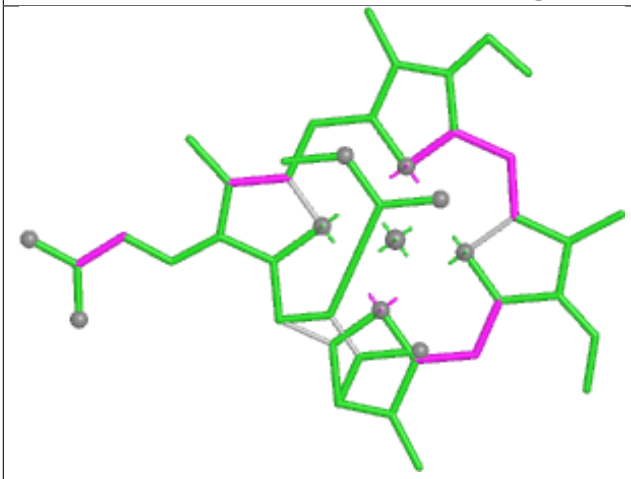


Rings

Ligand KC2 9 318



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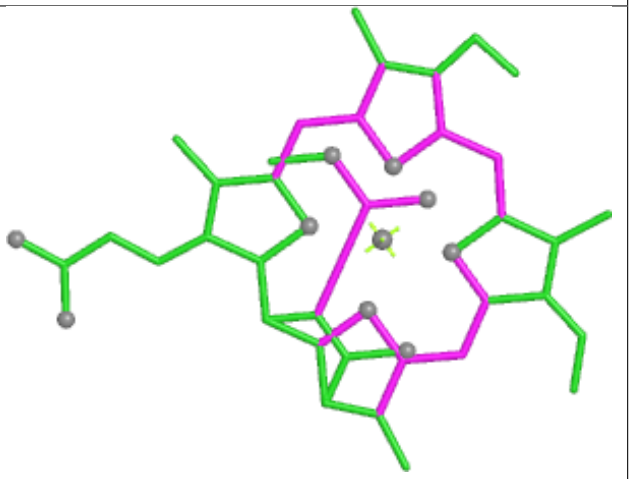
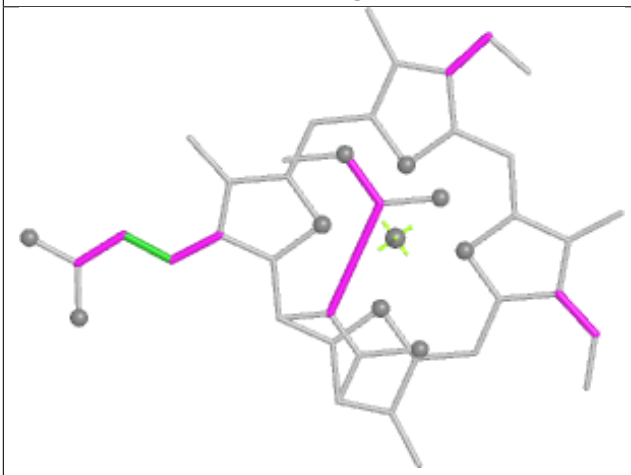


Bond angles



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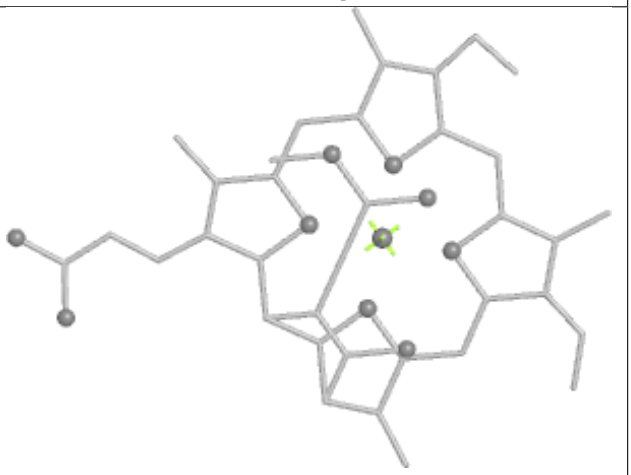
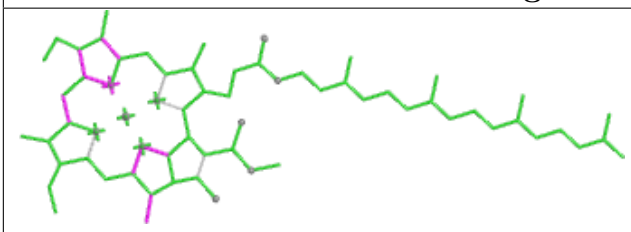


Rings

Ligand CLA R 307



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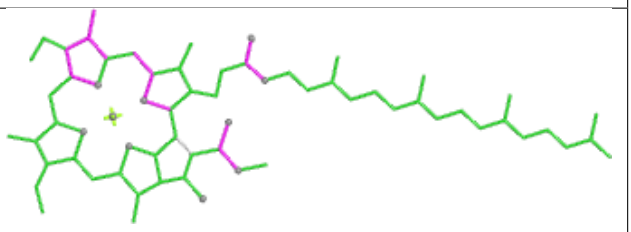

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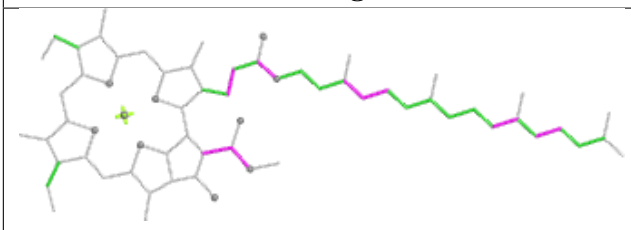

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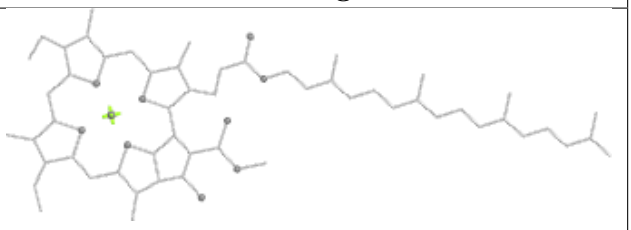
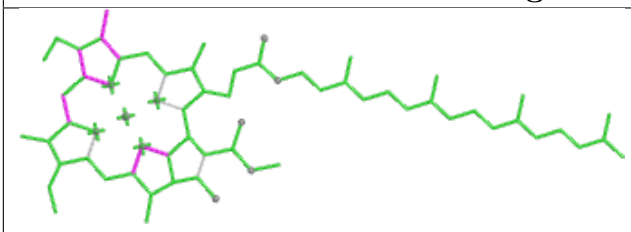


Rings

Ligand CLA F 312



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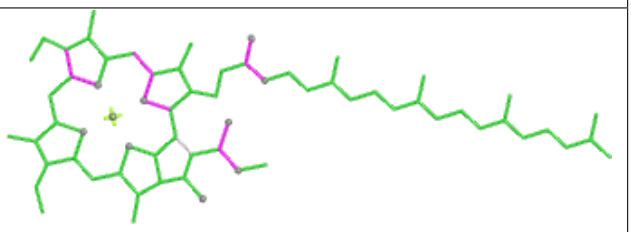

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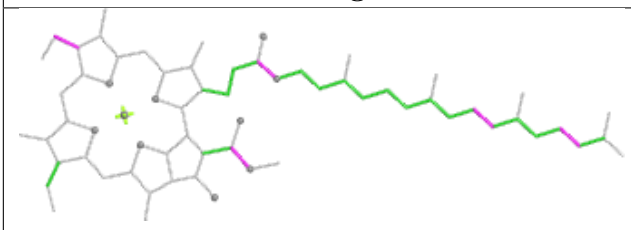

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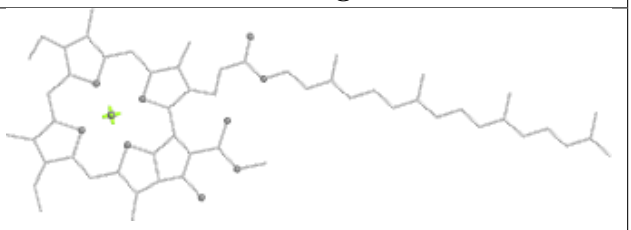
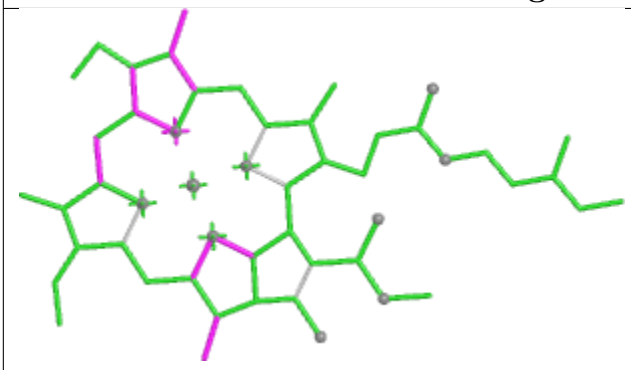


Rings

Ligand CLA a 820



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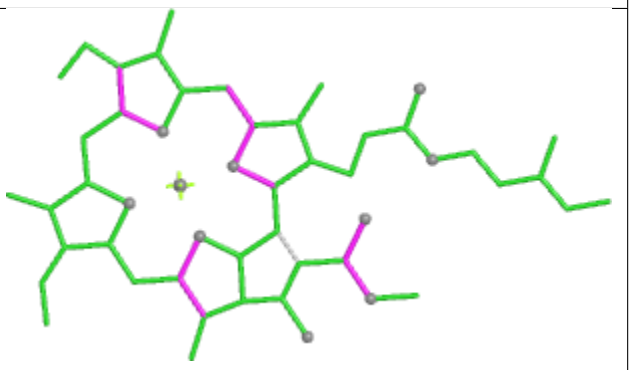
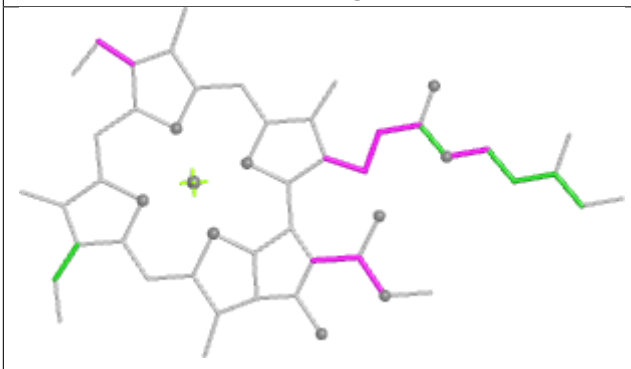


Bond angles



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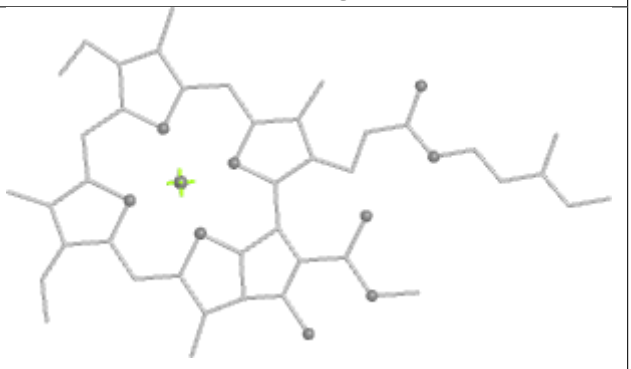
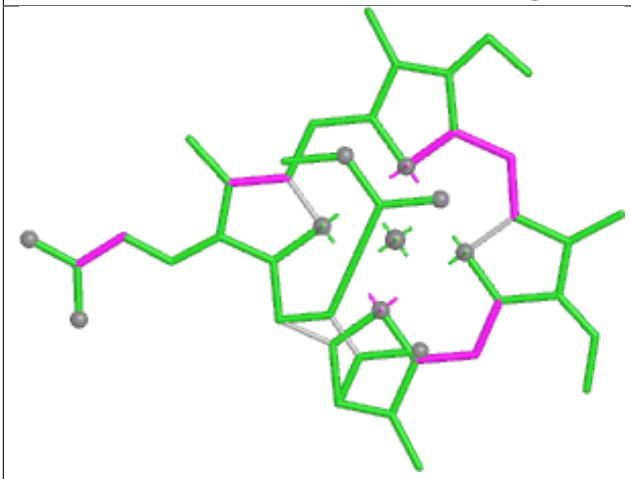


Rings

Ligand KC2 C 313



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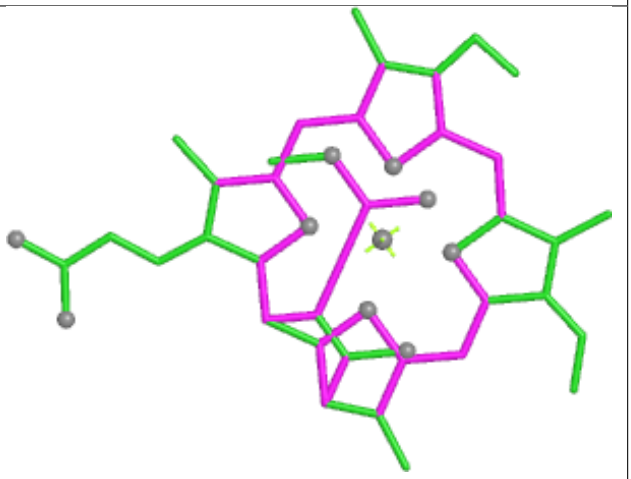
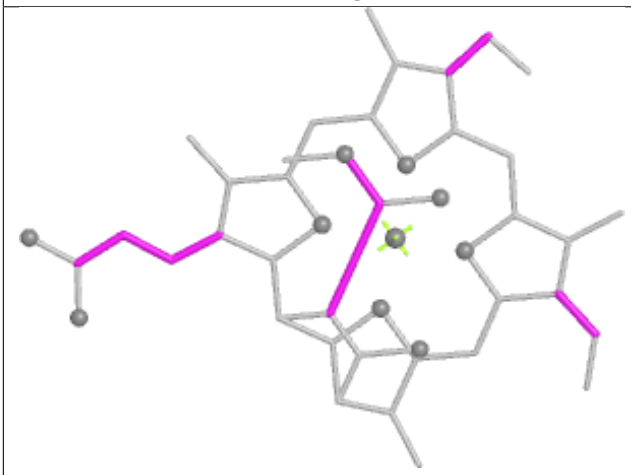


Bond angles



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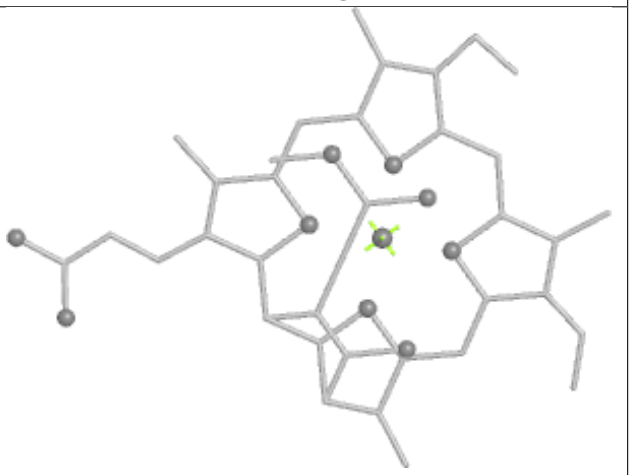
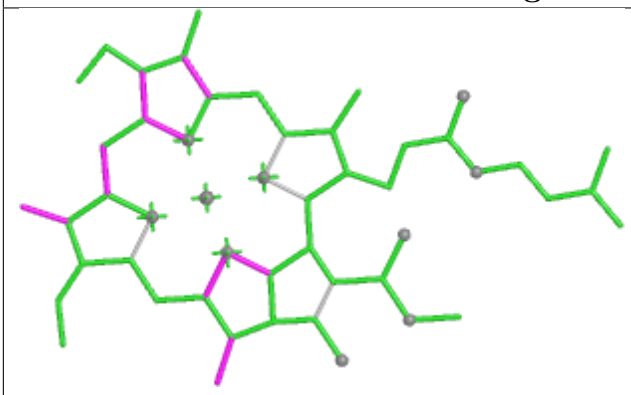


Rings

Ligand CLA R 311



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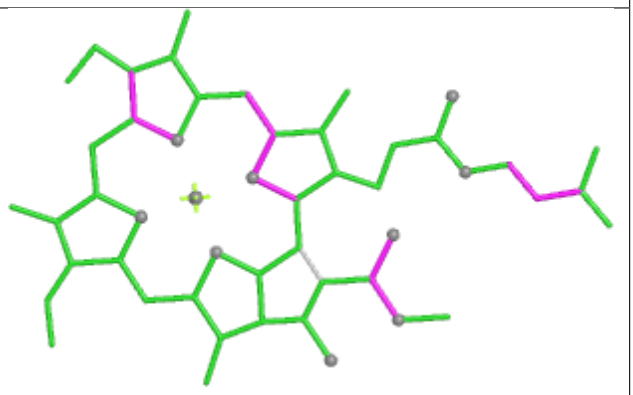
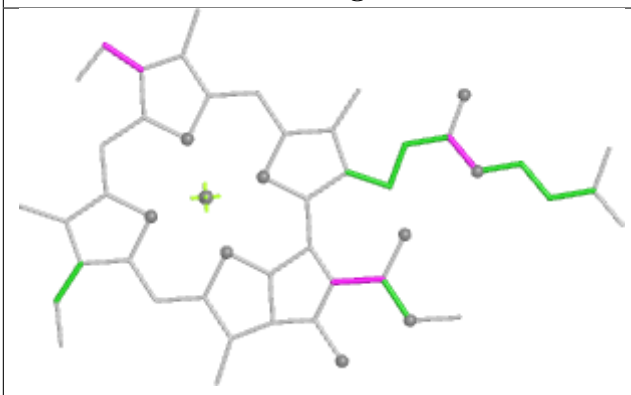


Bond angles



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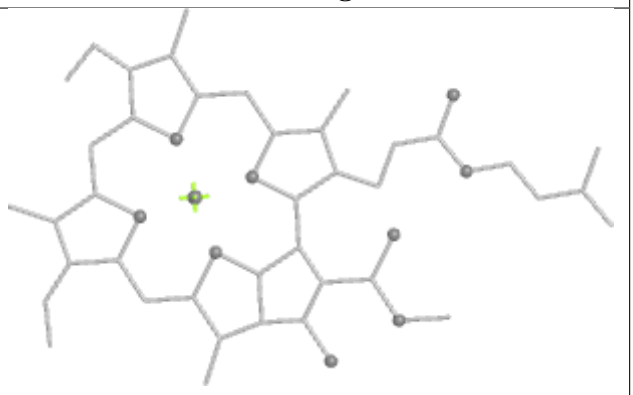
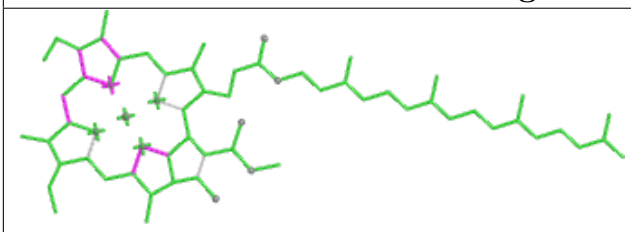


Rings

Ligand CLA W 311



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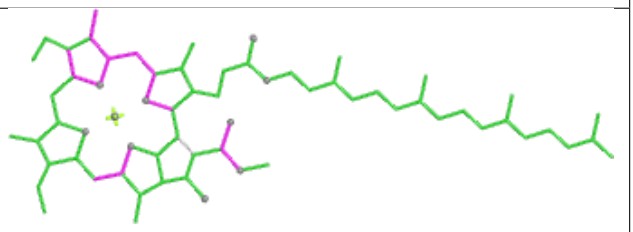
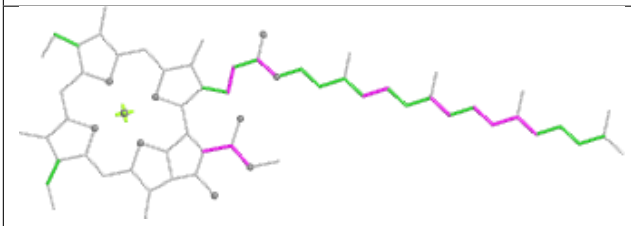


Bond angles



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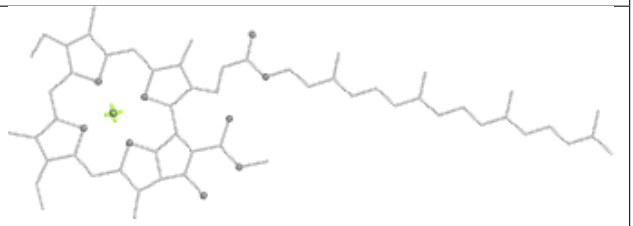
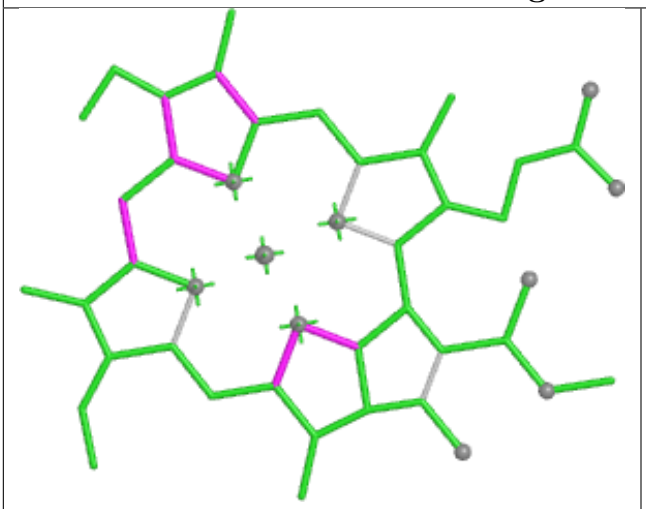


Rings

Ligand CLA 8 310



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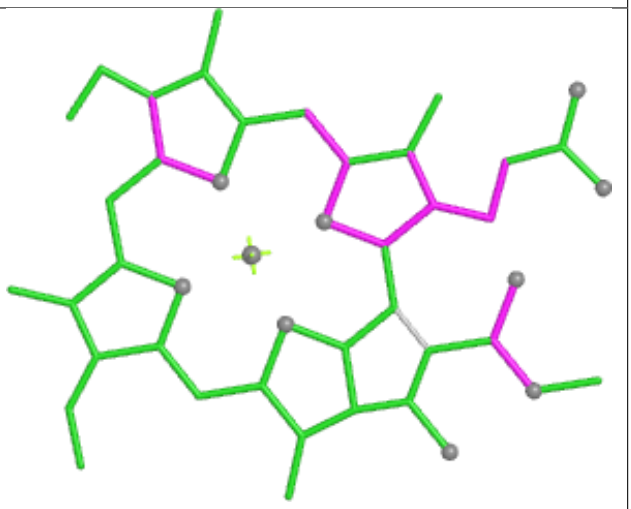
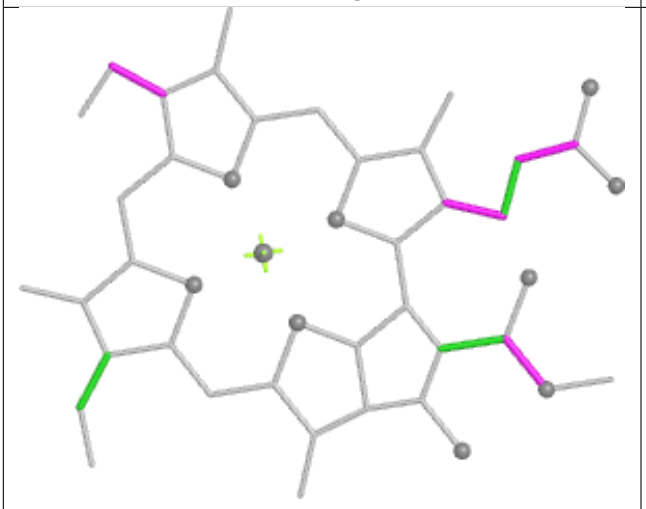


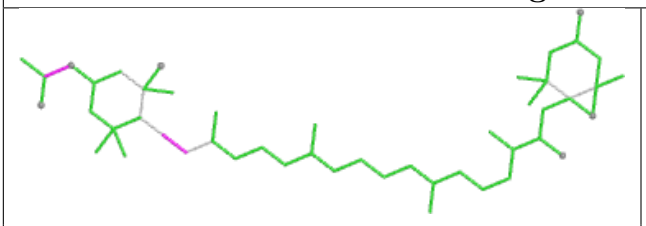
Bond angles



Torsions

Rings

Ligand A86 G 305



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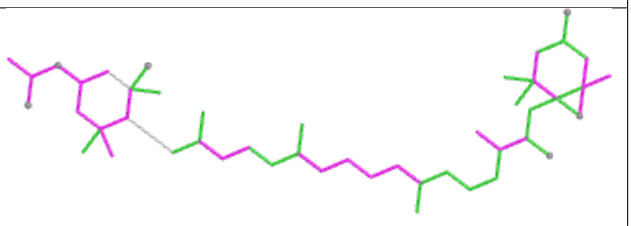
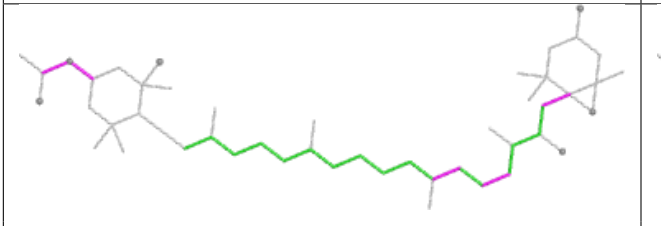
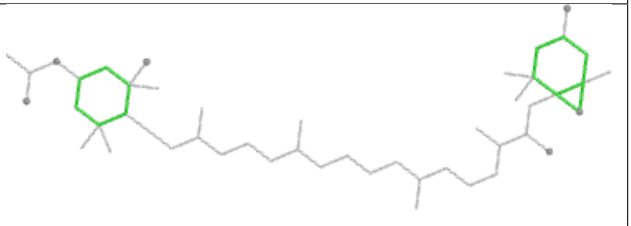


Bond angles

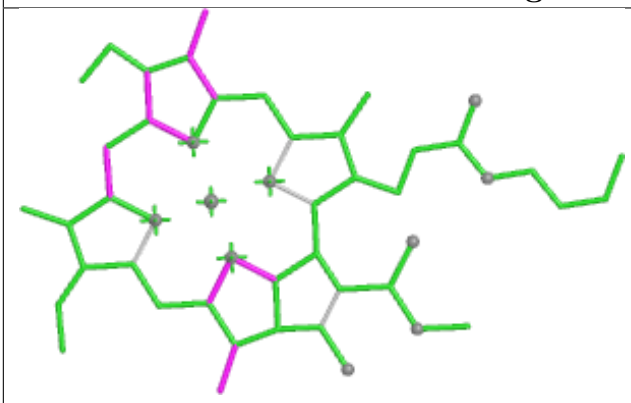


Torsions

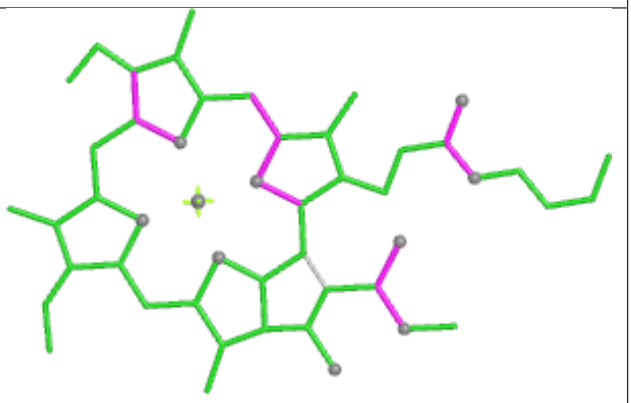


Rings

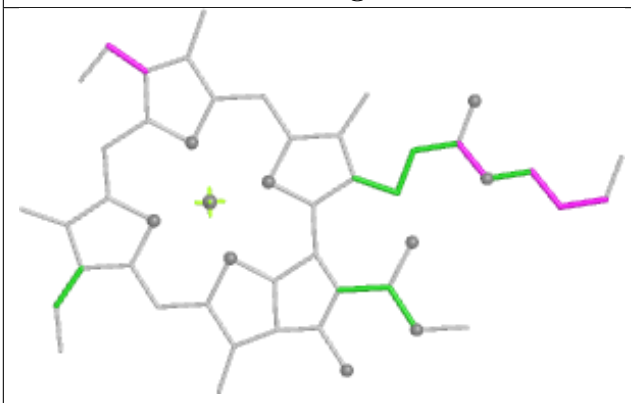
Ligand CLA E 306



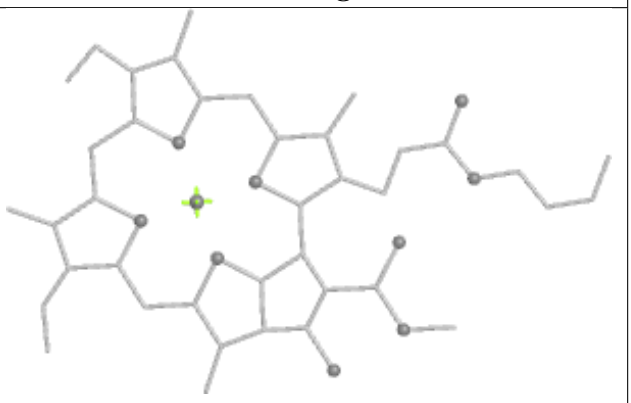
Bond lengths



Bond angles

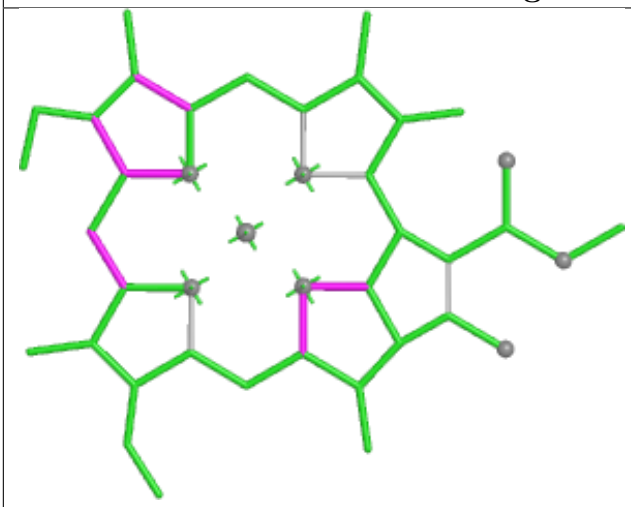


Torsions

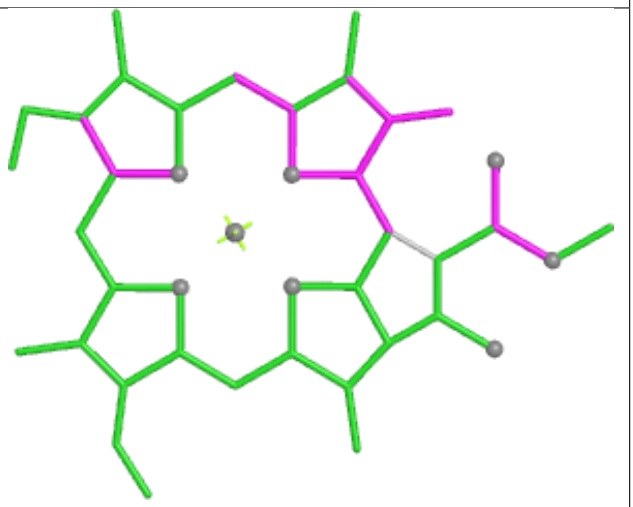


Rings

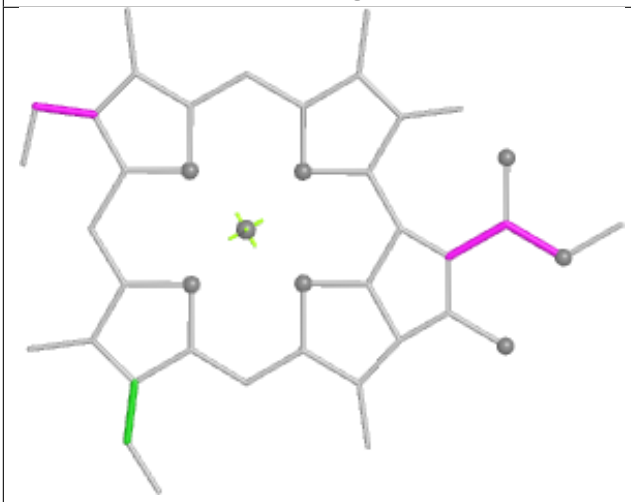
Ligand CLA Y 314



Bond lengths



Bond angles



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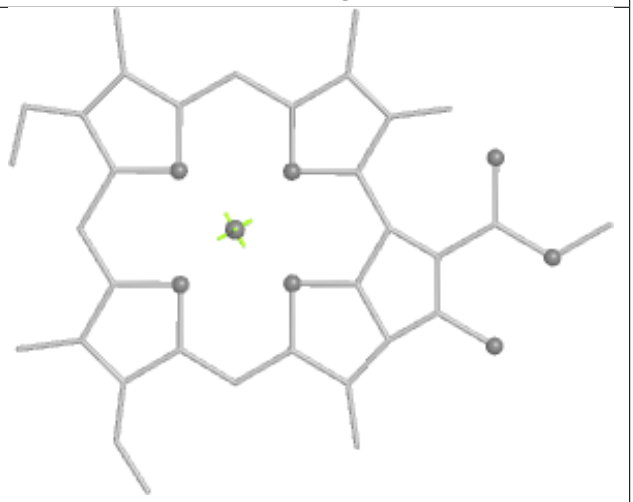
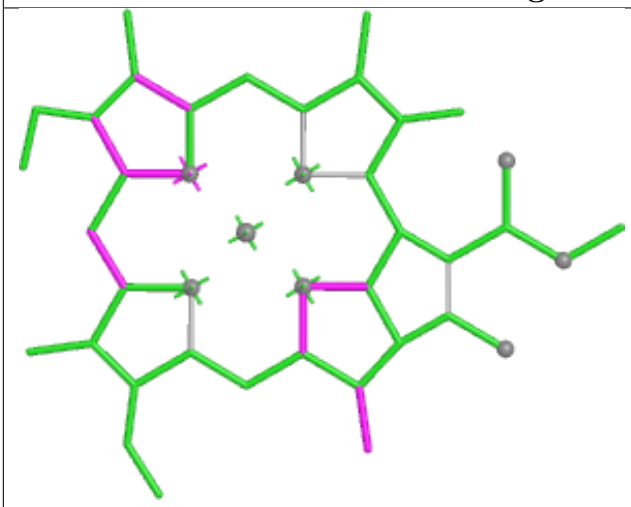
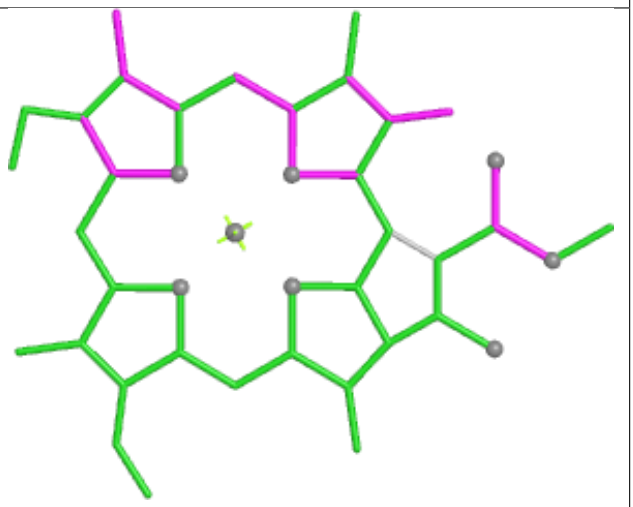


Rings

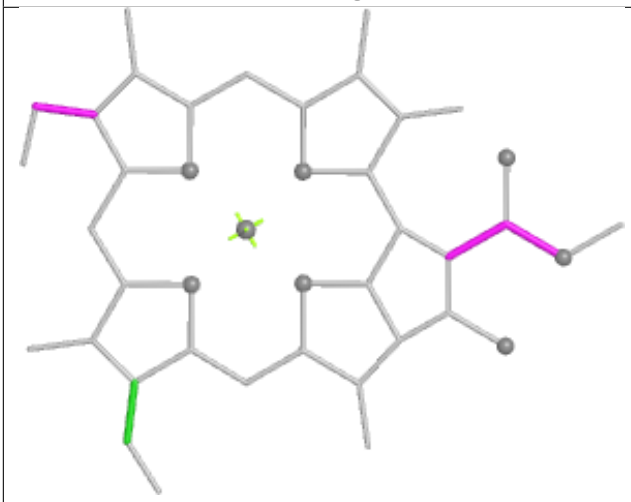
Ligand CLA x 309



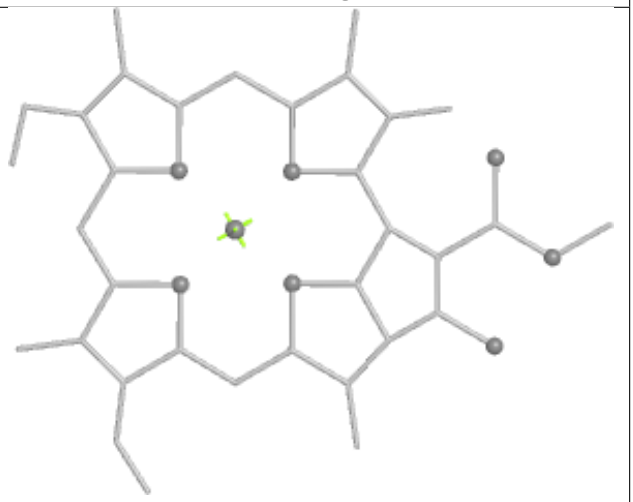
Bond lengths



Bond angles

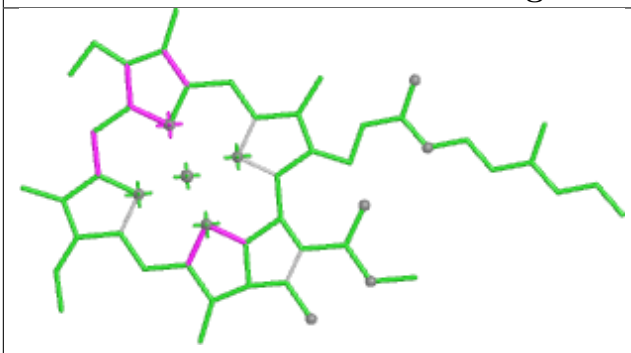


Torsions

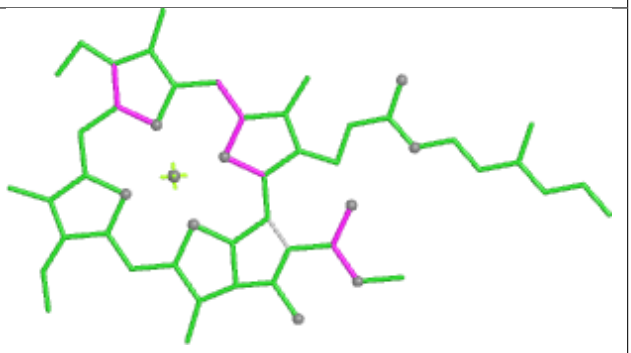


Rings

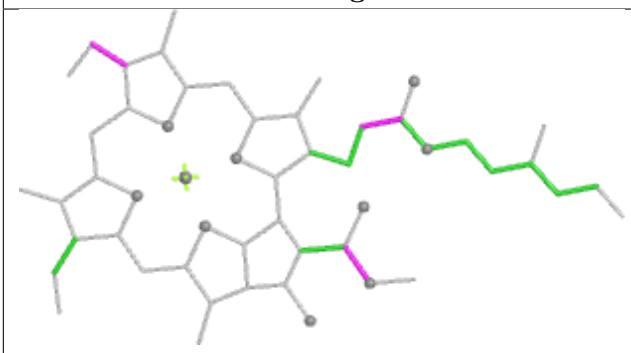
Ligand CLA F 309



Bond lengths



Bond angles



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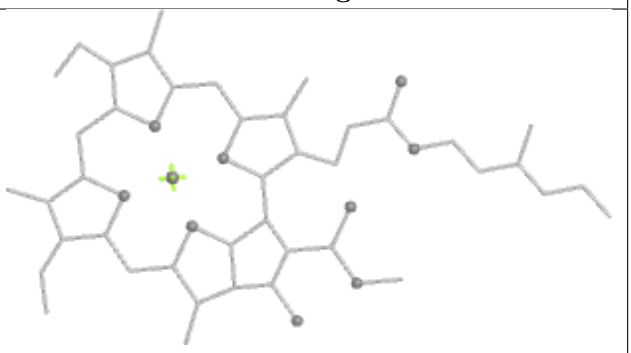
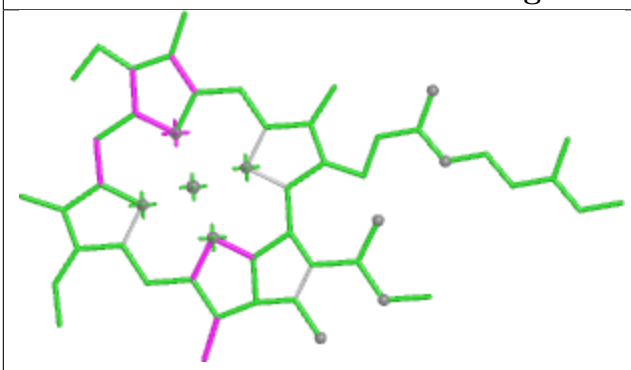


Rings

Ligand CLA A 308



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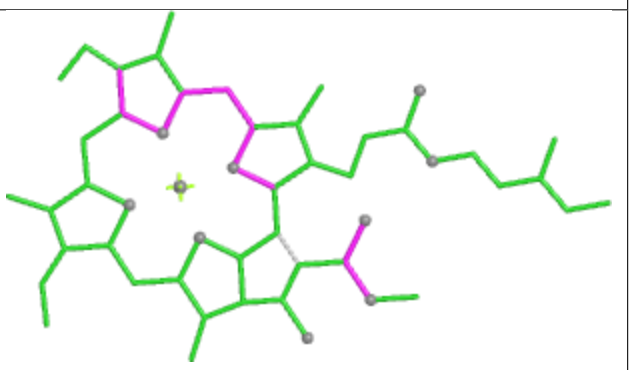
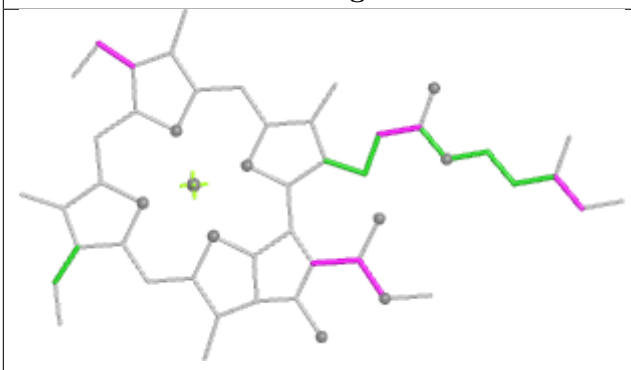


Bond angles



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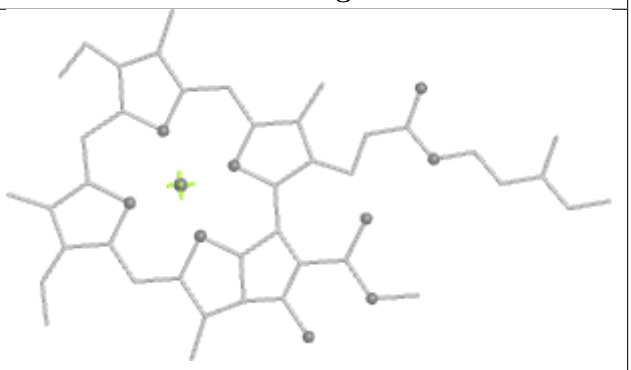
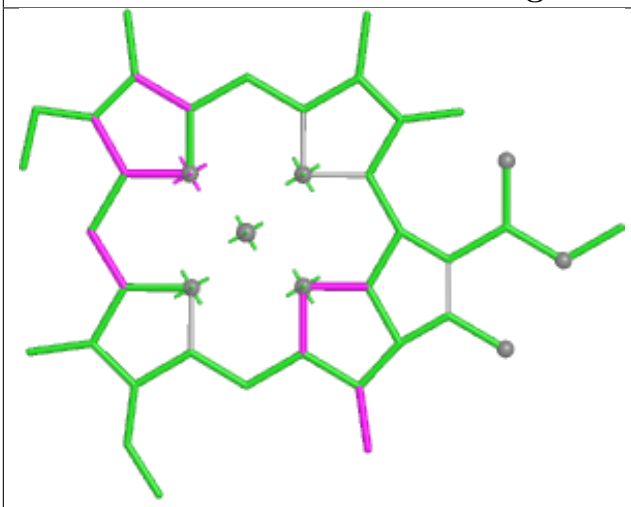


Rings

Ligand CLA Z 307



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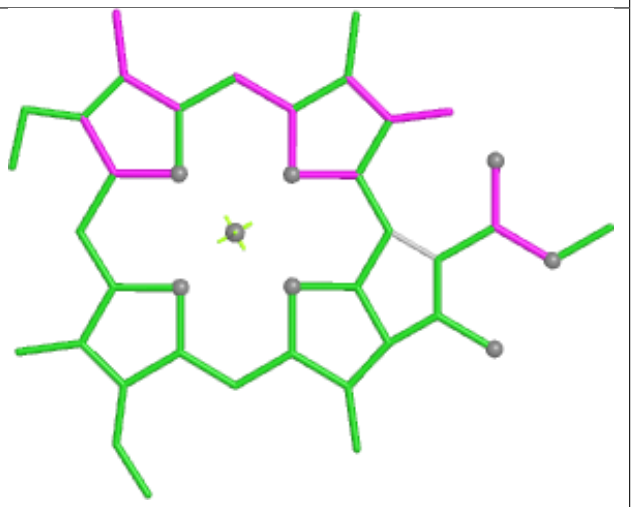
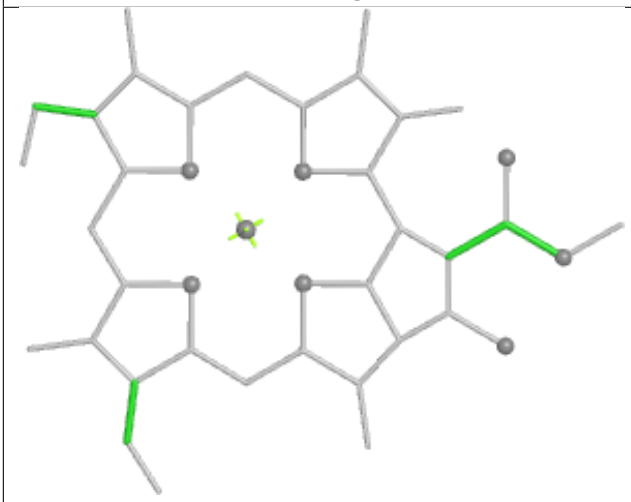


Bond angles



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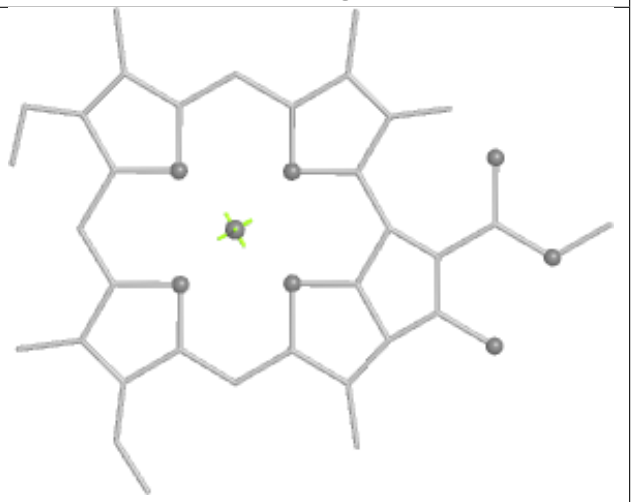
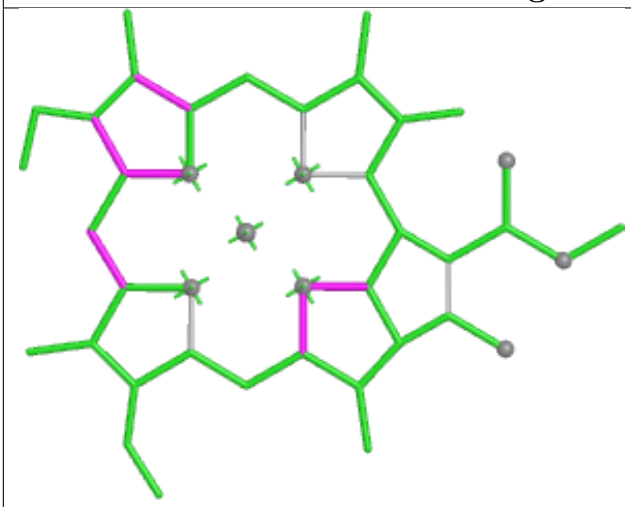


Rings

Ligand CLA 1 320



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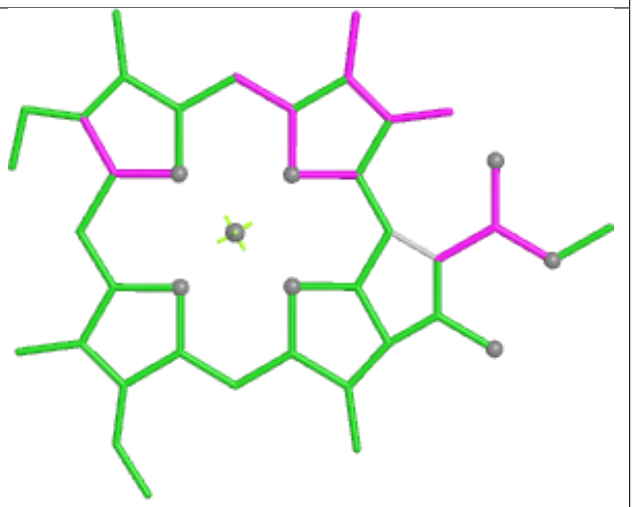
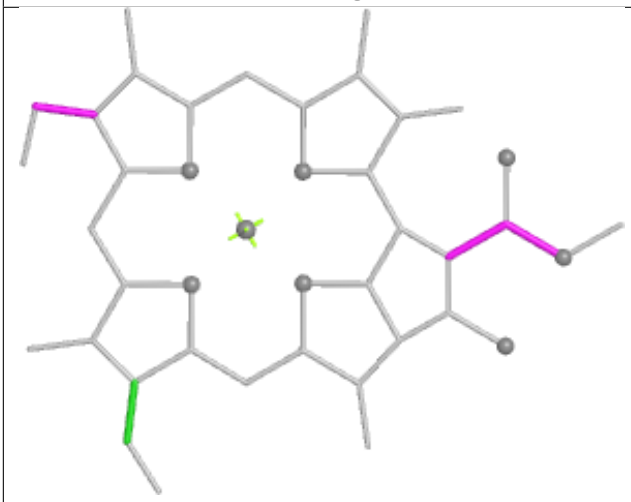


Bond angles



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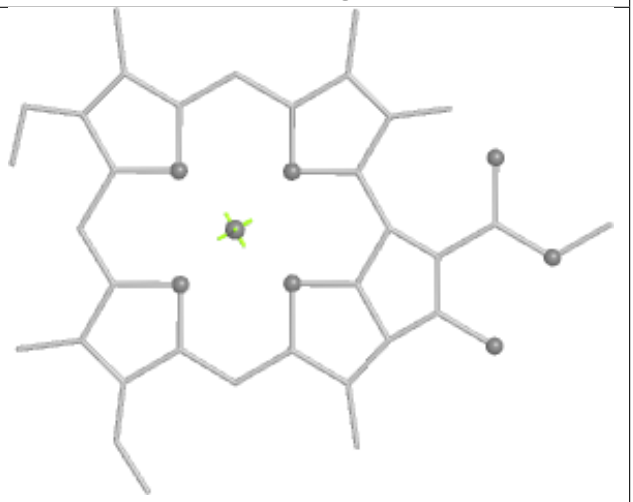
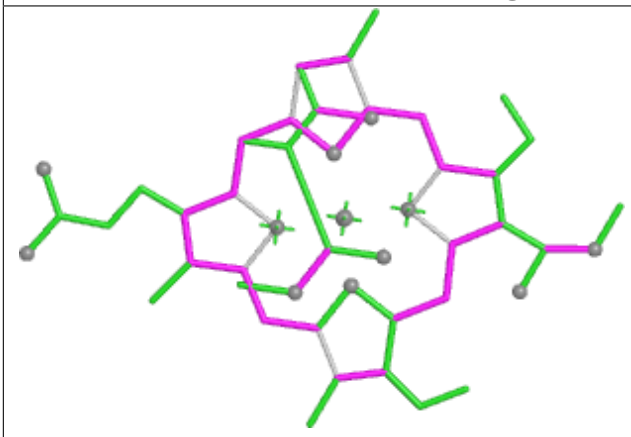


Rings

Ligand A1ECV S 318



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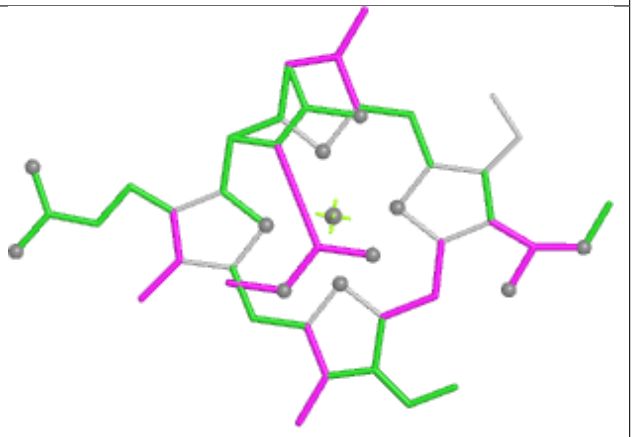
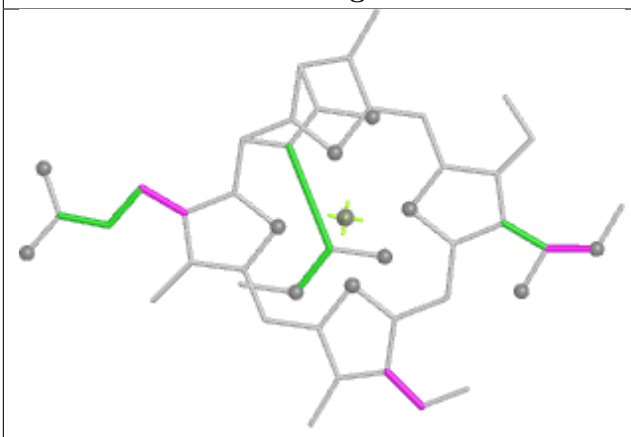


Bond angles



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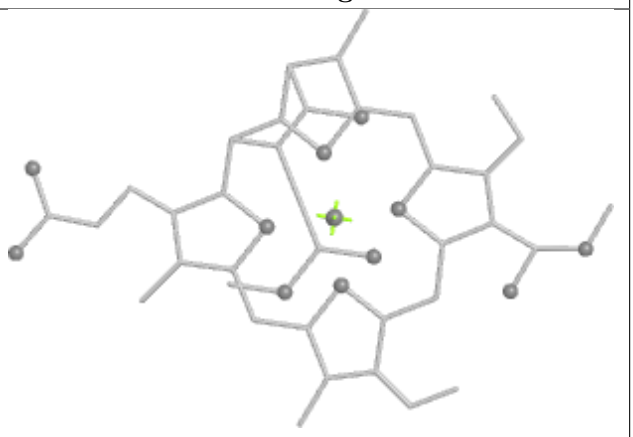
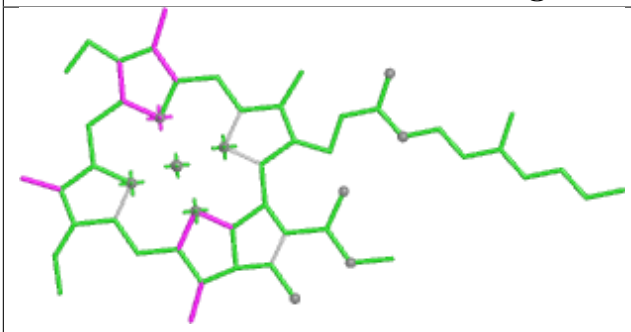
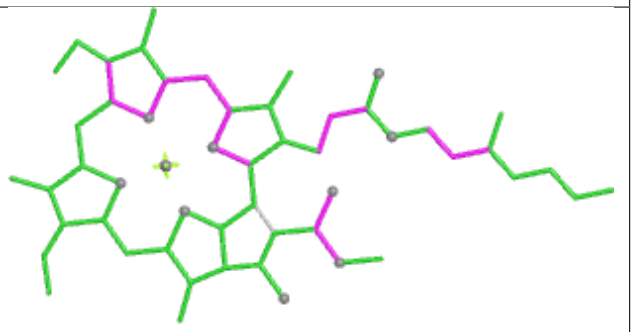


Rings

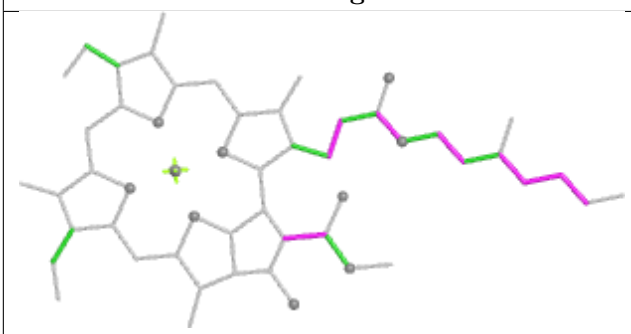
Ligand CLA 0 312



Bond lengths



Bond angles



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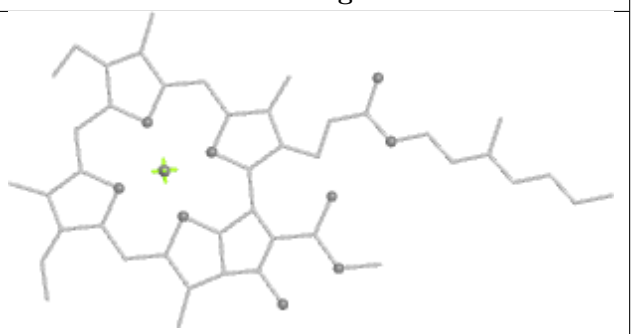
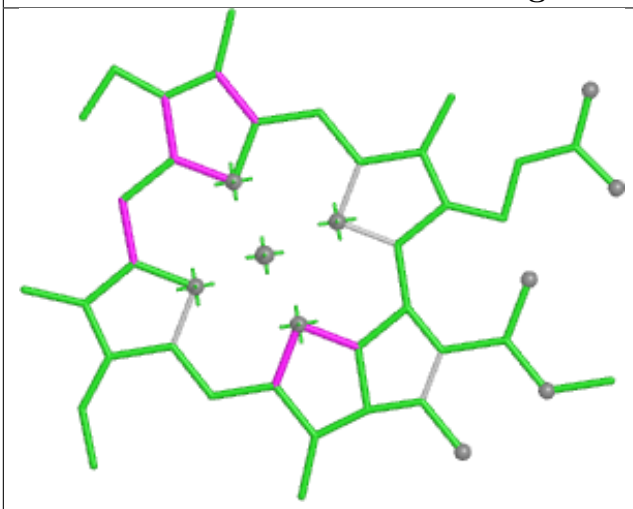


Rings

Ligand CLA 0 320



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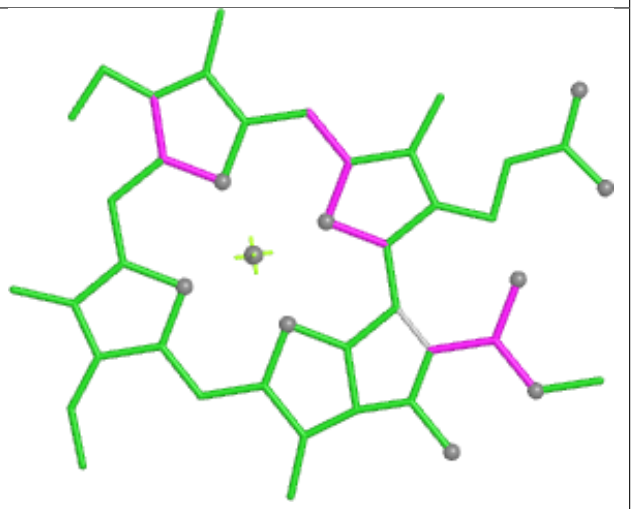

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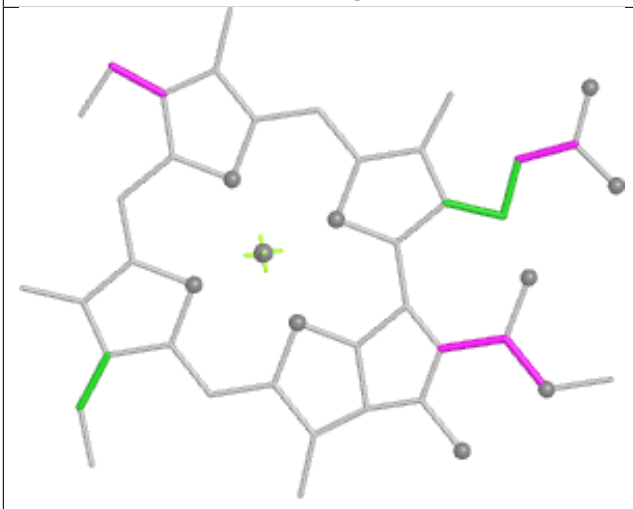
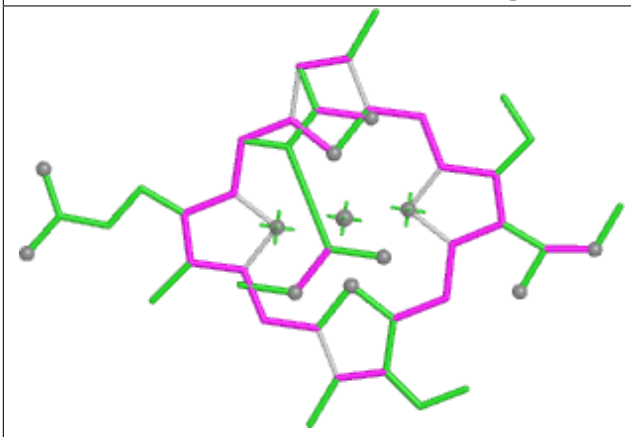


Torsions

Rings

Ligand A1ECV y 311



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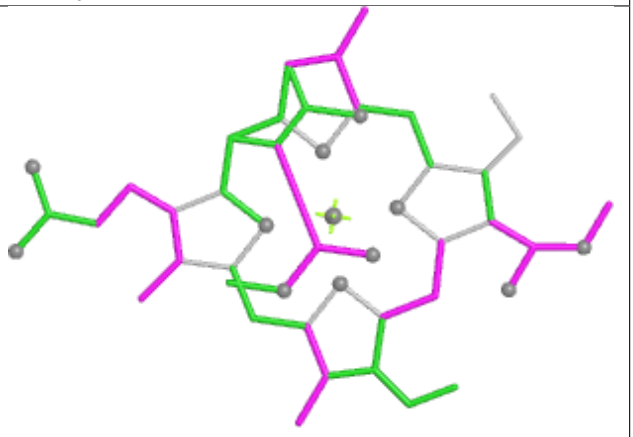
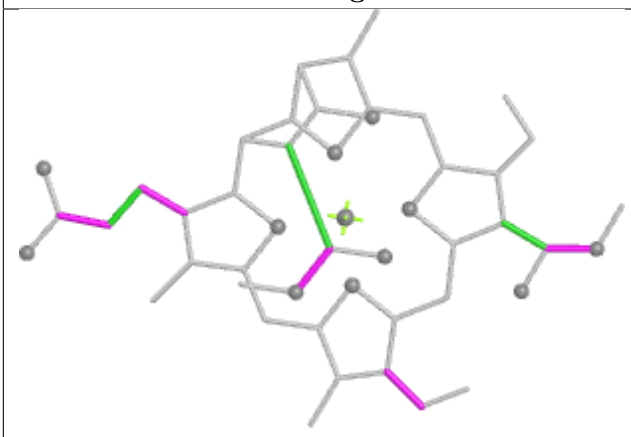


Bond angles



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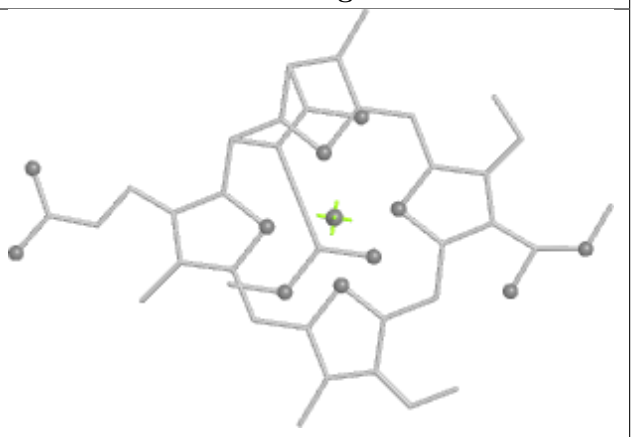
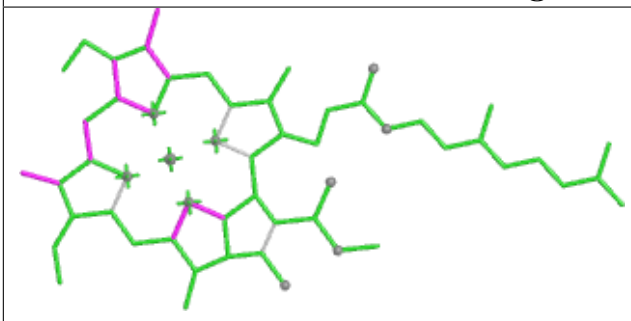


Rings

Ligand CLA a 821



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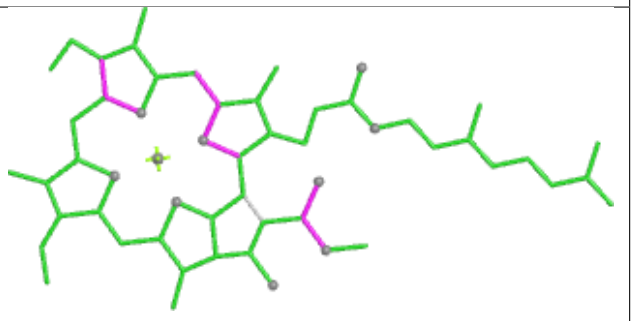
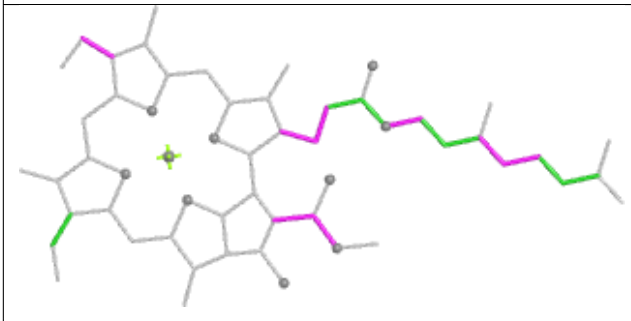


Bond angles



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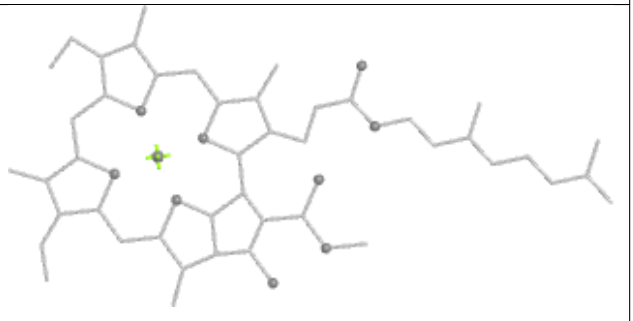
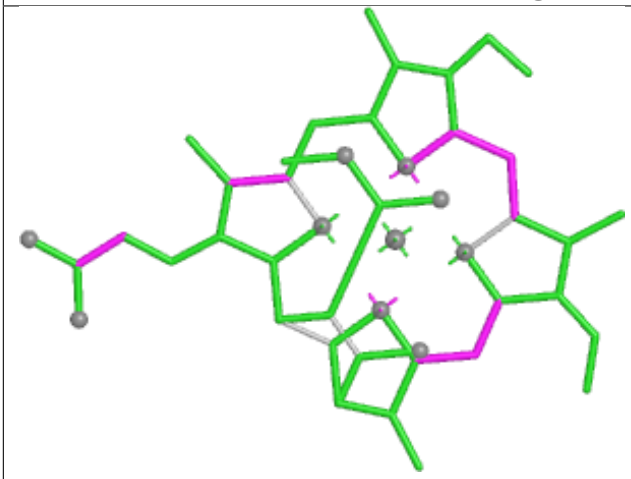


Rings

Ligand KC2 x 315



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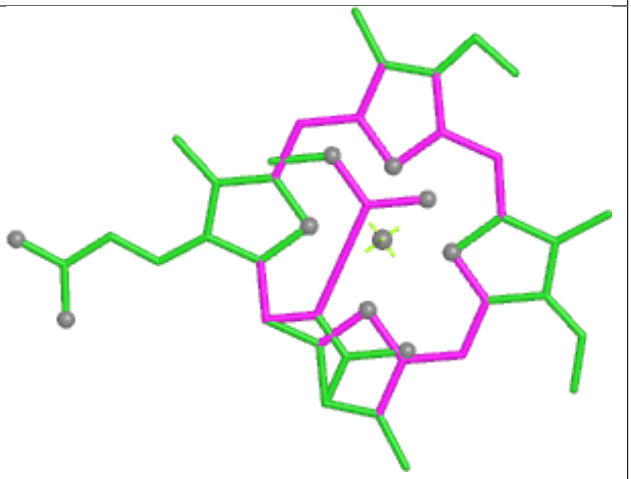
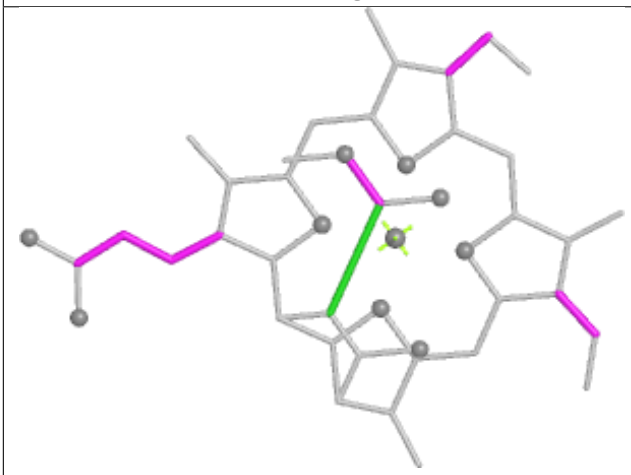
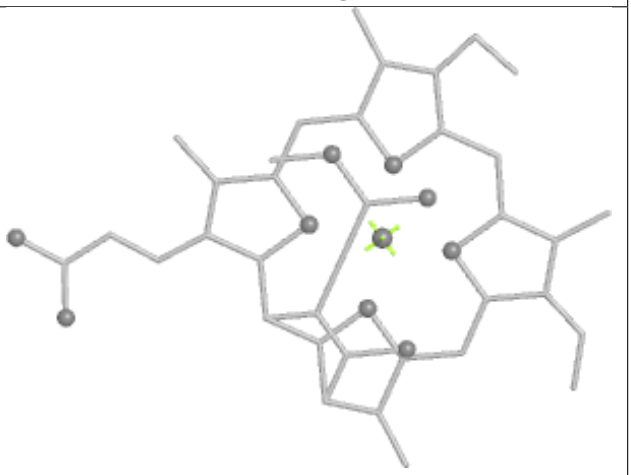


Bond angles

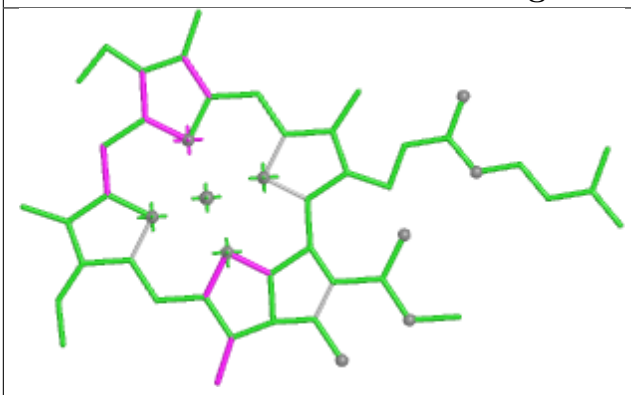


Torsions



Rings

Ligand CLA 7 315



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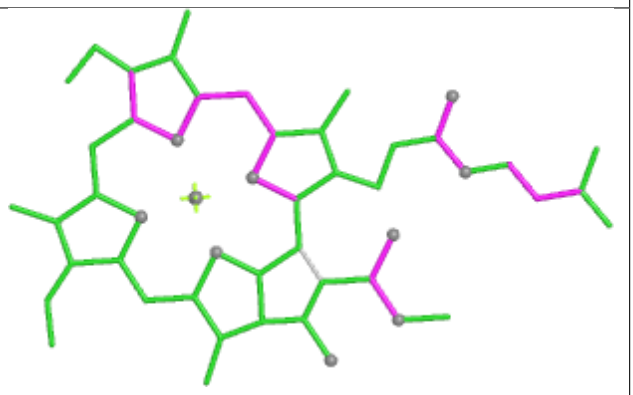
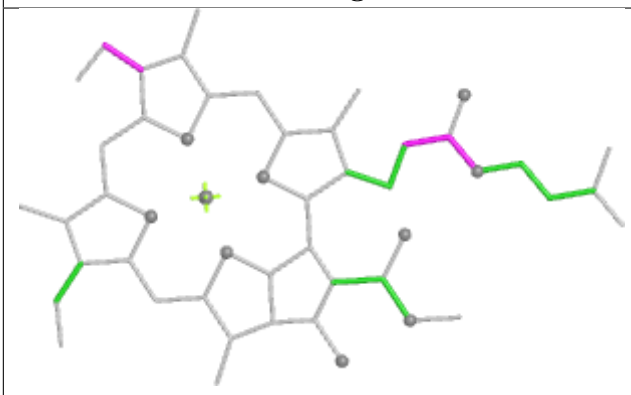
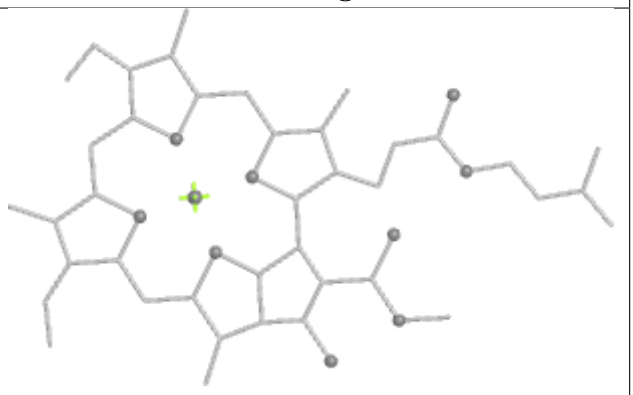


Bond angles

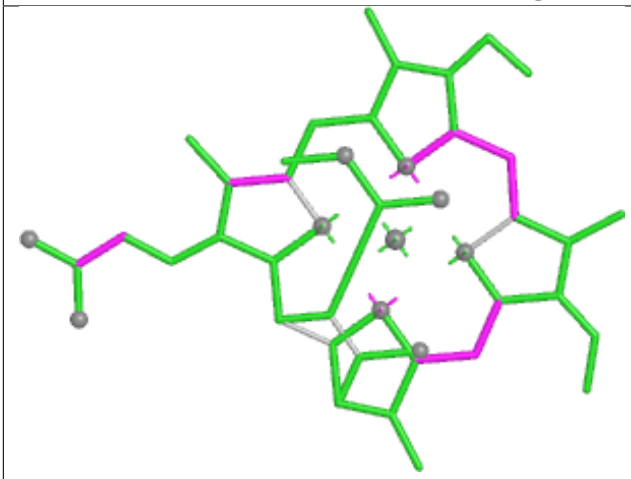


Torsions

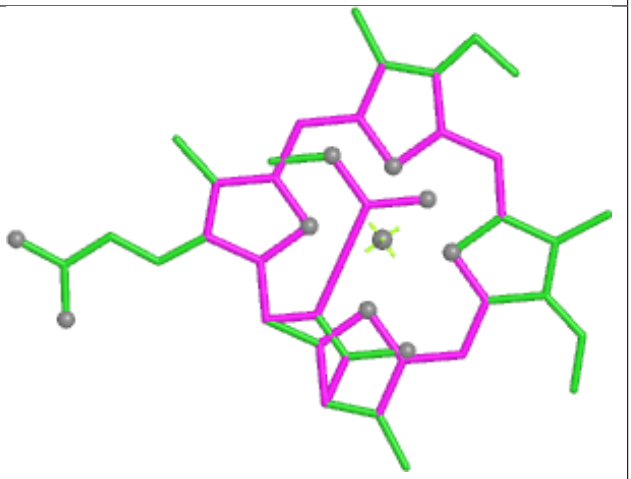


Rings

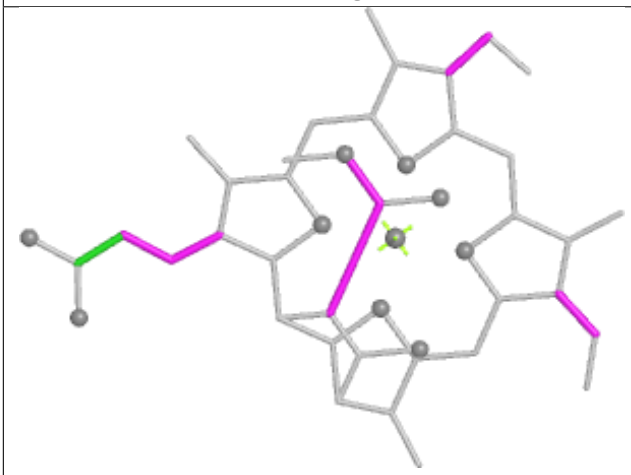
Ligand KC2 J 315



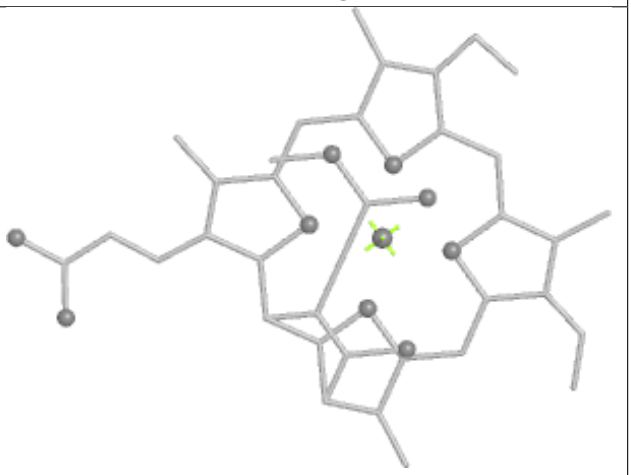
Bond lengths



Bond angles

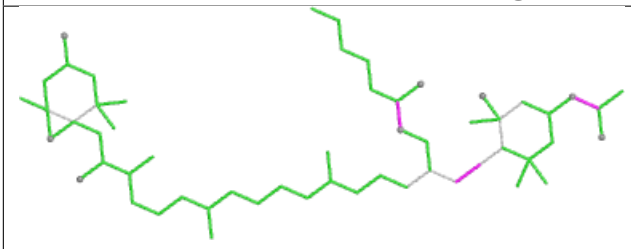


Torsions



Rings

Ligand A1EB1 4 303



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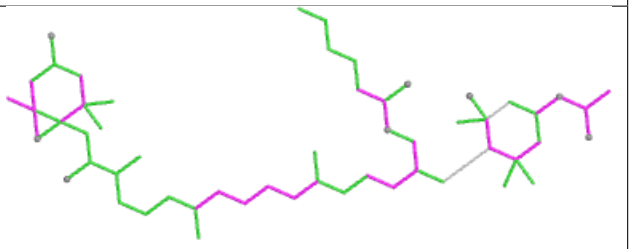

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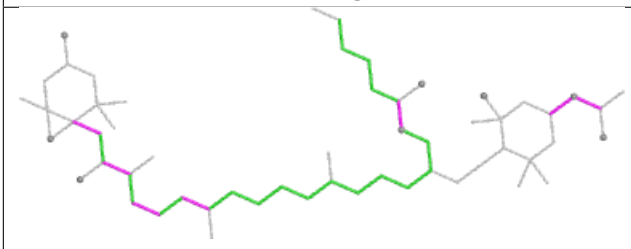
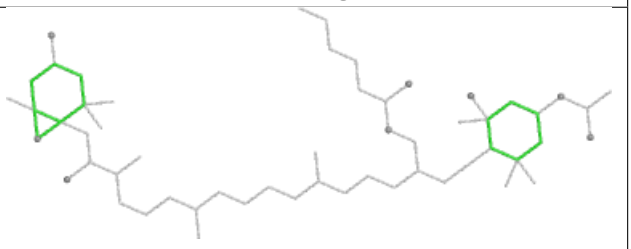
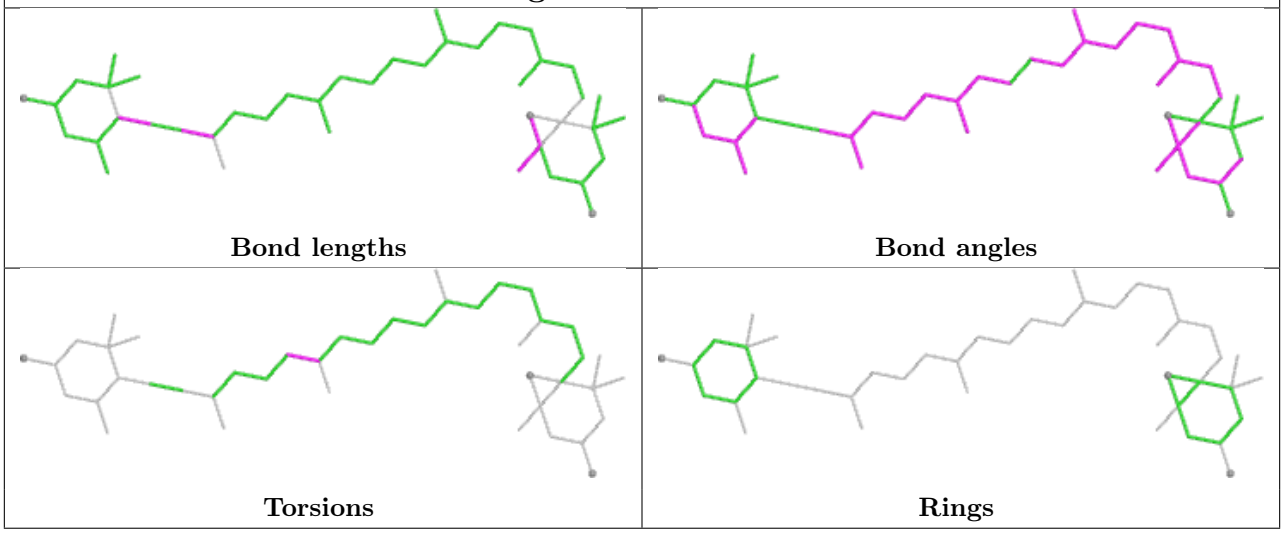


Torsions

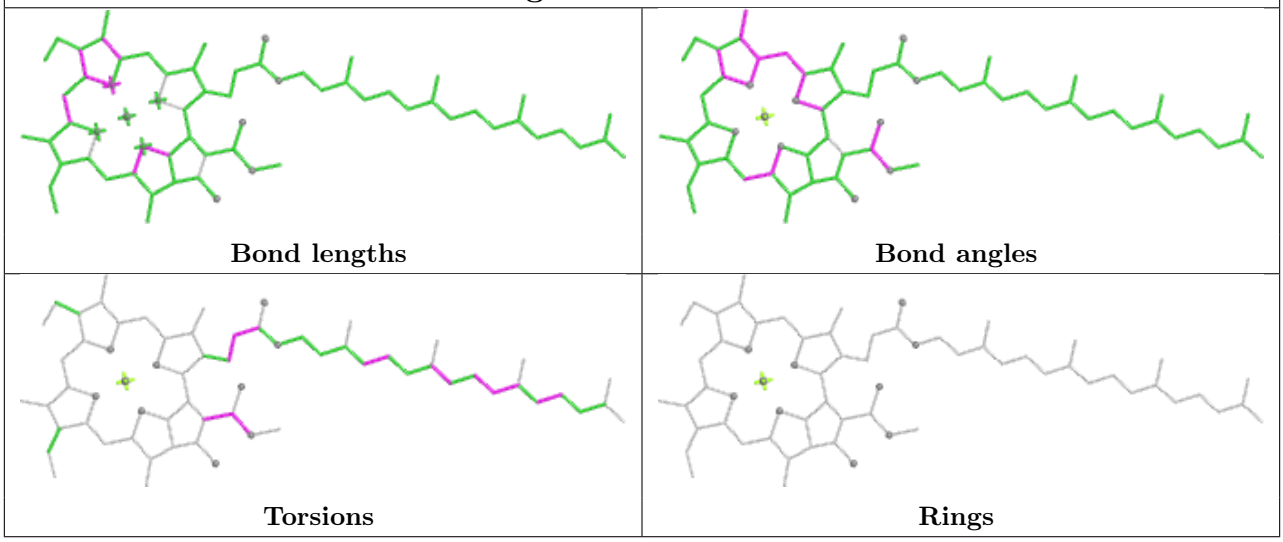


Rings

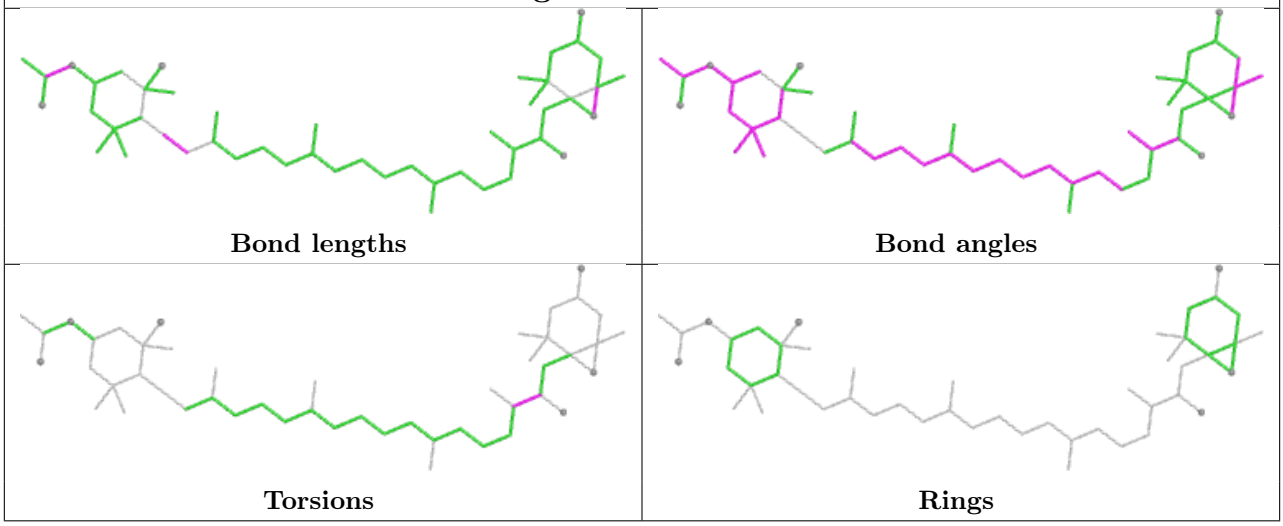
Ligand DD6 Z 302



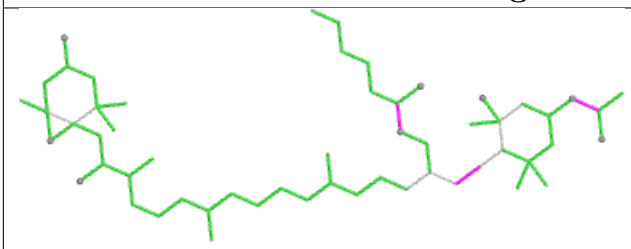
Ligand CLA P 309



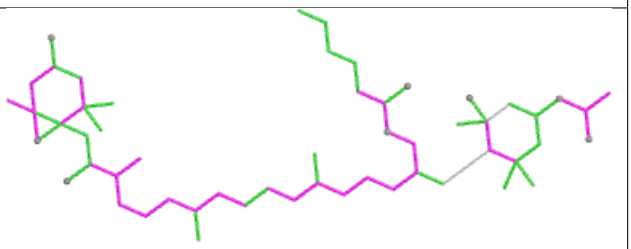
Ligand A86 L 305



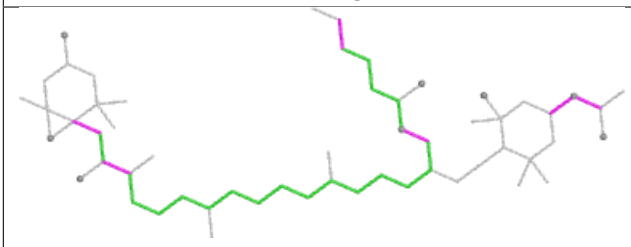
Ligand A1EB1 0 307



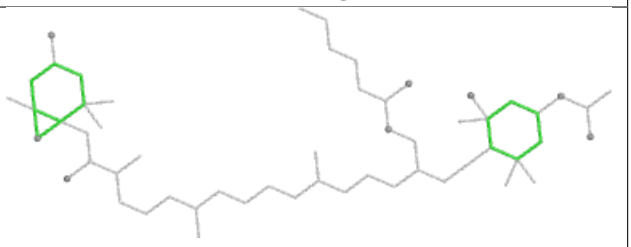
Bond lengths



Bond angles

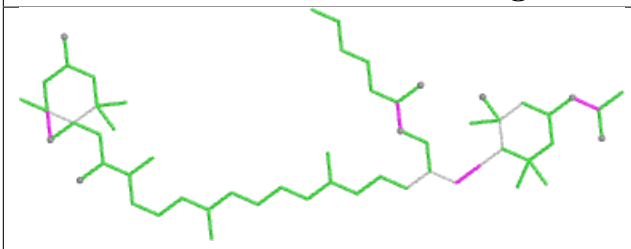


Torsions

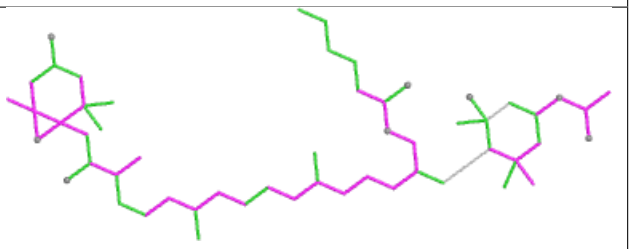


Rings

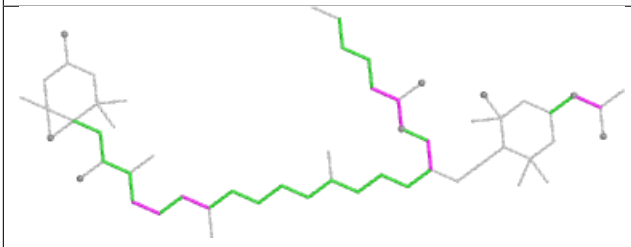
Ligand A1EB1 4 302



Bond lengths



Bond angles



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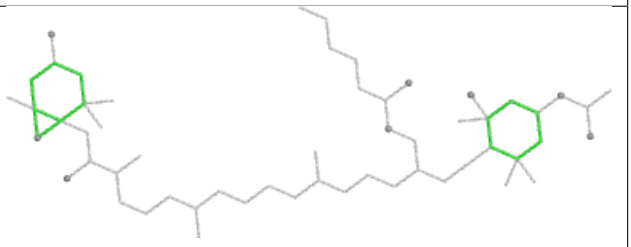
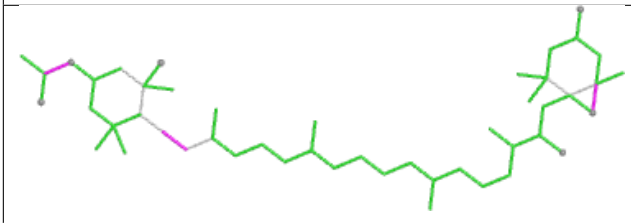


Rings

Ligand A86 U 202



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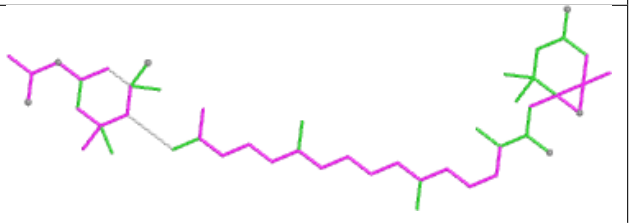
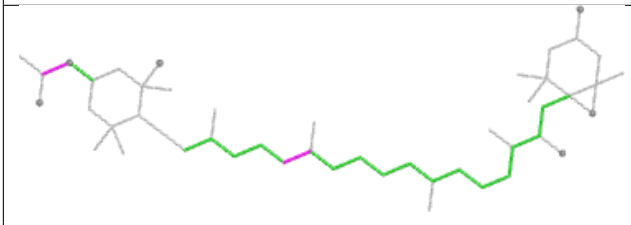


Bond angles



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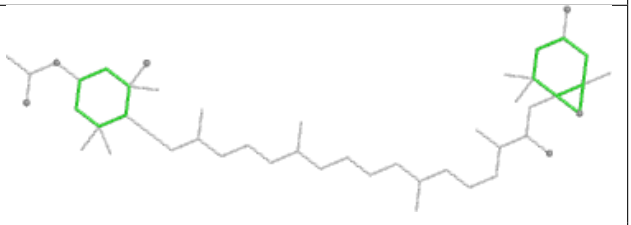
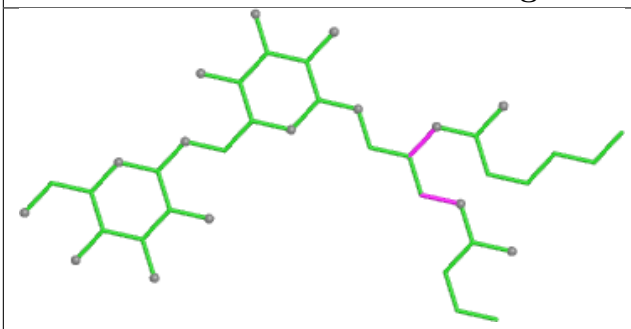


Rings

Ligand DGD C 314



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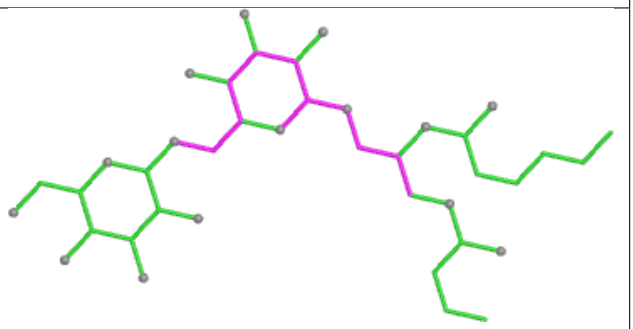
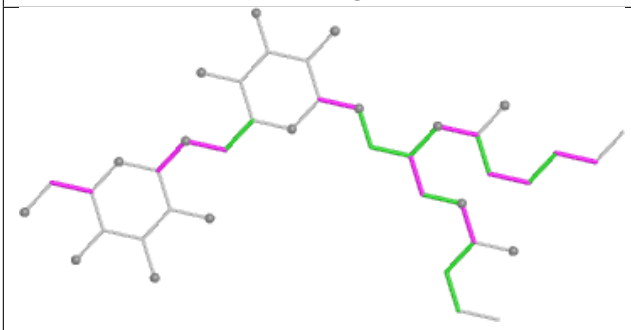


Bond angles



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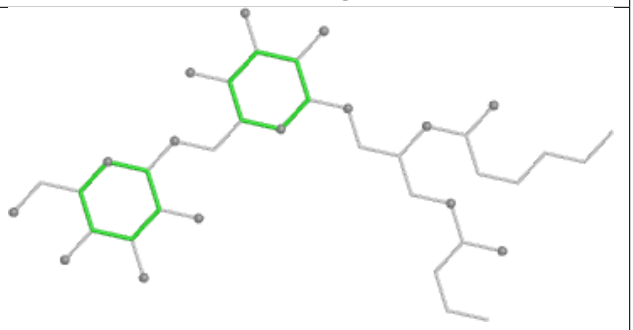
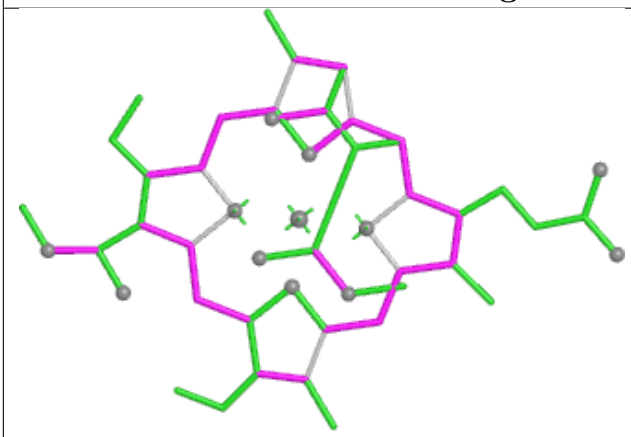


Rings

Ligand A1ECV G 316



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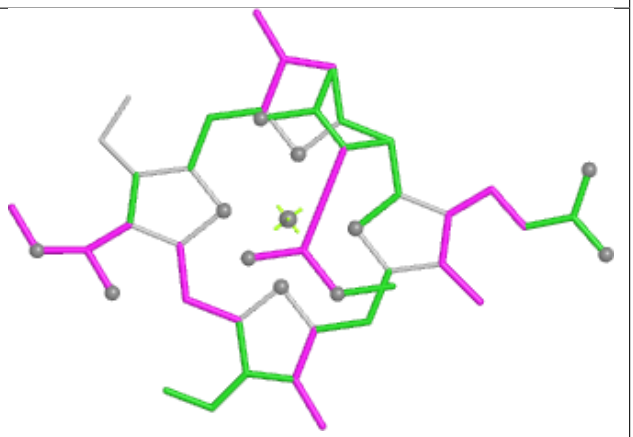
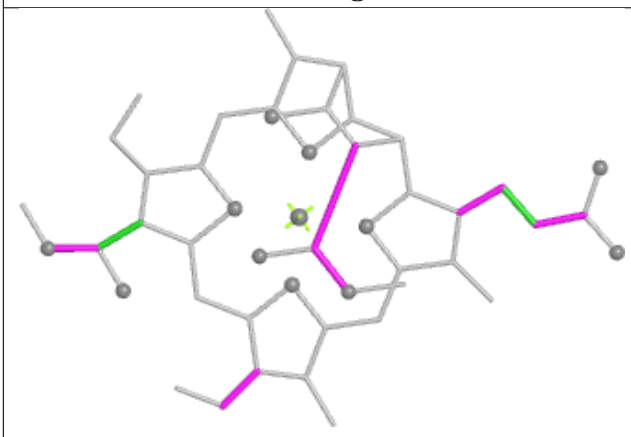


Bond angles



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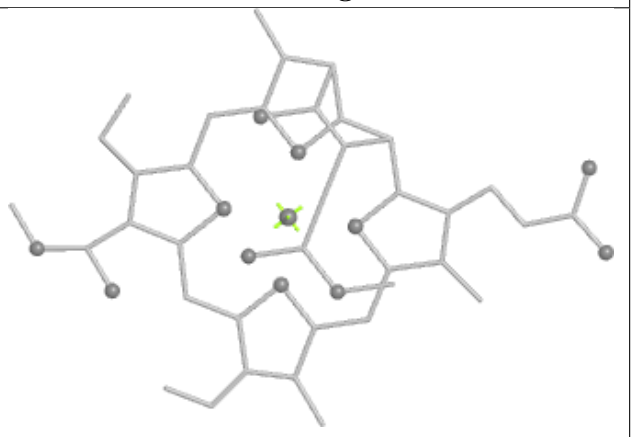
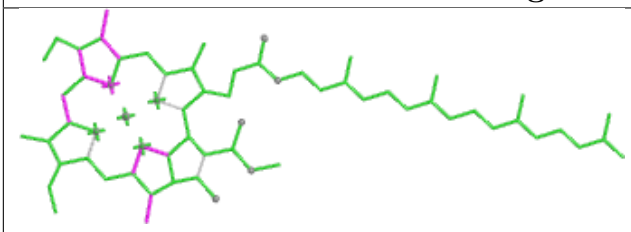


Rings

Ligand CLA b 812



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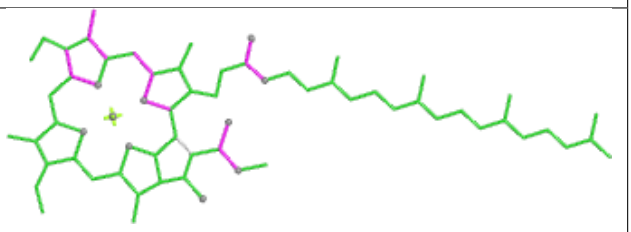
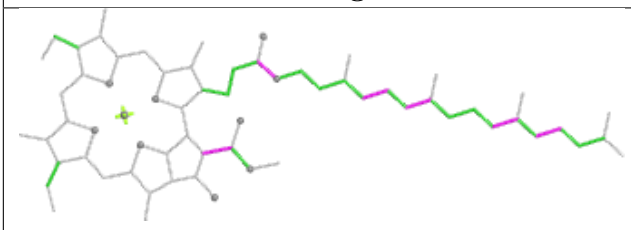
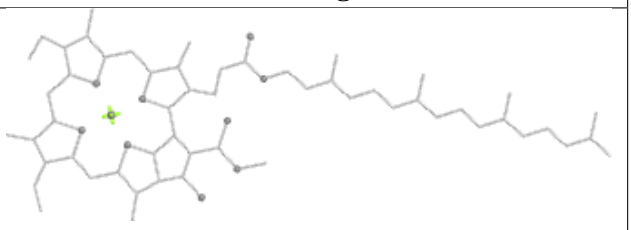


Bond angles

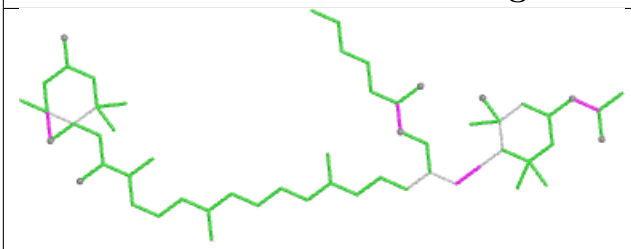


Torsions



Rings

Ligand A1EB1 x 301



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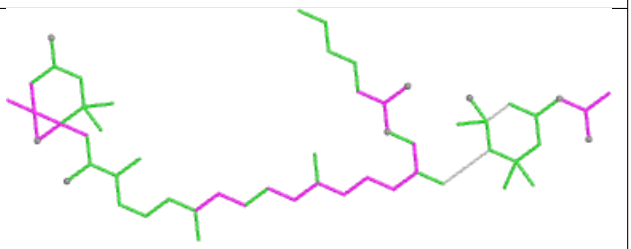
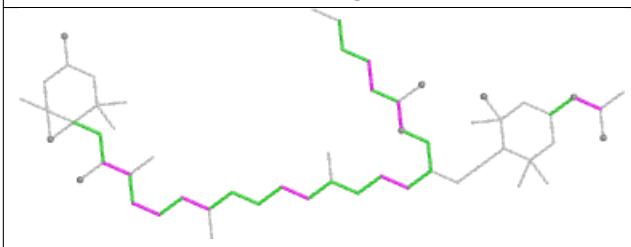


Bond angles



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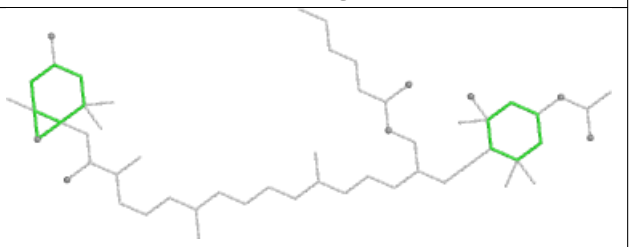
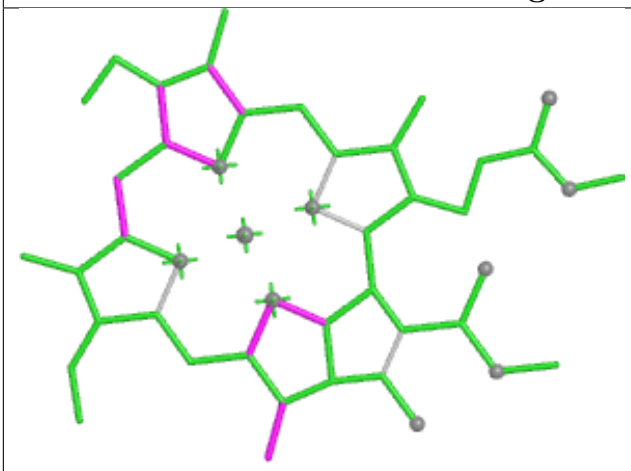


Rings

Ligand CLA 2 319



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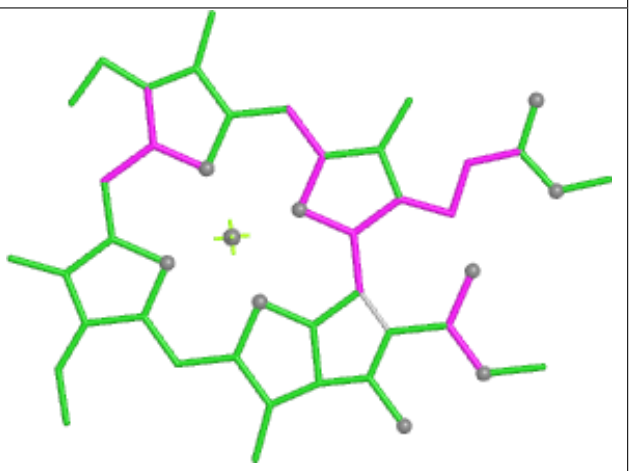
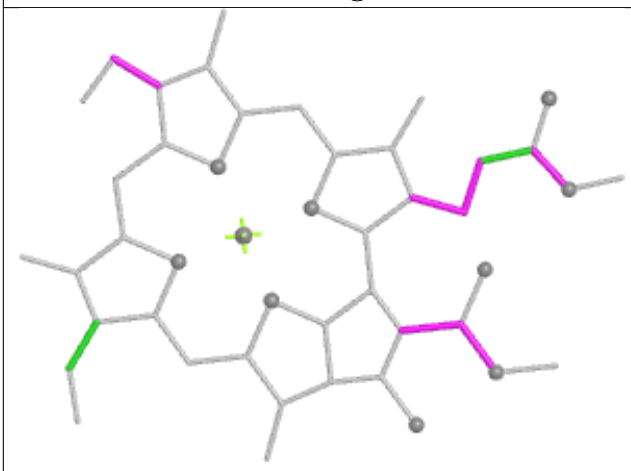
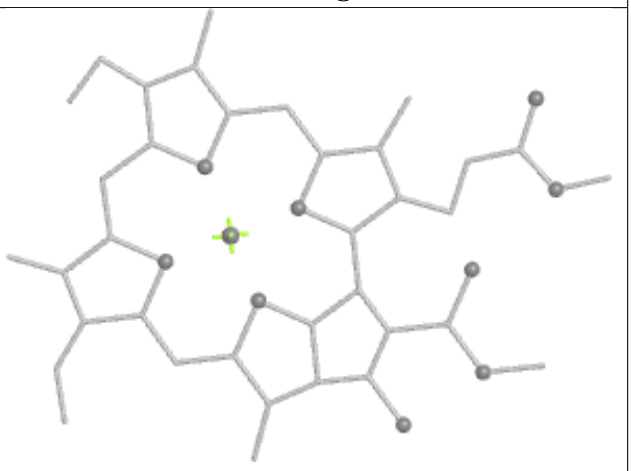


Bond angles

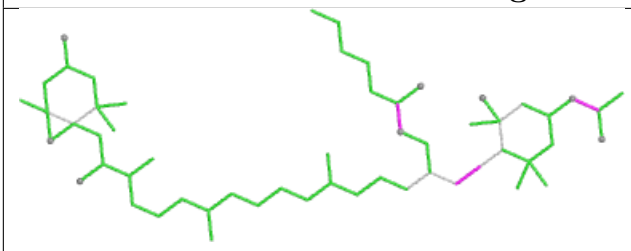


Torsions



Rings

Ligand A1EB1 4 304



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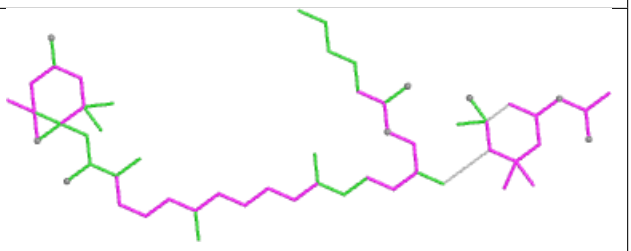
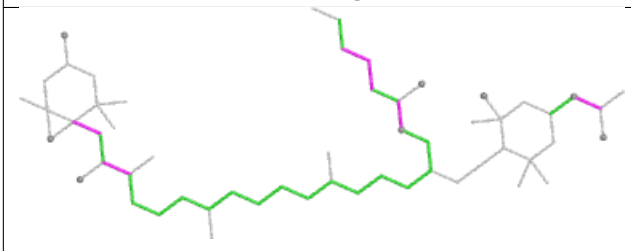


Bond angles



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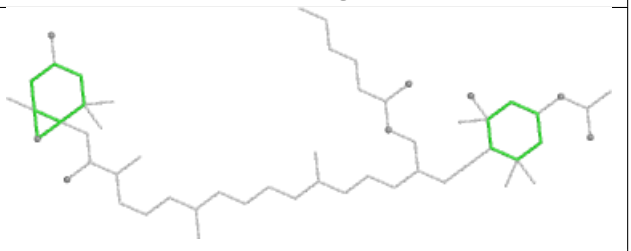
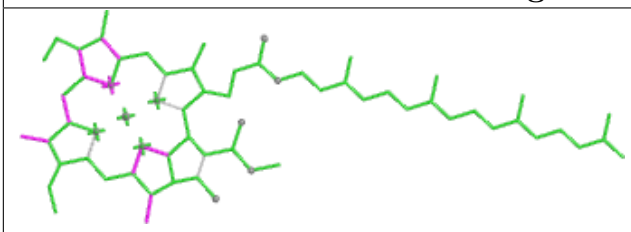
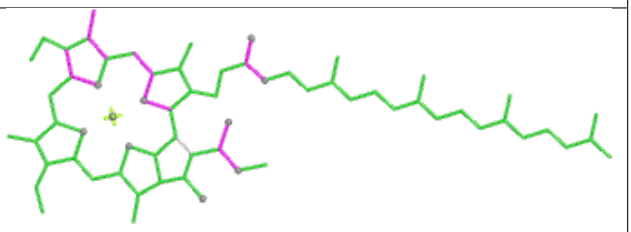


Rings

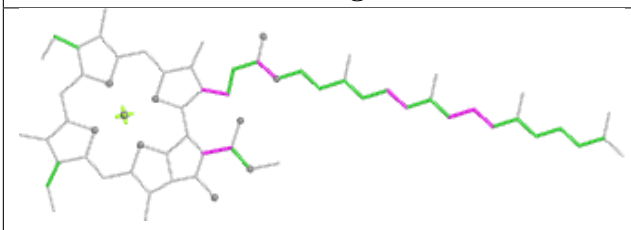
Ligand CLA S 313



Bond lengths



Bond angles



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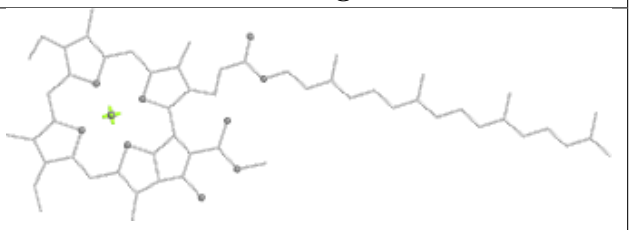
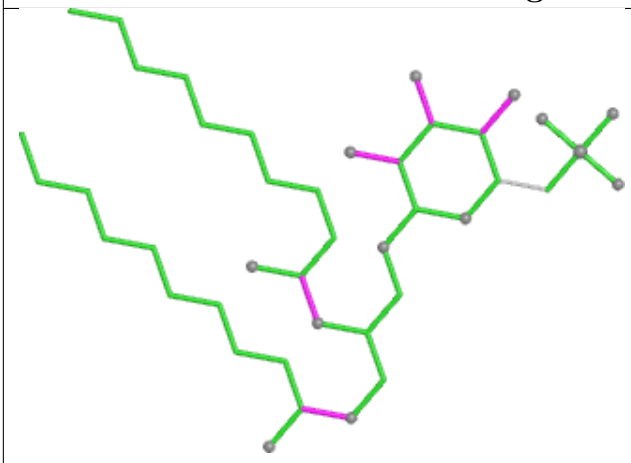
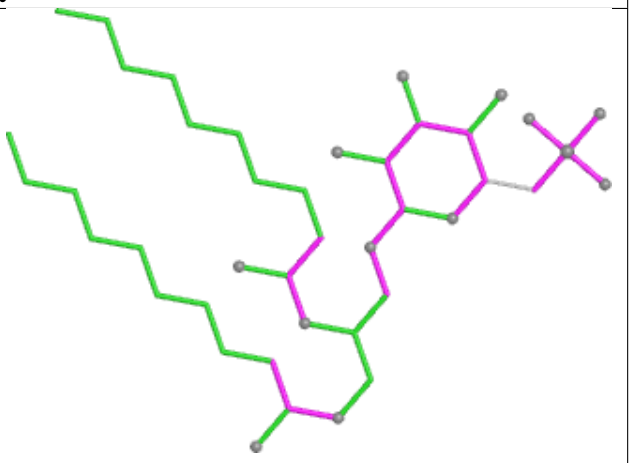


Rings

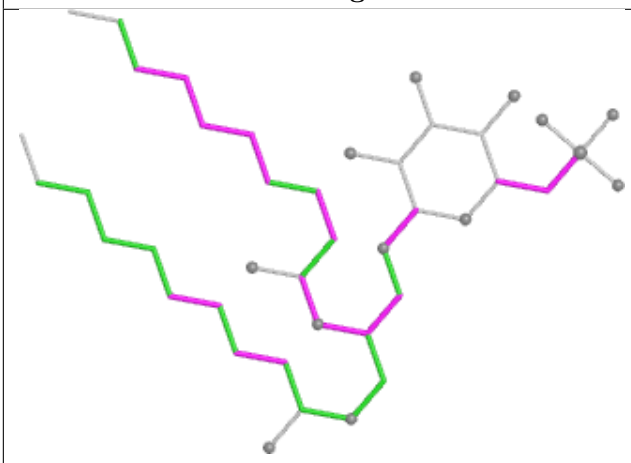
Ligand SQD F 318



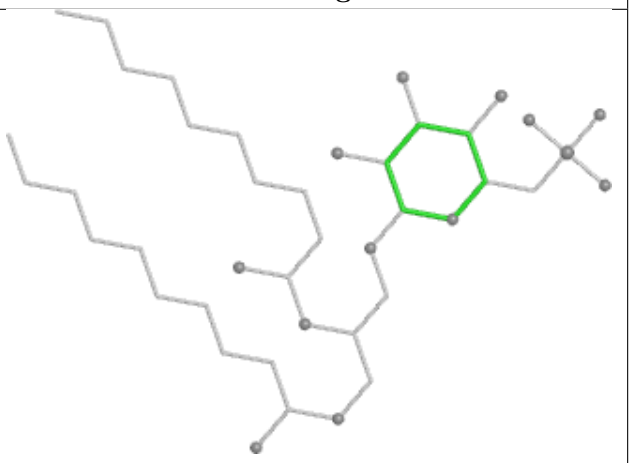
Bond lengths



Bond angles

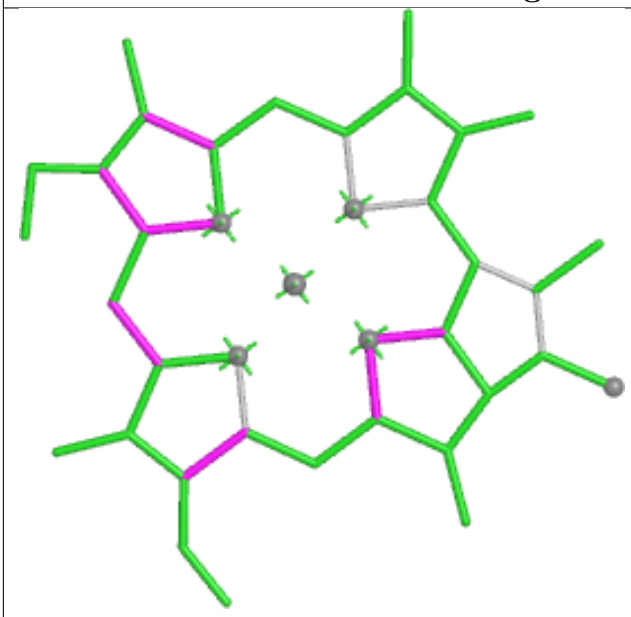


Torsions

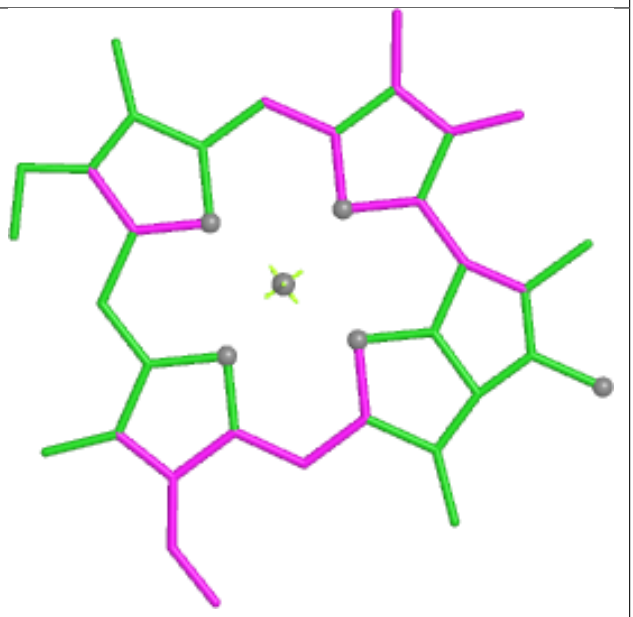


Rings

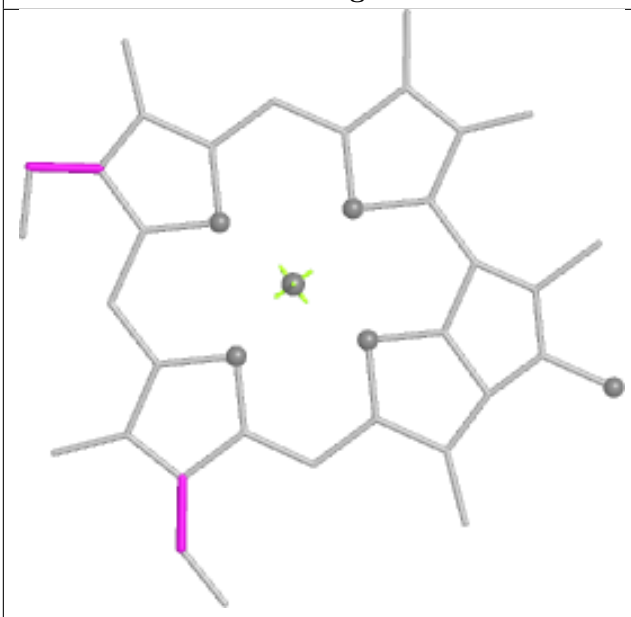
Ligand CLA O 308



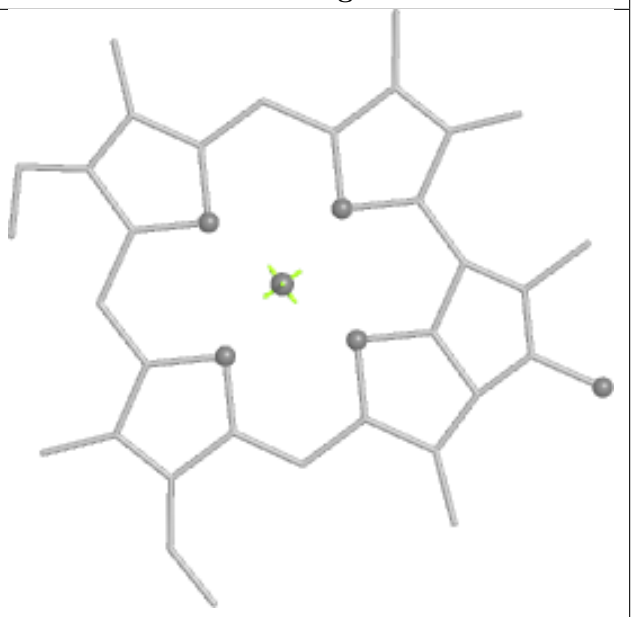
Bond lengths



Bond angles

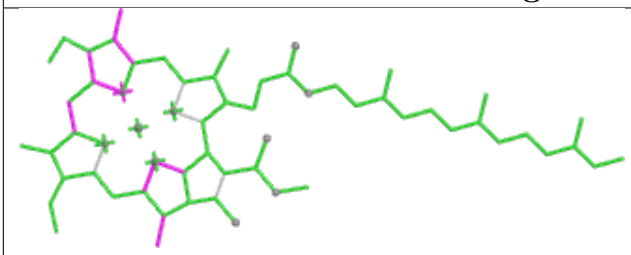


Torsions

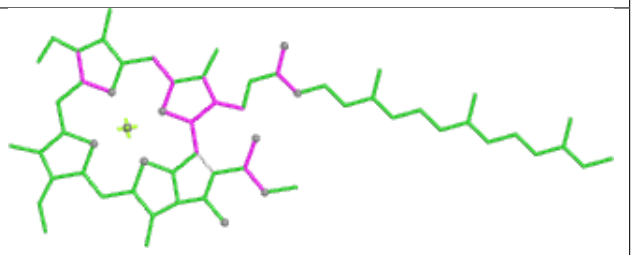


Rings

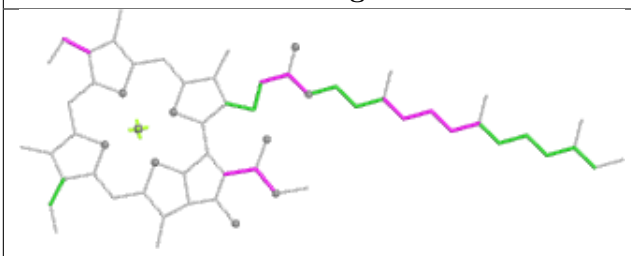
Ligand CLA K 306



Bond lengths



Bond angles



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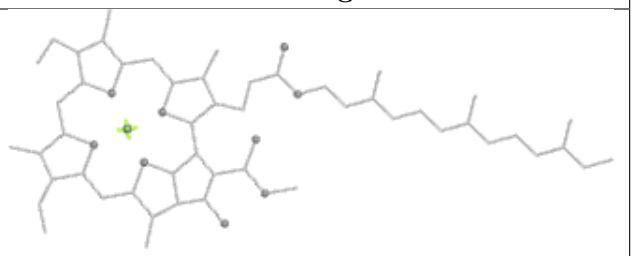
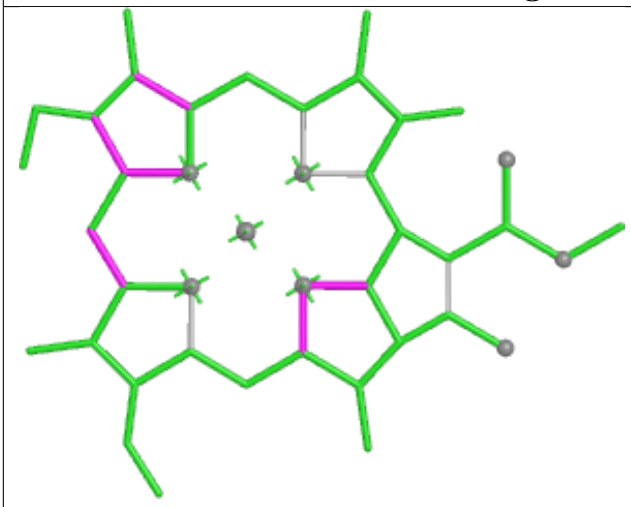


Rings

Ligand CLA Y 305



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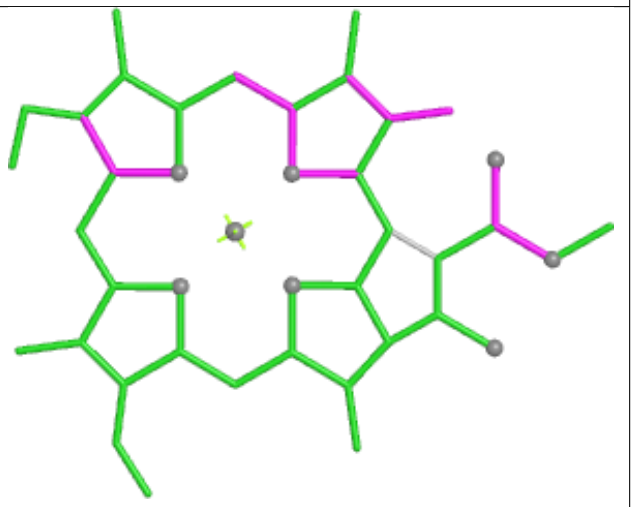
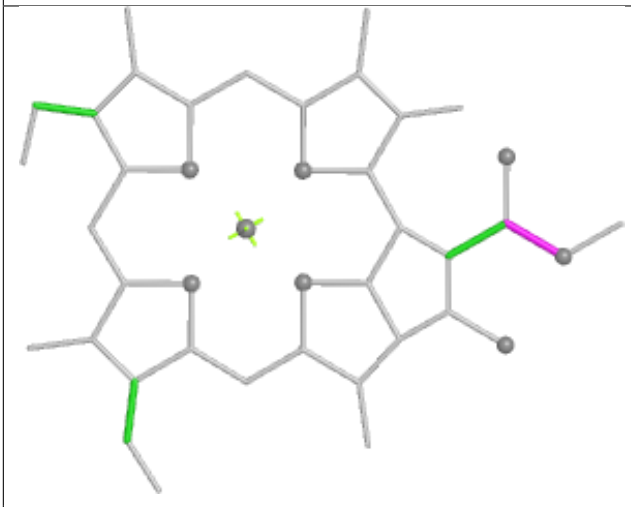


Bond angles



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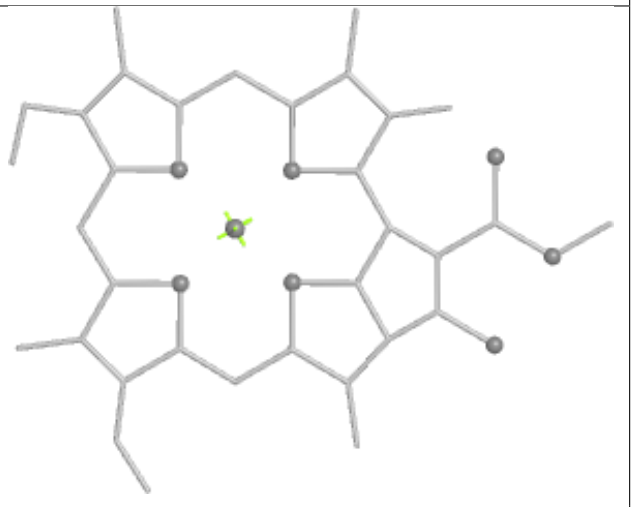
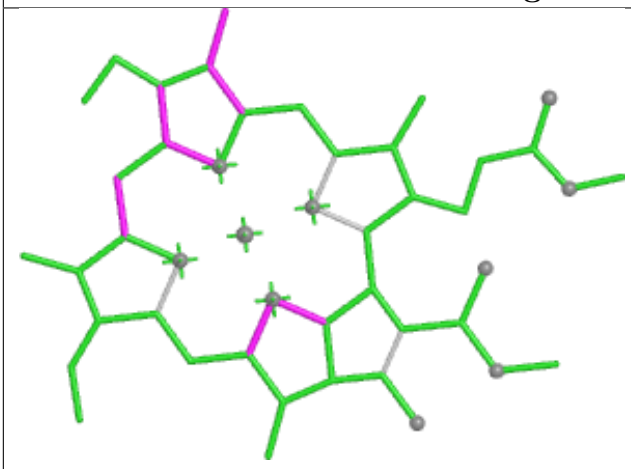


Rings

Ligand CLA Q 317



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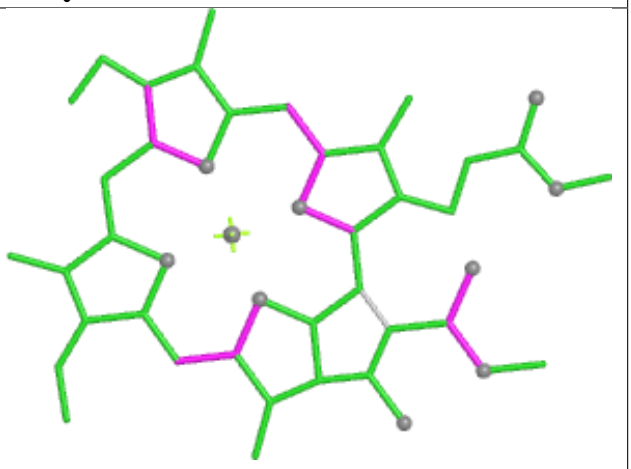
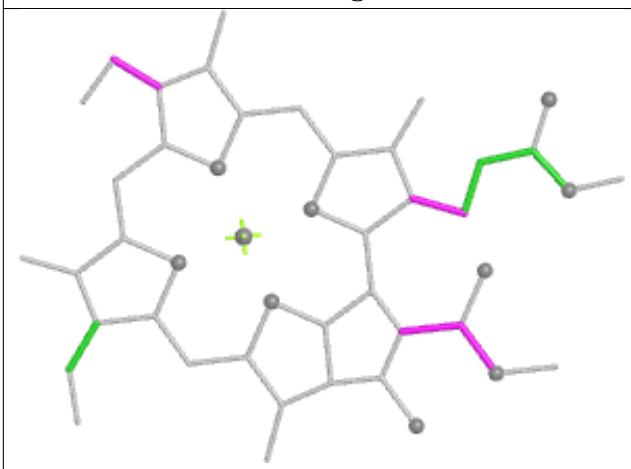


Bond angles



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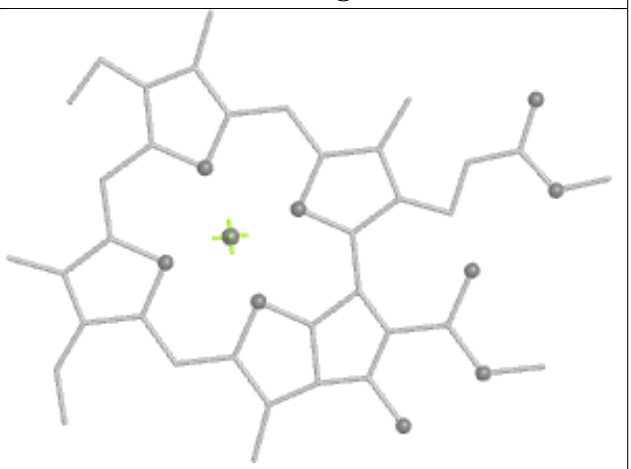
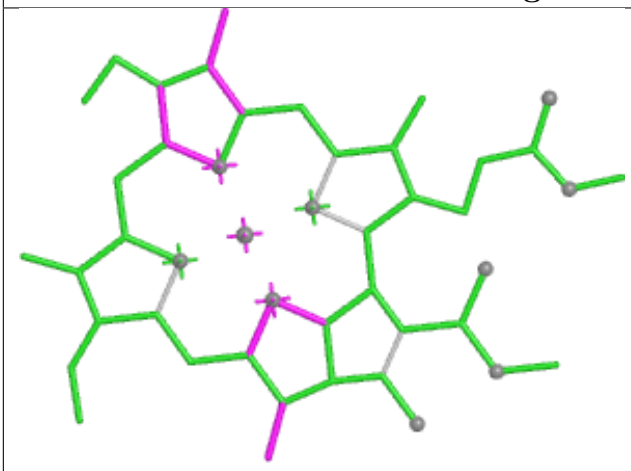


Rings

Ligand CLA U 201



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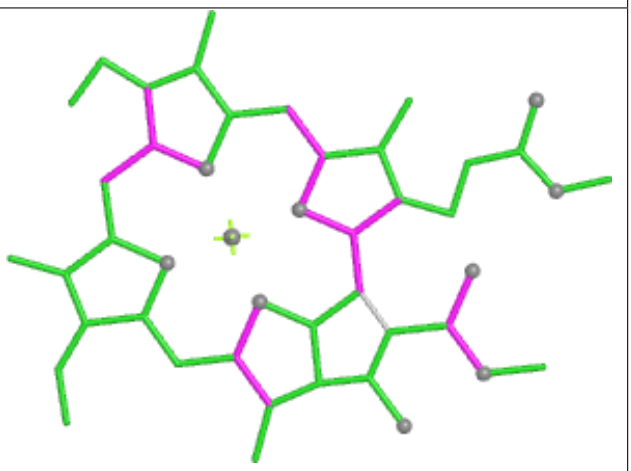
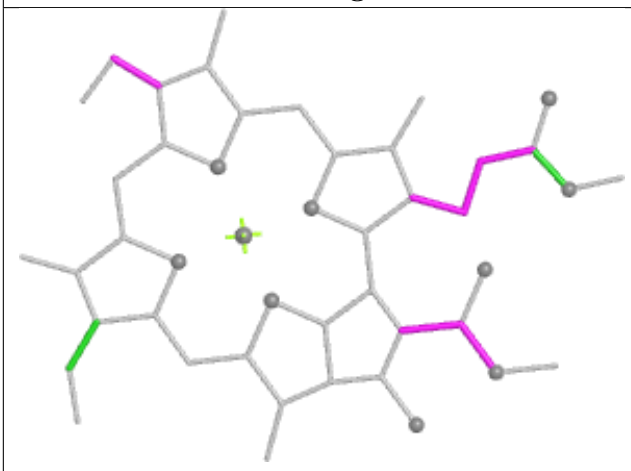


Bond angles



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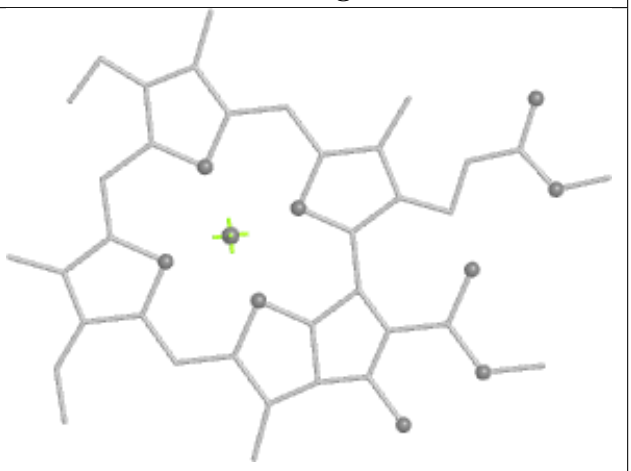
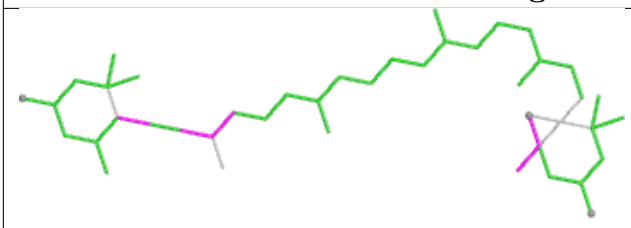


Rings

Ligand DD6 J 304



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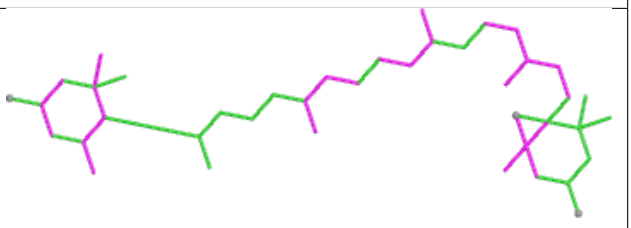
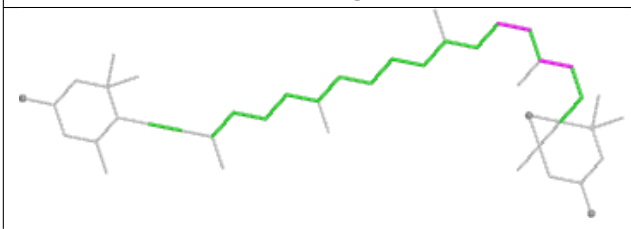


Bond angles



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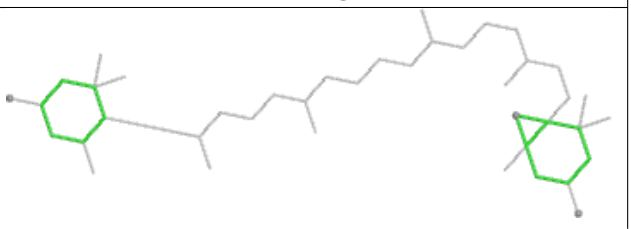
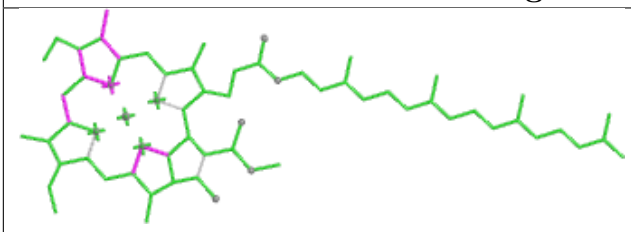


Rings

Ligand CLA E 313



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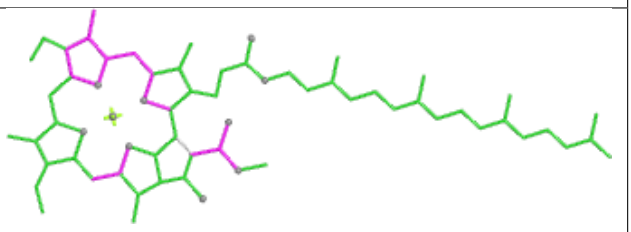
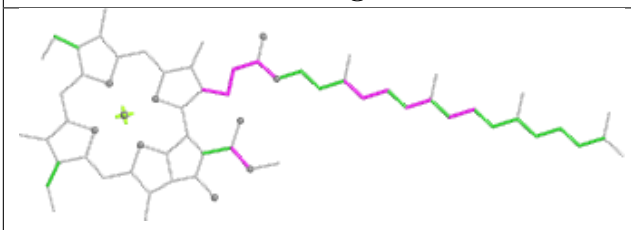


Bond angles



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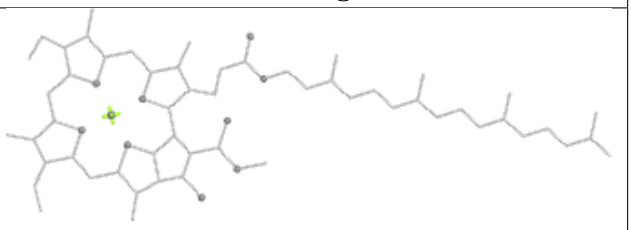
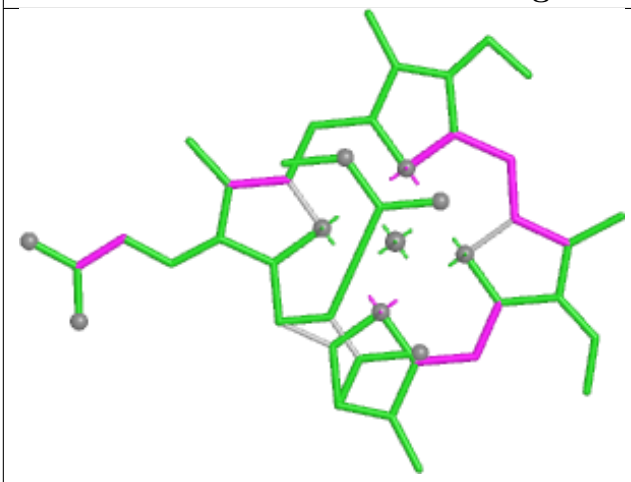


Rings

Ligand KC2 I 303



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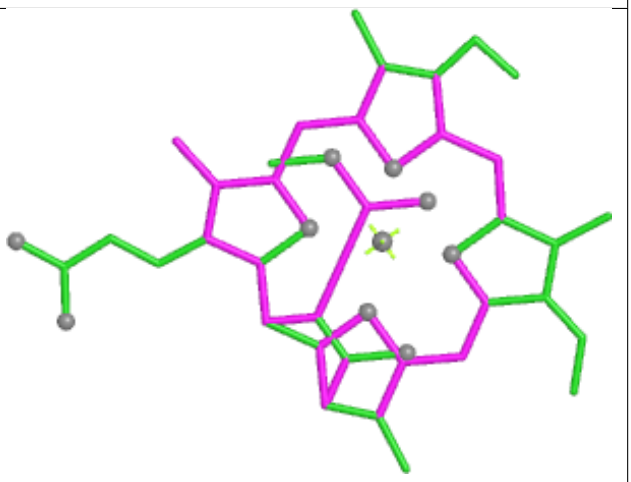
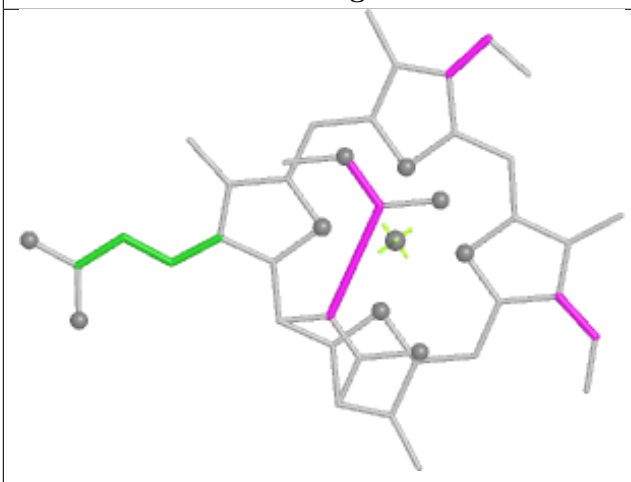


Bond angles



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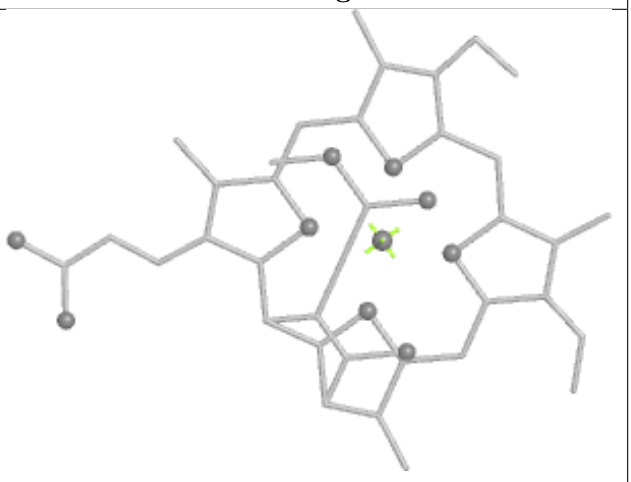
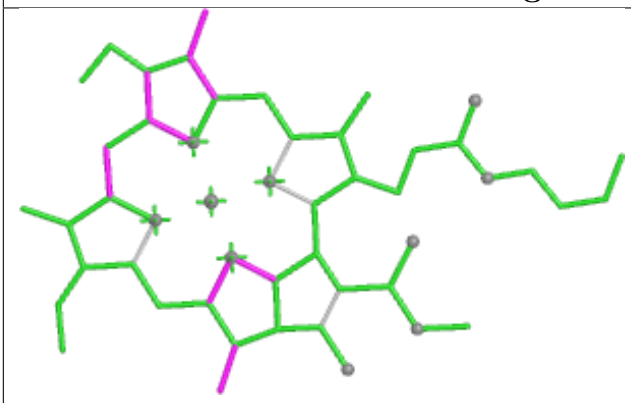


Rings

Ligand CLA A 305



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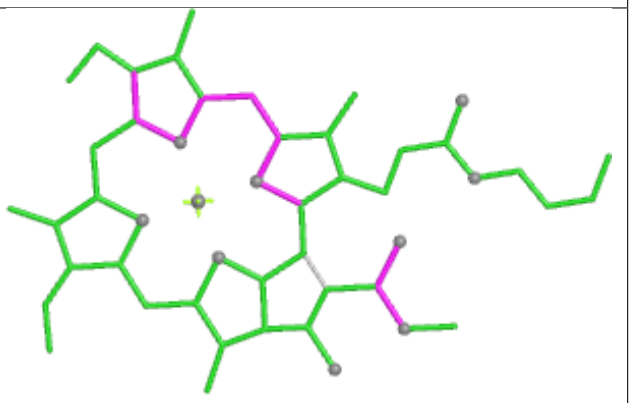
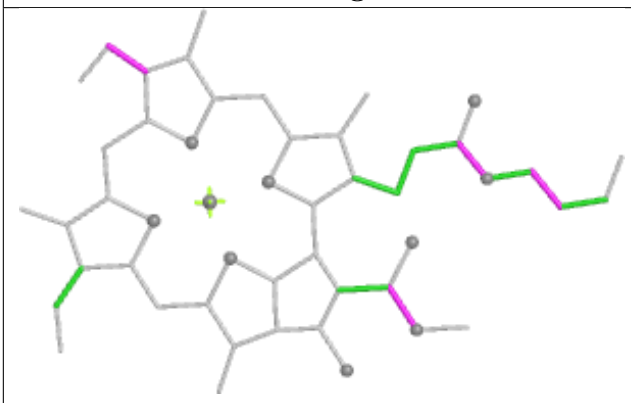


Bond angles



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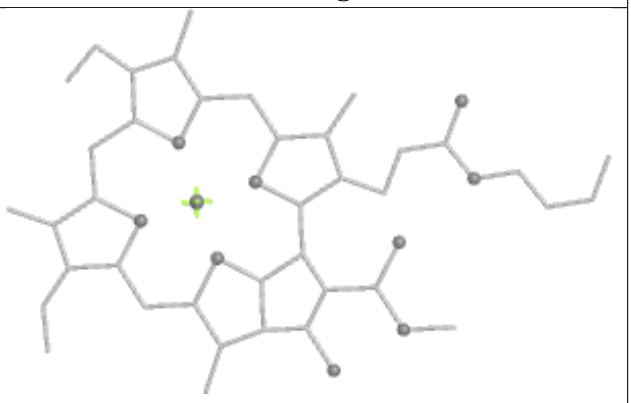
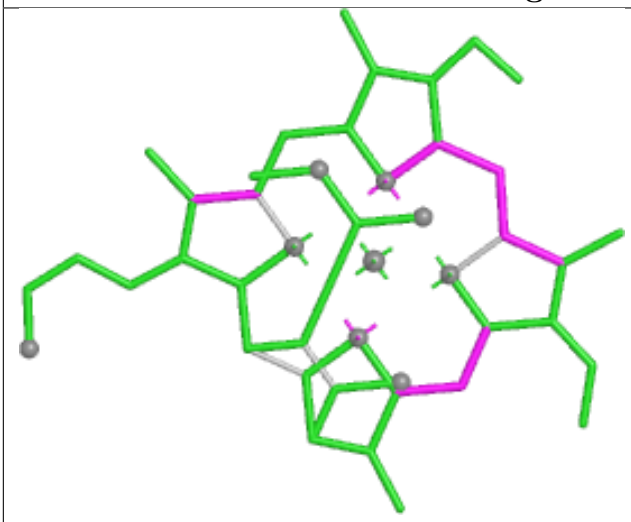


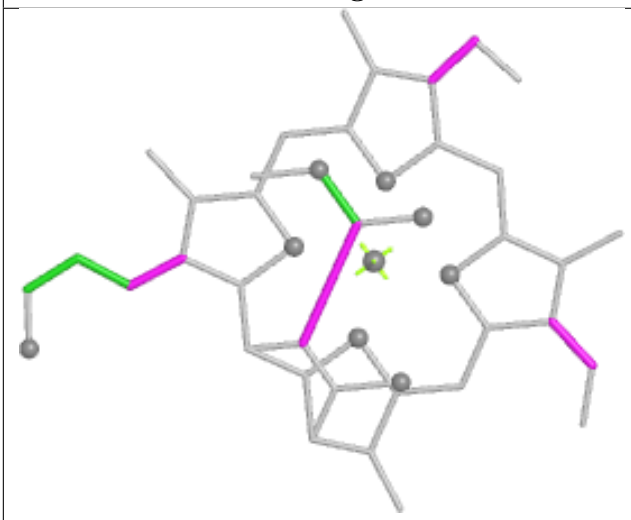
Rings

Ligand KC2 R 314



Bond lengths

Bond angles



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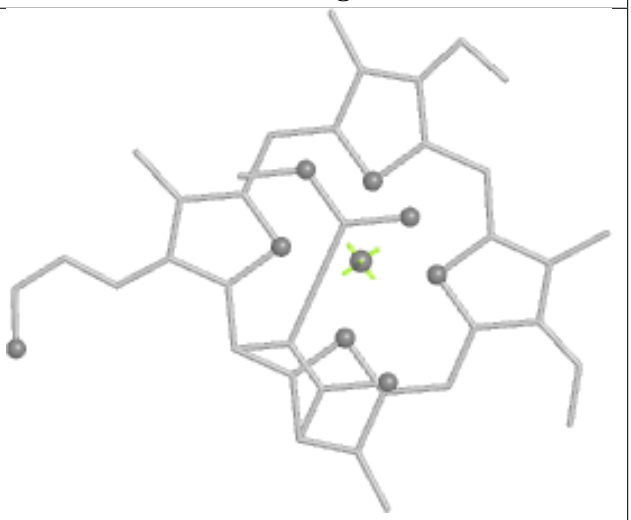
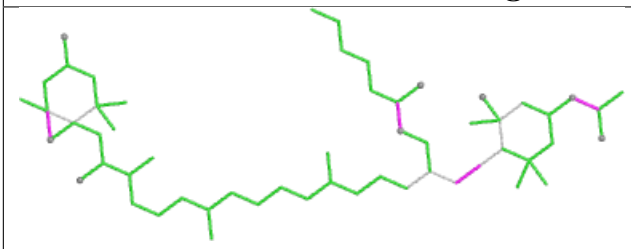


Rings

Ligand A1EB1 U 205



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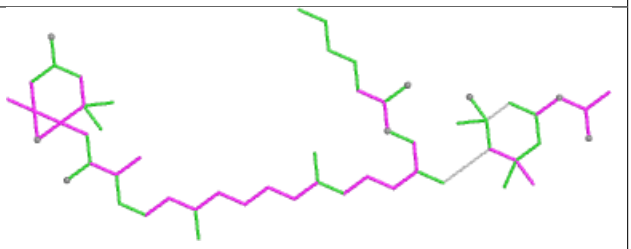
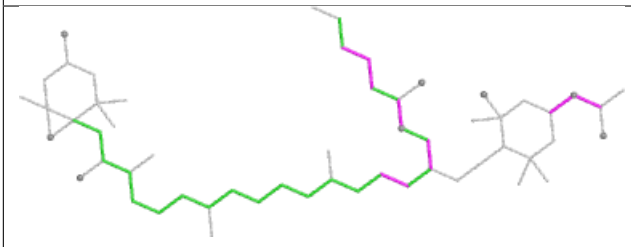


Bond angles



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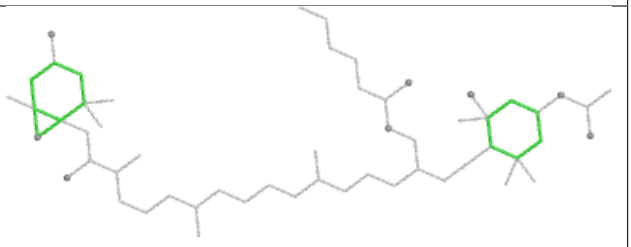
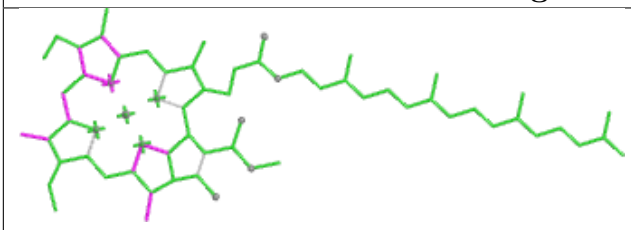


Rings

Ligand CLA I 314



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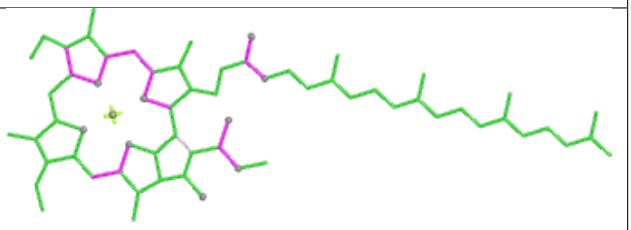
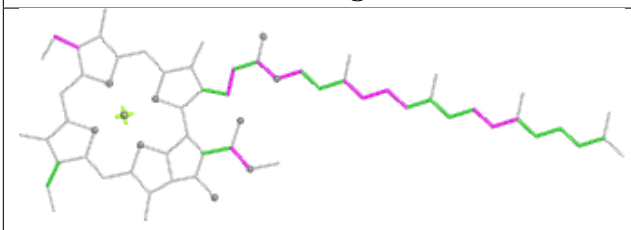
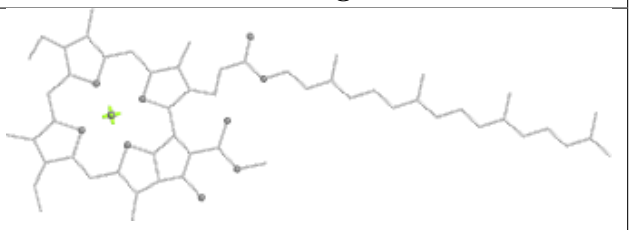


Bond angles

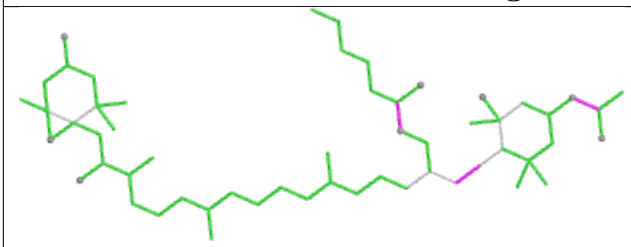


Torsions



Rings

Ligand A1EB1 Q 323



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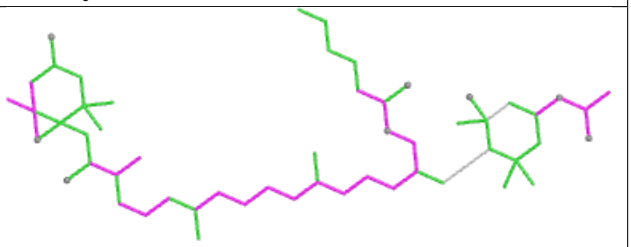
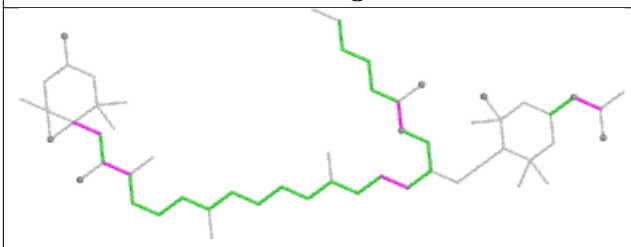


Bond angles



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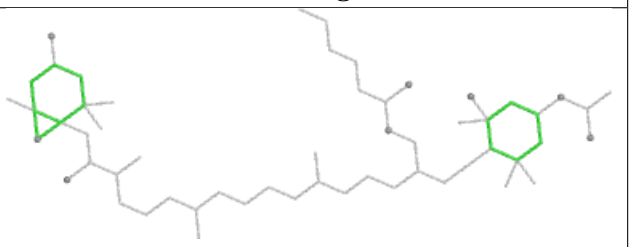
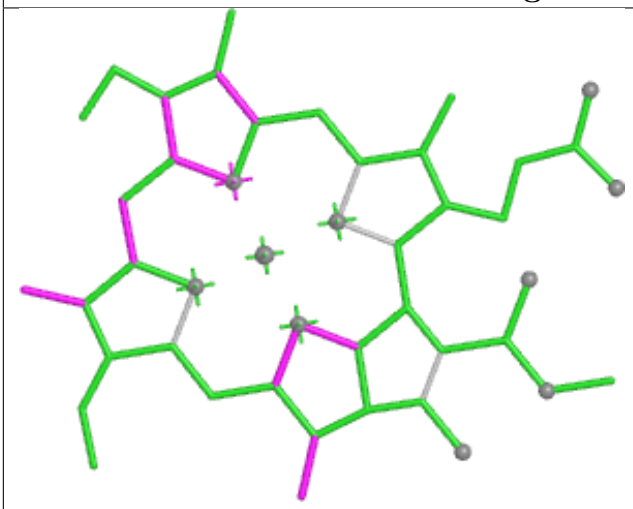


Rings

Ligand CLA O 309



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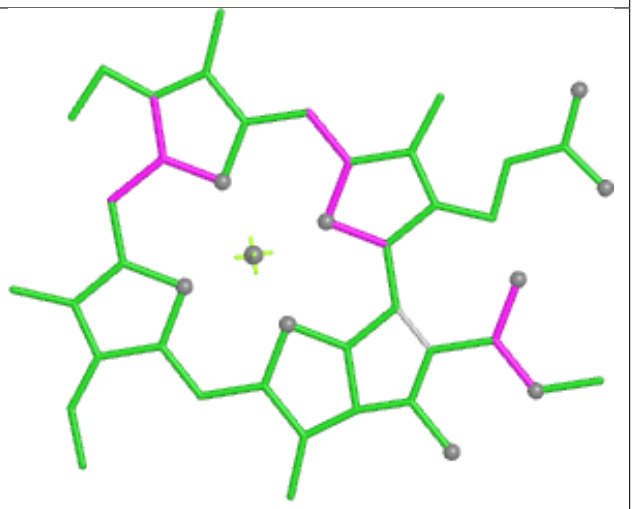
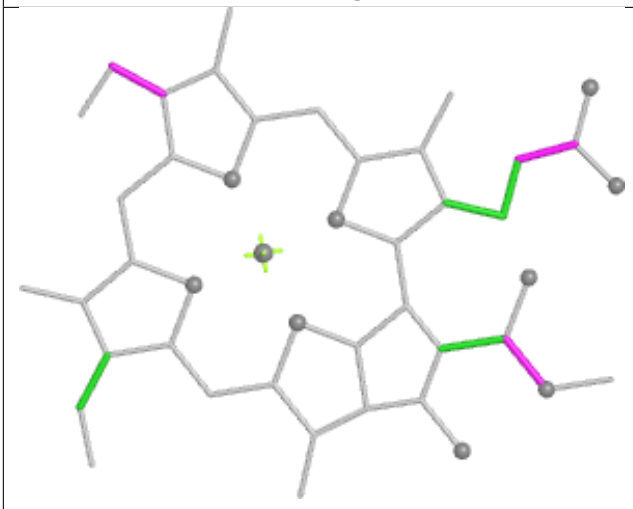


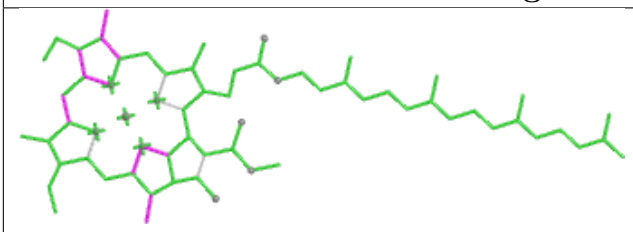
Bond angles



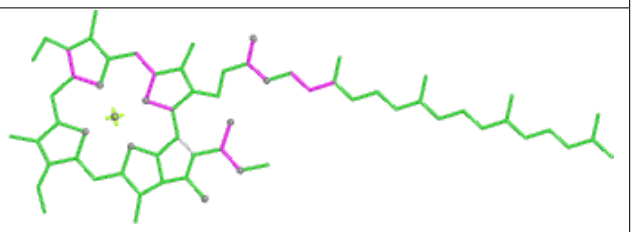
Torsions

Rings

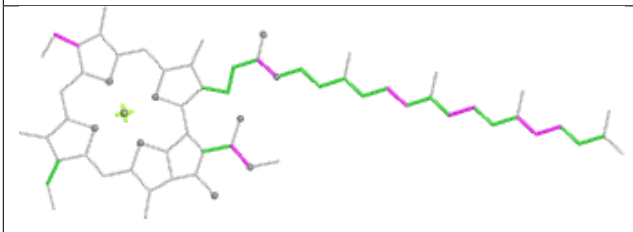
Ligand CLA D 314



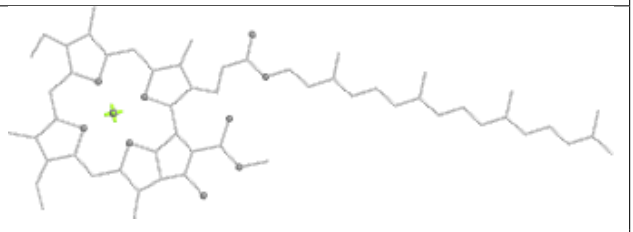
Bond lengths



Bond angles

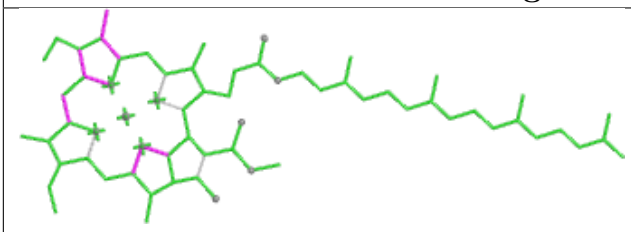


Torsions



Rings

Ligand CLA D 315



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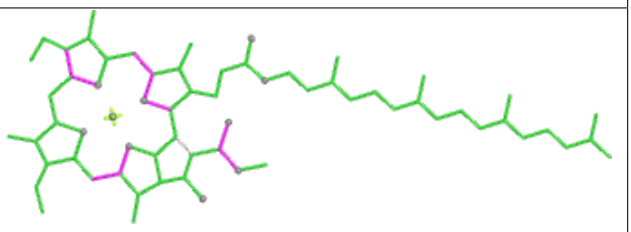

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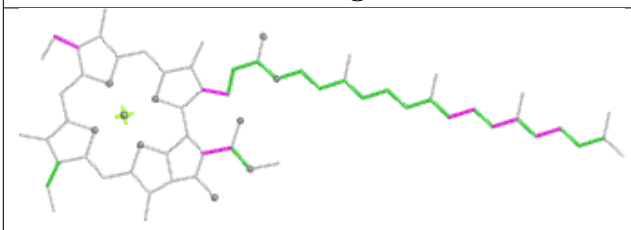

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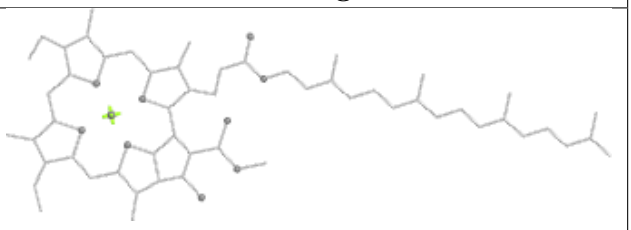
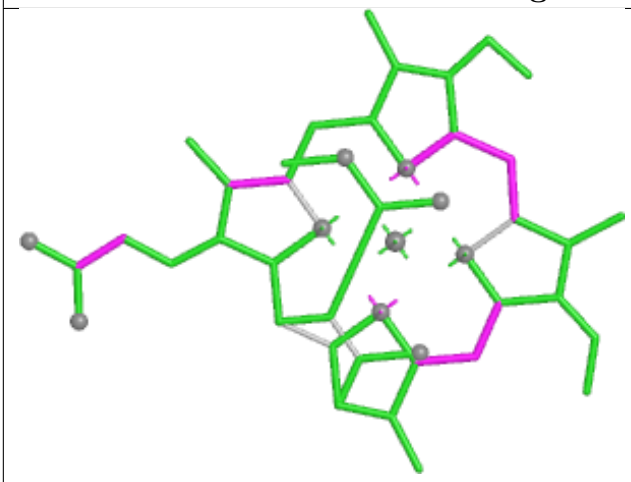


Rings

Ligand KC2 x 313



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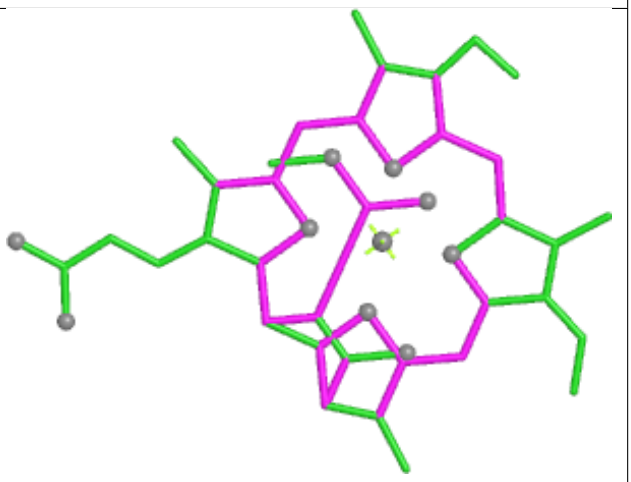

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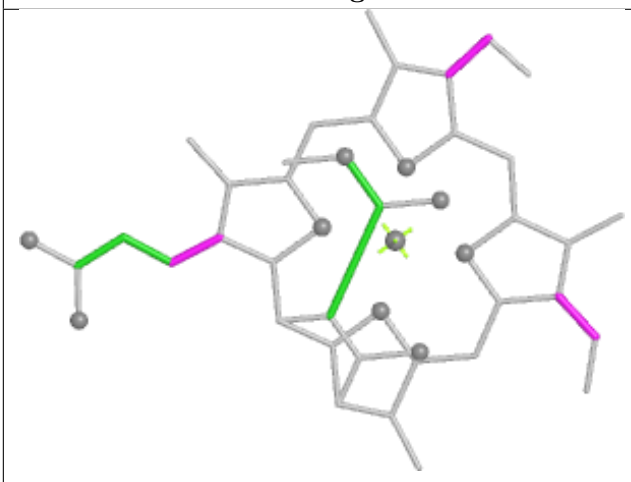
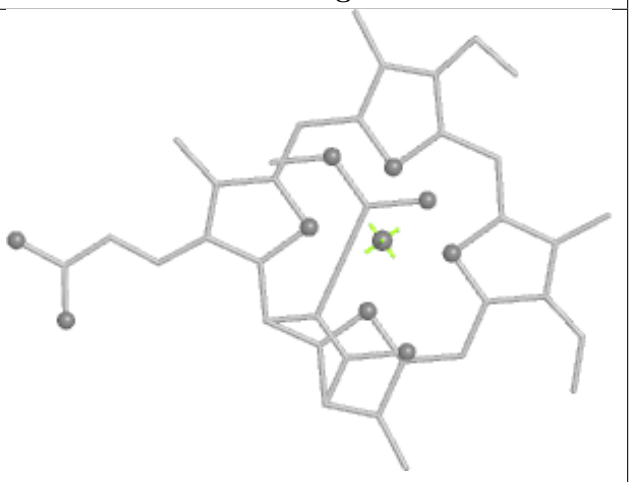
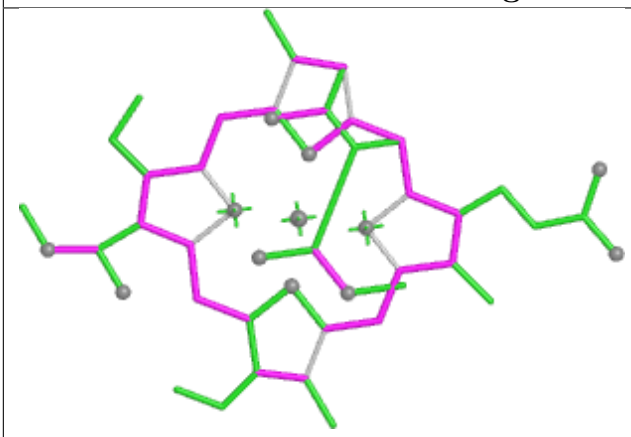


Torsions



Rings

Ligand A1ECV Z 308



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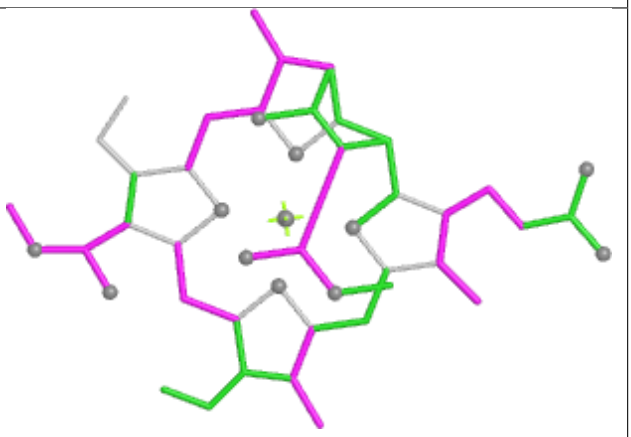
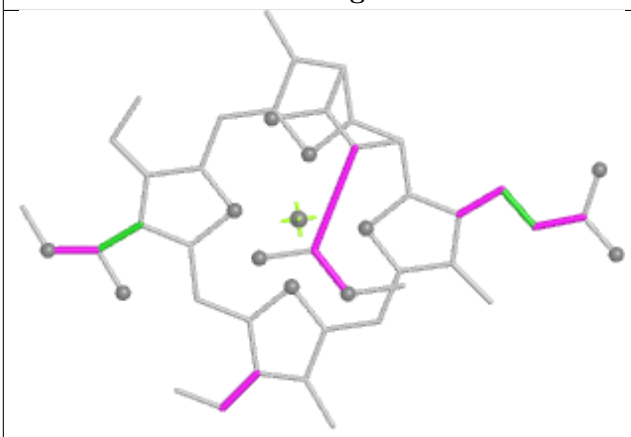


Bond angles



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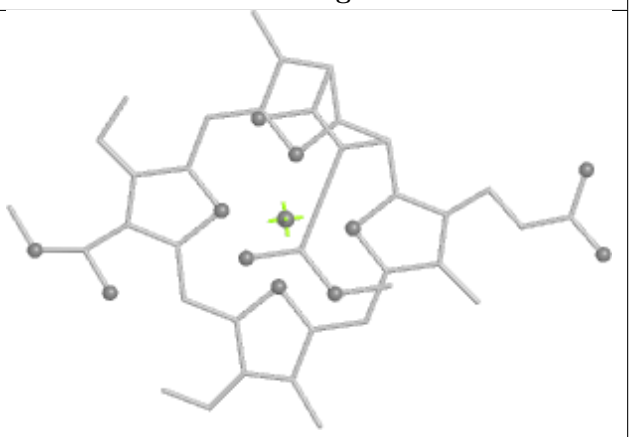
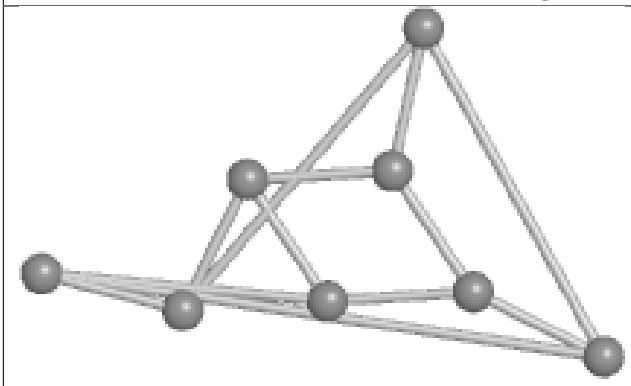


Rings

Ligand SF4 c 102



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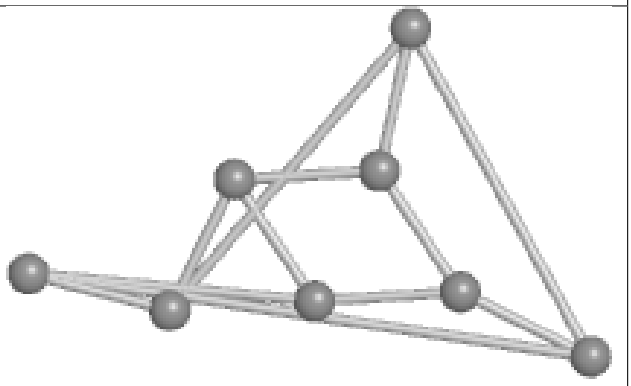
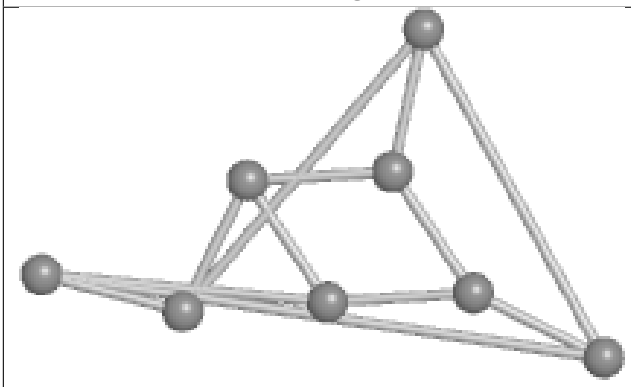


Bond angles



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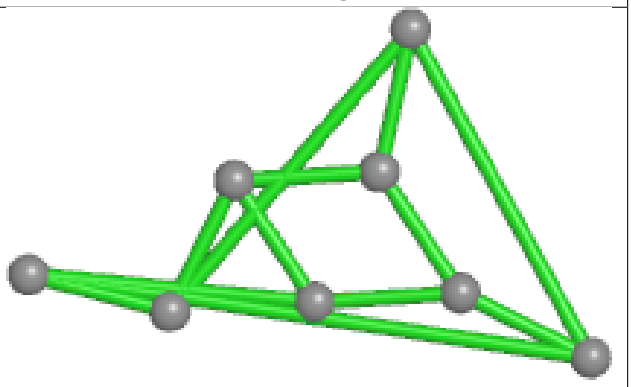
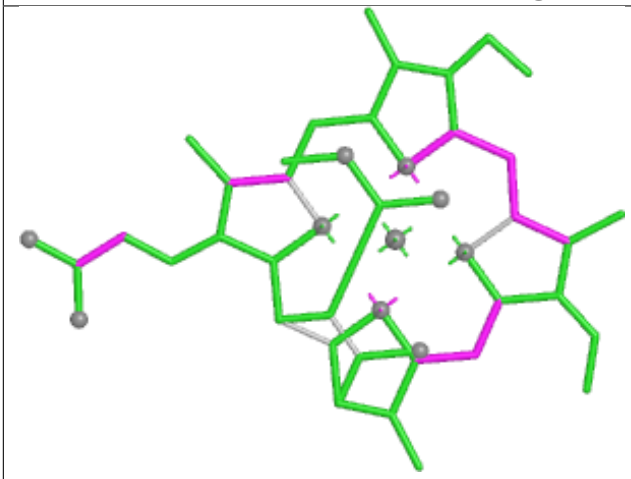


Rings

Ligand KC2 5 311



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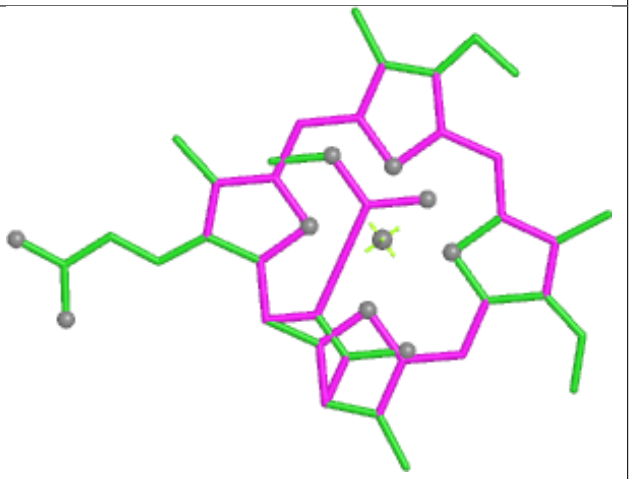
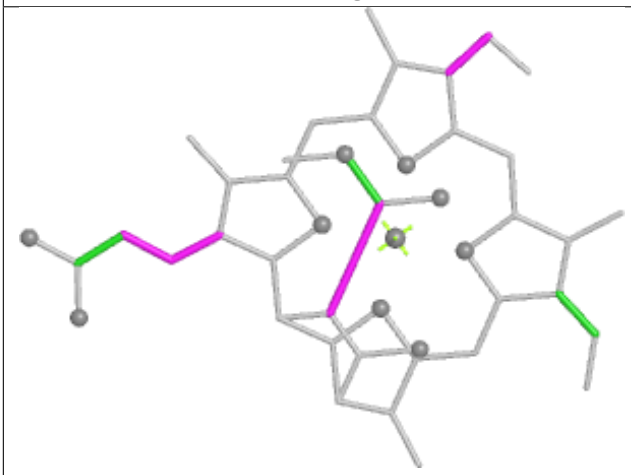


Bond angles



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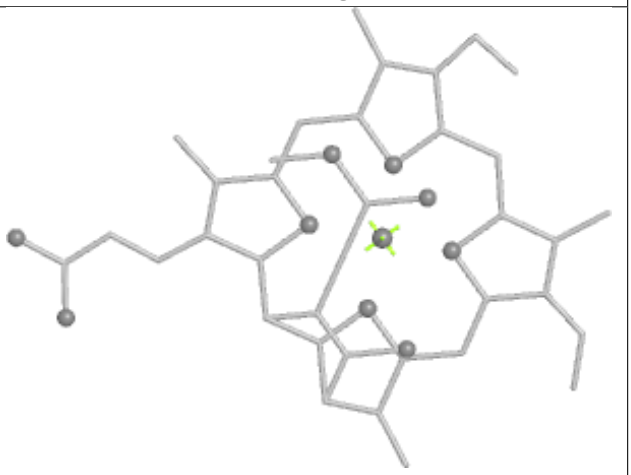
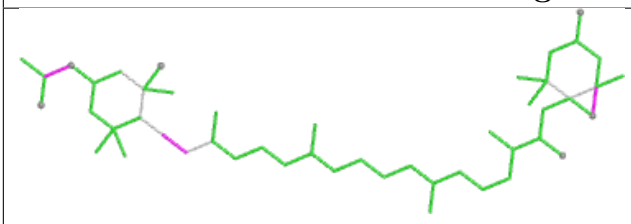


Rings

Ligand A86 6 302



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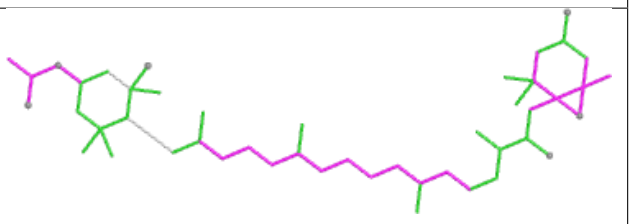
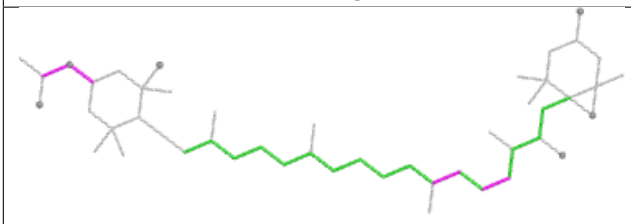


Bond angles



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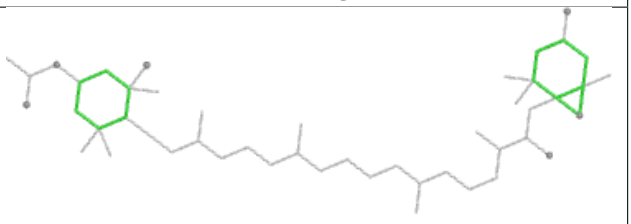
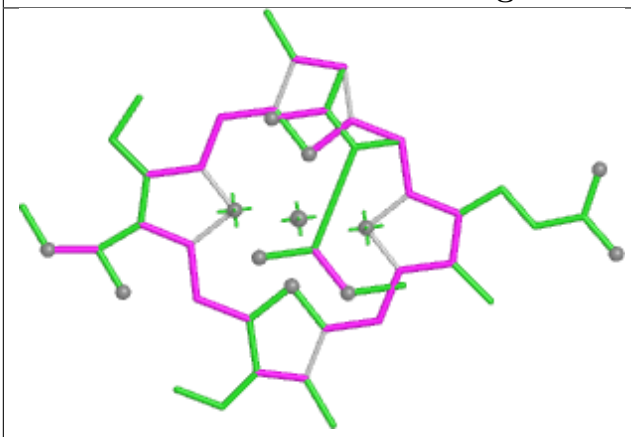


Rings

Ligand A1ECV M 316



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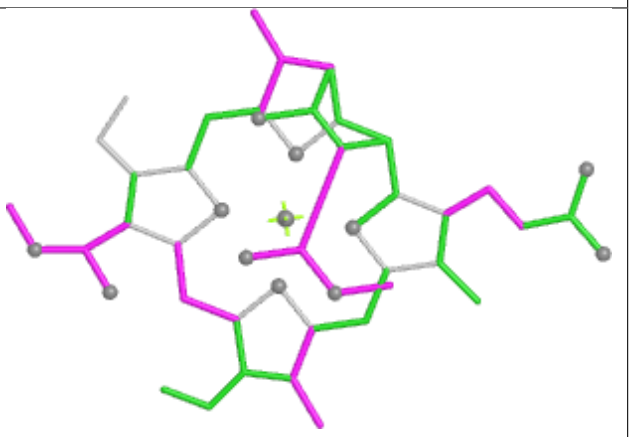
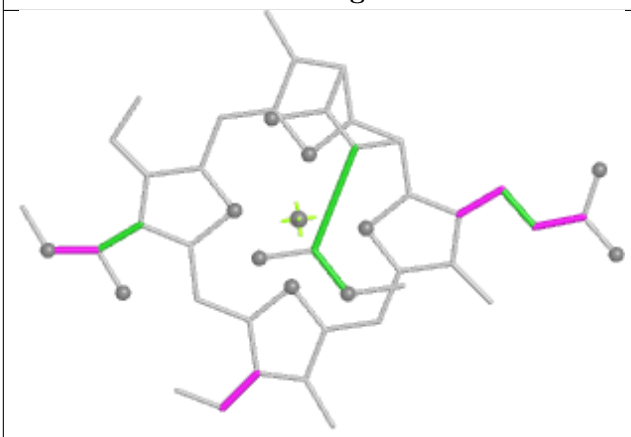


Bond angles



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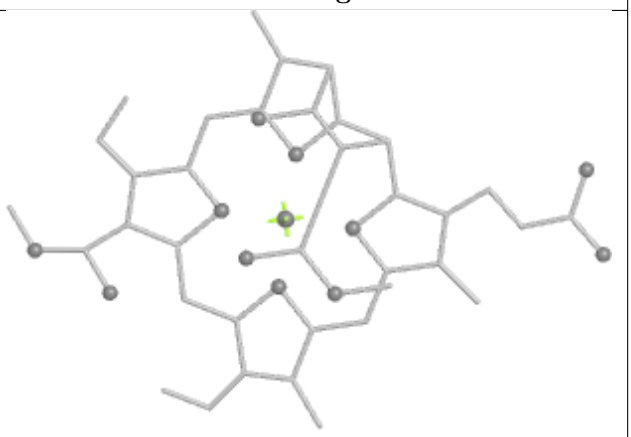
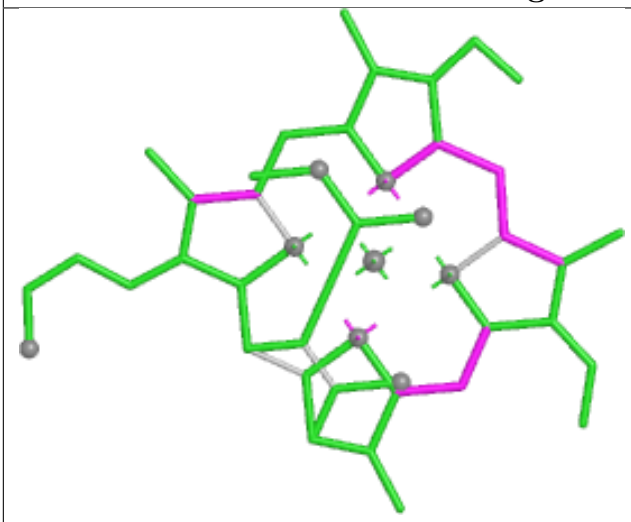


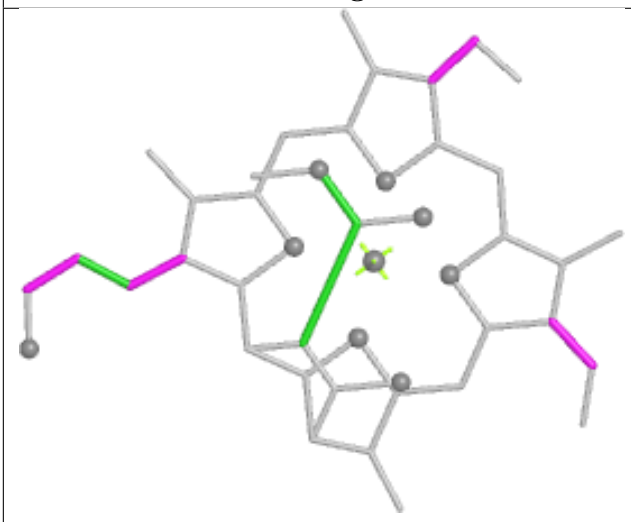
Rings

Ligand KC2 F 311



Bond lengths

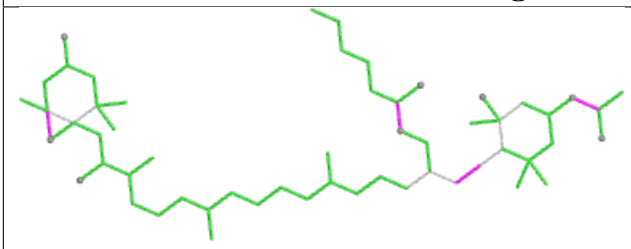
Bond angles



Torsions

Rings

Ligand A1EB1 3 302



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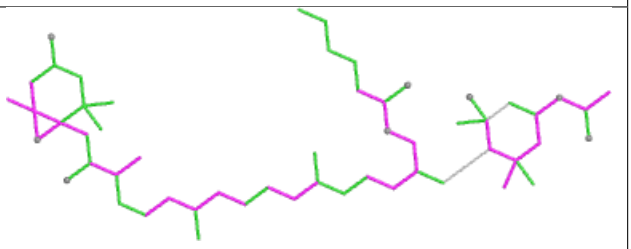
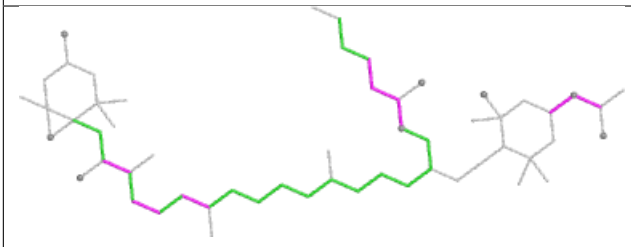
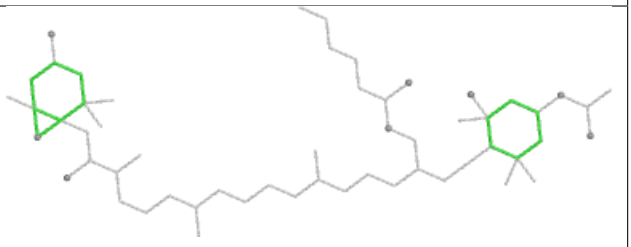


Bond angles

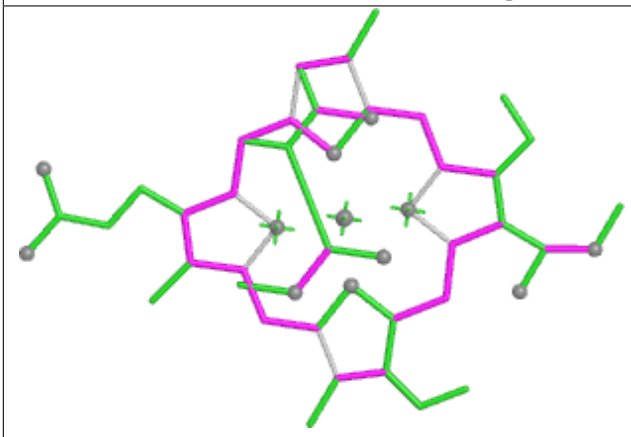


Torsions



Rings

Ligand A1ECV R 310



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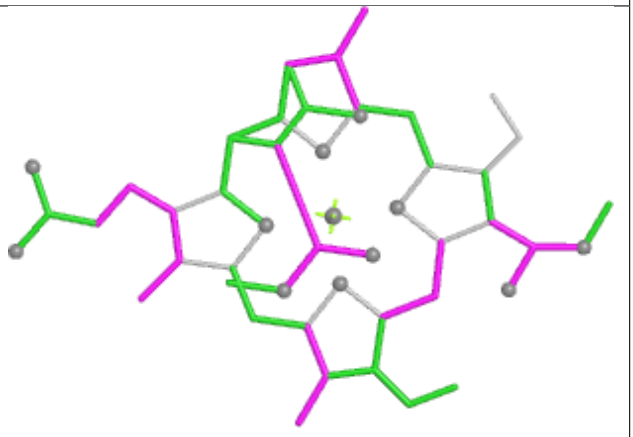
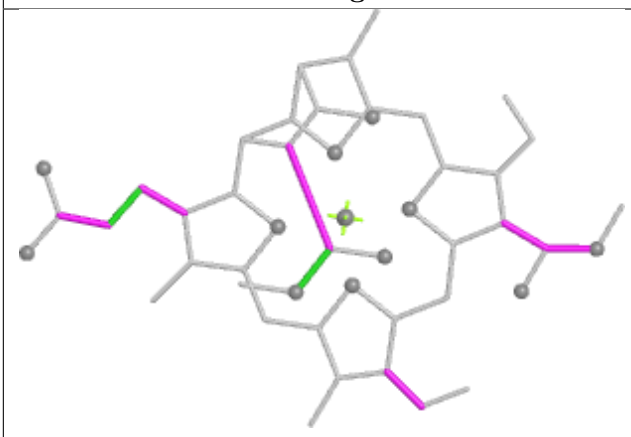
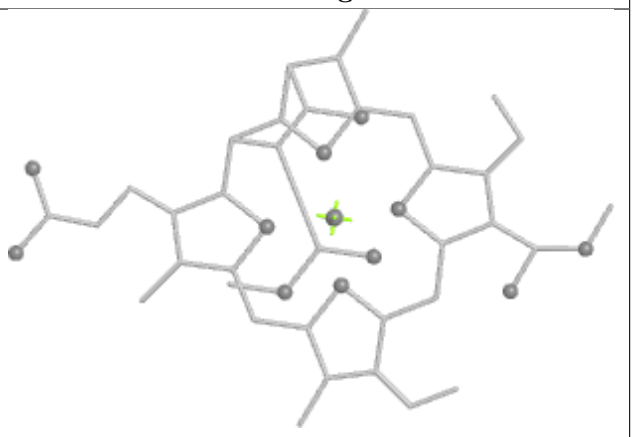


Bond angles

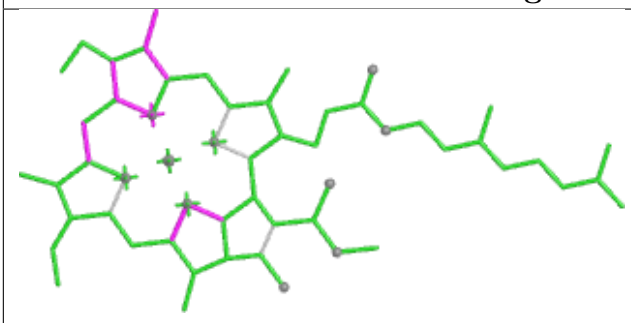


Torsions



Rings

Ligand CLA B 207



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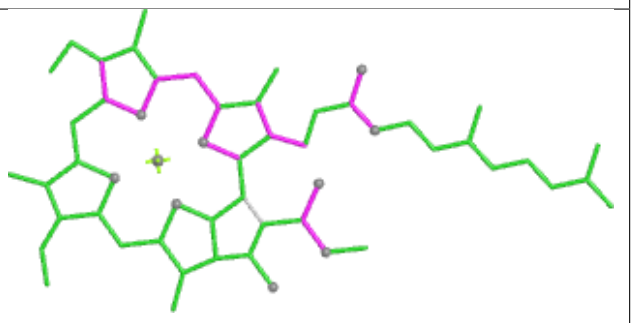
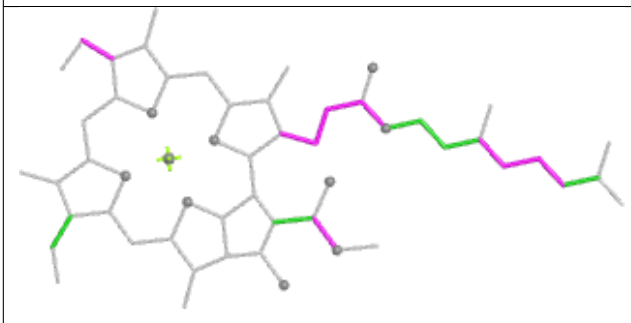


Bond angles



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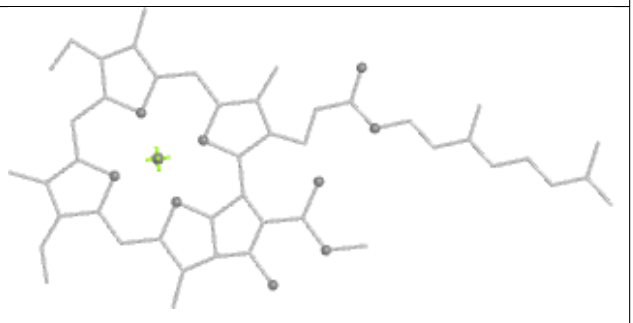
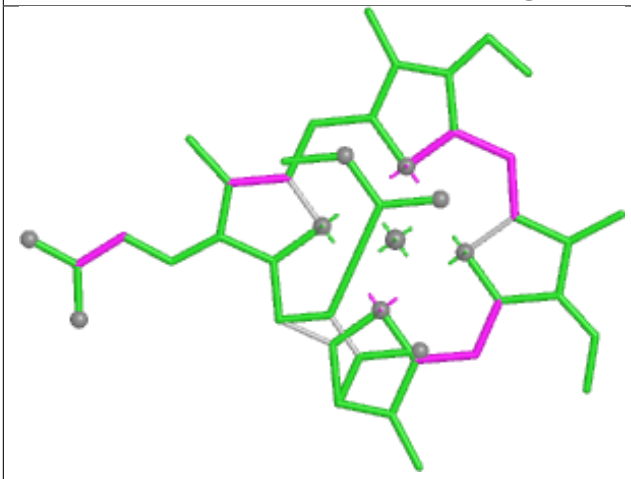


Rings

Ligand KC2 W 314



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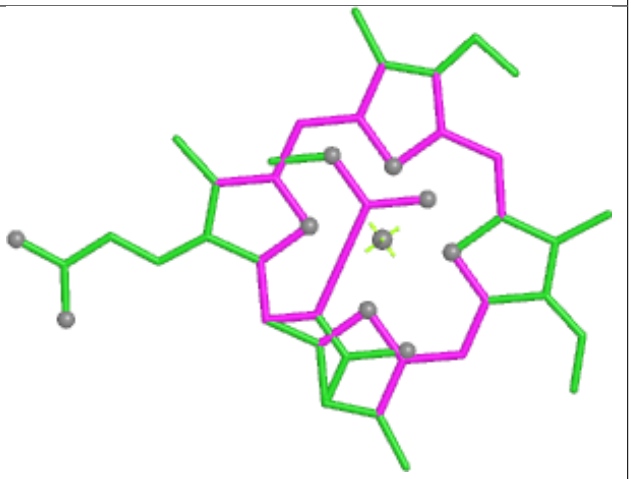
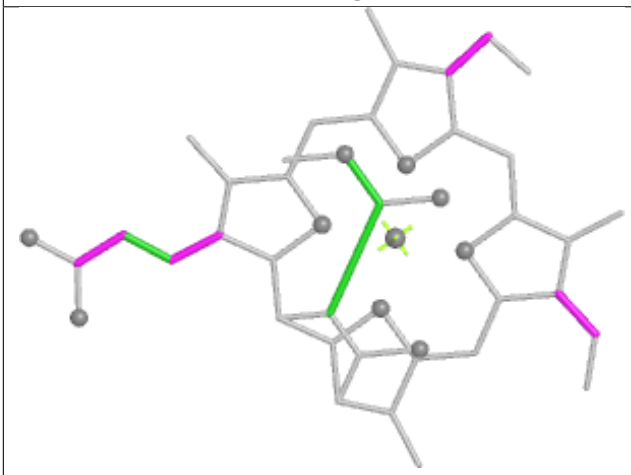


Bond angles



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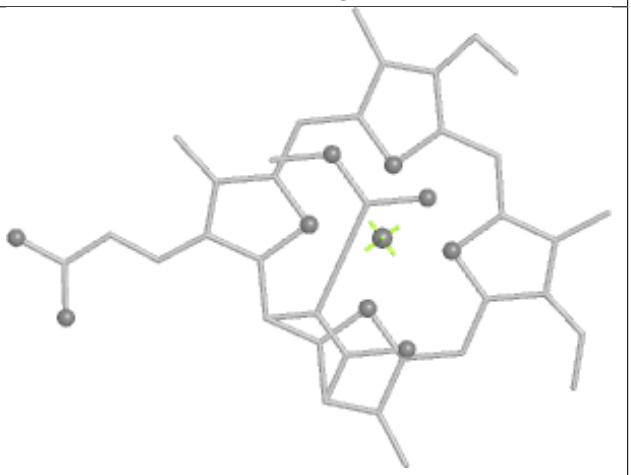
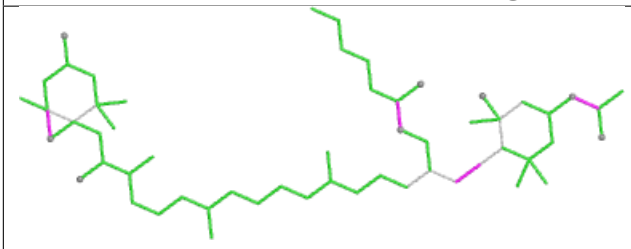


Rings

Ligand A1EB1 K 302



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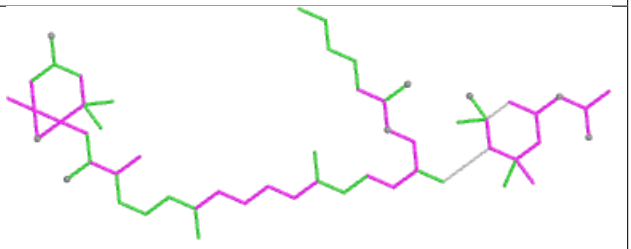
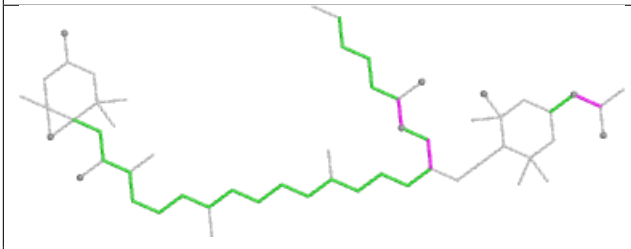


Bond angles



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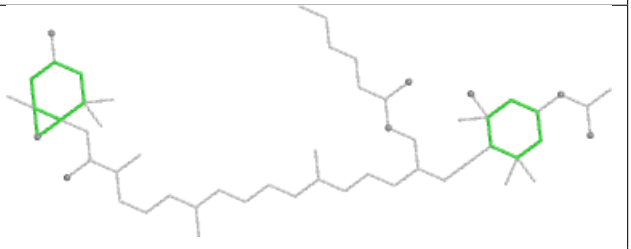
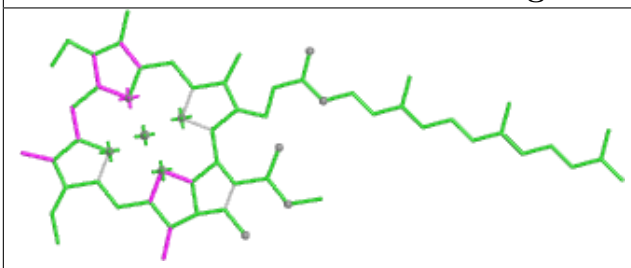
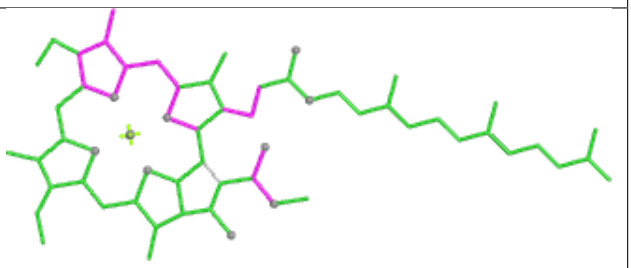
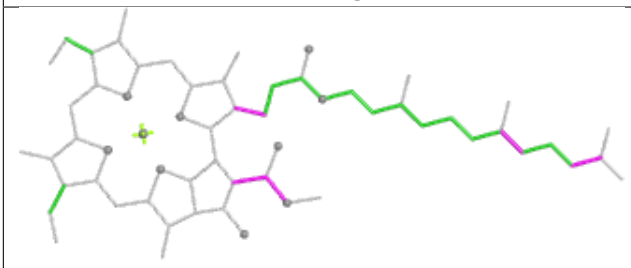
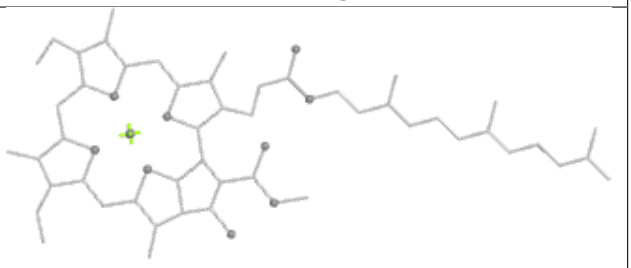
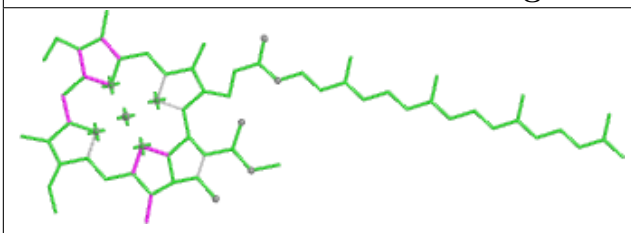
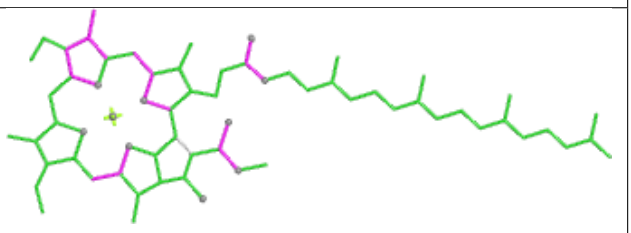
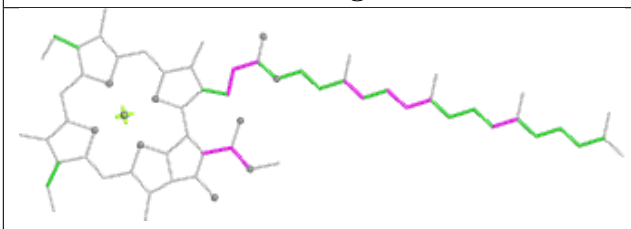
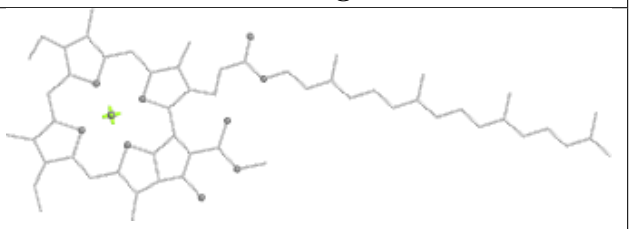
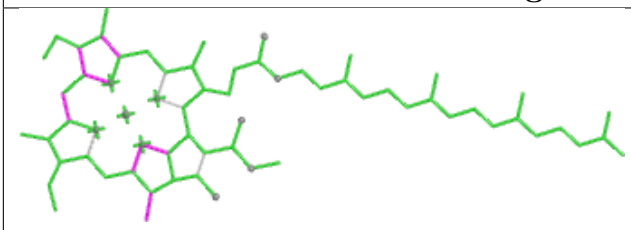


Rings

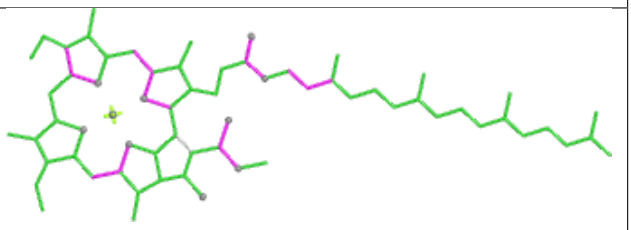
Ligand CLA b 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

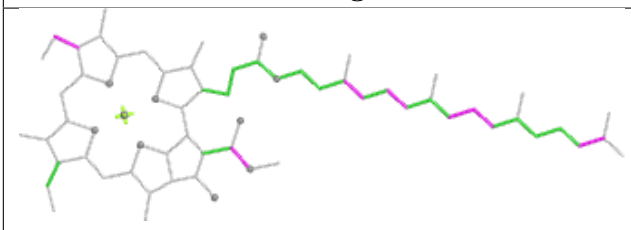
Ligand CLA E 310



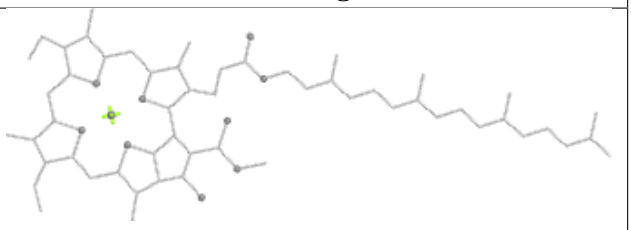
Bond lengths



Bond angles

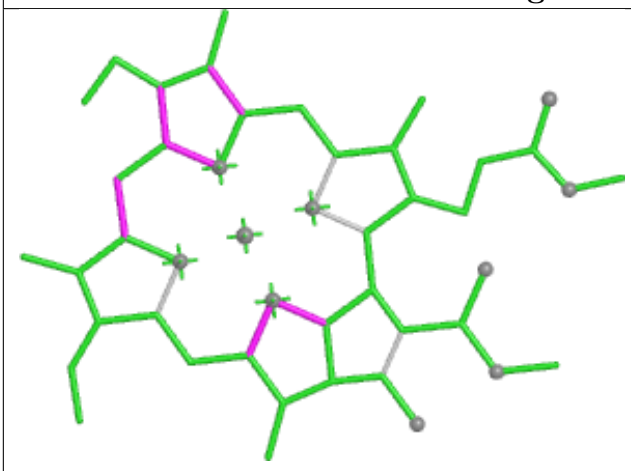


Torsions



Rings

Ligand CLA b 823



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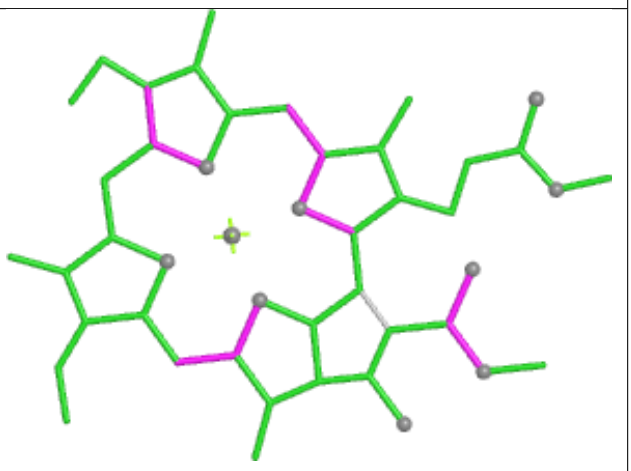
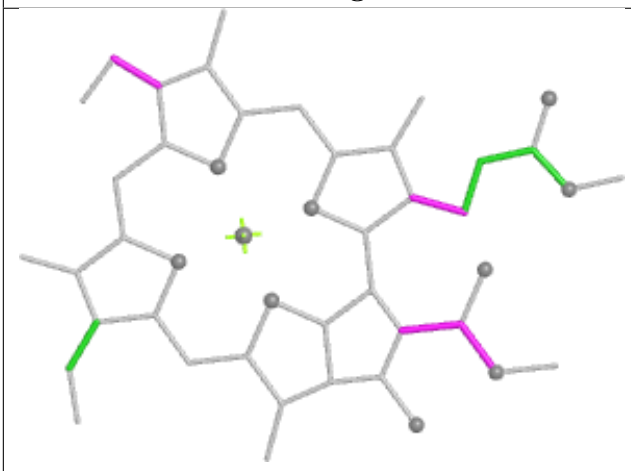


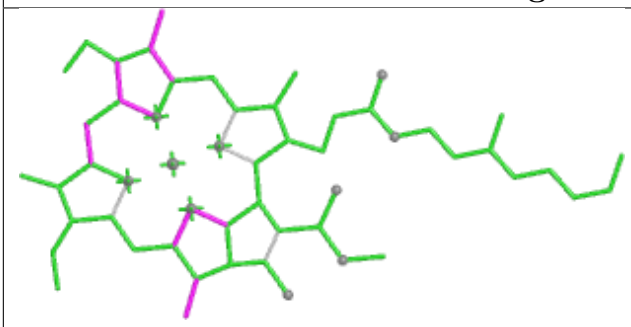
Bond angles



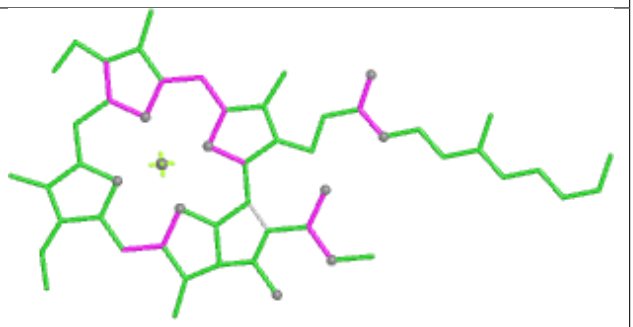
Torsions

Rings

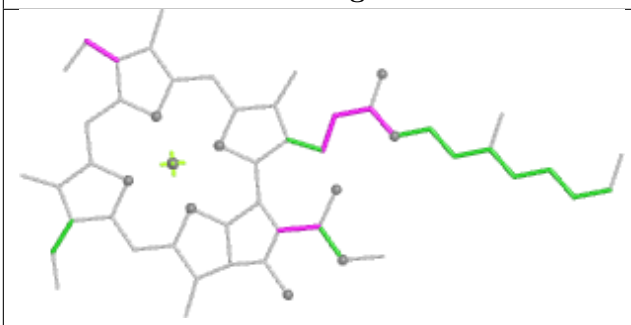
Ligand CLA a 810



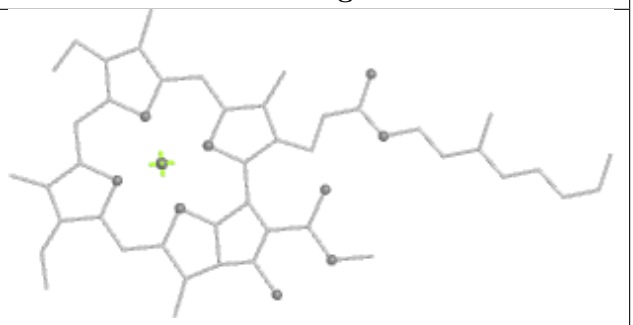
Bond lengths



Bond angles

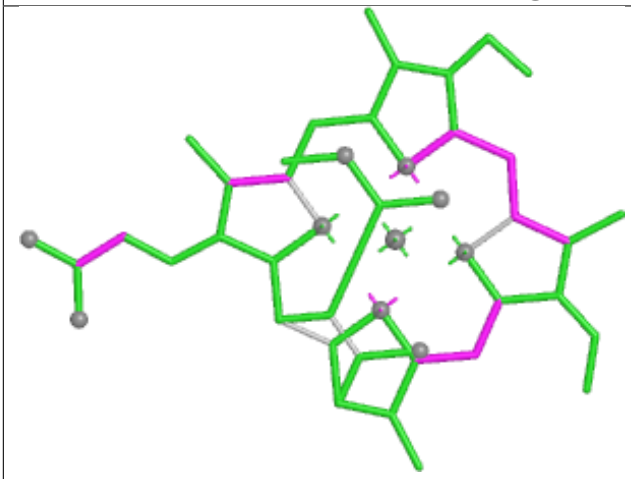


Torsions



Rings

Ligand KC2 T 312



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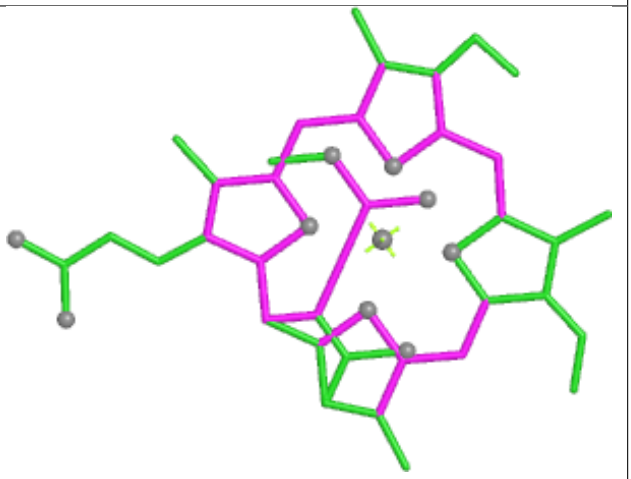
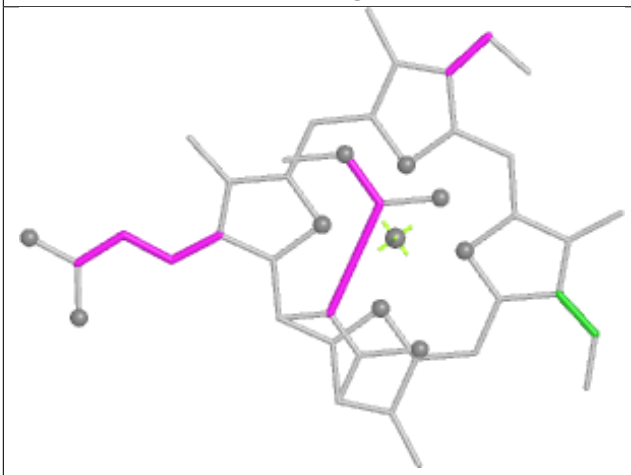


Bond angles



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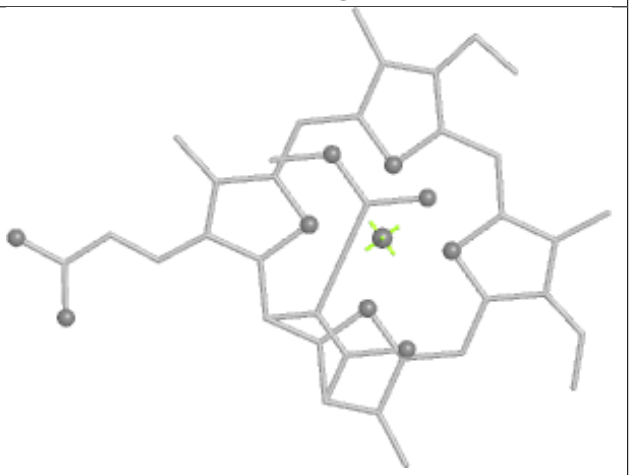
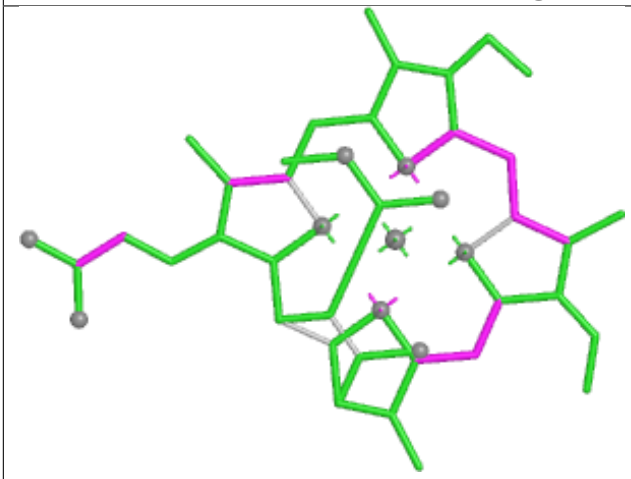


Rings

Ligand KC2 1 315



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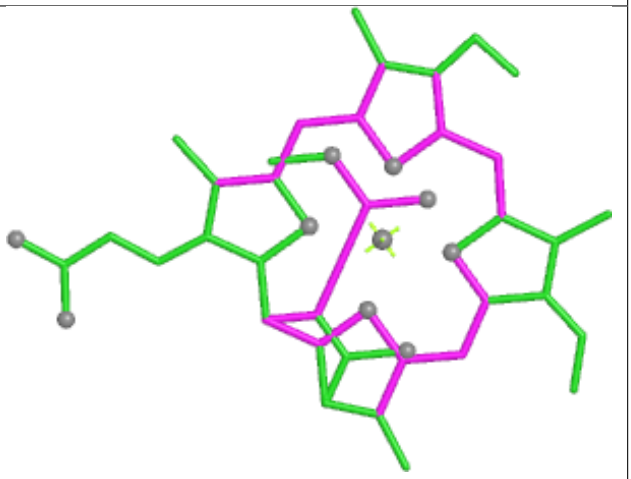
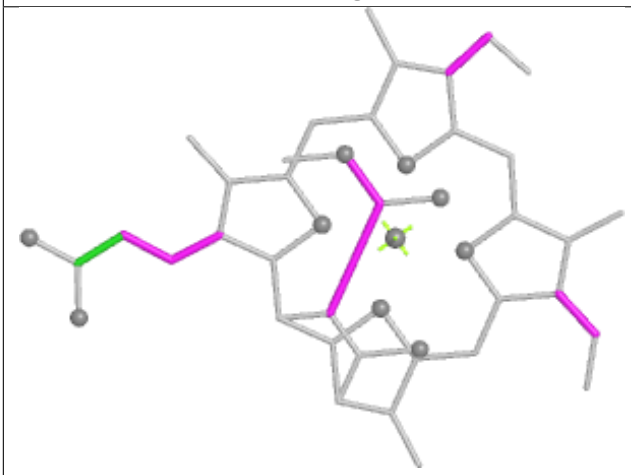


Bond angles



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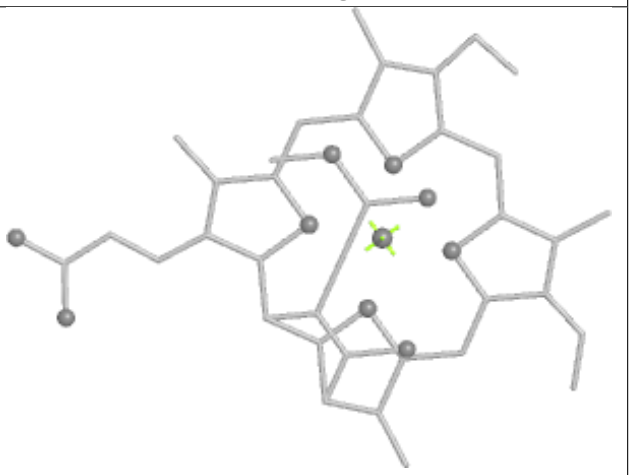
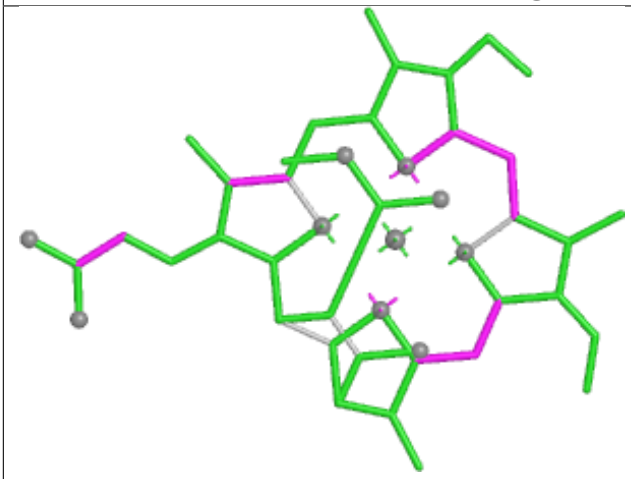


Rings

Ligand KC2 Z 311



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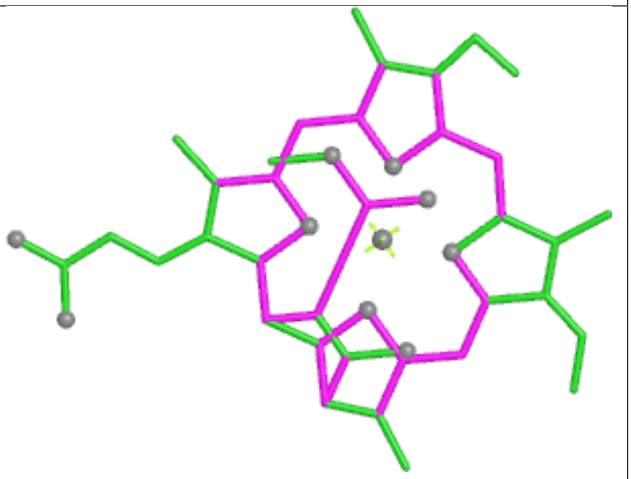
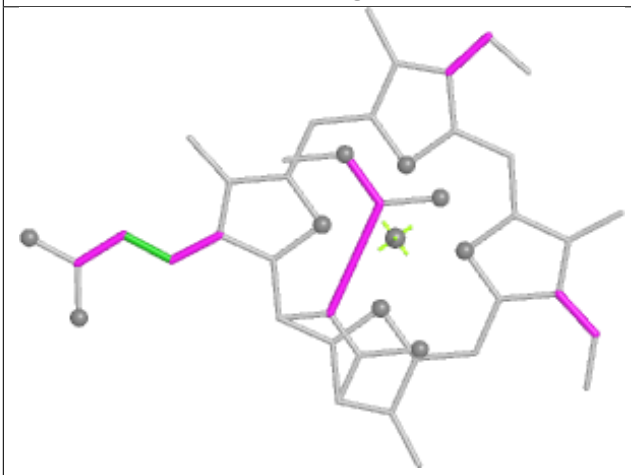


Bond angles



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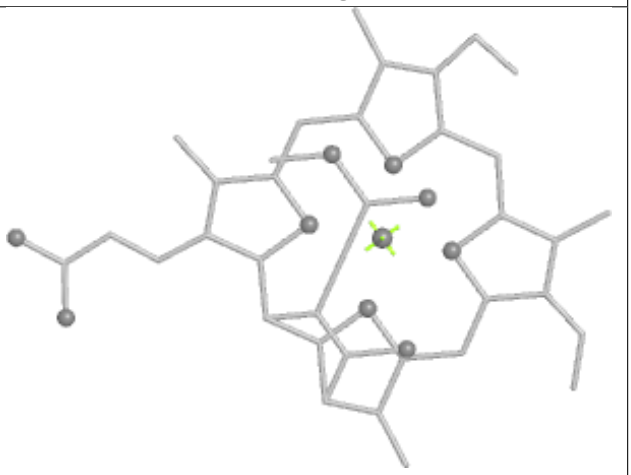
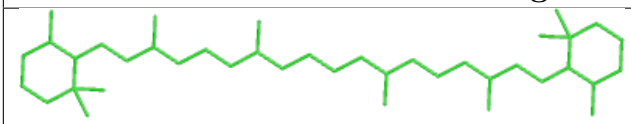


Rings

Ligand BCR i 102



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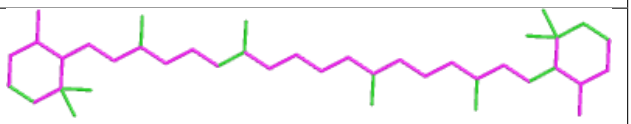
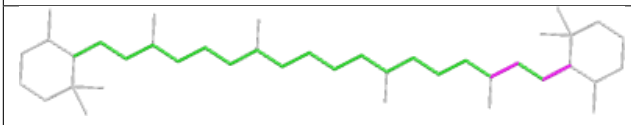


Bond angles



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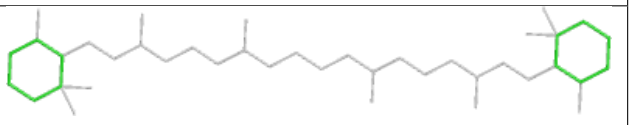
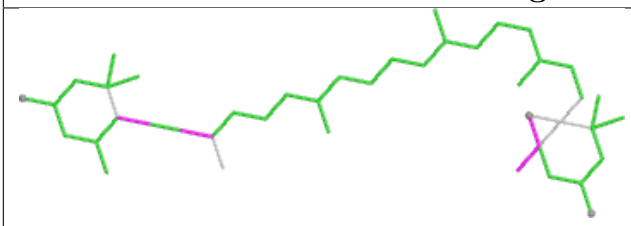


Rings

Ligand DD6 2 303



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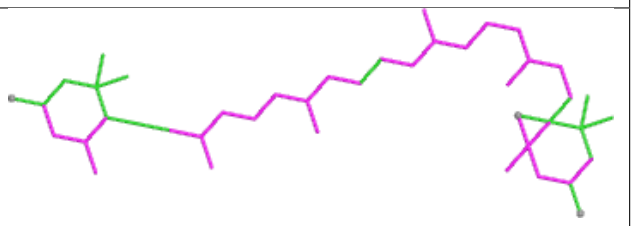
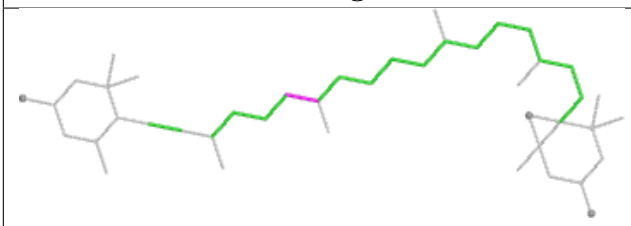
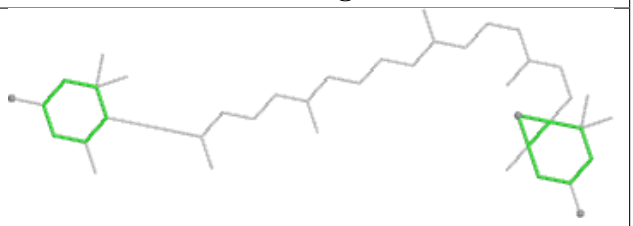


Bond angles

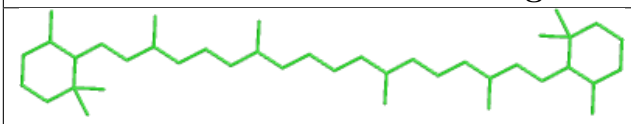


Torsions



Rings

Ligand BCR b 844



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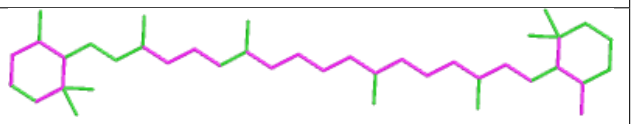
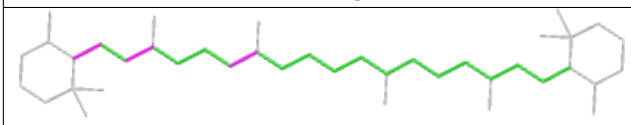
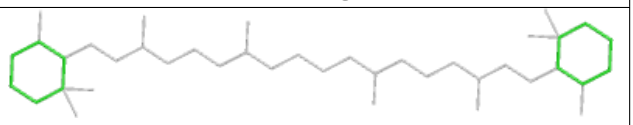


Bond angles

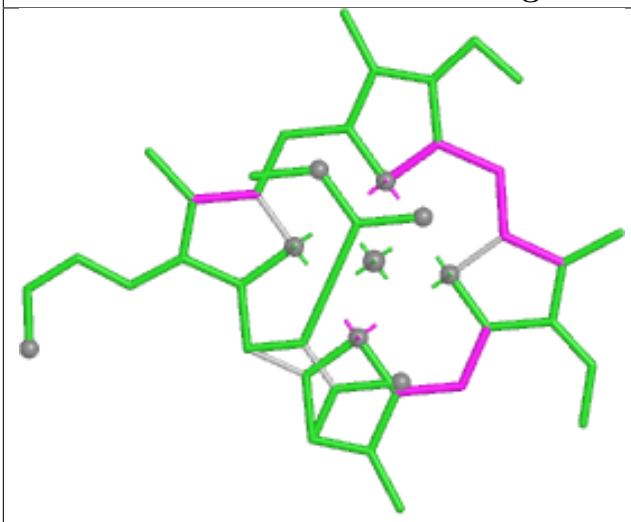


Torsions



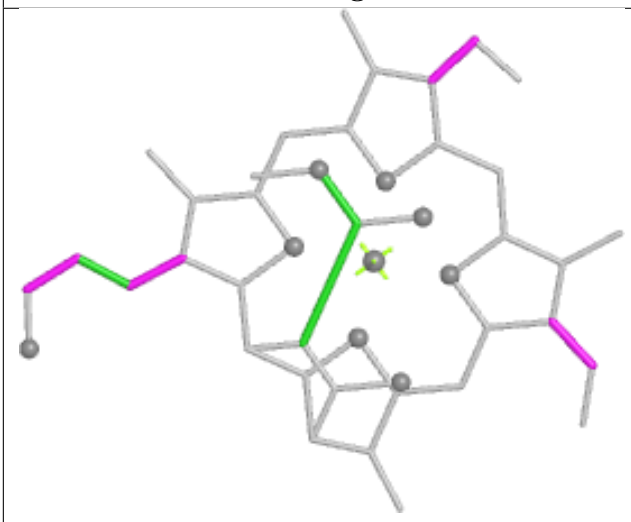
Rings

Ligand KC2 M 311



Bond lengths

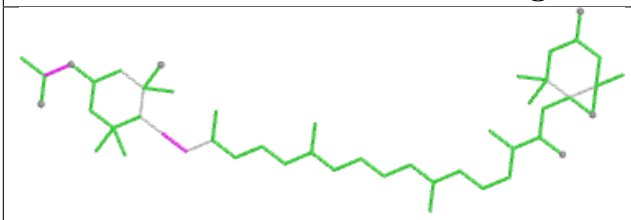
Bond angles



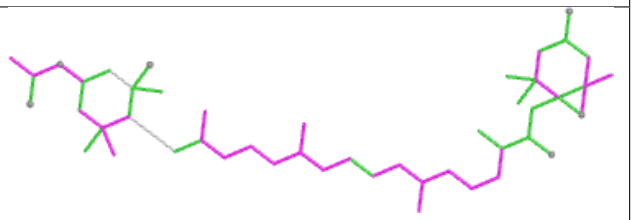
Torsions

Rings

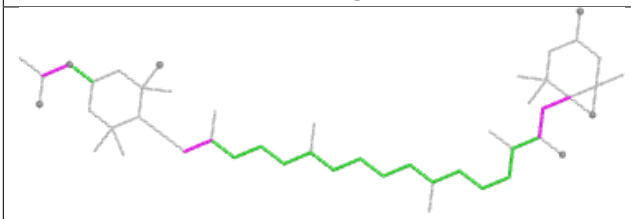
Ligand A86 X 302



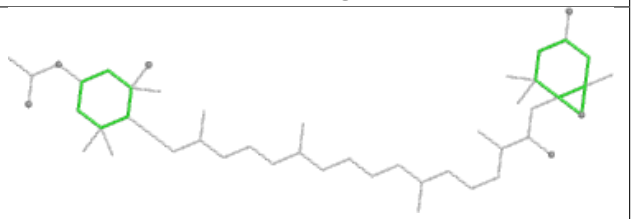
Bond lengths



Bond angles

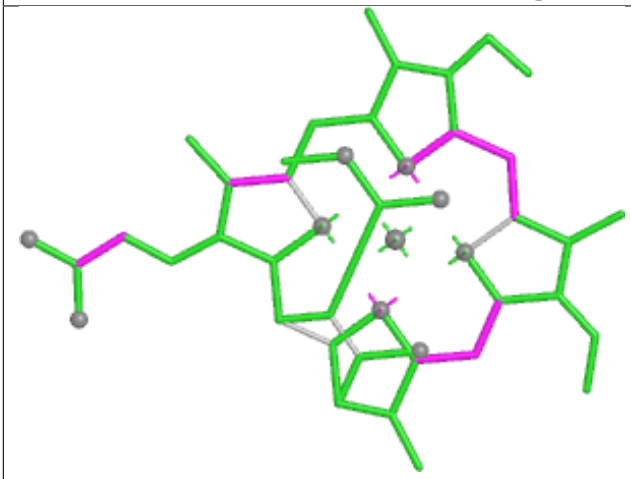


Torsions

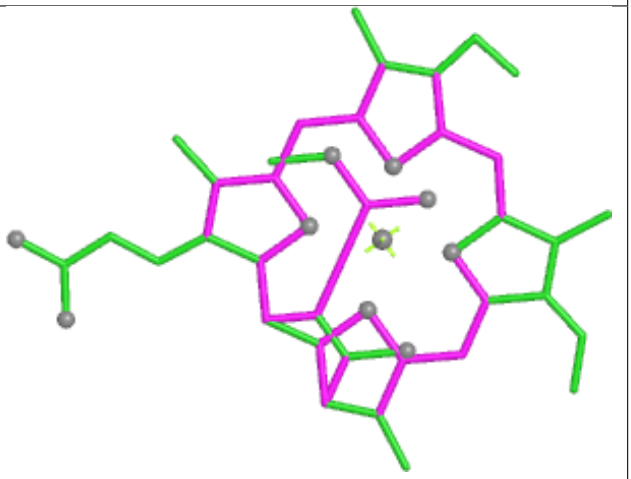


Rings

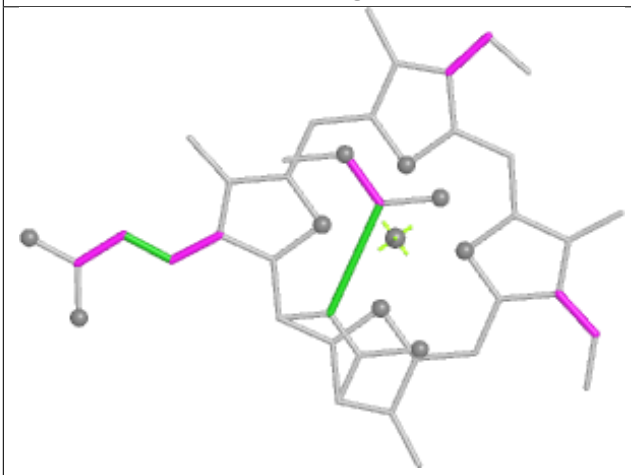
Ligand KC2 6 316



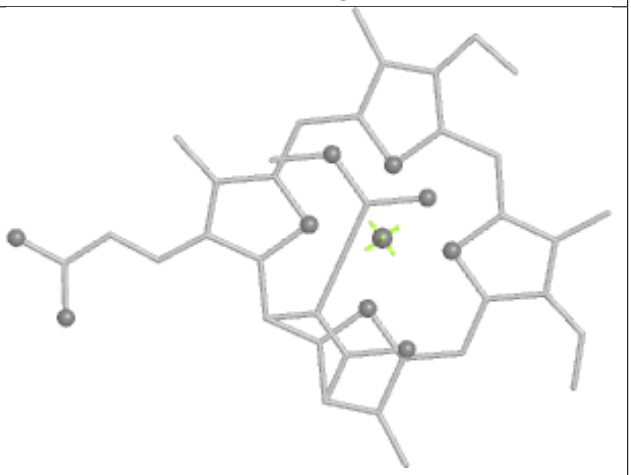
Bond lengths



Bond angles

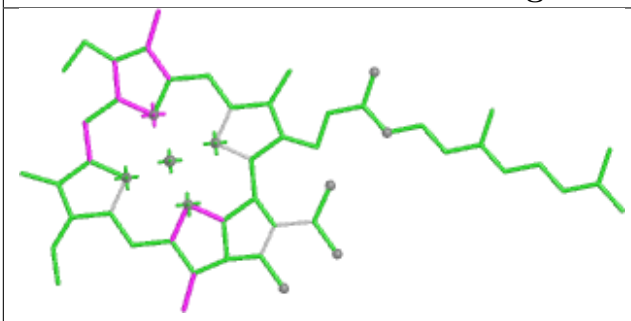


Torsions

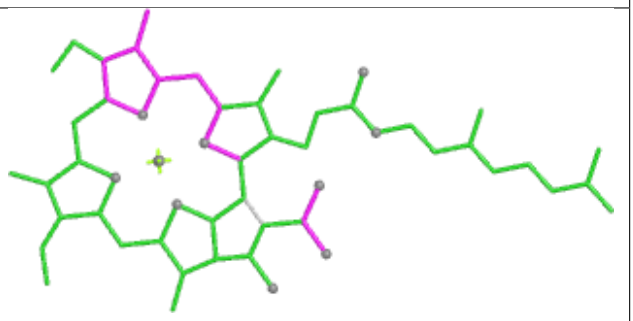


Rings

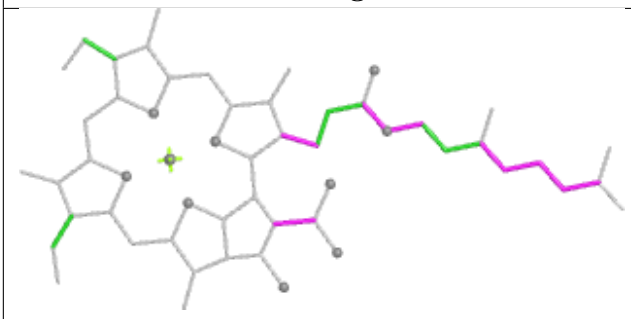
Ligand CLA L 309



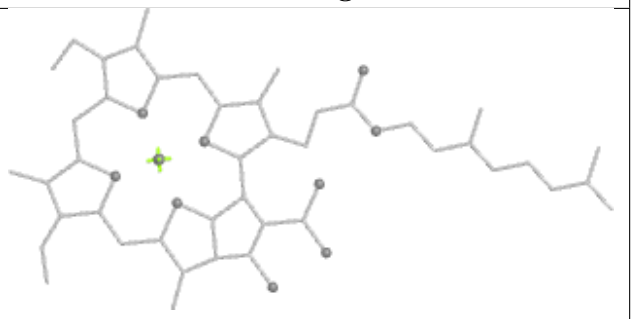
Bond lengths



Bond angles

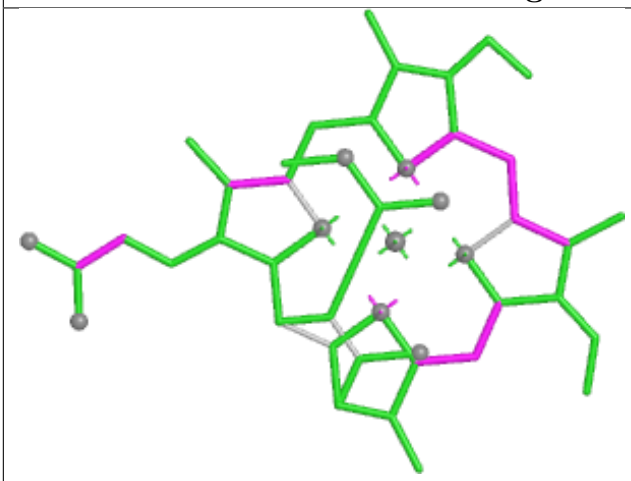


Torsions



Rings

Ligand KC2 Q 318



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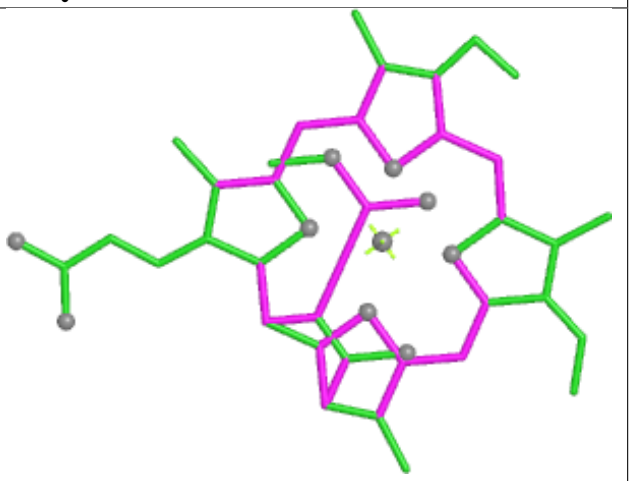

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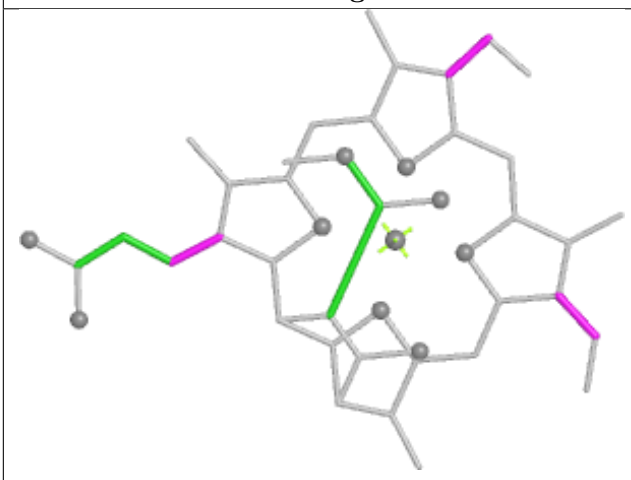

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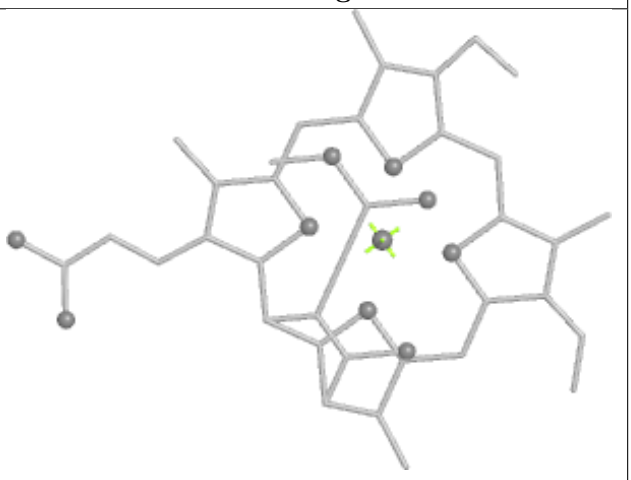
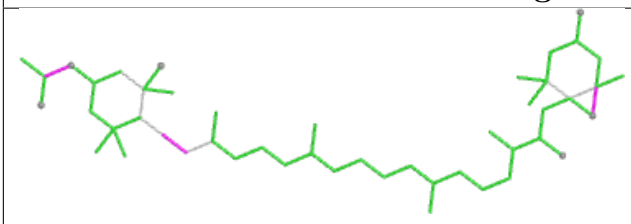


Rings

Ligand A86 1 303



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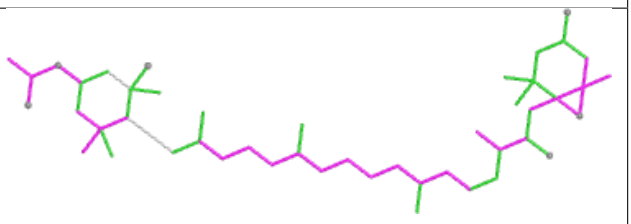

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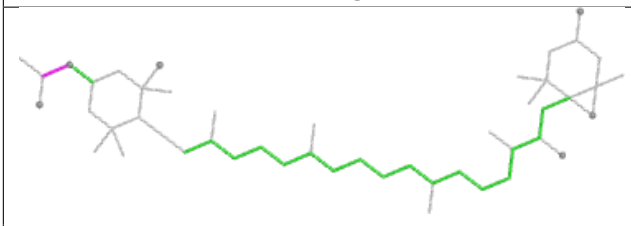

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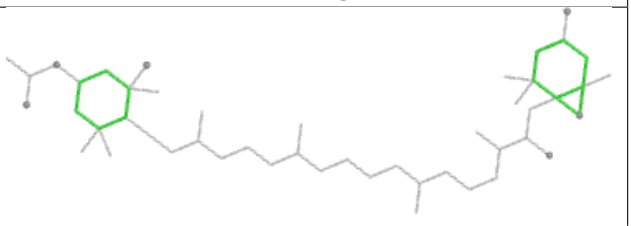
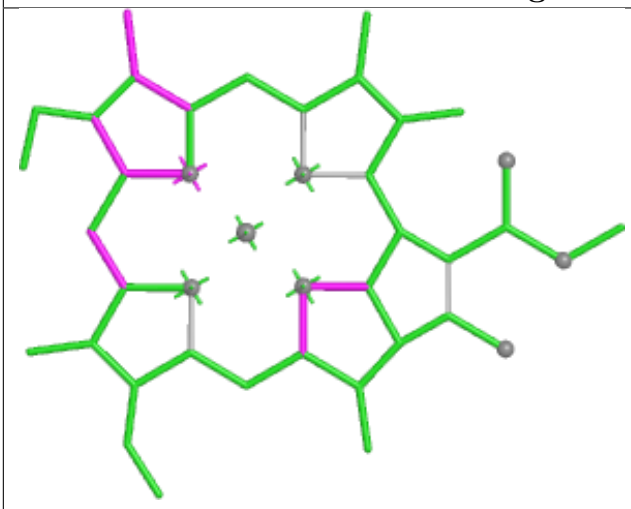


Rings

Ligand CLA 7 324



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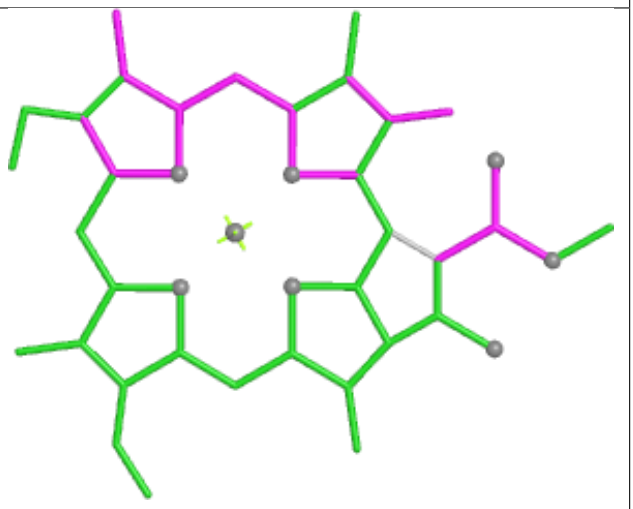
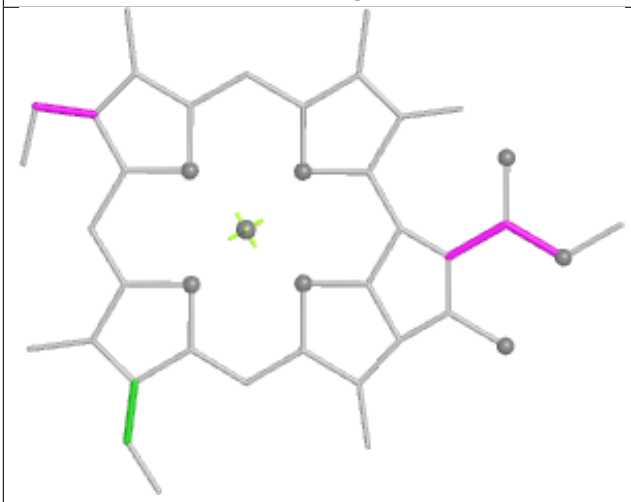


Bond angles



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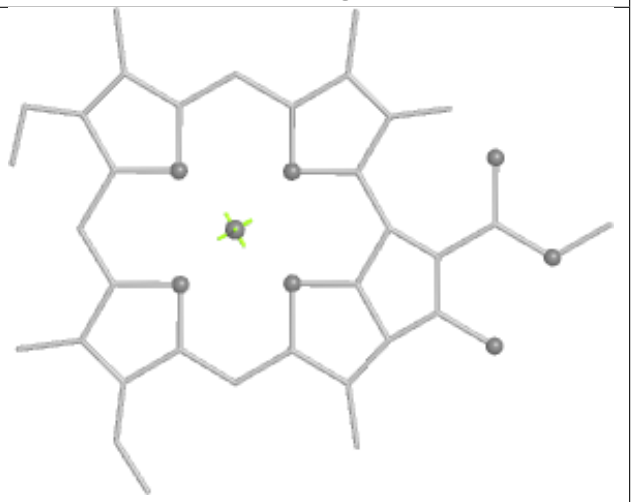
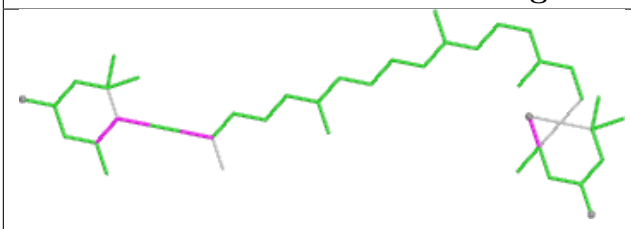


Rings

Ligand DD6 z 304



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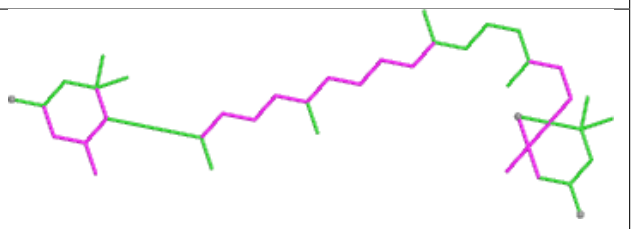

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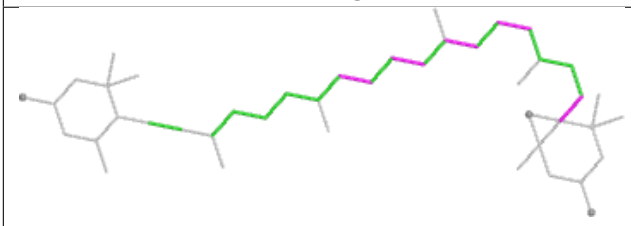
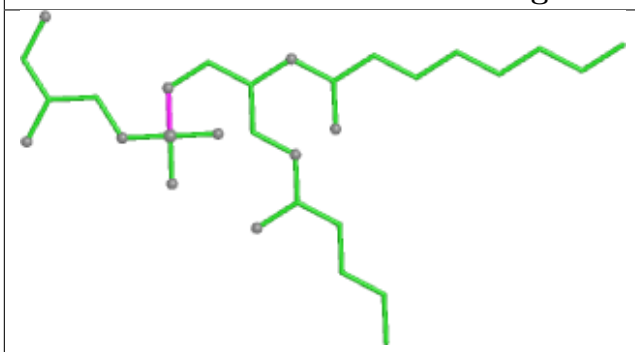


Torsions

Rings

Ligand LHG j 104



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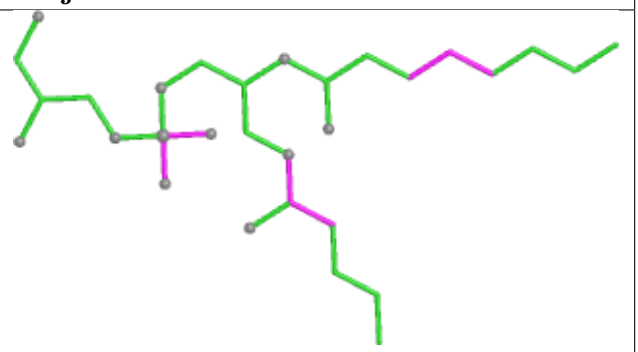

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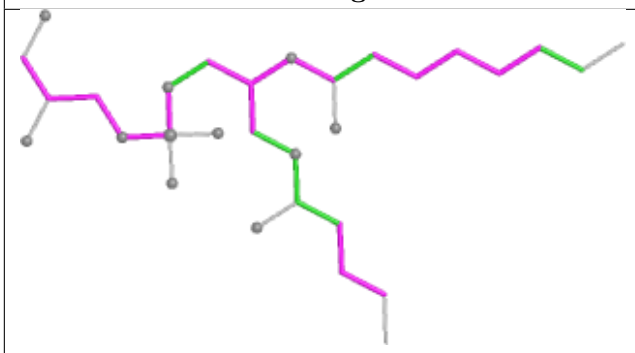

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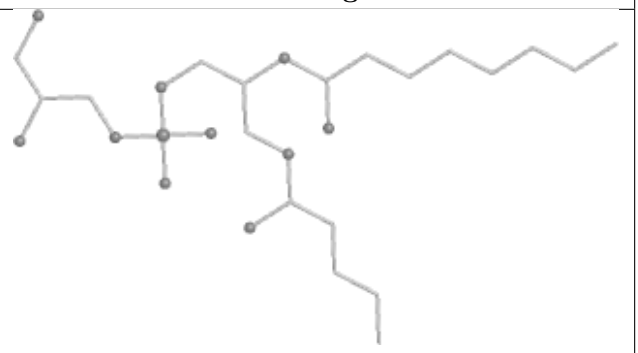
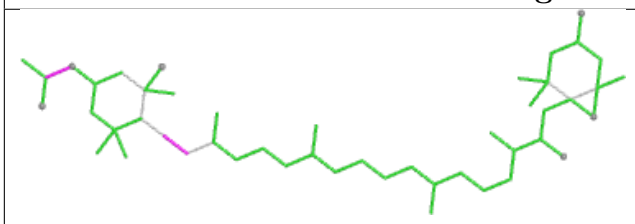


Rings

Ligand A86 4 310



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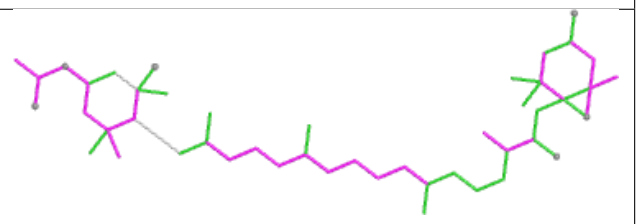

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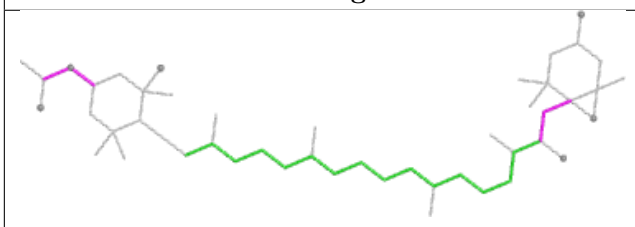

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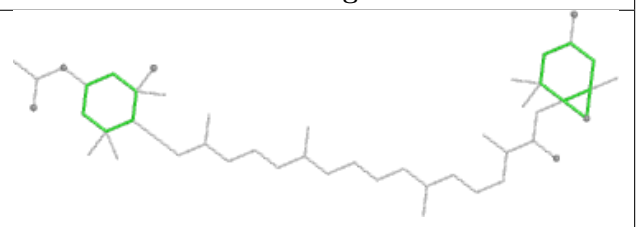
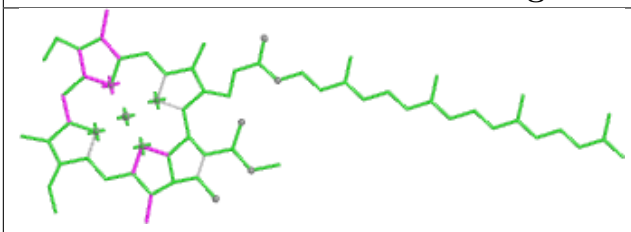


Rings

Ligand CLA S 309



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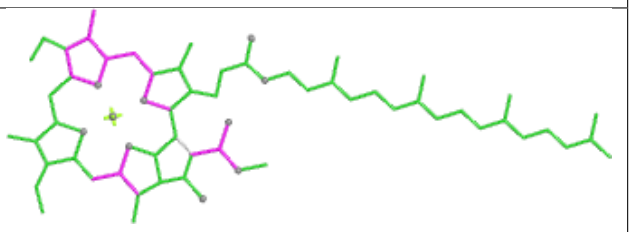

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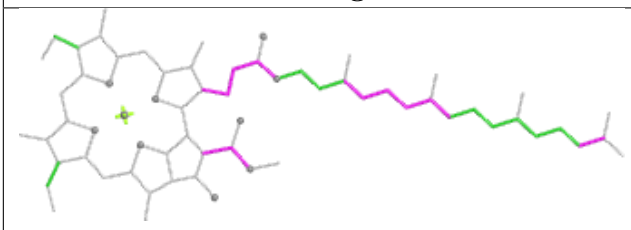

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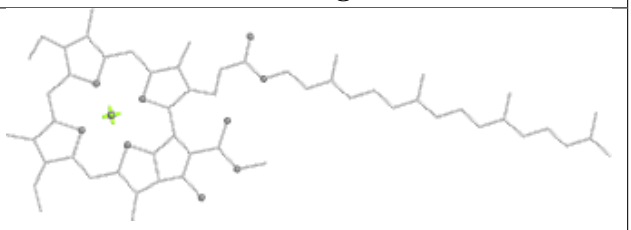
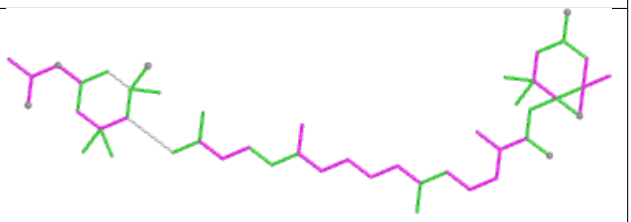


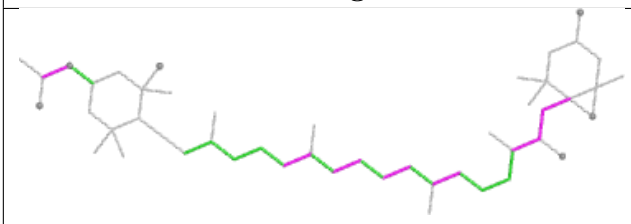
Rings

Ligand A86 4 328

Bond lengths



Bond angles



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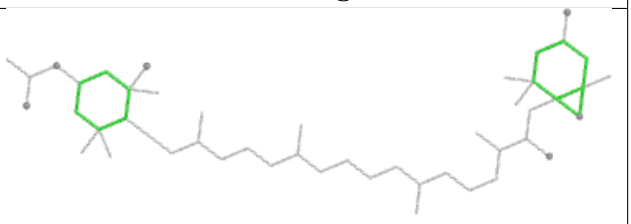
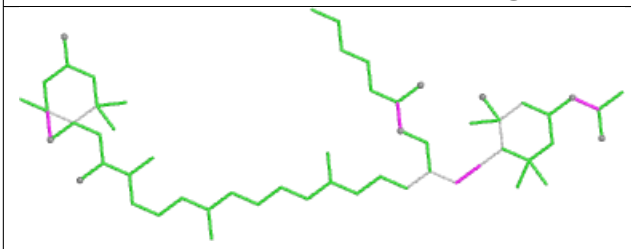


Rings

Ligand A1EB1 V 307



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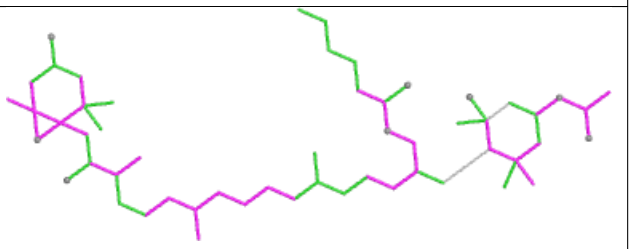
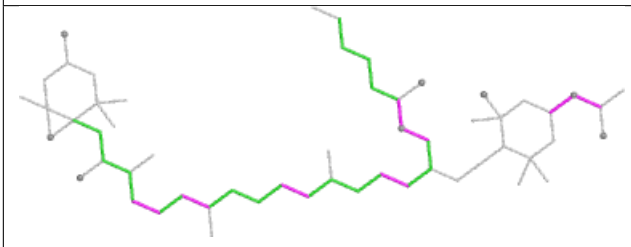


Bond angles



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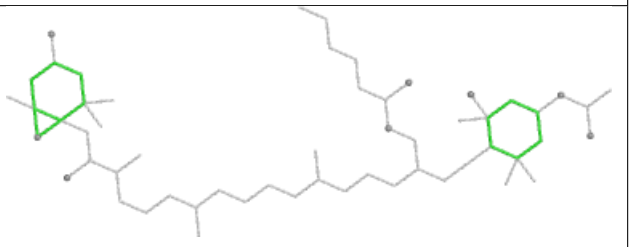
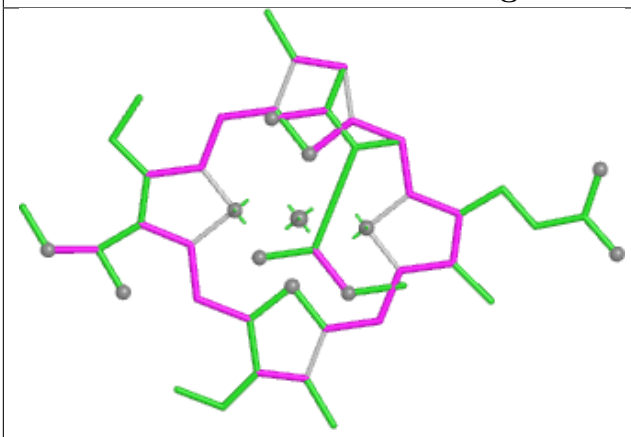
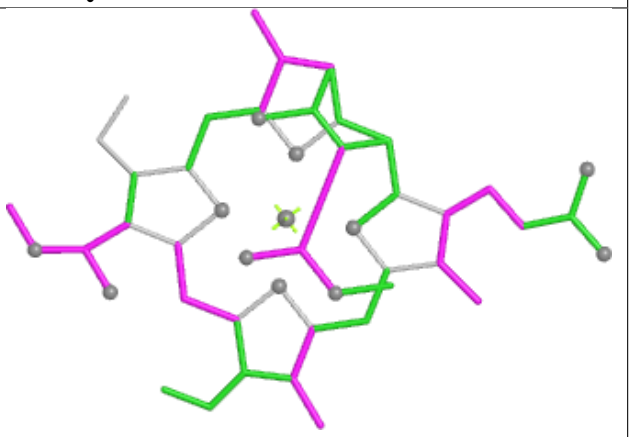


Rings

Ligand A1ECV Q 319	
	
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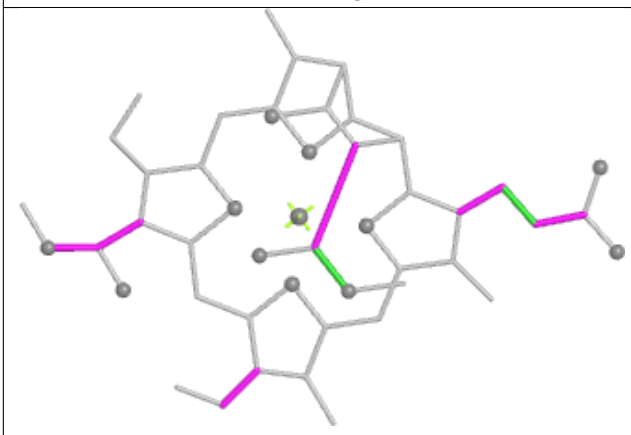
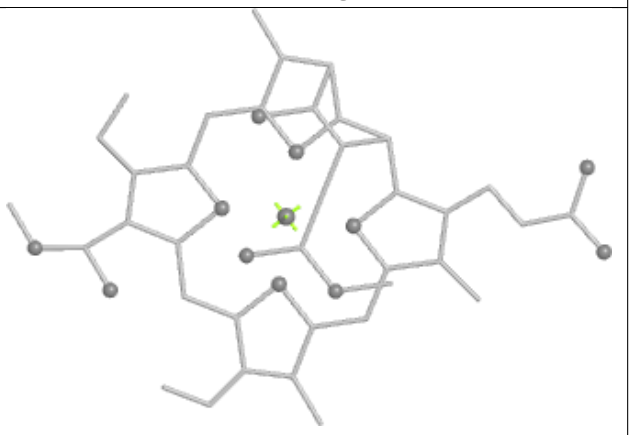
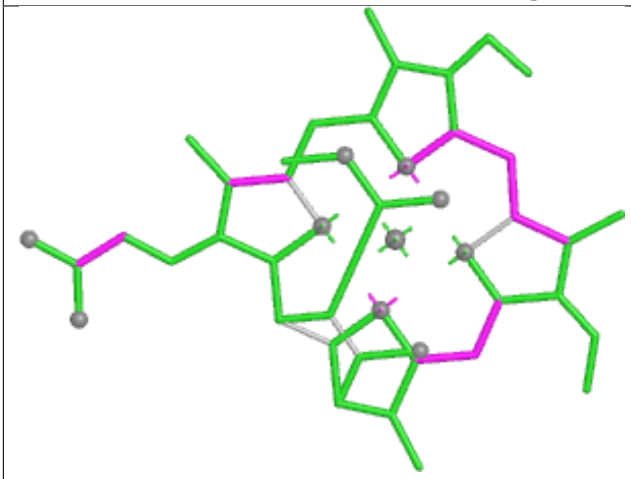
	
Torsions	**Rings**

Ligand KC2 H 314



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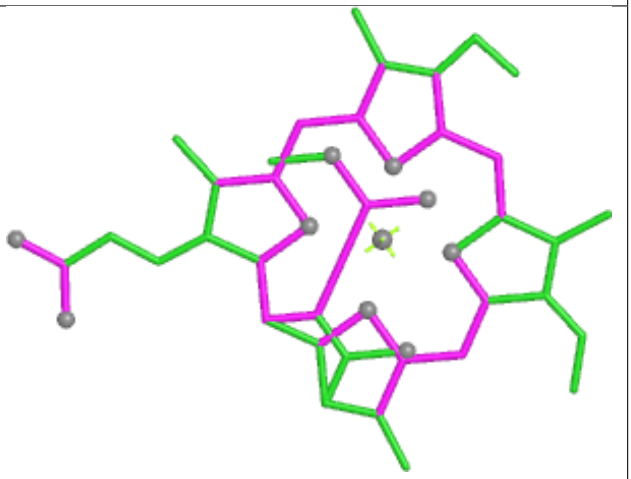
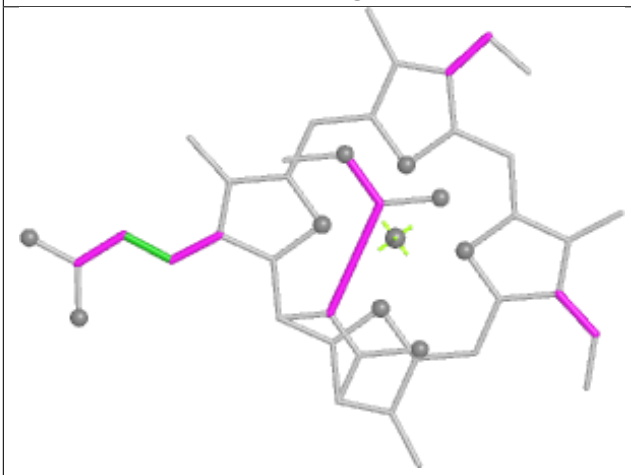
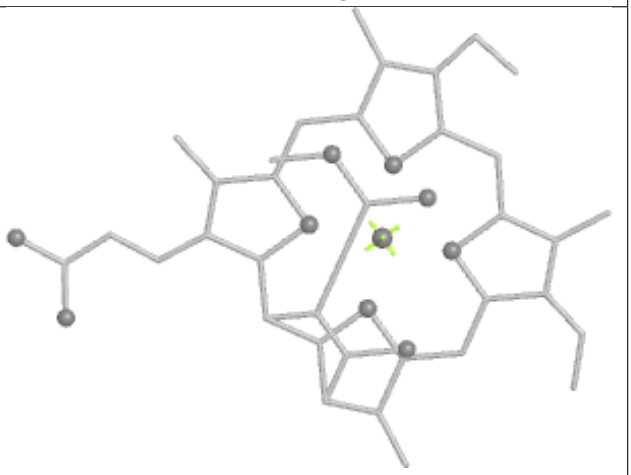


Bond angles

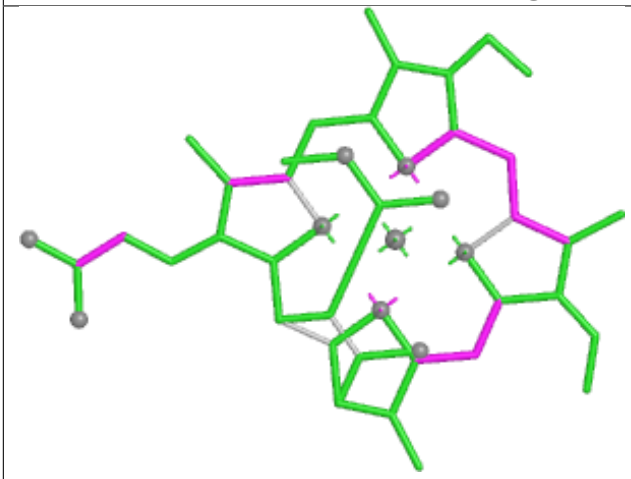


Torsions



Rings

Ligand KC2 H 311



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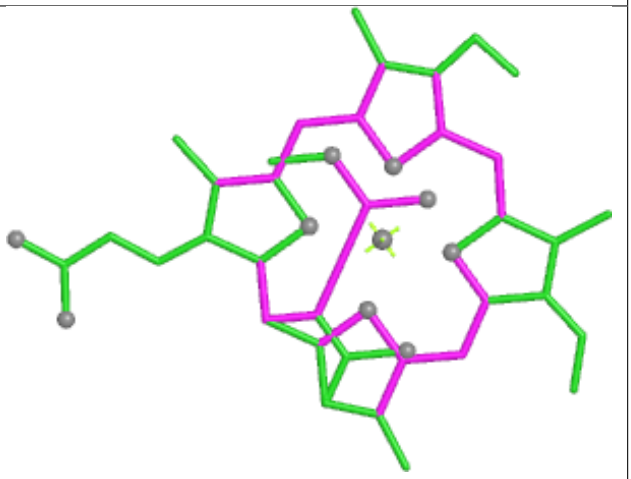
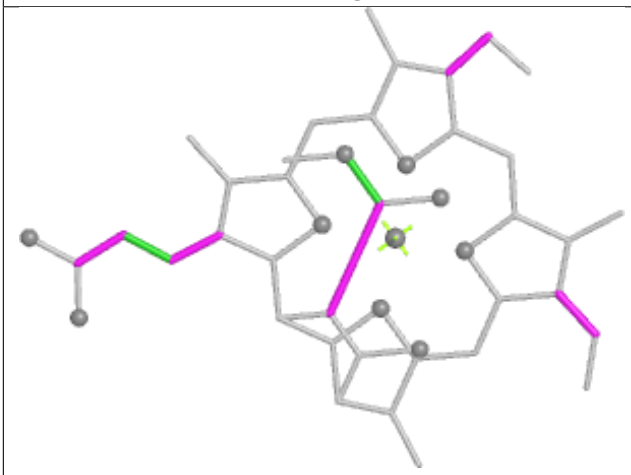


Bond angles



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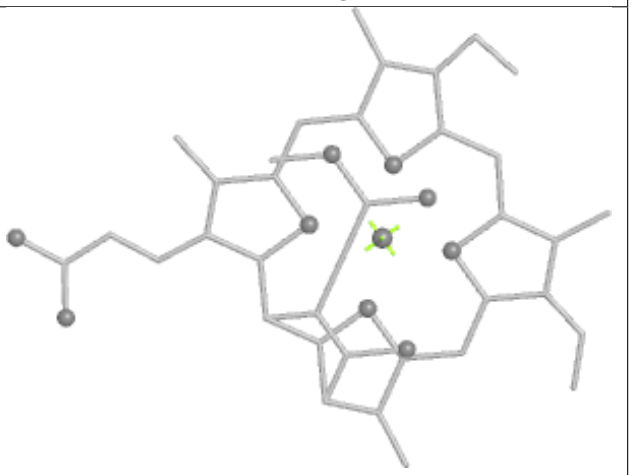
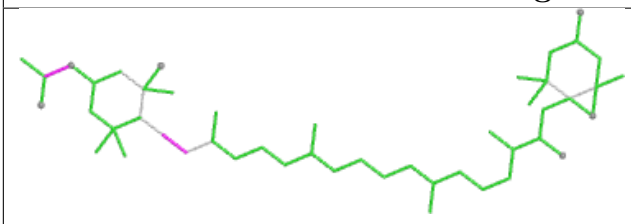


Rings

Ligand A86 0 304



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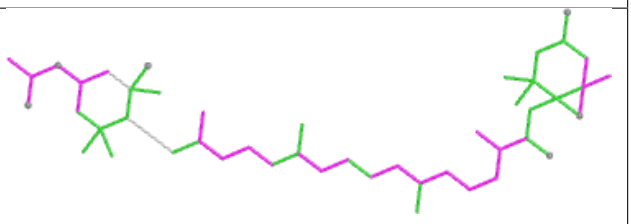
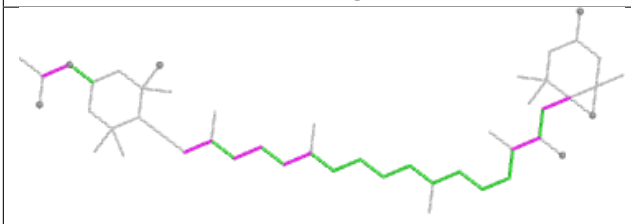


Bond angles



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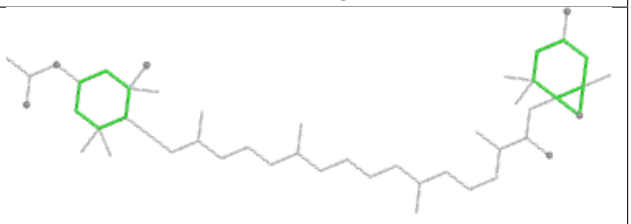
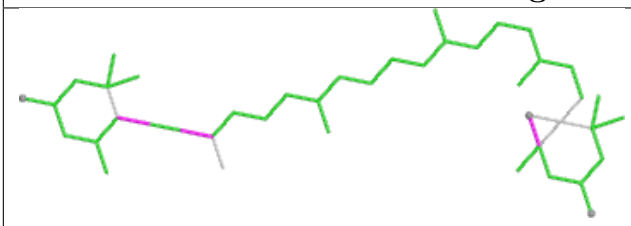


Rings

Ligand DD6 7 310



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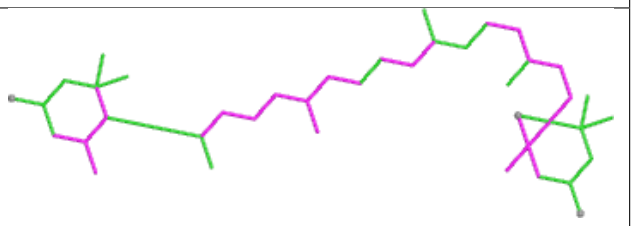
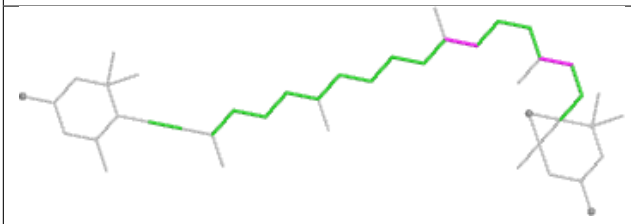
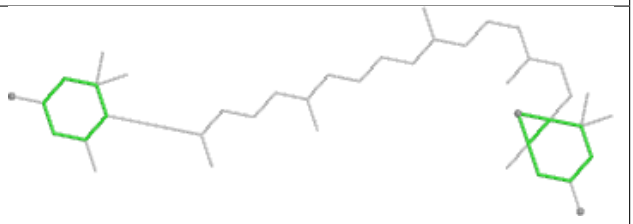


Bond angles

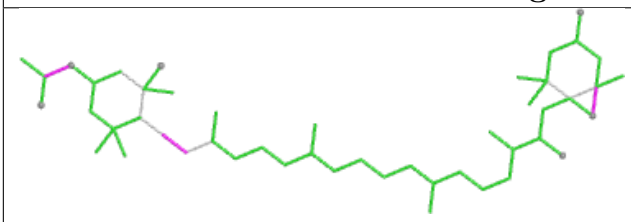


Torsions

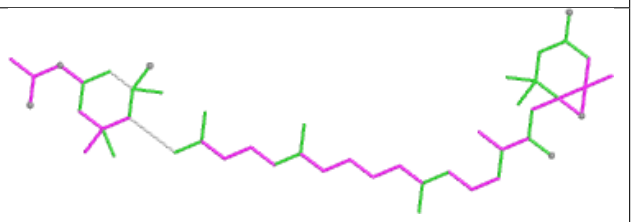


Rings

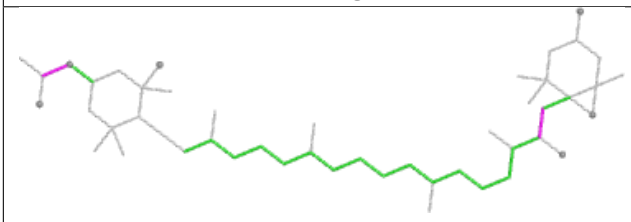
Ligand A86 V 304



Bond lengths



Bond angles



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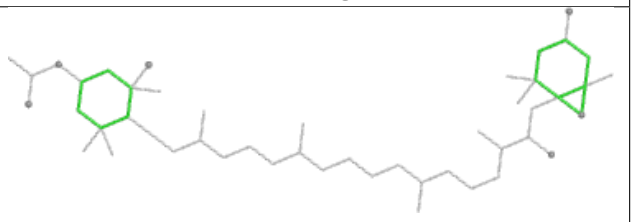
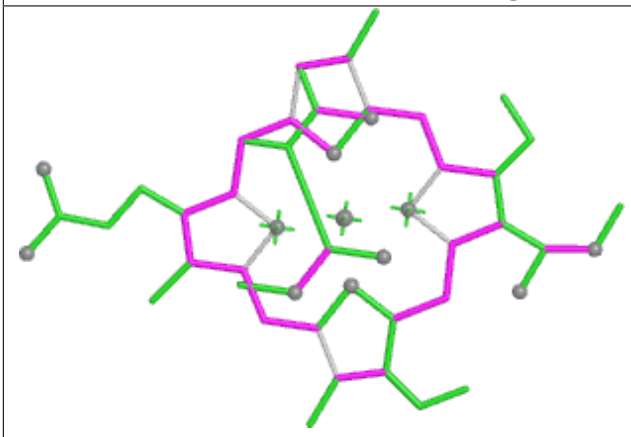


Rings

Ligand A1ECV 5 309



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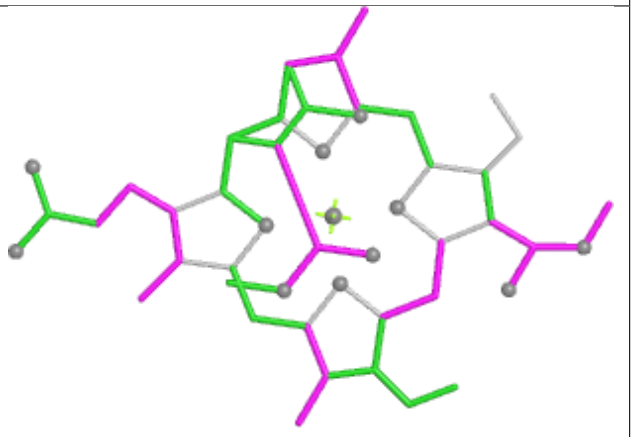

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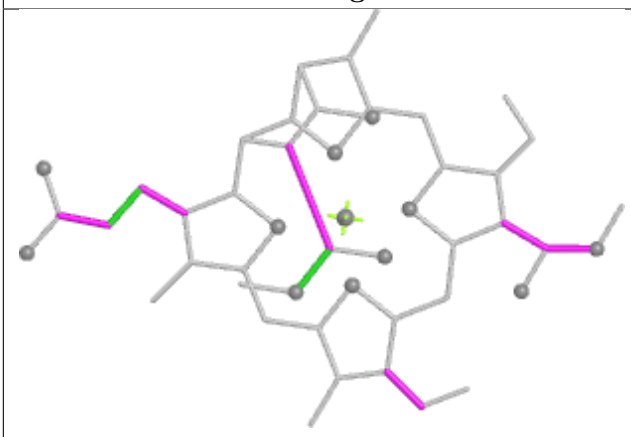

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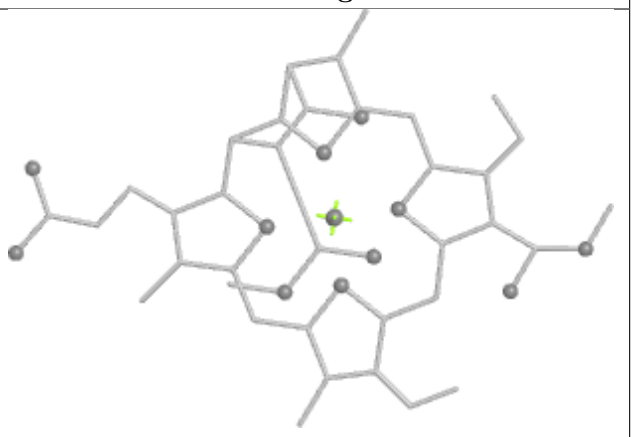
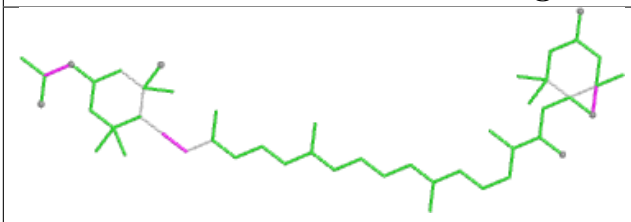


Rings

Ligand A86 0 308



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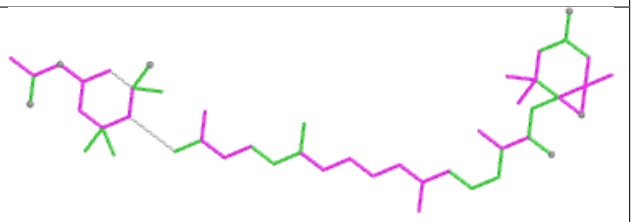
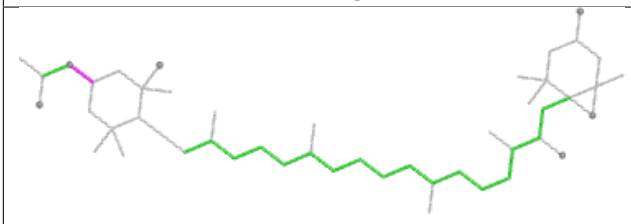


Bond angles



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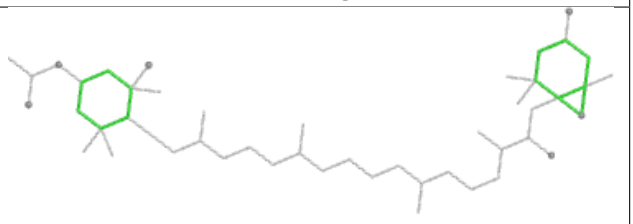
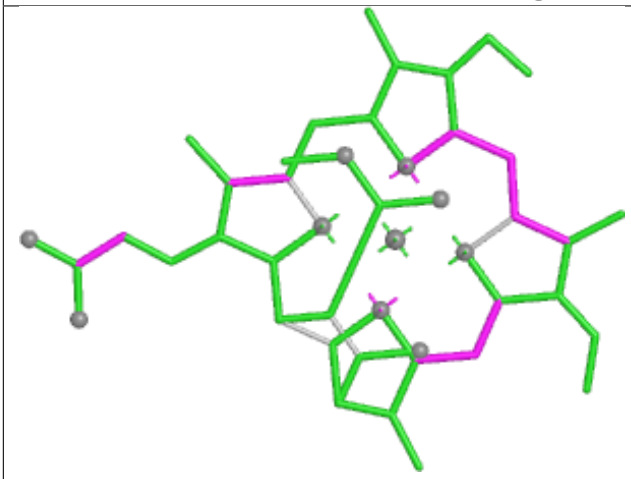


Rings

Ligand KC2 8 316



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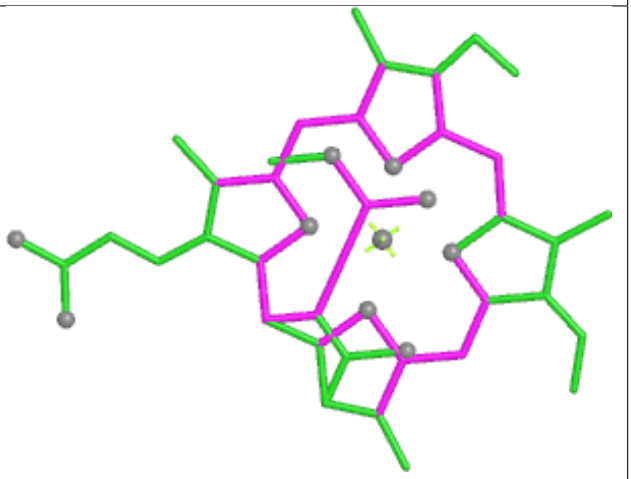
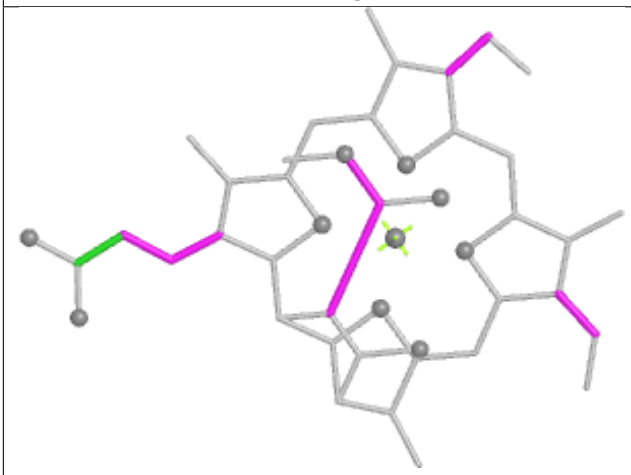


Bond angles



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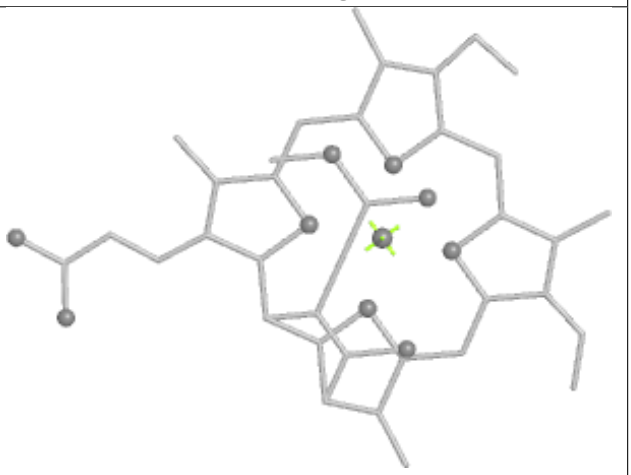
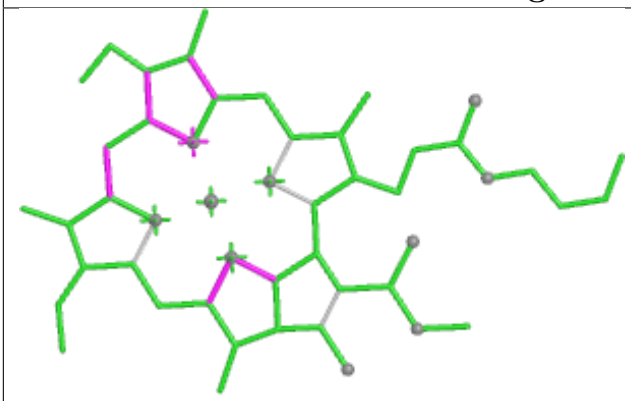


Rings

Ligand CLA a 819



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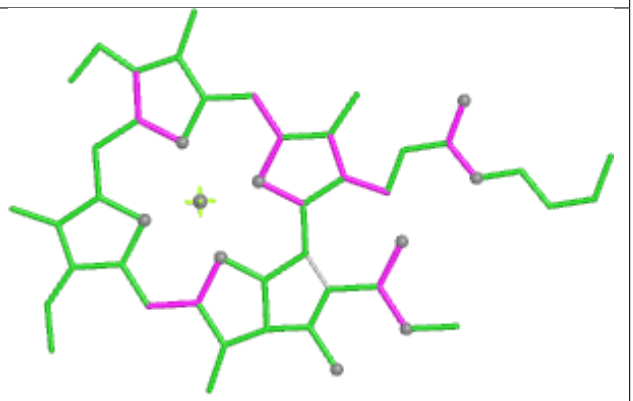
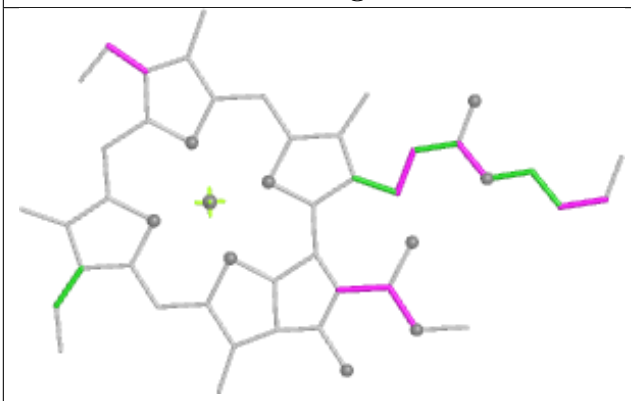


Bond angles



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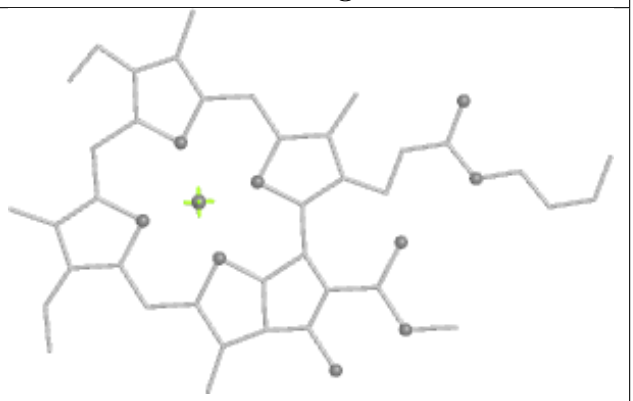
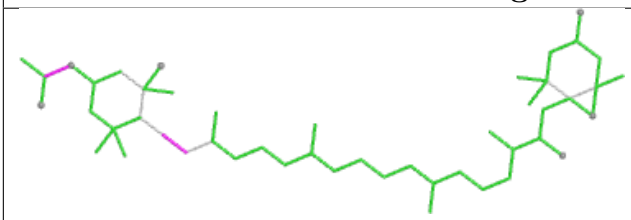


Rings

Ligand A1EB1 z 301



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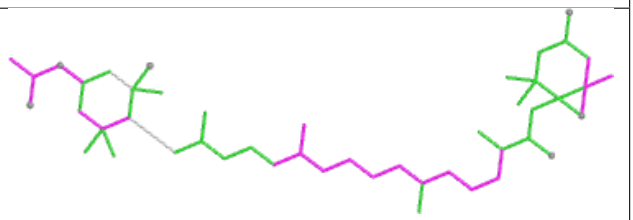
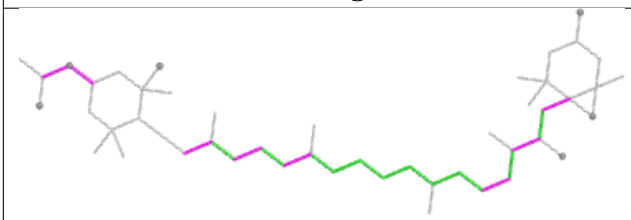


Bond angles



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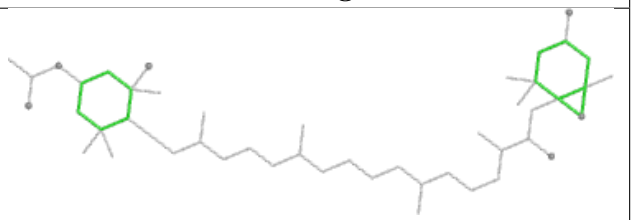
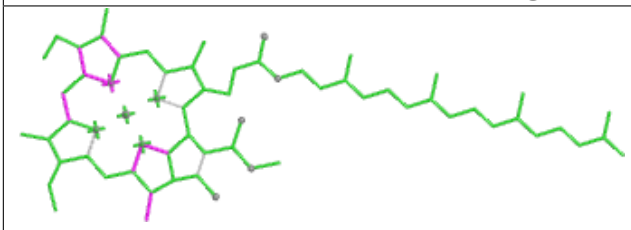


Rings

Ligand CLA C 307



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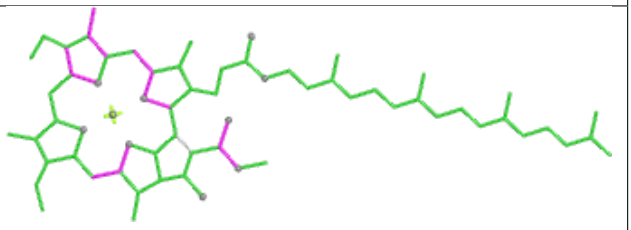

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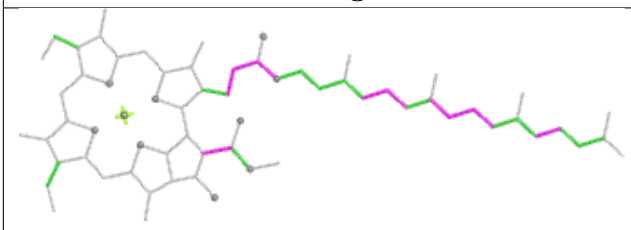

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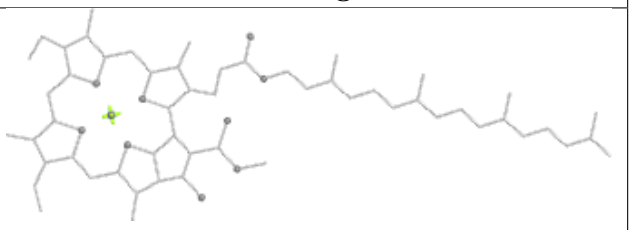
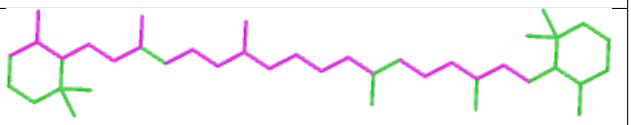


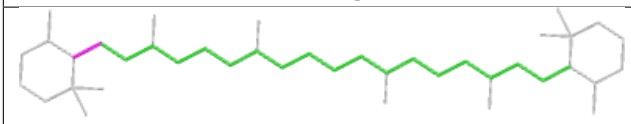
Rings

Ligand BCR b 848

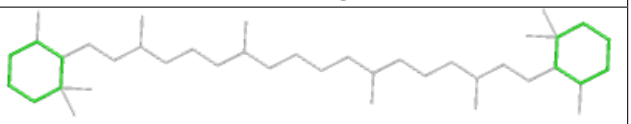
Bond lengths



Bond angles

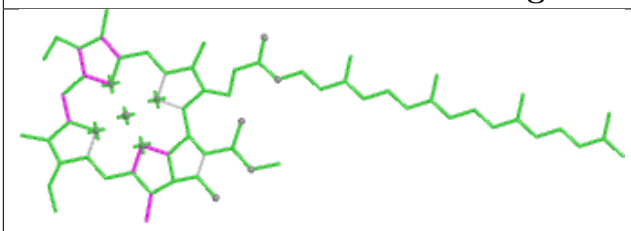


Torsions



Rings

Ligand CLA b 806



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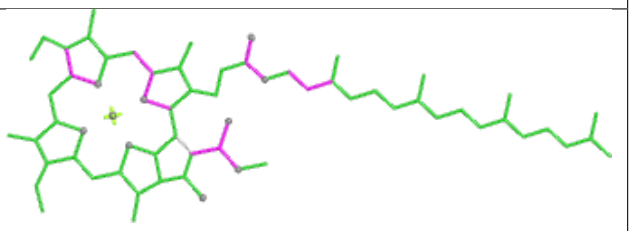
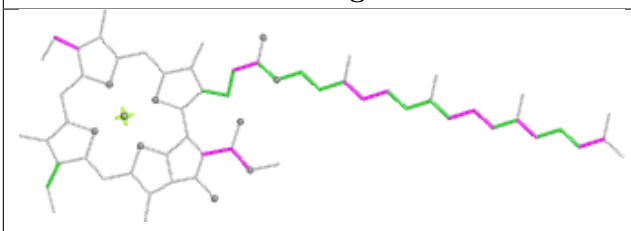
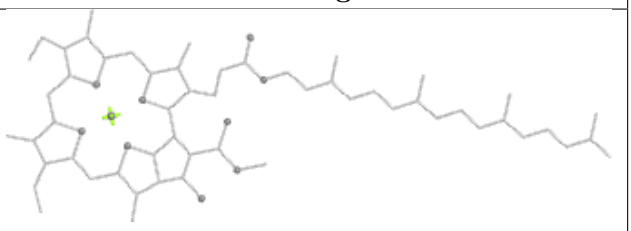


Bond angles

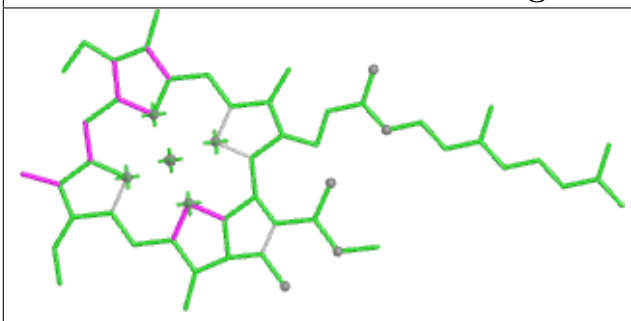


Torsions



Rings

Ligand CLA 0 313



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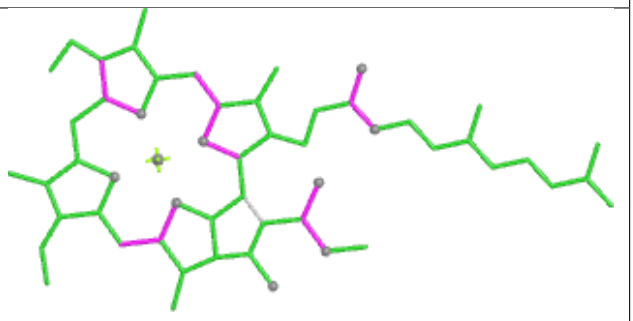
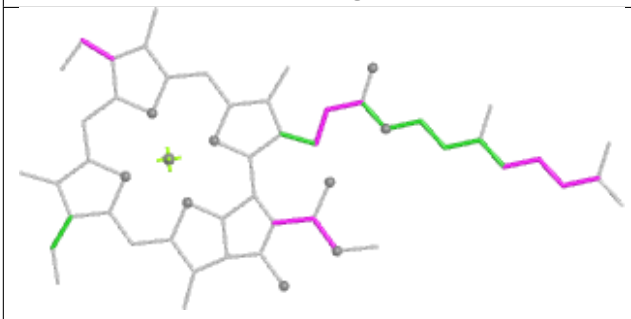


Bond angles



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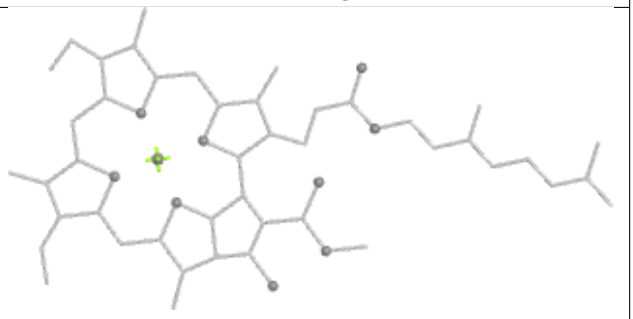
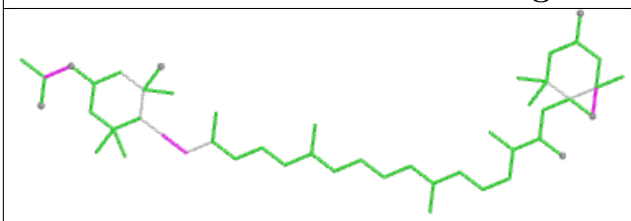


Rings

Ligand A86 L 304



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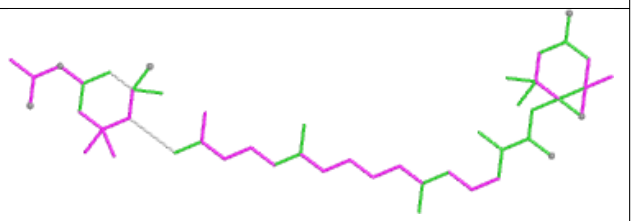
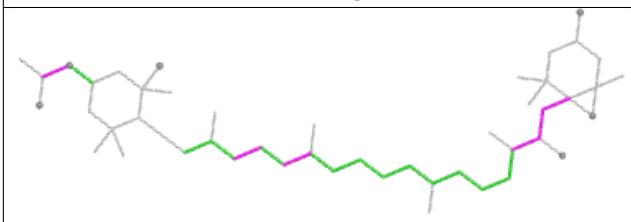


Bond angles



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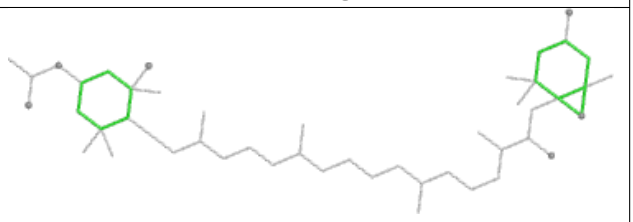
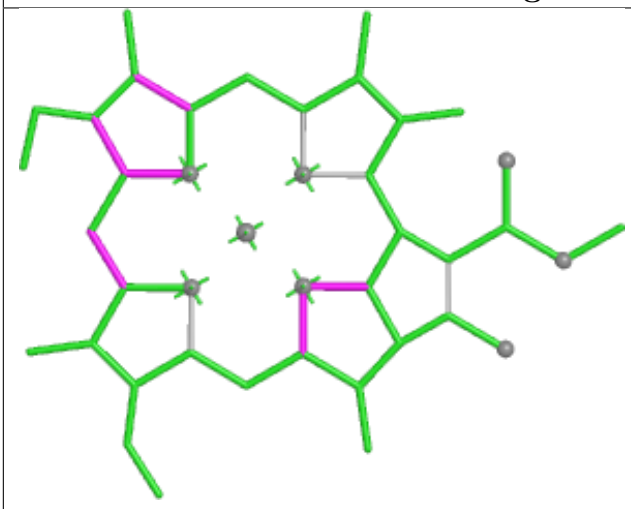
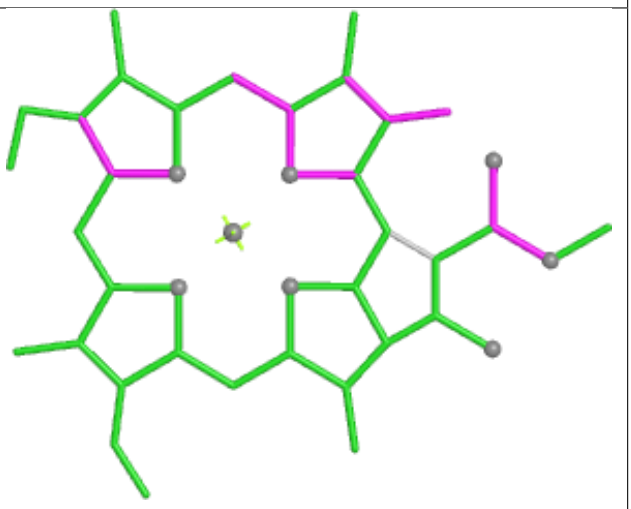


Rings

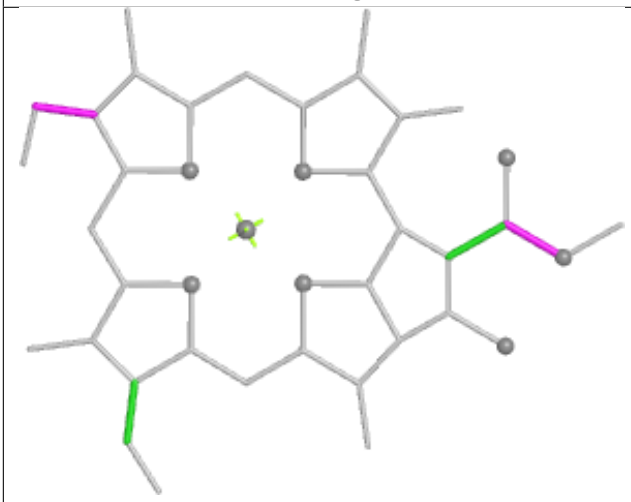
Ligand CLA Y 310



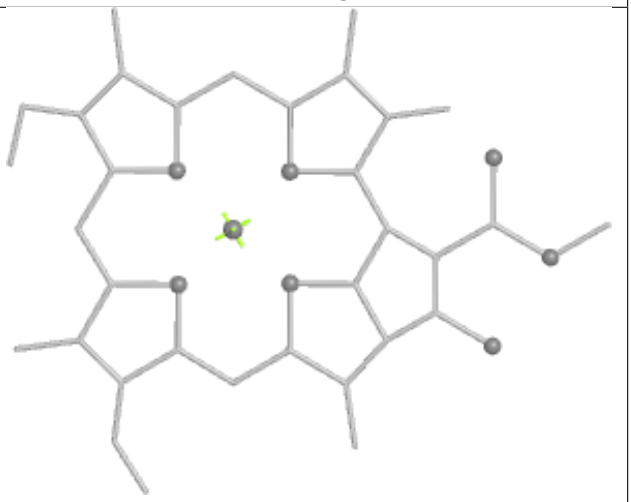
Bond lengths



Bond angles

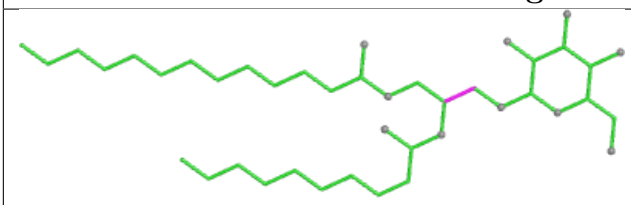


Torsions



Rings

Ligand LMG I 302



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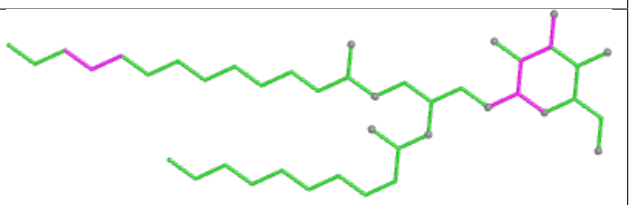
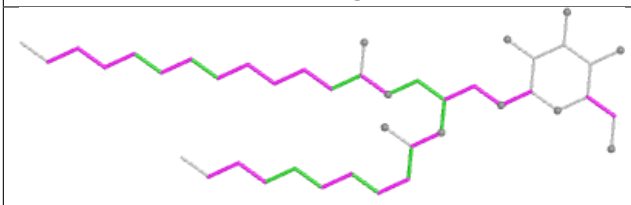
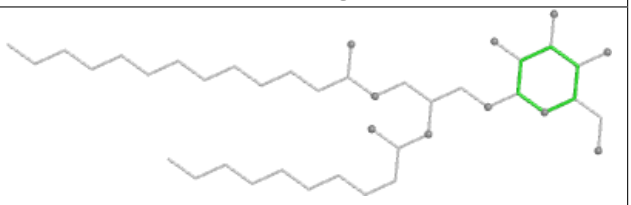


Bond angles

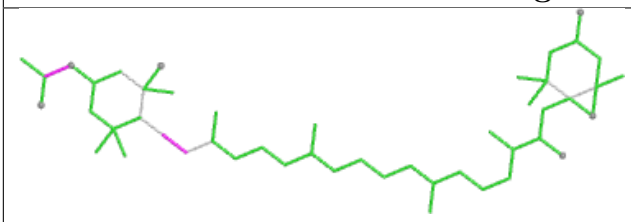


Torsions

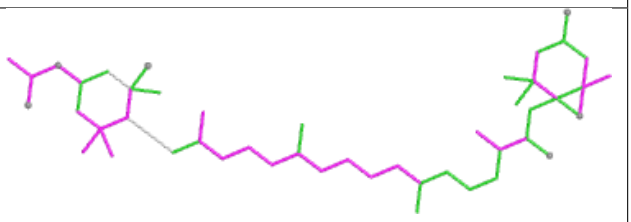


Rings

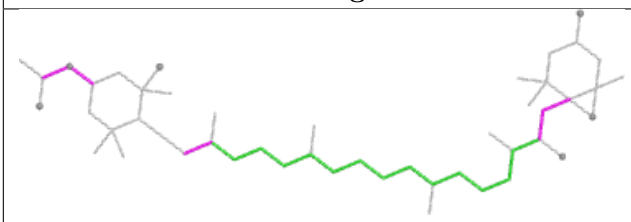
Ligand A86 0 309



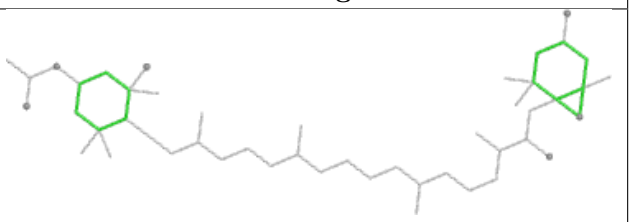
Bond lengths



Bond angles

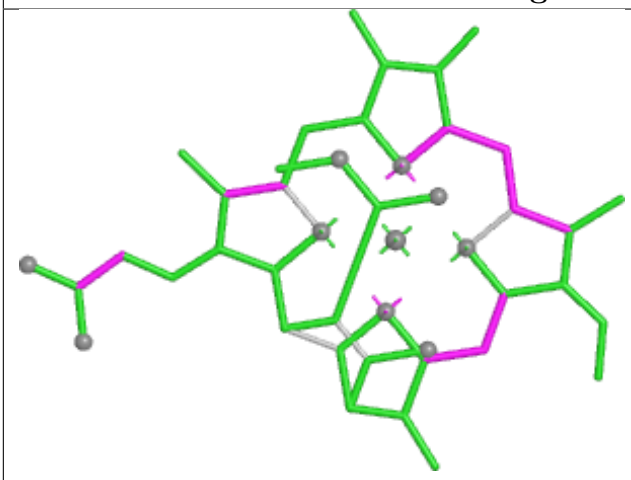


Torsions



Rings

Ligand KC2 2 313



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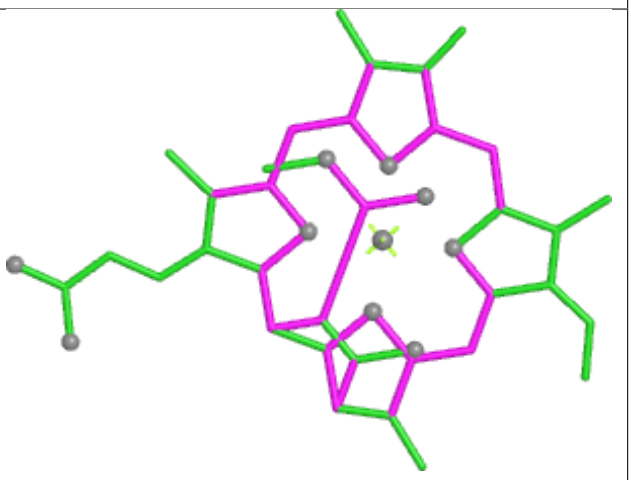
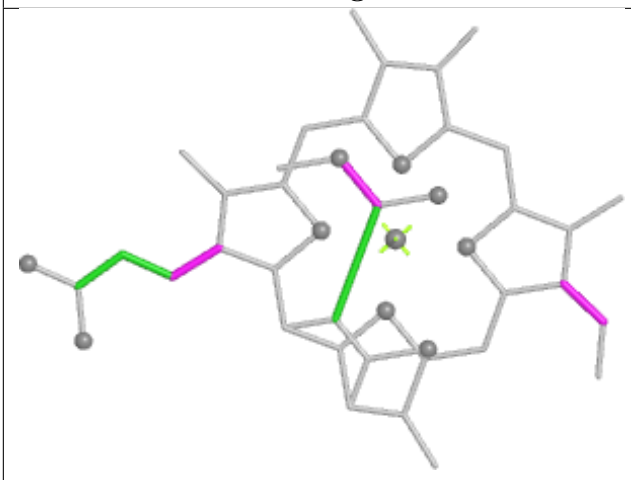


Bond angles



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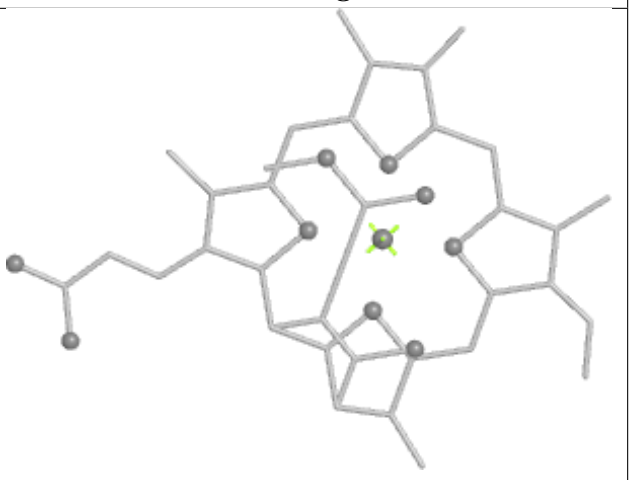
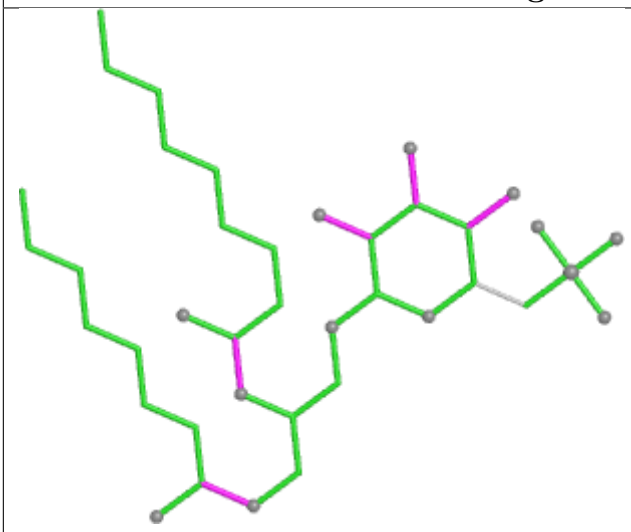
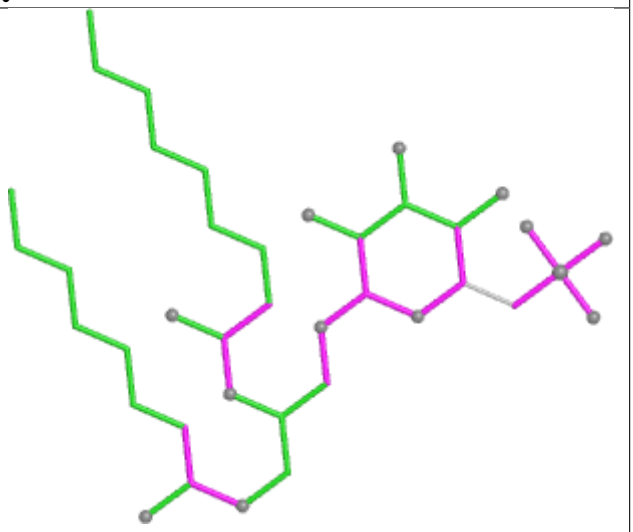


Rings

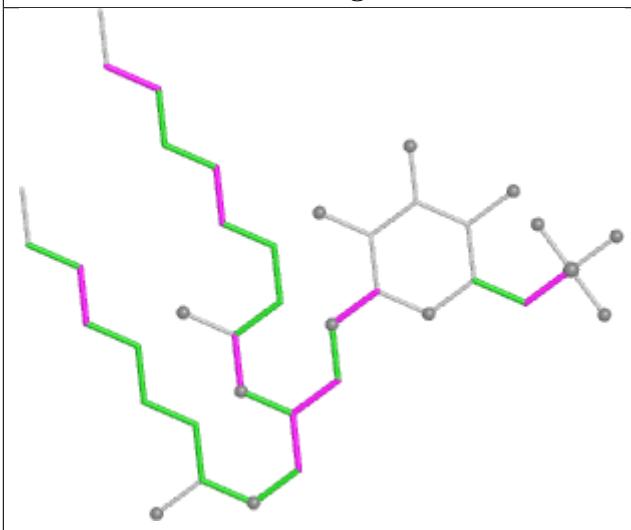
Ligand SQD S 301



Bond lengths



Bond angles



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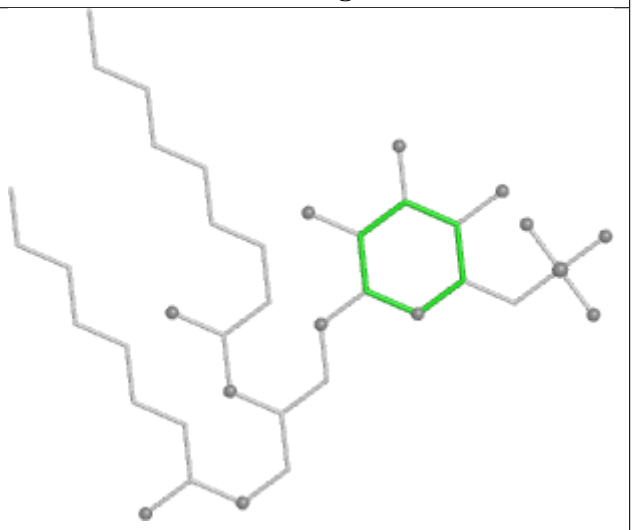
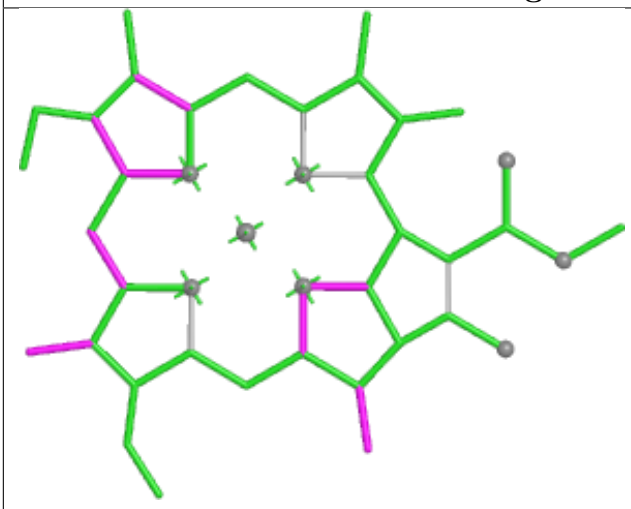


Rings

Ligand CLA P 314



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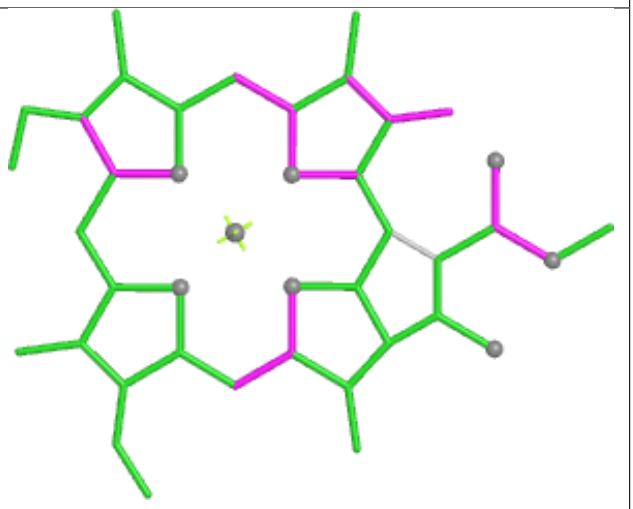
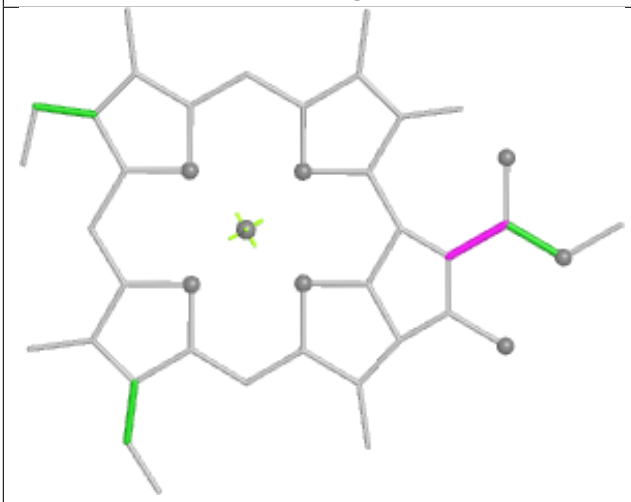


Bond angles



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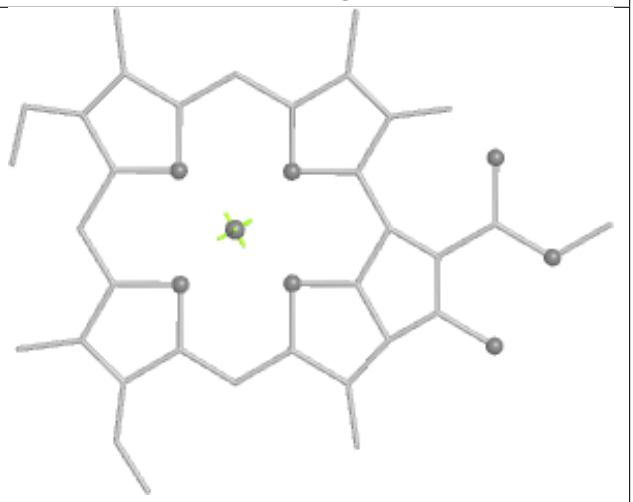
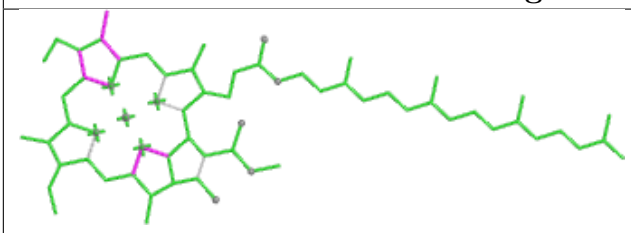


Rings

Ligand CLA P 311



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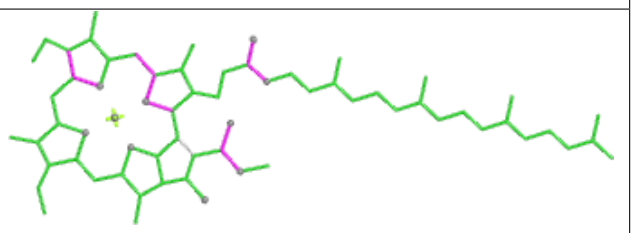
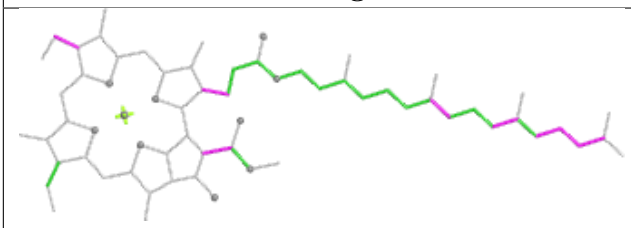


Bond angles



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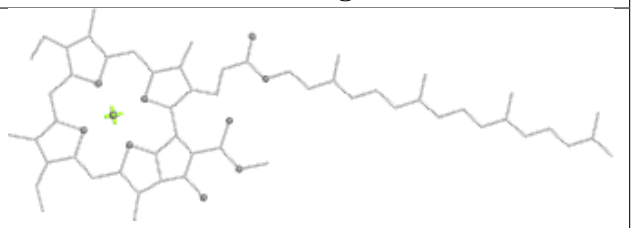
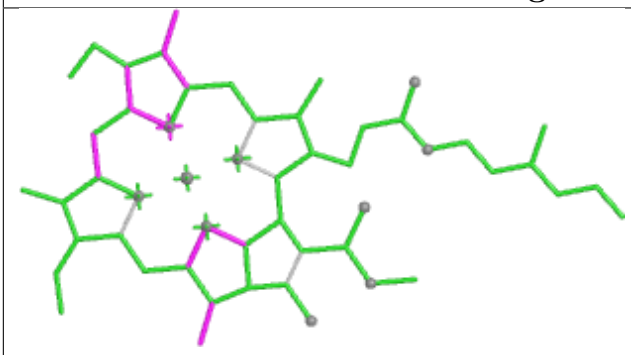


Rings

Ligand CLA 4 322



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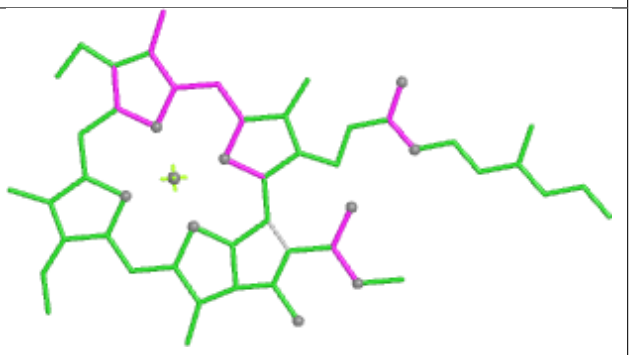
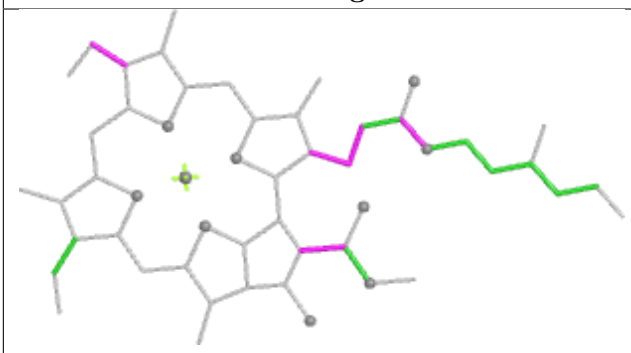


Bond angles



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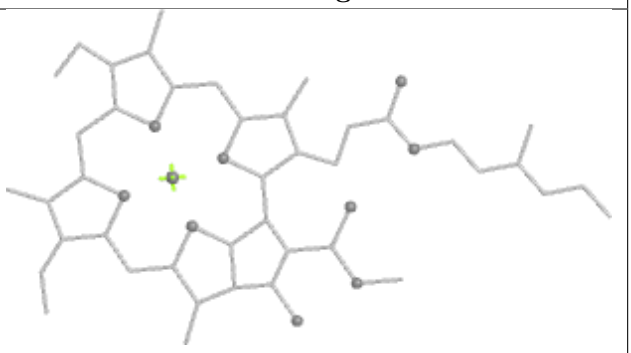
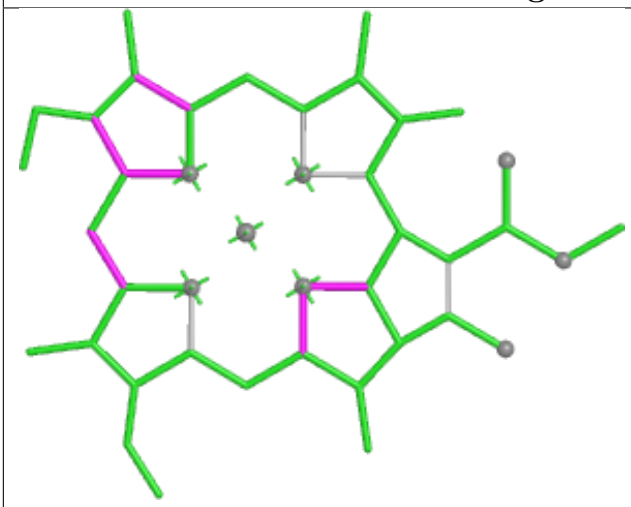
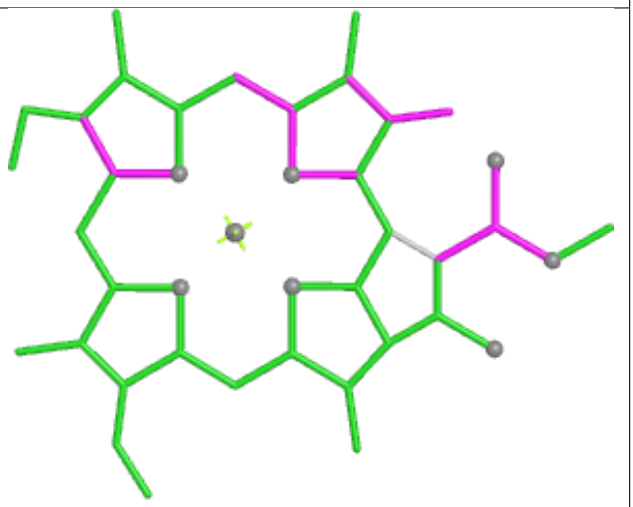


Rings

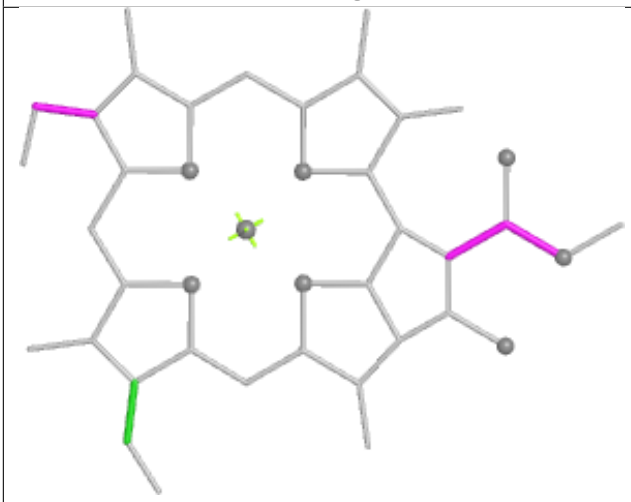
Ligand CLA x 317



Bond lengths



Bond angles



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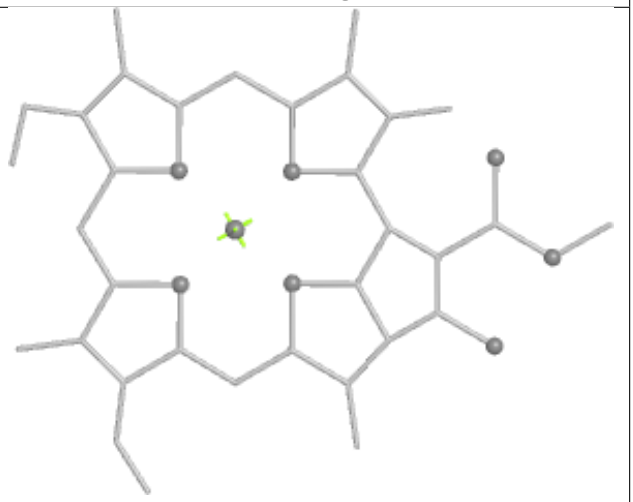
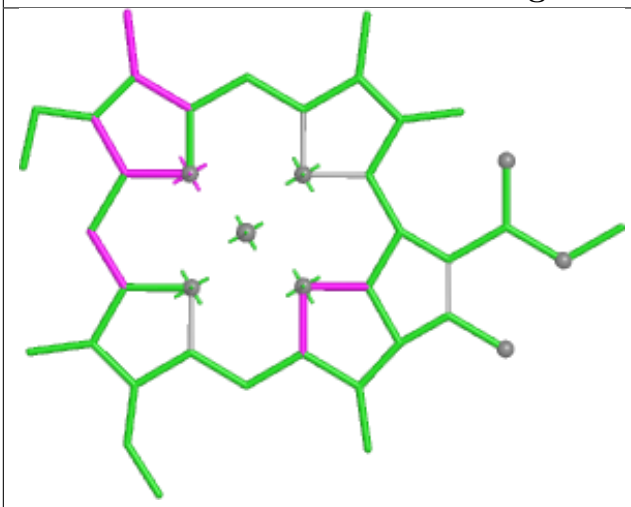


Rings

Ligand CLA 6 321



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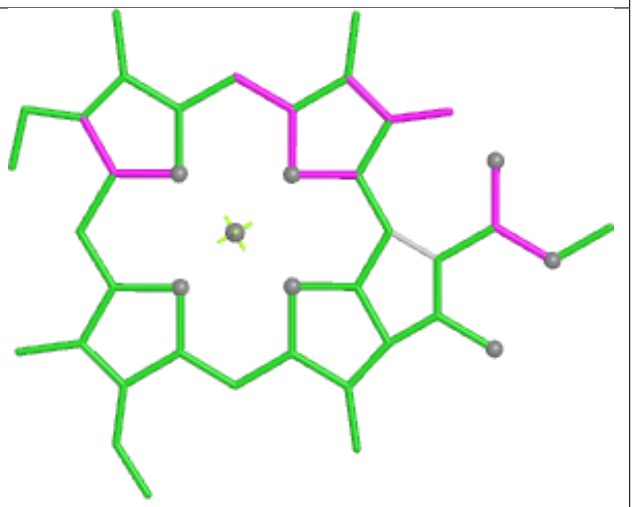
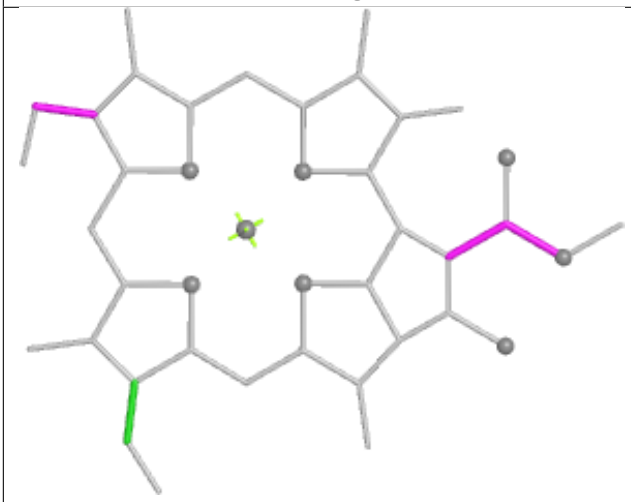


Bond angles



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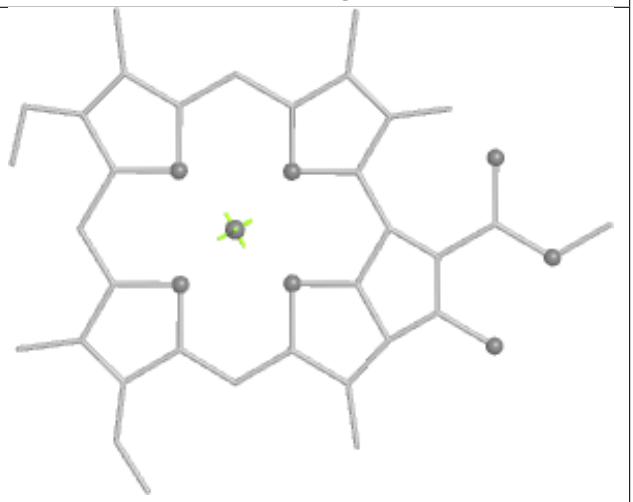
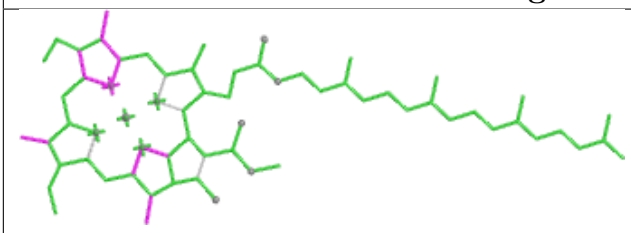


Rings

Ligand CLA a 827



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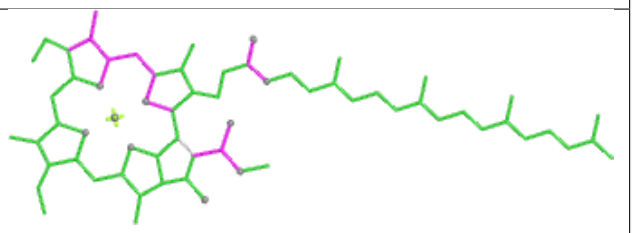
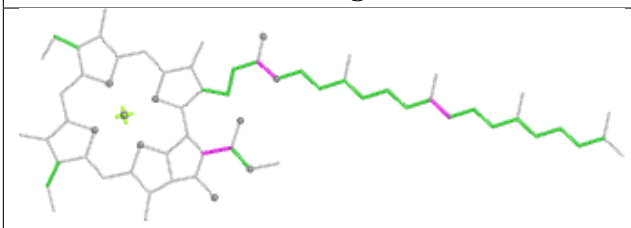
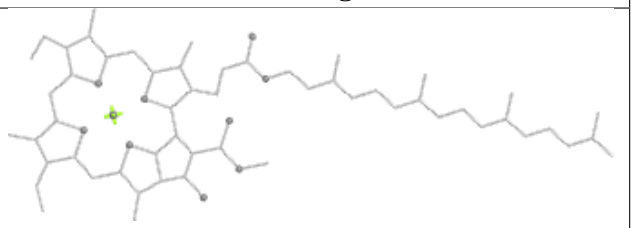


Bond angles

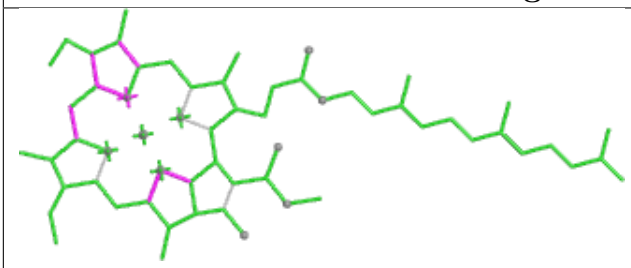


Torsions



Rings

Ligand CLA R 308



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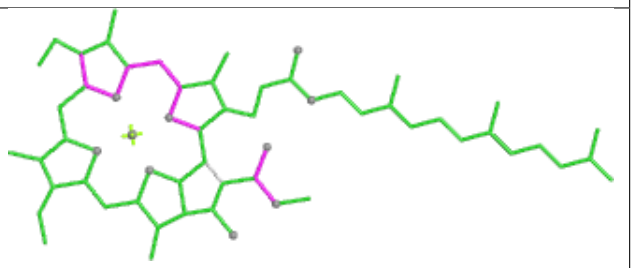

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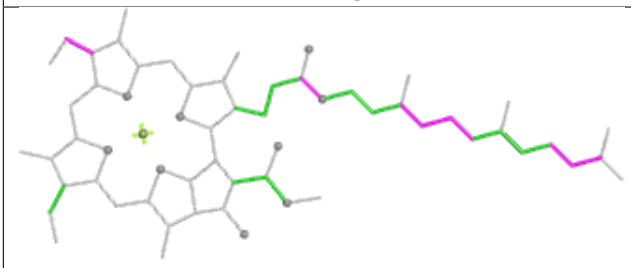

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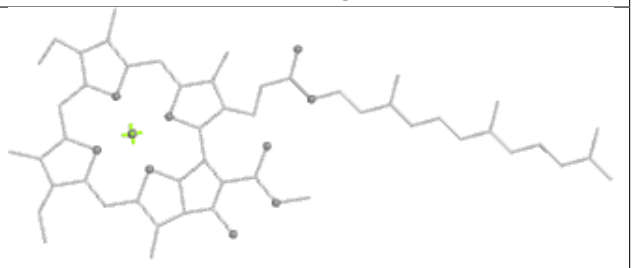
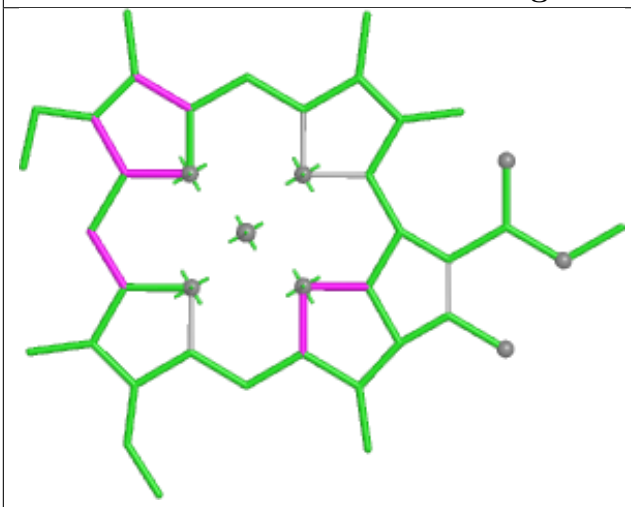


Rings

Ligand CLA I 316



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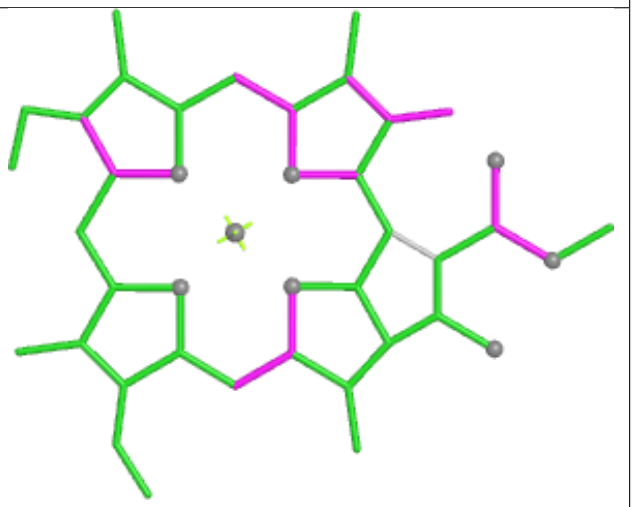
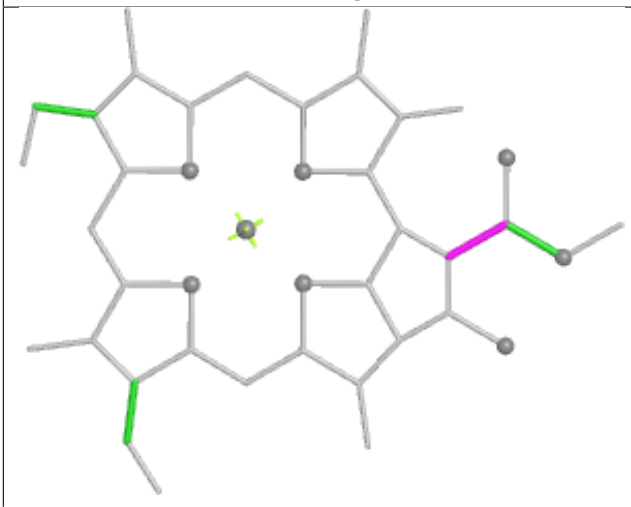


Bond angles



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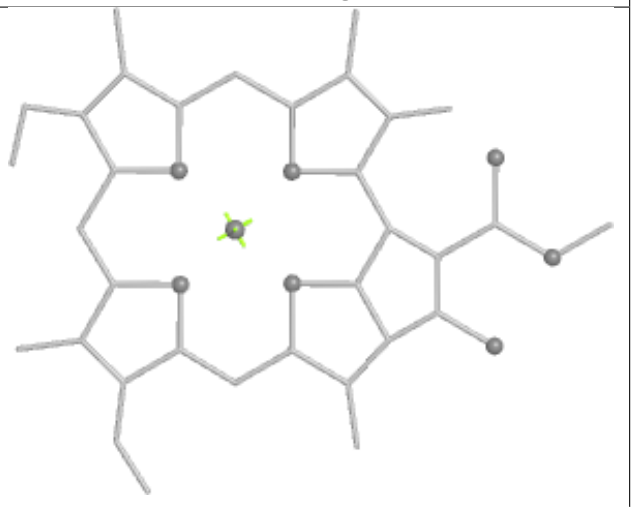
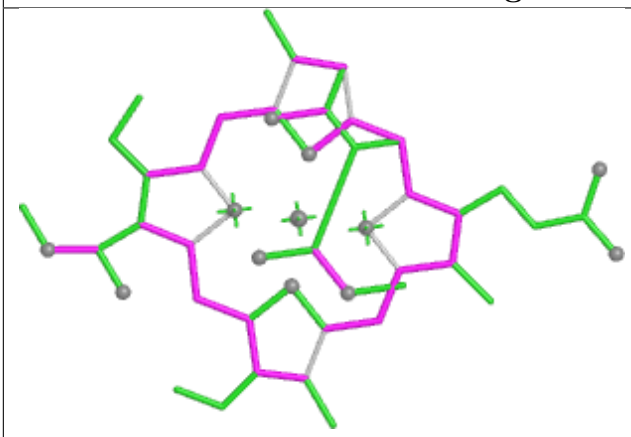


Rings

Ligand A1ECV 6 320



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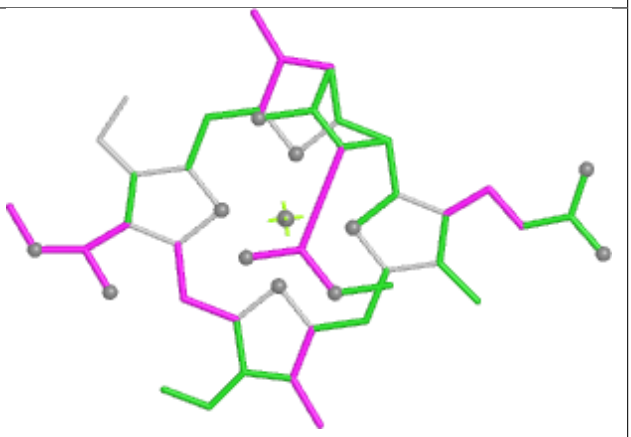
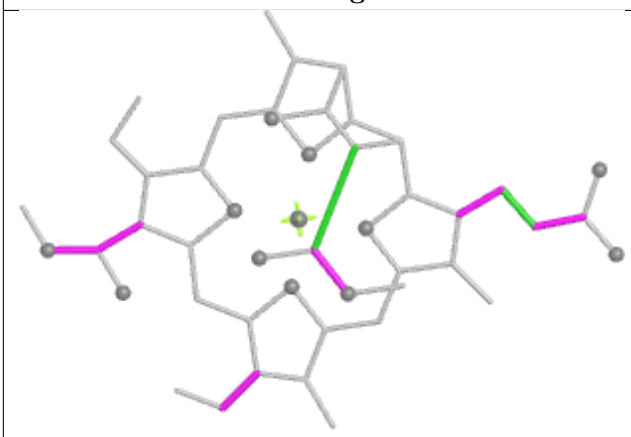


Bond angles



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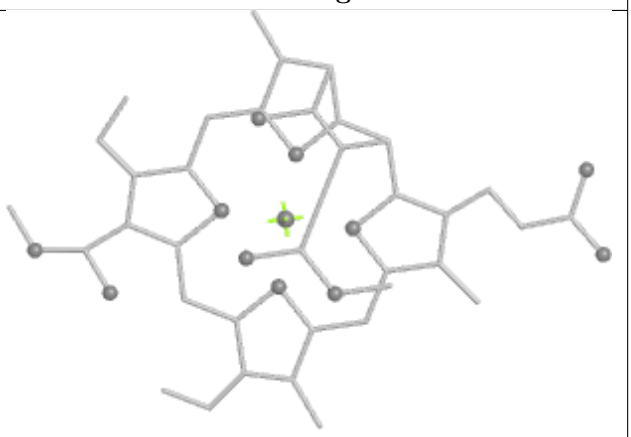
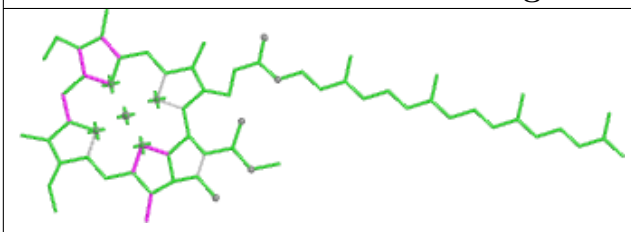


Rings

Ligand CLA D 316



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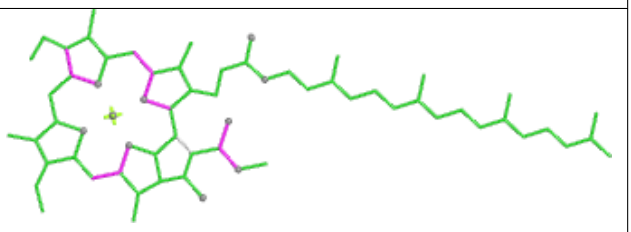
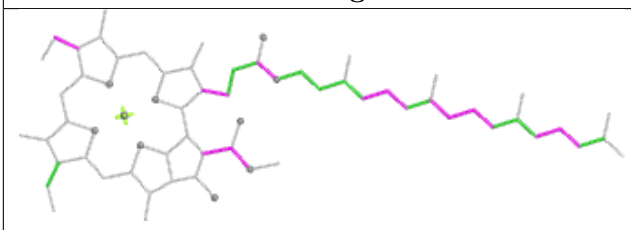


Bond angles



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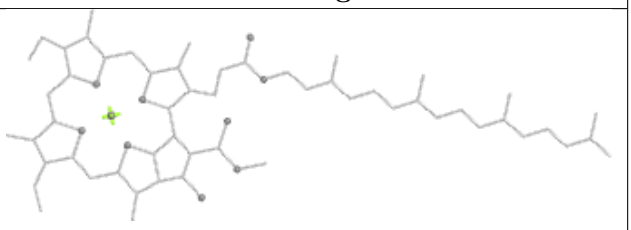
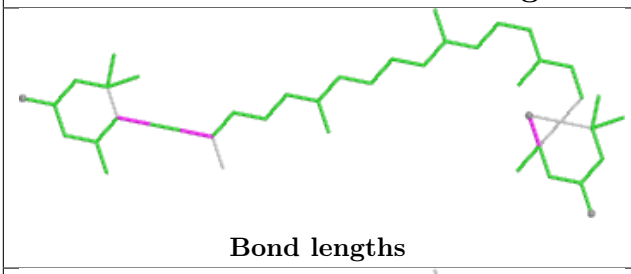


Rings

Ligand DD6 M 304



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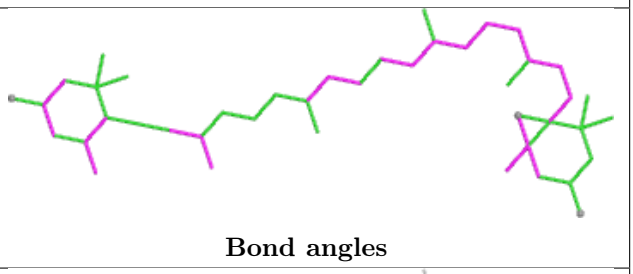
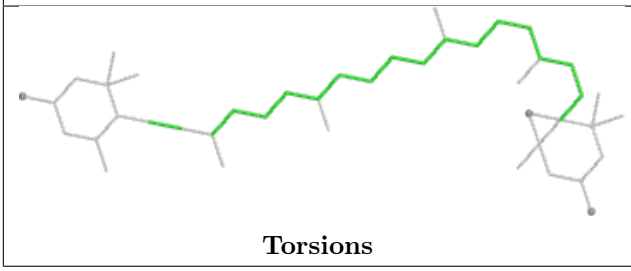
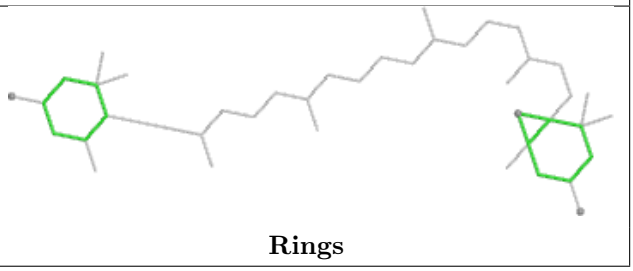


Bond angles

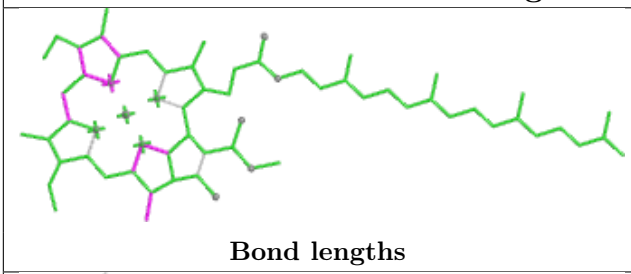


Torsions

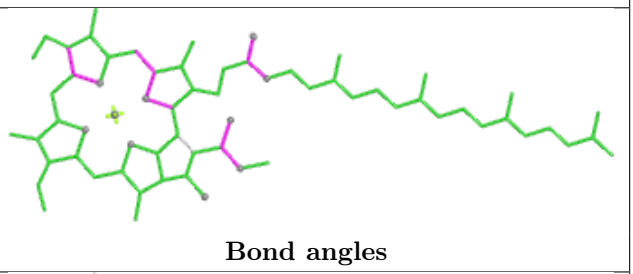


Rings

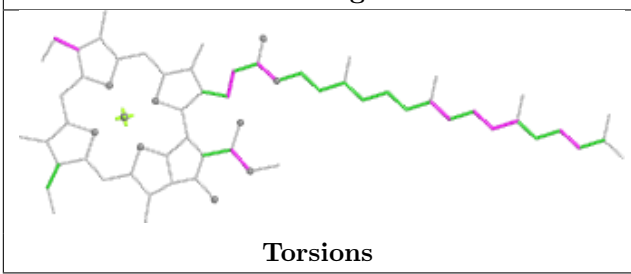
Ligand CLA P 307



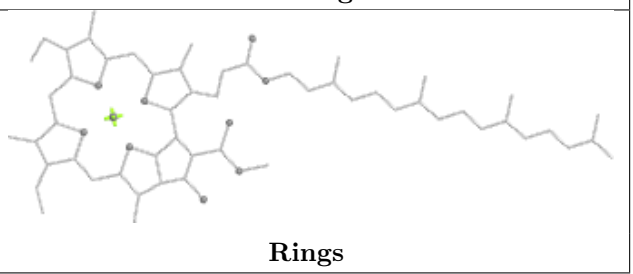
Bond lengths



Bond angles

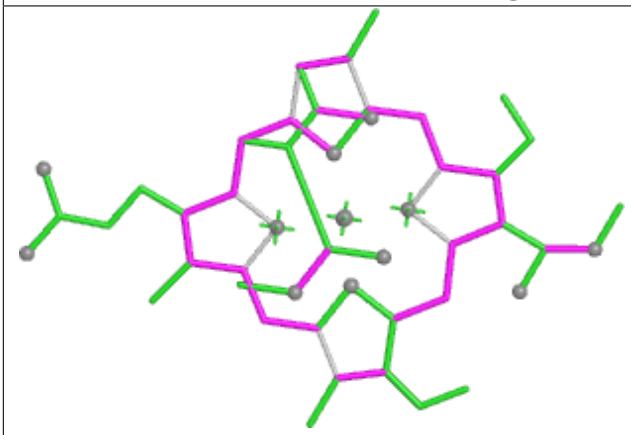


Torsions



Rings

Ligand A1ECV 9 317



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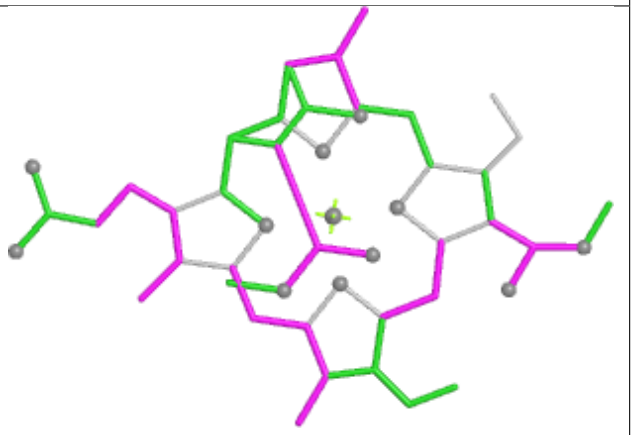
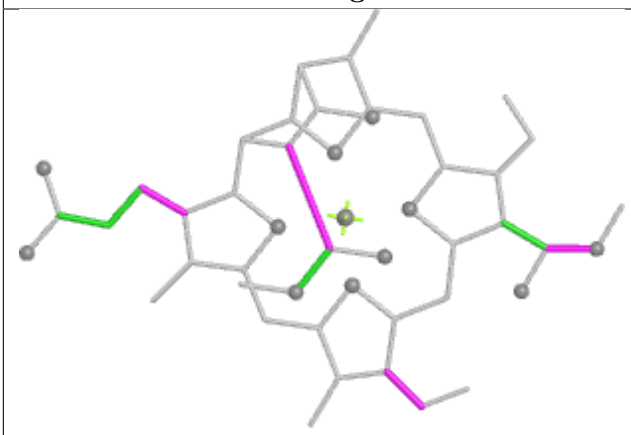


Bond angles



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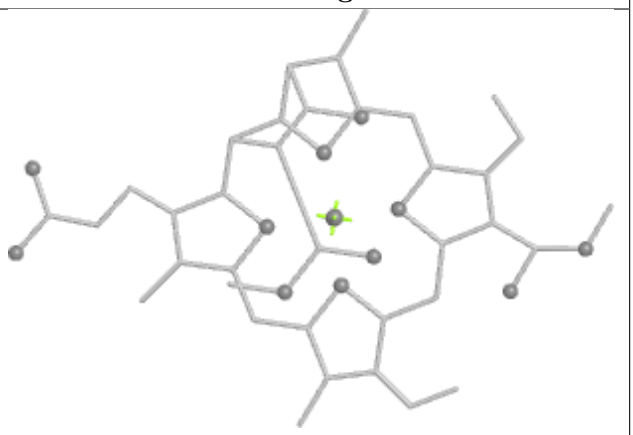
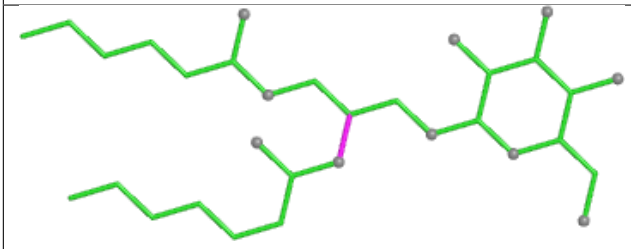


Rings

Ligand LMG 7 326



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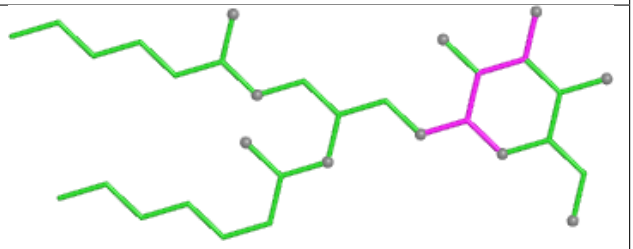
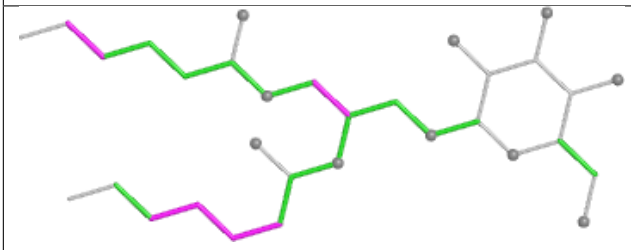
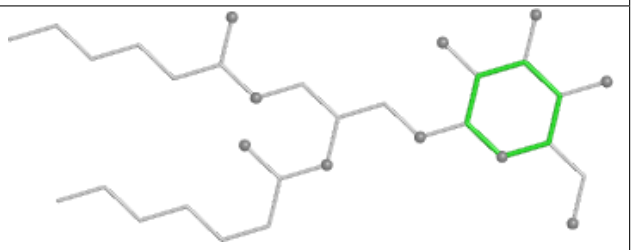


Bond angles

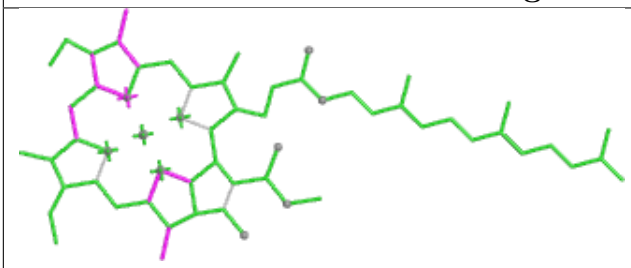


Torsions



Rings

Ligand CLA O 310



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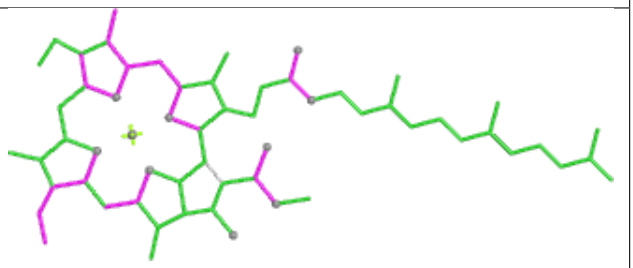
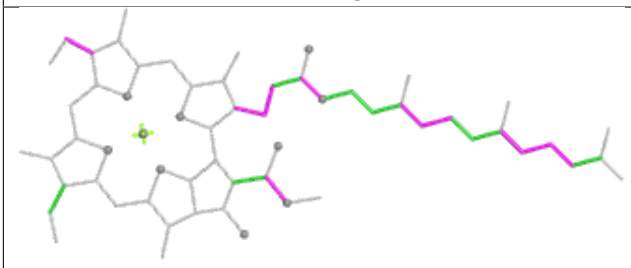


Bond angles



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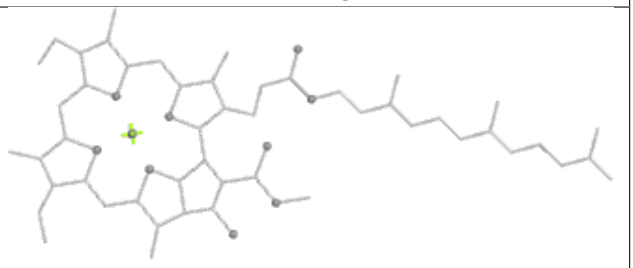
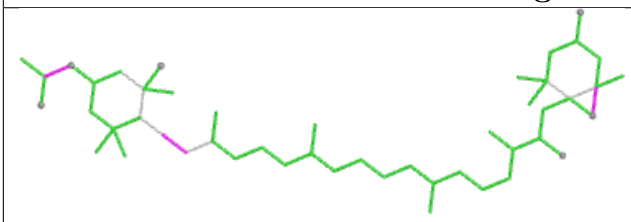


Rings

Ligand A86 7 311



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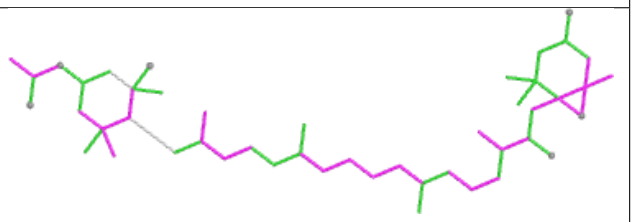
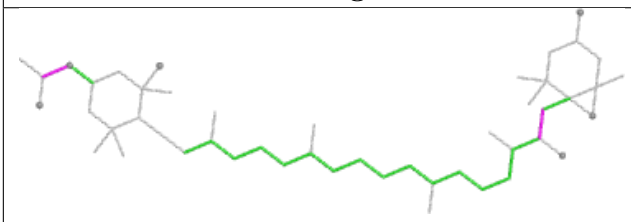


Bond angles



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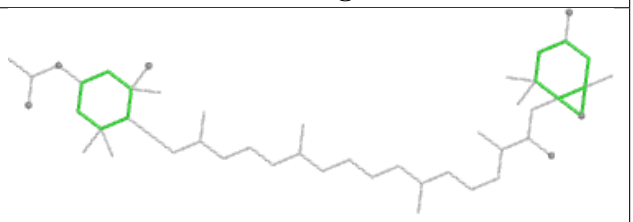
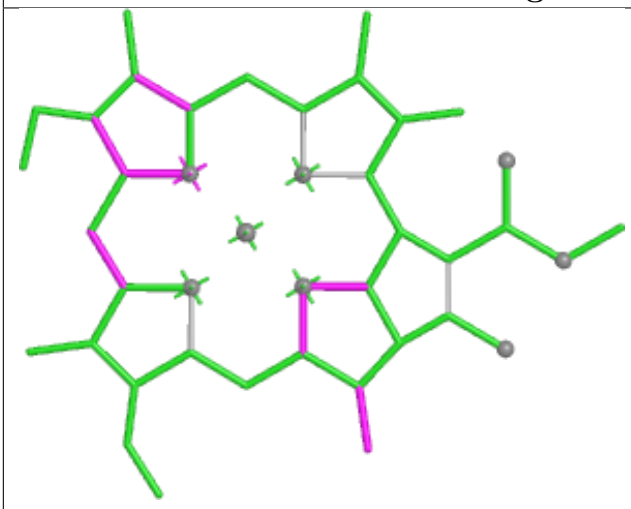


Rings

Ligand CLA Z 304



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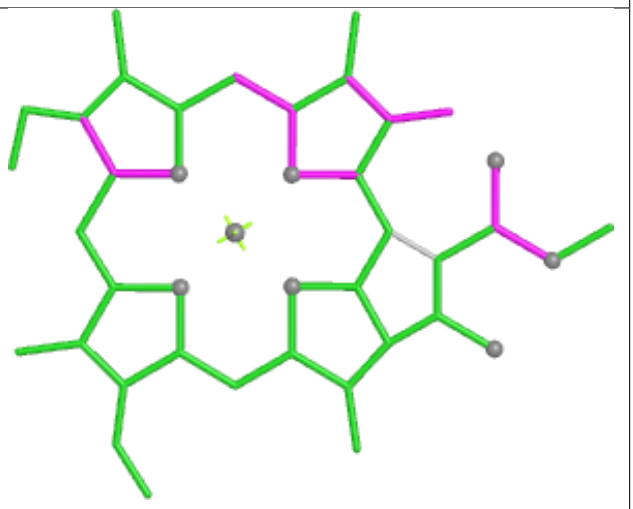
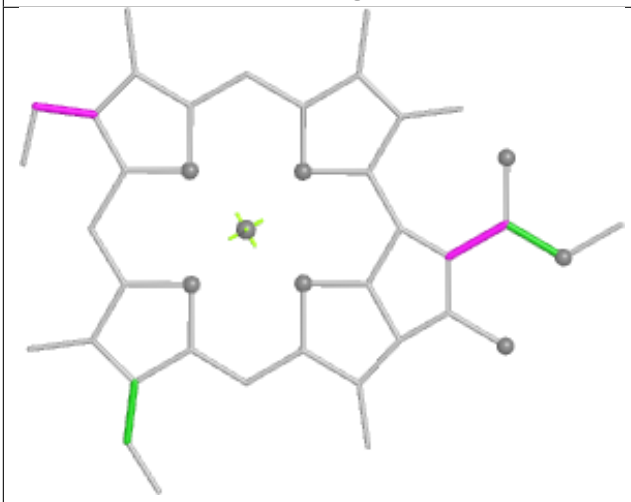


Bond angles



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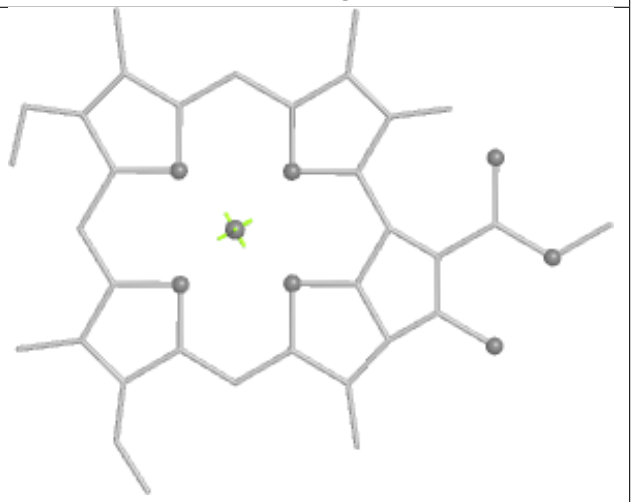
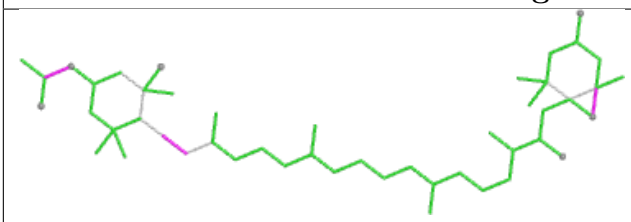


Rings

Ligand A86 Z 303



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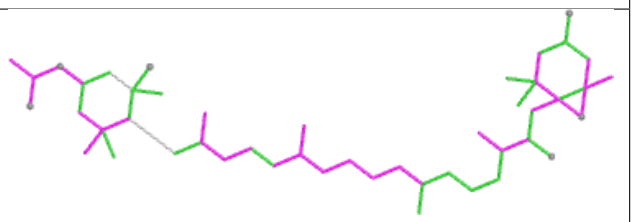
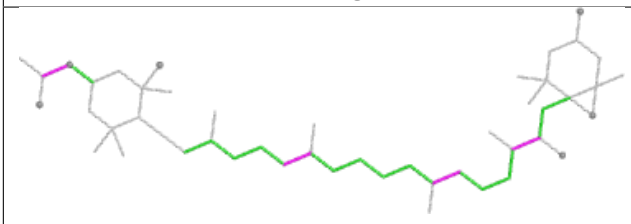


Bond angles



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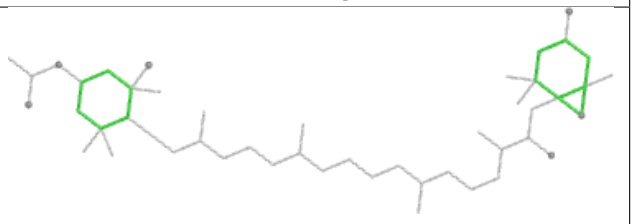
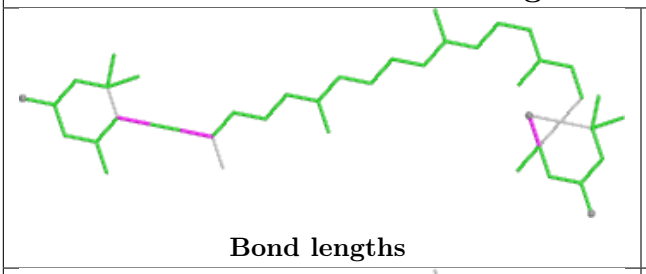


Rings

Ligand DD6 G 303



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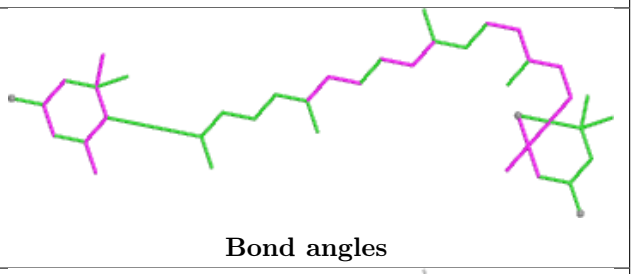
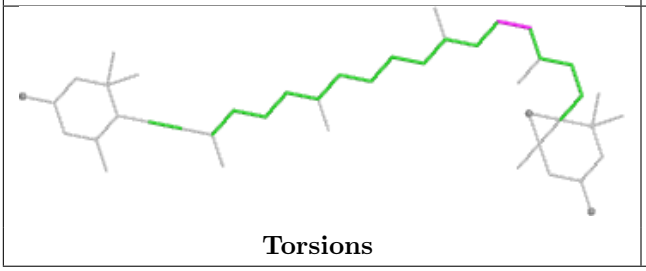
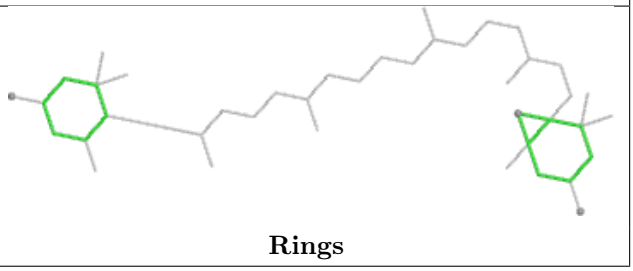


Bond angles

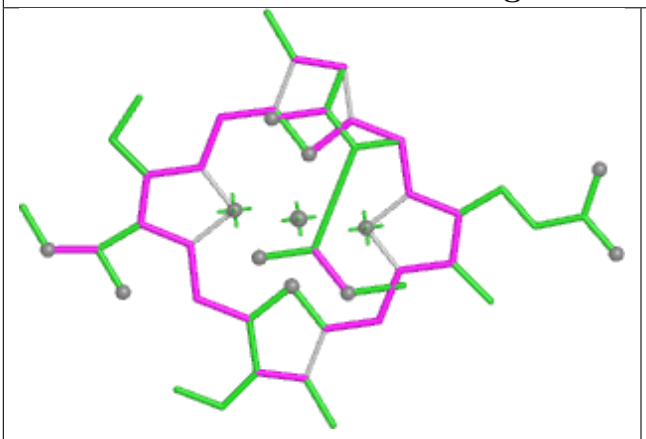


Torsions



Rings

Ligand A1ECV S 312



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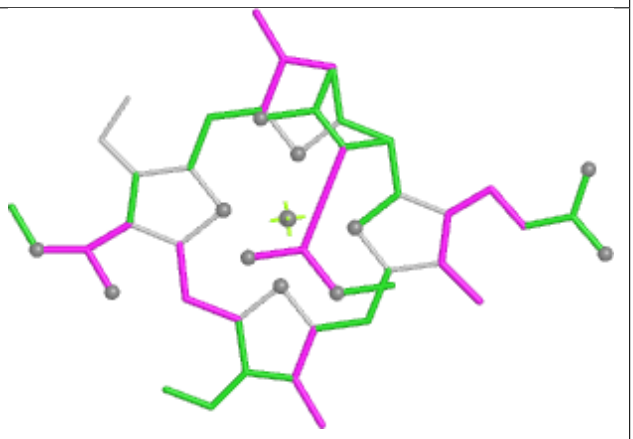
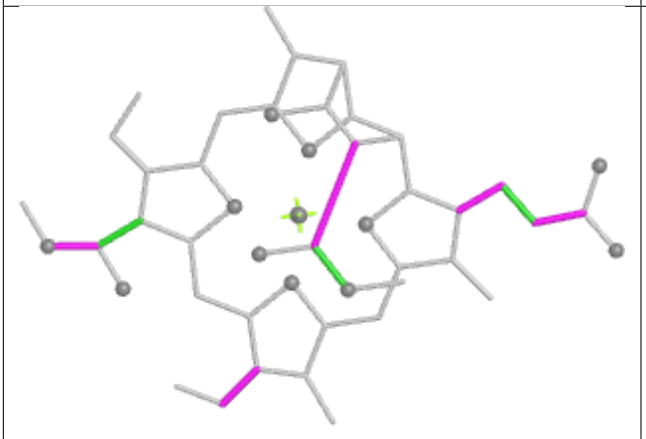


Bond angles



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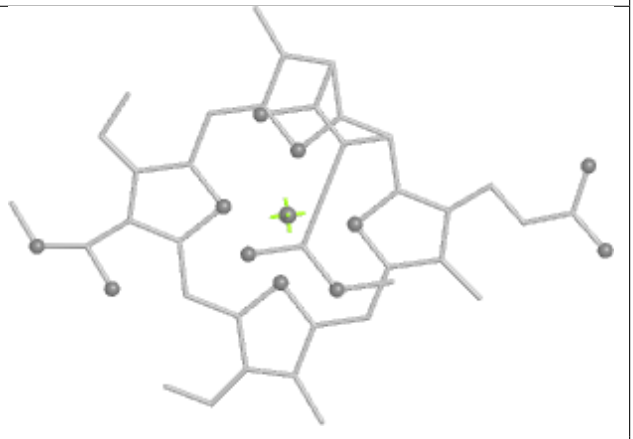
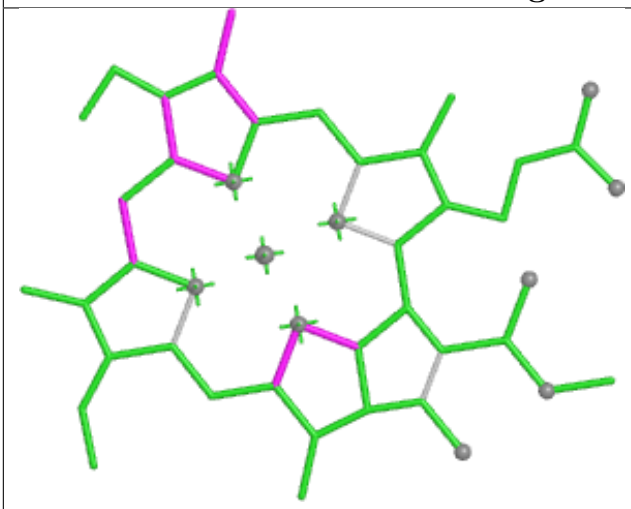


Rings

Ligand CLA a 833



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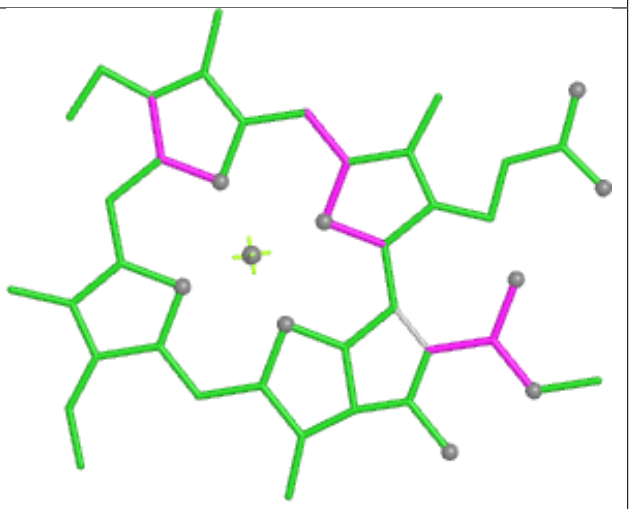
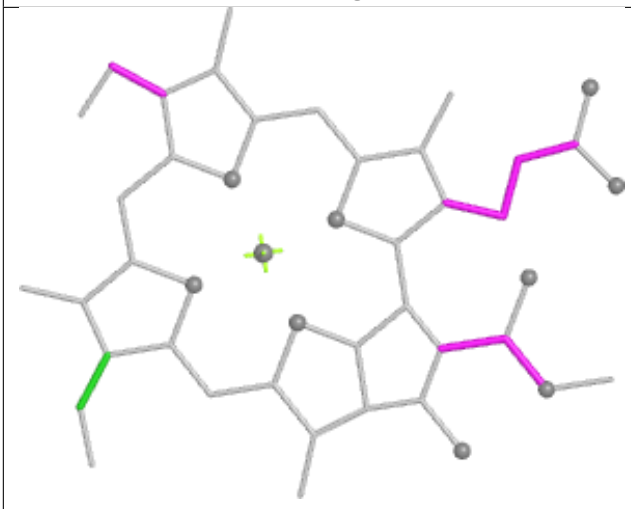


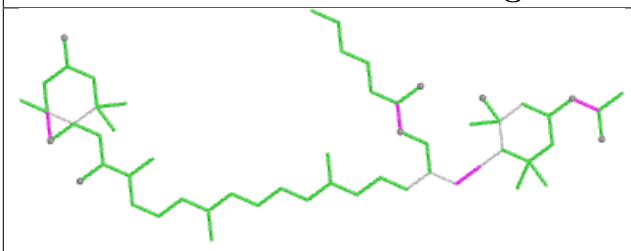
Bond angles



Torsions

Rings

Ligand A1EB1 K 304



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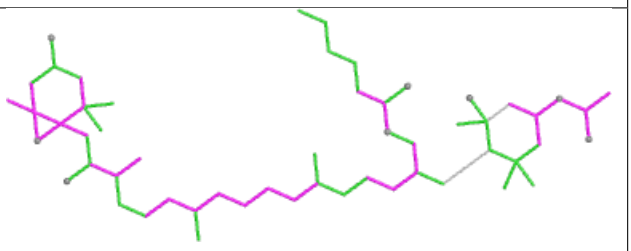
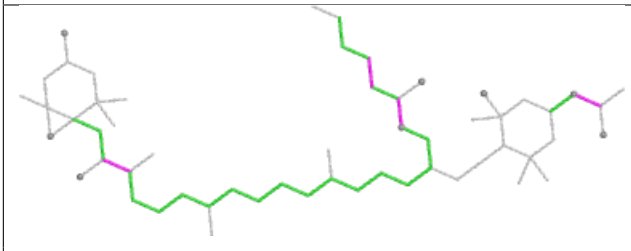
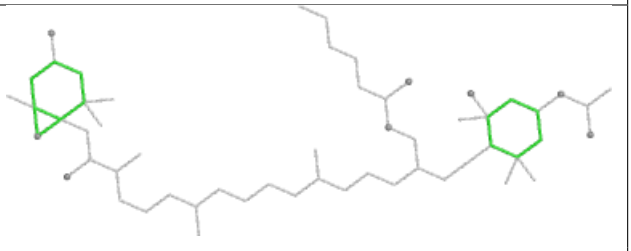


Bond angles

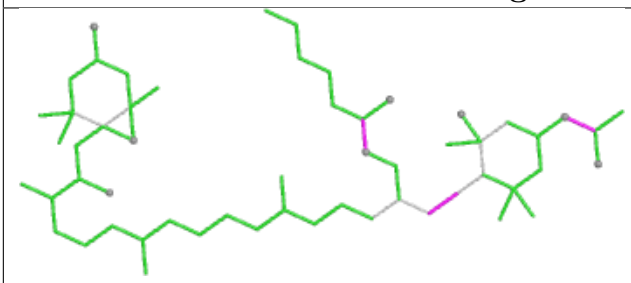


Torsions



Rings

Ligand A1EB1 6 301



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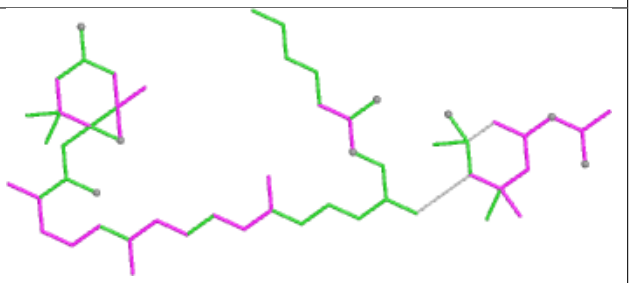
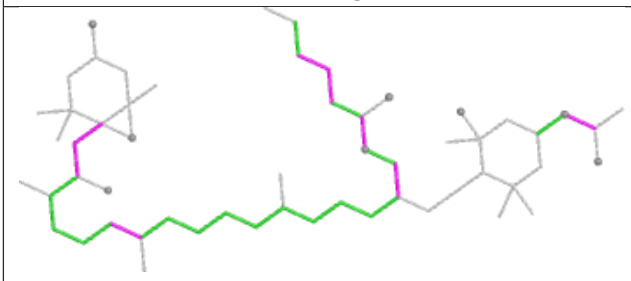
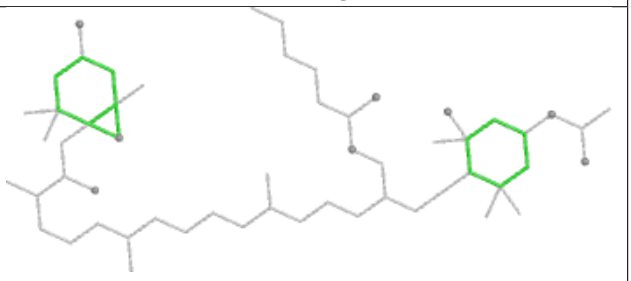


Bond angles



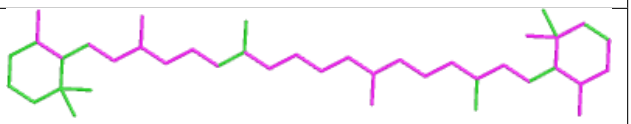
Torsions



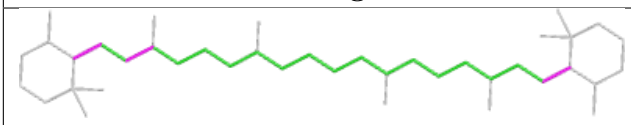
Rings

Ligand BCR h 202

Bond lengths



Bond angles



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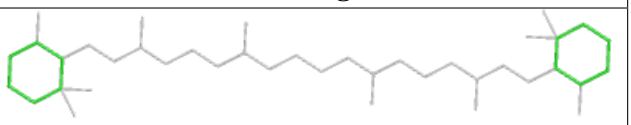
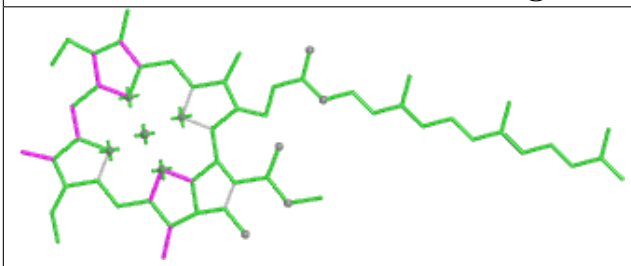


Rings

Ligand CLA b 824



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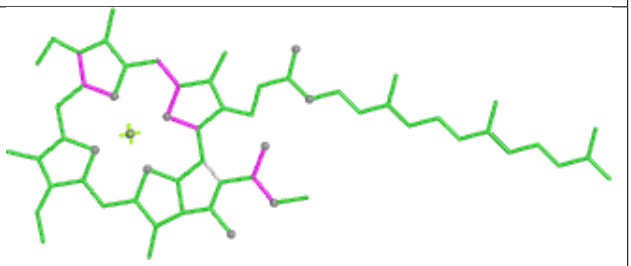
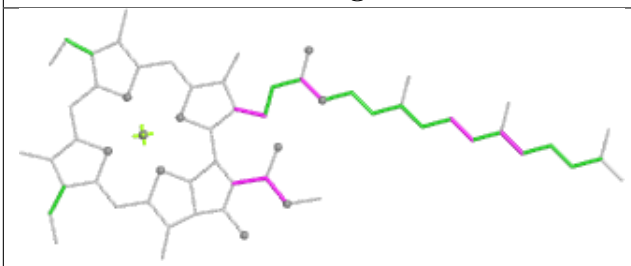
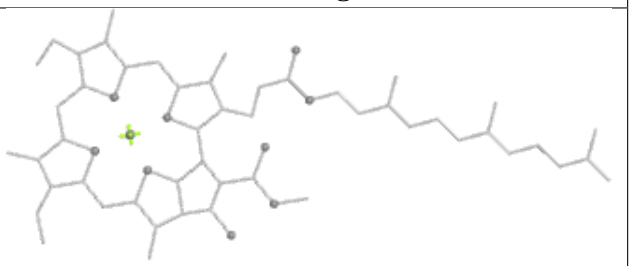


Bond angles

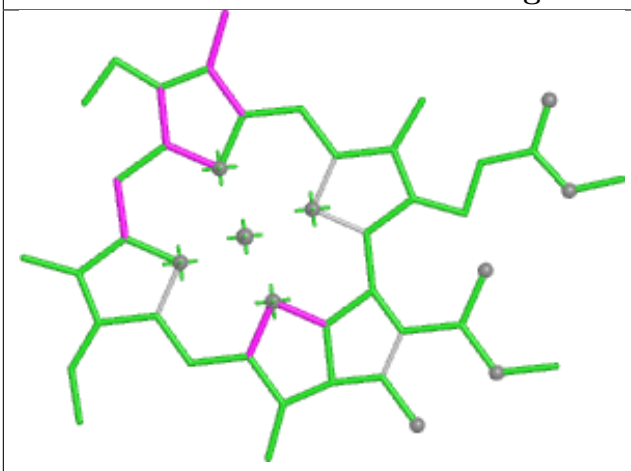


Torsions

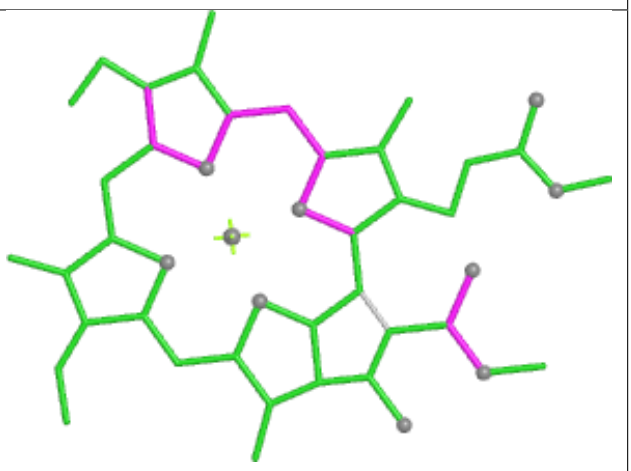


Rings

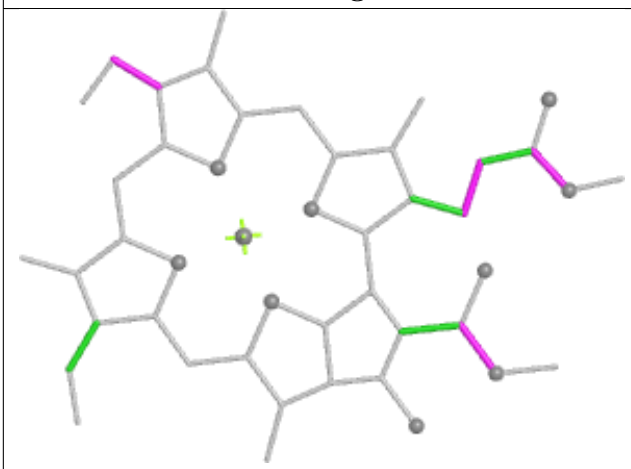
Ligand CLA U 212



Bond lengths



Bond angles



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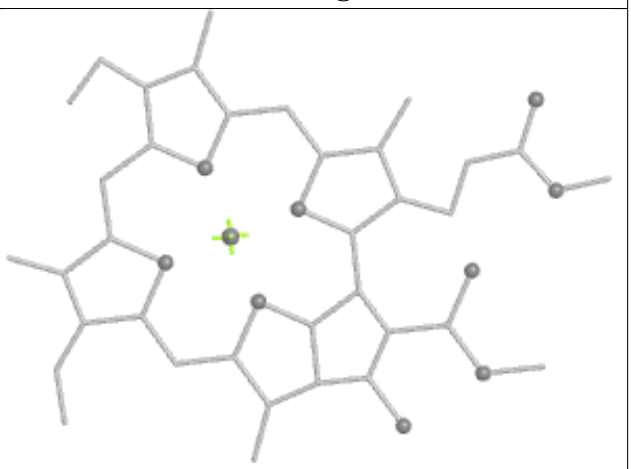
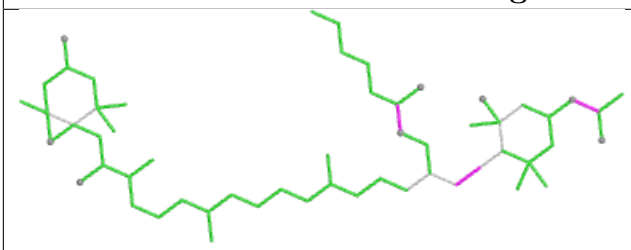


Rings

Ligand A1EB1 0 303



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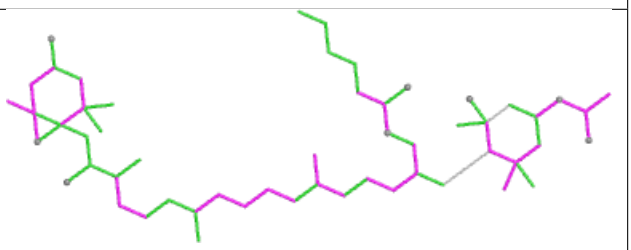

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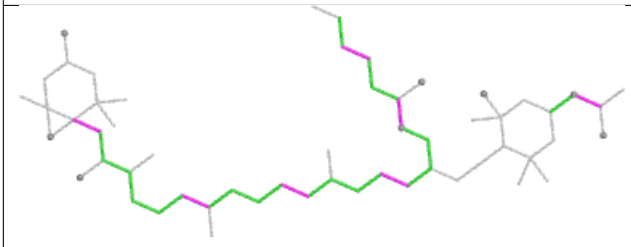

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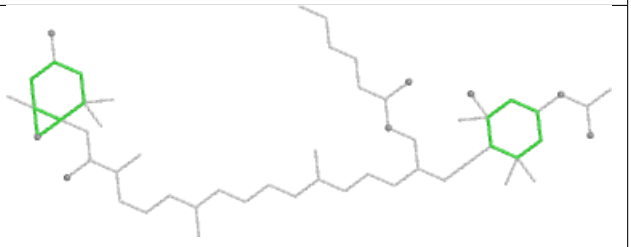
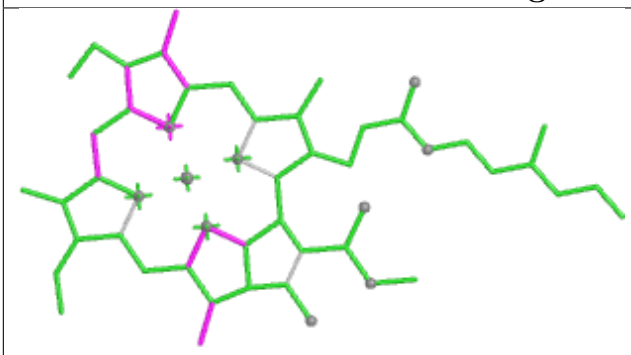


Rings

Ligand CLA 5 316



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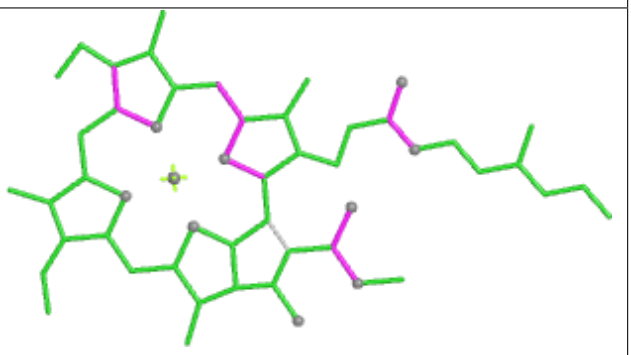
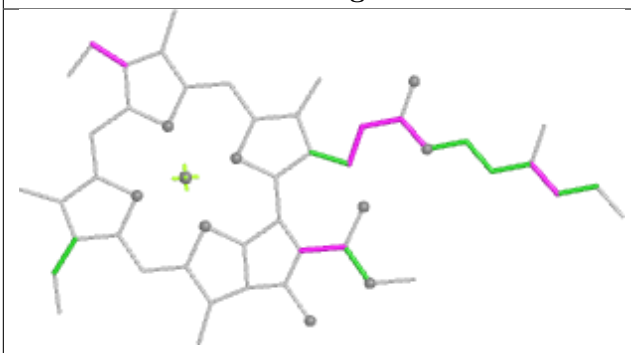


Bond angles



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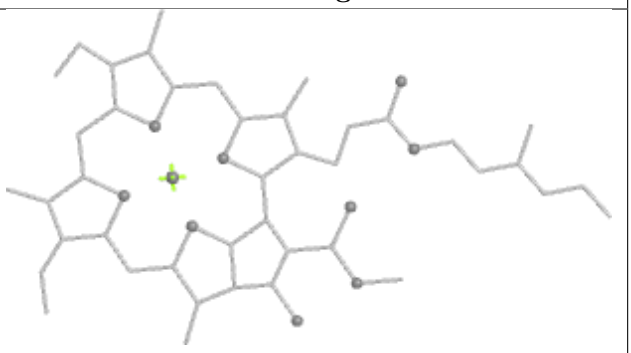
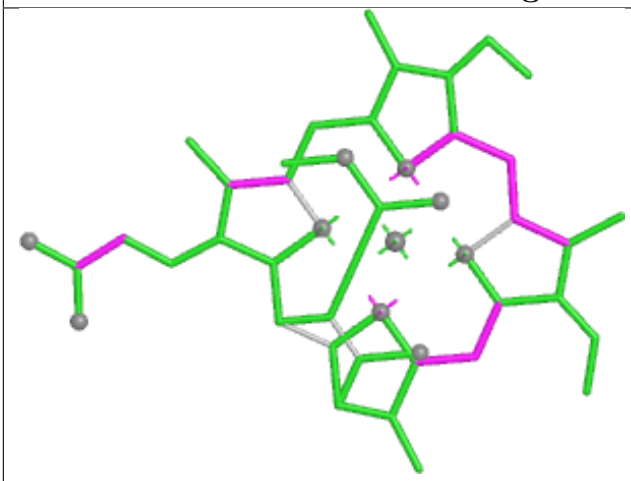


Rings

Ligand KC2 M 307



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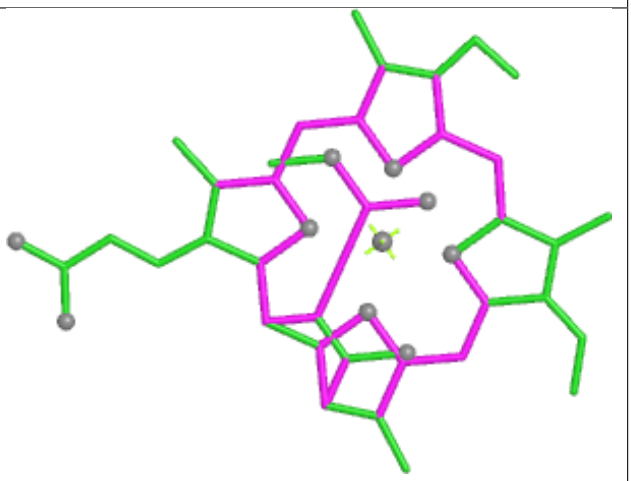

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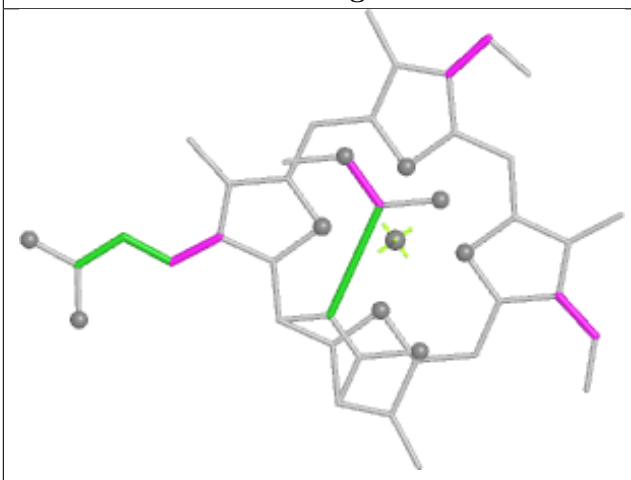

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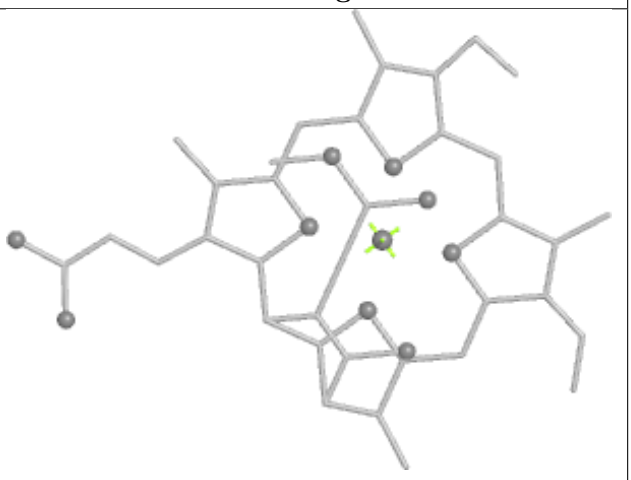
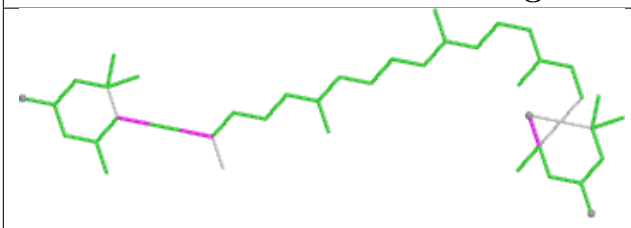


Rings

Ligand DD6 X 304



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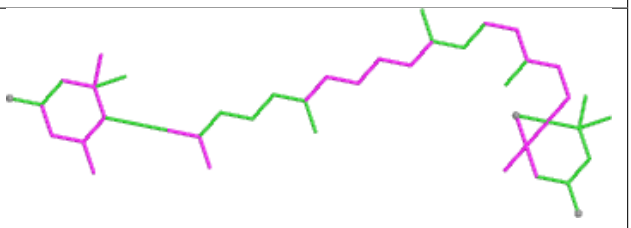

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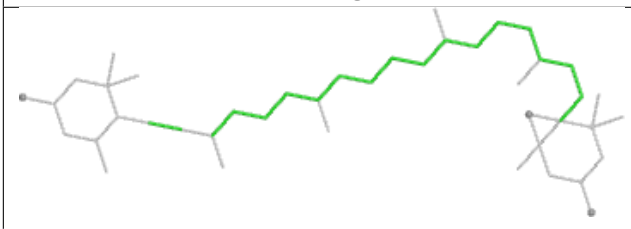
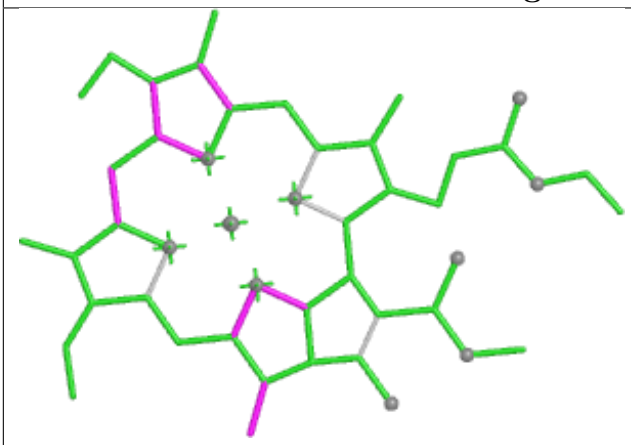


Torsions

Rings

Ligand CLA Q 320



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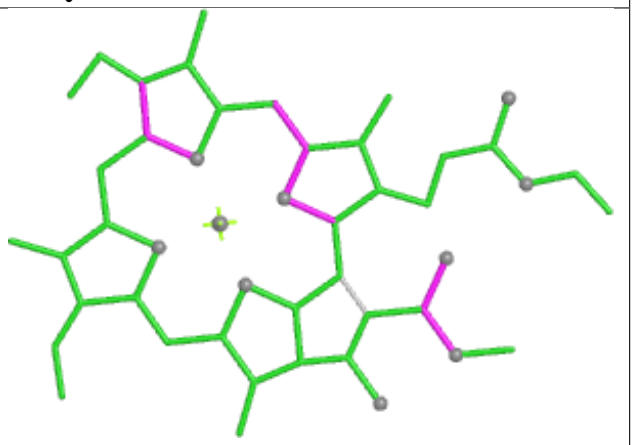
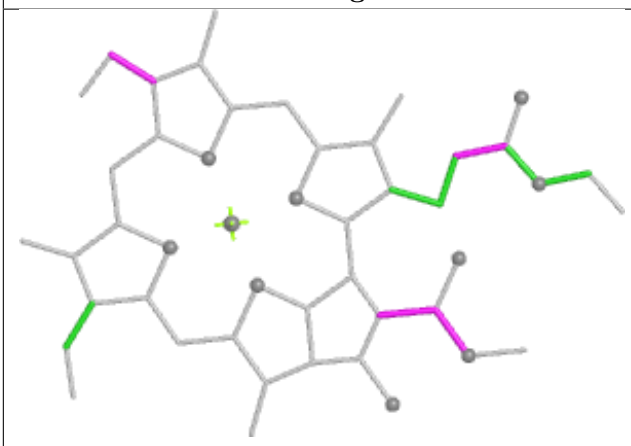


Bond angles



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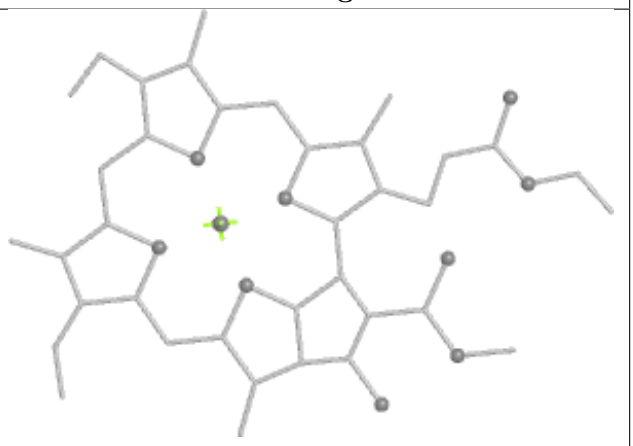
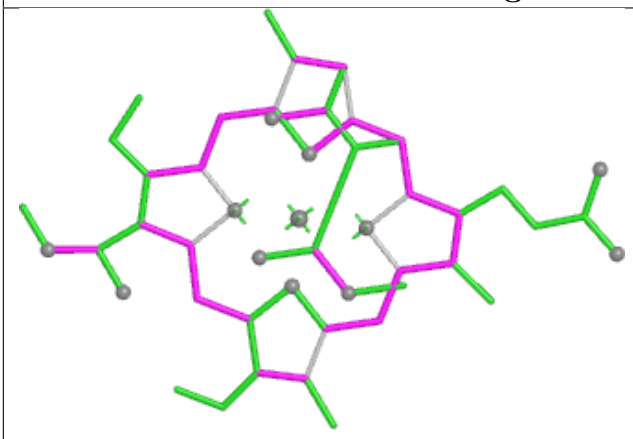


Rings

Ligand A1ECV x 316



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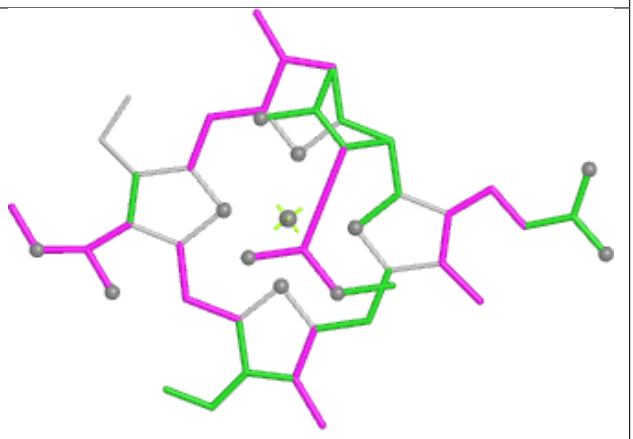
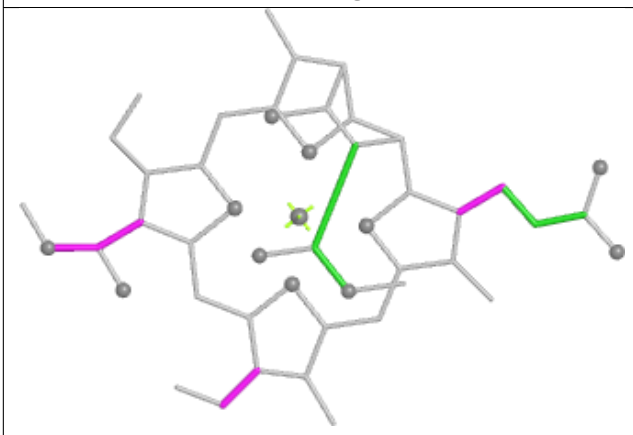


Bond angles



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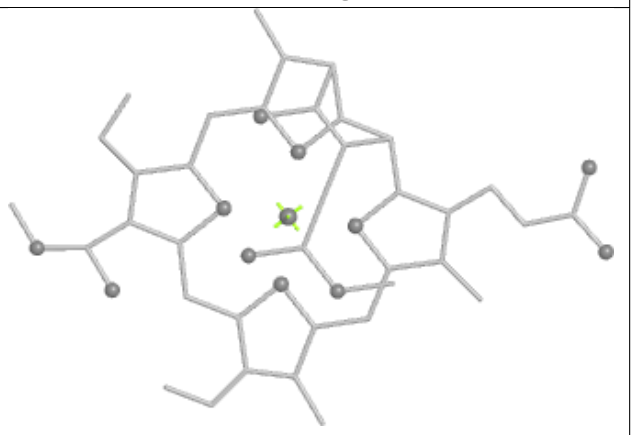
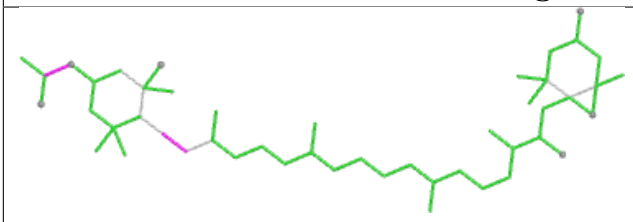


Rings

Ligand A86 7 308



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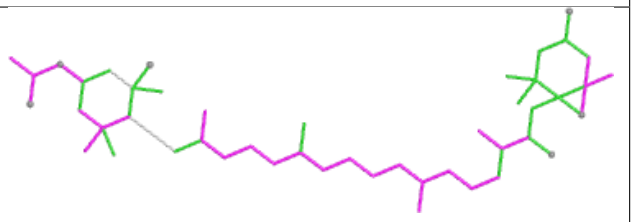

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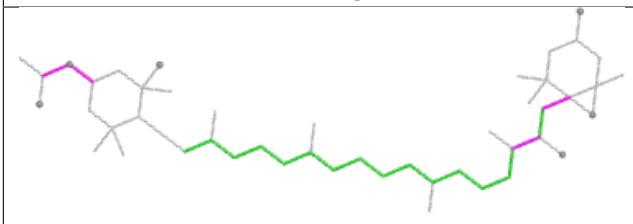

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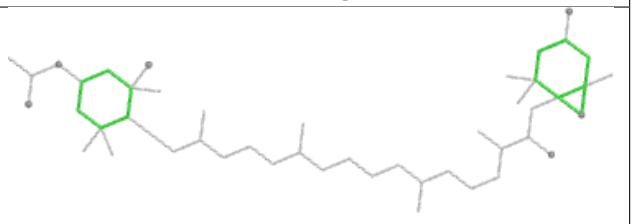
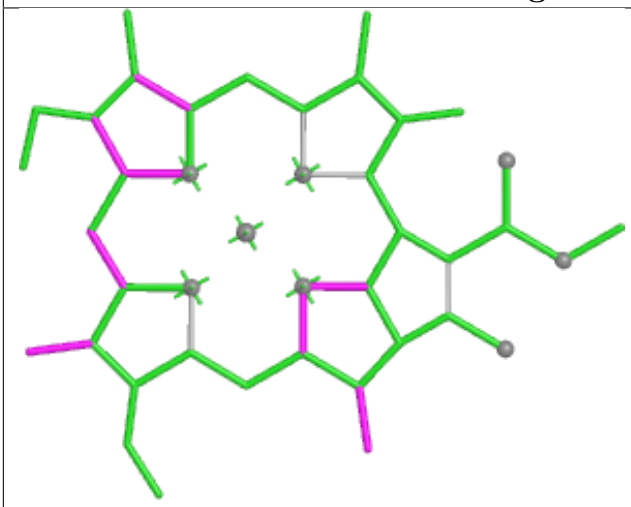


Rings

Ligand CLA 2 315



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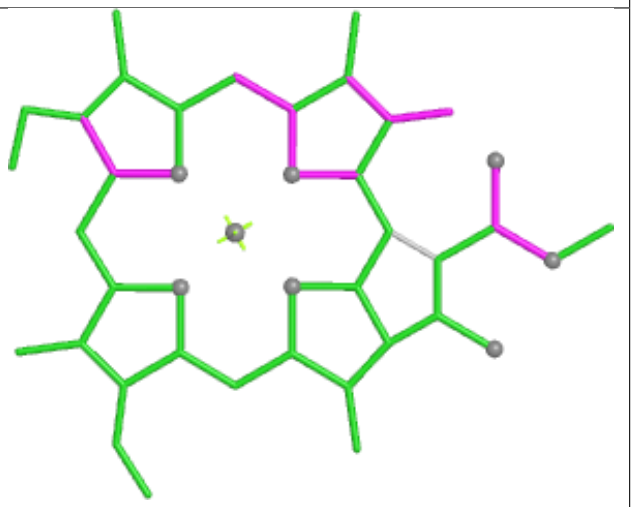
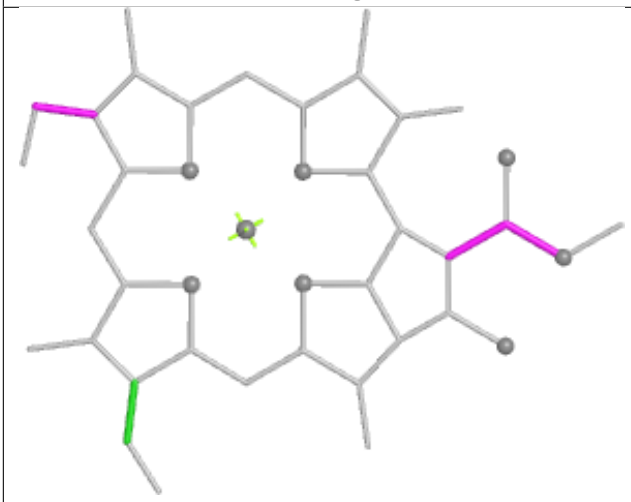


Bond angles



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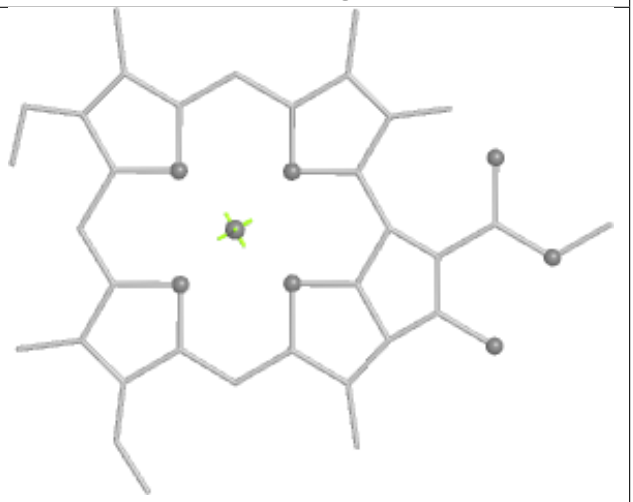
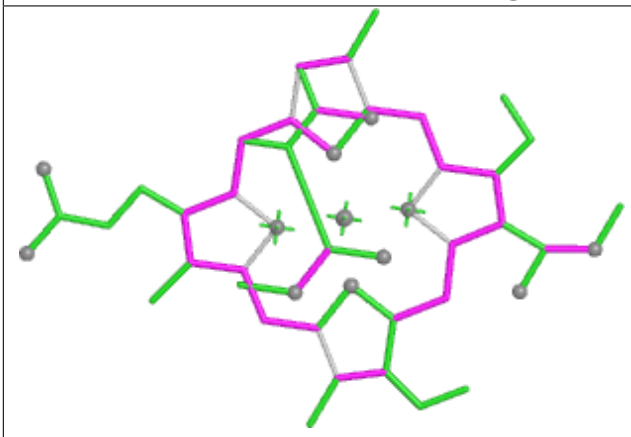


Rings

Ligand A1ECV 2 311



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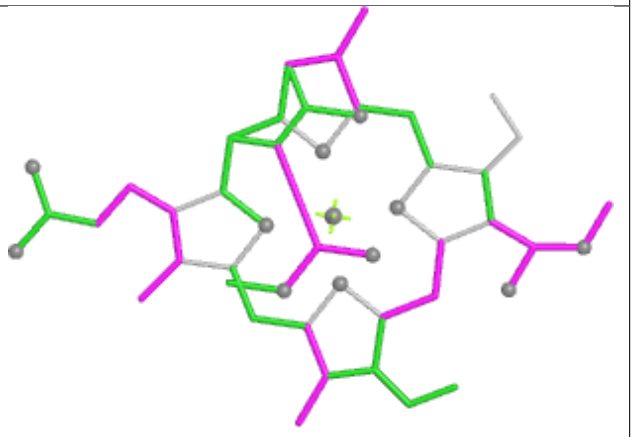
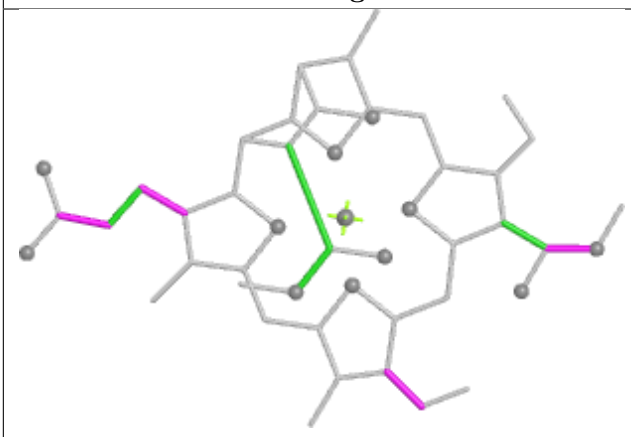
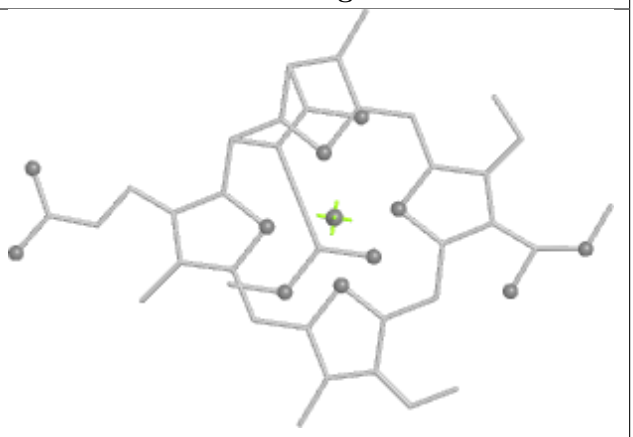


Bond angles

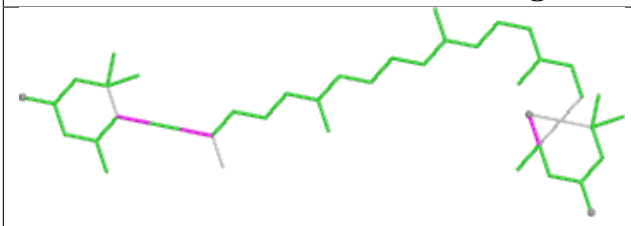


Torsions



Rings

Ligand DD6 J 306



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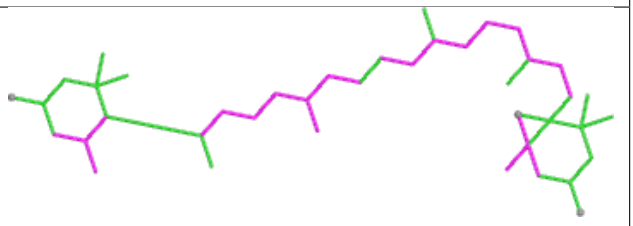
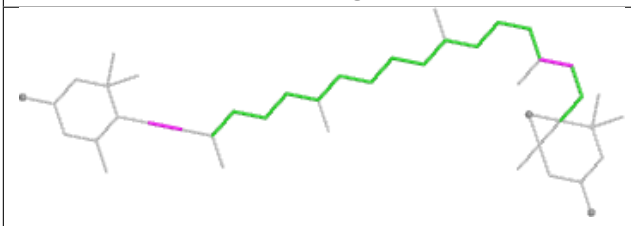


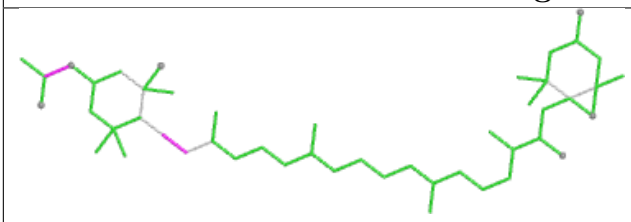
Bond angles



Torsions

Rings

Ligand A86 4 306



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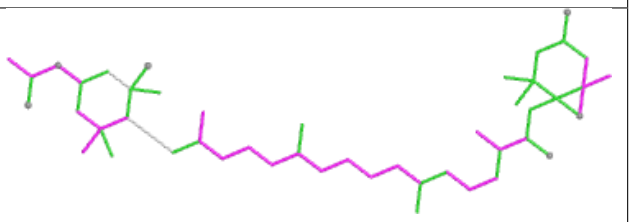
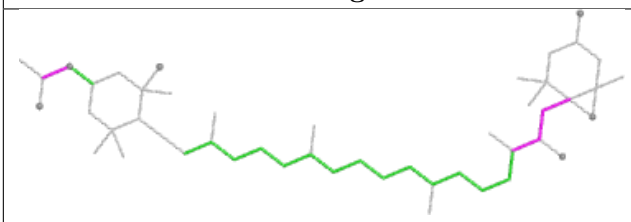


Bond angles



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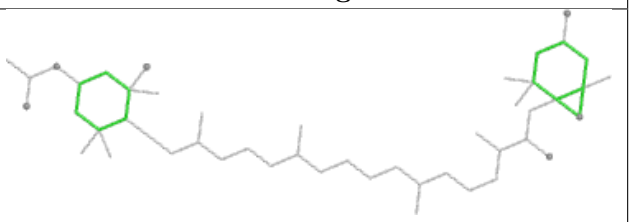
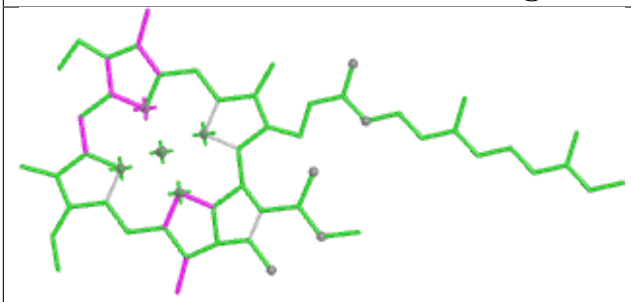


Rings

Ligand CLA G 309



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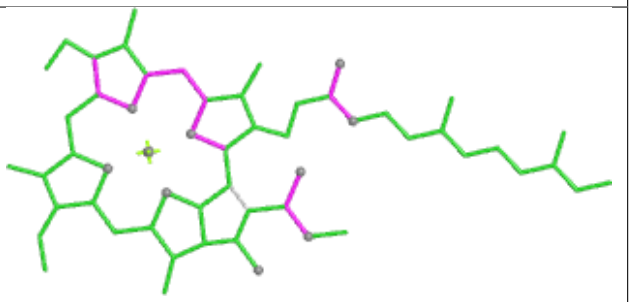
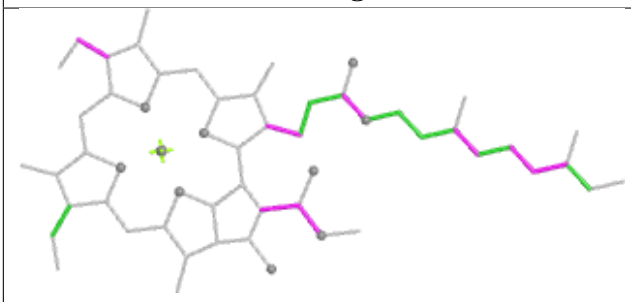


Bond angles



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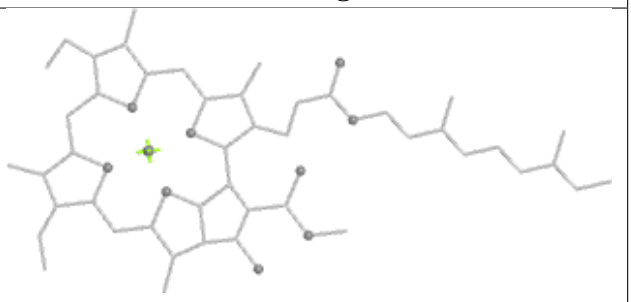
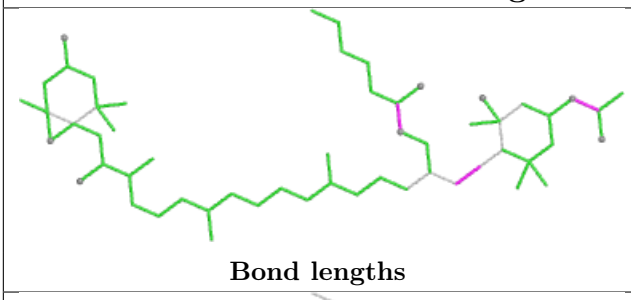


Rings

Ligand A1EB1 S 303



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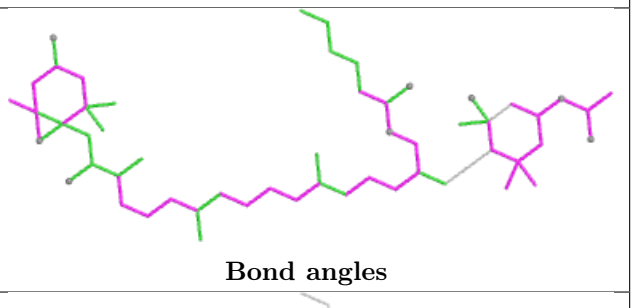
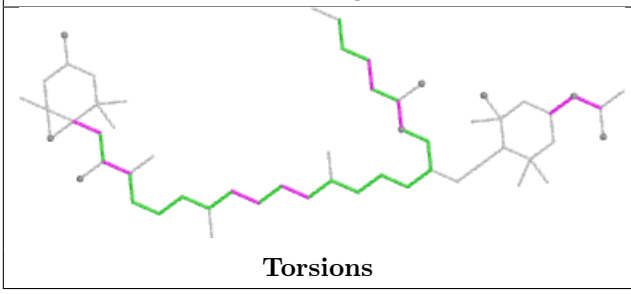
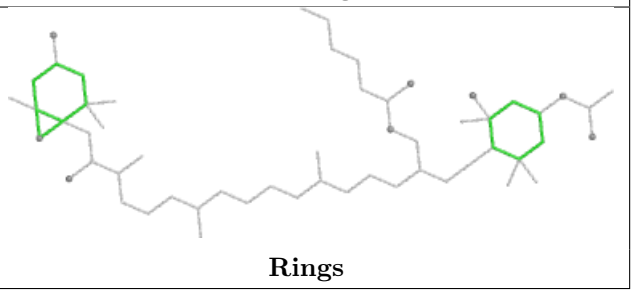


Bond angles

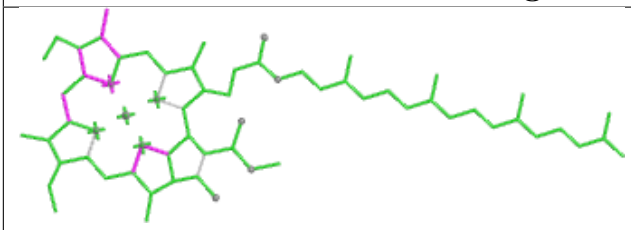


Torsions

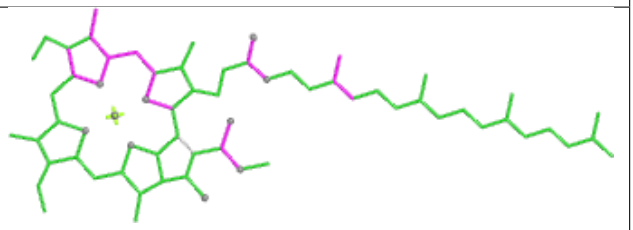


Rings

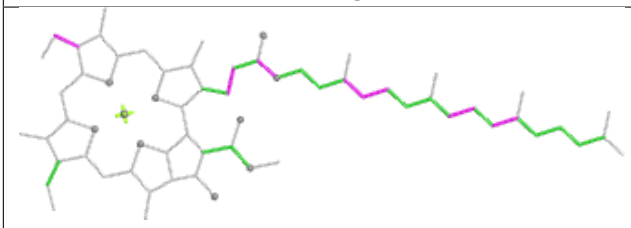
Ligand CLA V 309



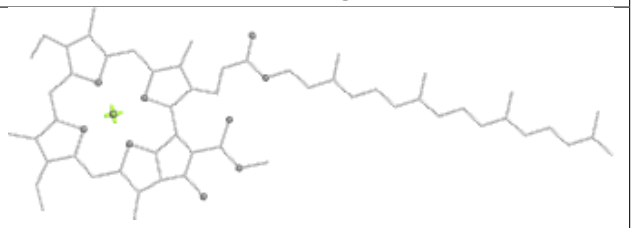
Bond lengths



Bond angles

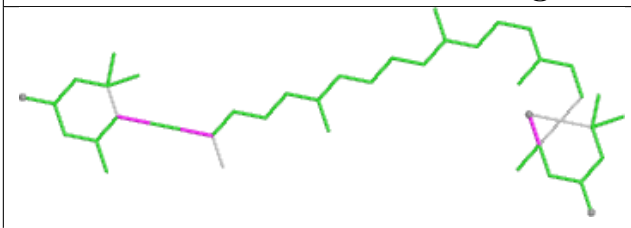


Torsions



Rings

Ligand DD6 I 307



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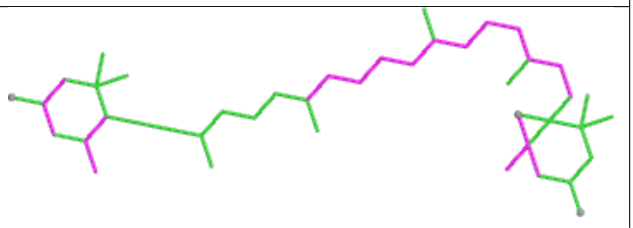
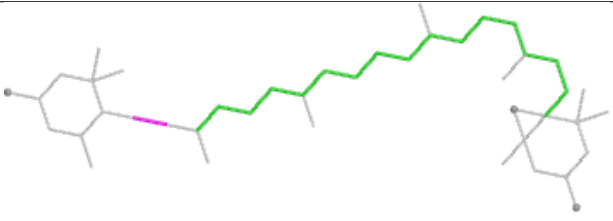
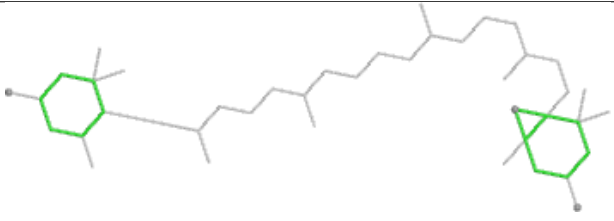


Bond angles

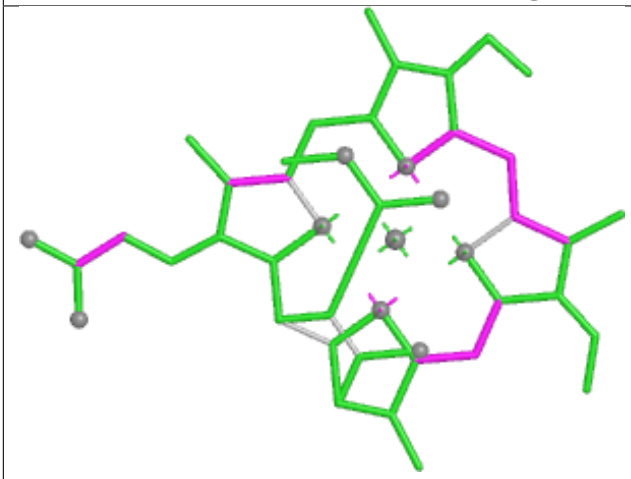


Torsions



Rings

Ligand KC2 V 308



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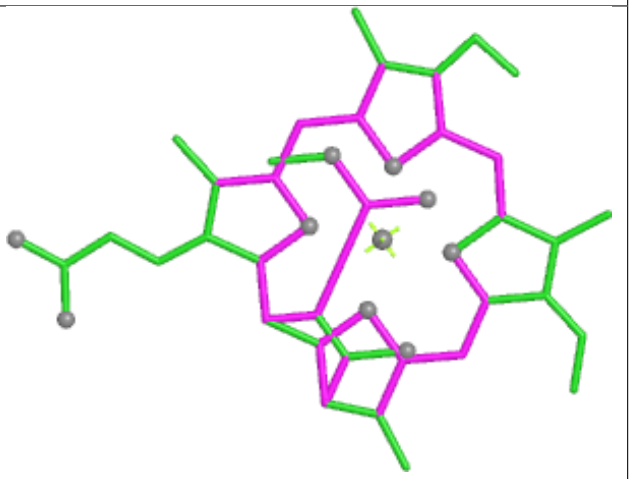
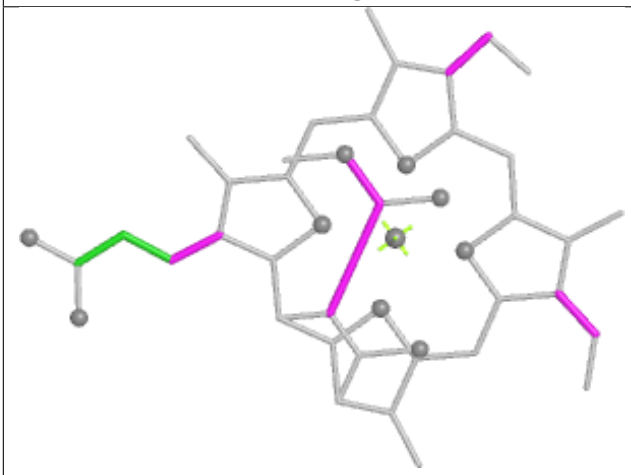


Bond angles



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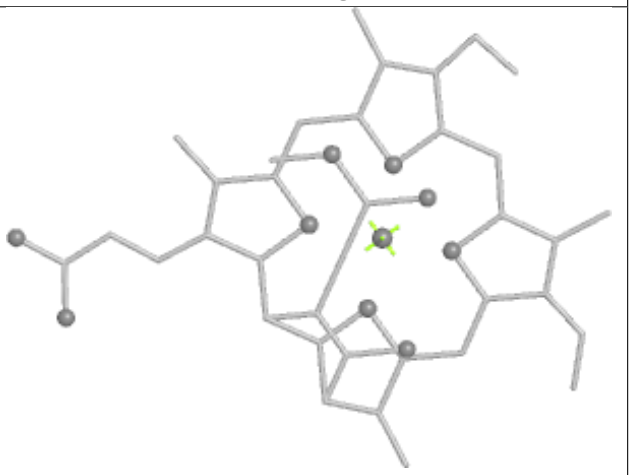
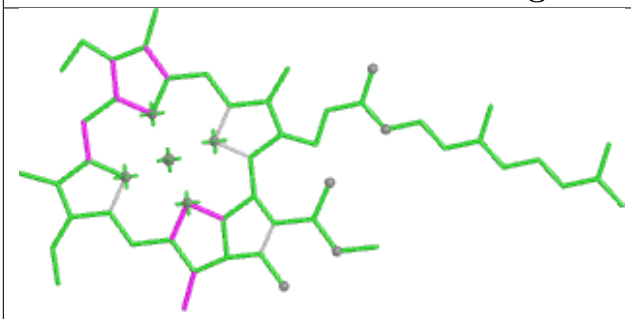


Rings

Ligand CLA a 802



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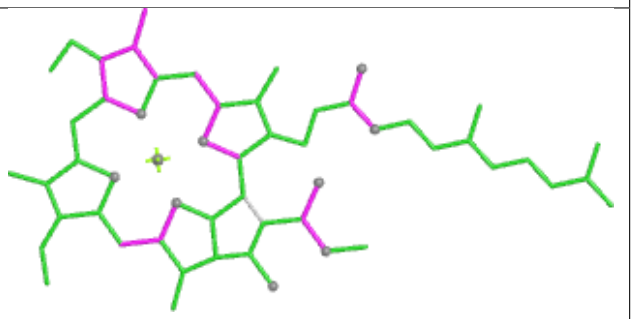
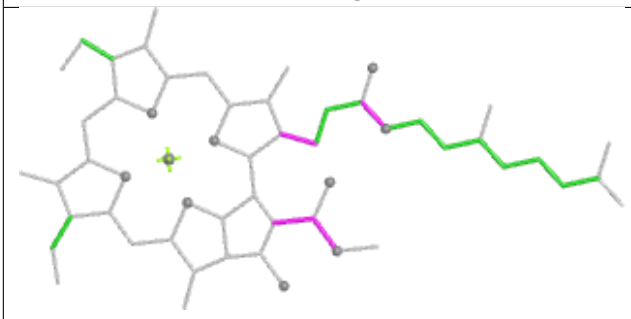


Bond angles



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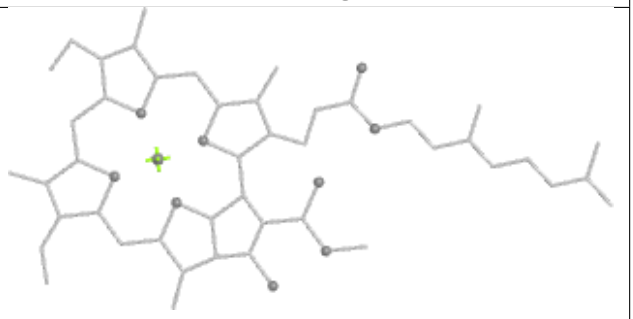
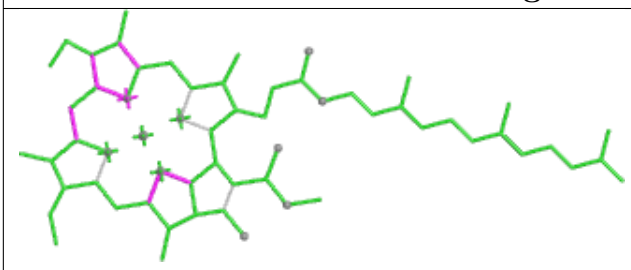


Rings

Ligand CLA H 308



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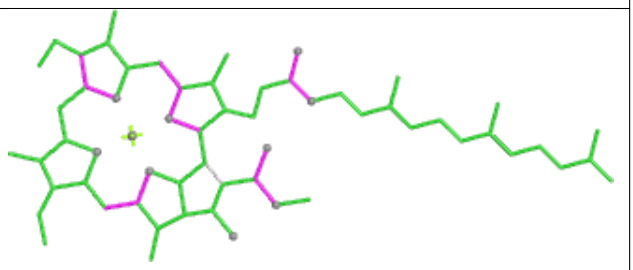
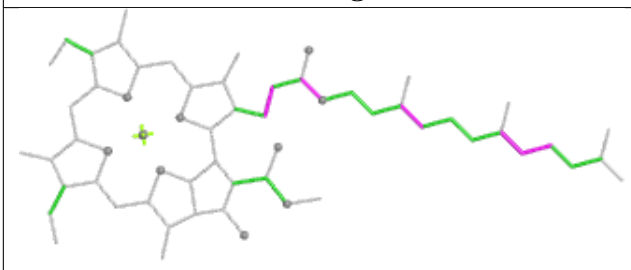


Bond angles



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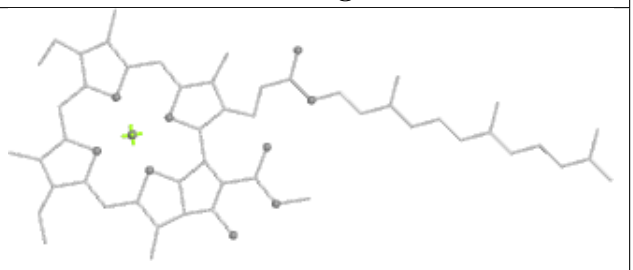
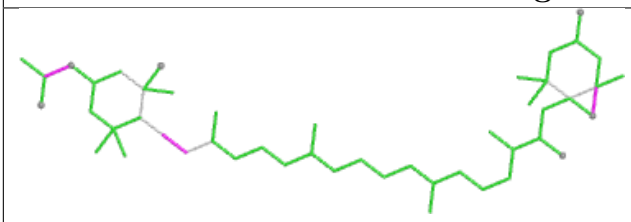


Rings

Ligand A86 4 309



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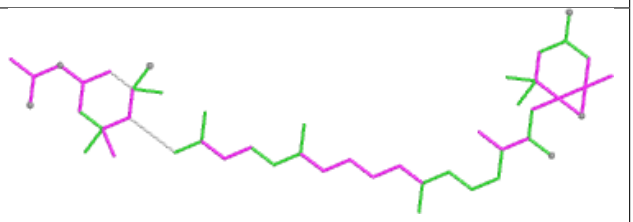

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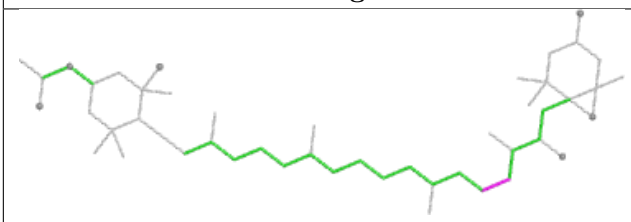

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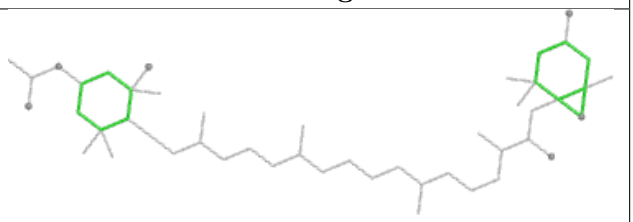
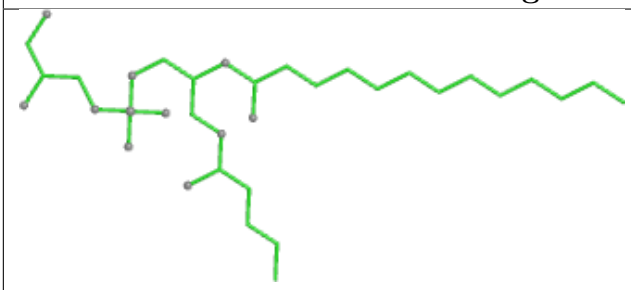


Rings

Ligand LHG D 302



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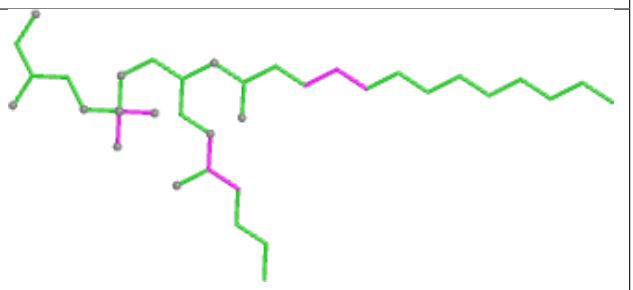
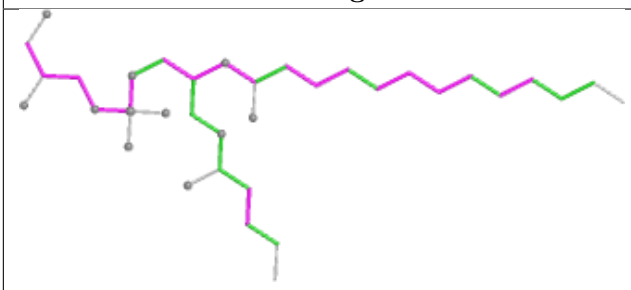


Bond angles



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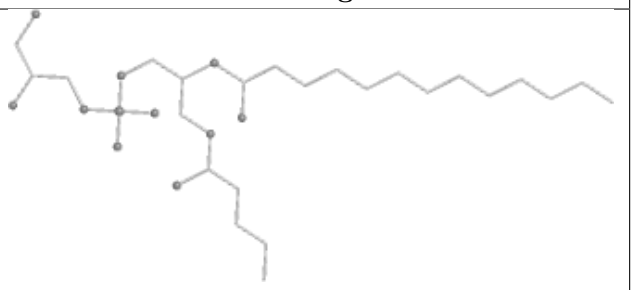
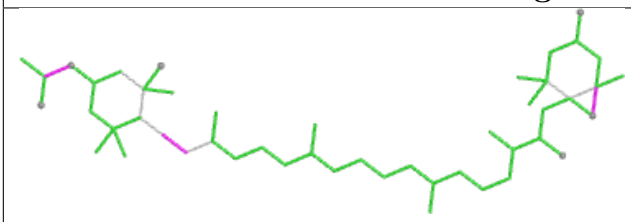


Rings

Ligand A86 8 302



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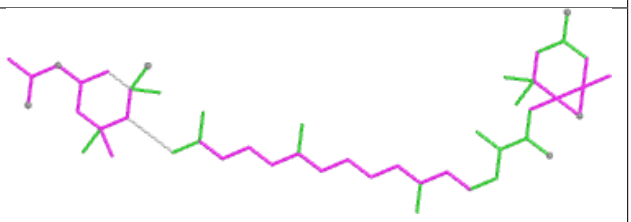

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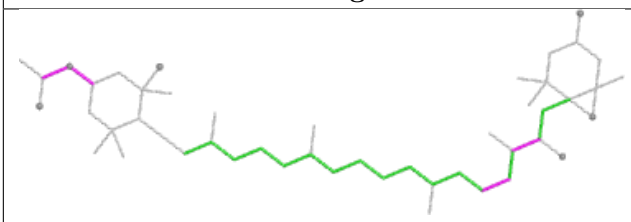

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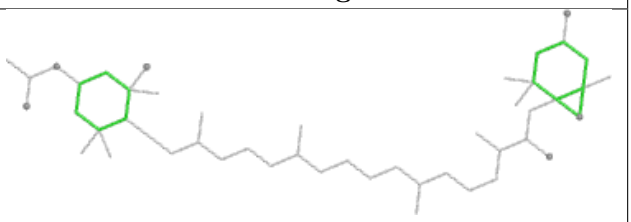
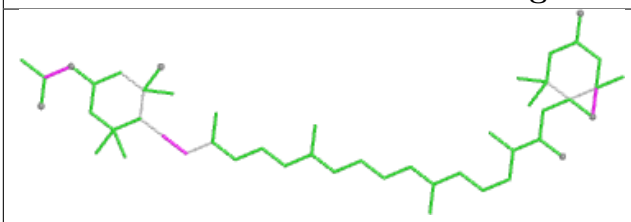


Rings

Ligand A86 Q 302



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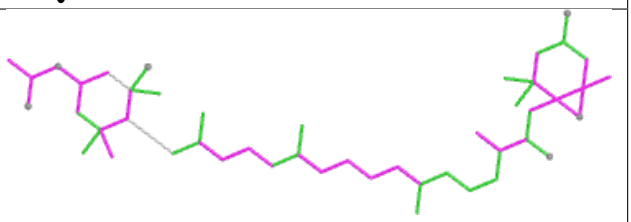

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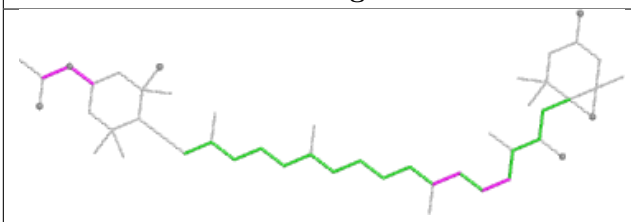

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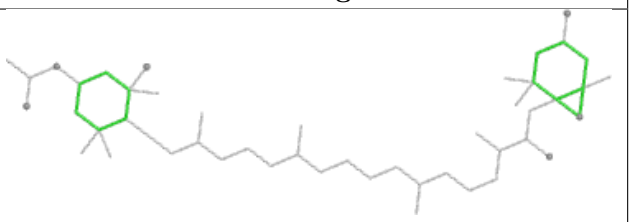
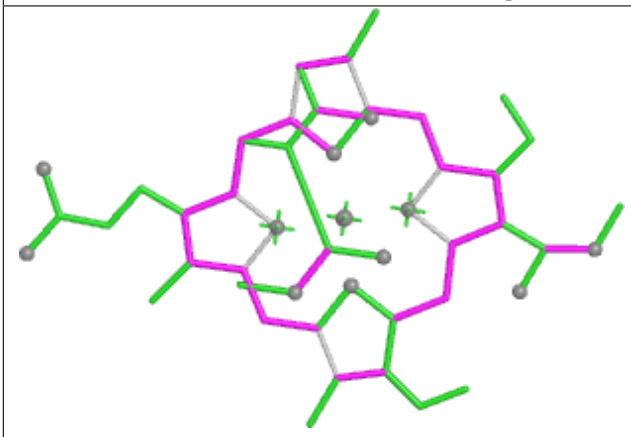


Rings

Ligand A1ECV X 313



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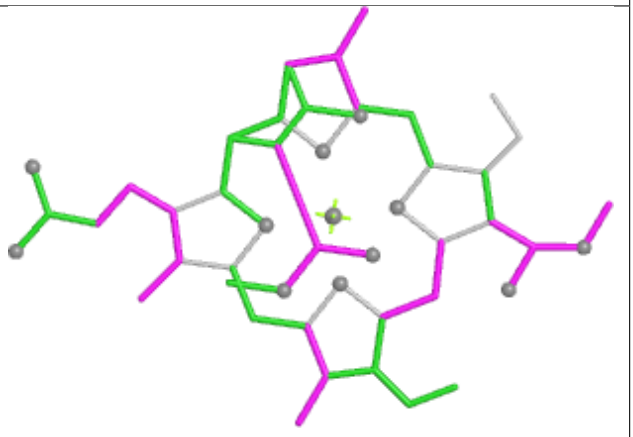
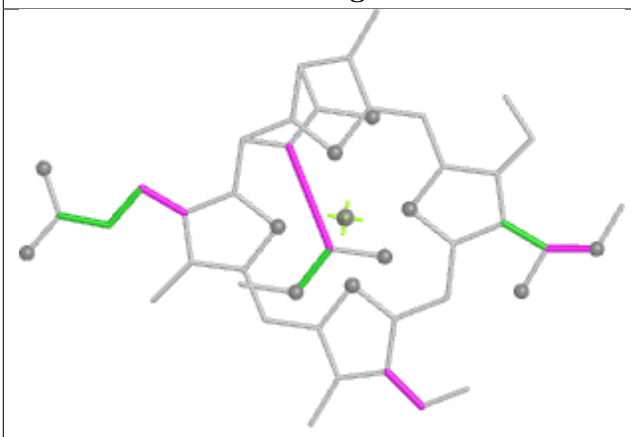


Bond angles



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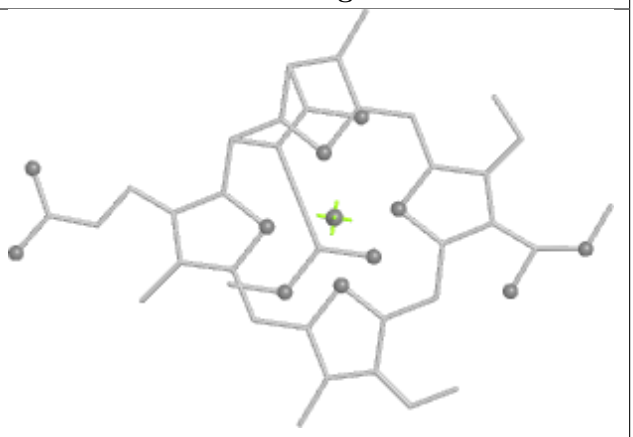
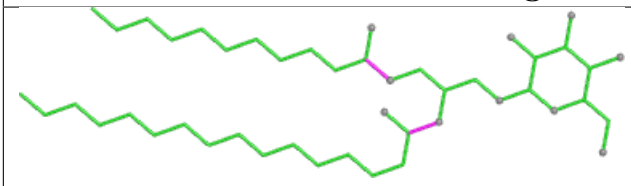


Rings

Ligand LMG 4 326



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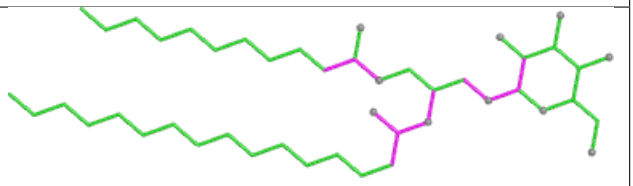
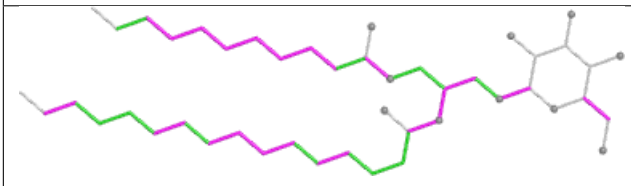


Bond angles



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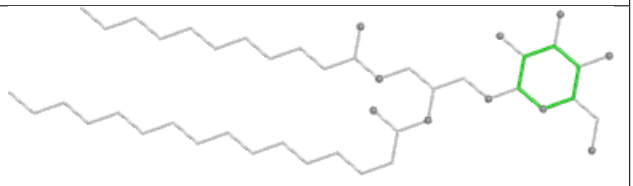
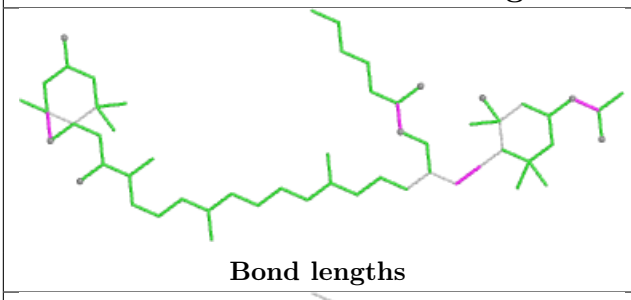


Rings

Ligand A1EB1 T 307



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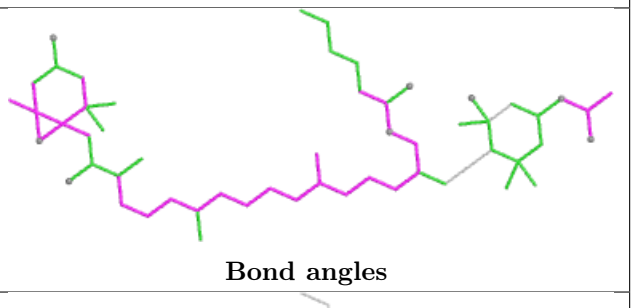
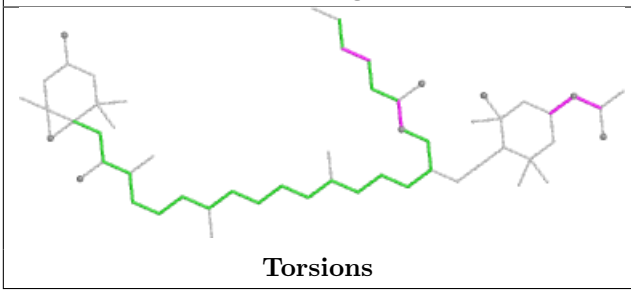
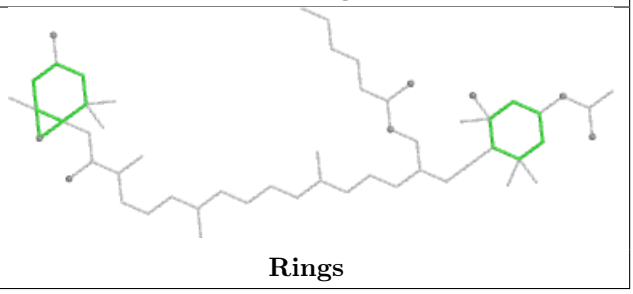


Bond angles

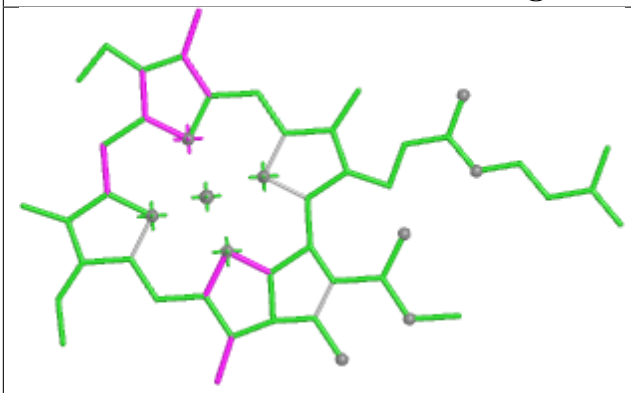


Torsions

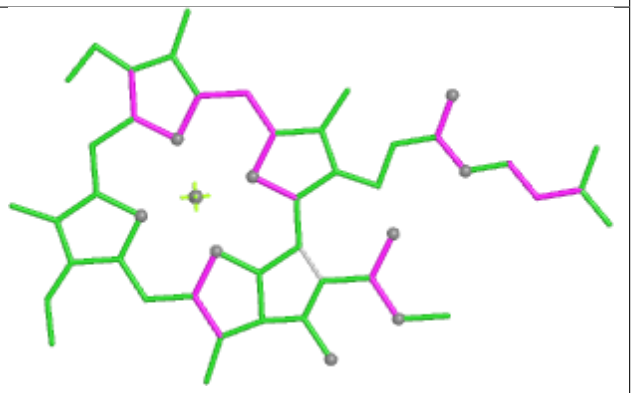


Rings

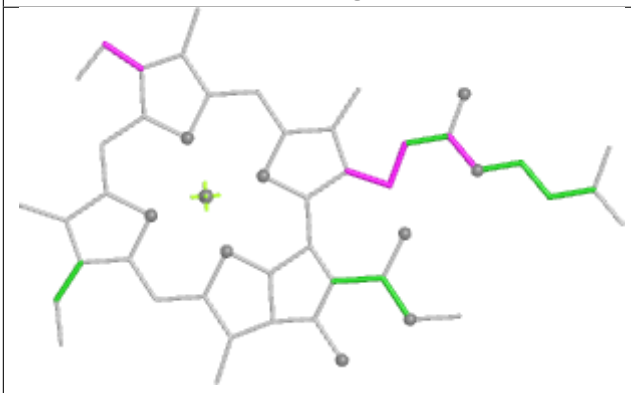
Ligand CLA b 831



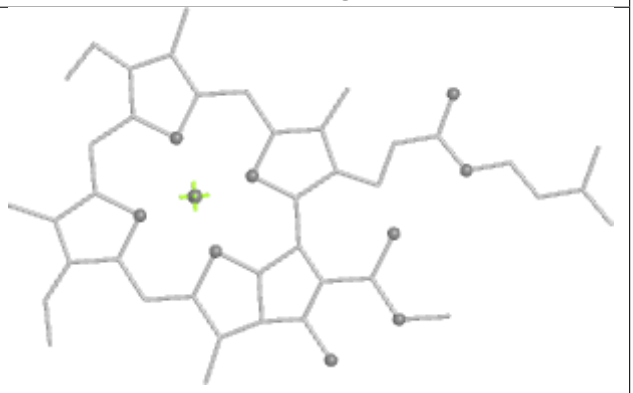
Bond lengths



Bond angles

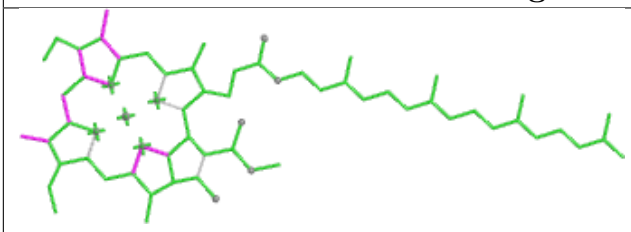


Torsions

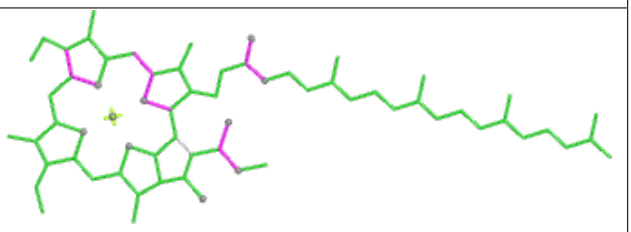


Rings

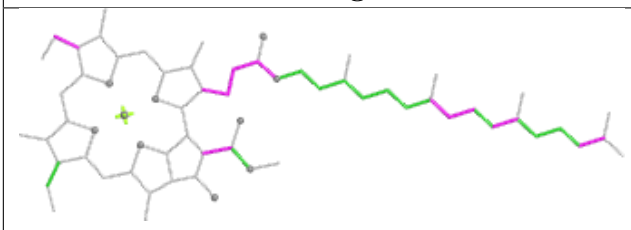
Ligand CLA a 815



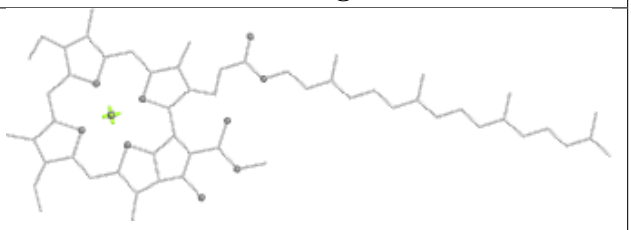
Bond lengths



Bond angles

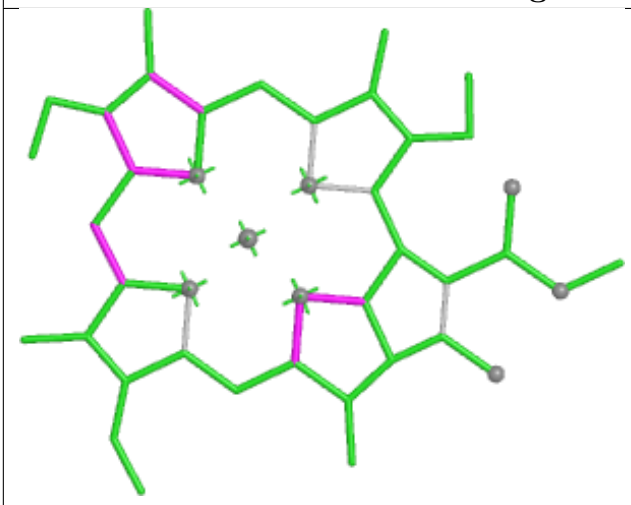


Torsions



Rings

Ligand CLA z 317



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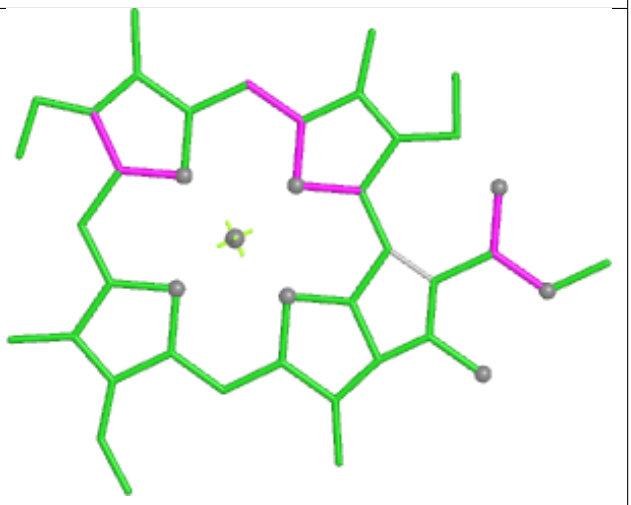
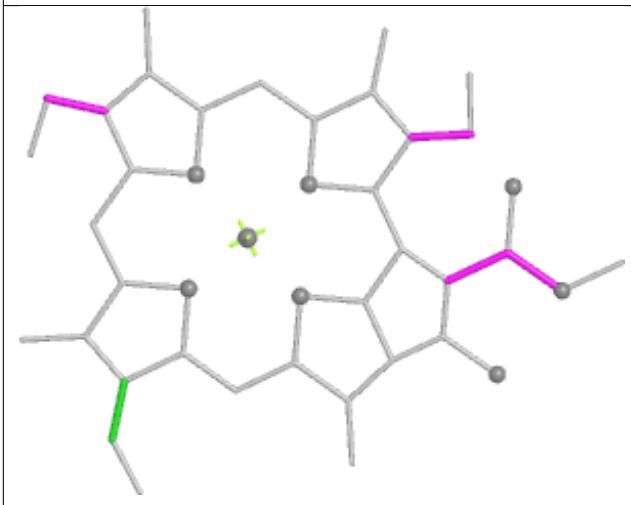


Bond angles



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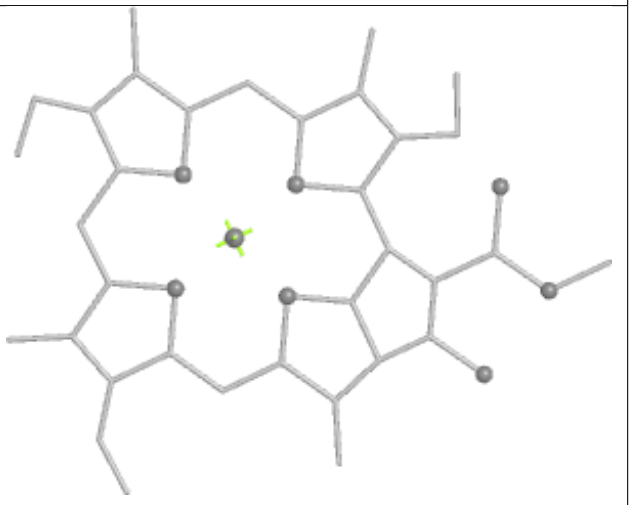
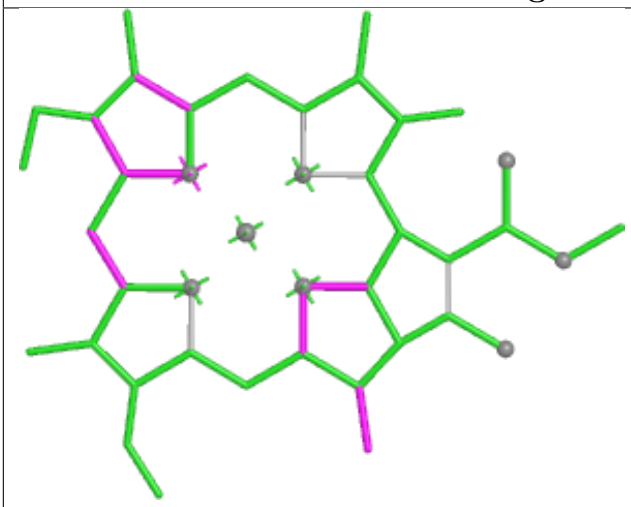


Rings

Ligand CLA 6 315



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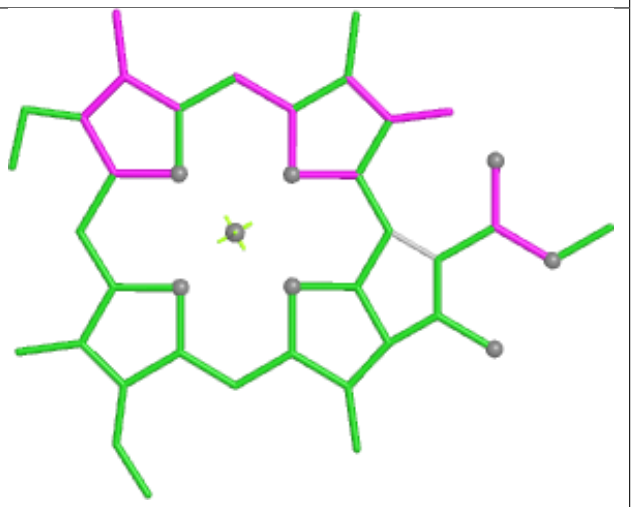

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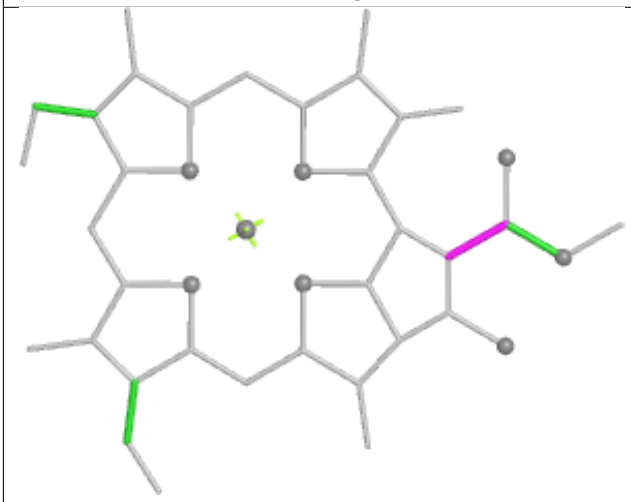

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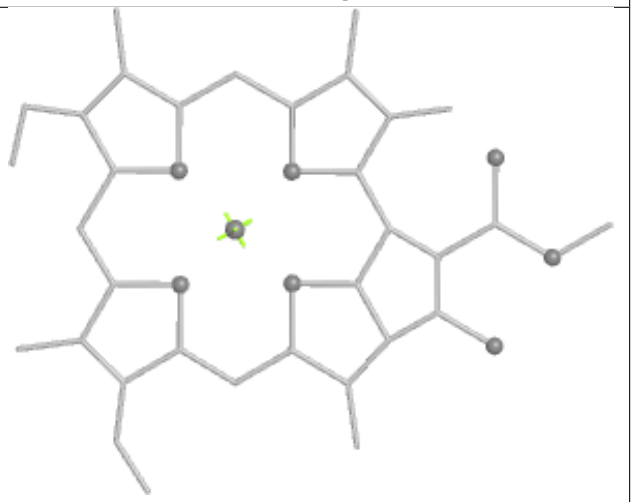
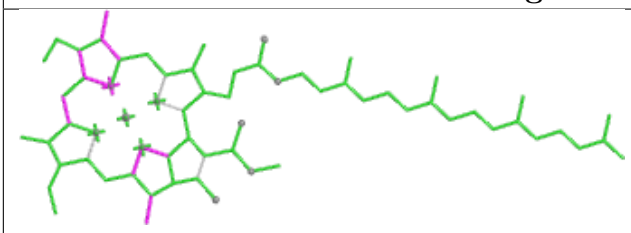


Rings

Ligand CLA E 307



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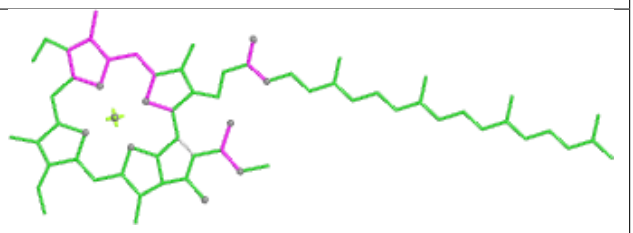
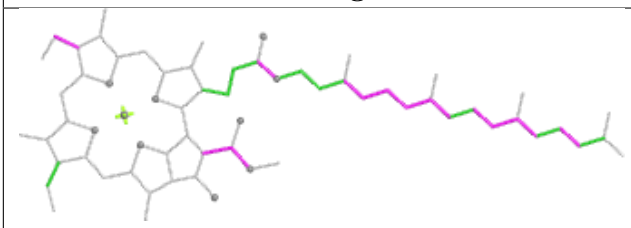


Bond angles



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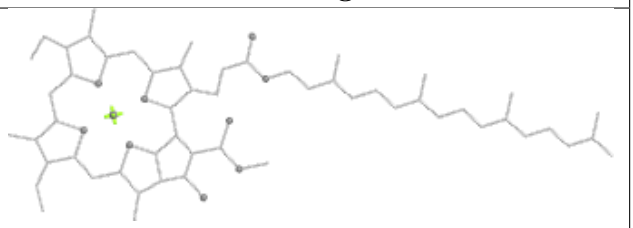
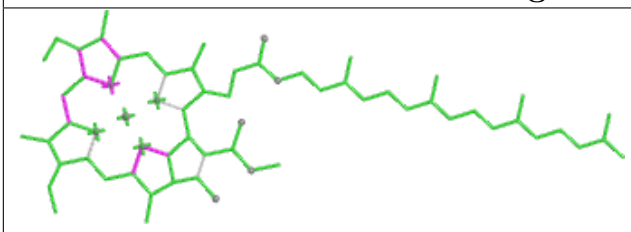
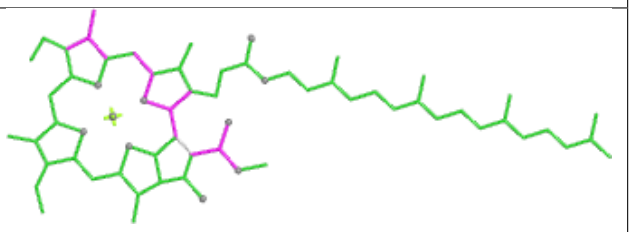


Rings

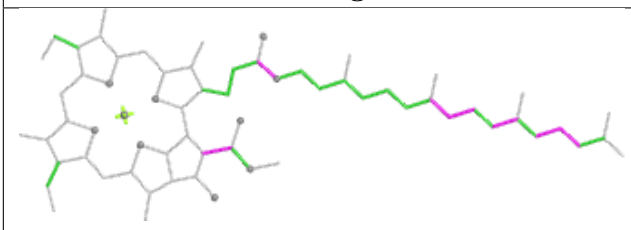
Ligand CLA a 822



Bond lengths



Bond angles



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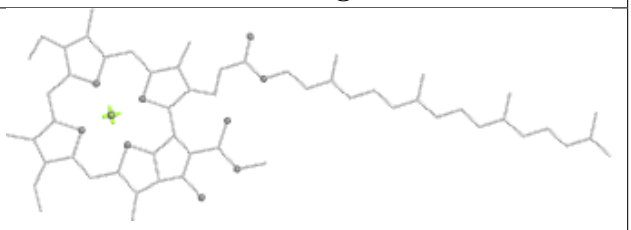
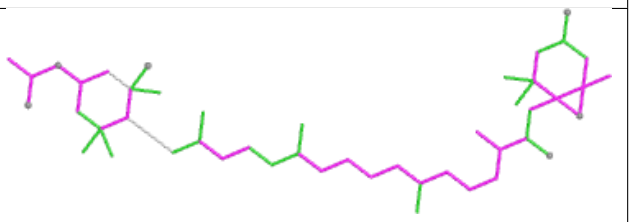


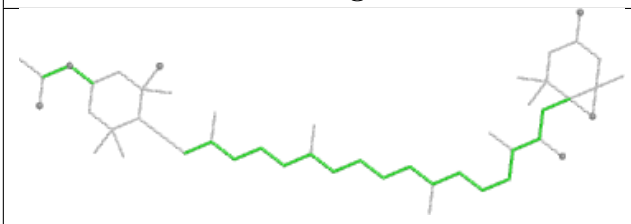
Rings

Ligand A86 M 303

Bond lengths



Bond angles



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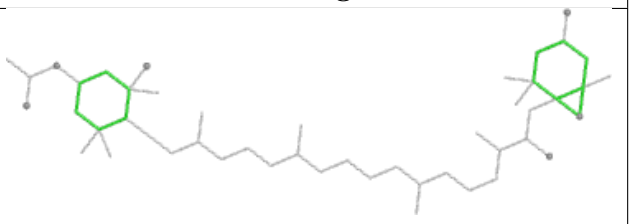
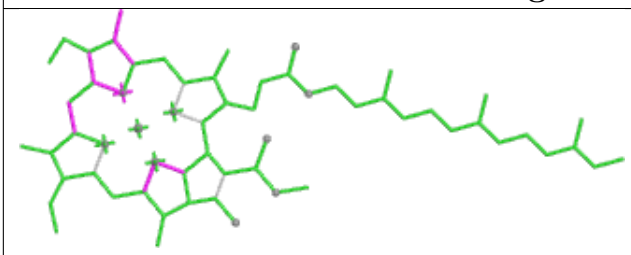
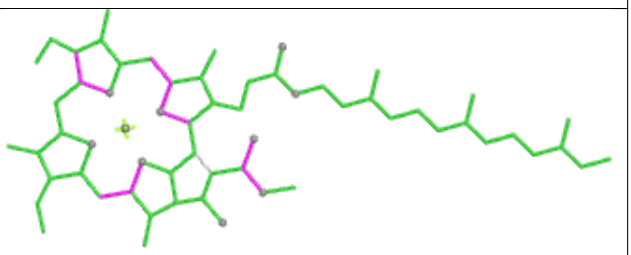


Rings

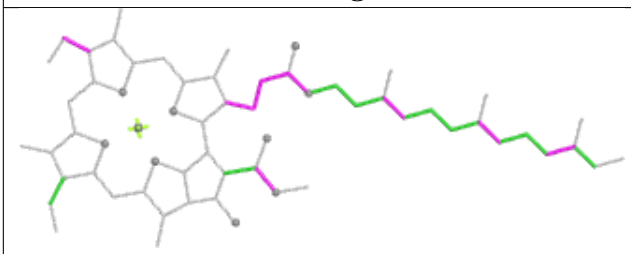
Ligand CLA 3 311



Bond lengths



Bond angles



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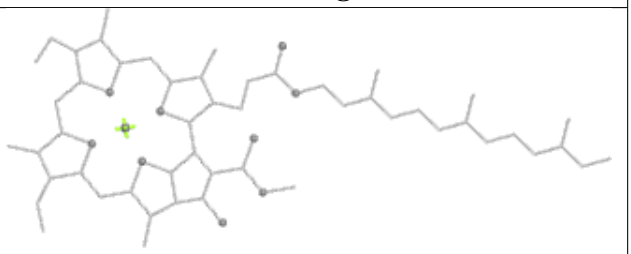
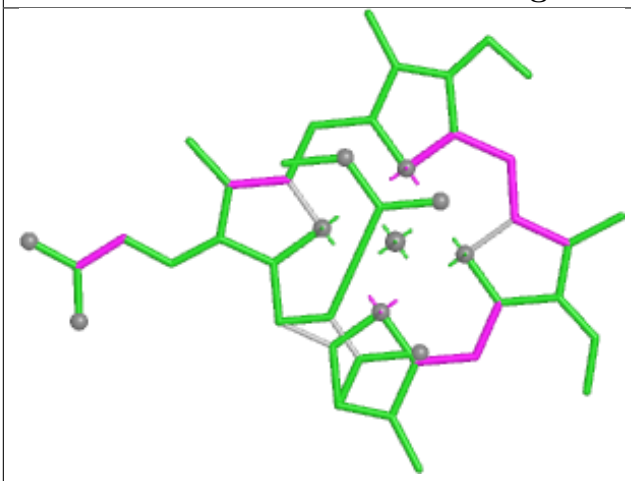


Rings

Ligand KC2 8 319



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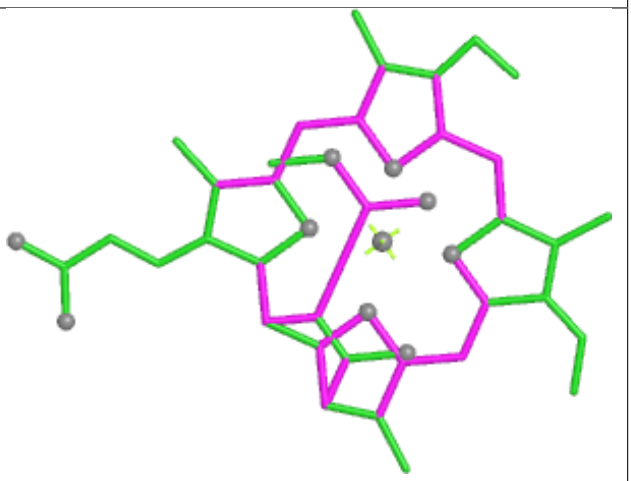
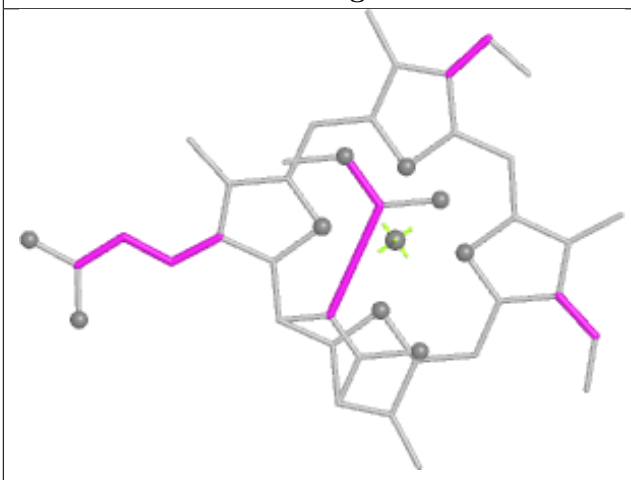


Bond angles



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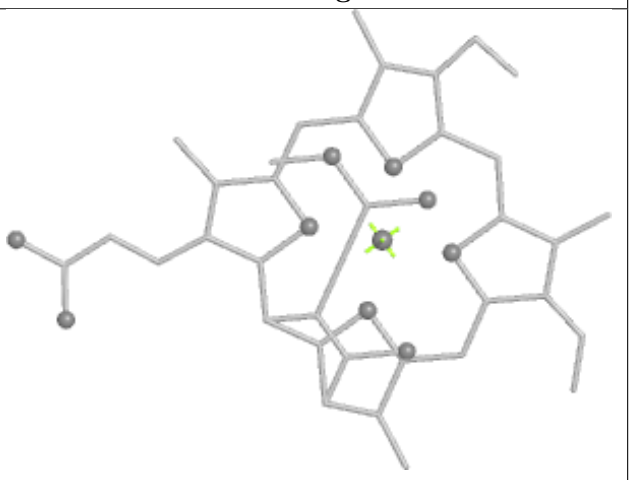
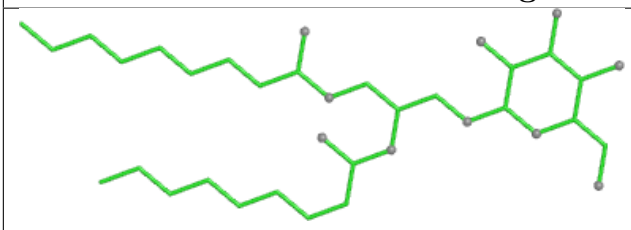


Rings

Ligand LMG D 322



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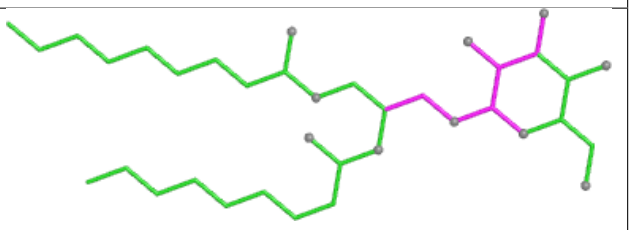
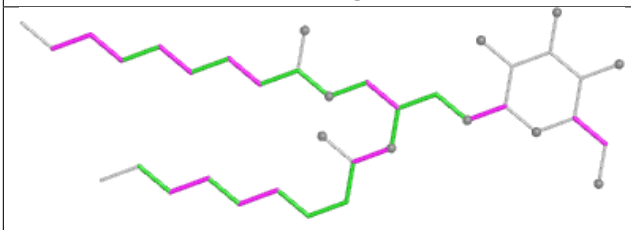
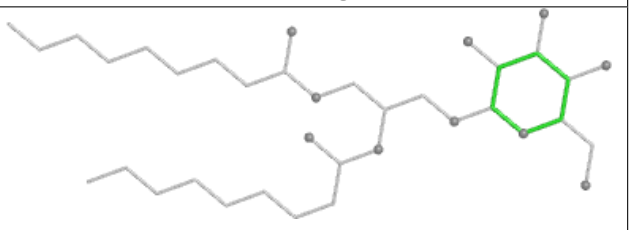


Bond angles

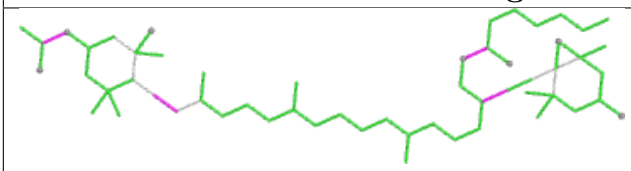


Torsions



Rings

Ligand A1EB4 P 305



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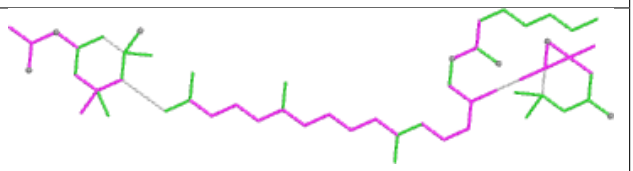
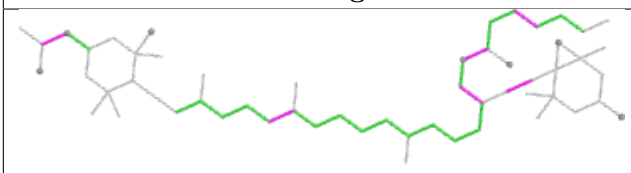


Bond angles



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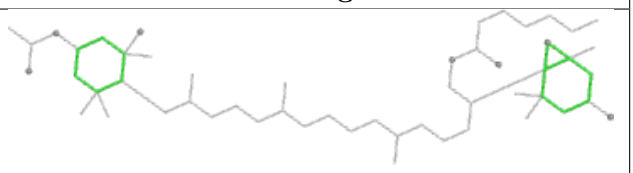
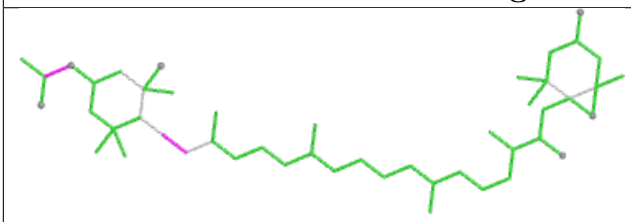


Rings

Ligand A1EB1 6 306



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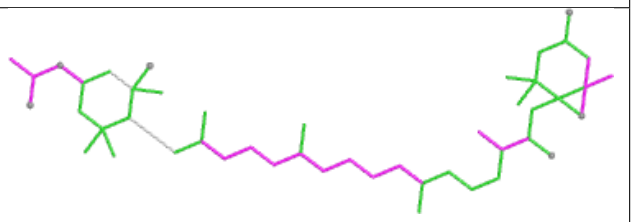
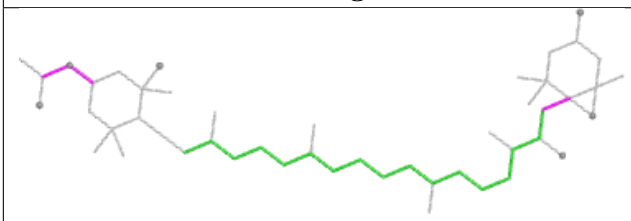
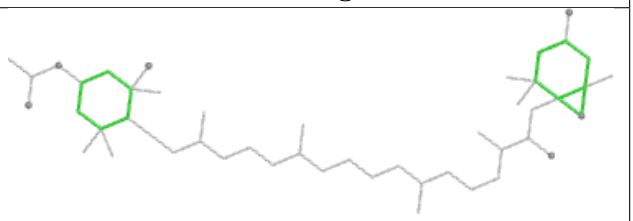


Bond angles

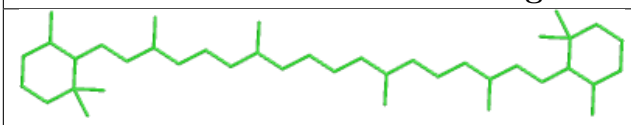


Torsions



Rings

Ligand BCR b 847



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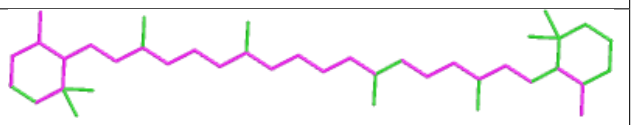
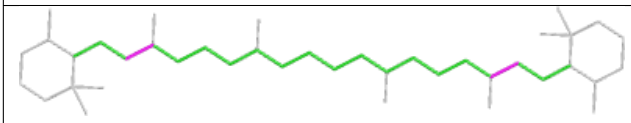
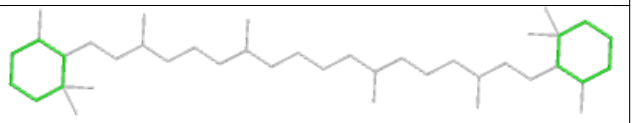


Bond angles

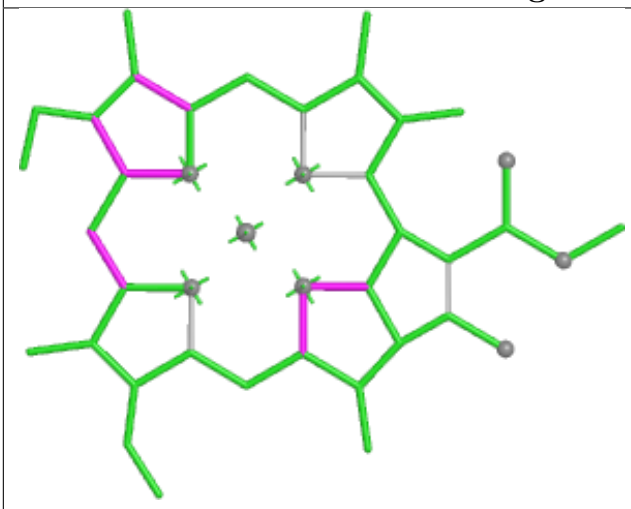


Torsions



Rings

Ligand CLA 3 319



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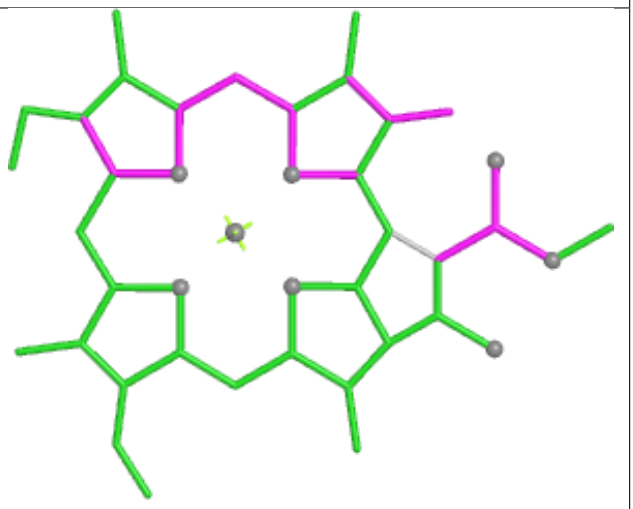
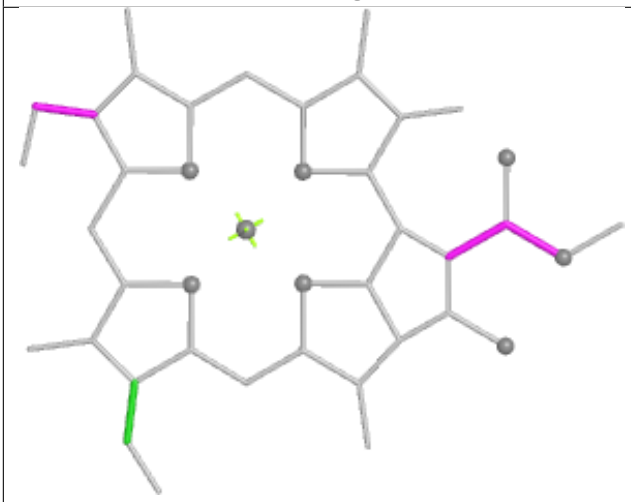
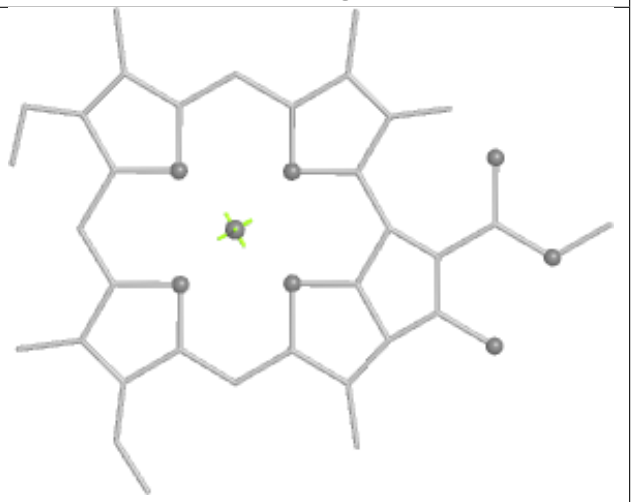


Bond angles



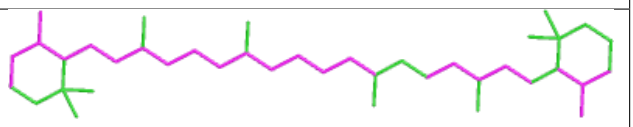
Torsions



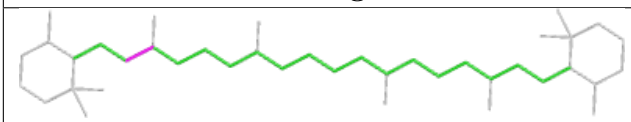
Rings

Ligand BCR k 204

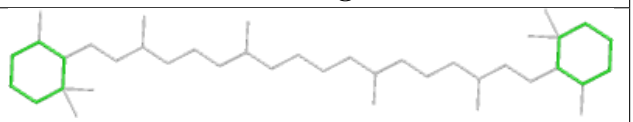
Bond lengths



Bond angles

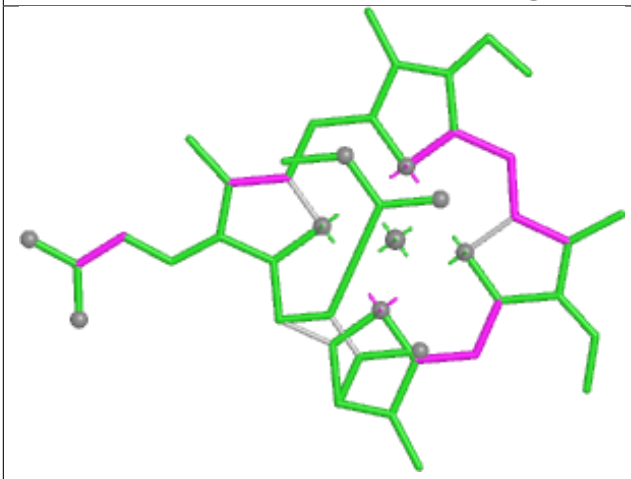


Torsions

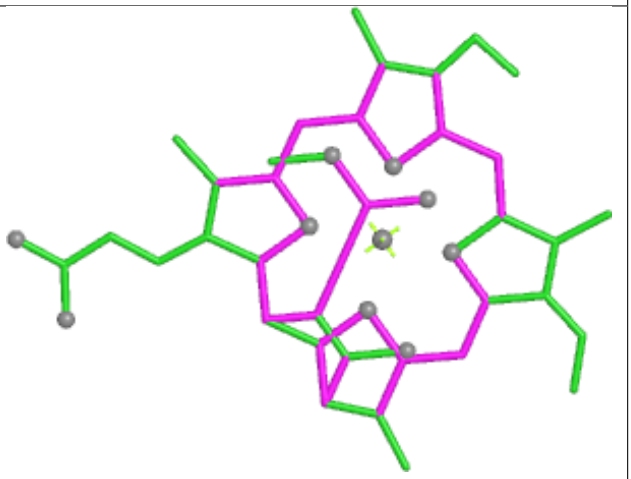


Rings

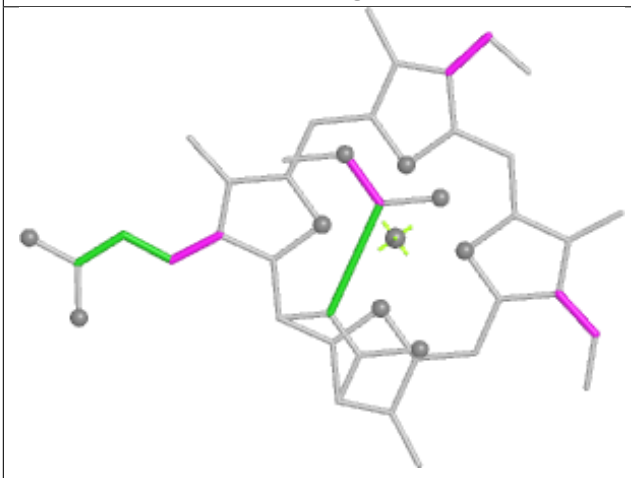
Ligand KC2 K 310



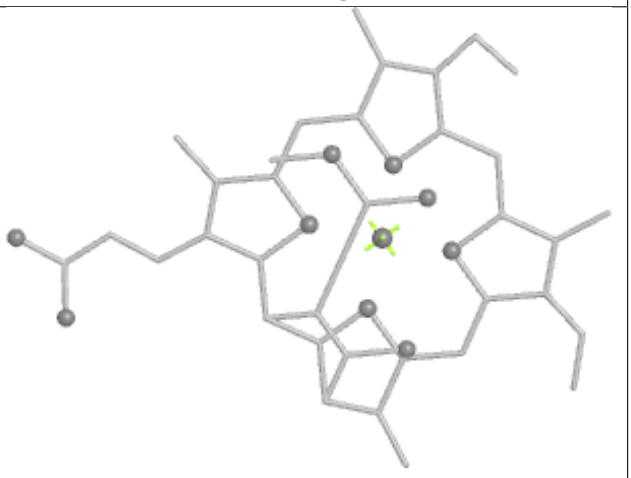
Bond lengths



Bond angles

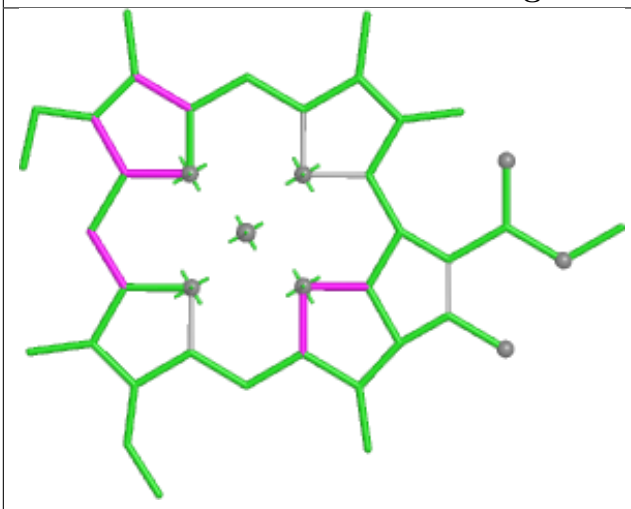


Torsions



Rings

Ligand CLA Y 311



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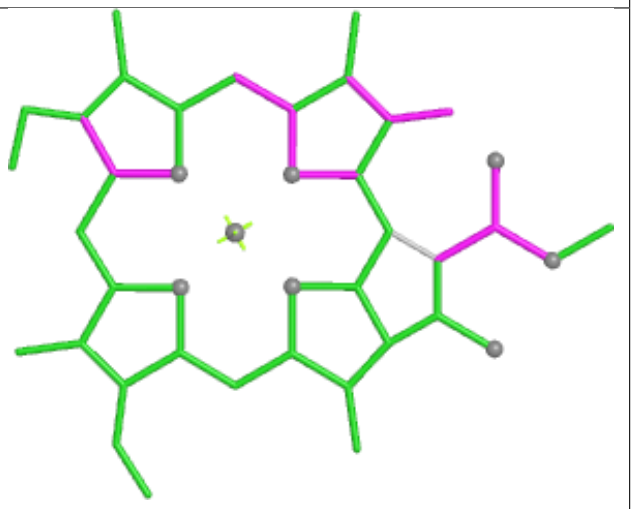
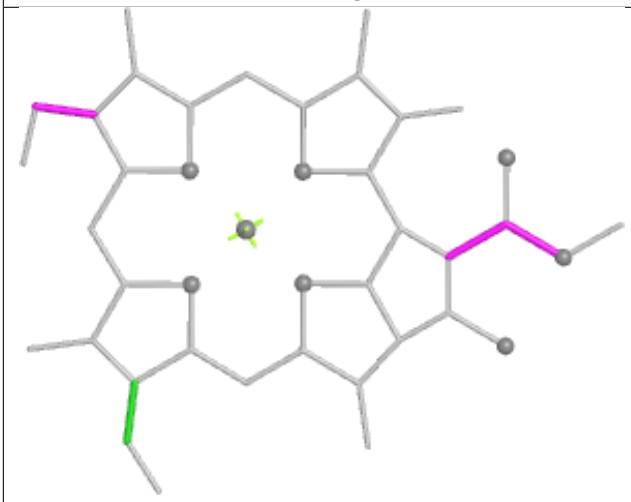


Bond angles



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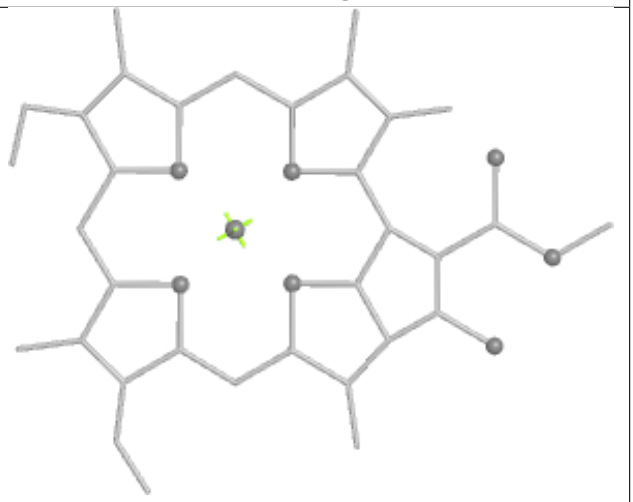
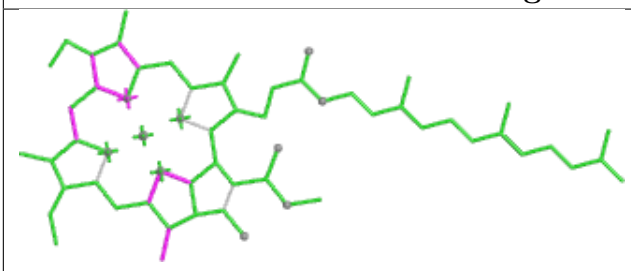


Rings

Ligand CLA A 307



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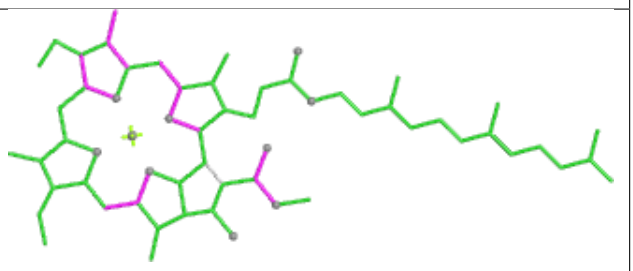
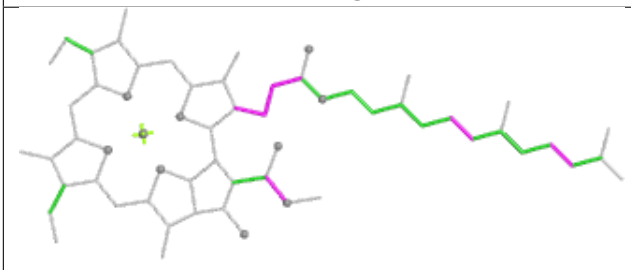
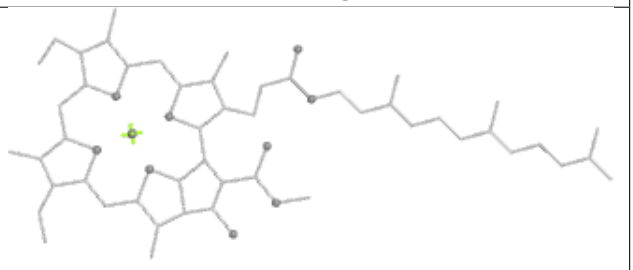


Bond angles

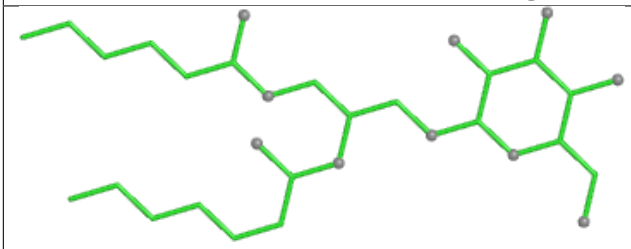


Torsions



Rings

Ligand LMG S 321



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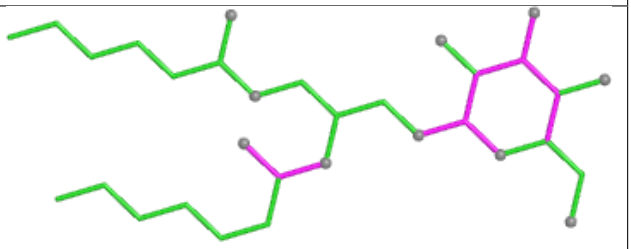
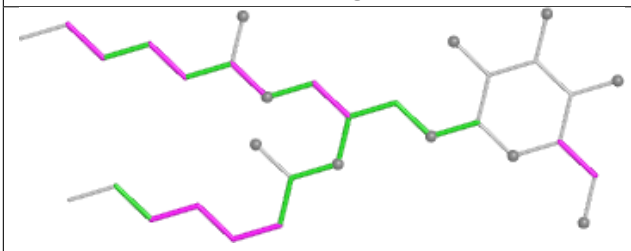


Bond angles



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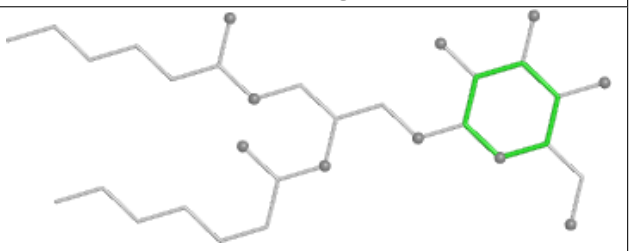
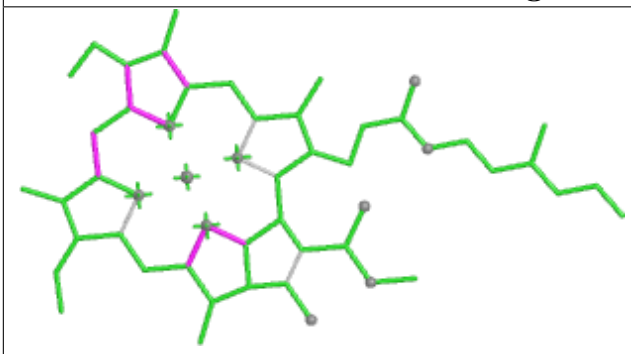


Rings

Ligand CLA E 317



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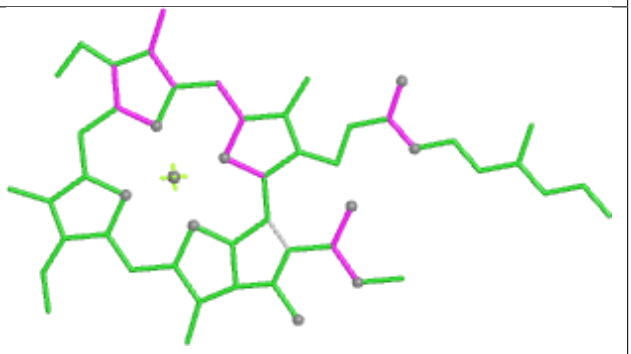
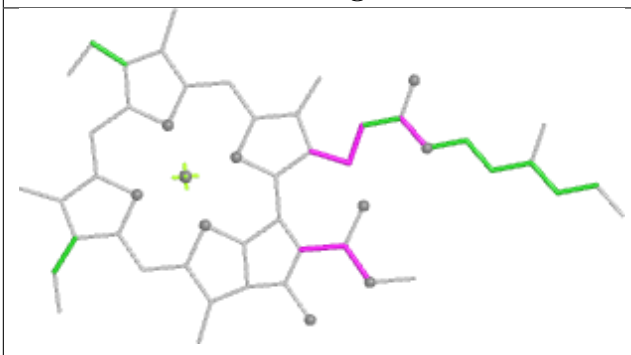


Bond angles



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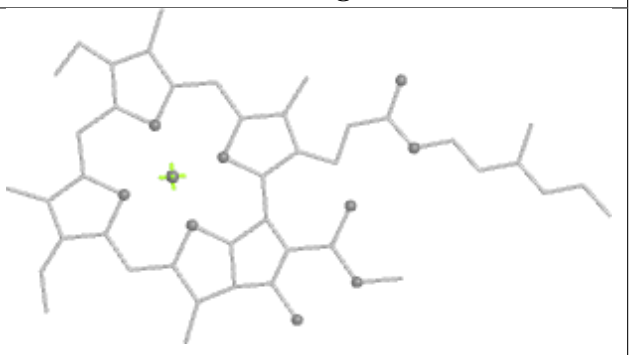
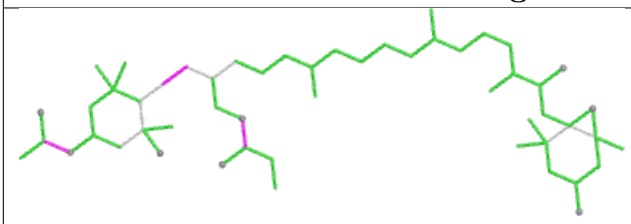


Rings

Ligand A1EB1 6 304



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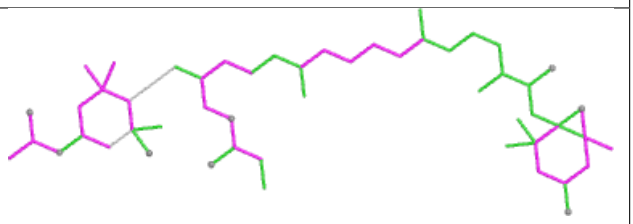
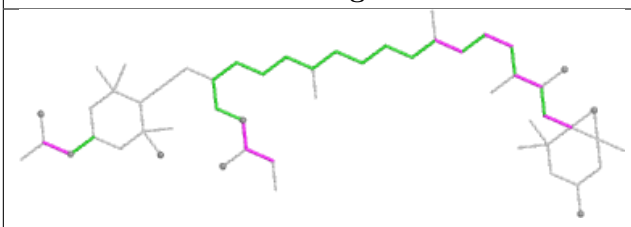


Bond angles



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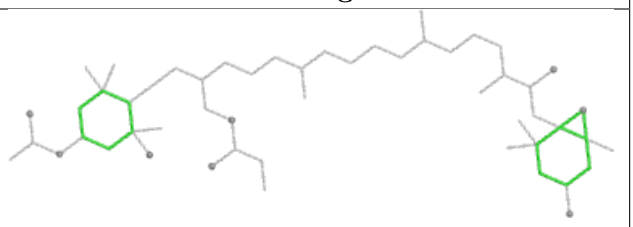
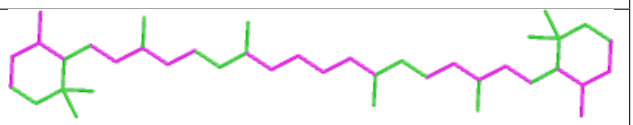


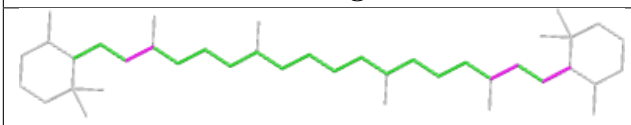
Rings

Ligand BCR b 850

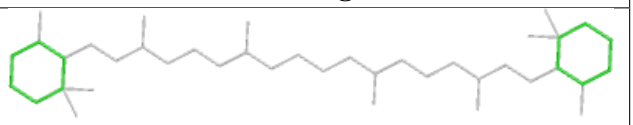
Bond lengths



Bond angles

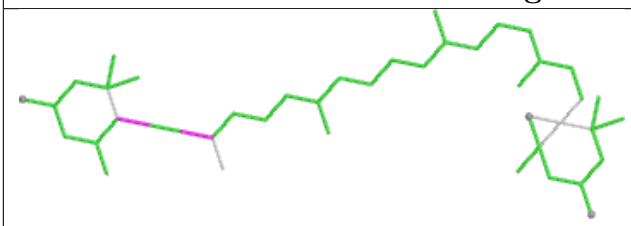


Torsions



Rings

Ligand DD6 D 303



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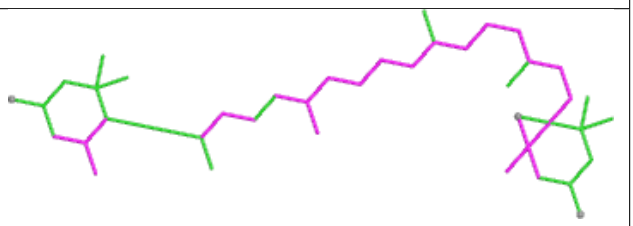

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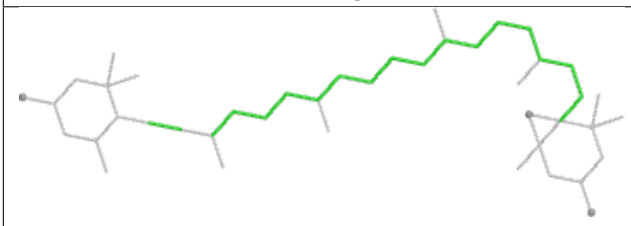

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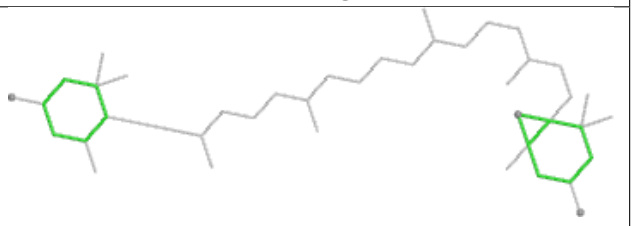
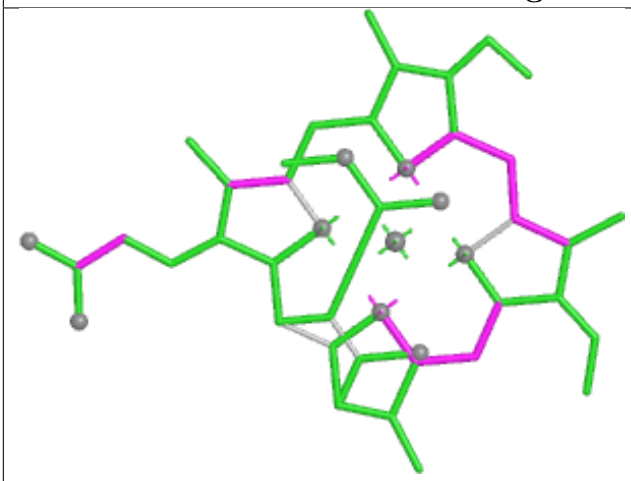
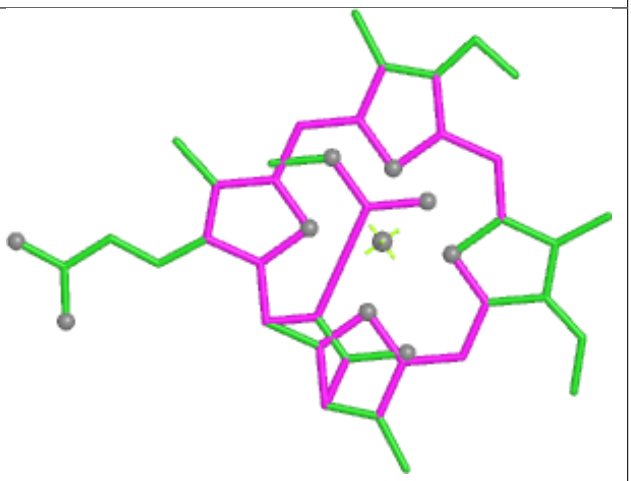


Rings

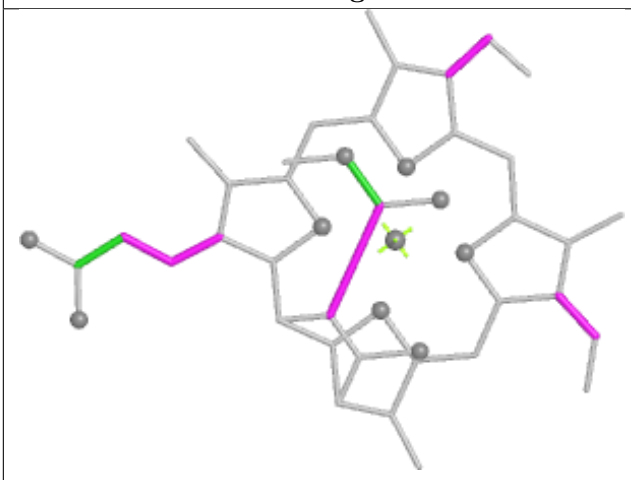
Ligand KC2 R 312



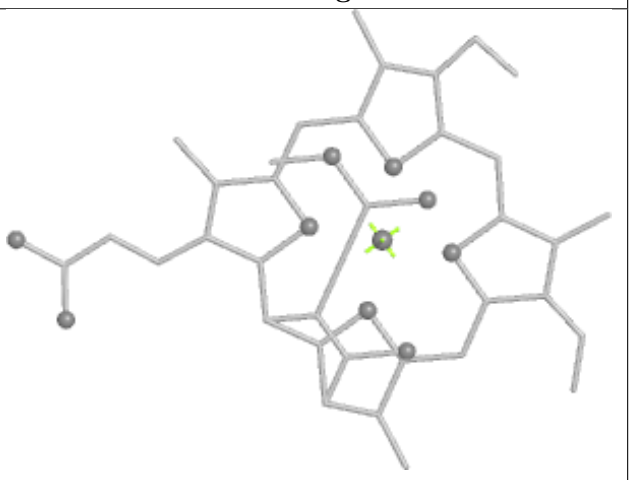
Bond lengths



Bond angles

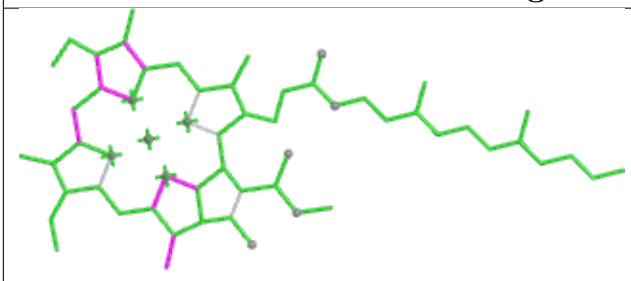


Torsions



Rings

Ligand CLA b 834



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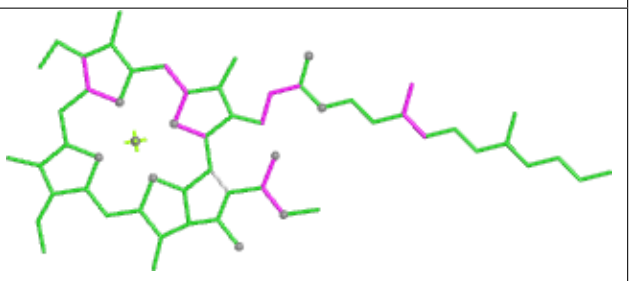
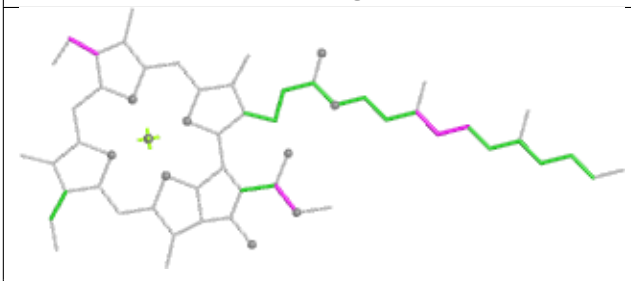


Bond angles



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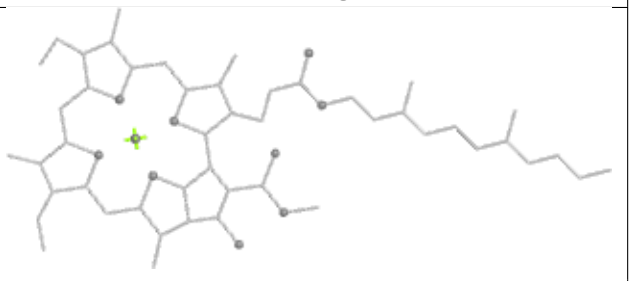
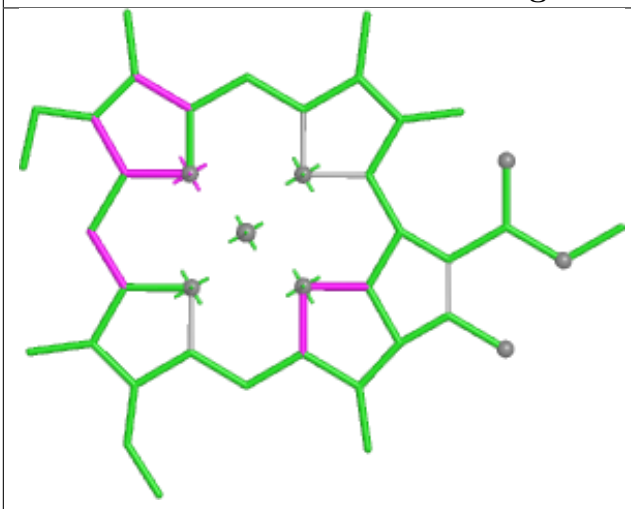
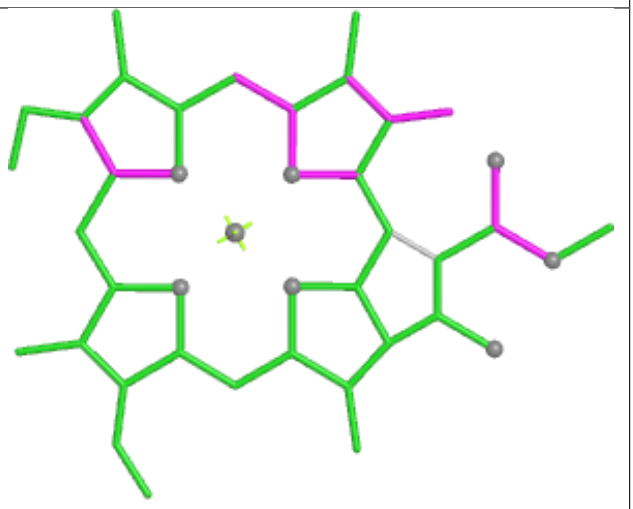


Rings

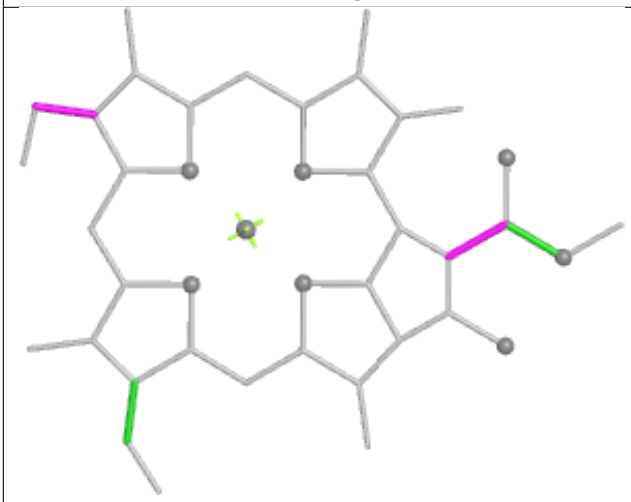
Ligand CLA z 314



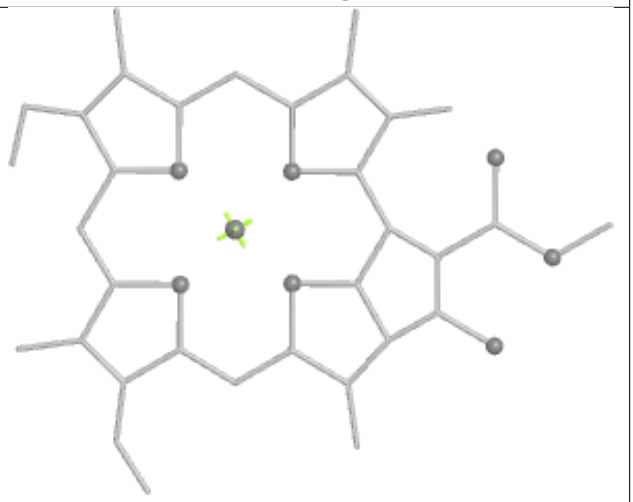
Bond lengths



Bond angles



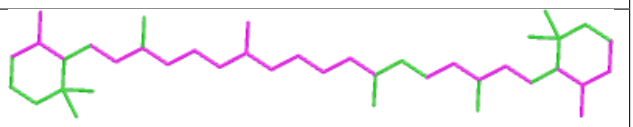
Torsions



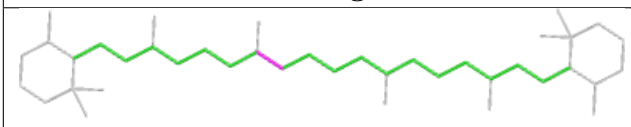
Rings

Ligand BCR f 804

Bond lengths



Bond angles



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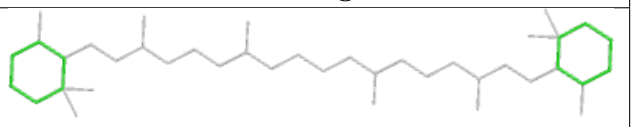
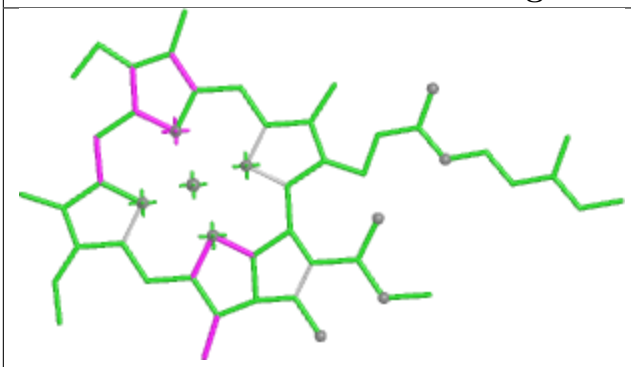
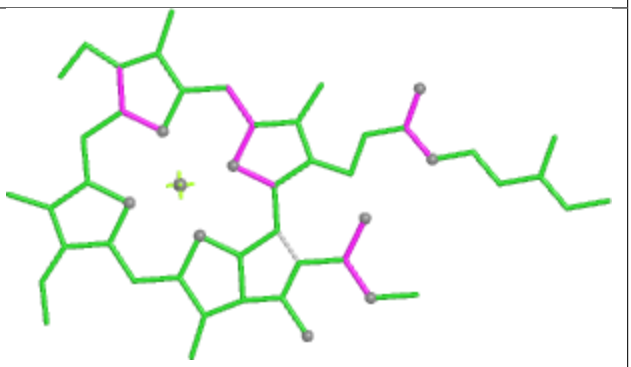


Rings

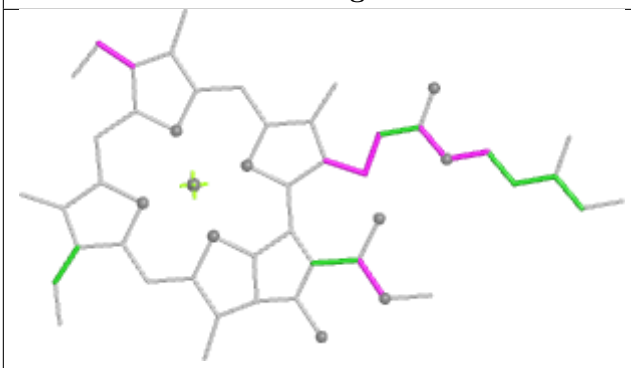
Ligand CLA F 316



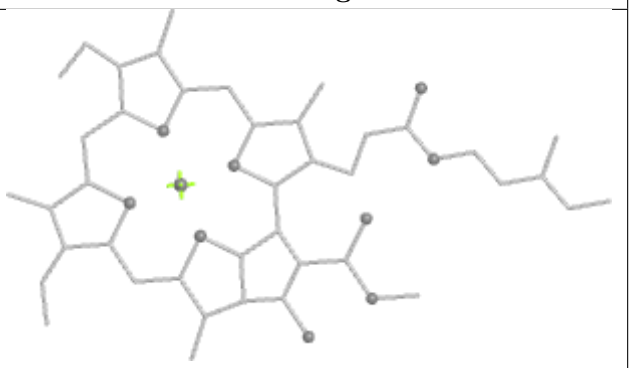
Bond lengths



Bond angles

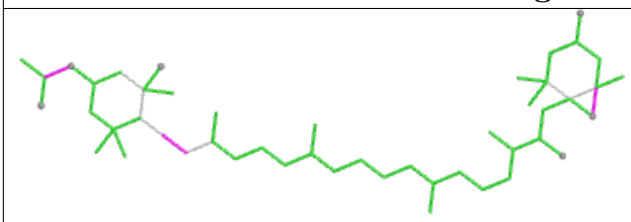


Torsions

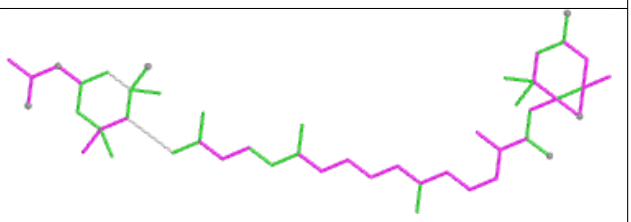


Rings

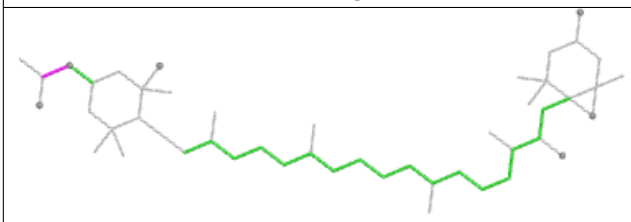
Ligand A86 0 306



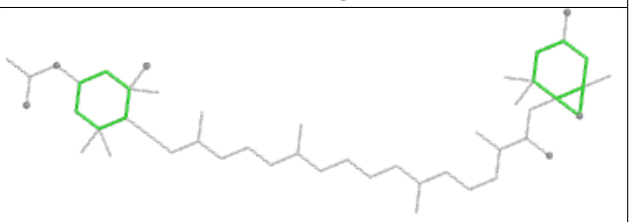
Bond lengths



Bond angles

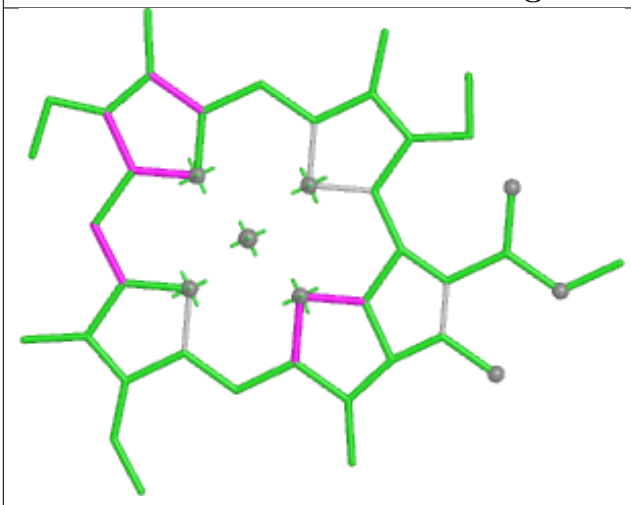


Torsions

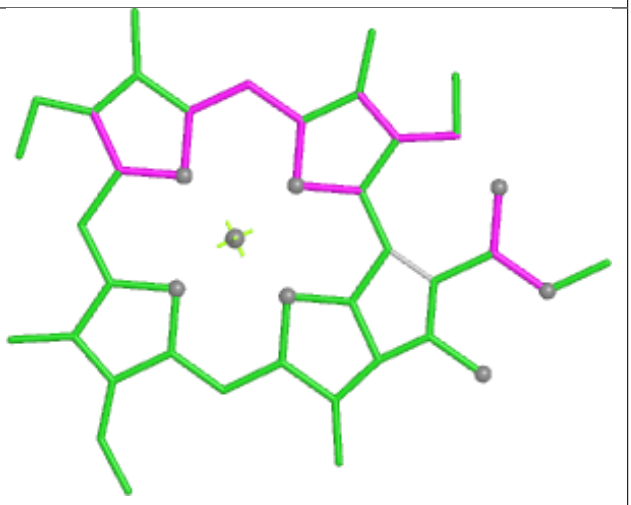


Rings

Ligand CLA B 205



Bond lengths



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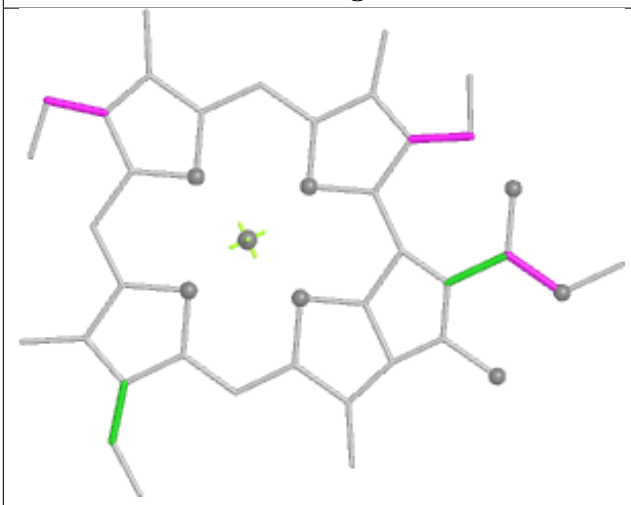
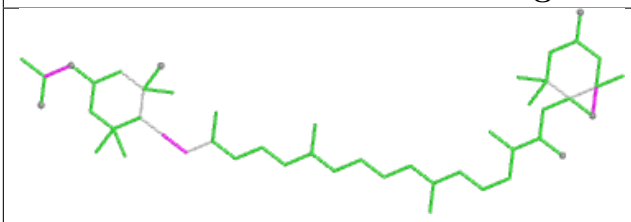


Torsions

Rings

Ligand A86 3 307



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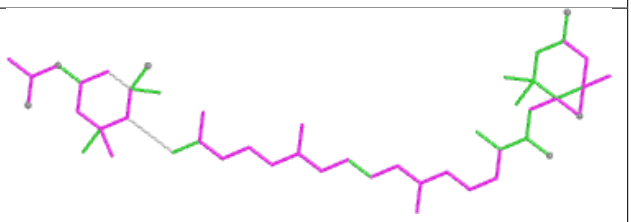

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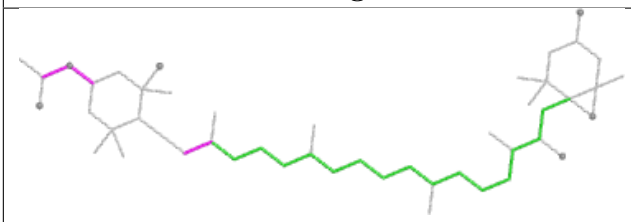
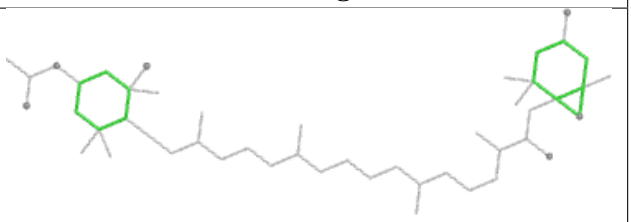
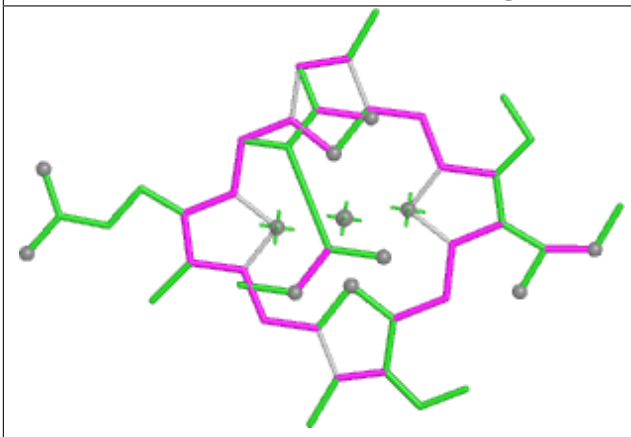


Torsions



Rings

Ligand A1ECV Y 306



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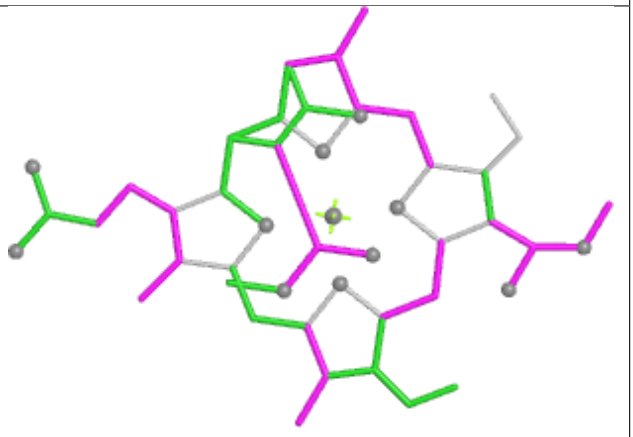

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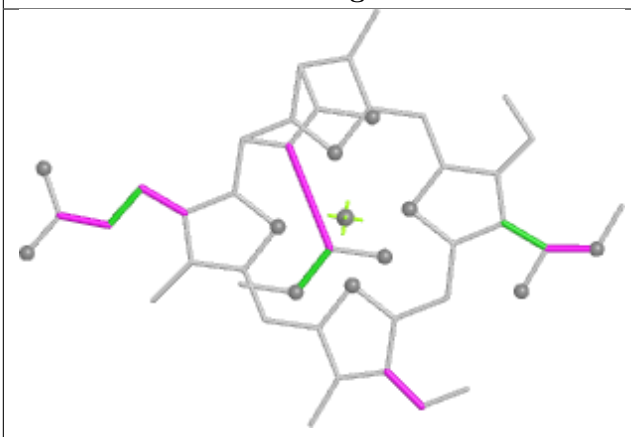

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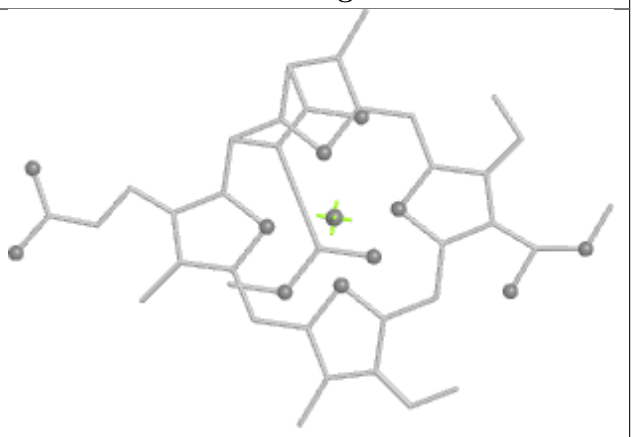
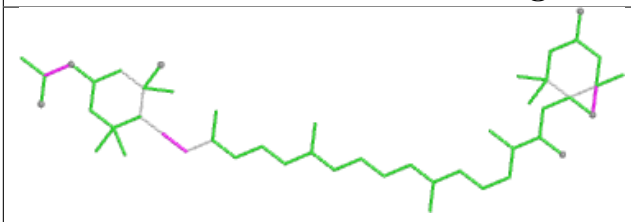


Rings

Ligand A86 D 305



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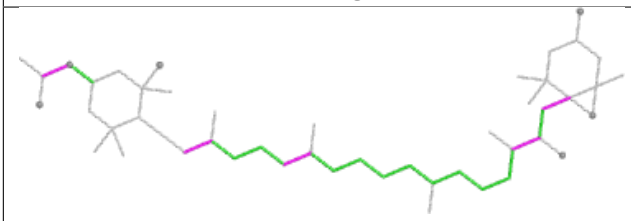

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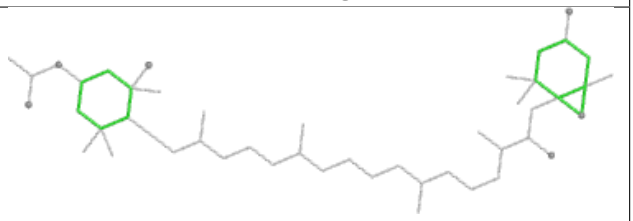
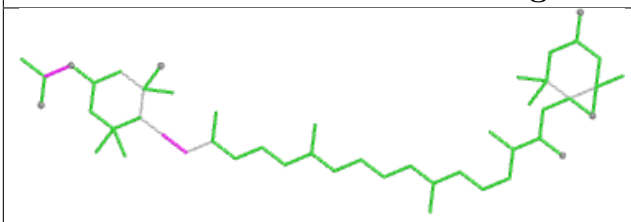


Rings

Ligand A86 O 307



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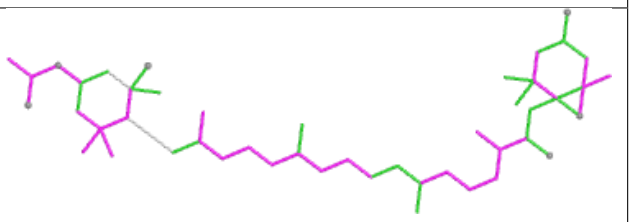

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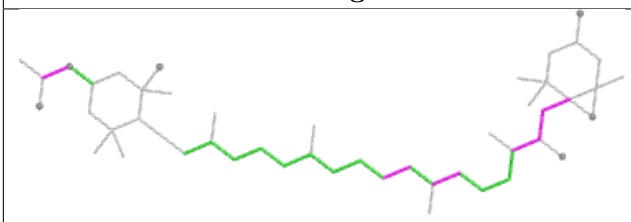

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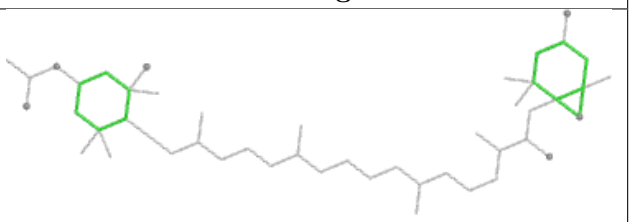
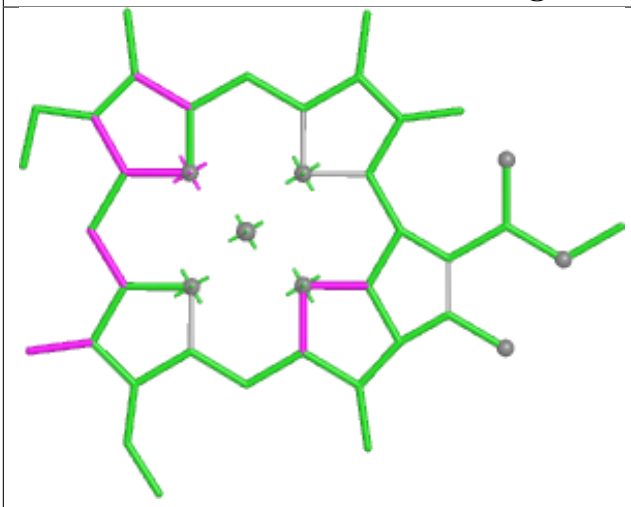


Rings

Ligand CLA 9 310



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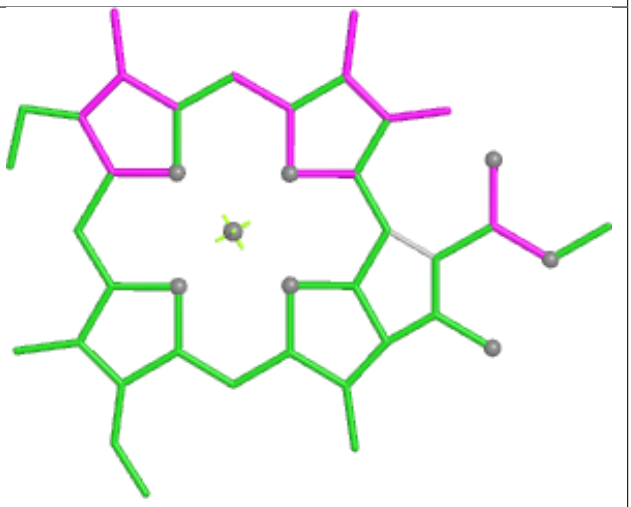

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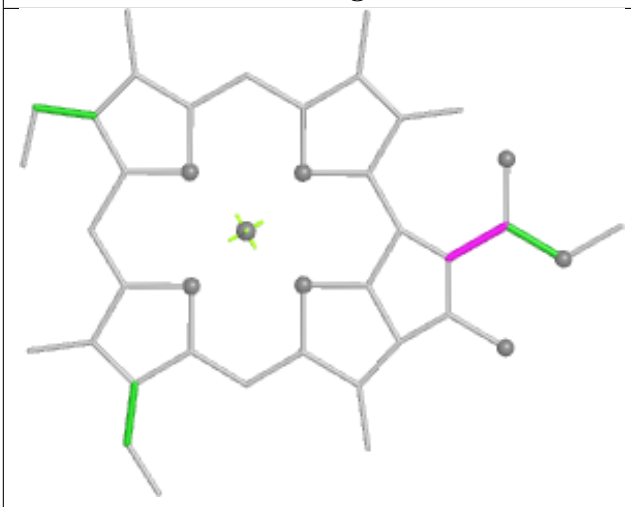

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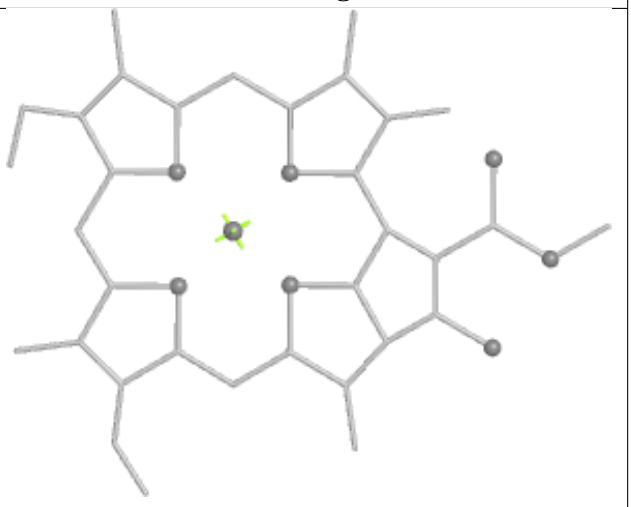

Rings

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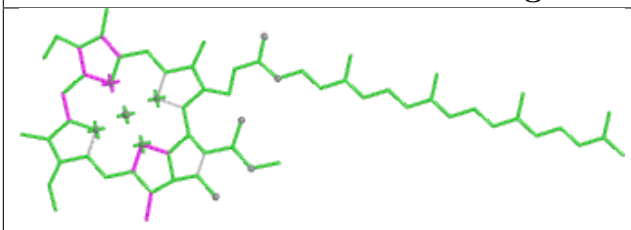

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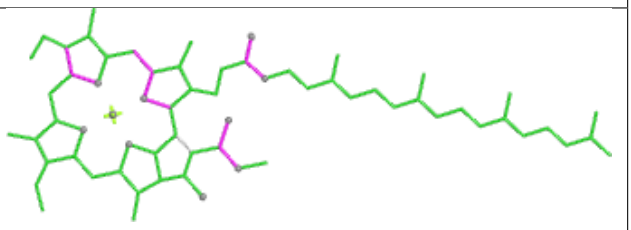

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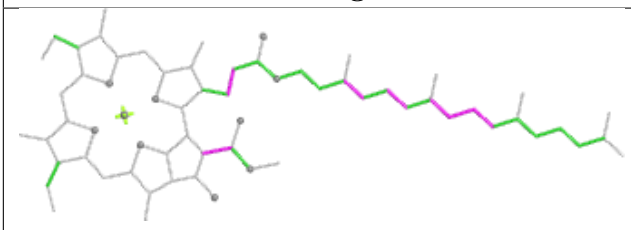

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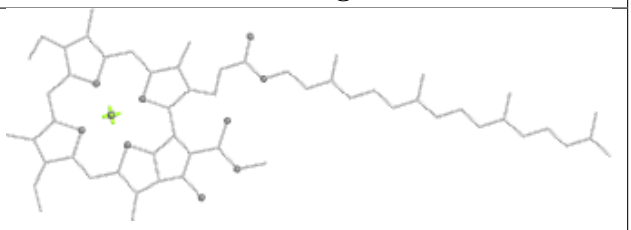
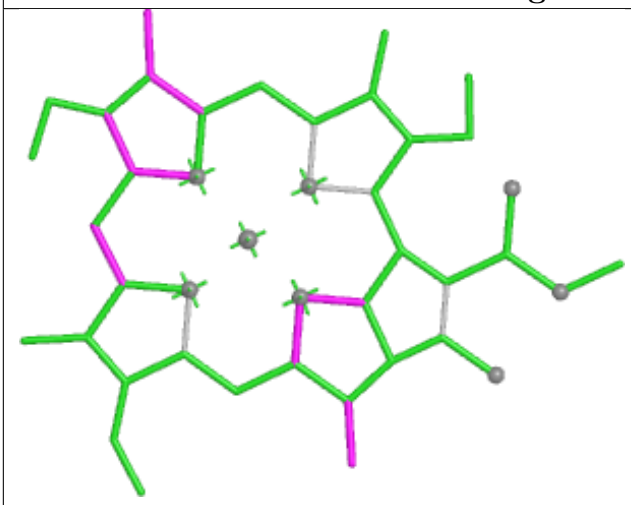


Rings

Ligand CLA 9 312



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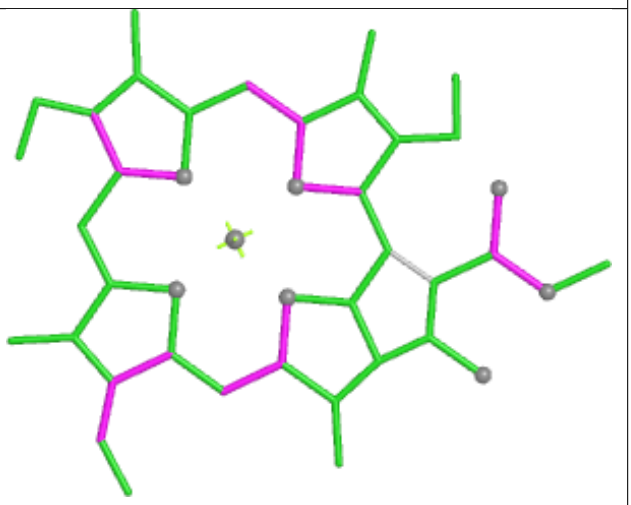

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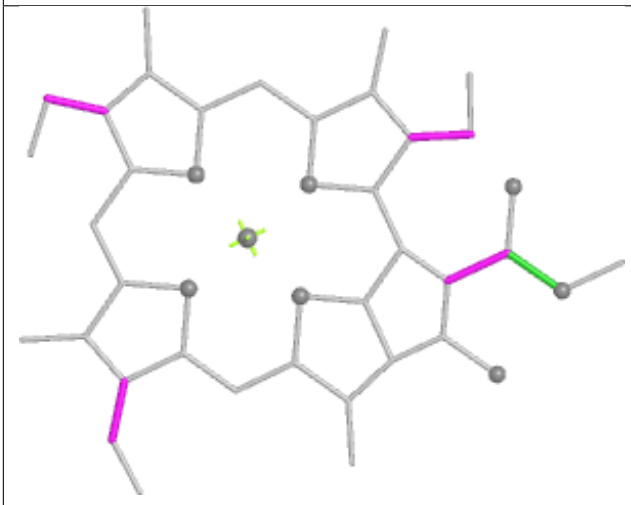

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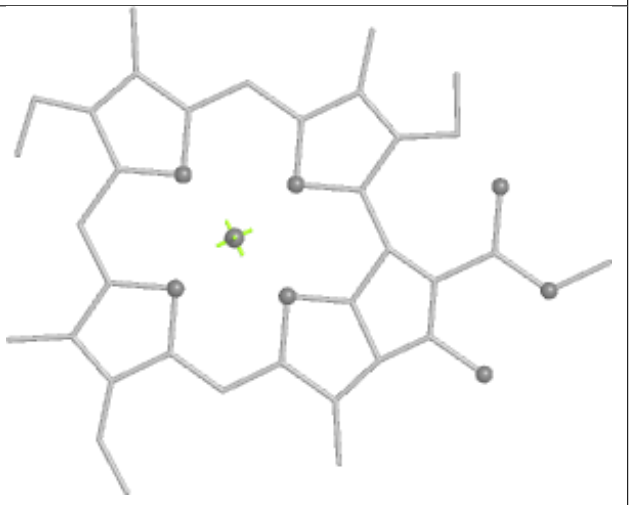
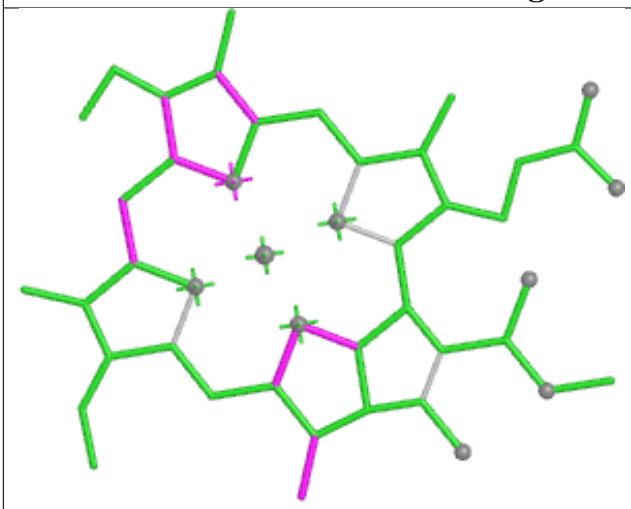


Rings

Ligand CLA y 308



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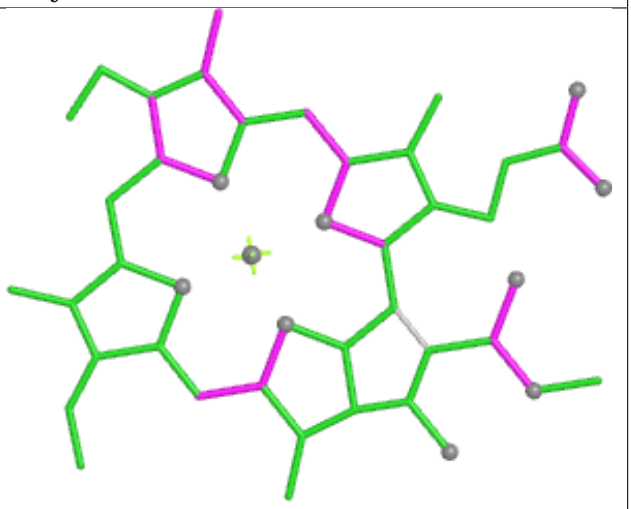

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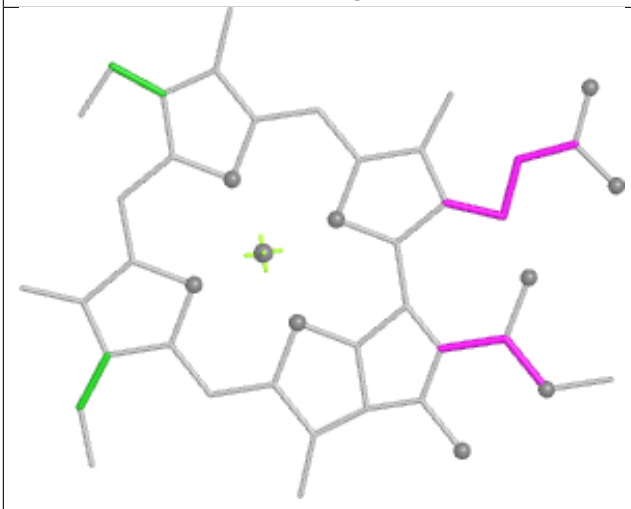
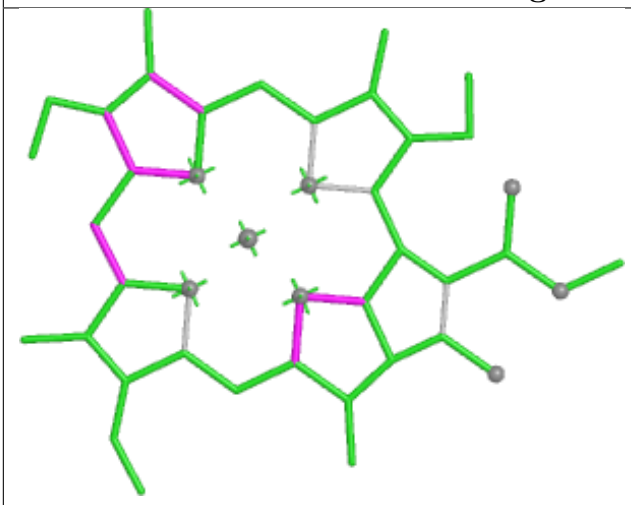


Torsions

Rings

Ligand CLA z 307



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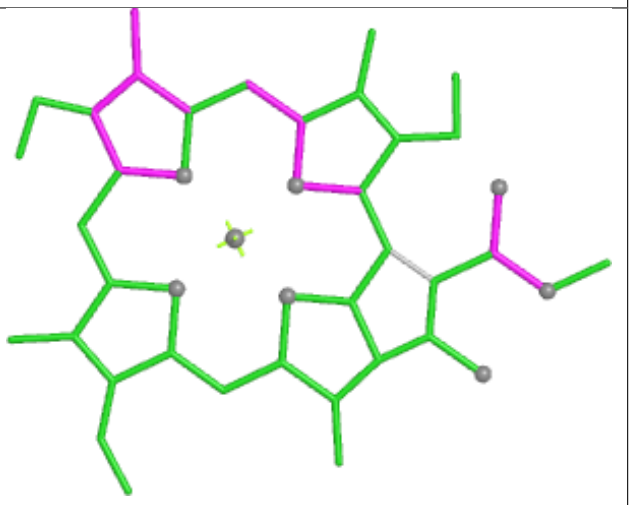

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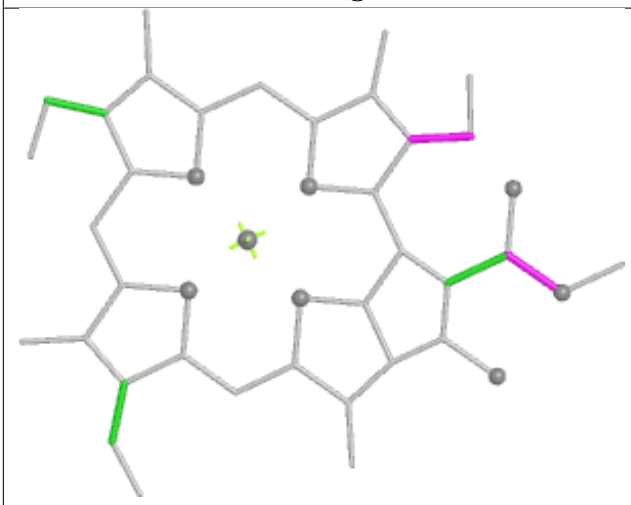
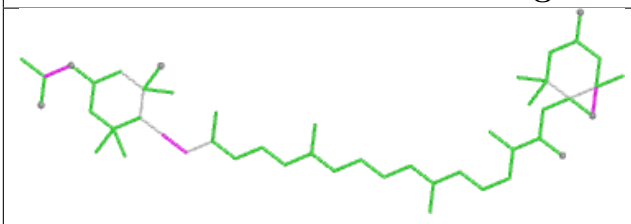


Torsions

Rings

Ligand A86 1 302



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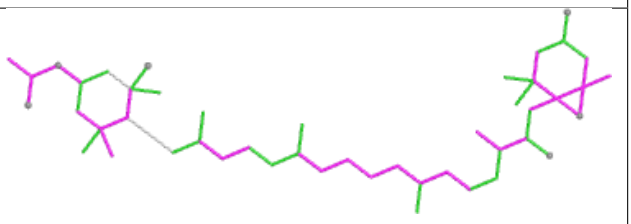

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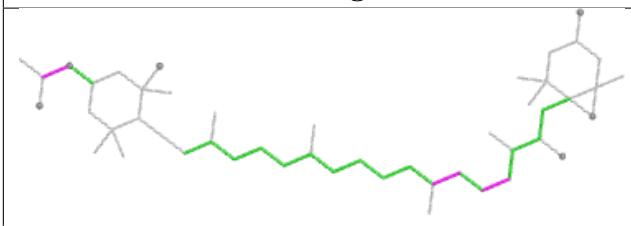

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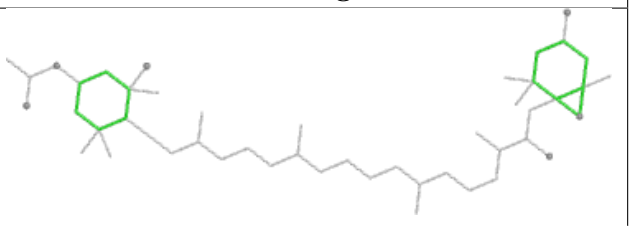
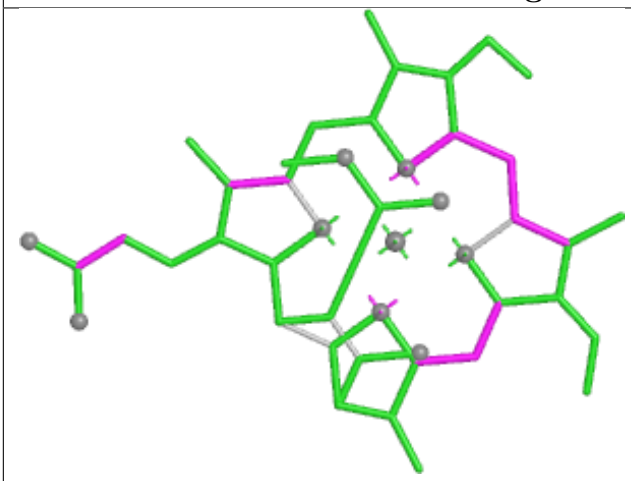


Rings

Ligand KC2 G 311



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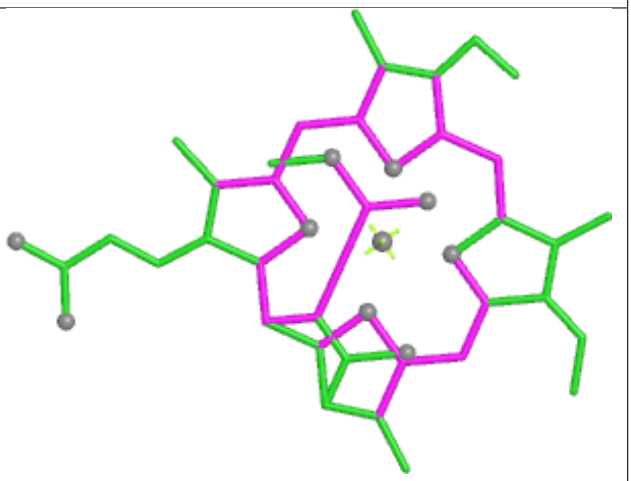

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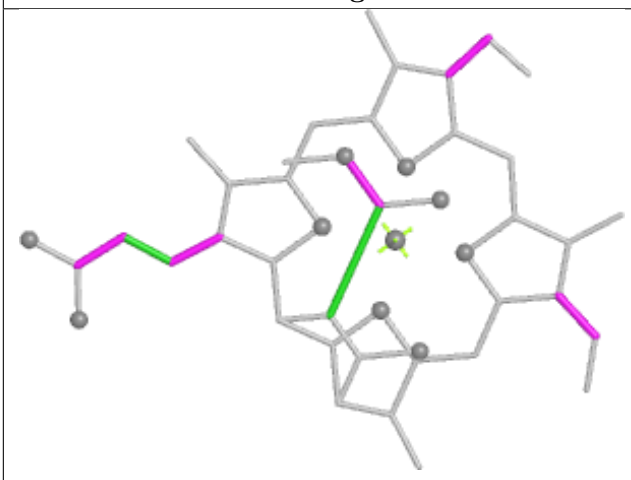

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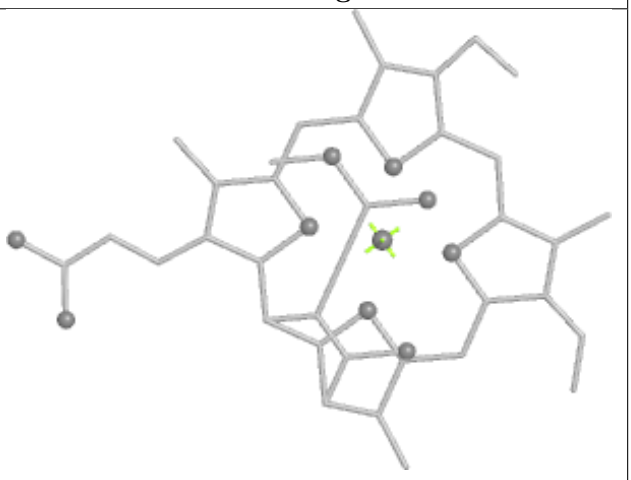
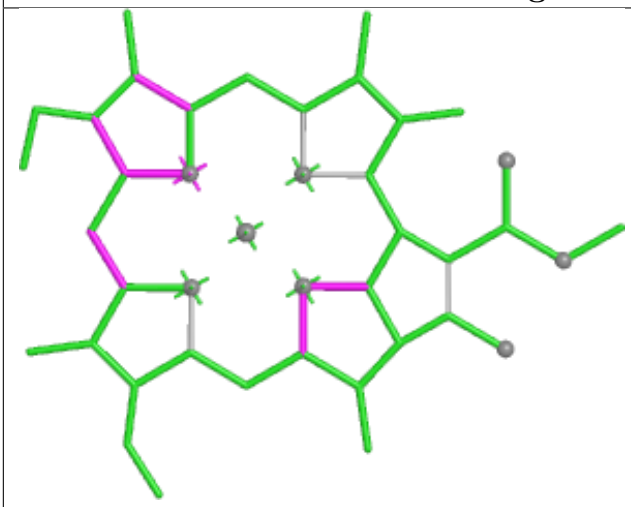


Rings

Ligand CLA 8 322



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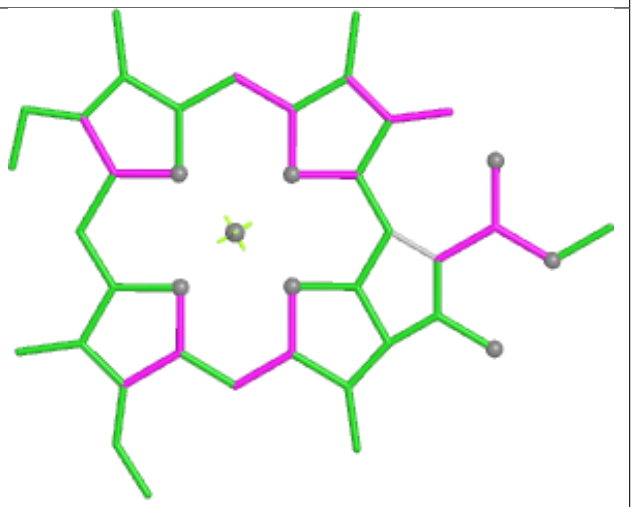

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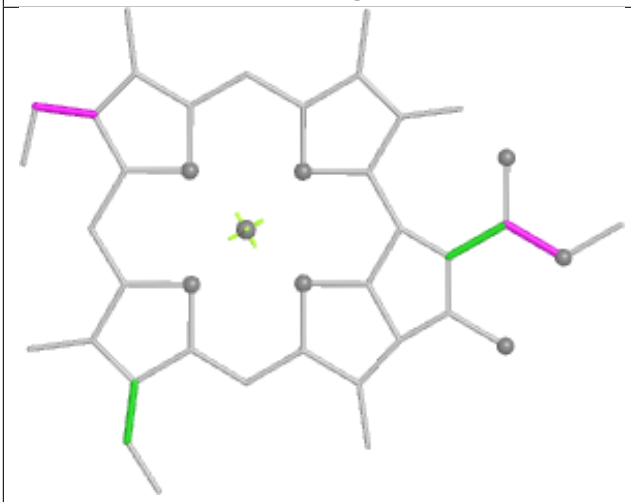

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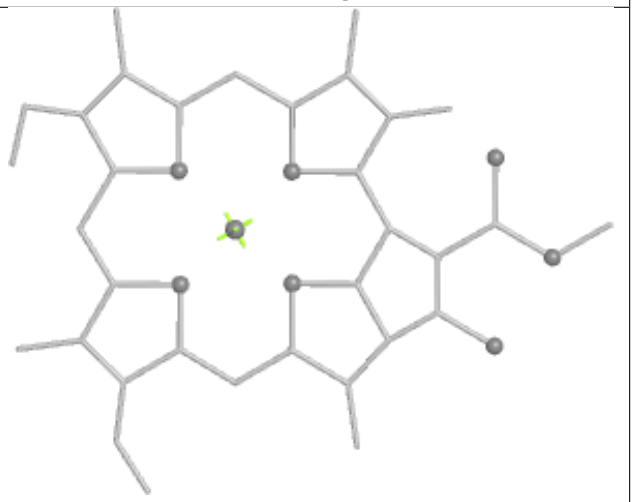
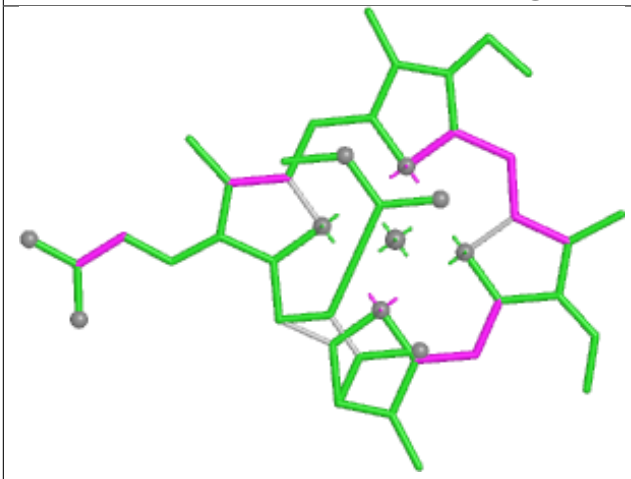


Rings

Ligand KC2 T 314



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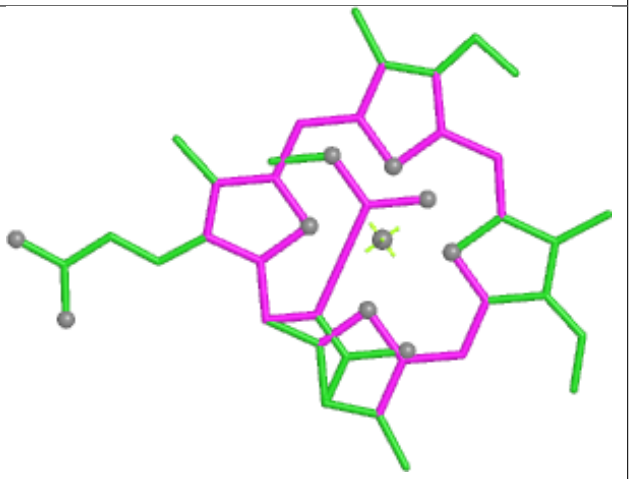
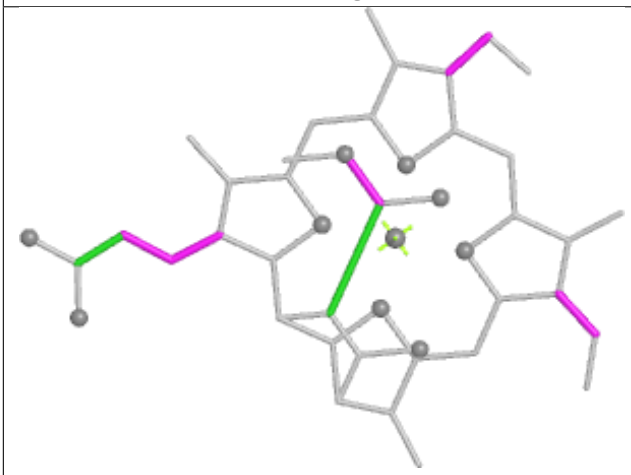


Bond angles



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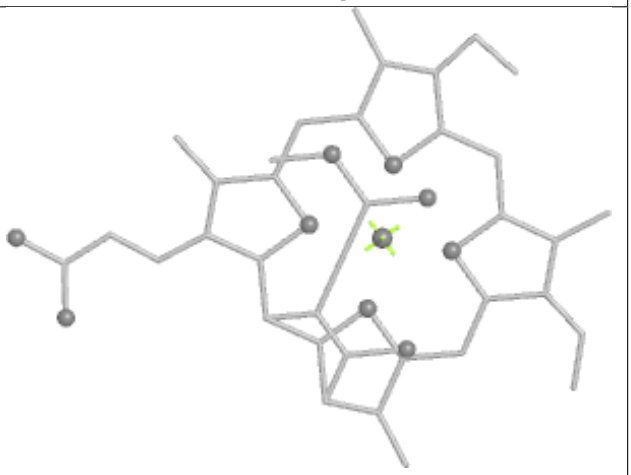
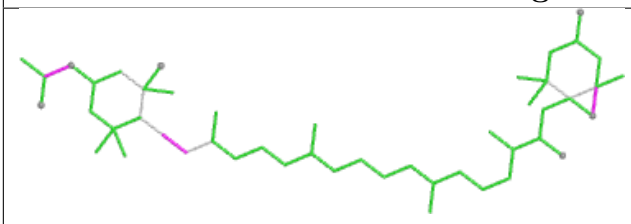


Rings

Ligand A86 F 301



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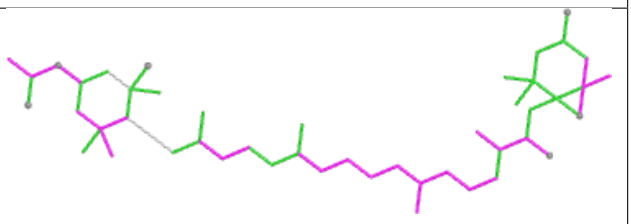
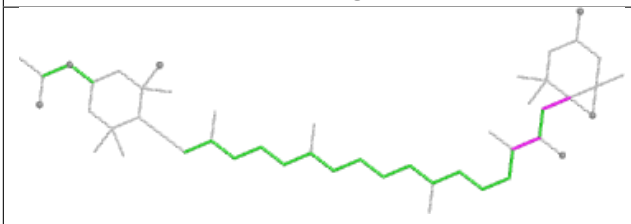
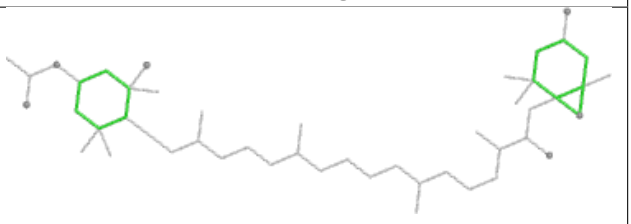


Bond angles

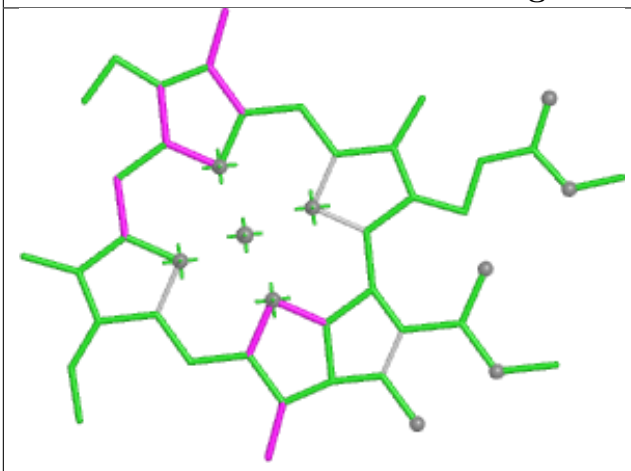


Torsions

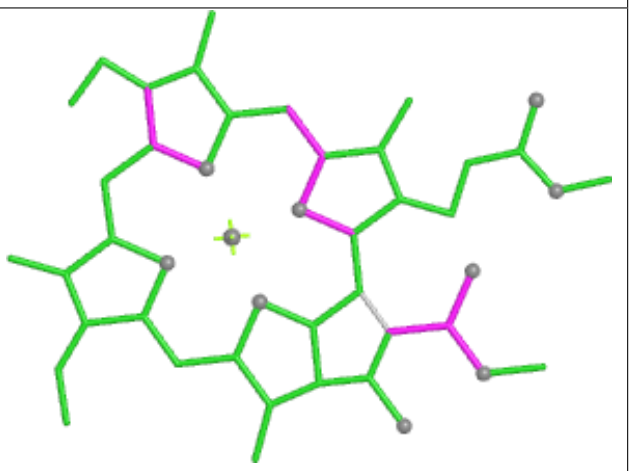


Rings

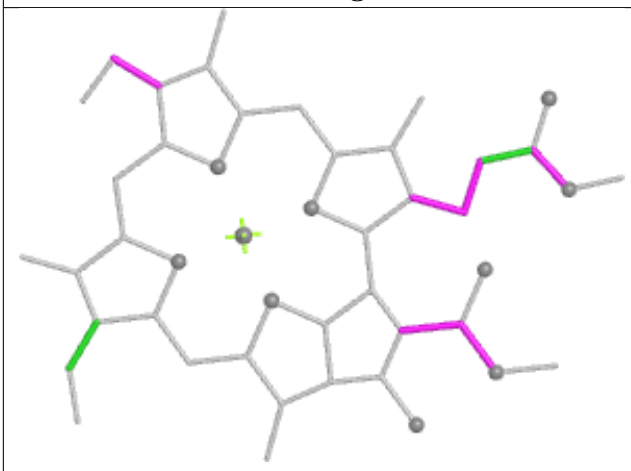
Ligand CLA 0 323



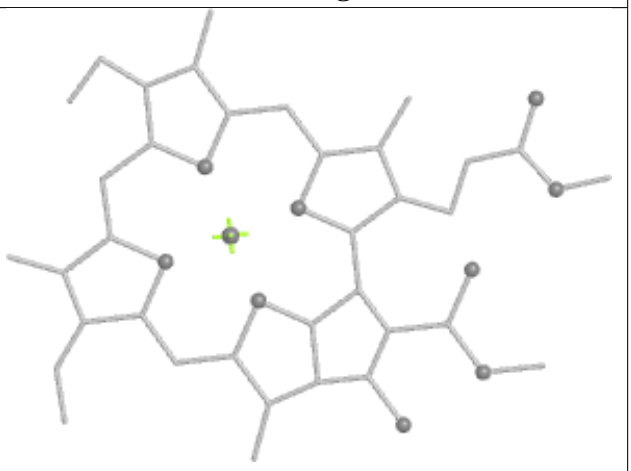
Bond lengths



Bond angles

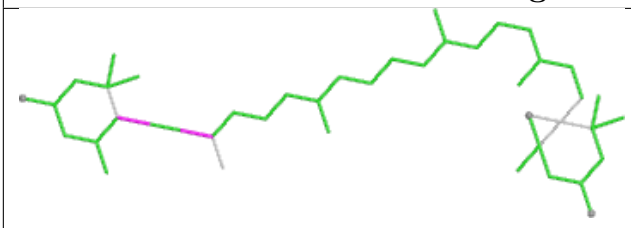


Torsions



Rings

Ligand DD6 o 204



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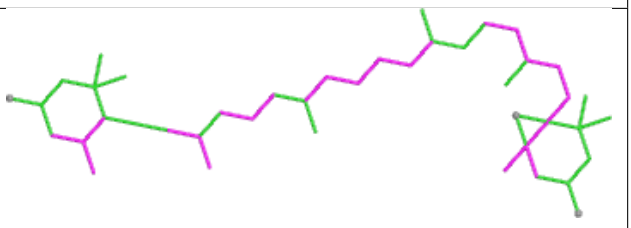

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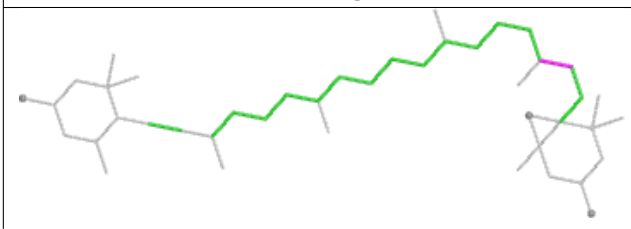

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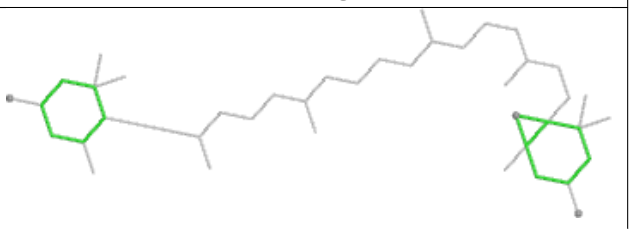
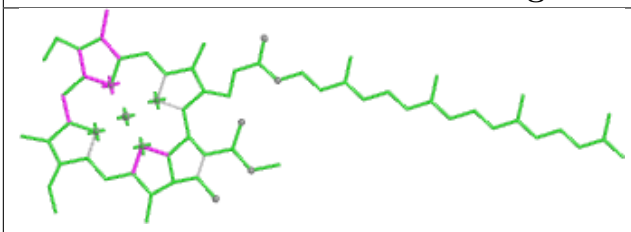


Rings

Ligand CLA b 821



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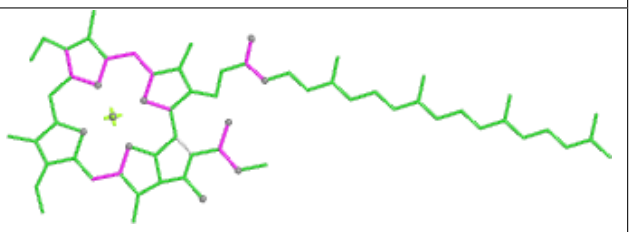
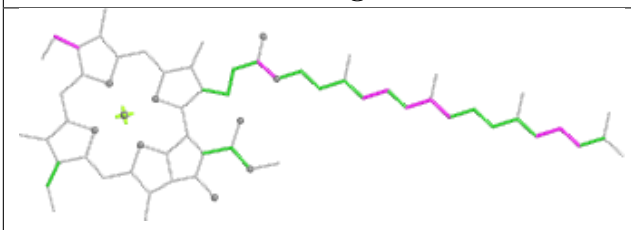


Bond angles



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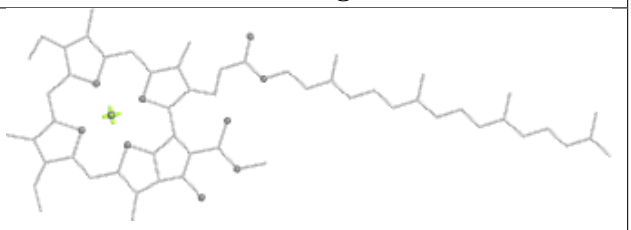
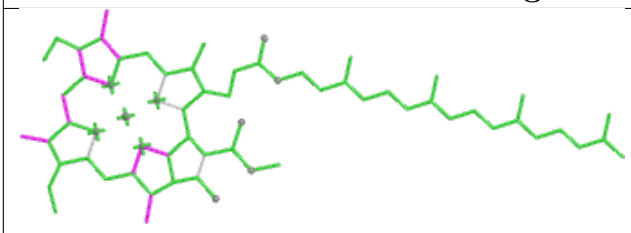


Rings

Ligand CLA V 313



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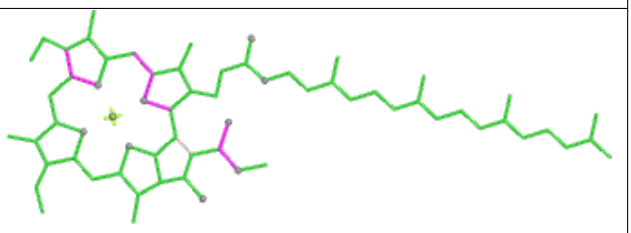
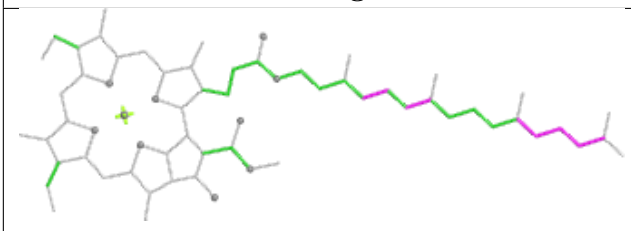


Bond angles



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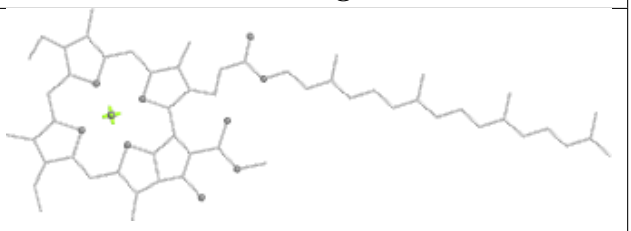
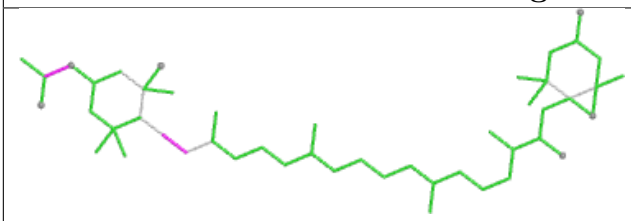


Rings

Ligand A86 C 303



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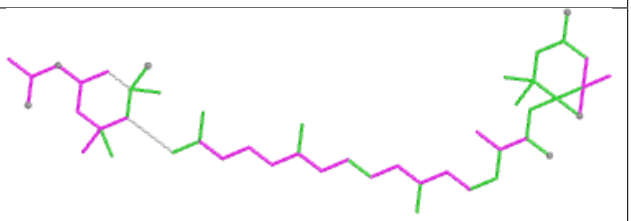
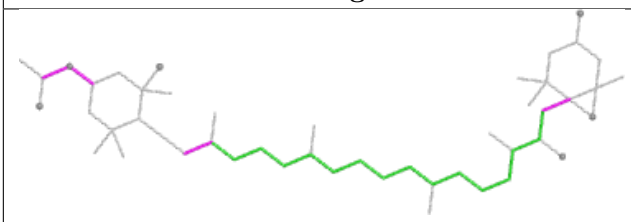


Bond angles



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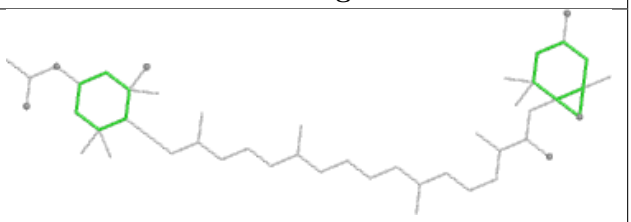
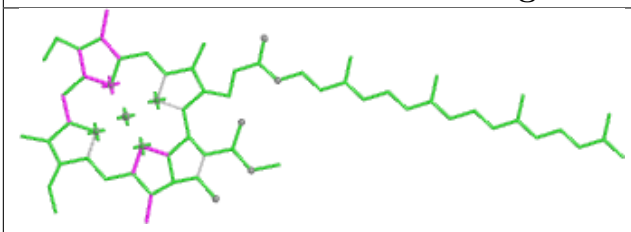
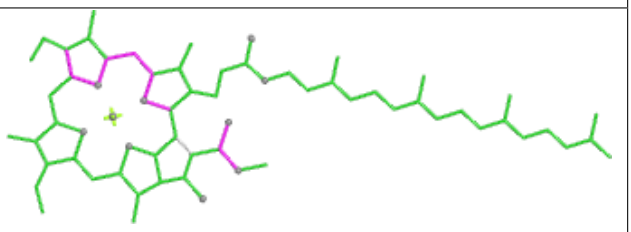


Rings

Ligand CLA W 310



Bond lengths



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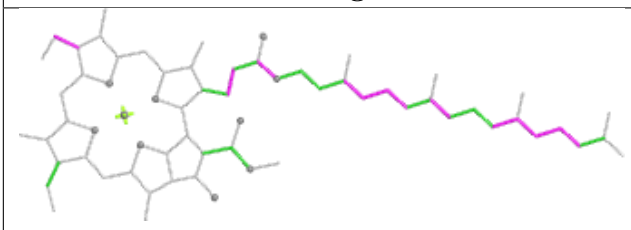

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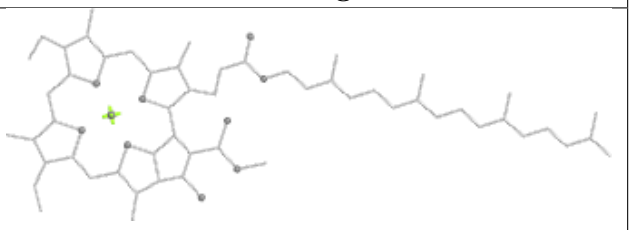
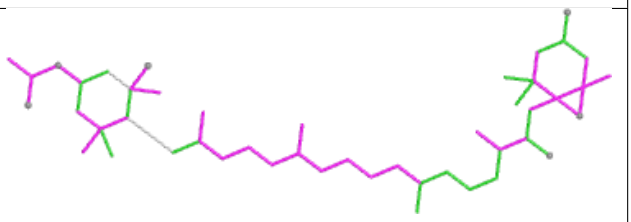


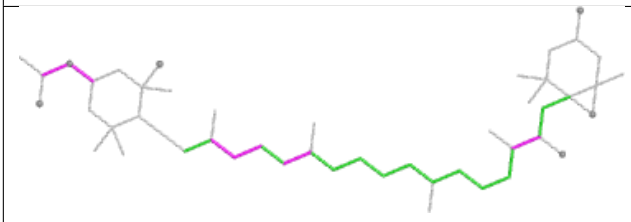
Rings

Ligand A86 L 302

Bond lengths



Bond angles



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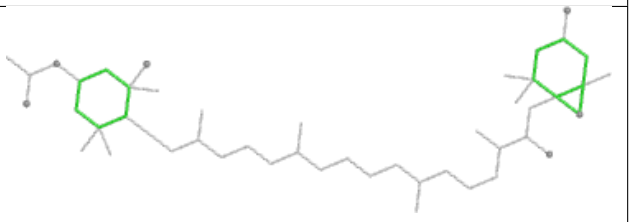
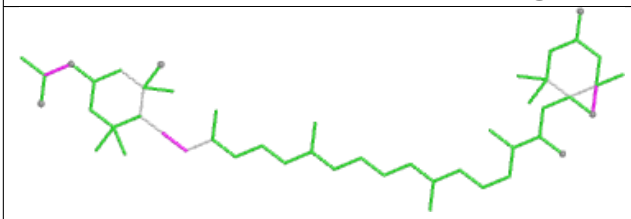


Rings

Ligand A86 T 305



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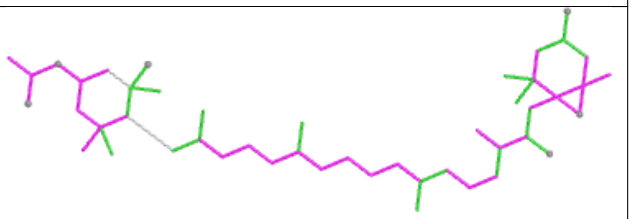
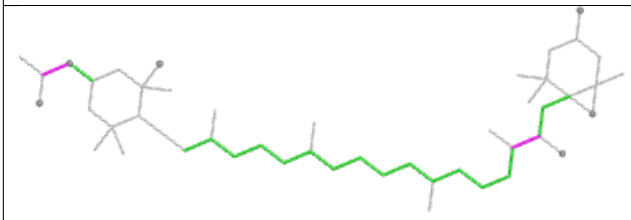


Bond angles



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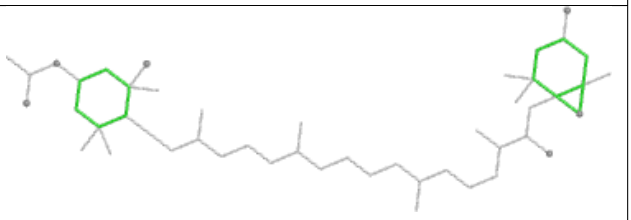
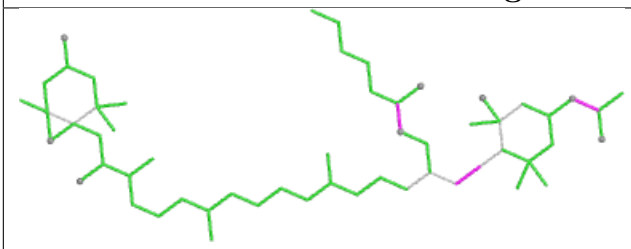


Rings

Ligand A1EB1 G 308



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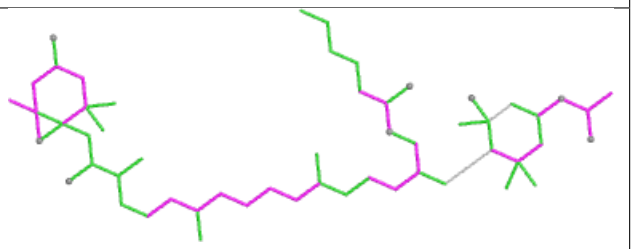
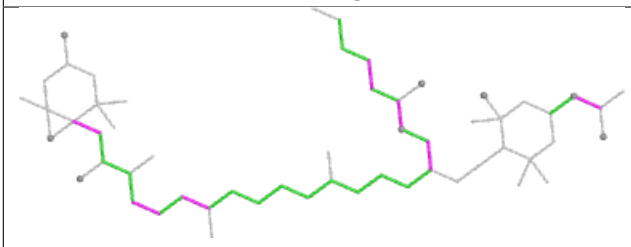


Bond angles



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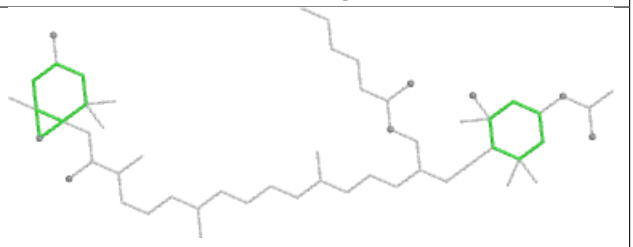
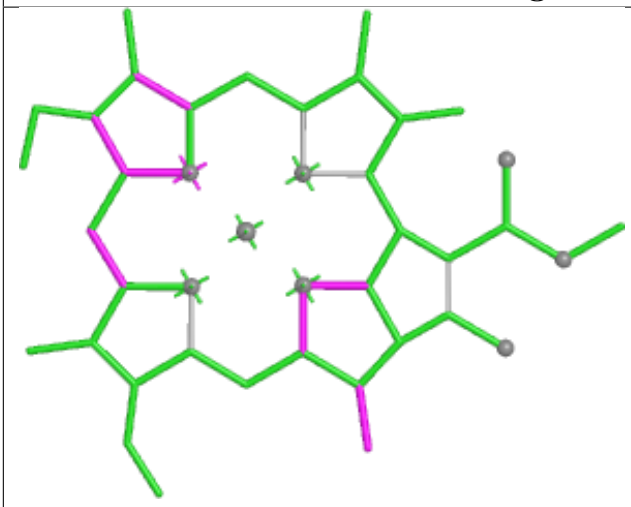


Rings

Ligand CLA 6 318



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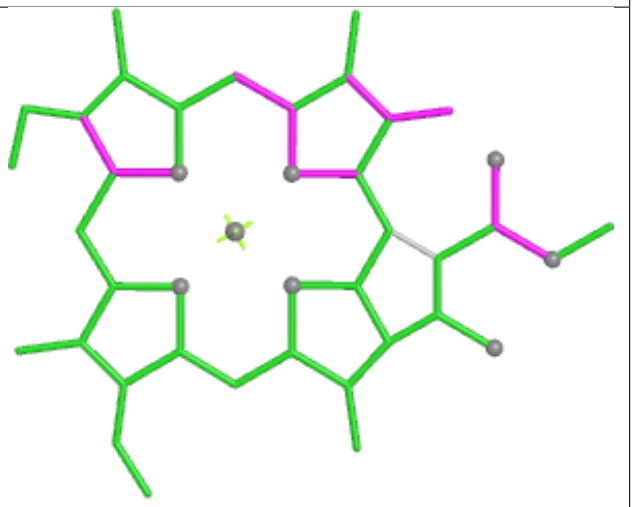
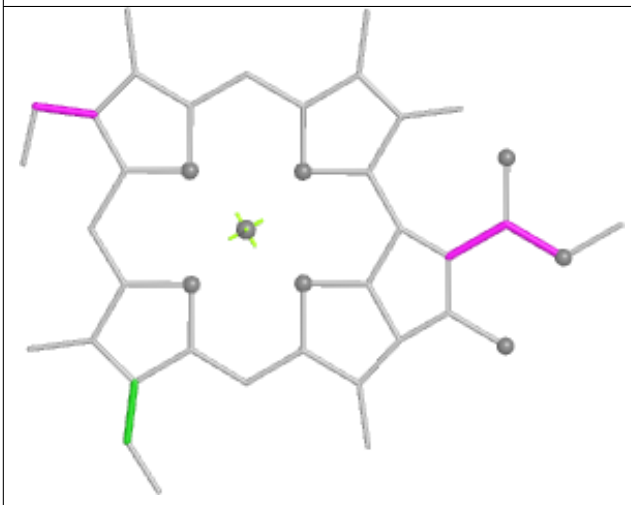


Bond angles



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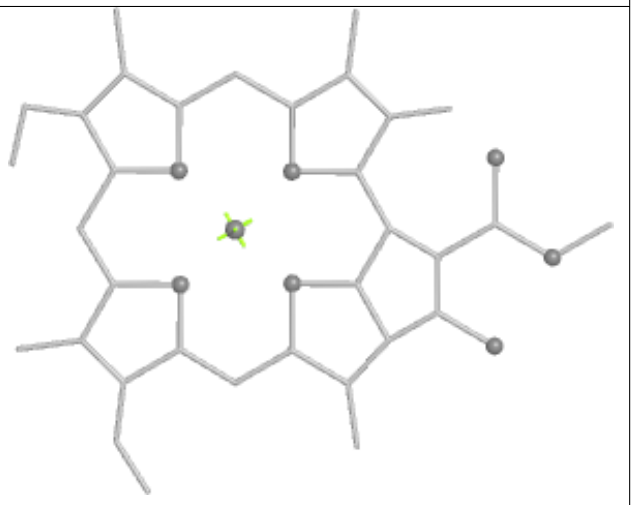
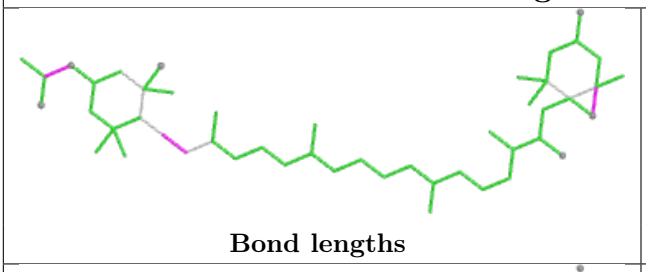


Rings

Ligand A86 2 302



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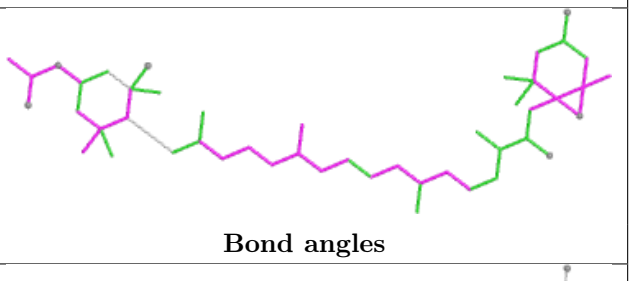
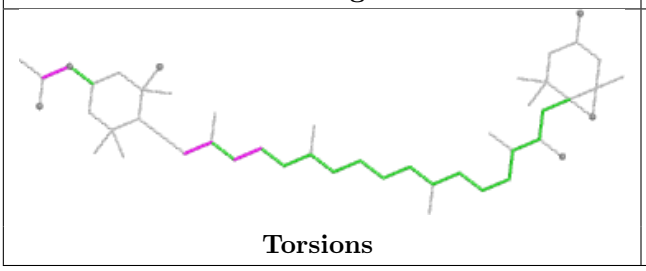


Bond angles



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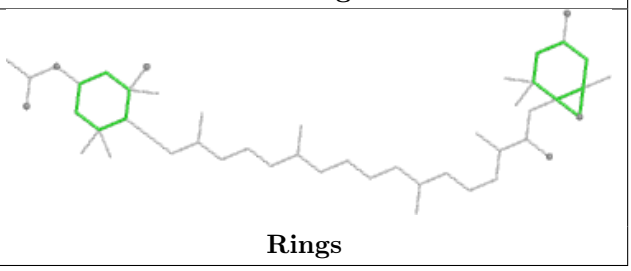
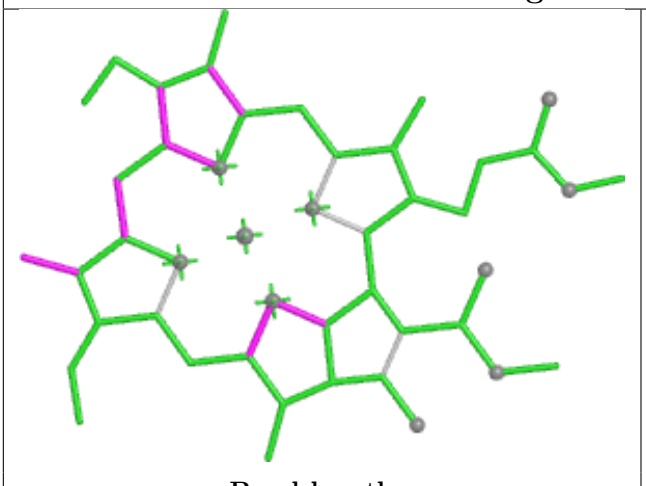
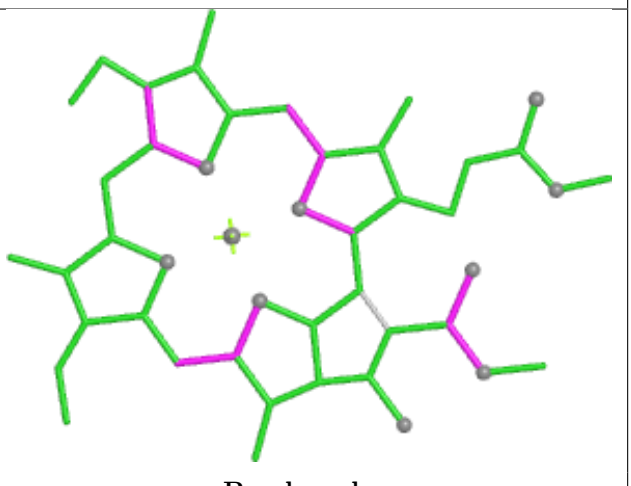


Rings

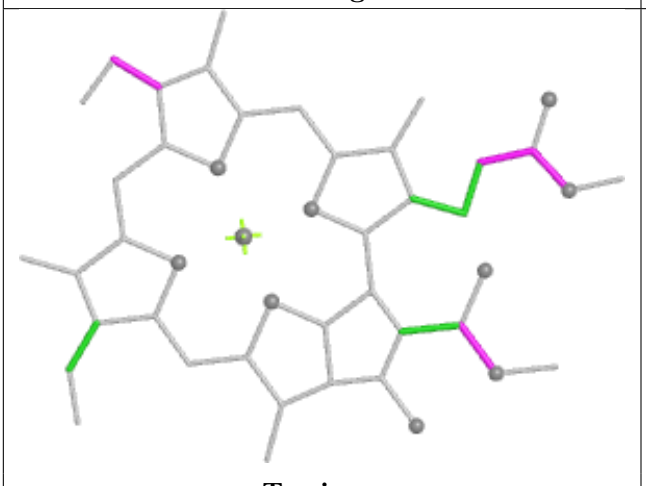
Ligand CLA F 306



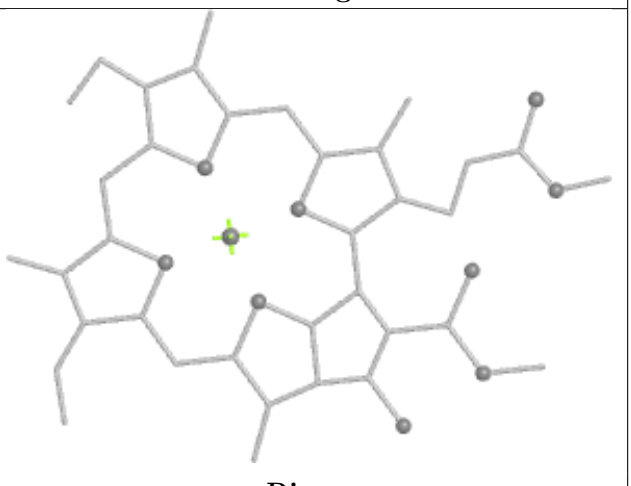
Bond lengths



Bond angles

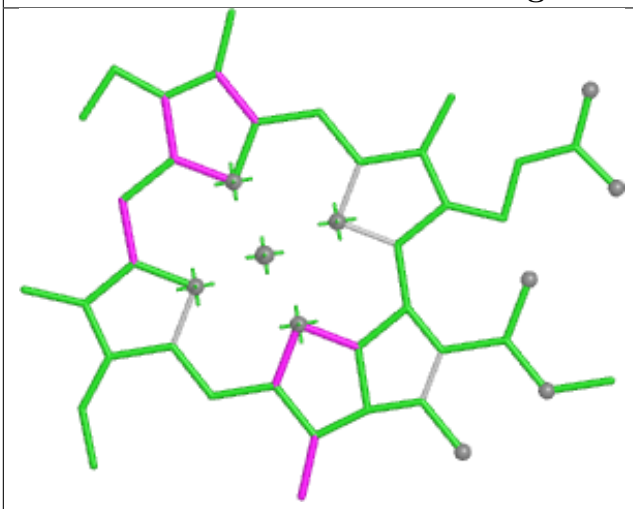


Torsions



Rings

Ligand CLA b 808



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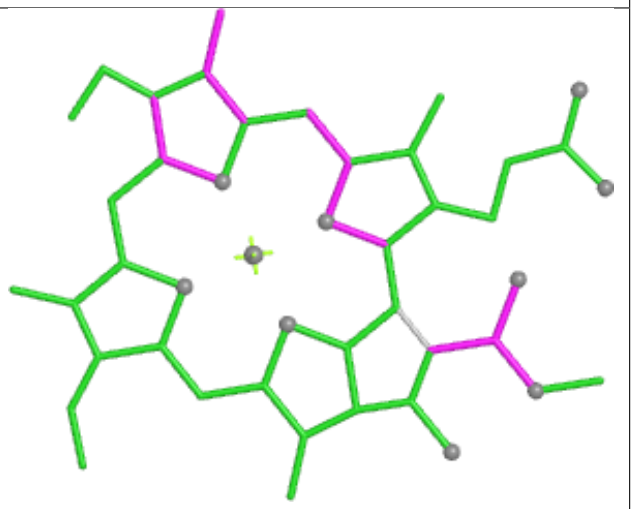
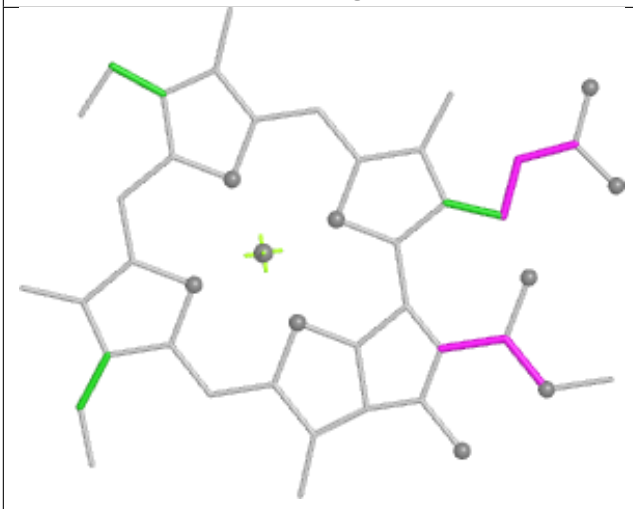


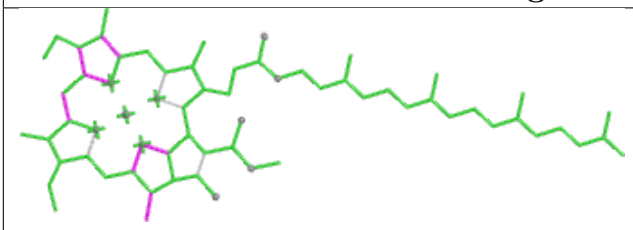
Bond angles



Torsions

Rings

Ligand CLA b 835



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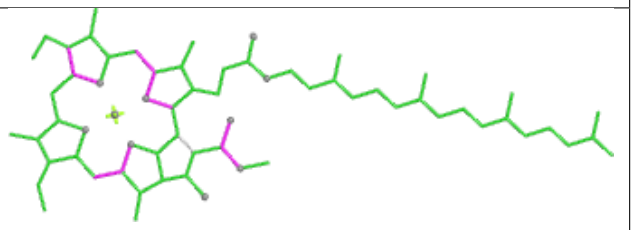
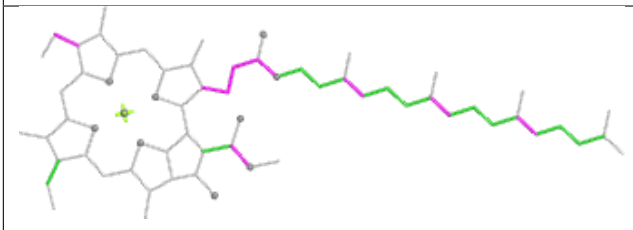
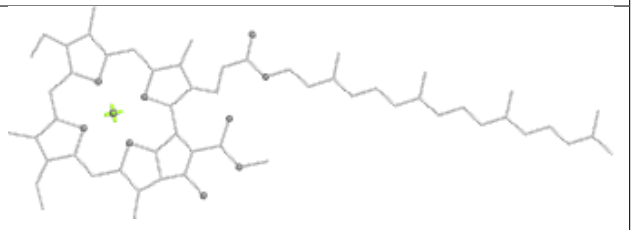


Bond angles

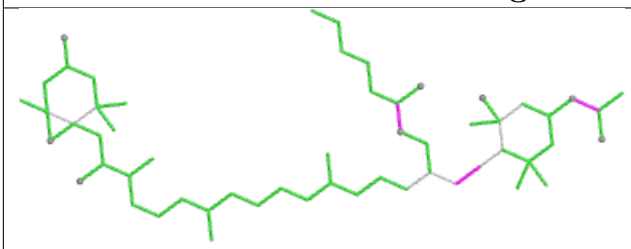


Torsions

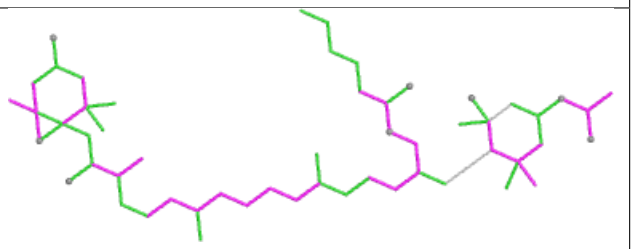


Rings

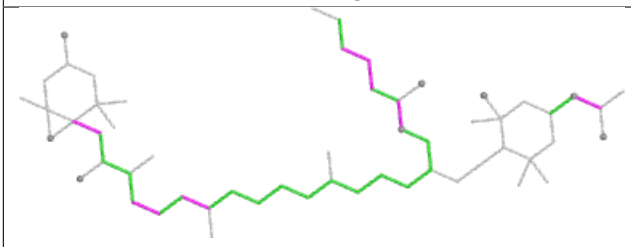
Ligand A1EB1 8 304



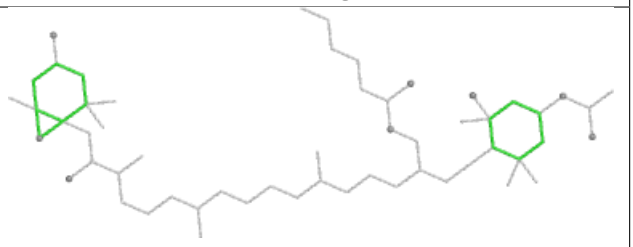
Bond lengths



Bond angles

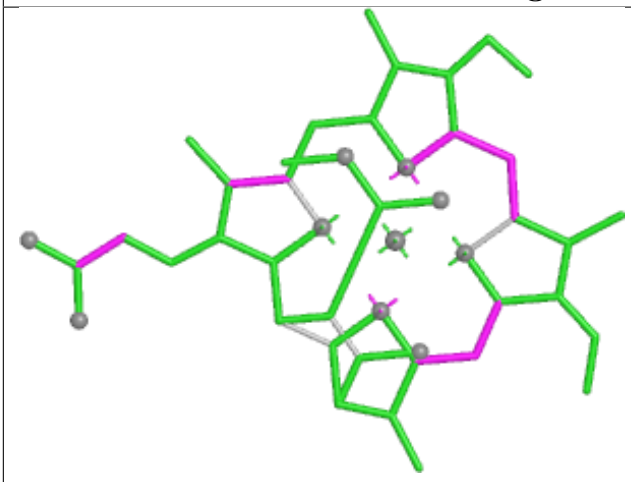


Torsions

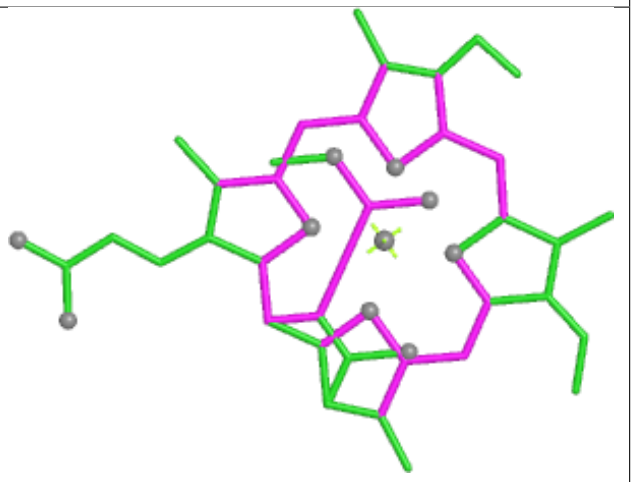


Rings

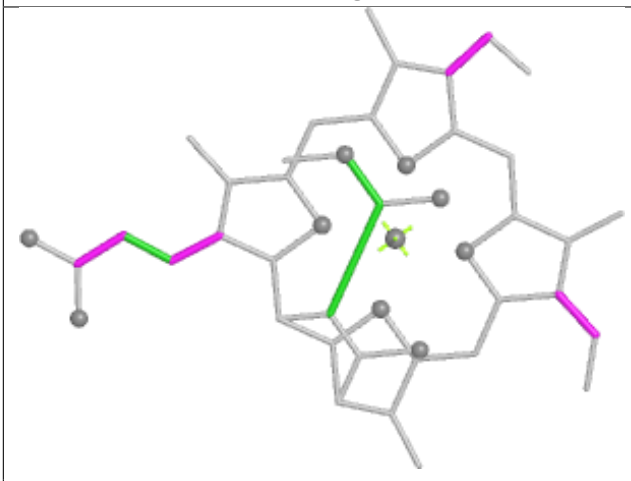
Ligand KC2 T 316



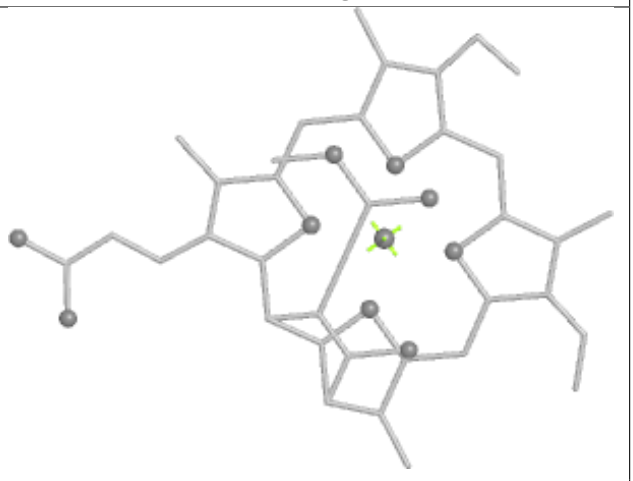
Bond lengths



Bond angles

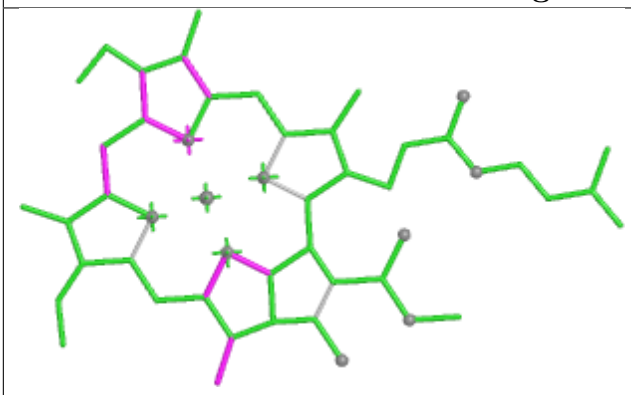


Torsions

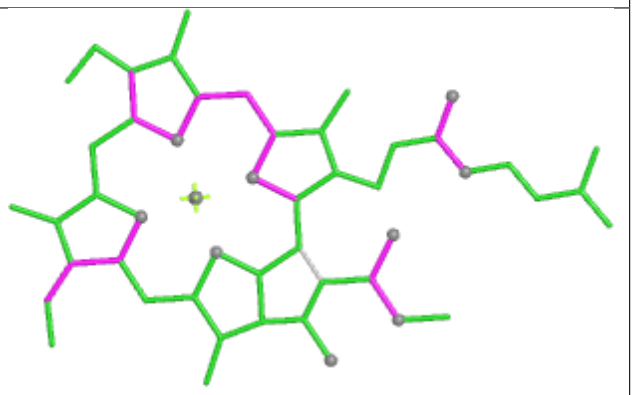


Rings

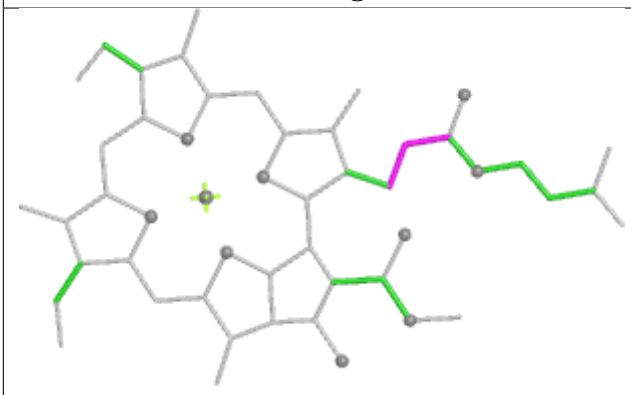
Ligand CLA l 205



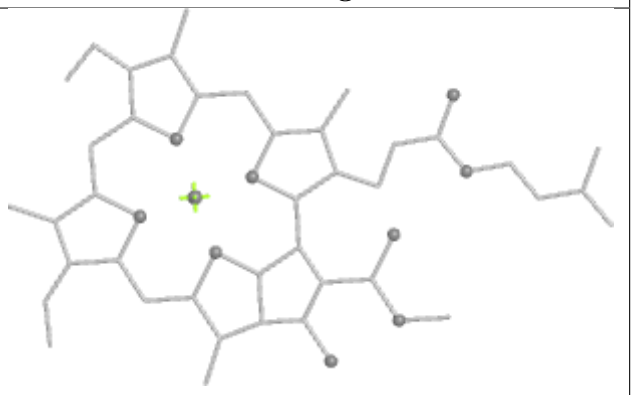
Bond lengths



Bond angles

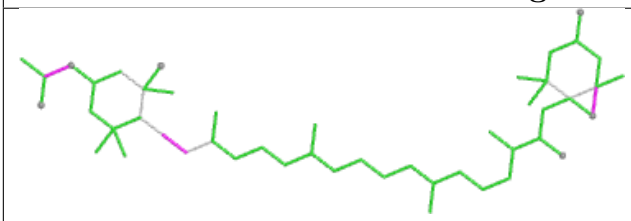


Torsions

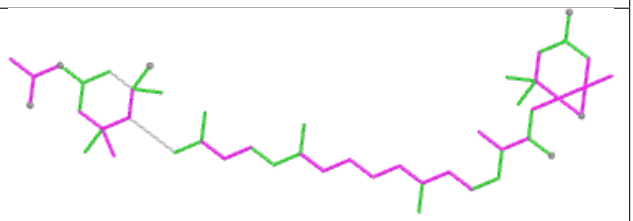


Rings

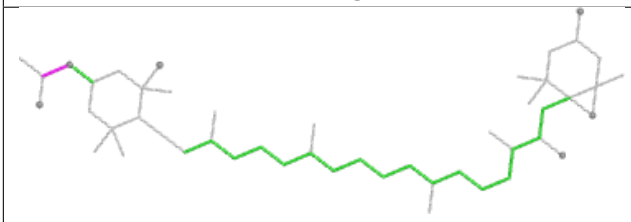
Ligand A86 V 301



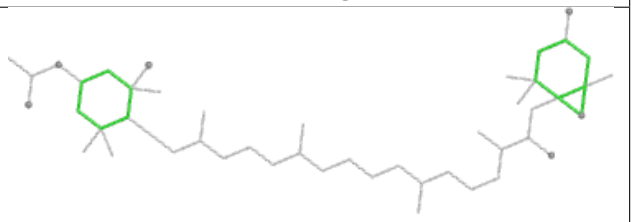
Bond lengths



Bond angles

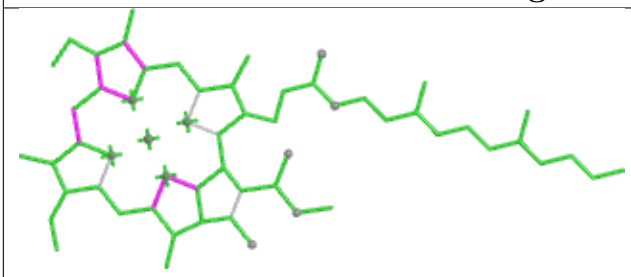


Torsions

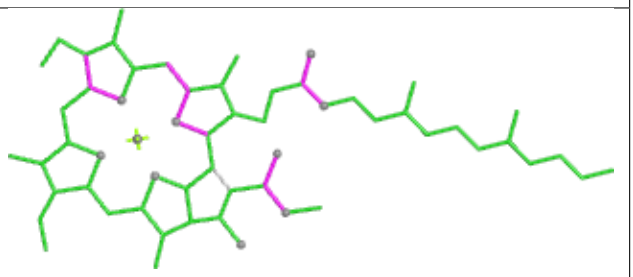


Rings

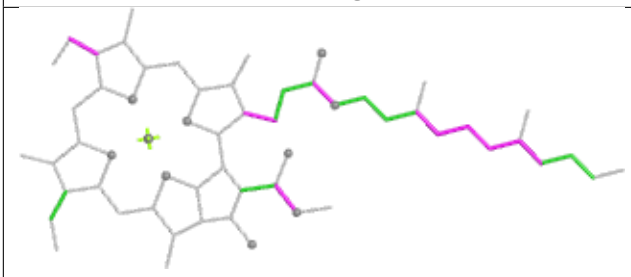
Ligand CLA o 206



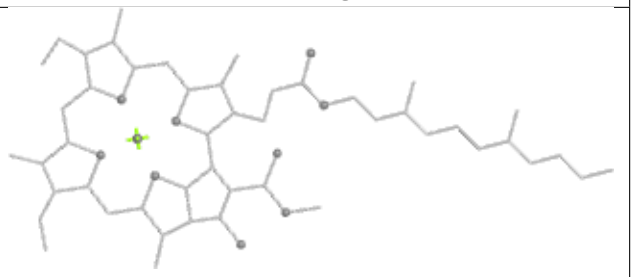
Bond lengths



Bond angles

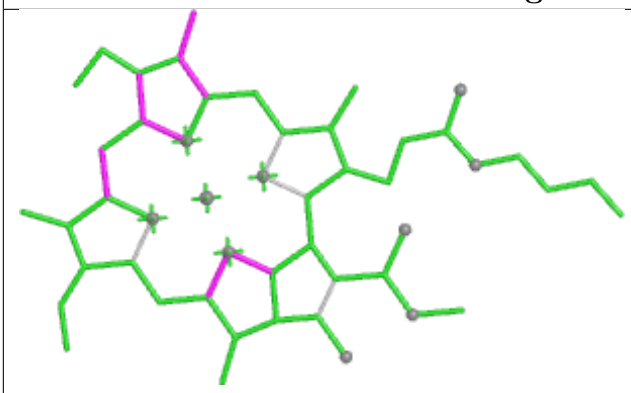


Torsions



Rings

Ligand CLA E 319



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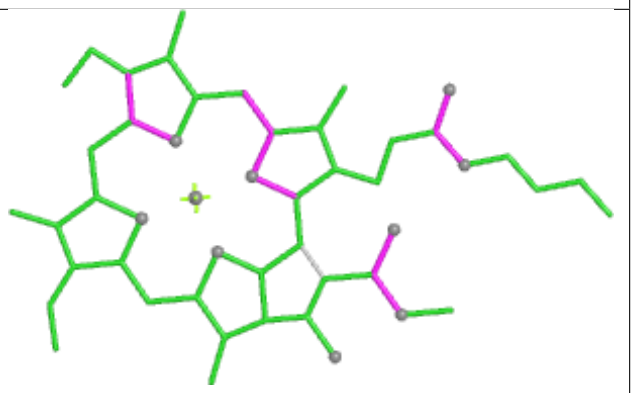
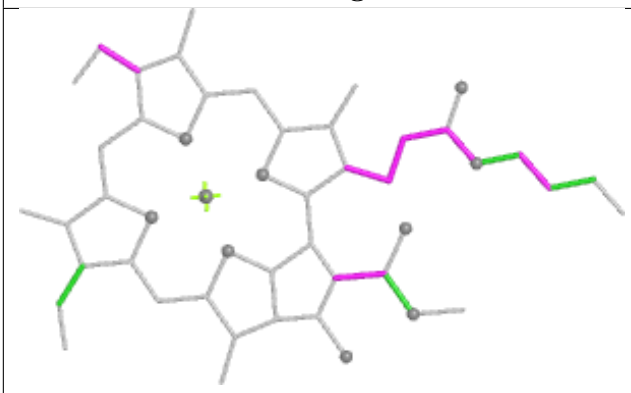
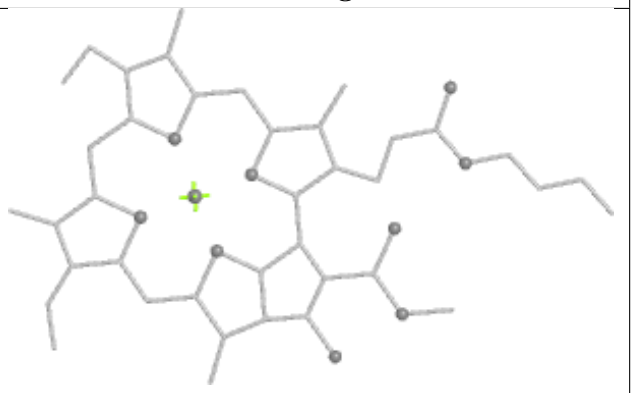


Bond angles

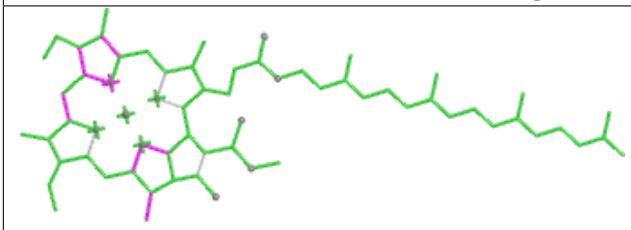


Torsions

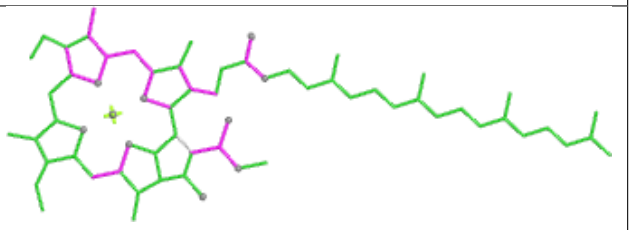


Rings

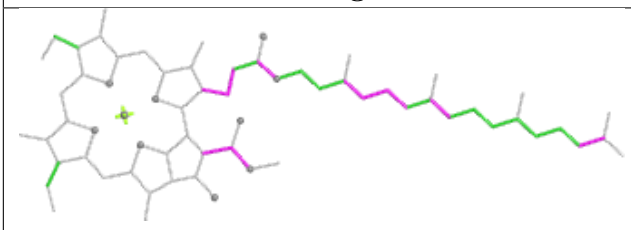
Ligand CLA 4 312



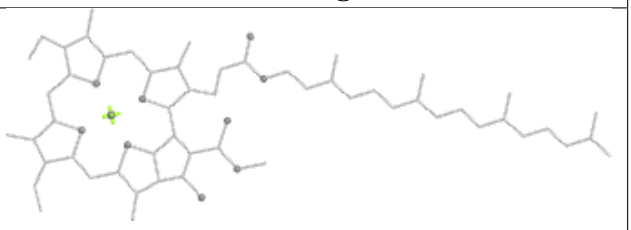
Bond lengths



Bond angles

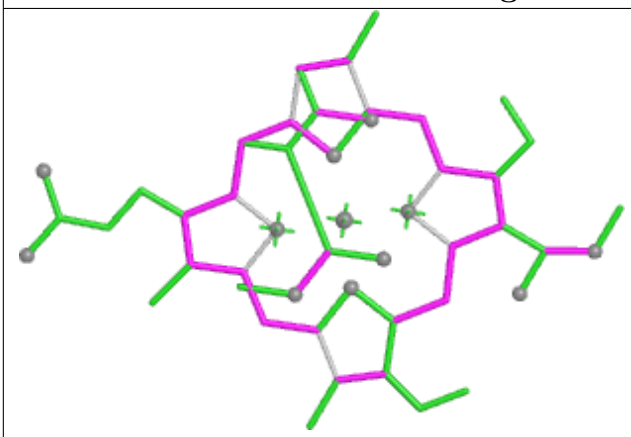


Torsions

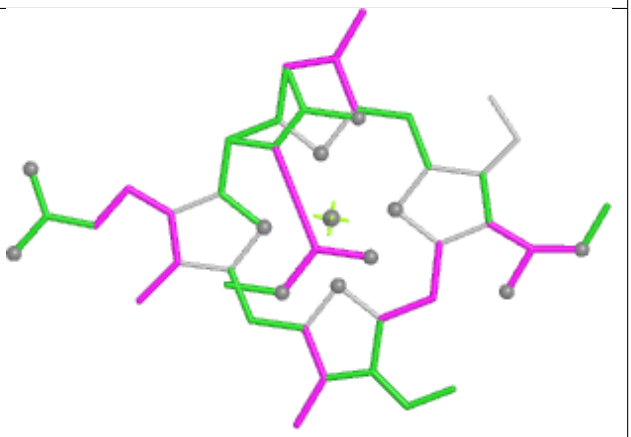


Rings

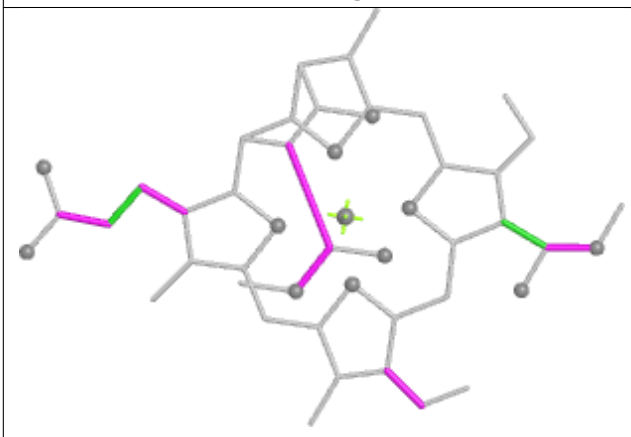
Ligand A1ECV V 317



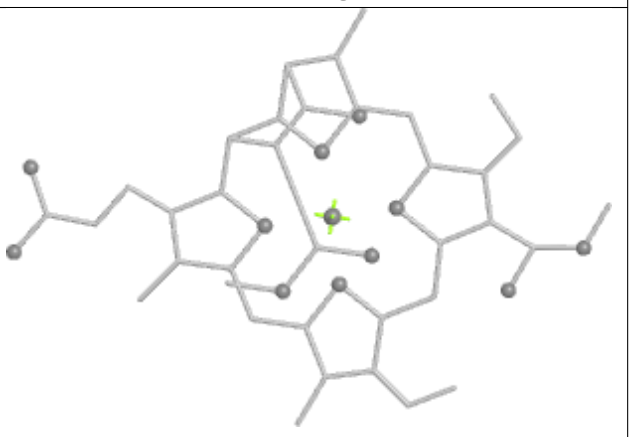
Bond lengths



Bond angles

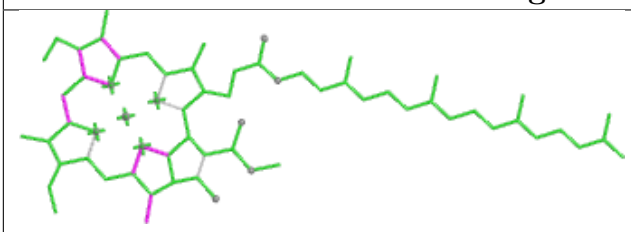


Torsions

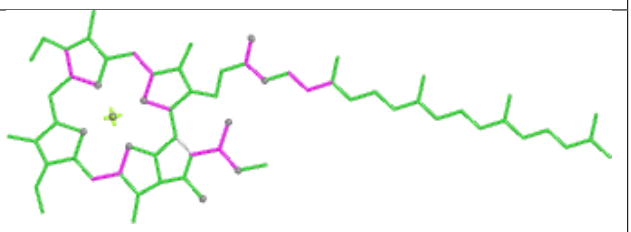


Rings

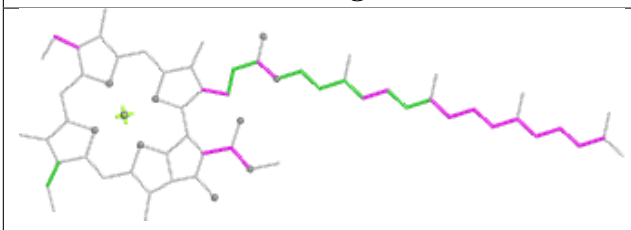
Ligand CLA 3 312



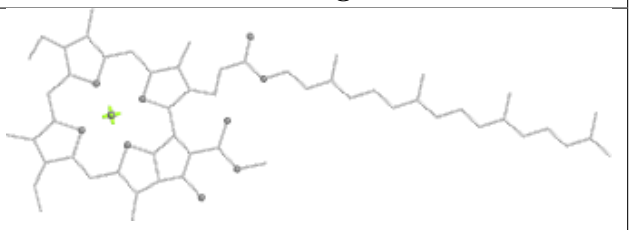
Bond lengths



Bond angles

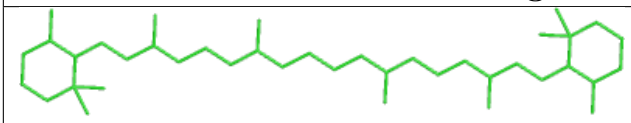


Torsions

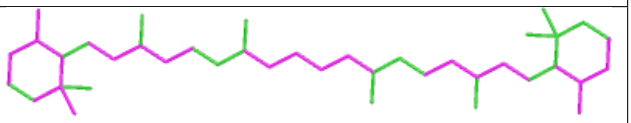


Rings

Ligand BCR a 842

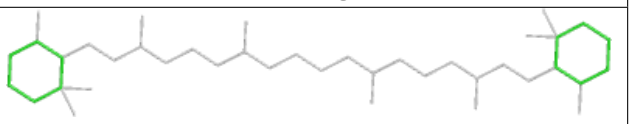


Bond lengths



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.

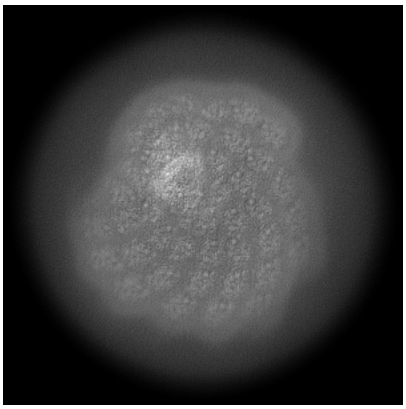
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61519. These allow visual inspection of the internal detail of the map and identification of artifacts.

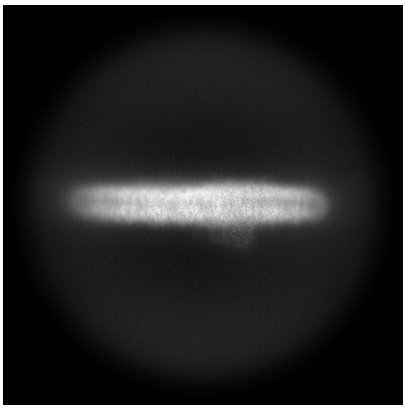
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

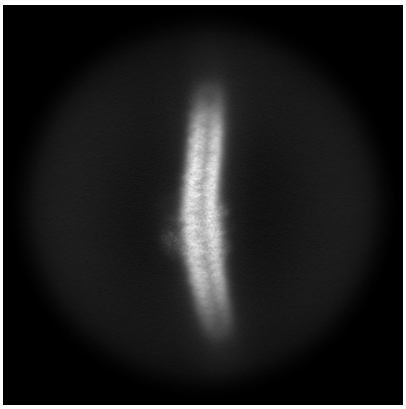
6.1.1 Primary map



X

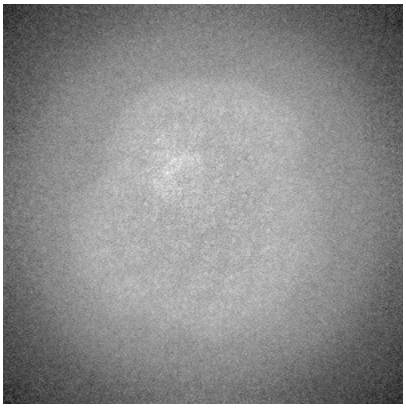


Y

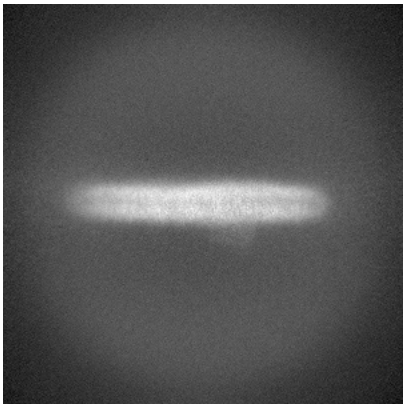


Z

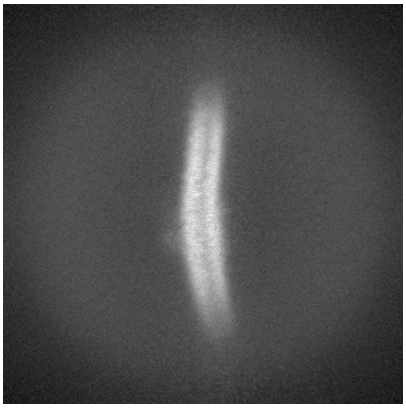
6.1.2 Raw map



X



Y

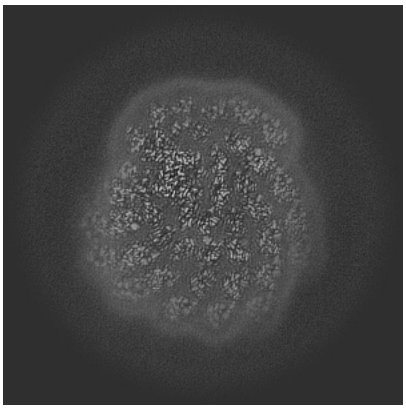


Z

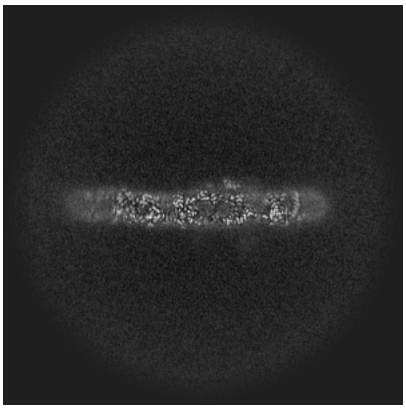
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

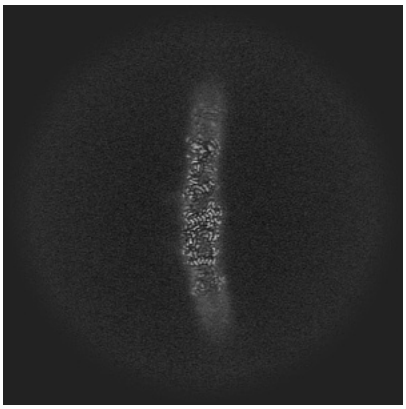
6.2.1 Primary map



X Index: 330

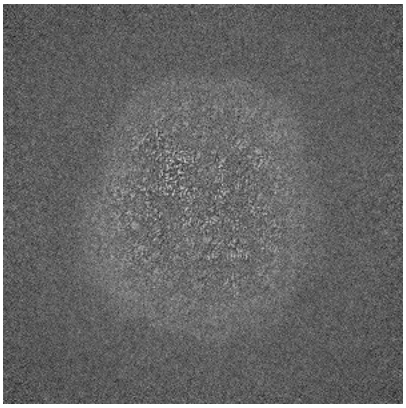


Y Index: 330

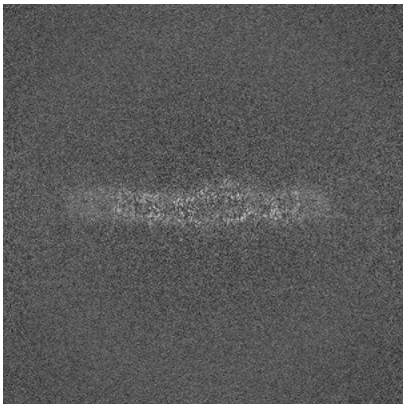


Z Index: 330

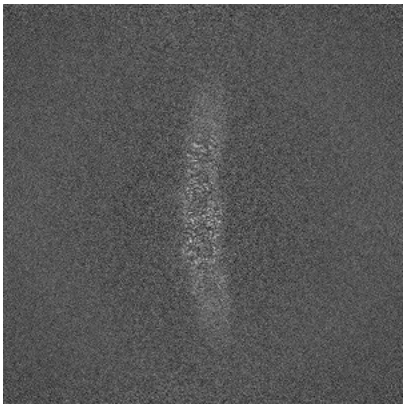
6.2.2 Raw map



X Index: 330



Y Index: 330

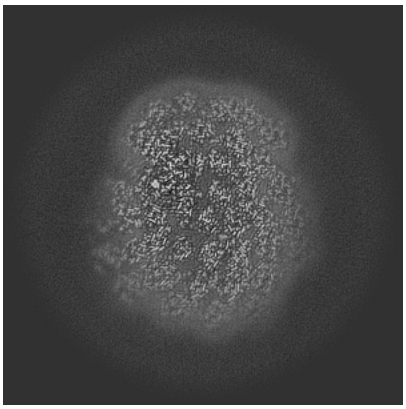


Z Index: 330

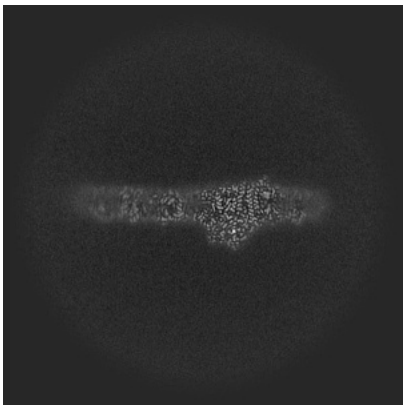
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

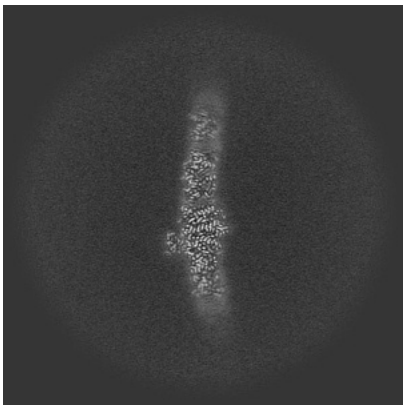
6.3.1 Primary map



X Index: 318

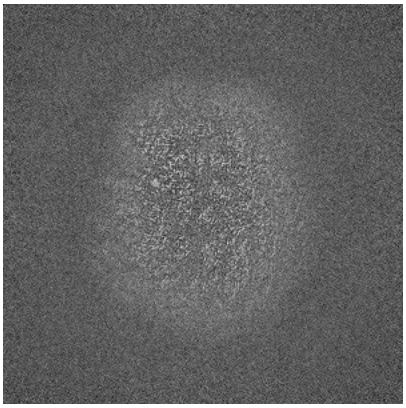


Y Index: 272

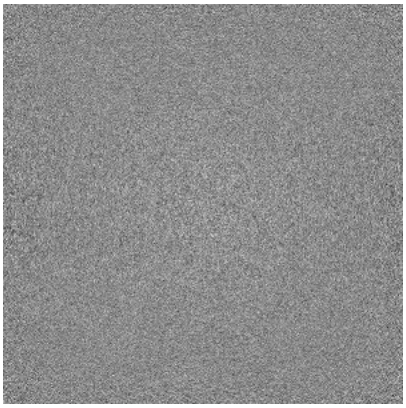


Z Index: 354

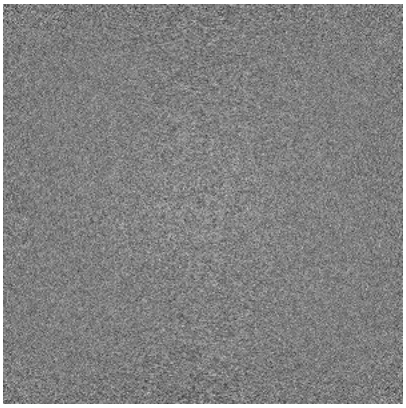
6.3.2 Raw map



X Index: 318



Y Index: 0

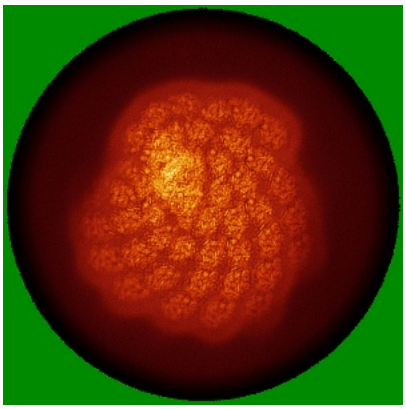


Z Index: 0

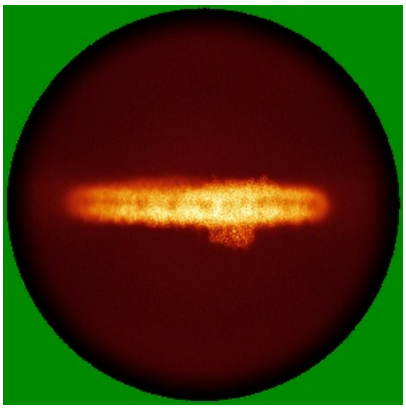
The images above show the largest variance slices of the map in three orthogonal directions.

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

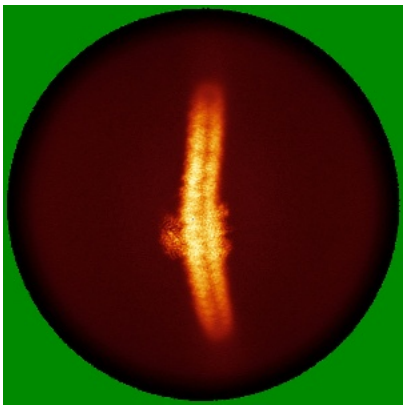
6.4.1 Primary map



X

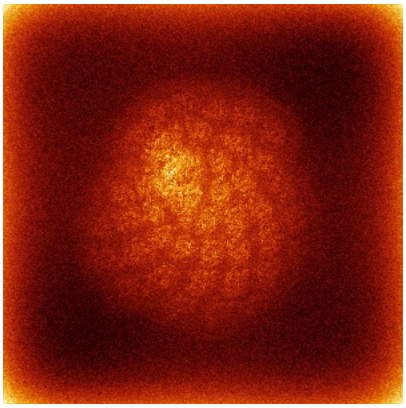


Y

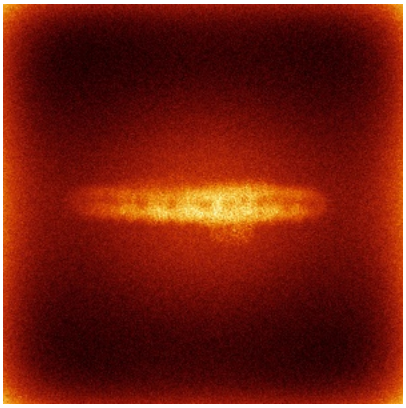


Z

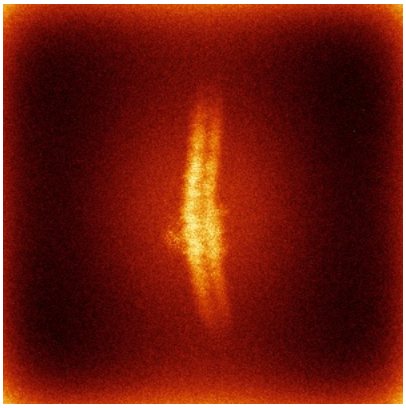
6.4.2 Raw map



X



Y

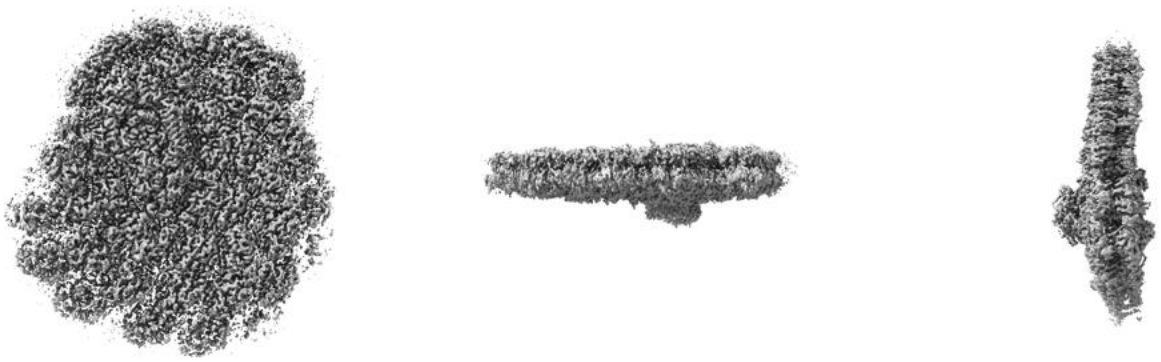


Z

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 0.066. 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.

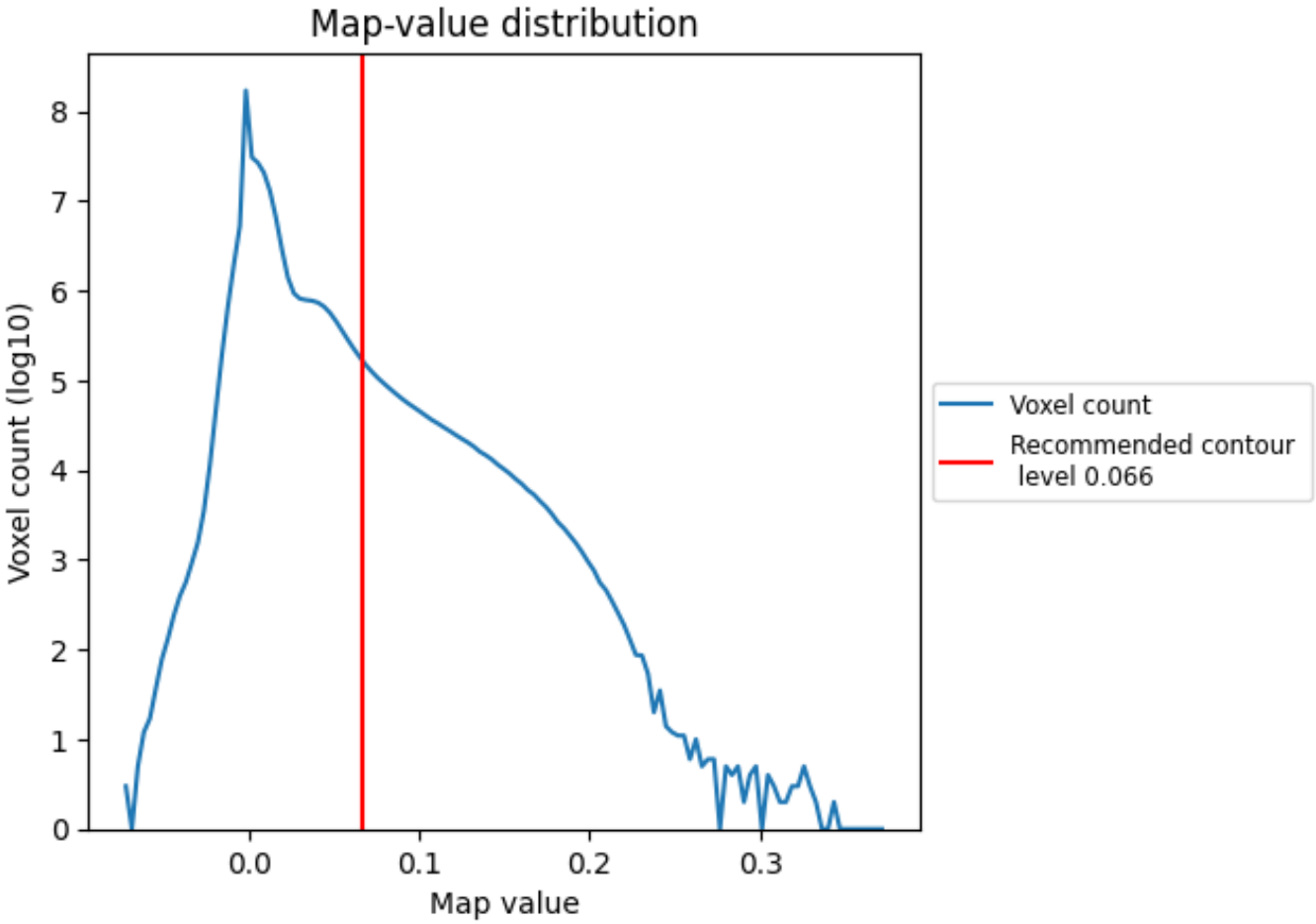
6.6 Mask visualisation (i)

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

7 Map analysis

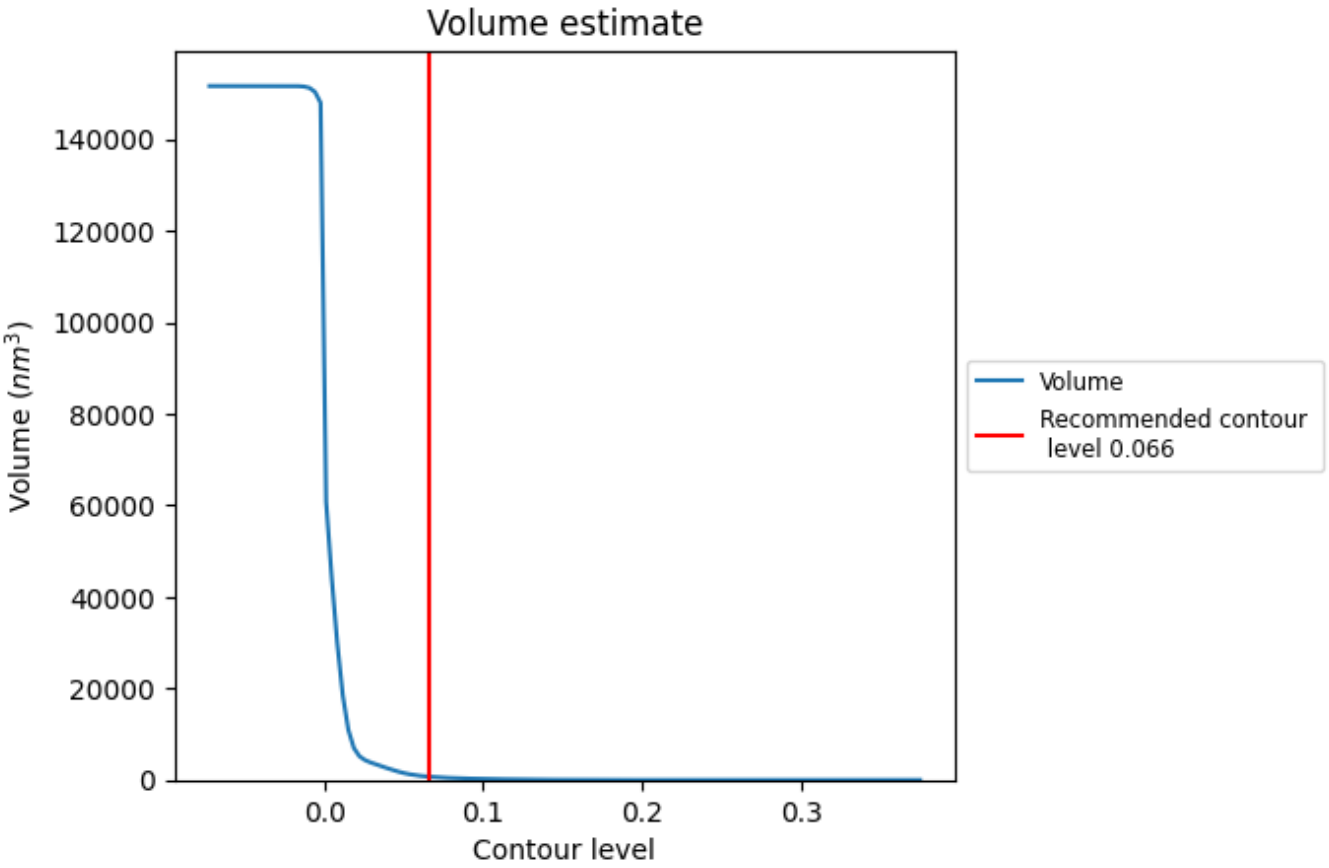
This section contains the results of statistical analysis of the map.

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.

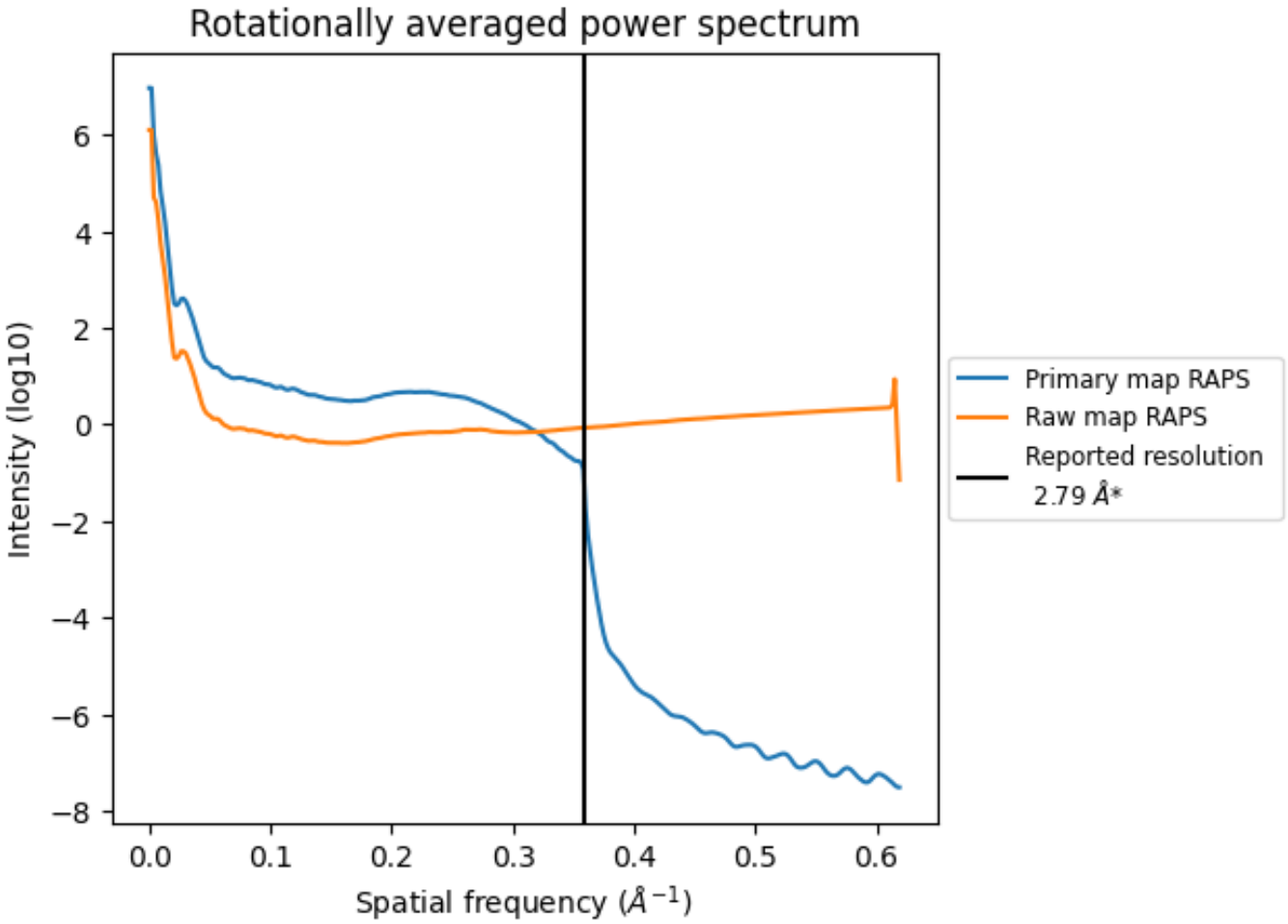
7.2 Volume estimate



The volume at the recommended contour level is 712 nm^3; this corresponds to an approximate mass of 643 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)

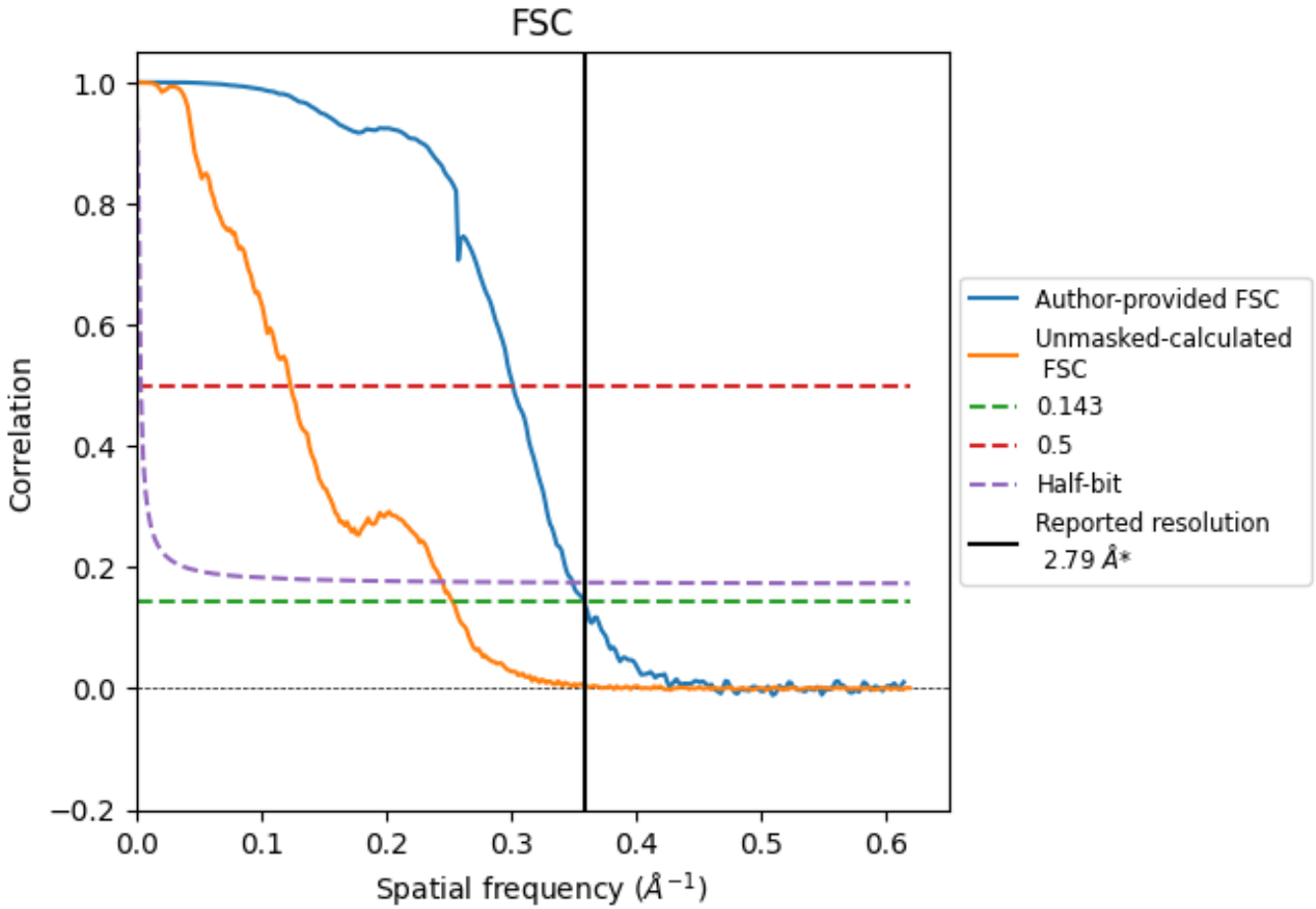


*Reported resolution corresponds to spatial frequency of 0.358 Å^{-1}

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 0.358 Å^{-1}

8.2 Resolution estimates (i)

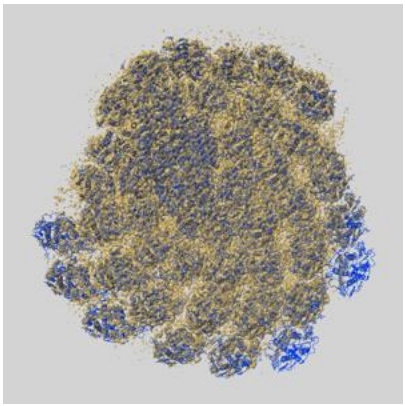
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.32	2.86
Unmasked-calculated*	3.95	8.10	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 2.79 by more than 10 %

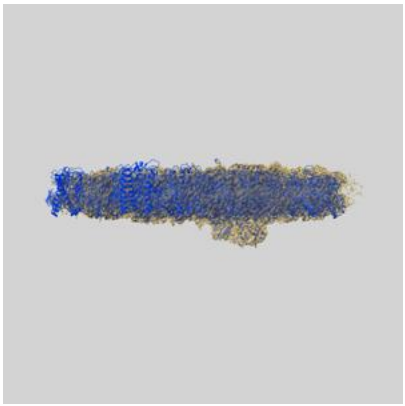
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61519 and PDB model 9JJ8. Per-residue inclusion information can be found in section 3 on page 62.

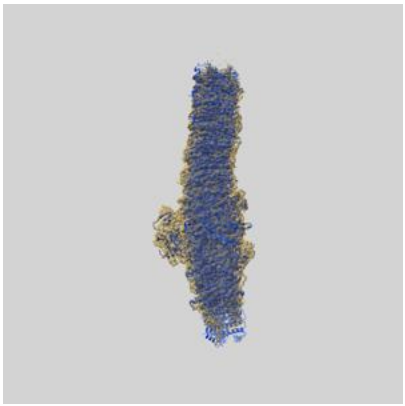
9.1 Map-model overlay



X



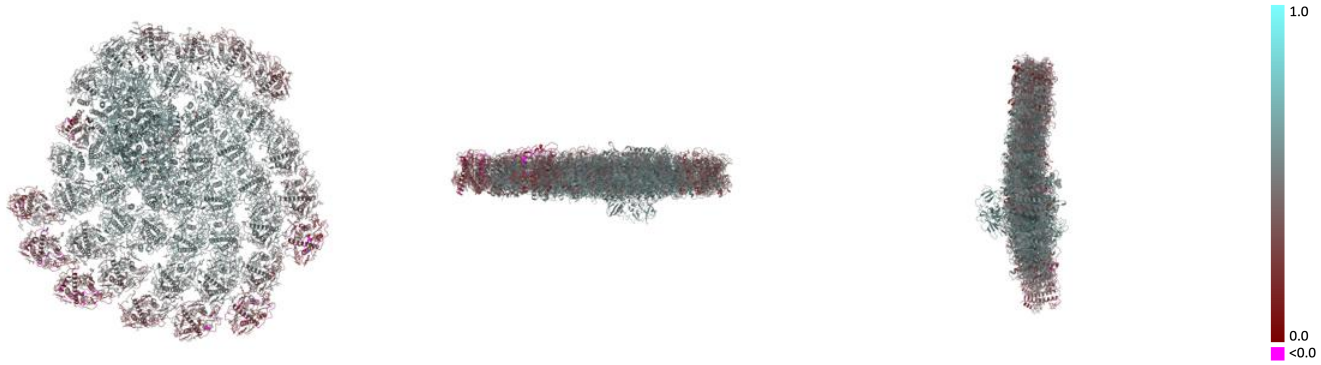
Y



Z

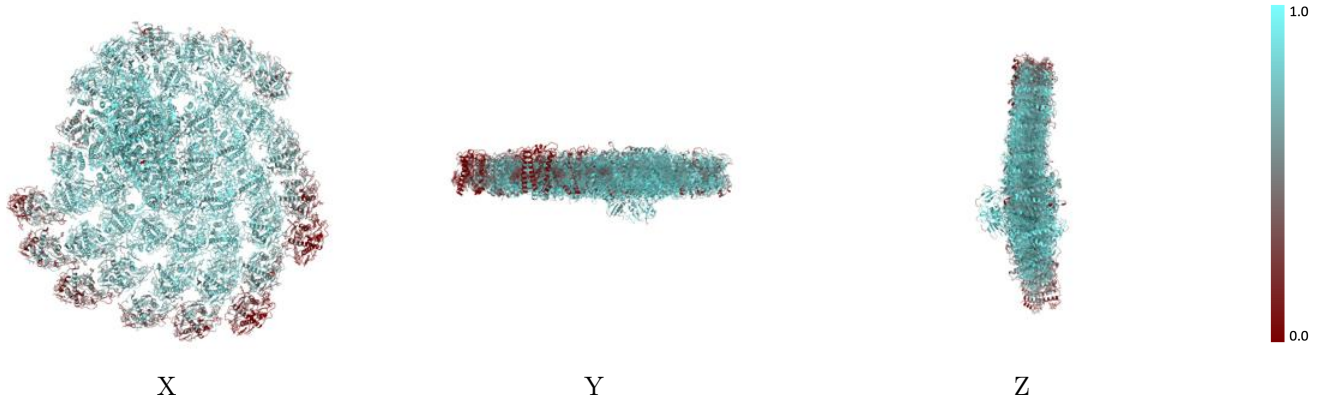
The images above show the 3D surface view of the map at the recommended contour level 0.066 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



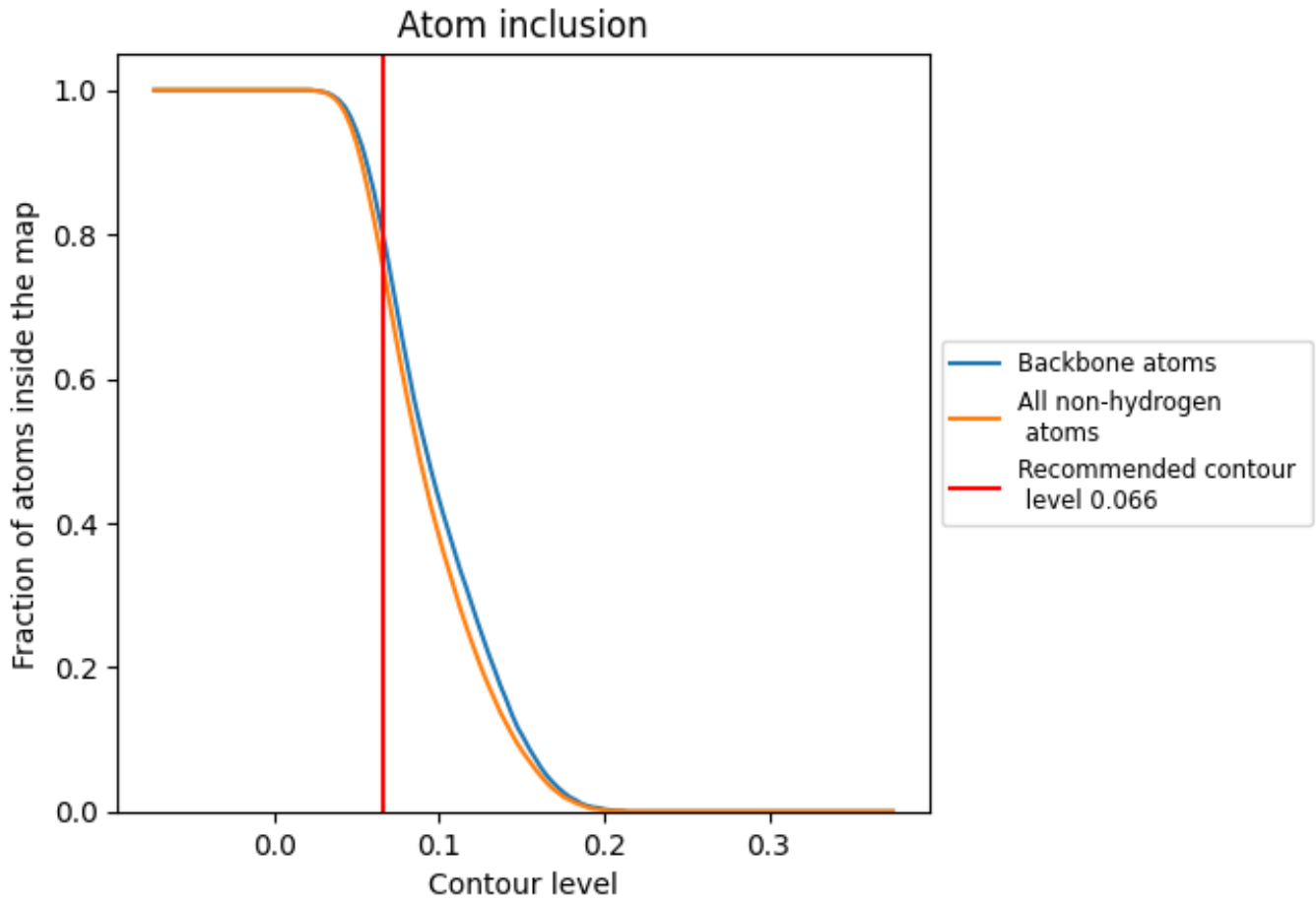
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.066).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.066) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7580	0.4970
0	0.7730	0.4850
1	0.5320	0.3590
2	0.3860	0.3210
3	0.6050	0.4440
4	0.7900	0.5080
5	0.8680	0.5370
6	0.4230	0.4270
7	0.6570	0.4750
8	0.6230	0.3800
9	0.7070	0.4130
A	0.8990	0.5670
B	0.6160	0.3650
C	0.7300	0.4910
D	0.9090	0.5770
E	0.9140	0.5810
F	0.8440	0.5350
G	0.8770	0.5490
H	0.7460	0.5100
I	0.9040	0.5730
J	0.6160	0.4410
K	0.8850	0.5630
L	0.7380	0.4540
M	0.9150	0.5810
O	0.7290	0.4320
P	0.8980	0.5700
Q	0.7920	0.4910
R	0.8830	0.5470
S	0.7930	0.5050
T	0.8170	0.5200
U	0.7860	0.5060
V	0.8500	0.5200
W	0.9100	0.5700
X	0.8410	0.5180
Y	0.0510	0.2320

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Chain	Atom inclusion	Q-score
Z	0.0890	0.2370
a	0.9340	0.5960
b	0.9310	0.5920
c	0.9500	0.5810
d	0.8370	0.5680
e	0.8070	0.5750
f	0.8570	0.5590
h	0.8640	0.5510
i	0.9040	0.5730
j	0.9040	0.5690
k	0.8880	0.5540
l	0.9100	0.5760
m	0.8620	0.5300
o	0.7770	0.5290
x	0.3510	0.2530
y	0.4260	0.2940
z	0.3600	0.3220