Full wwPDB EM Validation Report ⓘ

Sep 14, 2026 – 01:42 PM JST

PDB ID	:	7Y7B / pdb_00007y7b
EMDB ID	:	EMD-33659
Title	:	Cryo-EM structure of cryptophyte photosystem I
Authors	:	Zhao, L.S.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on	:	2022-06-22
Resolution	:	2.66 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:

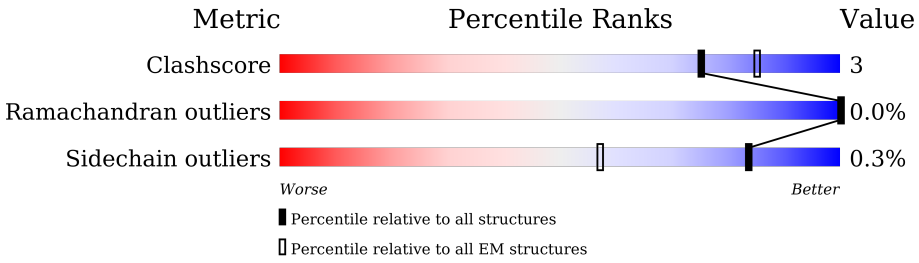
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

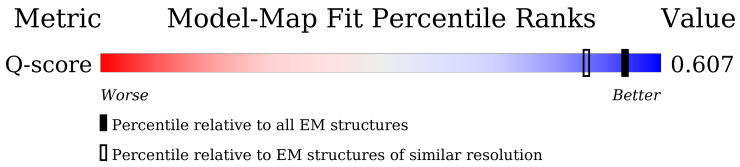
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.66 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	9119 (2.16 - 3.16)

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	1	222	5% 66% 14% 19%
2	2	216	70% 7% 22%
3	3	236	72% 5% 24%
4	4	217	76% 5% 19%

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Mol	Chain	Length	Quality of chain
5	5	229	71% 11% 18%
6	6	215	72% 8% 20%
7	7	230	70% 7% 23%
8	8	227	70% 6% 24%
9	9	220	72% 10% 18%
10	A	752	92% 7%
11	B	734	92% 7%
12	C	81	81% 15%
13	D	141	89% 8%
14	E	64	89% 6% 5%
15	F	183	83% 13%
16	I	36	75% 17% 8%
17	J	42	98%
18	K	87	86% 10%
19	L	153	93% 5%
20	M	30	97%
21	O	99	89% 11%
22	R	133	62% 8% 31%
23	X	164	22% 79% 9% 12%
24	Z	242	59% 37%
25	a	215	74% 5% 20%
25	d	215	76% 20%
26	b	218	76% 5% 19%
27	c	257	72% 11% 16%
28	e	208	73% 7% 19%

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 60515 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 ACPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	179	1338	861	227	242	8	0	0

- Molecule 2 is a protein called ACPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	168	1320	872	215	230	3	0	0

- Molecule 3 is a protein called ACPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	180	1362	875	231	246	10	0	0

- Molecule 4 is a protein called ACPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	176	1366	891	224	245	6	0	0

- Molecule 5 is a protein called ACPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	188	1403	908	234	253	8	0	0

- Molecule 6 is a protein called ACPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	173	1305	846	217	232	10	0	0

- Molecule 7 is a protein called ACPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	177	Total	C	N	O	S	0	0
			1337	861	230	238	8		

- Molecule 8 is a protein called ACPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	173	Total	C	N	O	S	0	0
			1298	842	217	235	4		

- Molecule 9 is a protein called ACPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	180	Total	C	N	O	S	0	0
			1349	864	230	243	12		

- Molecule 10 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	741	Total	C	N	O	S	0	0
			5824	3804	992	1000	28		

- Molecule 11 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	731	Total	C	N	O	S	0	0
			5828	3847	982	984	15		

- Molecule 12 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	80	Total	C	N	O	S	0	0
			591	361	103	115	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	137	Total	C	N	O	S	0	0
			1070	685	184	198	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	E	61	Total	C	N	O	0	0
			491	312	85	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	160	Total	C	N	O	S	0	0
			1258	814	214	228	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	33	Total	C	N	O	S	0	0
			258	180	34	42	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	42	Total	C	N	O	S	0	0
			342	232	49	58	3		

- Molecule 18 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	78	Total	C	N	O	S	0	0
			553	358	90	102	3		

- Molecule 19 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	150	Total	C	N	O	S	0	0
			1143	746	184	211	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	30	Total	C	N	O	S	0	0
			227	152	35	39	1		

- Molecule 21 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	99	Total	C	N	O	S	0	0
			766	518	113	134	1		

- Molecule 22 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	92	Total	C	N	O	S	0	0
			680	439	112	127	2		

- Molecule 23 is a protein called Unk1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	145	Total	C	N	O	0	0
			725	435	145	145		

- Molecule 24 is a protein called ACPI-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	153	Total	C	N	O	S	0	0
			1130	721	188	211	10		

- Molecule 25 is a protein called ACPI-13/10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	171	Total	C	N	O	S	0	0
			1271	823	207	231	10		
25	d	171	Total	C	N	O	S	0	0
			1271	823	207	231	10		

- Molecule 26 is a protein called ACPI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	176	Total	C	N	O	S	0	0
			1368	891	224	244	9		

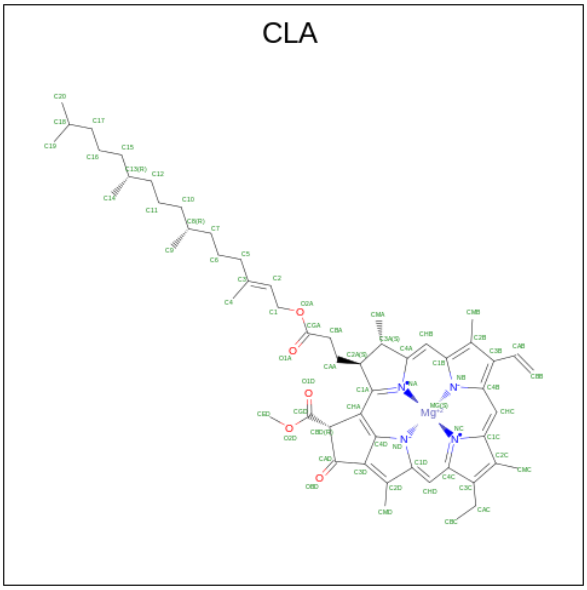
- Molecule 27 is a protein called ACPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	215	Total	C	N	O	S	0	0
			1615	1053	265	283	14		

- Molecule 28 is a protein called ACPI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	168	Total	C	N	O	S	0	0
			1288	840	209	227	12		

- Molecule 29 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
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	2	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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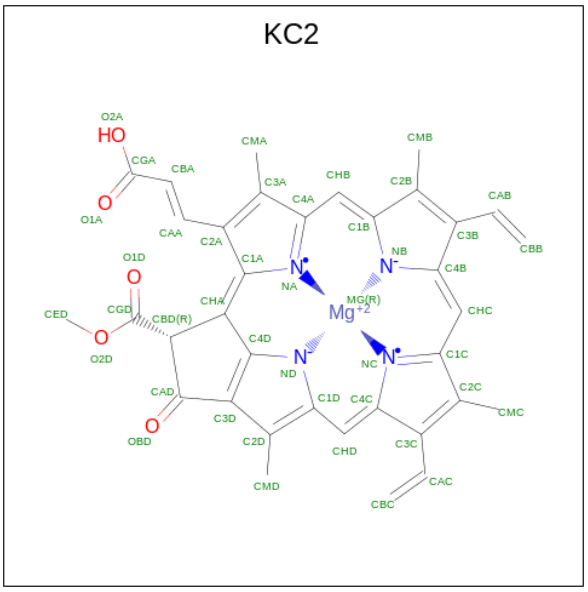
Mol	Chain	Residues	Atoms					AltConf
29	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	d	1	Total 63	C 53	Mg 1	N 4	O 5	0
29	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	e	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	e	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	e	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	e	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 30 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
30	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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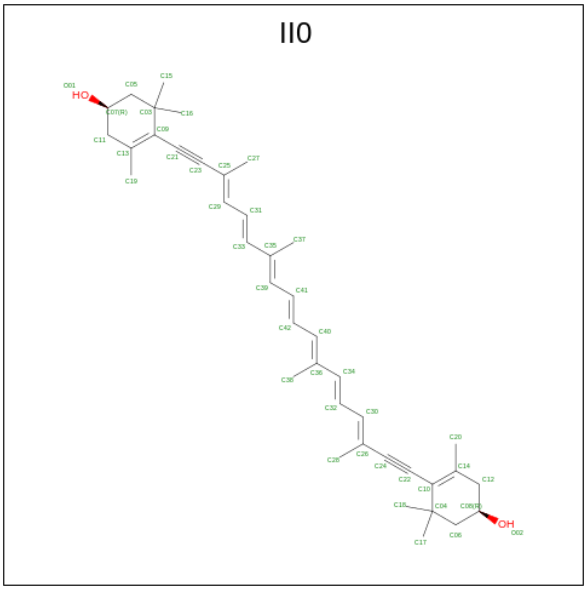
Mol	Chain	Residues	Atoms					AltConf
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 31 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: $C_{40}H_{52}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
31	2	1	Total C O 42 40 2	0
31	2	1	Total C O 42 40 2	0
31	2	1	Total C O 42 40 2	0
31	3	1	Total C O 42 40 2	0
31	3	1	Total C O 42 40 2	0
31	3	1	Total C O 42 40 2	0
31	3	1	Total C O 42 40 2	0
31	3	1	Total C O 42 40 2	0
31	4	1	Total C O 42 40 2	0
31	4	1	Total C O 42 40 2	0
31	4	1	Total C O 42 40 2	0
31	4	1	Total C O 42 40 2	0
31	5	1	Total C O 42 40 2	0
31	5	1	Total C O 42 40 2	0
31	5	1	Total C O 42 40 2	0
31	5	1	Total C O 42 40 2	0
31	5	1	Total C O 42 40 2	0
31	6	1	Total C O 42 40 2	0
31	6	1	Total C O 42 40 2	0
31	6	1	Total C O 42 40 2	0
31	7	1	Total C O 42 40 2	0

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Mol	Chain	Residues	Atoms			AltConf
31	7	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	9	1	Total	C	O	0
			42	40	2	
31	9	1	Total	C	O	0
			42	40	2	
31	9	1	Total	C	O	0
			42	40	2	
31	9	1	Total	C	O	0
			42	40	2	
31	B	1	Total	C	O	0
			42	40	2	
31	J	1	Total	C	O	0
			42	40	2	
31	O	1	Total	C	O	0
			42	40	2	
31	O	1	Total	C	O	0
			42	40	2	
31	R	1	Total	C	O	0
			42	40	2	
31	a	1	Total	C	O	0
			42	40	2	
31	a	1	Total	C	O	0
			42	40	2	
31	a	1	Total	C	O	0
			42	40	2	
31	a	1	Total	C	O	0
			42	40	2	
31	a	1	Total	C	O	0
			42	40	2	

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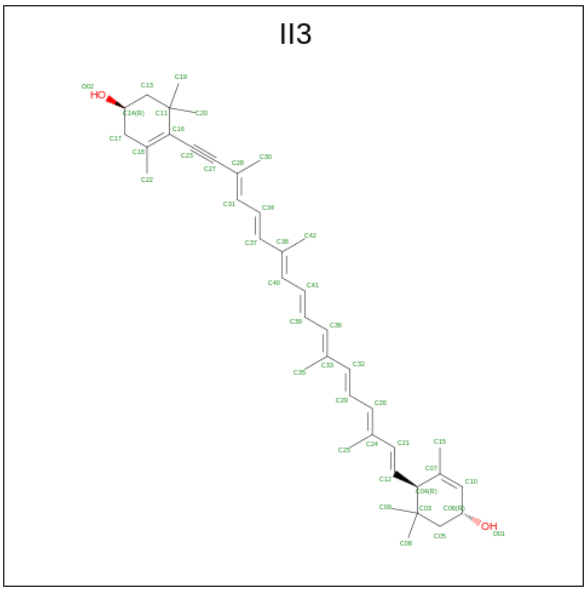
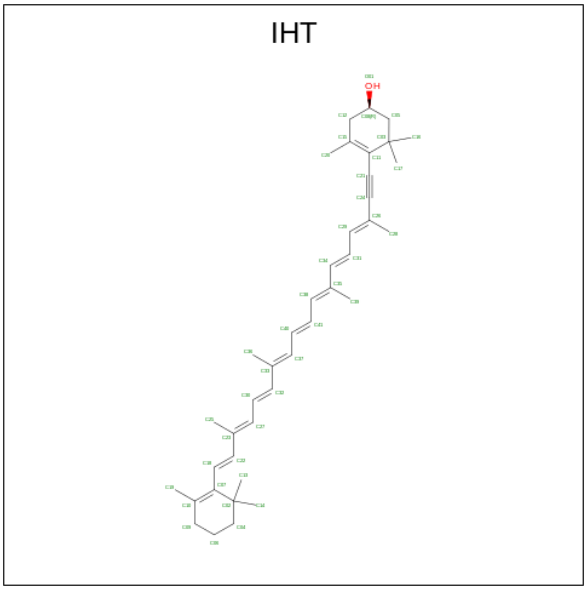
Mol	Chain	Residues	Atoms	AltConf
31	b	1	Total C O 42 40 2	0
31	b	1	Total C O 42 40 2	0
31	c	1	Total C O 42 40 2	0
31	c	1	Total C O 42 40 2	0
31	c	1	Total C O 42 40 2	0
31	c	1	Total C O 42 40 2	0
31	d	1	Total C O 42 40 2	0
31	d	1	Total C O 42 40 2	0
31	d	1	Total C O 42 40 2	0
31	d	1	Total C O 42 40 2	0
31	e	1	Total C O 42 40 2	0
31	e	1	Total C O 42 40 2	0
31	e	1	Total C O 42 40 2	0

- Molecule 32 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: II3) (formula: $C_{40}H_{54}O_2$) (labeled as "Ligand of Interest" by depositor).



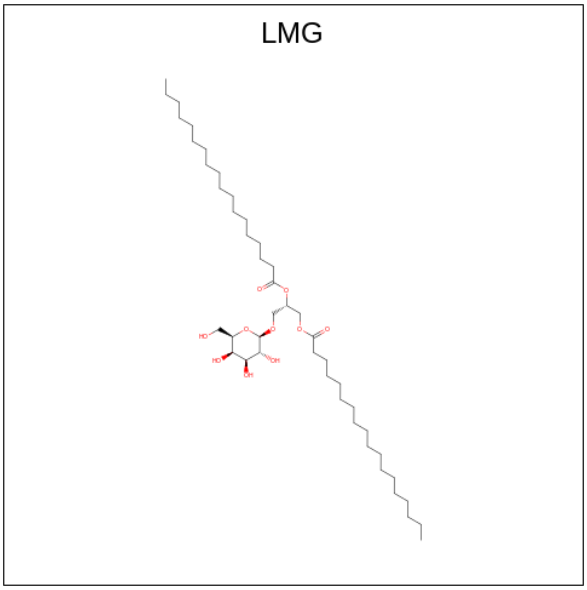
Mol	Chain	Residues	Atoms			AltConf
32	1	1	Total	C	O	0
			42	40	2	
32	b	1	Total	C	O	0
			42	40	2	
32	e	1	Total	C	O	0
			42	40	2	

- Molecule 33 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: $C_{40}H_{54}O$) (labeled as "Ligand of Interest" by depositor).



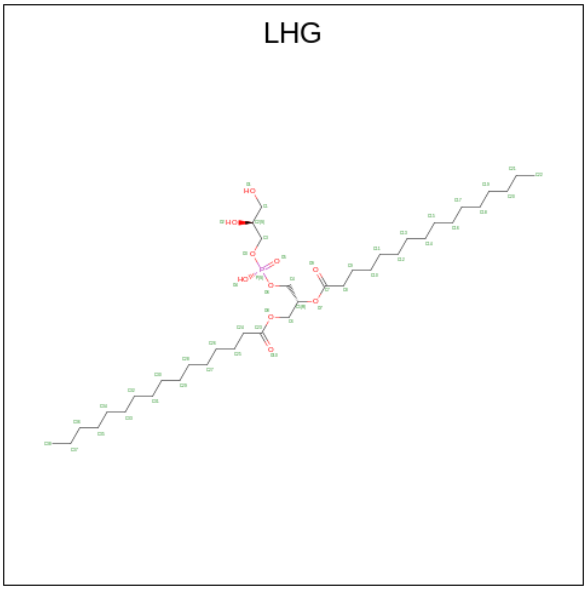
Mol	Chain	Residues	Atoms			AltConf
33	1	1	Total	C	O	0
			41	40	1	
33	2	1	Total	C	O	0
			41	40	1	
33	5	1	Total	C	O	0
			41	40	1	
33	6	1	Total	C	O	0
			41	40	1	
33	8	1	Total	C	O	0
			41	40	1	
33	9	1	Total	C	O	0
			41	40	1	
33	K	1	Total	C	O	0
			41	40	1	
33	L	1	Total	C	O	0
			41	40	1	
33	Z	1	Total	C	O	0
			41	40	1	
33	a	1	Total	C	O	0
			41	40	1	
33	c	1	Total	C	O	0
			41	40	1	
33	d	1	Total	C	O	0
			41	40	1	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
34	2	1	Total C O 36 26 10	0
34	3	1	Total C O 30 20 10	0
34	3	1	Total C O 32 22 10	0
34	6	1	Total C O 32 22 10	0
34	8	1	Total C O 52 42 10	0
34	F	1	Total C O 32 22 10	0
34	I	1	Total C O 51 41 10	0

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
35	2	1	Total C O P 22 12 9 1	0
35	2	1	Total C O P 39 28 10 1	0
35	2	1	Total C O P 42 31 10 1	0
35	3	1	Total C O P 49 38 10 1	0

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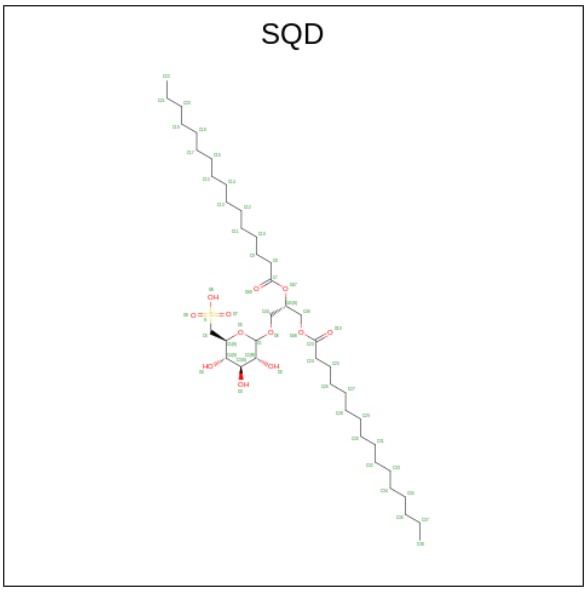
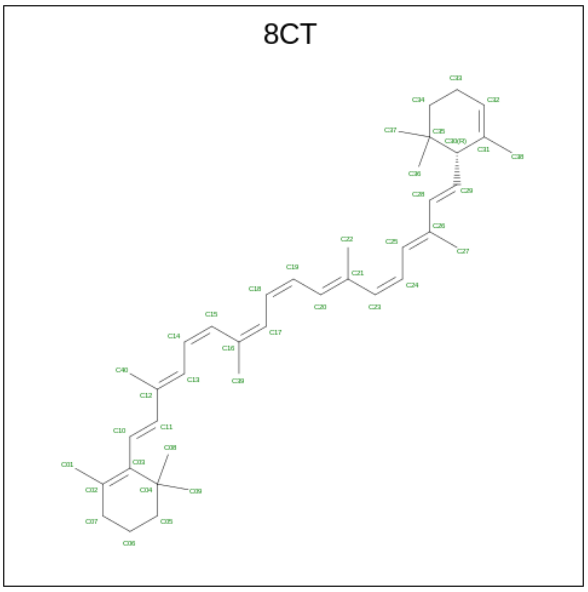
Mol	Chain	Residues	Atoms				AltConf
35	3	1	Total	C	O	P	0
			34	23	10	1	
35	3	1	Total	C	O	P	0
			49	38	10	1	
35	4	1	Total	C	O	P	0
			47	36	10	1	
35	4	1	Total	C	O	P	0
			45	34	10	1	
35	5	1	Total	C	O	P	0
			23	12	10	1	
35	6	1	Total	C	O	P	0
			35	24	10	1	
35	7	1	Total	C	O	P	0
			31	20	10	1	
35	7	1	Total	C	O	P	0
			39	28	10	1	
35	8	1	Total	C	O	P	0
			33	22	10	1	
35	A	1	Total	C	O	P	0
			49	38	10	1	
35	A	1	Total	C	O	P	0
			39	28	10	1	
35	B	1	Total	C	O	P	0
			45	34	10	1	
35	L	1	Total	C	O	P	0
			34	23	10	1	
35	Z	1	Total	C	O	P	0
			46	35	10	1	
35	a	1	Total	C	O	P	0
			29	18	10	1	
35	b	1	Total	C	O	P	0
			49	38	10	1	
35	c	1	Total	C	O	P	0
			29	18	10	1	
35	d	1	Total	C	O	P	0
			23	13	9	1	
35	d	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 36 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
36	3	1	Total 42	C 29	O 12	S 1	0
36	O	1	Total 29	C 16	O 12	S 1	0

- Molecule 37 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
37	4	1	Total 40	C 40	0

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Mol	Chain	Residues	Atoms	AltConf
37	7	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	F	1	Total C 40 40	0
37	I	1	Total C 40 40	0
37	J	1	Total C 40 40	0
37	K	1	Total C 40 40	0
37	L	1	Total C 40 40	0
37	M	1	Total C 40 40	0
37	R	1	Total C 40 40	0
37	R	1	Total C 40 40	0
37	Z	1	Total C 40 40	0

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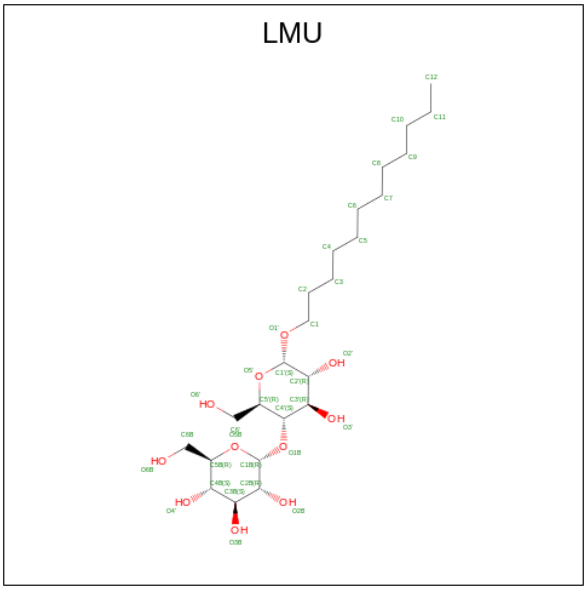
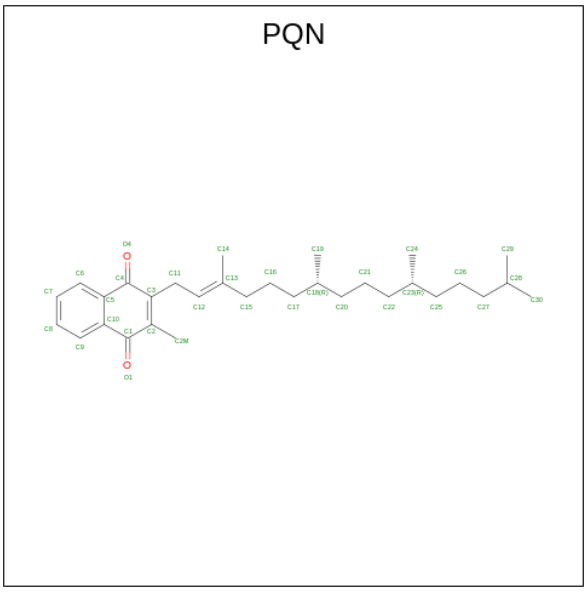
Mol	Chain	Residues	Atoms	AltConf
37	Z	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	e	1	Total C 40 40	0

- Molecule 38 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



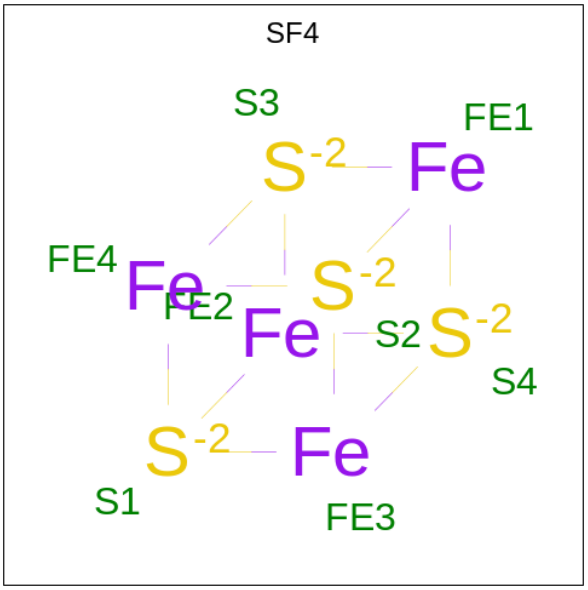
Mol	Chain	Residues	Atoms	AltConf
38	4	1	Total C O 35 24 11	0
38	7	1	Total C O 35 24 11	0
38	J	1	Total C O 31 20 11	0
38	O	1	Total C O 30 19 11	0
38	e	1	Total C O 31 20 11	0

- Molecule 39 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 40 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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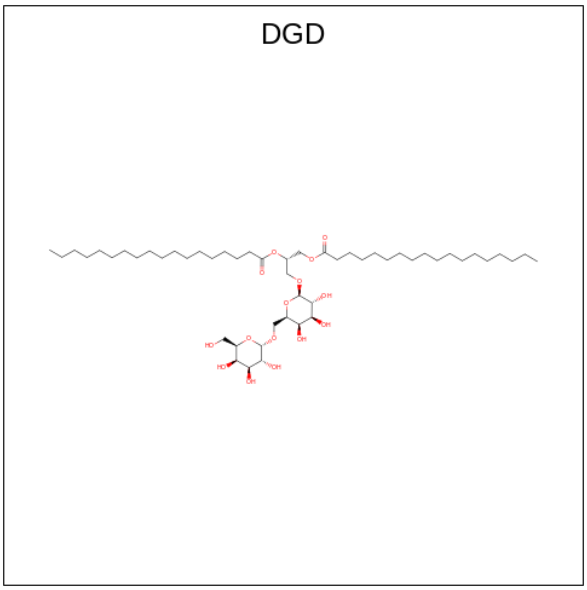
Mol	Chain	Residues	Atoms			AltConf
40	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 41 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
41	B	1	Total	C	O	0
			59	44	15	
41	Z	1	Total	C	O	0
			60	45	15	

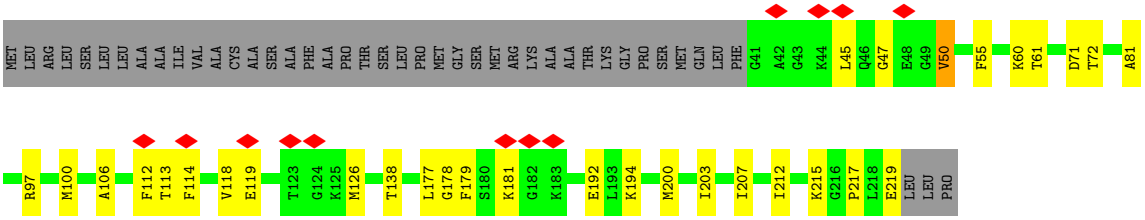
3 Residue-property plots (i)

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

• Molecule 1: ACPI-1

Chain 1:

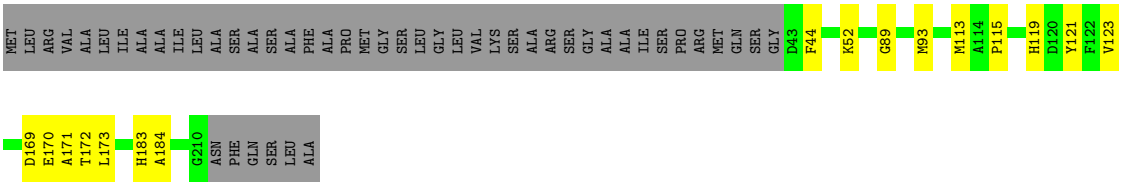




• Molecule 2: ACPI-2

Chain 2:

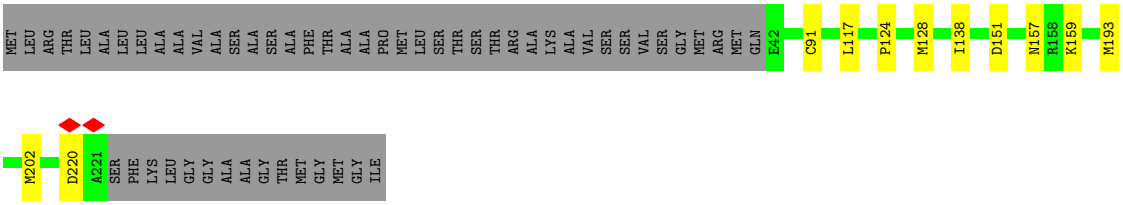




• Molecule 3: ACPI-3

Chain 3:





• Molecule 4: ACPI-4

Chain 4:



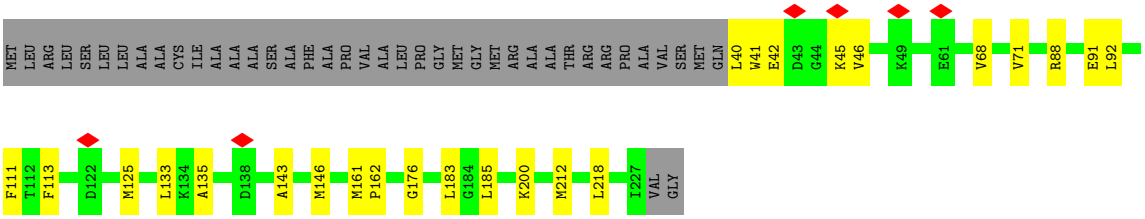




• Molecule 5: ACPI-5

Chain 5:

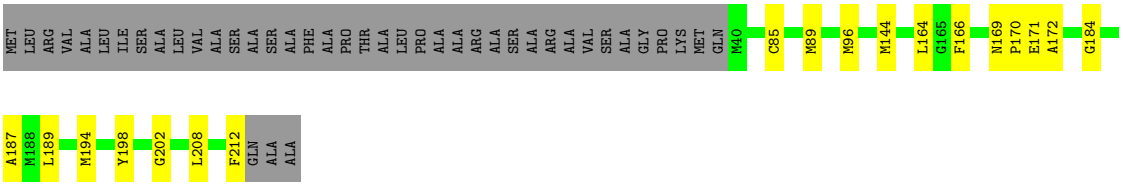




• Molecule 6: ACPI-6

Chain 6:

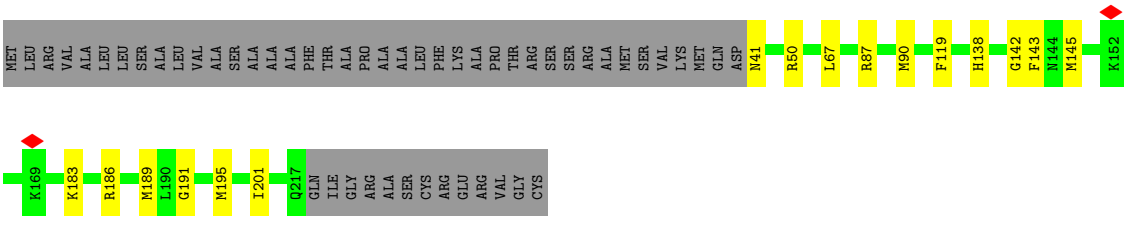




• Molecule 7: ACPI-7

Chain 7:

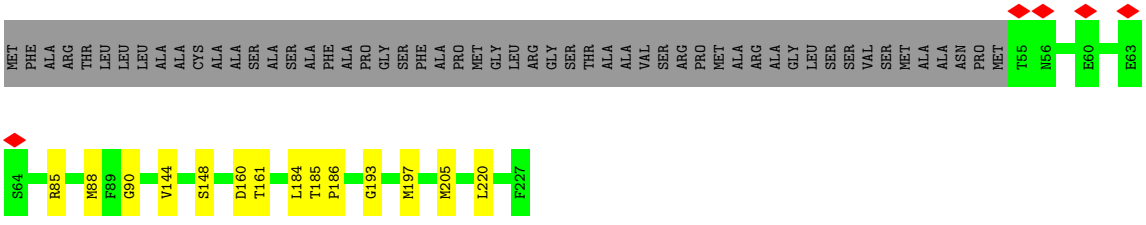




• Molecule 8: ACPI-8

Chain 8:

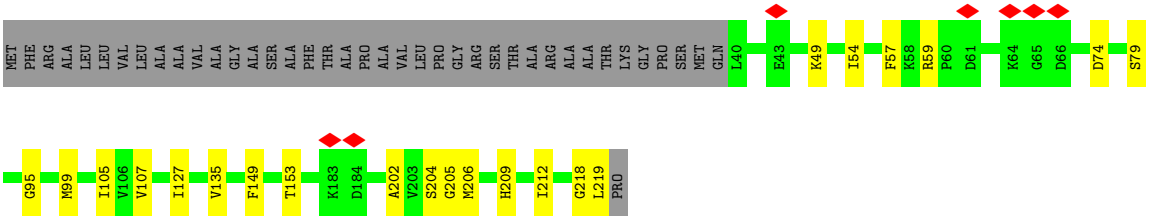




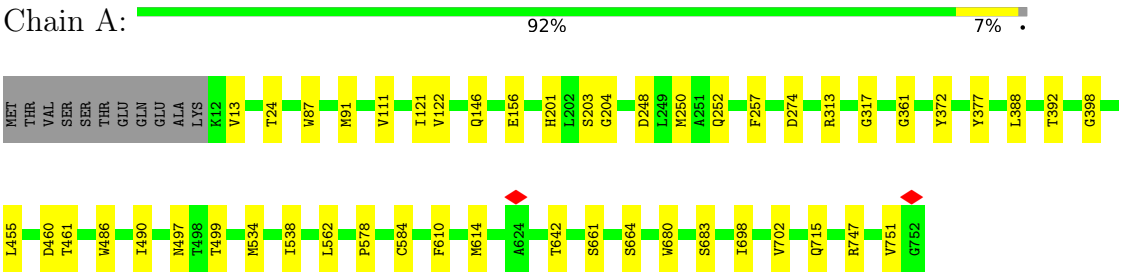
• Molecule 9: ACPI-12

Chain 9:

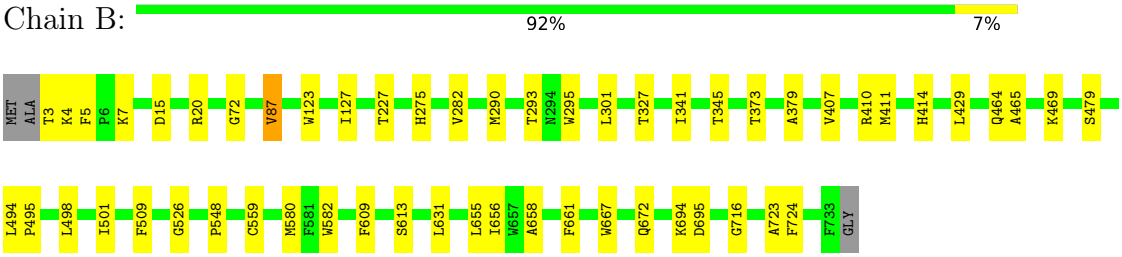




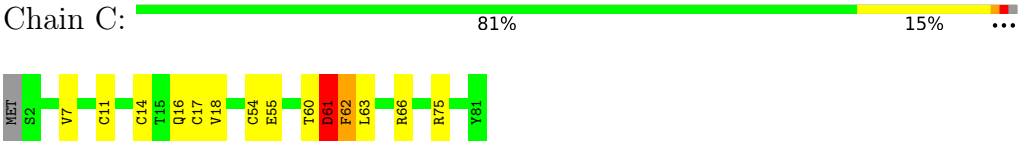
• Molecule 10: Photosystem I P700 chlorophyll a apoprotein A1



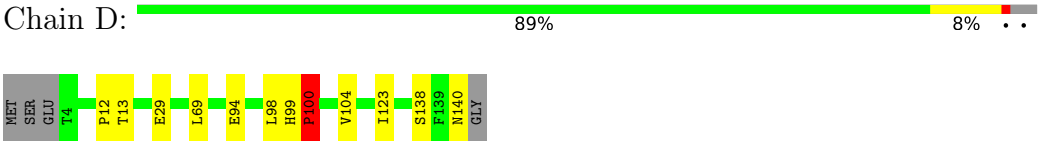
• Molecule 11: Photosystem I P700 chlorophyll a apoprotein A2



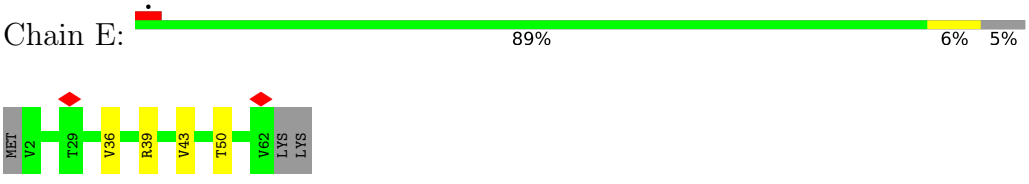
• Molecule 12: Photosystem I iron-sulfur center



• Molecule 13: Photosystem I reaction center subunit II



• Molecule 14: Photosystem I reaction center subunit IV



• Molecule 15: Photosystem I reaction center subunit III

Chain F:

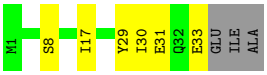




• Molecule 16: Photosystem I reaction center subunit VIII

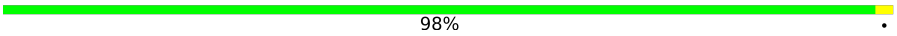
Chain I:





• Molecule 17: Photosystem I reaction center subunit IX

Chain J:

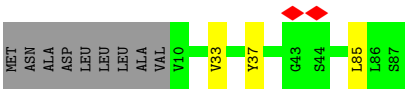




• Molecule 18: Photosystem I reaction center subunit PsaK

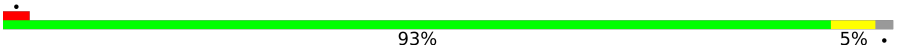
Chain K:

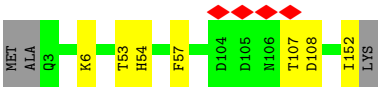




• Molecule 19: Photosystem I reaction center subunit XI

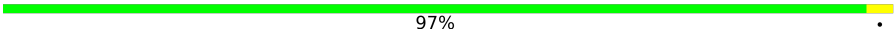
Chain L:





• Molecule 20: Photosystem I reaction center subunit XII

Chain M:





• Molecule 21: PsaO

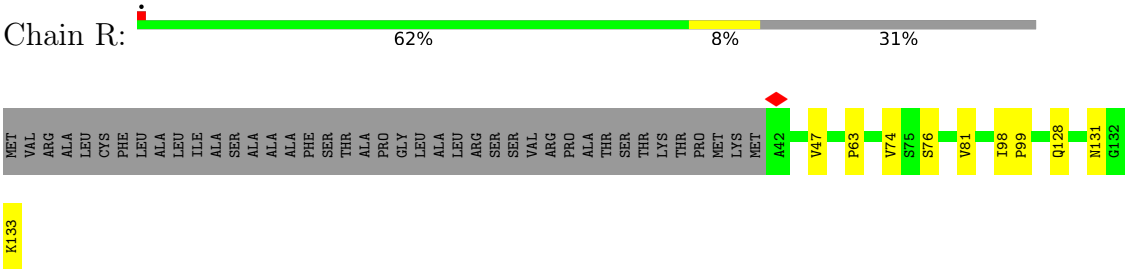
Chain O:





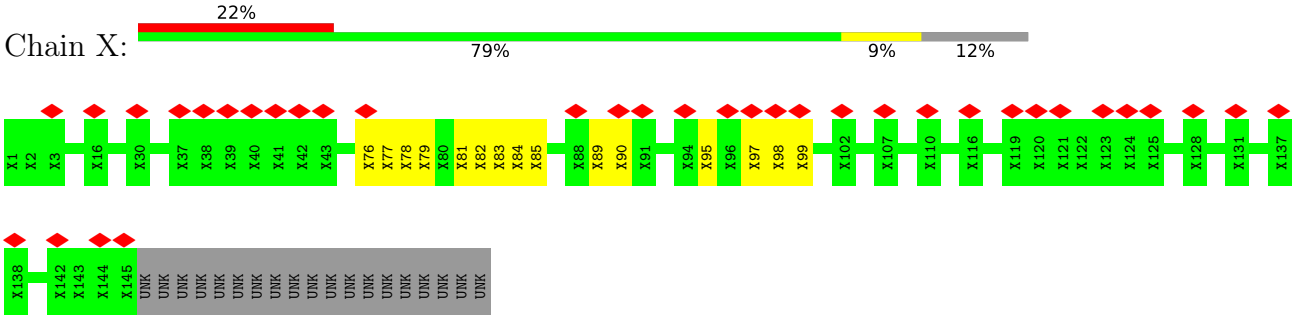
• Molecule 22: PsaR

Chain R:



• Molecule 23: Unk1

Chain X:

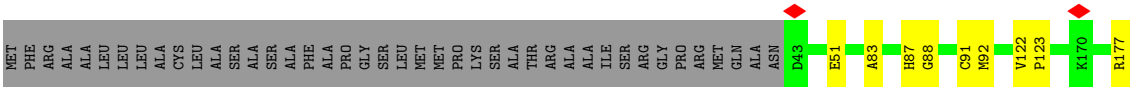

22%
79%
9%
12%
X1 X2 X3 X16 X30 X37 X38 X39 X40 X41 X42 X43 X76 X77 X78 X79 X80 X81 X82 X83 X84 X85 X88 X89 X90 X91 X94 X95 X96 X97 X98 X99 X102 X107 X110 X116 X119 X120 X121 X122 X123 X124 X125 X128 X131 X137
X138 X142 X143 X144 X145 UNK UNK UNK



• Molecule 26: ACPI-14

Chain b:





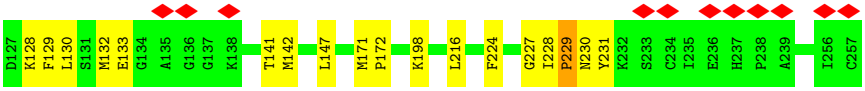


• Molecule 27: ACPI-9

Chain c:



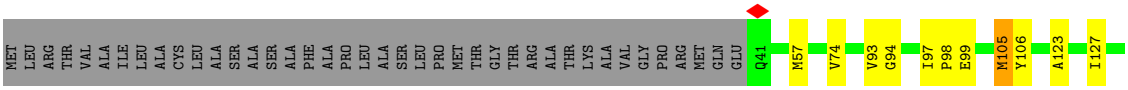




• Molecule 28: ACPI-11

Chain e:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133521	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.411	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.032	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, KC2, CLA, II0, IHT, DGD, 8CT, LHG, II3, SQD, SF4, LMU, LMG

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	1	0.33	0/1371	0.51	1/1854 (0.1%)
2	2	0.23	0/1356	0.31	0/1835
3	3	0.18	0/1392	0.29	0/1883
4	4	0.18	0/1406	0.32	0/1900
5	5	0.32	0/1438	0.45	0/1940
6	6	0.36	0/1334	0.39	0/1796
7	7	0.22	0/1373	0.35	0/1858
8	8	0.22	0/1326	0.35	0/1804
9	9	0.20	0/1376	0.34	0/1846
10	A	0.23	0/6019	0.35	0/8204
11	B	0.26	0/6046	0.37	1/8254 (0.0%)
12	C	0.48	1/600 (0.2%)	0.64	4/812 (0.5%)
13	D	0.22	0/1094	0.41	0/1476
14	E	0.21	0/499	0.33	0/677
15	F	0.22	0/1290	0.33	0/1745
16	I	0.23	0/266	0.34	0/362
17	J	0.26	0/353	0.34	0/481
18	K	0.23	0/563	0.36	0/768
19	L	0.31	0/1171	0.40	0/1594
20	M	0.19	0/228	0.26	0/310
21	O	0.22	0/796	0.36	0/1091
22	R	0.17	0/700	0.31	0/963
24	Z	0.20	0/1163	0.32	0/1572
25	a	0.21	0/1299	0.33	0/1747
25	d	0.24	0/1299	0.33	0/1747
26	b	0.21	0/1404	0.33	0/1902
27	c	0.29	0/1658	0.45	1/2241 (0.0%)
28	e	0.24	0/1325	0.36	0/1793
All	All	0.25	1/40145 (0.0%)	0.37	7/54455 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	61	ASP	CA-C	-5.09	1.46	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	61	ASP	CA-C-N	-6.23	112.87	122.09
12	C	61	ASP	C-N-CA	-6.23	112.87	122.09
1	1	50	VAL	N-CA-C	6.07	117.42	109.58
27	c	229	PRO	N-CA-C	-5.95	103.24	113.70
12	C	62	PHE	N-CA-CB	5.34	118.88	110.23
11	B	580	MET	O-C-N	-5.33	116.12	122.20
12	C	63	LEU	N-CA-C	5.03	117.76	110.42

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	1	1338	0	1329	26	0
2	2	1320	0	1309	12	0
3	3	1362	0	1389	8	0
4	4	1366	0	1349	7	0
5	5	1403	0	1398	20	0
6	6	1305	0	1324	16	0
7	7	1337	0	1317	11	0
8	8	1298	0	1322	9	0
9	9	1349	0	1358	15	0
10	A	5824	0	5672	36	0
11	B	5828	0	5626	44	0
12	C	591	0	568	11	0
13	D	1070	0	1076	17	0
14	E	491	0	491	2	0
15	F	1258	0	1266	5	0
16	I	258	0	268	6	0
17	J	342	0	344	1	0
18	K	553	0	581	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	1143	0	1145	5	0
20	M	227	0	257	2	0
21	O	766	0	752	10	0
22	R	680	0	674	6	0
23	X	725	0	152	11	0
24	Z	1130	0	1088	6	0
25	a	1271	0	1281	13	0
25	d	1271	0	1281	5	0
26	b	1368	0	1346	10	0
27	c	1615	0	1646	27	0
28	e	1288	0	1282	10	0
29	1	584	0	476	7	0
29	2	547	0	456	1	0
29	3	625	0	596	0	0
29	4	598	0	597	2	0
29	5	563	0	442	6	0
29	6	581	0	514	1	0
29	7	509	0	431	4	0
29	8	496	0	471	4	0
29	9	642	0	539	6	0
29	A	2679	0	2767	11	0
29	B	2406	0	2458	13	0
29	F	160	0	141	0	0
29	J	41	0	29	0	0
29	K	120	0	121	0	0
29	L	267	0	240	2	0
29	O	165	0	147	4	0
29	R	55	0	49	0	0
29	Z	225	0	206	2	0
29	a	645	0	632	1	0
29	b	530	0	525	2	0
29	c	666	0	632	7	0
29	d	589	0	538	1	0
29	e	472	0	414	3	0
30	1	45	0	0	0	0
30	2	45	0	0	0	0
30	3	45	0	0	0	0
30	4	45	0	0	0	0
30	5	45	0	0	0	0
30	6	90	0	0	0	0
30	7	90	0	0	0	0
30	9	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Z	45	0	0	0	0
30	a	45	0	0	0	0
30	b	90	0	0	1	0
30	c	135	0	0	3	0
30	d	45	0	0	0	0
30	e	90	0	0	0	0
31	1	168	0	0	2	0
31	2	126	0	0	1	0
31	3	210	0	0	1	0
31	4	168	0	0	2	0
31	5	210	0	0	3	0
31	6	126	0	0	0	0
31	7	168	0	0	0	0
31	8	168	0	0	1	0
31	9	168	0	0	0	0
31	B	42	0	0	0	0
31	J	42	0	0	0	0
31	O	84	0	0	0	0
31	R	42	0	0	0	0
31	a	210	0	0	2	0
31	b	84	0	0	0	0
31	c	168	0	0	0	0
31	d	168	0	0	0	0
31	e	126	0	0	0	0
32	1	42	0	0	0	0
32	b	42	0	0	1	0
32	e	42	0	0	0	0
33	1	41	0	0	0	0
33	2	41	0	0	1	0
33	5	41	0	0	0	0
33	6	41	0	0	1	0
33	8	41	0	0	0	0
33	9	41	0	0	1	0
33	K	41	0	0	0	0
33	L	41	0	0	0	0
33	Z	41	0	0	0	0
33	a	41	0	0	1	0
33	c	41	0	0	1	0
33	d	41	0	0	1	0
34	2	36	0	42	0	0
34	3	62	0	64	0	0
34	6	32	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	8	52	0	77	0	0
34	F	32	0	34	0	0
34	I	51	0	75	0	0
35	2	103	0	125	0	0
35	3	132	0	186	0	0
35	4	92	0	130	0	0
35	5	23	0	16	0	0
35	6	35	0	40	0	0
35	7	70	0	83	0	0
35	8	33	0	36	0	0
35	A	88	0	122	0	0
35	B	45	0	60	0	0
35	L	34	0	38	1	0
35	Z	46	0	65	0	0
35	a	29	0	28	0	0
35	b	49	0	74	0	0
35	c	29	0	28	0	0
35	d	62	0	73	0	0
36	3	42	0	48	0	0
36	O	29	0	22	0	0
37	4	40	0	0	1	0
37	7	40	0	0	1	0
37	A	200	0	0	0	0
37	B	240	0	0	0	0
37	F	40	0	0	1	0
37	I	40	0	0	0	0
37	J	40	0	0	0	0
37	K	40	0	0	0	0
37	L	40	0	0	0	0
37	M	40	0	0	0	0
37	R	80	0	0	0	0
37	Z	80	0	0	0	0
37	b	40	0	0	0	0
37	e	40	0	0	0	0
38	4	35	0	46	1	0
38	7	35	0	46	1	0
38	J	31	0	35	1	0
38	O	30	0	33	4	0
38	e	31	0	35	0	0
39	A	33	0	46	0	0
39	B	33	0	46	0	0
40	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	C	16	0	0	1	0
41	B	59	0	79	0	0
41	Z	60	0	78	1	0
All	All	60515	0	54256	360	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 3.

All (360) 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)
25:a:127:THR:HG23	26:b:218:MET:HE1	1.50	0.93
26:b:177:ARG:NH2	30:b:609:KC2:O1A	2.13	0.81
11:B:609:PHE:O	11:B:613:SER:OG	2.00	0.80
6:6:89:MET:HE3	6:6:184:GLY:HA2	1.64	0.78
38:J:104:LMU:O5B	38:J:104:LMU:O3'	2.03	0.76
6:6:89:MET:HE3	6:6:184:GLY:CA	2.17	0.73
38:O:207:LMU:O2'	38:O:207:LMU:H5'	1.87	0.72
22:R:74:VAL:O	22:R:128:GLN:NE2	2.23	0.71
9:9:107:VAL:HG11	29:9:604:CLA:HBC3	1.72	0.71
13:D:99:HIS:O	13:D:100:PRO:C	2.32	0.70
27:c:228:ILE:HB	27:c:229:PRO:HD3	1.72	0.70
10:A:680:TRP:O	10:A:683:SER:OG	2.11	0.69
4:4:43:SER:OG	4:4:64:GLY:O	2.12	0.68
12:C:7:VAL:CG1	12:C:11:CYS:SG	2.83	0.67
27:c:216:LEU:HD13	27:c:231:TYR:OH	1.95	0.66
1:1:97:ARG:NH1	1:1:192:GLU:OE2	2.27	0.65
2:2:170:GLU:O	2:2:173:LEU:N	2.30	0.65
5:5:40:LEU:HD21	5:5:46:VAL:HG21	1.78	0.65
13:D:99:HIS:CB	13:D:100:PRO:HD2	2.28	0.64
13:D:99:HIS:CG	13:D:100:PRO:HD2	2.32	0.64
1:1:60:LYS:HD2	1:1:60:LYS:N	2.14	0.62
9:9:135:VAL:O	41:Z:303:DGD:O2D	2.16	0.62
11:B:275:HIS:HB3	29:B:816:CLA:HMB2	1.82	0.62
28:e:57:MET:HE1	28:e:74:VAL:HG11	1.82	0.62
13:D:99:HIS:CD2	13:D:100:PRO:HD2	2.34	0.61
9:9:218:GLY:O	9:9:219:LEU:C	2.42	0.61
1:1:61:THR:CG2	1:1:81:ALA:HB2	2.30	0.61
9:9:49:LYS:HD2	9:9:59:ARG:HE	1.65	0.61
13:D:99:HIS:CD2	13:D:100:PRO:CD	2.84	0.60
10:A:392:THR:HG21	29:A:826:CLA:HMB1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:47:GLY:O	1:1:50:VAL:HG12	2.03	0.59
23:X:77:UNK:O	23:X:81:UNK:N	2.36	0.59
13:D:99:HIS:HB3	13:D:100:PRO:HD2	1.83	0.59
1:1:50:VAL:HG11	1:1:71:ASP:O	2.03	0.59
27:c:133:GLU:OE2	27:c:142:MET:N	2.35	0.58
38:4:618:LMU:O5B	38:4:618:LMU:O3'	2.21	0.58
9:9:212:ILE:HD11	29:9:611:CLA:HMD1	1.84	0.58
13:D:99:HIS:CG	13:D:100:PRO:CD	2.86	0.58
3:3:193:MET:HE2	3:3:193:MET:HA	1.86	0.58
26:b:51:GLU:HA	26:b:51:GLU:OE1	2.02	0.58
1:1:119:GLU:OE1	1:1:119:GLU:N	2.35	0.57
12:C:60:THR:O	12:C:61:ASP:C	2.47	0.57
11:B:465:ALA:O	11:B:479:SER:OG	2.21	0.57
25:a:124:LEU:HA	25:a:127:THR:HB	1.85	0.57
2:2:169:ASP:OD1	2:2:172:THR:OG1	2.22	0.56
5:5:183:LEU:HB3	5:5:185:LEU:HD21	1.88	0.56
18:K:85:LEU:HD11	29:e:611:CLA:HED1	1.87	0.56
23:X:81:UNK:O	23:X:82:UNK:C	2.53	0.56
5:5:41:TRP:O	5:5:42:GLU:C	2.48	0.56
25:a:127:THR:HG23	26:b:218:MET:CE	2.32	0.56
1:1:112:PHE:O	29:1:604:CLA:HMD1	2.06	0.55
6:6:89:MET:HA	6:6:187:ALA:HB1	1.87	0.55
10:A:455:LEU:HB3	10:A:534:MET:HE3	1.89	0.55
23:X:95:UNK:C	23:X:97:UNK:H	2.19	0.55
25:a:127:THR:CG2	25:a:129:THR:HG23	2.37	0.55
27:c:133:GLU:OE2	27:c:141:THR:N	2.40	0.55
4:4:181:ARG:HA	4:4:184:MET:HE3	1.90	0.54
2:2:89:GLY:HA3	2:2:184:ALA:HB1	1.90	0.54
29:4:611:CLA:HMB1	37:4:616:8CT:C39	2.38	0.54
1:1:194:LYS:HB3	29:1:609:CLA:HMD2	1.89	0.54
10:A:661:SER:O	10:A:664:SER:OG	2.25	0.54
23:X:84:UNK:O	23:X:85:UNK:C	2.54	0.54
9:9:105:ILE:HG21	9:9:206:MET:HE3	1.90	0.54
10:A:584:CYS:HB2	11:B:667:TRP:HB3	1.90	0.54
27:c:126:HIS:CD2	27:c:142:MET:HE2	2.43	0.53
4:4:82:ALA:O	4:4:86:HIS:ND1	2.40	0.53
6:6:169:ASN:O	6:6:170:PRO:C	2.49	0.53
1:1:100:MET:HG3	31:1:614:II0:C41	2.39	0.53
11:B:345:THR:HG23	11:B:379:ALA:HB2	1.90	0.53
4:4:211:TYR:OH	29:Z:304:CLA:OBD	2.26	0.53
8:8:205:MET:HA	8:8:205:MET:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:372:TYR:CD1	10:A:372:TYR:C	2.87	0.53
18:K:85:LEU:HD11	29:e:611:CLA:CED	2.39	0.52
27:c:198:LYS:HB3	29:c:609:CLA:HMD2	1.91	0.52
5:5:40:LEU:HD23	5:5:40:LEU:O	2.09	0.52
29:L:201:CLA:H2A	29:L:201:CLA:O2A	2.09	0.52
5:5:40:LEU:HD22	29:5:609:CLA:HED3	1.91	0.52
12:C:14:CYS:SG	12:C:16:GLN:HG2	2.50	0.52
15:F:150:SER:O	15:F:154:THR:HG23	2.10	0.51
23:X:82:UNK:O	23:X:83:UNK:CB	2.57	0.51
24:Z:125:GLN:HB2	24:Z:126:PRO:HD3	1.92	0.51
23:X:76:UNK:O	23:X:78:UNK:N	2.42	0.51
28:e:105:MET:HG2	28:e:106:TYR:CD2	2.46	0.51
11:B:290:MET:HE1	29:B:818:CLA:HMD1	1.92	0.51
38:O:207:LMU:O1B	38:O:207:LMU:O6'	2.11	0.51
13:D:99:HIS:CD2	13:D:100:PRO:HD3	2.46	0.51
23:X:77:UNK:C	23:X:79:UNK:N	2.68	0.51
2:2:113:MET:HE1	2:2:121:TYR:HB2	1.93	0.50
28:e:93:VAL:O	28:e:97:ILE:HG12	2.10	0.50
8:8:144:VAL:O	8:8:148:SER:OG	2.23	0.50
27:c:48:PRO:HG2	29:c:601:CLA:HMB2	1.94	0.50
11:B:498:LEU:HA	11:B:501:ILE:HG22	1.94	0.50
27:c:228:ILE:C	27:c:230:ASN:H	2.19	0.50
2:2:115:PRO:O	31:2:614:II0:O01	2.30	0.50
25:a:127:THR:HG22	25:a:129:THR:HG23	1.94	0.50
2:2:170:GLU:O	2:2:171:ALA:C	2.55	0.49
25:d:103:PHE:CZ	25:d:105:PHE:HA	2.47	0.49
14:E:39:ARG:HG2	14:E:50:THR:HG22	1.92	0.49
2:2:170:GLU:OE2	2:2:170:GLU:C	2.54	0.49
29:B:808:CLA:C1A	29:B:808:CLA:CGA	2.90	0.49
13:D:94:GLU:O	13:D:94:GLU:HG2	2.12	0.49
21:O:69:LEU:HD21	25:d:148:LEU:HD23	1.94	0.49
22:R:76:SER:OG	22:R:133:LYS:O	2.23	0.49
24:Z:205:PHE:CD2	24:Z:209:MET:HE2	2.47	0.49
28:e:144:THR:CG2	28:e:145:PRO:HD2	2.43	0.49
2:2:170:GLU:O	2:2:170:GLU:OE2	2.30	0.49
11:B:15:ASP:HB3	11:B:20:ARG:HB2	1.94	0.49
12:C:75:ARG:NH1	13:D:29:GLU:OE2	2.45	0.49
6:6:85:CYS:O	6:6:89:MET:HG2	2.13	0.49
29:8:615:CLA:O1D	16:I:8:SER:OG	2.18	0.49
9:9:74:ASP:OD2	9:9:79:SER:OG	2.29	0.49
27:c:224:PHE:CZ	30:c:611:KC2:O1D	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:147:ASN:C	28:e:147:ASN:OD1	2.55	0.49
26:b:83:ALA:O	26:b:87:HIS:ND1	2.45	0.49
27:c:171:MET:HA	27:c:171:MET:HE3	1.95	0.49
29:B:818:CLA:HMB2	29:B:823:CLA:CED	2.42	0.49
10:A:610:PHE:O	10:A:614:MET:HG2	2.13	0.48
11:B:407:VAL:O	11:B:411:MET:HG2	2.12	0.48
9:9:205:GLY:O	9:9:209:HIS:CG	2.66	0.48
10:A:392:THR:CG2	29:A:826:CLA:HMB1	2.43	0.48
11:B:123:TRP:O	11:B:127:ILE:HG12	2.13	0.48
11:B:548:PRO:HD2	12:C:62:PHE:CE1	2.48	0.48
27:c:228:ILE:C	27:c:230:ASN:N	2.71	0.48
1:1:106:ALA:HB1	1:1:217:PRO:HG3	1.95	0.48
6:6:164:LEU:HB2	6:6:166:PHE:CE2	2.48	0.48
27:c:43:LYS:O	27:c:44:SER:C	2.55	0.48
23:X:76:UNK:C	23:X:78:UNK:N	2.77	0.48
1:1:177:LEU:HB2	1:1:179:PHE:CE2	2.48	0.48
5:5:71:VAL:HG12	5:5:71:VAL:O	2.14	0.48
8:8:148:SER:HB3	29:8:605:CLA:NC	2.29	0.48
27:c:126:HIS:HD2	27:c:142:MET:HE2	1.79	0.48
1:1:212:ILE:CD1	29:1:611:CLA:HMD2	2.44	0.48
4:4:90:CYS:SG	31:4:613:II0:C39	3.02	0.48
19:L:152:ILE:HD13	21:O:112:PRO:HB2	1.95	0.48
22:R:98:ILE:HB	22:R:99:PRO:HD3	1.96	0.48
12:C:54:CYS:SG	12:C:55:GLU:N	2.87	0.47
3:3:117:LEU:HG	3:3:202:MET:HE3	1.97	0.47
5:5:200:LYS:HB3	29:5:609:CLA:HMD2	1.96	0.47
38:O:207:LMU:O2B	38:O:207:LMU:H5B	2.14	0.47
5:5:161:MET:HE3	22:R:81:VAL:HG21	1.96	0.47
8:8:90:GLY:HA3	31:8:610:II0:C14	2.44	0.47
11:B:429:LEU:HD11	29:B:835:CLA:HMB1	1.96	0.47
12:C:7:VAL:HG13	12:C:11:CYS:SG	2.54	0.47
10:A:461:THR:HG23	29:B:809:CLA:HMC3	1.96	0.47
2:2:119:HIS:O	2:2:123:VAL:HG23	2.15	0.47
11:B:373:THR:HB	29:B:826:CLA:HMB1	1.96	0.47
16:I:29:TYR:OH	20:M:29:TYR:OH	2.19	0.47
3:3:220:ASP:OD1	3:3:220:ASP:O	2.33	0.47
5:5:135:ALA:HB3	5:5:143:ALA:CB	2.45	0.47
29:A:810:CLA:H42	29:A:810:CLA:O1A	2.15	0.47
11:B:410:ARG:O	11:B:414:HIS:ND1	2.40	0.47
18:K:33:VAL:O	18:K:37:TYR:HD1	1.97	0.47
21:O:141:ILE:HG12	29:O:201:CLA:ND	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:122:VAL:HG23	26:b:123:PRO:HD2	1.97	0.47
27:c:128:LYS:O	27:c:132:MET:HG3	2.15	0.47
28:e:94:GLY:O	28:e:98:PRO:HG2	2.15	0.47
5:5:218:LEU:HG	29:5:612:CLA:HED2	1.96	0.47
29:9:606:CLA:HMB1	33:9:619:IHT:C26	2.44	0.47
15:F:145:VAL:HG22	15:F:146:PRO:HD3	1.97	0.47
27:c:126:HIS:CE1	27:c:130:LEU:HD12	2.50	0.47
21:O:69:LEU:HD22	25:d:145:THR:HG23	1.96	0.47
29:a:603:CLA:HBB2	33:a:617:IHT:C40	2.45	0.47
9:9:107:VAL:HG11	29:9:604:CLA:CBC	2.42	0.46
10:A:274:ASP:N	10:A:274:ASP:OD1	2.47	0.46
10:A:460:ASP:OD1	10:A:642:THR:HB	2.15	0.46
13:D:138:SER:C	13:D:140:ASN:H	2.23	0.46
11:B:3:THR:HG21	11:B:20:ARG:CZ	2.45	0.46
5:5:92:LEU:HD13	5:5:176:GLY:HA3	1.97	0.46
23:X:89:UNK:O	23:X:90:UNK:C	2.63	0.46
4:4:149:ASP:OD1	4:4:149:ASP:O	2.33	0.46
10:A:388:LEU:O	10:A:392:THR:HG22	2.15	0.46
13:D:98:LEU:HD12	13:D:98:LEU:N	2.30	0.46
11:B:526:GLY:HA2	11:B:582:TRP:CZ3	2.50	0.46
1:1:100:MET:HG3	31:1:614:II0:C42	2.46	0.46
9:9:204:SER:HB2	29:9:611:CLA:HMC1	1.98	0.46
24:Z:206:LEU:HA	24:Z:209:MET:HE3	1.97	0.46
4:4:180:GLY:O	4:4:184:MET:HG3	2.15	0.46
8:8:185:THR:HB	8:8:186:PRO:HD2	1.97	0.46
11:B:723:ALA:O	11:B:724:PHE:C	2.59	0.46
27:c:74:MET:HE1	29:c:602:CLA:H91	1.98	0.46
1:1:50:VAL:HG21	1:1:72:THR:HG23	1.98	0.46
5:5:212:MET:HE3	31:5:614:II0:C09	2.46	0.45
27:c:171:MET:HE3	27:c:172:PRO:HD3	1.98	0.45
27:c:227:GLY:O	27:c:230:ASN:ND2	2.50	0.45
29:A:821:CLA:CGA	29:O:203:CLA:H42	2.46	0.45
10:A:361:GLY:HA2	10:A:398:GLY:HA2	1.99	0.45
12:C:66:ARG:HG2	13:D:123:ILE:HD11	1.99	0.45
11:B:469:LYS:NZ	11:B:509:PHE:O	2.43	0.45
5:5:161:MET:HB3	5:5:162:PRO:HD3	1.99	0.45
26:b:91:CYS:SG	32:b:613:II3:C40	3.04	0.45
27:c:47:ILE:HD11	29:c:601:CLA:HBC3	1.98	0.45
27:c:147:LEU:HB2	29:c:614:CLA:HMD3	1.98	0.45
2:2:89:GLY:O	2:2:93:MET:HG3	2.17	0.45
6:6:89:MET:CE	6:6:184:GLY:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:203:SER:OG	10:A:204:GLY:N	2.50	0.45
1:1:212:ILE:HD11	29:1:611:CLA:HMD2	1.99	0.45
9:9:202:ALA:O	9:9:206:MET:HG3	2.16	0.45
11:B:5:PHE:HB2	16:I:30:ILE:HA	1.99	0.45
11:B:694:LYS:NZ	16:I:33:GLU:OE2	2.48	0.45
27:c:47:ILE:HD13	27:c:50:LEU:HD12	1.99	0.45
6:6:169:ASN:O	6:6:172:ALA:N	2.51	0.45
1:1:126:MET:HE1	1:1:207:ILE:HD13	1.99	0.44
5:5:88:ARG:NH1	5:5:91:GLU:OE1	2.51	0.44
11:B:548:PRO:HD2	12:C:62:PHE:CZ	2.52	0.44
24:Z:132:MET:HE3	24:Z:143:LYS:HE3	1.98	0.44
31:5:620:II0:C30	6:6:189:LEU:HD13	2.47	0.44
10:A:698:ILE:O	10:A:702:VAL:HG23	2.18	0.44
7:7:119:PHE:CD1	23:X:81:UNK:CB	3.00	0.44
38:7:620:LMU:O5B	38:7:620:LMU:O6'	2.33	0.44
29:A:844:CLA:HBA2	11:B:655:LEU:HB2	2.00	0.44
11:B:464:GLN:NE2	29:B:834:CLA:OBD	2.38	0.44
29:2:612:CLA:HMB2	33:2:616:IHT:C36	2.48	0.43
12:C:17:CYS:SG	12:C:18:VAL:N	2.90	0.43
2:2:93:MET:HE3	2:2:183:HIS:HB3	2.00	0.43
19:L:53:THR:HG23	29:L:202:CLA:HAB	2.00	0.43
26:b:210:GLN:NE2	29:b:610:CLA:O1D	2.51	0.43
9:9:95:GLY:O	9:9:99:MET:HG3	2.19	0.43
10:A:121:ILE:HG13	10:A:122:VAL:HG13	2.00	0.43
29:A:836:CLA:C1A	29:A:836:CLA:CGA	2.96	0.43
3:3:151:ASP:OD1	3:3:151:ASP:C	2.61	0.43
10:A:201:HIS:ND1	29:A:823:CLA:OBD	2.50	0.43
25:d:190:GLY:O	25:d:194:MET:HG3	2.18	0.43
29:d:612:CLA:HMB1	33:d:617:IHT:C36	2.48	0.43
29:5:604:CLA:CGA	29:5:604:CLA:C1A	2.97	0.43
7:7:201:ILE:CD1	29:7:611:CLA:HMD1	2.48	0.43
10:A:250:MET:HE2	10:A:257:PHE:CZ	2.54	0.43
3:3:91:CYS:SG	31:3:614:II0:C39	3.07	0.43
9:9:105:ILE:HG23	9:9:127:ILE:HG21	2.01	0.43
10:A:578:PRO:HB3	11:B:559:CYS:SG	2.58	0.43
29:B:832:CLA:O1A	29:B:832:CLA:C2	2.66	0.43
25:a:42:MET:N	25:a:50:LYS:HZ2	2.17	0.43
1:1:45:LEU:HD12	1:1:45:LEU:N	2.33	0.43
1:1:138:THR:O	29:1:605:CLA:HMD1	2.18	0.43
10:A:562:LEU:HD13	11:B:672:GLN:CG	2.49	0.43
11:B:656:ILE:HG23	11:B:716:GLY:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:108:TYR:CE1	31:a:616:II0:C20	3.01	0.43
11:B:7:LYS:HD2	20:M:29:TYR:CZ	2.54	0.43
11:B:282:VAL:HG21	29:B:815:CLA:HMC1	2.01	0.43
7:7:191:GLY:O	7:7:195:MET:HG3	2.18	0.43
8:8:184:LEU:HD23	8:8:184:LEU:HA	1.94	0.43
11:B:658:ALA:O	11:B:661:PHE:HB2	2.19	0.43
38:O:207:LMU:O2B	38:O:207:LMU:H4'	2.19	0.43
24:Z:92:THR:HG23	24:Z:109:GLY:C	2.44	0.43
7:7:41:ASN:HB3	7:7:50:ARG:H	1.83	0.42
8:8:193:GLY:O	8:8:197:MET:HG3	2.18	0.42
11:B:301:LEU:HD23	29:B:818:CLA:HED3	2.00	0.42
11:B:327:THR:HG21	22:R:47:VAL:HG13	2.01	0.42
37:F:201:8CT:C28	37:F:201:8CT:C36	2.97	0.42
21:O:82:GLY:O	21:O:96:LEU:N	2.51	0.42
22:R:63:PRO:O	22:R:131:ASN:ND2	2.51	0.42
27:c:231:TYR:CZ	30:c:611:KC2:CED	3.02	0.42
29:c:612:CLA:HMB2	33:c:620:IHT:C36	2.48	0.42
5:5:42:GLU:HB3	5:5:45:LYS:HB2	2.00	0.42
26:b:88:GLY:O	26:b:92:MET:HG3	2.18	0.42
6:6:208:LEU:CD2	6:6:212:PHE:HD1	2.33	0.42
8:8:85:ARG:HA	8:8:88:MET:HE3	2.01	0.42
10:A:146:GLN:HB3	10:A:377:TYR:HB3	2.01	0.42
25:a:118:THR:O	25:a:121:HIS:HB3	2.19	0.42
28:e:123:ALA:O	28:e:127:ILE:HG12	2.19	0.42
7:7:138:HIS:CE1	7:7:145:MET:HE1	2.55	0.42
10:A:486:TRP:CE2	10:A:490:ILE:HD11	2.55	0.42
29:B:803:CLA:CGA	29:B:803:CLA:H3A	2.49	0.42
19:L:107:THR:O	19:L:108:ASP:C	2.62	0.42
35:L:208:LHG:HC82	29:c:614:CLA:HMC1	2.01	0.42
1:1:126:MET:CE	1:1:207:ILE:HD13	2.50	0.42
29:5:608:CLA:H41	29:5:608:CLA:C7	2.50	0.42
19:L:57:PHE:CD1	19:L:57:PHE:C	2.97	0.42
28:e:99:GLU:OE1	28:e:195:GLY:HA3	2.20	0.42
28:e:144:THR:HG23	28:e:145:PRO:HD2	2.02	0.42
2:2:44:PHE:HA	2:2:52:LYS:HA	2.02	0.42
11:B:5:PHE:CD1	11:B:5:PHE:C	2.98	0.42
11:B:123:TRP:CD1	11:B:127:ILE:HD11	2.55	0.42
3:3:124:PRO:O	3:3:128:MET:HG2	2.19	0.42
5:5:111:PHE:CZ	5:5:113:PHE:HA	2.54	0.42
10:A:499:THR:HG22	29:A:834:CLA:HED3	2.01	0.42
11:B:494:LEU:N	11:B:495:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:12:PRO:O	13:D:13:THR:C	2.63	0.42
15:F:158:TRP:N	15:F:159:PRO:CD	2.83	0.42
24:Z:177:PRO:HB2	25:a:134:LEU:HD23	2.02	0.42
27:c:129:PHE:O	27:c:133:GLU:HG3	2.20	0.42
29:4:611:CLA:HMA2	31:4:614:II0:C29	2.50	0.42
10:A:121:ILE:HG23	10:A:122:VAL:N	2.34	0.42
12:C:17:CYS:HB3	40:C:102:SF4:S4	2.59	0.42
21:O:151:THR:HG23	21:O:152:THR:N	2.35	0.42
27:c:47:ILE:CG2	27:c:49:PHE:CZ	3.03	0.42
6:6:144:MET:HE3	7:7:67:LEU:HA	2.02	0.42
7:7:183:LYS:HB3	29:7:609:CLA:HMD1	2.02	0.42
10:A:24:THR:O	10:A:24:THR:HG23	2.20	0.42
11:B:227:THR:O	11:B:227:THR:HG22	2.20	0.42
19:L:54:HIS:HA	19:L:57:PHE:CE2	2.55	0.42
21:O:136:MET:HE2	29:O:201:CLA:C2	2.49	0.42
7:7:87:ARG:HA	7:7:90:MET:HE3	2.01	0.41
7:7:201:ILE:HD11	29:7:611:CLA:HMD1	2.02	0.41
8:8:160:ASP:OD1	8:8:161:THR:N	2.53	0.41
29:8:603:CLA:H43	16:I:17:ILE:HG21	2.02	0.41
10:A:87:TRP:O	10:A:91:MET:HG2	2.20	0.41
29:B:816:CLA:O2A	29:B:816:CLA:H42	2.20	0.41
13:D:138:SER:C	13:D:140:ASN:N	2.78	0.41
5:5:212:MET:HE3	31:5:614:II0:C21	2.50	0.41
29:9:608:CLA:H61	29:9:608:CLA:H41	1.86	0.41
27:c:75:LEU:HB2	27:c:80:TRP:CG	2.55	0.41
1:1:55:PHE:CD1	1:1:55:PHE:C	2.98	0.41
3:3:157:ASN:O	3:3:159:LYS:NZ	2.51	0.41
5:5:133:LEU:HD22	5:5:146:MET:HG3	2.02	0.41
13:D:99:HIS:CB	13:D:100:PRO:CD	2.98	0.41
25:a:190:GLY:O	25:a:194:MET:HG3	2.20	0.41
10:A:460:ASP:OD1	10:A:642:THR:CB	2.69	0.41
26:b:122:VAL:HB	29:b:604:CLA:HED1	2.03	0.41
11:B:127:ILE:N	11:B:127:ILE:HD13	2.35	0.41
25:a:50:LYS:HD2	25:a:50:LYS:HA	1.90	0.41
6:6:198:TYR:O	6:6:202:GLY:N	2.45	0.41
29:7:612:CLA:HMB1	37:7:617:8CT:C22	2.50	0.41
11:B:293:THR:O	11:B:295:TRP:N	2.53	0.41
15:F:30:CYS:SG	15:F:36:PHE:CG	3.13	0.41
1:1:113:THR:HG21	1:1:118:VAL:HB	2.03	0.41
1:1:178:GLY:HA2	1:1:181:LYS:HE2	2.03	0.41
6:6:89:MET:CE	6:6:184:GLY:CA	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:13:VAL:HG12	29:A:810:CLA:O1D	2.21	0.41
11:B:341:ILE:O	11:B:345:THR:HG22	2.21	0.41
1:1:114:PHE:CD2	29:1:613:CLA:HMC1	2.56	0.41
5:5:68:VAL:O	5:5:88:ARG:NH2	2.53	0.41
6:6:89:MET:CE	6:6:184:GLY:HA2	2.41	0.41
29:6:612:CLA:HMB1	33:6:617:IHT:C36	2.51	0.41
9:9:149:PHE:O	9:9:153:THR:OG1	2.35	0.41
10:A:156:GLU:OE1	10:A:156:GLU:N	2.54	0.41
10:A:248:ASP:O	10:A:252:GLN:HG3	2.21	0.41
10:A:497:ASN:HA	21:O:89:PRO:HD2	2.03	0.41
10:A:584:CYS:CB	11:B:667:TRP:HB3	2.50	0.41
10:A:715:GLN:NE2	14:E:43:VAL:O	2.49	0.41
10:A:747:ARG:NH1	10:A:751:VAL:HG11	2.35	0.41
11:B:72:GLY:HA2	11:B:87:VAL:CG2	2.51	0.41
13:D:69:LEU:HD21	13:D:99:HIS:CE1	2.56	0.41
23:X:98:UNK:O	23:X:99:UNK:C	2.69	0.41
1:1:50:VAL:HG23	29:1:601:CLA:HED3	2.03	0.41
5:5:111:PHE:CE2	29:5:604:CLA:HMD3	2.56	0.41
10:A:313:ARG:HD3	10:A:317:GLY:O	2.21	0.41
11:B:631:LEU:HD22	11:B:724:PHE:HA	2.02	0.41
25:d:81:GLU:HG2	25:d:148:LEU:HD13	2.02	0.41
1:1:215:LYS:HB2	1:1:219:GLU:OE1	2.20	0.40
6:6:169:ASN:C	6:6:171:GLU:N	2.78	0.40
7:7:186:ARG:HA	7:7:189:MET:HE3	2.03	0.40
25:a:127:THR:CG2	25:a:129:THR:CG2	2.99	0.40
25:a:189:LEU:HD13	31:a:615:II0:C30	2.51	0.40
1:1:200:MET:O	1:1:203:ILE:HG22	2.21	0.40
7:7:142:GLY:O	7:7:143:PHE:HB2	2.21	0.40
15:F:145:VAL:N	15:F:146:PRO:CD	2.84	0.40
27:c:87:ALA:O	27:c:91:HIS:ND1	2.54	0.40
28:e:204:LYS:O	29:e:610:CLA:HED1	2.21	0.40
29:A:824:CLA:C2	29:A:836:CLA:HBA1	2.51	0.40
11:B:695:ASP:OD2	16:I:31:GLU:OE2	2.38	0.40
3:3:138:ILE:HA	29:Z:306:CLA:CED	2.52	0.40
6:6:96:MET:HE3	6:6:194:MET:CE	2.52	0.40
29:8:608:CLA:CGA	29:8:608:CLA:C1A	2.99	0.40
10:A:562:LEU:HD13	11:B:672:GLN:HG3	2.04	0.40
29:A:842:CLA:HED2	17:J:16:LEU:HD22	2.04	0.40
9:9:54:ILE:HG21	9:9:57:PHE:CE2	2.57	0.40
11:B:3:THR:HG22	11:B:4:LYS:N	2.36	0.40
21:O:146:TYR:CD2	29:O:203:CLA:HBD	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:152:THR:HG21	21:O:154:TYR:CE1	2.57	0.40
27:c:224:PHE:CE2	30:c:611:KC2:O1D	2.74	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	1	177/222 (80%)	172 (97%)	5 (3%)	0	100	100
2	2	166/216 (77%)	161 (97%)	5 (3%)	0	100	100
3	3	178/236 (75%)	174 (98%)	4 (2%)	0	100	100
4	4	174/217 (80%)	173 (99%)	1 (1%)	0	100	100
5	5	186/229 (81%)	176 (95%)	10 (5%)	0	100	100
6	6	171/215 (80%)	163 (95%)	8 (5%)	0	100	100
7	7	175/230 (76%)	172 (98%)	3 (2%)	0	100	100
8	8	171/227 (75%)	168 (98%)	3 (2%)	0	100	100
9	9	178/220 (81%)	174 (98%)	4 (2%)	0	100	100
10	A	739/752 (98%)	713 (96%)	26 (4%)	0	100	100
11	B	729/734 (99%)	706 (97%)	23 (3%)	0	100	100
12	C	78/81 (96%)	73 (94%)	4 (5%)	1 (1%)	9	16
13	D	135/141 (96%)	124 (92%)	10 (7%)	1 (1%)	18	30
14	E	59/64 (92%)	57 (97%)	2 (3%)	0	100	100
15	F	158/183 (86%)	152 (96%)	6 (4%)	0	100	100
16	I	31/36 (86%)	29 (94%)	2 (6%)	0	100	100
17	J	40/42 (95%)	40 (100%)	0	0	100	100
18	K	76/87 (87%)	72 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	L	148/153 (97%)	143 (97%)	5 (3%)	0	100	100
20	M	28/30 (93%)	28 (100%)	0	0	100	100
21	O	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
22	R	90/133 (68%)	88 (98%)	2 (2%)	0	100	100
24	Z	151/242 (62%)	150 (99%)	1 (1%)	0	100	100
25	a	169/215 (79%)	165 (98%)	4 (2%)	0	100	100
25	d	169/215 (79%)	166 (98%)	3 (2%)	0	100	100
26	b	174/218 (80%)	171 (98%)	3 (2%)	0	100	100
27	c	213/257 (83%)	203 (95%)	10 (5%)	0	100	100
28	e	166/208 (80%)	165 (99%)	1 (1%)	0	100	100
All	All	5026/5902 (85%)	4871 (97%)	153 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	D	100	PRO
12	C	61	ASP

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	1	130/163 (80%)	130 (100%)	0	100	100
2	2	134/167 (80%)	134 (100%)	0	100	100
3	3	145/183 (79%)	145 (100%)	0	100	100
4	4	139/167 (83%)	139 (100%)	0	100	100
5	5	139/166 (84%)	138 (99%)	1 (1%)	76	86
6	6	134/160 (84%)	134 (100%)	0	100	100
7	7	137/176 (78%)	137 (100%)	0	100	100
8	8	134/169 (79%)	133 (99%)	1 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	9	138/164 (84%)	138 (100%)	0	100	100
10	A	607/617 (98%)	605 (100%)	2 (0%)	86	94
11	B	592/593 (100%)	591 (100%)	1 (0%)	87	95
12	C	66/67 (98%)	66 (100%)	0	100	100
13	D	114/117 (97%)	112 (98%)	2 (2%)	51	72
14	E	56/59 (95%)	55 (98%)	1 (2%)	51	72
15	F	133/154 (86%)	133 (100%)	0	100	100
16	I	27/29 (93%)	27 (100%)	0	100	100
17	J	38/38 (100%)	38 (100%)	0	100	100
18	K	62/69 (90%)	62 (100%)	0	100	100
19	L	126/128 (98%)	125 (99%)	1 (1%)	73	85
20	M	25/25 (100%)	25 (100%)	0	100	100
21	O	81/81 (100%)	81 (100%)	0	100	100
22	R	74/105 (70%)	74 (100%)	0	100	100
24	Z	117/180 (65%)	117 (100%)	0	100	100
25	a	128/153 (84%)	127 (99%)	1 (1%)	73	85
25	d	128/153 (84%)	128 (100%)	0	100	100
26	b	144/173 (83%)	144 (100%)	0	100	100
27	c	169/195 (87%)	169 (100%)	0	100	100
28	e	133/162 (82%)	132 (99%)	1 (1%)	73	85
All	All	4050/4613 (88%)	4039 (100%)	11 (0%)	84	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	5	125	MET
8	8	220	LEU
10	A	111	VAL
10	A	538	ILE
11	B	87	VAL
13	D	100	PRO
13	D	104	VAL
14	E	36	VAL
19	L	6	LYS
25	a	129	THR

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Mol	Chain	Res	Type
28	e	105	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	208	GLN
3	3	157	ASN
4	4	129	GLN
6	6	130	GLN
6	6	211	ASN
7	7	99	GLN
7	7	111	ASN
7	7	120	GLN
9	9	52	ASN
10	A	80	GLN
10	A	182	HIS
10	A	394	HIS
10	A	705	HIS
10	A	715	GLN
11	B	10	GLN
11	B	14	GLN
11	B	53	HIS
11	B	610	ASN
13	D	99	HIS
13	D	126	ASN
15	F	37	GLN
24	Z	171	ASN
24	Z	190	ASN
25	a	172	ASN
26	b	199	GLN
27	c	144	GLN
27	c	199	ASN
27	c	223	GLN
25	d	183	ASN
28	e	48	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

417 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	$\#\|Z\| > 2$
31	II0	4	615	-	39,43,43	2.67	4 (10%)	50,60,60	1.43	6 (12%)
31	II0	O	205	-	39,43,43	2.72	4 (10%)	50,60,60	1.51	11 (22%)
36	SQD	O	206	-	28,29,54	1.63	5 (17%)	37,40,65	1.52	5 (13%)
29	CLA	L	204	-	54,58,73	1.97	9 (16%)	65,95,113	1.65	10 (15%)
29	CLA	Z	305	24	54,58,73	1.96	9 (16%)	65,95,113	1.56	9 (13%)
31	II0	3	614	-	39,43,43	2.71	4 (10%)	50,60,60	1.40	6 (12%)
29	CLA	4	608	35	69,73,73	1.75	9 (13%)	83,113,113	1.37	8 (9%)
37	8CT	b	615	-	40,41,41	0.20	0	50,56,56	0.33	0
29	CLA	5	612	5	49,53,73	2.09	9 (18%)	59,89,113	1.69	10 (16%)
29	CLA	d	605	25	49,53,73	2.12	9 (18%)	59,89,113	1.67	8 (13%)
29	CLA	B	823	-	69,73,73	1.77	9 (13%)	83,113,113	1.38	10 (12%)
31	II0	5	614	-	39,43,43	2.67	4 (10%)	50,60,60	1.39	8 (16%)
29	CLA	c	607	27	69,73,73	1.76	9 (13%)	83,113,113	1.38	9 (10%)
29	CLA	Z	304	24	59,63,73	1.91	9 (15%)	71,101,113	1.47	9 (12%)
35	LHG	b	616	-	48,48,48	0.57	1 (2%)	51,54,54	1.14	4 (7%)
29	CLA	c	605	-	49,53,73	2.08	9 (18%)	59,89,113	1.62	8 (13%)
30	KC2	7	610	7	49,53,53	1.85	4 (8%)	62,89,89	1.39	6 (9%)
30	KC2	6	610	6	49,53,53	1.85	4 (8%)	62,89,89	1.39	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	4	602	4	63,67,73	1.84	9 (14%)	75,105,113	1.50	11 (14%)
36	SQD	3	621	-	41,42,54	1.34	4 (9%)	50,53,65	1.12	3 (6%)
40	SF4	C	101	12	0,12,12	-	-	-		
29	CLA	K	101	-	69,73,73	1.76	9 (13%)	83,113,113	1.36	7 (8%)
29	CLA	1	607	1	49,53,73	2.12	9 (18%)	59,89,113	1.64	9 (15%)
29	CLA	B	834	11	59,63,73	1.91	9 (15%)	71,101,113	1.54	10 (14%)
29	CLA	7	609	35	45,49,73	2.26	10 (22%)	54,84,113	1.73	8 (14%)
29	CLA	9	612	-	49,53,73	2.08	9 (18%)	59,89,113	1.62	9 (15%)
29	CLA	B	802	-	69,73,73	1.70	9 (13%)	83,113,113	1.37	9 (10%)
29	CLA	B	820	11	64,68,73	1.83	9 (14%)	77,107,113	1.44	10 (12%)
35	LHG	A	851	-	38,38,48	0.70	1 (2%)	41,44,54	1.25	3 (7%)
30	KC2	c	611	27	49,53,53	1.87	4 (8%)	62,89,89	1.39	8 (12%)
37	8CT	I	101	-	40,41,41	0.27	0	50,56,56	0.46	0
29	CLA	4	611	4	69,73,73	1.74	9 (13%)	83,113,113	1.38	9 (10%)
29	CLA	A	814	-	49,53,73	2.11	9 (18%)	59,89,113	1.65	8 (13%)
29	CLA	9	605	-	49,53,73	2.09	9 (18%)	59,89,113	1.66	9 (15%)
35	LHG	d	618	-	22,22,48	0.80	1 (4%)	24,27,54	1.28	3 (12%)
29	CLA	O	202	21	59,63,73	1.84	9 (15%)	71,101,113	1.55	10 (14%)
35	LHG	2	619	-	38,38,48	0.68	0	41,44,54	1.24	4 (9%)
29	CLA	Z	301	-	64,68,73	1.85	9 (14%)	77,107,113	1.46	10 (12%)
29	CLA	9	611	9	45,49,73	2.23	10 (22%)	54,84,113	1.74	9 (16%)
34	LMG	3	620	-	32,32,55	0.90	0	40,40,63	1.26	6 (15%)
29	CLA	8	604	8	69,73,73	1.77	9 (13%)	83,113,113	1.41	11 (13%)
29	CLA	B	839	35	69,73,73	1.80	9 (13%)	83,113,113	1.44	10 (12%)
29	CLA	B	816	11	63,67,73	1.84	9 (14%)	75,105,113	1.46	9 (12%)
29	CLA	L	202	19	55,59,73	1.97	9 (16%)	66,96,113	1.57	9 (13%)
29	CLA	3	602	3	59,63,73	1.92	9 (15%)	71,101,113	1.53	9 (12%)
31	II0	c	617	-	39,43,43	2.68	4 (10%)	50,60,60	1.40	7 (14%)
29	CLA	6	602	6	69,73,73	1.81	9 (13%)	83,113,113	1.47	7 (8%)
29	CLA	d	612	-	67,71,73	1.78	9 (13%)	80,110,113	1.37	10 (12%)
29	CLA	e	604	-	64,68,73	1.85	9 (14%)	77,107,113	1.44	8 (10%)
37	8CT	B	845	-	40,41,41	0.39	1 (2%)	50,56,56	0.64	1 (2%)
29	CLA	3	610	3	69,73,73	1.77	9 (13%)	83,113,113	1.44	10 (12%)
38	LMU	O	207	-	31,31,36	0.53	1 (3%)	42,42,47	1.08	2 (4%)
31	II0	d	615	-	39,43,43	2.77	4 (10%)	50,60,60	1.52	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LHG	7	618	-	30,30,48	0.74	0	33,36,54	1.19	3 (9%)
31	II0	c	616	-	39,43,43	2.67	4 (10%)	50,60,60	1.27	6 (12%)
41	DGD	B	848	-	60,60,67	0.90	1 (1%)	74,74,81	1.30	6 (8%)
31	II0	5	615	-	39,43,43	2.72	4 (10%)	50,60,60	1.46	7 (14%)
31	II0	2	614	-	39,43,43	2.68	4 (10%)	50,60,60	1.41	7 (14%)
29	CLA	c	601	27	49,53,73	2.14	9 (18%)	59,89,113	1.69	9 (15%)
29	CLA	2	609	-	45,49,73	2.30	10 (22%)	54,84,113	1.78	9 (16%)
29	CLA	B	807	11	69,73,73	1.72	9 (13%)	83,113,113	1.41	10 (12%)
30	KC2	5	610	5	49,53,53	1.86	4 (8%)	62,89,89	1.36	7 (11%)
29	CLA	5	613	5	45,49,73	2.25	10 (22%)	54,84,113	1.71	8 (14%)
31	II0	b	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.43	7 (14%)
29	CLA	7	604	7	57,61,73	1.96	9 (15%)	68,98,113	1.55	9 (13%)
31	II0	c	618	-	39,43,43	2.71	4 (10%)	50,60,60	1.42	8 (16%)
37	8CT	B	851	-	40,41,41	0.25	0	50,56,56	0.42	0
29	CLA	b	607	26	64,68,73	1.85	9 (14%)	77,107,113	1.46	9 (11%)
29	CLA	A	807	10	54,58,73	1.99	9 (16%)	65,95,113	1.60	10 (15%)
33	IHT	K	104	-	40,42,42	2.94	5 (12%)	53,58,58	2.01	18 (33%)
29	CLA	e	607	28	49,53,73	2.13	9 (18%)	59,89,113	1.68	9 (15%)
29	CLA	A	839	-	69,73,73	1.75	9 (13%)	83,113,113	1.43	10 (12%)
29	CLA	a	604	25	64,68,73	1.87	9 (14%)	77,107,113	1.48	7 (9%)
31	II0	e	614	-	39,43,43	2.78	4 (10%)	50,60,60	1.49	10 (20%)
37	8CT	K	103	-	40,41,41	0.16	0	50,56,56	0.34	0
29	CLA	A	843	10	69,73,73	1.79	9 (13%)	83,113,113	1.46	8 (9%)
40	SF4	C	102	12	0,12,12	-	-	-		
30	KC2	b	609	-	49,53,53	1.88	4 (8%)	62,89,89	1.37	8 (12%)
29	CLA	c	603	27	69,73,73	1.75	9 (13%)	83,113,113	1.41	10 (12%)
30	KC2	b	605	26	49,53,53	1.85	4 (8%)	62,89,89	1.41	9 (14%)
29	CLA	B	840	11	69,73,73	1.72	9 (13%)	83,113,113	1.36	8 (9%)
37	8CT	B	846	-	40,41,41	0.12	0	50,56,56	0.51	0
29	CLA	B	825	11	69,73,73	1.75	9 (13%)	83,113,113	1.38	10 (12%)
29	CLA	B	817	11	64,68,73	1.80	9 (14%)	77,107,113	1.45	8 (10%)
35	LHG	a	618	-	28,28,48	0.81	0	31,34,54	1.31	3 (9%)
29	CLA	a	605	25	59,63,73	1.88	9 (15%)	71,101,113	1.54	9 (12%)
29	CLA	9	601	9	49,53,73	2.10	9 (18%)	59,89,113	1.66	9 (15%)
29	CLA	B	836	11	51,55,73	2.03	9 (17%)	61,91,113	1.60	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	II0	4	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.34	7 (14%)
35	LHG	6	618	29	34,34,48	0.75	2 (5%)	37,40,54	1.18	3 (8%)
31	II0	2	613	-	39,43,43	2.77	4 (10%)	50,60,60	1.45	10 (20%)
29	CLA	B	805	11	69,73,73	1.75	9 (13%)	83,113,113	1.41	9 (10%)
29	CLA	1	606	-	49,53,73	2.09	9 (18%)	59,89,113	1.67	9 (15%)
29	CLA	A	829	10	54,58,73	1.98	9 (16%)	65,95,113	1.61	9 (13%)
37	8CT	4	616	-	40,41,41	0.20	0	50,56,56	0.35	0
35	LHG	4	619	-	44,44,48	0.65	2 (4%)	47,50,54	1.19	4 (8%)
29	CLA	8	607	8	45,49,73	2.24	10 (22%)	54,84,113	1.74	9 (16%)
33	IHT	5	618	-	40,42,42	2.81	5 (12%)	53,58,58	2.24	16 (30%)
29	CLA	A	809	29	64,68,73	1.87	9 (14%)	77,107,113	1.55	10 (12%)
29	CLA	B	833	-	49,53,73	2.08	9 (18%)	59,89,113	1.59	8 (13%)
29	CLA	c	608	27	64,68,73	1.84	9 (14%)	77,107,113	1.48	9 (11%)
31	II0	b	612	-	39,43,43	2.66	4 (10%)	50,60,60	1.39	8 (16%)
31	II0	O	204	-	39,43,43	2.75	4 (10%)	50,60,60	1.33	5 (10%)
37	8CT	M	101	-	40,41,41	0.19	0	50,56,56	0.87	1 (2%)
29	CLA	O	203	-	59,63,73	1.86	9 (15%)	71,101,113	1.60	10 (14%)
31	II0	a	615	-	39,43,43	2.72	4 (10%)	50,60,60	1.43	9 (18%)
29	CLA	2	601	2	46,50,73	2.19	9 (19%)	55,85,113	1.77	9 (16%)
29	CLA	2	611	-	49,53,73	2.11	9 (18%)	59,89,113	1.64	10 (16%)
35	LHG	3	622	30	33,33,48	0.71	0	36,39,54	1.25	3 (8%)
40	SF4	B	801	10,11	0,12,12	-	-	-		
34	LMG	8	614	-	52,52,55	0.84	3 (5%)	60,60,63	1.28	6 (10%)
29	CLA	a	606	-	69,73,73	1.75	9 (13%)	83,113,113	1.42	9 (10%)
29	CLA	A	834	10	59,63,73	1.89	9 (15%)	71,101,113	1.50	12 (16%)
29	CLA	5	607	5	49,53,73	2.08	9 (18%)	59,89,113	1.61	8 (13%)
29	CLA	4	609	4	64,68,73	1.84	9 (14%)	77,107,113	1.46	8 (10%)
33	IHT	6	617	-	40,42,42	2.81	4 (10%)	53,58,58	2.16	16 (30%)
29	CLA	e	602	28	59,63,73	1.93	9 (15%)	71,101,113	1.61	10 (14%)
29	CLA	Z	306	24	64,68,73	1.81	9 (14%)	77,107,113	1.47	8 (10%)
31	II0	d	614	-	39,43,43	2.71	4 (10%)	50,60,60	1.42	7 (14%)
29	CLA	e	610	-	55,59,73	2.00	9 (16%)	66,96,113	1.58	10 (15%)
29	CLA	c	614	-	59,63,73	1.90	9 (15%)	71,101,113	1.45	7 (9%)
29	CLA	a	607	25	69,73,73	1.75	9 (13%)	83,113,113	1.39	8 (9%)
29	CLA	c	613	27	49,53,73	2.13	9 (18%)	59,89,113	1.60	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	II0	e	612	-	39,43,43	2.69	4 (10%)	50,60,60	1.43	10 (20%)
29	CLA	B	821	-	64,68,73	1.80	9 (14%)	77,107,113	1.47	9 (11%)
35	LHG	d	619	-	38,38,48	0.70	1 (2%)	41,44,54	1.16	2 (4%)
31	II0	3	617	-	39,43,43	2.71	4 (10%)	50,60,60	1.35	5 (10%)
29	CLA	7	608	7	59,63,73	1.90	9 (15%)	71,101,113	1.62	8 (11%)
29	CLA	6	609	35	45,49,73	2.27	10 (22%)	54,84,113	1.75	8 (14%)
29	CLA	6	605	6	59,63,73	1.88	9 (15%)	71,101,113	1.46	9 (12%)
29	CLA	A	837	10	69,73,73	1.71	9 (13%)	83,113,113	1.37	8 (9%)
29	CLA	e	608	-	45,49,73	2.27	10 (22%)	54,84,113	1.73	9 (16%)
29	CLA	A	817	10	69,73,73	1.77	9 (13%)	83,113,113	1.51	9 (10%)
29	CLA	A	802	10,29	59,63,73	1.86	9 (15%)	71,101,113	1.49	9 (12%)
37	8CT	R	201	-	40,41,41	0.19	0	50,56,56	0.42	0
30	KC2	6	613	6	49,53,53	1.84	4 (8%)	62,89,89	1.37	7 (11%)
29	CLA	5	605	5	49,53,73	2.09	9 (18%)	59,89,113	1.61	9 (15%)
37	8CT	B	850	-	40,41,41	0.37	1 (2%)	50,56,56	0.74	1 (2%)
29	CLA	2	606	-	49,53,73	2.10	9 (18%)	59,89,113	1.62	9 (15%)
29	CLA	a	602	25	59,63,73	1.92	9 (15%)	71,101,113	1.58	9 (12%)
29	CLA	8	606	8	59,63,73	1.91	9 (15%)	71,101,113	1.51	9 (12%)
34	LMG	2	617	-	36,36,55	0.85	0	44,44,63	1.21	3 (6%)
38	LMU	4	618	-	36,36,36	0.48	1 (2%)	47,47,47	0.94	3 (6%)
37	8CT	A	848	-	40,41,41	0.37	0	50,56,56	0.57	0
29	CLA	d	609	-	45,49,73	2.24	10 (22%)	54,84,113	1.71	9 (16%)
29	CLA	c	609	-	45,49,73	2.25	10 (22%)	54,84,113	1.72	9 (16%)
31	II0	7	614	-	39,43,43	2.68	4 (10%)	50,60,60	1.48	7 (14%)
29	CLA	9	603	9	49,53,73	2.12	9 (18%)	59,89,113	1.65	9 (15%)
29	CLA	b	608	-	69,73,73	1.76	9 (13%)	83,113,113	1.37	9 (10%)
31	II0	9	617	-	39,43,43	2.71	4 (10%)	50,60,60	1.45	7 (14%)
29	CLA	5	606	-	49,53,73	2.09	9 (18%)	59,89,113	1.66	10 (16%)
31	II0	a	614	-	39,43,43	2.71	4 (10%)	50,60,60	1.40	7 (14%)
37	8CT	A	852	-	40,41,41	0.24	0	50,56,56	0.64	1 (2%)
29	CLA	5	611	5	49,53,73	2.10	9 (18%)	59,89,113	1.61	8 (13%)
29	CLA	3	603	3	64,68,73	1.83	9 (14%)	77,107,113	1.47	9 (11%)
31	II0	8	612	-	39,43,43	2.69	4 (10%)	50,60,60	1.39	6 (12%)
29	CLA	1	601	1	49,53,73	2.16	9 (18%)	59,89,113	1.74	10 (16%)
29	CLA	6	603	6	49,53,73	2.16	9 (18%)	59,89,113	1.67	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	B	819	11	64,68,73	1.85	9 (14%)	77,107,113	1.54	11 (14%)
29	CLA	9	607	9	69,73,73	1.73	9 (13%)	83,113,113	1.38	10 (12%)
29	CLA	3	605	3	59,63,73	1.91	9 (15%)	71,101,113	1.54	8 (11%)
29	CLA	L	201	11	69,73,73	1.78	9 (13%)	83,113,113	1.44	11 (13%)
31	II0	9	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.44	9 (18%)
33	IHT	a	617	-	40,42,42	2.81	4 (10%)	53,58,58	2.30	17 (32%)
37	8CT	A	847	-	40,41,41	0.24	0	50,56,56	0.76	1 (2%)
29	CLA	1	605	-	45,50,73	2.15	9 (20%)	53,85,113	1.65	7 (13%)
29	CLA	c	604	-	64,68,73	1.87	9 (14%)	77,107,113	1.47	9 (11%)
29	CLA	8	602	8	49,53,73	2.11	9 (18%)	59,89,113	1.55	6 (10%)
31	II0	6	615	-	39,43,43	2.69	4 (10%)	50,60,60	1.36	6 (12%)
29	CLA	9	606	-	68,72,73	1.75	9 (13%)	81,111,113	1.44	10 (12%)
29	CLA	B	815	11	69,73,73	1.80	9 (13%)	83,113,113	1.42	9 (10%)
35	LHG	3	619	-	48,48,48	0.60	0	51,54,54	1.21	6 (11%)
29	CLA	1	603	1	56,60,73	1.97	9 (16%)	67,97,113	1.52	9 (13%)
31	II0	5	617	-	39,43,43	2.70	4 (10%)	50,60,60	1.56	8 (16%)
29	CLA	6	606	-	59,63,73	1.93	9 (15%)	71,101,113	1.57	8 (11%)
29	CLA	A	833	10	69,73,73	1.76	9 (13%)	83,113,113	1.41	8 (9%)
29	CLA	5	602	5	59,63,73	1.93	9 (15%)	71,101,113	1.53	9 (12%)
37	8CT	L	206	-	40,41,41	0.21	0	50,56,56	0.44	0
29	CLA	2	605	2	64,68,73	1.80	9 (14%)	77,107,113	1.42	8 (10%)
37	8CT	e	616	-	40,41,41	0.16	0	50,56,56	0.36	0
39	PQN	B	842	-	34,34,34	0.37	0	42,45,45	0.65	1 (2%)
31	II0	a	616	-	39,43,43	2.80	4 (10%)	50,60,60	1.54	8 (16%)
30	KC2	d	610	25	49,53,53	1.87	4 (8%)	62,89,89	1.41	6 (9%)
29	CLA	A	818	10	69,73,73	1.75	9 (13%)	83,113,113	1.41	8 (9%)
31	II0	6	616	-	39,43,43	2.71	4 (10%)	50,60,60	1.60	11 (22%)
29	CLA	L	207	-	45,49,73	2.27	10 (22%)	54,84,113	1.78	8 (14%)
29	CLA	A	805	10	54,58,73	1.99	9 (16%)	65,95,113	1.60	9 (13%)
29	CLA	d	611	-	54,58,73	2.00	9 (16%)	65,95,113	1.63	10 (15%)
29	CLA	a	609	-	64,68,73	1.81	9 (14%)	77,107,113	1.50	9 (11%)
37	8CT	A	845	-	40,41,41	0.26	0	50,56,56	0.35	0
30	KC2	Z	307	24	49,53,53	1.84	4 (8%)	62,89,89	1.38	8 (12%)
29	CLA	8	603	-	69,73,73	1.78	9 (13%)	83,113,113	1.41	8 (9%)
29	CLA	9	604	-	59,63,73	1.92	9 (15%)	71,101,113	1.49	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	5	601	5	45,49,73	2.29	10 (22%)	54,84,113	1.82	9 (16%)
29	CLA	B	828	11	69,73,73	1.75	9 (13%)	83,113,113	1.36	8 (9%)
31	II0	c	619	-	39,43,43	2.72	4 (10%)	50,60,60	1.43	8 (16%)
33	IHT	8	609	-	40,42,42	2.80	4 (10%)	53,58,58	2.35	16 (30%)
29	CLA	d	606	-	45,49,73	2.22	10 (22%)	54,84,113	1.75	11 (20%)
29	CLA	6	601	6	49,53,73	2.08	9 (18%)	59,89,113	1.63	9 (15%)
29	CLA	3	612	3	49,53,73	2.07	9 (18%)	59,89,113	1.61	8 (13%)
33	IHT	9	619	-	40,42,42	2.80	4 (10%)	53,58,58	2.44	14 (26%)
34	LMG	3	618	-	30,30,55	0.96	1 (3%)	38,38,63	1.20	5 (13%)
29	CLA	A	831	10	69,73,73	1.74	9 (13%)	83,113,113	1.35	8 (9%)
31	II0	3	616	-	39,43,43	2.70	4 (10%)	50,60,60	1.38	6 (12%)
29	CLA	8	601	8	49,53,73	2.09	9 (18%)	59,89,113	1.61	8 (13%)
37	8CT	Z	308	-	40,41,41	0.16	0	50,56,56	0.32	0
29	CLA	1	611	1	49,53,73	2.15	9 (18%)	59,89,113	1.66	8 (13%)
29	CLA	5	603	5	49,53,73	2.10	9 (18%)	59,89,113	1.63	9 (15%)
32	II3	e	613	-	40,43,43	2.00	3 (7%)	47,60,60	1.66	13 (27%)
29	CLA	4	610	4	69,73,73	1.74	9 (13%)	83,113,113	1.38	8 (9%)
35	LHG	Z	310	-	45,45,48	0.63	0	48,51,54	1.19	4 (8%)
31	II0	R	204	-	39,43,43	2.71	4 (10%)	50,60,60	1.44	8 (16%)
29	CLA	B	835	11	69,73,73	1.80	9 (13%)	83,113,113	1.52	9 (10%)
29	CLA	3	601	3	49,53,73	2.11	9 (18%)	59,89,113	1.64	8 (13%)
29	CLA	A	813	10	46,50,73	2.16	9 (19%)	55,85,113	1.73	8 (14%)
29	CLA	c	606	-	69,73,73	1.77	9 (13%)	83,113,113	1.43	10 (12%)
29	CLA	A	815	10	66,70,73	1.82	9 (13%)	79,109,113	1.39	8 (10%)
29	CLA	3	611	3	54,58,73	2.00	9 (16%)	65,95,113	1.56	9 (13%)
29	CLA	B	826	11	69,73,73	1.73	9 (13%)	83,113,113	1.38	8 (9%)
31	II0	4	613	-	39,43,43	2.71	4 (10%)	50,60,60	1.37	6 (12%)
39	PQN	A	849	-	34,34,34	0.37	0	42,45,45	0.74	1 (2%)
33	IHT	Z	302	-	40,42,42	2.83	4 (10%)	53,58,58	2.15	15 (28%)
29	CLA	A	816	10	64,68,73	1.79	9 (14%)	77,107,113	1.46	8 (10%)
29	CLA	b	604	-	69,73,73	1.77	9 (13%)	83,113,113	1.37	9 (10%)
29	CLA	A	838	-	69,73,73	1.76	9 (13%)	83,113,113	1.38	8 (9%)
33	IHT	c	620	-	40,42,42	2.76	4 (10%)	53,58,58	2.17	15 (28%)
29	CLA	A	810	10	69,73,73	1.74	9 (13%)	83,113,113	1.40	11 (13%)
29	CLA	B	837	-	69,73,73	1.78	9 (13%)	83,113,113	1.36	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	IHT	L	205	-	40,42,42	2.85	4 (10%)	53,58,58	2.24	16 (30%)
29	CLA	7	612	7	54,58,73	2.00	9 (16%)	65,95,113	1.59	9 (13%)
29	CLA	B	831	11	59,63,73	1.94	9 (15%)	71,101,113	1.61	10 (14%)
35	LHG	8	613	-	32,32,48	0.76	1 (3%)	35,38,54	1.18	2 (5%)
29	CLA	1	613	-	49,53,73	2.15	9 (18%)	59,89,113	1.68	10 (16%)
29	CLA	A	804	10	69,73,73	1.76	9 (13%)	83,113,113	1.39	10 (12%)
29	CLA	A	832	-	69,73,73	1.75	9 (13%)	83,113,113	1.36	8 (9%)
29	CLA	B	806	11	69,73,73	1.75	9 (13%)	83,113,113	1.41	11 (13%)
31	II0	5	620	-	39,43,43	2.75	4 (10%)	50,60,60	1.55	8 (16%)
34	LMG	6	619	-	32,32,55	0.97	1 (3%)	40,40,63	1.22	4 (10%)
29	CLA	6	608	6	64,68,73	1.82	9 (14%)	77,107,113	1.49	10 (12%)
29	CLA	4	606	4	64,68,73	1.85	9 (14%)	77,107,113	1.44	9 (11%)
29	CLA	B	830	11	64,68,73	1.82	9 (14%)	77,107,113	1.47	8 (10%)
31	II0	9	616	-	39,43,43	2.70	4 (10%)	50,60,60	1.37	9 (18%)
29	CLA	A	825	10	69,73,73	1.76	9 (13%)	83,113,113	1.39	10 (12%)
29	CLA	A	811	10	69,73,73	1.79	9 (13%)	83,113,113	1.45	8 (9%)
41	DGD	Z	303	-	61,61,67	0.95	3 (4%)	75,75,81	1.36	8 (10%)
33	IHT	d	617	-	40,42,42	2.75	4 (10%)	53,58,58	2.25	15 (28%)
29	CLA	A	830	10	64,68,73	1.83	9 (14%)	77,107,113	1.45	8 (10%)
29	CLA	9	613	9	49,53,73	2.12	9 (18%)	59,89,113	1.61	9 (15%)
29	CLA	7	611	-	59,63,73	1.92	9 (15%)	71,101,113	1.50	8 (11%)
29	CLA	R	202	-	59,63,73	1.92	9 (15%)	71,101,113	1.65	11 (15%)
29	CLA	6	611	-	59,63,73	1.90	9 (15%)	71,101,113	1.53	10 (14%)
29	CLA	8	605	8	54,58,73	2.00	9 (16%)	65,95,113	1.65	11 (16%)
35	LHG	c	621	-	28,28,48	0.78	0	31,34,54	1.26	3 (9%)
31	II0	4	612	-	39,43,43	2.68	4 (10%)	50,60,60	1.42	8 (16%)
29	CLA	e	603	28	54,58,73	2.02	9 (16%)	65,95,113	1.61	8 (12%)
29	CLA	B	824	-	64,68,73	1.84	9 (14%)	77,107,113	1.51	9 (11%)
34	LMG	F	205	-	32,32,55	0.84	0	40,40,63	1.29	6 (15%)
31	II0	2	615	-	39,43,43	2.73	4 (10%)	50,60,60	1.57	10 (20%)
29	CLA	2	603	2	54,58,73	2.01	9 (16%)	65,95,113	1.56	10 (15%)
29	CLA	1	608	1	64,68,73	1.83	9 (14%)	77,107,113	1.48	9 (11%)
31	II0	d	613	-	39,43,43	2.69	4 (10%)	50,60,60	1.38	6 (12%)
30	KC2	3	606	35	49,53,53	1.83	4 (8%)	62,89,89	1.43	9 (14%)
29	CLA	A	824	-	69,73,73	1.78	9 (13%)	83,113,113	1.40	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	3	609	-	69,73,73	1.75	9 (13%)	83,113,113	1.34	7 (8%)
30	KC2	7	606	-	49,53,53	1.87	4 (8%)	62,89,89	1.45	8 (12%)
38	LMU	e	617	-	32,32,36	0.40	0	43,43,47	1.05	2 (4%)
29	CLA	9	614	-	45,49,73	2.30	10 (22%)	54,84,113	1.80	9 (16%)
29	CLA	B	808	11	69,73,73	1.73	9 (13%)	83,113,113	1.35	8 (9%)
31	II0	B	843	-	39,43,43	2.73	4 (10%)	50,60,60	1.37	5 (10%)
33	IHT	2	616	-	40,42,42	2.86	4 (10%)	53,58,58	2.27	17 (32%)
35	LHG	4	617	29	46,46,48	0.61	0	49,52,54	1.19	4 (8%)
29	CLA	A	836	10	59,63,73	1.89	9 (15%)	71,101,113	1.49	8 (11%)
29	CLA	B	811	11	59,63,73	1.90	9 (15%)	71,101,113	1.52	8 (11%)
35	LHG	5	619	-	22,22,48	0.88	1 (4%)	25,28,54	1.32	3 (12%)
29	CLA	A	821	10	59,63,73	1.89	9 (15%)	71,101,113	1.57	9 (12%)
29	CLA	1	602	1	63,67,73	1.85	9 (14%)	75,105,113	1.49	10 (13%)
29	CLA	A	808	10	59,63,73	1.89	9 (15%)	71,101,113	1.53	10 (14%)
29	CLA	A	822	10	69,73,73	1.76	9 (13%)	83,113,113	1.40	9 (10%)
29	CLA	d	607	25	69,73,73	1.75	9 (13%)	83,113,113	1.42	10 (12%)
37	8CT	F	201	-	40,41,41	0.46	1 (2%)	50,56,56	0.48	0
31	II0	a	619	-	39,43,43	2.69	4 (10%)	50,60,60	1.40	8 (16%)
37	8CT	B	847	-	40,41,41	0.16	0	50,56,56	0.49	0
29	CLA	4	604	-	59,63,73	1.91	9 (15%)	71,101,113	1.47	8 (11%)
29	CLA	F	203	-	49,53,73	2.09	9 (18%)	59,89,113	1.60	8 (13%)
29	CLA	2	607	2	49,53,73	2.09	9 (18%)	59,89,113	1.66	10 (16%)
35	LHG	7	619	29	38,38,48	0.65	0	41,44,54	1.16	3 (7%)
29	CLA	A	803	10	69,73,73	1.74	9 (13%)	83,113,113	1.45	10 (12%)
29	CLA	A	801	-	69,73,73	1.71	8 (11%)	83,113,113	1.35	10 (12%)
30	KC2	e	609	-	49,53,53	1.86	4 (8%)	62,89,89	1.38	7 (11%)
29	CLA	e	611	28	69,73,73	1.78	9 (13%)	83,113,113	1.36	10 (12%)
29	CLA	6	604	6	64,68,73	1.85	9 (14%)	77,107,113	1.47	9 (11%)
35	LHG	B	849	29	44,44,48	0.66	1 (2%)	47,50,54	1.20	5 (10%)
29	CLA	7	603	7	59,63,73	1.92	9 (15%)	71,101,113	1.52	9 (12%)
31	II0	7	613	-	39,43,43	2.67	4 (10%)	50,60,60	1.44	8 (16%)
31	II0	1	616	-	39,43,43	2.67	4 (10%)	50,60,60	1.46	8 (16%)
29	CLA	A	827	-	69,73,73	1.73	9 (13%)	83,113,113	1.36	9 (10%)
29	CLA	4	601	4	59,63,73	1.89	9 (15%)	71,101,113	1.47	9 (12%)
29	CLA	a	608	25	64,68,73	1.82	9 (14%)	77,107,113	1.49	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	8CT	B	844	-	40,41,41	0.23	0	50,56,56	0.62	0
29	CLA	b	603	26	64,68,73	1.83	9 (14%)	77,107,113	1.48	9 (11%)
29	CLA	3	604	-	69,73,73	1.77	9 (13%)	83,113,113	1.39	8 (9%)
29	CLA	A	842	10	69,73,73	1.77	9 (13%)	83,113,113	1.44	10 (12%)
38	LMU	7	620	-	36,36,36	0.39	0	47,47,47	1.05	3 (6%)
31	II0	8	610	-	39,43,43	2.78	4 (10%)	50,60,60	1.51	9 (18%)
29	CLA	A	812	10	59,63,73	1.89	9 (15%)	71,101,113	1.54	11 (15%)
29	CLA	2	608	2	64,68,73	1.83	9 (14%)	77,107,113	1.48	9 (11%)
29	CLA	d	603	25	54,58,73	2.00	9 (16%)	65,95,113	1.57	9 (13%)
29	CLA	d	604	-	64,68,73	1.87	9 (14%)	77,107,113	1.48	8 (10%)
29	CLA	5	609	-	45,49,73	2.26	10 (22%)	54,84,113	1.71	8 (14%)
29	CLA	9	609	-	45,49,73	2.26	10 (22%)	54,84,113	1.74	11 (20%)
30	KC2	e	605	28	49,53,53	1.86	4 (8%)	62,89,89	1.38	8 (12%)
31	II0	8	611	-	39,43,43	2.76	4 (10%)	50,60,60	1.39	7 (14%)
35	LHG	A	850	-	48,48,48	0.60	0	51,54,54	1.15	4 (7%)
29	CLA	3	607	3	64,68,73	1.83	9 (14%)	77,107,113	1.44	9 (11%)
29	CLA	O	201	-	59,63,73	1.89	9 (15%)	71,101,113	1.54	10 (14%)
29	CLA	2	602	2	63,67,73	1.86	9 (14%)	75,105,113	1.59	12 (16%)
37	8CT	7	617	-	40,41,41	0.40	1 (2%)	50,56,56	0.58	0
29	CLA	B	827	-	69,73,73	1.75	9 (13%)	83,113,113	1.40	8 (9%)
29	CLA	4	607	4	64,68,73	1.83	9 (14%)	77,107,113	1.47	10 (12%)
29	CLA	A	823	-	69,73,73	1.77	9 (13%)	83,113,113	1.36	9 (10%)
29	CLA	B	838	-	69,73,73	1.77	9 (13%)	83,113,113	1.43	11 (13%)
29	CLA	B	803	-	69,73,73	1.75	9 (13%)	83,113,113	1.34	11 (13%)
29	CLA	d	601	25	49,53,73	2.10	9 (18%)	59,89,113	1.64	8 (13%)
29	CLA	7	605	7	49,53,73	2.13	9 (18%)	59,89,113	1.65	8 (13%)
35	LHG	L	208	-	33,33,48	0.74	1 (3%)	36,39,54	1.19	2 (5%)
29	CLA	A	828	10	69,73,73	1.76	9 (13%)	83,113,113	1.35	8 (9%)
29	CLA	A	844	-	69,73,73	1.67	9 (13%)	83,113,113	1.45	9 (10%)
31	II0	e	615	-	39,43,43	2.71	4 (10%)	50,60,60	1.42	7 (14%)
29	CLA	1	612	1	64,68,73	1.81	9 (14%)	77,107,113	1.40	9 (11%)
29	CLA	b	611	26	59,63,73	1.88	9 (15%)	71,101,113	1.50	9 (12%)
29	CLA	8	608	-	69,73,73	1.78	9 (13%)	83,113,113	1.39	8 (9%)
29	CLA	B	829	11	49,53,73	2.13	9 (18%)	59,89,113	1.76	10 (16%)
29	CLA	K	102	18	59,63,73	1.92	9 (15%)	71,101,113	1.52	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	KC2	c	615	-	49,53,53	1.85	4 (8%)	62,89,89	1.39	8 (12%)
29	CLA	e	606	28	64,68,73	1.82	9 (14%)	77,107,113	1.40	10 (12%)
29	CLA	B	809	11	69,73,73	1.72	9 (13%)	83,113,113	1.36	8 (9%)
29	CLA	5	604	5	59,63,73	1.95	9 (15%)	71,101,113	1.55	8 (11%)
29	CLA	A	835	10	64,68,73	1.82	9 (14%)	77,107,113	1.44	8 (10%)
29	CLA	B	841	-	56,60,73	1.95	9 (16%)	67,97,113	1.55	9 (13%)
37	8CT	R	203	-	40,41,41	0.18	0	50,56,56	0.55	1 (2%)
29	CLA	7	607	7	49,53,73	2.12	9 (18%)	59,89,113	1.68	9 (15%)
29	CLA	A	806	10	69,73,73	1.75	9 (13%)	83,113,113	1.38	9 (10%)
31	II0	d	616	-	39,43,43	2.69	4 (10%)	50,60,60	1.65	11 (22%)
29	CLA	B	822	11	69,73,73	1.73	9 (13%)	83,113,113	1.40	10 (12%)
37	8CT	Z	309	-	40,41,41	0.24	0	50,56,56	0.67	1 (2%)
29	CLA	5	608	-	64,68,73	1.84	9 (14%)	77,107,113	1.61	10 (12%)
29	CLA	9	608	9	59,63,73	1.91	9 (15%)	71,101,113	1.56	10 (14%)
31	II0	7	615	-	39,43,43	2.74	4 (10%)	50,60,60	1.45	10 (20%)
30	KC2	c	610	27	49,53,53	1.82	4 (8%)	62,89,89	1.41	9 (14%)
29	CLA	3	608	3	64,68,73	1.85	9 (14%)	77,107,113	1.47	9 (11%)
31	II0	3	615	-	39,43,43	2.72	4 (10%)	50,60,60	1.38	7 (14%)
31	II0	1	617	-	39,43,43	2.73	4 (10%)	50,60,60	1.45	9 (18%)
29	CLA	c	612	27	59,63,73	1.89	9 (15%)	71,101,113	1.60	11 (15%)
29	CLA	A	820	10	69,73,73	1.78	9 (13%)	83,113,113	1.38	8 (9%)
29	CLA	A	819	-	69,73,73	1.77	9 (13%)	83,113,113	1.44	10 (12%)
29	CLA	e	601	28	49,53,73	2.10	9 (18%)	59,89,113	1.64	8 (13%)
29	CLA	B	812	11	69,73,73	1.75	9 (13%)	83,113,113	1.41	10 (12%)
29	CLA	2	604	2	59,63,73	1.93	9 (15%)	71,101,113	1.50	9 (12%)
31	II0	J	101	-	39,43,43	2.71	4 (10%)	50,60,60	1.47	9 (18%)
29	CLA	2	612	2	49,53,73	2.08	9 (18%)	59,89,113	1.66	8 (13%)
29	CLA	9	602	9	59,63,73	1.92	9 (15%)	71,101,113	1.57	10 (14%)
29	CLA	B	814	-	46,50,73	2.18	9 (19%)	55,85,113	1.73	9 (16%)
29	CLA	J	102	17	45,49,73	2.29	10 (22%)	54,84,113	1.75	10 (18%)
30	KC2	1	610	1	49,53,53	1.87	4 (8%)	62,89,89	1.36	7 (11%)
29	CLA	8	615	-	69,73,73	1.77	9 (13%)	83,113,113	1.40	10 (12%)
31	II0	1	614	-	39,43,43	2.71	4 (10%)	50,60,60	1.39	6 (12%)
29	CLA	a	603	25	64,68,73	1.83	9 (14%)	77,107,113	1.45	9 (11%)
29	CLA	7	602	7	69,73,73	1.78	9 (13%)	83,113,113	1.43	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	b	602	26	68,72,73	1.80	9 (13%)	81,111,113	1.50	11 (13%)
31	II0	a	613	-	39,43,43	2.70	4 (10%)	50,60,60	1.41	8 (16%)
29	CLA	1	609	-	45,49,73	2.26	10 (22%)	54,84,113	1.74	8 (14%)
35	LHG	2	618	-	21,21,48	0.76	0	23,26,54	1.24	2 (8%)
31	II0	8	616	-	39,43,43	2.63	4 (10%)	50,60,60	1.56	7 (14%)
30	KC2	9	610	9	49,53,53	1.85	4 (8%)	62,89,89	1.39	9 (14%)
29	CLA	d	608	25	69,73,73	1.78	9 (13%)	83,113,113	1.44	10 (12%)
32	II3	1	615	-	40,43,43	2.01	3 (7%)	47,60,60	1.61	12 (25%)
29	CLA	A	841	-	69,73,73	1.75	9 (13%)	83,113,113	1.39	9 (10%)
29	CLA	7	601	7	49,53,73	2.09	9 (18%)	59,89,113	1.62	8 (13%)
29	CLA	4	603	4	58,62,73	1.94	9 (15%)	69,99,113	1.56	8 (11%)
31	II0	9	618	-	39,43,43	2.69	4 (10%)	50,60,60	1.37	8 (16%)
31	II0	1	619	-	39,43,43	2.78	4 (10%)	50,60,60	1.53	11 (22%)
37	8CT	J	103	-	40,41,41	0.19	0	50,56,56	0.39	0
29	CLA	a	601	25	49,53,73	2.09	9 (18%)	59,89,113	1.64	8 (13%)
29	CLA	6	612	-	49,53,73	2.07	9 (18%)	59,89,113	1.63	8 (13%)
35	LHG	2	620	-	41,41,48	0.65	0	44,47,54	1.20	3 (6%)
31	II0	5	616	-	39,43,43	2.74	4 (10%)	50,60,60	1.44	9 (18%)
33	IHT	1	618	-	40,42,42	2.84	4 (10%)	53,58,58	2.09	14 (26%)
29	CLA	B	804	-	49,53,73	2.08	9 (18%)	59,89,113	1.60	9 (15%)
29	CLA	B	813	11	65,69,73	1.77	9 (13%)	78,108,113	1.45	9 (11%)
29	CLA	F	202	-	64,68,73	1.84	9 (14%)	77,107,113	1.44	10 (12%)
29	CLA	a	612	25	69,73,73	1.73	9 (13%)	83,113,113	1.38	9 (10%)
29	CLA	d	602	25	68,72,73	1.79	9 (13%)	81,111,113	1.46	11 (13%)
29	CLA	c	602	27	69,73,73	1.78	9 (13%)	83,113,113	1.42	9 (10%)
34	LMG	I	102	-	51,51,55	0.71	0	59,59,63	1.30	6 (10%)
29	CLA	L	203	-	64,68,73	1.85	9 (14%)	77,107,113	1.47	10 (12%)
30	KC2	a	610	-	49,53,53	1.86	4 (8%)	62,89,89	1.35	7 (11%)
29	CLA	F	204	15	59,63,73	1.90	9 (15%)	71,101,113	1.49	9 (12%)
29	CLA	B	818	-	64,68,73	1.82	9 (14%)	77,107,113	1.47	8 (10%)
29	CLA	b	601	26	49,53,73	2.09	9 (18%)	59,89,113	1.65	8 (13%)
30	KC2	2	610	2	49,53,53	1.86	4 (8%)	62,89,89	1.37	7 (11%)
31	II0	7	616	-	39,43,43	2.70	4 (10%)	50,60,60	1.46	9 (18%)
35	LHG	3	623	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
29	CLA	B	810	-	64,68,73	1.79	9 (14%)	77,107,113	1.47	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	1	604	1	49,53,73	2.15	9 (18%)	59,89,113	1.63	9 (15%)
29	CLA	b	610	26	55,59,73	2.00	9 (16%)	66,96,113	1.60	9 (13%)
29	CLA	a	611	-	59,63,73	1.92	9 (15%)	71,101,113	1.52	9 (12%)
30	KC2	4	605	4	49,53,53	1.86	4 (8%)	62,89,89	1.39	7 (11%)
29	CLA	A	840	-	59,63,73	1.85	9 (15%)	71,101,113	1.55	8 (11%)
38	LMU	J	104	-	32,32,36	0.41	0	43,43,47	1.04	2 (4%)
37	8CT	A	846	-	40,41,41	0.16	0	50,56,56	0.35	0
29	CLA	B	832	-	69,73,73	1.75	9 (13%)	83,113,113	1.38	9 (10%)
31	II0	3	613	-	39,43,43	2.67	4 (10%)	50,60,60	1.34	6 (12%)
29	CLA	6	607	6	59,63,73	1.89	9 (15%)	71,101,113	1.49	9 (12%)
31	II0	6	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.44	8 (16%)
29	CLA	A	826	10	69,73,73	1.72	9 (13%)	83,113,113	1.35	9 (10%)
29	CLA	b	606	26	69,73,73	1.76	9 (13%)	83,113,113	1.37	8 (9%)
32	II3	b	613	-	40,43,43	2.02	3 (7%)	47,60,60	1.68	14 (29%)

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
31	II0	4	615	-	-	1/21/67/67	0/2/2/2
31	II0	O	205	-	-	1/21/67/67	0/2/2/2
36	SQD	O	206	-	-	11/24/44/69	0/1/1/1
29	CLA	L	204	-	-	7/21/97/115	-
29	CLA	Z	305	24	-	3/21/97/115	-
31	II0	3	614	-	-	0/21/67/67	0/2/2/2
29	CLA	4	608	35	-	4/39/115/115	-
37	8CT	b	615	-	-	6/29/63/63	0/2/2/2
29	CLA	5	612	5	-	5/15/91/115	-
29	CLA	d	605	25	-	5/15/91/115	-
29	CLA	B	823	-	-	11/39/115/115	-
31	II0	5	614	-	-	2/21/67/67	0/2/2/2
29	CLA	c	607	27	-	11/39/115/115	-
29	CLA	Z	304	24	-	3/27/103/115	-
35	LHG	b	616	-	-	27/53/53/53	-
29	CLA	c	605	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	KC2	7	610	7	-	6/15/71/71	-
30	KC2	6	610	6	-	6/15/71/71	-
29	CLA	4	602	4	-	3/32/108/115	-
36	SQD	3	621	-	-	16/37/57/69	0/1/1/1
40	SF4	C	101	12	-	-	0/6/5/5
29	CLA	K	101	-	-	8/39/115/115	-
29	CLA	1	607	1	-	0/15/91/115	-
29	CLA	B	834	11	-	3/27/103/115	-
29	CLA	7	609	35	-	2/10/86/115	-
29	CLA	9	612	-	-	3/15/91/115	-
29	CLA	B	802	-	-	6/39/115/115	-
29	CLA	B	820	11	-	11/33/109/115	-
35	LHG	A	851	-	-	21/43/43/53	-
30	KC2	c	611	27	-	5/15/71/71	-
37	8CT	I	101	-	-	3/29/63/63	0/2/2/2
29	CLA	4	611	4	-	11/39/115/115	-
29	CLA	A	814	-	-	5/15/91/115	-
29	CLA	9	605	-	-	0/15/91/115	-
35	LHG	d	618	-	-	8/26/26/53	-
29	CLA	O	202	21	-	9/27/103/115	-
35	LHG	2	619	-	-	18/43/43/53	-
29	CLA	Z	301	-	-	13/33/109/115	-
29	CLA	9	611	9	-	3/10/86/115	-
34	LMG	3	620	-	-	12/27/47/70	0/1/1/1
29	CLA	8	604	8	-	7/39/115/115	-
29	CLA	B	839	35	-	5/39/115/115	-
29	CLA	B	816	11	-	14/32/108/115	-
29	CLA	L	202	19	-	1/23/99/115	-
29	CLA	3	602	3	-	4/27/103/115	-
31	II0	c	617	-	-	0/21/67/67	0/2/2/2
29	CLA	6	602	6	-	7/39/115/115	-
29	CLA	d	612	-	-	5/37/113/115	-
29	CLA	e	604	-	-	3/33/109/115	-
37	8CT	B	845	-	-	8/29/63/63	0/2/2/2
29	CLA	3	610	3	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LMU	O	207	-	-	9/16/56/61	0/2/2/2
31	II0	d	615	-	-	2/21/67/67	0/2/2/2
35	LHG	7	618	-	-	9/35/35/53	-
31	II0	c	616	-	-	2/21/67/67	0/2/2/2
41	DGD	B	848	-	-	17/48/88/95	0/2/2/2
31	II0	5	615	-	-	2/21/67/67	0/2/2/2
31	II0	2	614	-	-	0/21/67/67	0/2/2/2
29	CLA	c	601	27	-	2/15/91/115	-
29	CLA	2	609	-	-	1/10/86/115	-
29	CLA	B	807	11	-	7/39/115/115	-
30	KC2	5	610	5	-	4/15/71/71	-
29	CLA	5	613	5	-	3/10/86/115	-
31	II0	b	614	-	-	1/21/67/67	0/2/2/2
29	CLA	7	604	7	-	8/25/101/115	-
31	II0	c	618	-	-	2/21/67/67	0/2/2/2
37	8CT	B	851	-	-	9/29/63/63	0/2/2/2
29	CLA	b	607	26	-	7/33/109/115	-
29	CLA	A	807	10	-	2/21/97/115	-
33	IHT	K	104	-	-	2/25/65/65	0/2/2/2
29	CLA	e	607	28	-	3/15/91/115	-
29	CLA	A	839	-	-	12/39/115/115	-
29	CLA	a	604	25	-	13/33/109/115	-
31	II0	e	614	-	-	1/21/67/67	0/2/2/2
37	8CT	K	103	-	-	2/29/63/63	0/2/2/2
29	CLA	A	843	10	-	10/39/115/115	-
40	SF4	C	102	12	-	-	0/6/5/5
30	KC2	b	609	-	-	2/15/71/71	-
29	CLA	c	603	27	-	14/39/115/115	-
30	KC2	b	605	26	-	7/15/71/71	-
29	CLA	B	840	11	-	2/39/115/115	-
37	8CT	B	846	-	-	8/29/63/63	0/2/2/2
29	CLA	B	825	11	-	4/39/115/115	-
29	CLA	B	817	11	-	1/33/109/115	-
35	LHG	a	618	-	-	17/33/33/53	-
29	CLA	a	605	25	-	13/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	9	601	9	-	6/15/91/115	-
29	CLA	B	836	11	-	3/18/94/115	-
31	II0	4	614	-	-	1/21/67/67	0/2/2/2
35	LHG	6	618	29	-	15/39/39/53	-
31	II0	2	613	-	-	2/21/67/67	0/2/2/2
29	CLA	B	805	11	-	11/39/115/115	-
29	CLA	1	606	-	-	0/15/91/115	-
29	CLA	A	829	10	-	8/21/97/115	-
37	8CT	4	616	-	-	5/29/63/63	0/2/2/2
35	LHG	4	619	-	-	17/49/49/53	-
29	CLA	8	607	8	-	3/10/86/115	-
33	IHT	5	618	-	-	1/25/65/65	0/2/2/2
29	CLA	A	809	29	-	6/33/109/115	-
29	CLA	B	833	-	-	3/15/91/115	-
29	CLA	c	608	27	-	9/33/109/115	-
31	II0	b	612	-	-	1/21/67/67	0/2/2/2
31	II0	O	204	-	-	2/21/67/67	0/2/2/2
37	8CT	M	101	-	-	5/29/63/63	0/2/2/2
29	CLA	O	203	-	-	10/27/103/115	-
31	II0	a	615	-	-	1/21/67/67	0/2/2/2
29	CLA	2	601	2	-	5/12/88/115	-
29	CLA	2	611	-	-	2/15/91/115	-
35	LHG	3	622	30	-	13/38/38/53	-
40	SF4	B	801	10,11	-	-	0/6/5/5
34	LMG	8	614	-	-	23/47/67/70	0/1/1/1
29	CLA	a	606	-	-	7/39/115/115	-
29	CLA	A	834	10	-	7/27/103/115	-
29	CLA	5	607	5	-	2/15/91/115	-
29	CLA	4	609	4	-	5/33/109/115	-
33	IHT	6	617	-	-	3/25/65/65	0/2/2/2
29	CLA	e	602	28	-	10/27/103/115	-
29	CLA	Z	306	24	-	13/33/109/115	-
31	II0	d	614	-	-	2/21/67/67	0/2/2/2
29	CLA	e	610	-	-	6/23/99/115	-
29	CLA	c	614	-	-	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	a	607	25	-	4/39/115/115	-
29	CLA	c	613	27	-	9/15/91/115	-
31	II0	e	612	-	-	0/21/67/67	0/2/2/2
29	CLA	B	821	-	-	11/33/109/115	-
35	LHG	d	619	-	-	20/43/43/53	-
31	II0	3	617	-	-	2/21/67/67	0/2/2/2
29	CLA	7	608	7	-	12/27/103/115	-
29	CLA	6	609	35	-	2/10/86/115	-
29	CLA	6	605	6	-	7/27/103/115	-
29	CLA	A	837	10	-	12/39/115/115	-
29	CLA	e	608	-	-	2/10/86/115	-
29	CLA	A	817	10	-	13/39/115/115	-
29	CLA	A	802	10,29	-	5/27/103/115	-
37	8CT	R	201	-	-	7/29/63/63	0/2/2/2
30	KC2	6	613	6	-	7/15/71/71	-
29	CLA	5	605	5	-	4/15/91/115	-
37	8CT	B	850	-	-	4/29/63/63	0/2/2/2
29	CLA	2	606	-	-	1/15/91/115	-
29	CLA	a	602	25	-	10/27/103/115	-
29	CLA	8	606	8	-	4/27/103/115	-
34	LMG	2	617	-	-	8/31/51/70	0/1/1/1
38	LMU	4	618	-	-	12/21/61/61	0/2/2/2
37	8CT	A	848	-	-	0/29/63/63	0/2/2/2
29	CLA	d	609	-	-	0/10/86/115	-
29	CLA	c	609	-	-	2/10/86/115	-
31	II0	7	614	-	-	1/21/67/67	0/2/2/2
29	CLA	9	603	9	-	6/15/91/115	-
29	CLA	b	608	-	-	12/39/115/115	-
31	II0	9	617	-	-	2/21/67/67	0/2/2/2
29	CLA	5	606	-	-	5/15/91/115	-
31	II0	a	614	-	-	1/21/67/67	0/2/2/2
37	8CT	A	852	-	-	6/29/63/63	0/2/2/2
29	CLA	5	611	5	-	8/15/91/115	-
29	CLA	3	603	3	-	4/33/109/115	-
31	II0	8	612	-	-	1/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	1	601	1	-	6/15/91/115	-
29	CLA	6	603	6	-	7/15/91/115	-
29	CLA	B	819	11	-	9/33/109/115	-
29	CLA	9	607	9	-	11/39/115/115	-
29	CLA	3	605	3	-	4/27/103/115	-
29	CLA	L	201	11	-	10/39/115/115	-
31	II0	9	615	-	-	2/21/67/67	0/2/2/2
33	IHT	a	617	-	-	4/25/65/65	0/2/2/2
37	8CT	A	847	-	-	8/29/63/63	0/2/2/2
29	CLA	1	605	-	-	3/11/87/115	-
29	CLA	c	604	-	-	5/33/109/115	-
29	CLA	8	602	8	-	4/15/91/115	-
31	II0	6	615	-	-	2/21/67/67	0/2/2/2
29	CLA	9	606	-	-	11/38/114/115	-
29	CLA	B	815	11	-	10/39/115/115	-
35	LHG	3	619	-	-	23/53/53/53	-
29	CLA	1	603	1	-	6/24/100/115	-
31	II0	5	617	-	-	2/21/67/67	0/2/2/2
29	CLA	6	606	-	-	8/27/103/115	-
29	CLA	A	833	10	-	8/39/115/115	-
29	CLA	5	602	5	-	7/27/103/115	-
37	8CT	L	206	-	-	3/29/63/63	0/2/2/2
29	CLA	2	605	2	-	7/33/109/115	-
37	8CT	e	616	-	-	1/29/63/63	0/2/2/2
39	PQN	B	842	-	-	5/23/43/43	0/2/2/2
31	II0	a	616	-	-	1/21/67/67	0/2/2/2
30	KC2	d	610	25	-	5/15/71/71	-
29	CLA	A	818	10	-	9/39/115/115	-
31	II0	6	616	-	-	2/21/67/67	0/2/2/2
29	CLA	L	207	-	-	4/10/86/115	-
29	CLA	A	805	10	-	3/21/97/115	-
29	CLA	d	611	-	-	7/21/97/115	-
29	CLA	a	609	-	-	8/33/109/115	-
37	8CT	A	845	-	-	1/29/63/63	0/2/2/2
30	KC2	Z	307	24	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	8	603	-	-	11/39/115/115	-
29	CLA	9	604	-	-	3/27/103/115	-
29	CLA	5	601	5	-	2/10/86/115	-
29	CLA	B	828	11	-	10/39/115/115	-
31	II0	c	619	-	-	2/21/67/67	0/2/2/2
33	IHT	8	609	-	-	1/25/65/65	0/2/2/2
29	CLA	d	606	-	-	1/10/86/115	-
29	CLA	6	601	6	-	4/15/91/115	-
29	CLA	3	612	3	-	6/15/91/115	-
33	IHT	9	619	-	-	4/25/65/65	0/2/2/2
34	LMG	3	618	-	-	10/25/45/70	0/1/1/1
29	CLA	A	831	10	-	11/39/115/115	-
31	II0	3	616	-	-	2/21/67/67	0/2/2/2
29	CLA	8	601	8	-	2/15/91/115	-
37	8CT	Z	308	-	-	4/29/63/63	0/2/2/2
29	CLA	1	611	1	-	3/15/91/115	-
29	CLA	5	603	5	-	3/15/91/115	-
32	II3	e	613	-	-	3/25/67/67	0/2/2/2
29	CLA	4	610	4	-	7/39/115/115	-
35	LHG	Z	310	-	-	23/50/50/53	-
31	II0	R	204	-	-	1/21/67/67	0/2/2/2
29	CLA	B	835	11	-	8/39/115/115	-
29	CLA	3	601	3	-	5/15/91/115	-
29	CLA	A	813	10	-	0/12/88/115	-
29	CLA	c	606	-	-	14/39/115/115	-
29	CLA	A	815	10	-	2/36/112/115	-
29	CLA	3	611	3	-	4/21/97/115	-
29	CLA	B	826	11	-	12/39/115/115	-
31	II0	4	613	-	-	0/21/67/67	0/2/2/2
39	PQN	A	849	-	-	11/23/43/43	0/2/2/2
33	IHT	Z	302	-	-	2/25/65/65	0/2/2/2
29	CLA	A	816	10	-	9/33/109/115	-
29	CLA	b	604	-	-	17/39/115/115	-
29	CLA	A	838	-	-	7/39/115/115	-
33	IHT	c	620	-	-	1/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	810	10	-	20/39/115/115	-
29	CLA	B	837	-	-	6/39/115/115	-
33	IHT	L	205	-	-	2/25/65/65	0/2/2/2
29	CLA	7	612	7	-	8/21/97/115	-
29	CLA	B	831	11	-	10/27/103/115	-
35	LHG	8	613	-	-	23/37/37/53	-
29	CLA	1	613	-	-	6/15/91/115	-
29	CLA	A	804	10	-	15/39/115/115	-
29	CLA	A	832	-	-	8/39/115/115	-
29	CLA	B	806	11	-	12/39/115/115	-
31	II0	5	620	-	-	1/21/67/67	0/2/2/2
34	LMG	6	619	-	-	5/27/47/70	0/1/1/1
29	CLA	6	608	6	-	7/33/109/115	-
29	CLA	4	606	4	-	8/33/109/115	-
29	CLA	B	830	11	-	1/33/109/115	-
31	II0	9	616	-	-	2/21/67/67	0/2/2/2
29	CLA	A	825	10	-	9/39/115/115	-
29	CLA	A	811	10	-	13/39/115/115	-
41	DGD	Z	303	-	-	27/49/89/95	0/2/2/2
33	IHT	d	617	-	-	1/25/65/65	0/2/2/2
29	CLA	A	830	10	-	5/33/109/115	-
29	CLA	9	613	9	-	5/15/91/115	-
29	CLA	7	611	-	-	5/27/103/115	-
29	CLA	R	202	-	-	10/27/103/115	-
29	CLA	6	611	-	-	3/27/103/115	-
29	CLA	8	605	8	-	3/21/97/115	-
35	LHG	c	621	-	-	16/33/33/53	-
31	II0	4	612	-	-	2/21/67/67	0/2/2/2
29	CLA	e	603	28	-	6/21/97/115	-
29	CLA	B	824	-	-	5/33/109/115	-
34	LMG	F	205	-	-	13/27/47/70	0/1/1/1
31	II0	2	615	-	-	2/21/67/67	0/2/2/2
29	CLA	2	603	2	-	5/21/97/115	-
29	CLA	1	608	1	-	5/33/109/115	-
31	II0	d	613	-	-	2/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	KC2	3	606	35	-	9/15/71/71	-
29	CLA	A	824	-	-	7/39/115/115	-
29	CLA	3	609	-	-	3/39/115/115	-
30	KC2	7	606	-	-	8/15/71/71	-
38	LMU	e	617	-	-	8/17/57/61	0/2/2/2
29	CLA	9	614	-	-	3/10/86/115	-
29	CLA	B	808	11	-	13/39/115/115	-
31	II0	B	843	-	-	2/21/67/67	0/2/2/2
33	IHT	2	616	-	-	2/25/65/65	0/2/2/2
35	LHG	4	617	29	-	18/51/51/53	-
29	CLA	A	836	10	-	2/27/103/115	-
29	CLA	B	811	11	-	9/27/103/115	-
35	LHG	5	619	-	-	14/26/26/53	-
29	CLA	A	821	10	-	3/27/103/115	-
29	CLA	1	602	1	-	6/32/108/115	-
29	CLA	A	808	10	-	1/27/103/115	-
29	CLA	A	822	10	-	10/39/115/115	-
29	CLA	d	607	25	-	8/39/115/115	-
37	8CT	F	201	-	-	3/29/63/63	0/2/2/2
31	II0	a	619	-	-	1/21/67/67	0/2/2/2
37	8CT	B	847	-	-	3/29/63/63	0/2/2/2
29	CLA	4	604	-	-	11/27/103/115	-
29	CLA	F	203	-	-	3/15/91/115	-
29	CLA	2	607	2	-	2/15/91/115	-
35	LHG	7	619	29	-	19/43/43/53	-
29	CLA	A	803	10	-	9/39/115/115	-
29	CLA	A	801	-	-	8/39/115/115	-
30	KC2	e	609	-	-	7/15/71/71	-
29	CLA	e	611	28	-	11/39/115/115	-
29	CLA	6	604	6	-	5/33/109/115	-
35	LHG	B	849	29	-	22/49/49/53	-
29	CLA	7	603	7	-	3/27/103/115	-
31	II0	7	613	-	-	1/21/67/67	0/2/2/2
31	II0	1	616	-	-	1/21/67/67	0/2/2/2
29	CLA	A	827	-	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	4	601	4	-	7/27/103/115	-
29	CLA	a	608	25	-	4/33/109/115	-
37	8CT	B	844	-	-	4/29/63/63	0/2/2/2
29	CLA	b	603	26	-	7/33/109/115	-
29	CLA	3	604	-	-	4/39/115/115	-
29	CLA	A	842	10	-	5/39/115/115	-
38	LMU	7	620	-	-	8/21/61/61	0/2/2/2
31	II0	8	610	-	-	2/21/67/67	0/2/2/2
29	CLA	A	812	10	-	4/27/103/115	-
29	CLA	2	608	2	-	8/33/109/115	-
29	CLA	d	603	25	-	2/21/97/115	-
29	CLA	d	604	-	-	6/33/109/115	-
29	CLA	5	609	-	-	3/10/86/115	-
29	CLA	9	609	-	-	3/10/86/115	-
30	KC2	e	605	28	-	5/15/71/71	-
31	II0	8	611	-	-	2/21/67/67	0/2/2/2
35	LHG	A	850	-	-	22/53/53/53	-
29	CLA	3	607	3	-	5/33/109/115	-
29	CLA	O	201	-	-	3/27/103/115	-
29	CLA	2	602	2	-	14/32/108/115	-
37	8CT	7	617	-	-	9/29/63/63	0/2/2/2
29	CLA	B	827	-	-	5/39/115/115	-
29	CLA	4	607	4	-	7/33/109/115	-
29	CLA	A	823	-	-	13/39/115/115	-
29	CLA	B	838	-	-	5/39/115/115	-
29	CLA	B	803	-	-	12/39/115/115	-
29	CLA	d	601	25	-	5/15/91/115	-
29	CLA	7	605	7	-	6/15/91/115	-
35	LHG	L	208	-	-	15/38/38/53	-
29	CLA	A	828	10	-	7/39/115/115	-
29	CLA	A	844	-	-	7/39/115/115	-
31	II0	e	615	-	-	0/21/67/67	0/2/2/2
29	CLA	1	612	1	-	10/33/109/115	-
29	CLA	b	611	26	-	3/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	8	608	-	-	7/39/115/115	-
29	CLA	B	829	11	-	0/15/91/115	-
29	CLA	K	102	18	-	4/27/103/115	-
30	KC2	c	615	-	-	6/15/71/71	-
29	CLA	e	606	28	-	9/33/109/115	-
29	CLA	B	809	11	-	9/39/115/115	-
29	CLA	5	604	5	-	7/27/103/115	-
29	CLA	A	835	10	-	6/33/109/115	-
29	CLA	B	841	-	-	8/24/100/115	-
37	8CT	R	203	-	-	4/29/63/63	0/2/2/2
29	CLA	7	607	7	-	2/15/91/115	-
29	CLA	A	806	10	-	8/39/115/115	-
31	II0	d	616	-	-	4/21/67/67	0/2/2/2
29	CLA	B	822	11	-	12/39/115/115	-
37	8CT	Z	309	-	-	6/29/63/63	0/2/2/2
29	CLA	5	608	-	-	13/33/109/115	-
29	CLA	9	608	9	-	10/27/103/115	-
31	II0	7	615	-	-	2/21/67/67	0/2/2/2
30	KC2	c	610	27	-	4/15/71/71	-
29	CLA	3	608	3	-	6/33/109/115	-
31	II0	3	615	-	-	1/21/67/67	0/2/2/2
31	II0	1	617	-	-	1/21/67/67	0/2/2/2
29	CLA	c	612	27	-	5/27/103/115	-
29	CLA	A	820	10	-	7/39/115/115	-
29	CLA	A	819	-	-	8/39/115/115	-
29	CLA	e	601	28	-	5/15/91/115	-
29	CLA	B	812	11	-	16/39/115/115	-
29	CLA	2	604	2	-	2/27/103/115	-
31	II0	J	101	-	-	1/21/67/67	0/2/2/2
29	CLA	2	612	2	-	5/15/91/115	-
29	CLA	9	602	9	-	9/27/103/115	-
29	CLA	B	814	-	-	4/12/88/115	-
29	CLA	J	102	17	-	2/10/86/115	-
30	KC2	1	610	1	-	7/15/71/71	-
29	CLA	8	615	-	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	II0	1	614	-	-	1/21/67/67	0/2/2/2
29	CLA	a	603	25	-	8/33/109/115	-
29	CLA	7	602	7	-	8/39/115/115	-
29	CLA	b	602	26	-	16/38/114/115	-
31	II0	a	613	-	-	1/21/67/67	0/2/2/2
29	CLA	1	609	-	-	3/10/86/115	-
35	LHG	2	618	-	-	10/24/24/53	-
31	II0	8	616	-	-	0/21/67/67	0/2/2/2
30	KC2	9	610	9	-	5/15/71/71	-
29	CLA	d	608	25	-	5/39/115/115	-
32	II3	1	615	-	-	1/25/67/67	0/2/2/2
29	CLA	A	841	-	-	5/39/115/115	-
29	CLA	7	601	7	-	2/15/91/115	-
29	CLA	4	603	4	-	7/26/102/115	-
31	II0	9	618	-	-	2/21/67/67	0/2/2/2
31	II0	1	619	-	-	2/21/67/67	0/2/2/2
37	8CT	J	103	-	-	7/29/63/63	0/2/2/2
29	CLA	a	601	25	-	4/15/91/115	-
29	CLA	6	612	-	-	6/15/91/115	-
35	LHG	2	620	-	-	17/46/46/53	-
31	II0	5	616	-	-	0/21/67/67	0/2/2/2
33	IHT	1	618	-	-	2/25/65/65	0/2/2/2
29	CLA	B	804	-	-	3/15/91/115	-
29	CLA	B	813	11	-	11/35/111/115	-
29	CLA	F	202	-	-	13/33/109/115	-
29	CLA	a	612	25	-	7/39/115/115	-
29	CLA	d	602	25	-	11/38/114/115	-
29	CLA	c	602	27	-	10/39/115/115	-
34	LMG	I	102	-	-	22/46/66/70	0/1/1/1
29	CLA	L	203	-	-	9/33/109/115	-
30	KC2	a	610	-	-	2/15/71/71	-
29	CLA	F	204	15	-	7/27/103/115	-
29	CLA	B	818	-	-	7/33/109/115	-
29	CLA	b	601	26	-	4/15/91/115	-
30	KC2	2	610	2	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	II0	7	616	-	-	2/21/67/67	0/2/2/2
35	LHG	3	623	-	-	25/53/53/53	-
29	CLA	B	810	-	-	6/33/109/115	-
29	CLA	1	604	1	-	3/15/91/115	-
29	CLA	b	610	26	-	8/23/99/115	-
29	CLA	a	611	-	-	6/27/103/115	-
30	KC2	4	605	4	-	7/15/71/71	-
29	CLA	A	840	-	-	5/27/103/115	-
38	LMU	J	104	-	-	10/17/57/61	0/2/2/2
37	8CT	A	846	-	-	4/29/63/63	0/2/2/2
29	CLA	B	832	-	-	15/39/115/115	-
31	II0	3	613	-	-	2/21/67/67	0/2/2/2
29	CLA	6	607	6	-	4/27/103/115	-
31	II0	6	614	-	-	1/21/67/67	0/2/2/2
29	CLA	A	826	10	-	5/39/115/115	-
29	CLA	b	606	26	-	7/39/115/115	-
32	II3	b	613	-	-	1/25/67/67	0/2/2/2

All (2714) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	609	KC2	MG-ND	-10.26	1.85	2.05
33	K	104	IHT	C10-C07	10.23	1.52	1.34
30	3	606	KC2	MG-ND	-10.16	1.85	2.05
30	2	610	KC2	MG-ND	-10.14	1.85	2.05
30	6	613	KC2	MG-ND	-10.04	1.85	2.05
30	Z	307	KC2	MG-ND	-10.04	1.85	2.05
30	b	605	KC2	MG-ND	-10.03	1.85	2.05
30	c	610	KC2	MG-ND	-10.02	1.85	2.05
30	e	609	KC2	MG-ND	-10.02	1.85	2.05
30	d	610	KC2	MG-ND	-10.02	1.85	2.05
30	6	610	KC2	MG-ND	-10.00	1.86	2.05
30	7	606	KC2	MG-ND	-9.99	1.86	2.05
30	7	610	KC2	MG-ND	-9.99	1.86	2.05
30	5	610	KC2	MG-ND	-9.97	1.86	2.05
33	1	618	IHT	C10-C07	9.95	1.51	1.34
30	e	605	KC2	MG-ND	-9.94	1.86	2.05
30	a	610	KC2	MG-ND	-9.94	1.86	2.05
30	1	610	KC2	MG-ND	-9.93	1.86	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	611	KC2	MG-ND	-9.92	1.86	2.05
30	9	610	KC2	MG-ND	-9.92	1.86	2.05
30	c	615	KC2	MG-ND	-9.89	1.86	2.05
30	4	605	KC2	MG-ND	-9.85	1.86	2.05
33	Z	302	IHT	C10-C07	9.70	1.51	1.34
33	5	618	IHT	C10-C07	9.66	1.51	1.34
33	6	617	IHT	C10-C07	9.56	1.51	1.34
33	c	620	IHT	C10-C07	9.45	1.50	1.34
33	L	205	IHT	C10-C07	9.40	1.50	1.34
33	2	616	IHT	C10-C07	9.24	1.50	1.34
33	a	617	IHT	C10-C07	9.20	1.50	1.34
33	d	617	IHT	C10-C07	9.18	1.50	1.34
33	L	205	IHT	C24-C26	-9.03	1.25	1.42
33	8	609	IHT	C10-C07	9.03	1.50	1.34
33	K	104	IHT	C24-C26	-9.03	1.25	1.42
33	9	619	IHT	C10-C07	9.00	1.50	1.34
31	a	616	II0	C24-C26	-8.99	1.25	1.42
31	1	619	II0	C24-C26	-8.99	1.25	1.42
31	2	613	II0	C24-C26	-8.91	1.25	1.42
31	8	610	II0	C24-C26	-8.89	1.25	1.42
31	1	617	II0	C24-C26	-8.86	1.25	1.42
31	d	615	II0	C23-C25	-8.85	1.25	1.42
33	2	616	IHT	C24-C26	-8.83	1.25	1.42
33	2	616	IHT	C09-C10	-8.83	1.33	1.51
31	e	614	II0	C24-C26	-8.82	1.25	1.42
31	a	616	II0	C23-C25	-8.82	1.25	1.42
31	J	101	II0	C23-C25	-8.82	1.25	1.42
33	9	619	IHT	C09-C10	-8.81	1.33	1.51
31	a	615	II0	C23-C25	-8.80	1.25	1.42
31	7	615	II0	C23-C25	-8.80	1.25	1.42
31	8	611	II0	C23-C25	-8.80	1.25	1.42
31	8	611	II0	C24-C26	-8.80	1.25	1.42
31	O	204	II0	C23-C25	-8.79	1.25	1.42
31	B	843	II0	C24-C26	-8.79	1.25	1.42
31	5	615	II0	C24-C26	-8.78	1.25	1.42
31	c	619	II0	C23-C25	-8.77	1.25	1.42
31	3	614	II0	C24-C26	-8.77	1.25	1.42
33	6	617	IHT	C24-C26	-8.77	1.25	1.42
31	e	614	II0	C23-C25	-8.76	1.25	1.42
31	R	204	II0	C24-C26	-8.76	1.25	1.42
31	8	610	II0	C23-C25	-8.75	1.25	1.42
31	O	204	II0	C24-C26	-8.75	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	614	II0	C23-C25	-8.75	1.25	1.42
31	5	620	II0	C23-C25	-8.74	1.25	1.42
31	d	614	II0	C23-C25	-8.74	1.25	1.42
33	1	618	IHT	C24-C26	-8.74	1.25	1.42
31	2	613	II0	C23-C25	-8.74	1.25	1.42
31	d	615	II0	C24-C26	-8.74	1.25	1.42
31	a	613	II0	C24-C26	-8.73	1.25	1.42
33	a	617	IHT	C24-C26	-8.73	1.25	1.42
31	3	617	II0	C24-C26	-8.73	1.25	1.42
31	5	616	II0	C24-C26	-8.73	1.25	1.42
31	7	616	II0	C24-C26	-8.72	1.25	1.42
31	6	616	II0	C24-C26	-8.72	1.25	1.42
33	8	609	IHT	C09-C10	-8.71	1.33	1.51
31	4	613	II0	C24-C26	-8.71	1.25	1.42
31	1	614	II0	C23-C25	-8.70	1.25	1.42
31	c	618	II0	C23-C25	-8.70	1.25	1.42
33	8	609	IHT	C24-C26	-8.70	1.25	1.42
31	e	612	II0	C24-C26	-8.69	1.25	1.42
31	9	616	II0	C23-C25	-8.69	1.25	1.42
33	Z	302	IHT	C24-C26	-8.69	1.25	1.42
31	6	615	II0	C24-C26	-8.68	1.25	1.42
31	7	614	II0	C24-C26	-8.67	1.25	1.42
31	5	616	II0	C23-C25	-8.67	1.25	1.42
32	1	615	II3	C27-C28	-8.67	1.25	1.42
31	2	615	II0	C24-C26	-8.67	1.25	1.42
31	e	615	II0	C24-C26	-8.67	1.25	1.42
32	b	613	II3	C27-C28	-8.66	1.25	1.42
31	3	616	II0	C24-C26	-8.66	1.25	1.42
31	O	205	II0	C24-C26	-8.66	1.25	1.42
31	e	615	II0	C23-C25	-8.66	1.25	1.42
31	1	616	II0	C24-C26	-8.65	1.25	1.42
31	5	620	II0	C24-C26	-8.65	1.25	1.42
31	3	615	II0	C24-C26	-8.65	1.25	1.42
31	2	615	II0	C23-C25	-8.65	1.25	1.42
31	4	614	II0	C24-C26	-8.65	1.25	1.42
31	B	843	II0	C23-C25	-8.64	1.25	1.42
32	e	613	II3	C27-C28	-8.64	1.25	1.42
31	c	617	II0	C24-C26	-8.64	1.25	1.42
31	9	617	II0	C23-C25	-8.63	1.25	1.42
31	9	618	II0	C24-C26	-8.62	1.26	1.42
31	2	614	II0	C24-C26	-8.62	1.26	1.42
31	3	615	II0	C23-C25	-8.62	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	619	II0	C23-C25	-8.61	1.26	1.42
31	d	613	II0	C24-C26	-8.61	1.26	1.42
31	8	612	II0	C24-C26	-8.61	1.26	1.42
31	a	614	II0	C24-C26	-8.61	1.26	1.42
33	5	618	IHT	C24-C26	-8.60	1.26	1.42
31	3	616	II0	C23-C25	-8.60	1.26	1.42
31	9	617	II0	C24-C26	-8.60	1.26	1.42
31	c	619	II0	C24-C26	-8.60	1.26	1.42
31	1	614	II0	C24-C26	-8.60	1.26	1.42
31	a	615	II0	C24-C26	-8.60	1.26	1.42
31	1	619	II0	C23-C25	-8.60	1.26	1.42
31	9	615	II0	C23-C25	-8.60	1.26	1.42
31	O	205	II0	C23-C25	-8.60	1.26	1.42
31	3	617	II0	C23-C25	-8.60	1.26	1.42
31	4	612	II0	C24-C26	-8.59	1.26	1.42
31	7	615	II0	C24-C26	-8.59	1.26	1.42
31	b	612	II0	C24-C26	-8.59	1.26	1.42
31	5	614	II0	C24-C26	-8.58	1.26	1.42
33	9	619	IHT	C24-C26	-8.58	1.26	1.42
31	d	616	II0	C23-C25	-8.58	1.26	1.42
31	9	618	II0	C23-C25	-8.58	1.26	1.42
31	b	614	II0	C24-C26	-8.57	1.26	1.42
31	6	614	II0	C23-C25	-8.57	1.26	1.42
31	5	617	II0	C23-C25	-8.56	1.26	1.42
33	K	104	IHT	C09-C10	-8.56	1.34	1.51
31	b	614	II0	C23-C25	-8.55	1.26	1.42
31	1	617	II0	C23-C25	-8.55	1.26	1.42
31	c	616	II0	C23-C25	-8.55	1.26	1.42
31	3	614	II0	C23-C25	-8.55	1.26	1.42
31	c	618	II0	C24-C26	-8.55	1.26	1.42
31	J	101	II0	C24-C26	-8.54	1.26	1.42
31	5	617	II0	C24-C26	-8.54	1.26	1.42
31	3	613	II0	C24-C26	-8.54	1.26	1.42
31	9	615	II0	C24-C26	-8.54	1.26	1.42
31	R	204	II0	C23-C25	-8.54	1.26	1.42
31	d	614	II0	C24-C26	-8.54	1.26	1.42
31	9	616	II0	C24-C26	-8.53	1.26	1.42
31	4	615	II0	C24-C26	-8.53	1.26	1.42
31	a	619	II0	C24-C26	-8.52	1.26	1.42
31	7	616	II0	C23-C25	-8.52	1.26	1.42
31	4	613	II0	C23-C25	-8.51	1.26	1.42
31	6	616	II0	C23-C25	-8.51	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	614	II0	C23-C25	-8.50	1.26	1.42
31	8	612	II0	C23-C25	-8.50	1.26	1.42
31	e	612	II0	C23-C25	-8.50	1.26	1.42
31	4	615	II0	C23-C25	-8.49	1.26	1.42
31	d	613	II0	C23-C25	-8.49	1.26	1.42
33	d	617	IHT	C24-C26	-8.49	1.26	1.42
31	2	614	II0	C23-C25	-8.48	1.26	1.42
31	6	614	II0	C24-C26	-8.48	1.26	1.42
31	6	615	II0	C23-C25	-8.47	1.26	1.42
33	Z	302	IHT	C09-C10	-8.47	1.34	1.51
31	a	613	II0	C23-C25	-8.47	1.26	1.42
31	7	613	II0	C23-C25	-8.46	1.26	1.42
31	5	615	II0	C23-C25	-8.46	1.26	1.42
31	5	614	II0	C23-C25	-8.45	1.26	1.42
33	a	617	IHT	C09-C10	-8.45	1.34	1.51
31	7	613	II0	C24-C26	-8.45	1.26	1.42
31	4	612	II0	C23-C25	-8.44	1.26	1.42
31	c	617	II0	C23-C25	-8.44	1.26	1.42
31	c	616	II0	C24-C26	-8.43	1.26	1.42
31	3	613	II0	C23-C25	-8.42	1.26	1.42
31	7	614	II0	C23-C25	-8.42	1.26	1.42
33	c	620	IHT	C24-C26	-8.42	1.26	1.42
31	d	616	II0	C24-C26	-8.39	1.26	1.42
33	L	205	IHT	C09-C10	-8.39	1.34	1.51
31	1	616	II0	C23-C25	-8.37	1.26	1.42
31	b	612	II0	C23-C25	-8.36	1.26	1.42
31	8	616	II0	C24-C26	-8.36	1.26	1.42
33	5	618	IHT	C09-C10	-8.30	1.34	1.51
33	d	617	IHT	C09-C10	-8.29	1.34	1.51
33	c	620	IHT	C09-C10	-8.26	1.34	1.51
31	8	616	II0	C23-C25	-8.24	1.26	1.42
33	6	617	IHT	C09-C10	-8.17	1.34	1.51
31	a	616	II0	C22-C10	-8.14	1.25	1.42
31	1	619	II0	C22-C10	-8.09	1.25	1.42
33	1	618	IHT	C09-C10	-8.09	1.35	1.51
31	1	617	II0	C22-C10	-8.08	1.25	1.42
31	2	613	II0	C22-C10	-8.03	1.25	1.42
33	L	205	IHT	C21-C11	-8.02	1.25	1.42
31	e	614	II0	C22-C10	-8.01	1.25	1.42
33	K	104	IHT	C21-C11	-8.01	1.25	1.42
31	5	616	II0	C22-C10	-8.01	1.25	1.42
31	d	615	II0	C21-C09	-7.99	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	610	II0	C22-C10	-7.99	1.25	1.42
31	5	615	II0	C22-C10	-7.95	1.25	1.42
31	e	614	II0	C21-C09	-7.95	1.25	1.42
31	B	843	II0	C22-C10	-7.95	1.25	1.42
31	8	611	II0	C22-C10	-7.95	1.25	1.42
31	R	204	II0	C22-C10	-7.94	1.25	1.42
31	a	613	II0	C22-C10	-7.94	1.25	1.42
33	6	617	IHT	C21-C11	-7.94	1.25	1.42
33	2	616	IHT	C21-C11	-7.94	1.25	1.42
31	8	611	II0	C21-C09	-7.93	1.25	1.42
31	7	615	II0	C21-C09	-7.93	1.25	1.42
31	d	614	II0	C21-C09	-7.93	1.25	1.42
31	d	615	II0	C22-C10	-7.92	1.25	1.42
31	4	613	II0	C22-C10	-7.92	1.25	1.42
31	O	204	II0	C22-C10	-7.92	1.25	1.42
31	5	620	II0	C21-C09	-7.92	1.25	1.42
31	8	610	II0	C21-C09	-7.91	1.25	1.42
31	O	204	II0	C21-C09	-7.90	1.25	1.42
31	a	615	II0	C21-C09	-7.90	1.25	1.42
33	1	618	IHT	C21-C11	-7.90	1.25	1.42
31	a	614	II0	C21-C09	-7.89	1.25	1.42
31	3	617	II0	C22-C10	-7.89	1.25	1.42
31	2	613	II0	C21-C09	-7.89	1.25	1.42
31	a	616	II0	C21-C09	-7.89	1.25	1.42
33	8	609	IHT	C21-C11	-7.88	1.25	1.42
31	c	618	II0	C21-C09	-7.87	1.25	1.42
31	3	614	II0	C22-C10	-7.87	1.25	1.42
31	6	616	II0	C22-C10	-7.87	1.25	1.42
31	4	614	II0	C22-C10	-7.86	1.25	1.42
31	7	616	II0	C22-C10	-7.86	1.25	1.42
31	J	101	II0	C21-C09	-7.86	1.25	1.42
31	e	615	II0	C22-C10	-7.86	1.25	1.42
31	1	614	II0	C21-C09	-7.86	1.26	1.42
31	d	613	II0	C22-C10	-7.85	1.26	1.42
31	3	616	II0	C22-C10	-7.84	1.26	1.42
31	5	620	II0	C22-C10	-7.84	1.26	1.42
33	a	617	IHT	C21-C11	-7.84	1.26	1.42
31	6	615	II0	C22-C10	-7.84	1.26	1.42
31	e	612	II0	C22-C10	-7.83	1.26	1.42
31	7	614	II0	C22-C10	-7.83	1.26	1.42
31	3	615	II0	C22-C10	-7.83	1.26	1.42
31	c	619	II0	C21-C09	-7.82	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	619	II0	C21-C09	-7.82	1.26	1.42
31	9	617	II0	C22-C10	-7.82	1.26	1.42
31	2	615	II0	C22-C10	-7.82	1.26	1.42
31	O	205	II0	C22-C10	-7.81	1.26	1.42
31	c	617	II0	C22-C10	-7.81	1.26	1.42
31	7	615	II0	C22-C10	-7.80	1.26	1.42
31	8	612	II0	C22-C10	-7.80	1.26	1.42
31	1	614	II0	C22-C10	-7.79	1.26	1.42
29	c	613	CLA	C1D-ND	7.79	1.47	1.37
32	b	613	II3	C23-C16	-7.79	1.26	1.42
31	9	616	II0	C21-C09	-7.79	1.26	1.42
31	B	843	II0	C21-C09	-7.79	1.26	1.42
33	Z	302	IHT	C21-C11	-7.78	1.26	1.42
31	c	618	II0	C22-C10	-7.78	1.26	1.42
31	a	615	II0	C22-C10	-7.78	1.26	1.42
31	1	616	II0	C22-C10	-7.78	1.26	1.42
33	5	618	IHT	C21-C11	-7.78	1.26	1.42
31	5	616	II0	C21-C09	-7.78	1.26	1.42
31	e	615	II0	C21-C09	-7.77	1.26	1.42
31	9	618	II0	C22-C10	-7.77	1.26	1.42
31	2	615	II0	C21-C09	-7.77	1.26	1.42
32	1	615	II3	C23-C16	-7.77	1.26	1.42
31	c	619	II0	C22-C10	-7.77	1.26	1.42
31	O	205	II0	C21-C09	-7.76	1.26	1.42
31	7	613	II0	C22-C10	-7.76	1.26	1.42
31	b	612	II0	C22-C10	-7.76	1.26	1.42
31	6	614	II0	C21-C09	-7.76	1.26	1.42
31	5	617	II0	C22-C10	-7.75	1.26	1.42
31	1	617	II0	C21-C09	-7.75	1.26	1.42
33	9	619	IHT	C21-C11	-7.75	1.26	1.42
32	e	613	II3	C23-C16	-7.75	1.26	1.42
31	9	618	II0	C21-C09	-7.74	1.26	1.42
31	a	614	II0	C22-C10	-7.74	1.26	1.42
31	4	612	II0	C22-C10	-7.74	1.26	1.42
31	2	614	II0	C22-C10	-7.74	1.26	1.42
31	a	619	II0	C21-C09	-7.74	1.26	1.42
31	5	614	II0	C22-C10	-7.74	1.26	1.42
31	3	615	II0	C21-C09	-7.74	1.26	1.42
31	3	616	II0	C21-C09	-7.74	1.26	1.42
31	4	615	II0	C22-C10	-7.73	1.26	1.42
31	9	615	II0	C21-C09	-7.73	1.26	1.42
31	d	614	II0	C22-C10	-7.73	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	9	615	II0	C22-C10	-7.73	1.26	1.42
31	9	616	II0	C22-C10	-7.72	1.26	1.42
31	d	616	II0	C21-C09	-7.72	1.26	1.42
31	3	613	II0	C22-C10	-7.72	1.26	1.42
31	e	612	II0	C21-C09	-7.72	1.26	1.42
31	b	614	II0	C22-C10	-7.71	1.26	1.42
31	b	614	II0	C21-C09	-7.71	1.26	1.42
31	3	614	II0	C21-C09	-7.71	1.26	1.42
31	5	617	II0	C21-C09	-7.71	1.26	1.42
31	4	613	II0	C21-C09	-7.69	1.26	1.42
31	J	101	II0	C22-C10	-7.69	1.26	1.42
31	a	619	II0	C22-C10	-7.69	1.26	1.42
31	c	616	II0	C21-C09	-7.68	1.26	1.42
31	6	616	II0	C21-C09	-7.68	1.26	1.42
31	5	615	II0	C21-C09	-7.68	1.26	1.42
31	d	613	II0	C21-C09	-7.67	1.26	1.42
33	d	617	IHT	C21-C11	-7.67	1.26	1.42
31	9	617	II0	C21-C09	-7.67	1.26	1.42
31	3	617	II0	C21-C09	-7.66	1.26	1.42
29	e	611	CLA	C1D-ND	7.66	1.47	1.37
31	c	616	II0	C22-C10	-7.65	1.26	1.42
31	2	614	II0	C21-C09	-7.65	1.26	1.42
31	6	614	II0	C22-C10	-7.65	1.26	1.42
31	4	615	II0	C21-C09	-7.64	1.26	1.42
31	7	616	II0	C21-C09	-7.64	1.26	1.42
31	a	613	II0	C21-C09	-7.64	1.26	1.42
31	8	616	II0	C22-C10	-7.63	1.26	1.42
31	4	614	II0	C21-C09	-7.63	1.26	1.42
31	3	613	II0	C21-C09	-7.63	1.26	1.42
31	c	617	II0	C21-C09	-7.62	1.26	1.42
31	R	204	II0	C21-C09	-7.61	1.26	1.42
31	4	612	II0	C21-C09	-7.61	1.26	1.42
31	8	612	II0	C21-C09	-7.61	1.26	1.42
31	7	613	II0	C21-C09	-7.60	1.26	1.42
31	d	616	II0	C22-C10	-7.60	1.26	1.42
31	6	615	II0	C21-C09	-7.60	1.26	1.42
29	7	605	CLA	C1D-ND	7.59	1.47	1.37
29	5	613	CLA	C1D-ND	7.58	1.47	1.37
31	1	616	II0	C21-C09	-7.57	1.26	1.42
31	7	614	II0	C21-C09	-7.56	1.26	1.42
33	c	620	IHT	C21-C11	-7.56	1.26	1.42
29	Z	301	CLA	C1D-ND	7.55	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	609	CLA	C1D-ND	7.53	1.47	1.37
29	5	611	CLA	C1D-ND	7.53	1.47	1.37
31	5	614	II0	C21-C09	-7.53	1.26	1.42
29	B	823	CLA	C1D-ND	7.53	1.47	1.37
31	b	612	II0	C21-C09	-7.52	1.26	1.42
29	9	613	CLA	C1D-ND	7.51	1.47	1.37
29	A	823	CLA	C1D-ND	7.51	1.47	1.37
31	8	616	II0	C21-C09	-7.50	1.26	1.42
29	8	607	CLA	C1D-ND	7.50	1.47	1.37
29	1	604	CLA	C1D-ND	7.48	1.47	1.37
29	1	609	CLA	C1D-ND	7.47	1.47	1.37
29	e	604	CLA	C1D-ND	7.45	1.46	1.37
29	1	613	CLA	C1D-ND	7.45	1.46	1.37
29	9	609	CLA	C1D-ND	7.45	1.46	1.37
29	F	204	CLA	C1D-ND	7.44	1.46	1.37
29	b	608	CLA	C1D-ND	7.44	1.46	1.37
29	8	604	CLA	C1D-ND	7.44	1.46	1.37
29	8	606	CLA	C1D-ND	7.44	1.46	1.37
29	A	807	CLA	C1D-ND	7.42	1.46	1.37
29	9	614	CLA	C1D-ND	7.42	1.46	1.37
29	9	604	CLA	C1D-ND	7.42	1.46	1.37
29	B	837	CLA	C1D-ND	7.42	1.46	1.37
29	1	611	CLA	C1D-ND	7.42	1.46	1.37
29	c	609	CLA	C1D-ND	7.41	1.46	1.37
29	K	101	CLA	C1D-ND	7.41	1.46	1.37
29	e	610	CLA	C1D-ND	7.40	1.46	1.37
29	5	609	CLA	C1D-ND	7.39	1.46	1.37
29	7	611	CLA	C1D-ND	7.39	1.46	1.37
29	e	603	CLA	C1D-ND	7.39	1.46	1.37
29	F	203	CLA	C1D-ND	7.39	1.46	1.37
29	d	601	CLA	C1D-ND	7.38	1.46	1.37
29	3	601	CLA	C1D-ND	7.38	1.46	1.37
29	B	841	CLA	C1D-ND	7.38	1.46	1.37
29	7	601	CLA	C1D-ND	7.37	1.46	1.37
29	7	609	CLA	C1D-ND	7.37	1.46	1.37
29	8	615	CLA	C1D-ND	7.37	1.46	1.37
29	6	601	CLA	C1D-ND	7.37	1.46	1.37
29	b	610	CLA	C1D-ND	7.36	1.46	1.37
29	B	820	CLA	C1D-ND	7.36	1.46	1.37
29	c	607	CLA	C1D-ND	7.36	1.46	1.37
29	d	603	CLA	C1D-ND	7.36	1.46	1.37
29	2	604	CLA	C1D-ND	7.36	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	e	607	CLA	C1D-ND	7.36	1.46	1.37
29	K	102	CLA	C1D-ND	7.35	1.46	1.37
29	J	102	CLA	C1D-ND	7.35	1.46	1.37
29	8	601	CLA	C1D-ND	7.35	1.46	1.37
29	A	842	CLA	C1D-ND	7.34	1.46	1.37
29	9	601	CLA	C1D-ND	7.34	1.46	1.37
29	d	609	CLA	C1D-ND	7.34	1.46	1.37
29	e	601	CLA	C1D-ND	7.34	1.46	1.37
29	c	603	CLA	C1D-ND	7.33	1.46	1.37
29	6	609	CLA	C1D-ND	7.32	1.46	1.37
29	4	603	CLA	C1D-ND	7.32	1.46	1.37
29	A	835	CLA	C1D-ND	7.32	1.46	1.37
29	c	604	CLA	C1D-ND	7.31	1.46	1.37
29	1	612	CLA	C1D-ND	7.31	1.46	1.37
29	B	829	CLA	C1D-ND	7.30	1.46	1.37
29	7	603	CLA	C1D-ND	7.30	1.46	1.37
29	d	611	CLA	C1D-ND	7.30	1.46	1.37
29	9	603	CLA	C1D-ND	7.30	1.46	1.37
29	e	602	CLA	C1D-ND	7.30	1.46	1.37
29	4	601	CLA	C1D-ND	7.30	1.46	1.37
29	7	607	CLA	C1D-ND	7.30	1.46	1.37
29	Z	304	CLA	C1D-ND	7.30	1.46	1.37
29	1	603	CLA	C1D-ND	7.29	1.46	1.37
29	c	601	CLA	C1D-ND	7.29	1.46	1.37
29	2	609	CLA	C1D-ND	7.29	1.46	1.37
29	5	601	CLA	C1D-ND	7.29	1.46	1.37
29	3	604	CLA	C1D-ND	7.29	1.46	1.37
29	2	611	CLA	C1D-ND	7.29	1.46	1.37
29	A	813	CLA	C1D-ND	7.29	1.46	1.37
29	B	825	CLA	C1D-ND	7.29	1.46	1.37
29	3	608	CLA	C1D-ND	7.28	1.46	1.37
29	A	805	CLA	C1D-ND	7.28	1.46	1.37
29	B	815	CLA	C1D-ND	7.28	1.46	1.37
29	B	834	CLA	C1D-ND	7.27	1.46	1.37
29	A	830	CLA	C1D-ND	7.27	1.46	1.37
29	L	201	CLA	C1D-ND	7.27	1.46	1.37
29	d	604	CLA	C1D-ND	7.27	1.46	1.37
29	6	604	CLA	C1D-ND	7.27	1.46	1.37
29	b	604	CLA	C1D-ND	7.27	1.46	1.37
29	1	601	CLA	C1D-ND	7.27	1.46	1.37
29	3	610	CLA	C1D-ND	7.27	1.46	1.37
29	4	610	CLA	C1D-ND	7.27	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	820	CLA	C1D-ND	7.27	1.46	1.37
29	3	612	CLA	C1D-ND	7.26	1.46	1.37
29	b	603	CLA	C1D-ND	7.26	1.46	1.37
29	1	607	CLA	C1D-ND	7.26	1.46	1.37
29	B	839	CLA	C1D-ND	7.26	1.46	1.37
29	5	604	CLA	C1D-ND	7.26	1.46	1.37
29	d	612	CLA	C1D-ND	7.25	1.46	1.37
29	e	608	CLA	C1D-ND	7.25	1.46	1.37
29	6	603	CLA	C1D-ND	7.25	1.46	1.37
29	A	828	CLA	C1D-ND	7.25	1.46	1.37
29	A	825	CLA	C1D-ND	7.25	1.46	1.37
29	F	202	CLA	C1D-ND	7.25	1.46	1.37
29	2	612	CLA	C1D-ND	7.24	1.46	1.37
29	4	606	CLA	C1D-ND	7.24	1.46	1.37
29	9	612	CLA	C1D-ND	7.24	1.46	1.37
29	8	608	CLA	C1D-ND	7.23	1.46	1.37
29	A	814	CLA	C1D-ND	7.22	1.46	1.37
29	6	612	CLA	C1D-ND	7.22	1.46	1.37
29	A	836	CLA	C1D-ND	7.22	1.46	1.37
29	b	601	CLA	C1D-ND	7.22	1.46	1.37
29	a	601	CLA	C1D-ND	7.21	1.46	1.37
29	5	612	CLA	C1D-ND	7.21	1.46	1.37
29	4	608	CLA	C1D-ND	7.21	1.46	1.37
29	A	831	CLA	C1D-ND	7.21	1.46	1.37
29	A	832	CLA	C1D-ND	7.21	1.46	1.37
29	B	811	CLA	C1D-ND	7.21	1.46	1.37
29	a	611	CLA	C1D-ND	7.21	1.46	1.37
29	b	607	CLA	C1D-ND	7.20	1.46	1.37
29	5	603	CLA	C1D-ND	7.20	1.46	1.37
29	L	204	CLA	C1D-ND	7.20	1.46	1.37
29	5	607	CLA	C1D-ND	7.20	1.46	1.37
29	A	810	CLA	C1D-ND	7.20	1.46	1.37
29	B	816	CLA	C1D-ND	7.19	1.46	1.37
29	c	602	CLA	C1D-ND	7.19	1.46	1.37
29	B	805	CLA	C1D-ND	7.19	1.46	1.37
29	2	603	CLA	C1D-ND	7.19	1.46	1.37
29	4	607	CLA	C1D-ND	7.19	1.46	1.37
29	7	604	CLA	C1D-ND	7.19	1.46	1.37
29	5	606	CLA	C1D-ND	7.19	1.46	1.37
29	A	804	CLA	C1D-ND	7.18	1.46	1.37
29	Z	305	CLA	C1D-ND	7.18	1.46	1.37
29	c	614	CLA	C1D-ND	7.18	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	604	CLA	C1D-ND	7.18	1.46	1.37
29	3	607	CLA	C1D-ND	7.18	1.46	1.37
29	d	606	CLA	C1D-ND	7.17	1.46	1.37
29	a	604	CLA	C1D-ND	7.16	1.46	1.37
29	B	819	CLA	C1D-ND	7.16	1.46	1.37
29	B	806	CLA	C1D-ND	7.16	1.46	1.37
29	3	609	CLA	C1D-ND	7.16	1.46	1.37
29	d	608	CLA	C1D-ND	7.16	1.46	1.37
29	9	602	CLA	C1D-ND	7.15	1.46	1.37
29	3	605	CLA	C1D-ND	7.15	1.46	1.37
29	a	609	CLA	C1D-ND	7.15	1.46	1.37
29	3	611	CLA	C1D-ND	7.14	1.46	1.37
29	6	606	CLA	C1D-ND	7.14	1.46	1.37
29	B	833	CLA	C1D-ND	7.13	1.46	1.37
29	6	607	CLA	C1D-ND	7.13	1.46	1.37
29	A	829	CLA	C1D-ND	7.13	1.46	1.37
29	A	821	CLA	C1D-ND	7.12	1.46	1.37
29	7	602	CLA	C1D-ND	7.12	1.46	1.37
29	B	838	CLA	C1D-ND	7.12	1.46	1.37
29	B	812	CLA	C1D-ND	7.12	1.46	1.37
29	A	833	CLA	C1D-ND	7.12	1.46	1.37
29	2	606	CLA	C1D-ND	7.11	1.46	1.37
29	B	835	CLA	C1D-ND	7.11	1.46	1.37
29	2	601	CLA	C1D-ND	7.11	1.46	1.37
29	a	607	CLA	C1D-ND	7.11	1.46	1.37
29	8	603	CLA	C1D-ND	7.10	1.46	1.37
29	b	611	CLA	C1D-ND	7.10	1.46	1.37
29	1	602	CLA	C1D-ND	7.10	1.46	1.37
29	a	606	CLA	C1D-ND	7.09	1.46	1.37
29	2	608	CLA	C1D-ND	7.09	1.46	1.37
29	2	607	CLA	C1D-ND	7.09	1.46	1.37
29	7	612	CLA	C1D-ND	7.09	1.46	1.37
29	9	606	CLA	C1D-ND	7.09	1.46	1.37
29	c	606	CLA	C1D-ND	7.09	1.46	1.37
29	B	814	CLA	C1D-ND	7.08	1.46	1.37
29	B	826	CLA	C1D-ND	7.08	1.46	1.37
29	6	611	CLA	C1D-ND	7.08	1.46	1.37
29	9	611	CLA	C1D-ND	7.08	1.46	1.37
29	3	603	CLA	C1D-ND	7.08	1.46	1.37
29	4	611	CLA	C1D-ND	7.07	1.46	1.37
29	A	818	CLA	C1D-ND	7.07	1.46	1.37
29	B	836	CLA	C1D-ND	7.07	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	608	CLA	C1D-ND	7.07	1.46	1.37
29	A	824	CLA	C1D-ND	7.07	1.46	1.37
29	1	606	CLA	C1D-ND	7.06	1.46	1.37
29	A	834	CLA	C1D-ND	7.06	1.46	1.37
29	9	607	CLA	C1D-ND	7.06	1.46	1.37
29	a	612	CLA	C1D-ND	7.06	1.46	1.37
29	5	608	CLA	C1D-ND	7.05	1.46	1.37
29	B	810	CLA	C1D-ND	7.05	1.46	1.37
29	c	608	CLA	C1D-ND	7.04	1.46	1.37
29	7	608	CLA	C1D-ND	7.04	1.46	1.37
29	B	817	CLA	C1D-ND	7.04	1.46	1.37
29	a	603	CLA	C1D-ND	7.04	1.46	1.37
29	9	605	CLA	C1D-ND	7.04	1.46	1.37
29	A	838	CLA	C1D-ND	7.04	1.46	1.37
29	B	840	CLA	C1D-ND	7.04	1.46	1.37
29	c	612	CLA	C1D-ND	7.04	1.46	1.37
29	d	607	CLA	C1D-ND	7.04	1.46	1.37
29	e	606	CLA	C1D-ND	7.03	1.46	1.37
29	B	832	CLA	C1D-ND	7.02	1.46	1.37
29	A	811	CLA	C1D-ND	7.02	1.46	1.37
29	5	602	CLA	C1D-ND	7.02	1.46	1.37
29	2	602	CLA	C1D-ND	7.02	1.46	1.37
29	Z	306	CLA	C1D-ND	7.01	1.46	1.37
29	A	803	CLA	C1D-ND	7.01	1.46	1.37
29	A	827	CLA	C1D-ND	7.00	1.46	1.37
29	B	804	CLA	C1D-ND	6.98	1.46	1.37
29	A	802	CLA	C1D-ND	6.98	1.46	1.37
29	L	203	CLA	C1D-ND	6.98	1.46	1.37
29	A	822	CLA	C1D-ND	6.97	1.46	1.37
29	A	815	CLA	C1D-ND	6.97	1.46	1.37
29	A	837	CLA	C1D-ND	6.96	1.46	1.37
29	9	608	CLA	C1D-ND	6.96	1.46	1.37
29	B	813	CLA	C1D-ND	6.96	1.46	1.37
29	b	606	CLA	C1D-ND	6.96	1.46	1.37
29	B	824	CLA	C1D-ND	6.95	1.46	1.37
29	a	608	CLA	C1D-ND	6.95	1.46	1.37
29	A	808	CLA	C1D-ND	6.94	1.46	1.37
29	b	602	CLA	C1D-ND	6.94	1.46	1.37
29	A	816	CLA	C1D-ND	6.94	1.46	1.37
29	B	828	CLA	C1D-ND	6.94	1.46	1.37
29	2	605	CLA	C1D-ND	6.93	1.46	1.37
29	8	602	CLA	C1D-ND	6.93	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	602	CLA	C1D-ND	6.92	1.46	1.37
29	A	843	CLA	C1D-ND	6.92	1.46	1.37
29	B	830	CLA	C1D-ND	6.92	1.46	1.37
29	c	605	CLA	C1D-ND	6.92	1.46	1.37
29	L	202	CLA	C1D-ND	6.92	1.46	1.37
29	A	819	CLA	C1D-ND	6.91	1.46	1.37
29	a	605	CLA	C1D-ND	6.90	1.46	1.37
29	B	807	CLA	C1D-ND	6.89	1.46	1.37
29	B	827	CLA	C1D-ND	6.88	1.46	1.37
29	A	817	CLA	C1D-ND	6.87	1.46	1.37
29	B	821	CLA	C1D-ND	6.87	1.46	1.37
29	B	818	CLA	C1D-ND	6.85	1.46	1.37
29	O	201	CLA	C1D-ND	6.84	1.46	1.37
29	B	809	CLA	C1D-ND	6.84	1.46	1.37
29	5	605	CLA	C1D-ND	6.83	1.46	1.37
29	4	602	CLA	C1D-ND	6.81	1.46	1.37
29	8	605	CLA	C1D-ND	6.81	1.46	1.37
29	6	602	CLA	C1D-ND	6.81	1.46	1.37
29	O	203	CLA	C1D-ND	6.79	1.46	1.37
29	6	608	CLA	C1D-ND	6.78	1.46	1.37
29	3	602	CLA	C1D-ND	6.77	1.46	1.37
29	B	831	CLA	C1D-ND	6.77	1.46	1.37
29	A	812	CLA	C1D-ND	6.77	1.46	1.37
29	d	605	CLA	C1D-ND	6.75	1.46	1.37
29	a	602	CLA	C1D-ND	6.75	1.46	1.37
29	A	806	CLA	C1D-ND	6.73	1.46	1.37
29	6	605	CLA	C1D-ND	6.73	1.46	1.37
29	A	809	CLA	C1D-ND	6.70	1.46	1.37
29	1	605	CLA	C1D-ND	6.69	1.46	1.37
29	A	839	CLA	C1D-ND	6.66	1.46	1.37
29	B	822	CLA	C1D-ND	6.66	1.46	1.37
29	A	801	CLA	MG-ND	-6.65	1.92	2.05
29	B	803	CLA	C1D-ND	6.62	1.45	1.37
29	A	826	CLA	C1D-ND	6.58	1.45	1.37
29	B	808	CLA	C1D-ND	6.57	1.45	1.37
29	A	841	CLA	C1D-ND	6.50	1.45	1.37
29	L	207	CLA	C1D-ND	6.50	1.45	1.37
29	O	202	CLA	C1D-ND	6.45	1.45	1.37
29	B	802	CLA	C1D-ND	6.43	1.45	1.37
29	R	202	CLA	C1D-ND	6.41	1.45	1.37
29	A	844	CLA	MG-ND	-6.23	1.93	2.05
29	A	840	CLA	MG-ND	-6.13	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	605	CLA	MG-ND	-6.11	1.93	2.05
30	c	611	KC2	C4B-NB	6.09	1.45	1.37
29	B	802	CLA	MG-ND	-6.07	1.93	2.05
29	A	840	CLA	C1D-ND	6.04	1.45	1.37
30	a	610	KC2	C4B-NB	6.04	1.45	1.37
29	A	844	CLA	C1D-ND	6.02	1.45	1.37
30	d	610	KC2	C4B-NB	6.01	1.45	1.37
29	B	803	CLA	MG-ND	-5.98	1.93	2.05
29	8	605	CLA	MG-NA	-5.96	1.92	2.06
30	1	610	KC2	C4B-NB	5.92	1.45	1.37
29	A	801	CLA	MG-NB	-5.91	1.94	2.05
30	e	605	KC2	C4B-NB	5.91	1.45	1.37
29	R	202	CLA	MG-ND	-5.90	1.94	2.05
29	O	203	CLA	MG-ND	-5.90	1.94	2.05
30	4	605	KC2	C4B-NB	5.88	1.45	1.37
30	b	605	KC2	C4B-NB	5.86	1.45	1.37
30	7	606	KC2	C4B-NB	5.84	1.45	1.37
29	A	826	CLA	MG-ND	-5.81	1.94	2.05
29	A	809	CLA	MG-NA	-5.81	1.92	2.06
30	5	610	KC2	C4B-NB	5.80	1.44	1.37
29	5	605	CLA	MG-ND	-5.79	1.94	2.05
29	A	811	CLA	C1B-NB	5.79	1.44	1.37
29	6	603	CLA	MG-NB	-5.78	1.94	2.05
30	e	609	KC2	C4B-NB	5.77	1.44	1.37
29	d	605	CLA	MG-ND	-5.76	1.94	2.05
29	6	605	CLA	MG-ND	-5.75	1.94	2.05
29	L	207	CLA	MG-NB	-5.75	1.94	2.05
29	1	611	CLA	C1B-NB	5.75	1.44	1.37
29	2	605	CLA	MG-ND	-5.74	1.94	2.05
29	a	604	CLA	C1B-NB	5.74	1.44	1.37
29	R	202	CLA	MG-NA	-5.73	1.92	2.06
29	A	806	CLA	MG-ND	-5.73	1.94	2.05
29	B	822	CLA	MG-ND	-5.73	1.94	2.05
30	6	610	KC2	C4B-NB	5.73	1.44	1.37
30	c	615	KC2	C4B-NB	5.73	1.44	1.37
29	1	608	CLA	C1B-NB	5.72	1.44	1.37
29	6	603	CLA	MG-ND	-5.72	1.94	2.05
29	1	601	CLA	C1B-NB	5.71	1.44	1.37
29	1	607	CLA	C1B-NB	5.71	1.44	1.37
29	5	601	CLA	C1B-NB	5.71	1.44	1.37
30	9	610	KC2	C4B-NB	5.71	1.44	1.37
29	A	843	CLA	MG-NA	-5.70	1.92	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	827	CLA	MG-ND	-5.70	1.94	2.05
29	9	607	CLA	MG-ND	-5.69	1.94	2.05
29	A	809	CLA	MG-ND	-5.69	1.94	2.05
29	B	833	CLA	MG-ND	-5.69	1.94	2.05
29	b	606	CLA	MG-ND	-5.69	1.94	2.05
29	A	812	CLA	MG-ND	-5.69	1.94	2.05
29	B	839	CLA	MG-ND	-5.68	1.94	2.05
29	B	827	CLA	MG-ND	-5.68	1.94	2.05
29	d	604	CLA	C1B-NB	5.68	1.44	1.37
29	c	605	CLA	MG-ND	-5.67	1.94	2.05
29	9	608	CLA	C1B-NB	5.67	1.44	1.37
29	2	606	CLA	MG-ND	-5.67	1.94	2.05
29	1	609	CLA	C1B-NB	5.67	1.44	1.37
30	7	610	KC2	C4B-NB	5.67	1.44	1.37
29	8	602	CLA	MG-ND	-5.67	1.94	2.05
29	B	821	CLA	MG-ND	-5.67	1.94	2.05
29	9	614	CLA	C1B-NB	5.66	1.44	1.37
29	A	831	CLA	MG-ND	-5.66	1.94	2.05
29	B	815	CLA	C1B-NB	5.66	1.44	1.37
29	5	608	CLA	C1B-NB	5.66	1.44	1.37
29	d	612	CLA	MG-ND	-5.66	1.94	2.05
29	e	606	CLA	MG-ND	-5.66	1.94	2.05
29	A	801	CLA	C1D-ND	5.65	1.44	1.37
29	B	812	CLA	C1B-NB	5.65	1.44	1.37
29	A	841	CLA	MG-NA	-5.65	1.92	2.06
29	A	809	CLA	MG-NB	-5.64	1.94	2.05
29	9	605	CLA	MG-ND	-5.64	1.94	2.05
29	6	602	CLA	MG-ND	-5.63	1.94	2.05
29	B	839	CLA	MG-NB	-5.63	1.94	2.05
29	a	605	CLA	MG-ND	-5.63	1.94	2.05
29	7	612	CLA	MG-ND	-5.63	1.94	2.05
29	B	809	CLA	MG-ND	-5.62	1.94	2.05
29	A	841	CLA	MG-ND	-5.62	1.94	2.05
29	a	603	CLA	MG-ND	-5.62	1.94	2.05
29	1	613	CLA	MG-NB	-5.62	1.94	2.05
29	9	601	CLA	C1B-NB	5.62	1.44	1.37
29	c	601	CLA	C1B-NB	5.62	1.44	1.37
29	d	602	CLA	C1B-NB	5.62	1.44	1.37
29	2	609	CLA	C1B-NB	5.62	1.44	1.37
29	A	810	CLA	MG-ND	-5.61	1.94	2.05
29	e	610	CLA	C1B-NB	5.61	1.44	1.37
29	d	607	CLA	MG-ND	-5.61	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	608	CLA	C1B-NB	5.61	1.44	1.37
29	6	607	CLA	C1B-NB	5.61	1.44	1.37
29	9	611	CLA	MG-ND	-5.60	1.94	2.05
29	e	602	CLA	C1B-NB	5.60	1.44	1.37
29	L	202	CLA	MG-ND	-5.60	1.94	2.05
30	b	609	KC2	C4B-NB	5.60	1.44	1.37
29	B	819	CLA	C1B-NB	5.60	1.44	1.37
29	L	207	CLA	MG-ND	-5.60	1.94	2.05
29	4	611	CLA	MG-ND	-5.60	1.94	2.05
29	1	604	CLA	C1B-NB	5.60	1.44	1.37
29	e	603	CLA	C1B-NB	5.60	1.44	1.37
29	8	603	CLA	C1B-NB	5.60	1.44	1.37
29	a	607	CLA	MG-ND	-5.59	1.94	2.05
29	B	831	CLA	MG-NA	-5.59	1.93	2.06
29	Z	305	CLA	MG-ND	-5.59	1.94	2.05
29	c	608	CLA	C1B-NB	5.59	1.44	1.37
29	7	605	CLA	C1B-NB	5.58	1.44	1.37
29	e	608	CLA	C1B-NB	5.58	1.44	1.37
29	B	835	CLA	MG-NA	-5.58	1.93	2.06
29	B	816	CLA	MG-ND	-5.58	1.94	2.05
29	3	608	CLA	C1B-NB	5.58	1.44	1.37
29	7	607	CLA	C1B-NB	5.57	1.44	1.37
29	B	818	CLA	MG-ND	-5.57	1.94	2.05
29	2	601	CLA	C1B-NB	5.57	1.44	1.37
29	A	832	CLA	MG-ND	-5.57	1.94	2.05
29	2	607	CLA	MG-ND	-5.57	1.94	2.05
29	L	203	CLA	MG-NA	-5.57	1.93	2.06
29	Z	301	CLA	C1B-NB	5.57	1.44	1.37
29	c	609	CLA	C1B-NB	5.57	1.44	1.37
29	A	819	CLA	MG-ND	-5.57	1.94	2.05
29	A	804	CLA	MG-ND	-5.56	1.94	2.05
29	a	608	CLA	C1B-NB	5.56	1.44	1.37
29	A	839	CLA	MG-ND	-5.56	1.94	2.05
29	1	601	CLA	MG-ND	-5.56	1.94	2.05
29	4	602	CLA	C1B-NB	5.56	1.44	1.37
29	L	203	CLA	MG-NB	-5.56	1.94	2.05
29	B	831	CLA	C1B-NB	5.55	1.44	1.37
29	L	201	CLA	MG-ND	-5.55	1.94	2.05
29	2	604	CLA	C1B-NB	5.55	1.44	1.37
29	d	608	CLA	C1B-NB	5.55	1.44	1.37
29	c	604	CLA	MG-NB	-5.55	1.94	2.05
29	4	601	CLA	MG-ND	-5.55	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	840	CLA	MG-NB	-5.55	1.94	2.05
29	B	826	CLA	MG-ND	-5.55	1.94	2.05
29	A	844	CLA	MG-NB	-5.55	1.94	2.05
29	1	602	CLA	C1B-NB	5.54	1.44	1.37
29	7	609	CLA	C1B-NB	5.54	1.44	1.37
29	B	824	CLA	MG-ND	-5.54	1.94	2.05
29	d	611	CLA	C1B-NB	5.54	1.44	1.37
29	B	806	CLA	MG-ND	-5.54	1.94	2.05
29	4	606	CLA	MG-ND	-5.54	1.94	2.05
30	6	613	KC2	C4B-NB	5.54	1.44	1.37
29	c	606	CLA	MG-ND	-5.54	1.94	2.05
29	7	604	CLA	C1B-NB	5.54	1.44	1.37
29	d	601	CLA	C1B-NB	5.54	1.44	1.37
29	b	602	CLA	C1B-NB	5.53	1.44	1.37
29	B	808	CLA	MG-ND	-5.53	1.94	2.05
29	A	842	CLA	C1B-NB	5.53	1.44	1.37
29	A	829	CLA	MG-ND	-5.53	1.94	2.05
29	e	611	CLA	MG-ND	-5.53	1.94	2.05
29	e	601	CLA	C1B-NB	5.53	1.44	1.37
29	B	832	CLA	MG-ND	-5.53	1.94	2.05
29	b	602	CLA	MG-ND	-5.52	1.94	2.05
29	2	608	CLA	C1B-NB	5.52	1.44	1.37
29	4	608	CLA	MG-ND	-5.52	1.94	2.05
29	5	612	CLA	MG-ND	-5.52	1.94	2.05
29	9	614	CLA	MG-ND	-5.52	1.94	2.05
29	F	203	CLA	MG-ND	-5.52	1.94	2.05
29	a	609	CLA	C1B-NB	5.52	1.44	1.37
30	2	610	KC2	C4B-NB	5.52	1.44	1.37
29	5	607	CLA	MG-ND	-5.52	1.94	2.05
29	B	825	CLA	MG-ND	-5.52	1.94	2.05
29	5	612	CLA	C1B-NB	5.52	1.44	1.37
29	d	609	CLA	C1B-NB	5.52	1.44	1.37
29	9	612	CLA	MG-ND	-5.52	1.94	2.05
29	3	603	CLA	C1B-NB	5.52	1.44	1.37
29	B	829	CLA	C1B-NB	5.52	1.44	1.37
29	6	602	CLA	MG-NB	-5.52	1.94	2.05
29	9	609	CLA	C1B-NB	5.52	1.44	1.37
29	J	102	CLA	MG-ND	-5.51	1.94	2.05
29	6	606	CLA	MG-ND	-5.51	1.94	2.05
29	B	824	CLA	MG-NA	-5.51	1.93	2.06
29	a	611	CLA	C1B-NB	5.51	1.44	1.37
29	7	608	CLA	C1B-NB	5.51	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	823	CLA	MG-ND	-5.51	1.94	2.05
29	1	604	CLA	MG-NB	-5.51	1.94	2.05
29	c	614	CLA	MG-ND	-5.51	1.94	2.05
29	B	814	CLA	MG-ND	-5.51	1.94	2.05
29	5	604	CLA	C1B-NB	5.51	1.44	1.37
29	Z	306	CLA	MG-ND	-5.51	1.94	2.05
29	6	604	CLA	C1B-NB	5.51	1.44	1.37
29	B	835	CLA	MG-ND	-5.50	1.94	2.05
29	B	836	CLA	MG-ND	-5.50	1.94	2.05
29	6	611	CLA	MG-ND	-5.50	1.94	2.05
29	4	607	CLA	C1B-NB	5.50	1.44	1.37
29	B	830	CLA	MG-ND	-5.50	1.94	2.05
29	A	843	CLA	MG-ND	-5.50	1.94	2.05
29	a	612	CLA	MG-ND	-5.50	1.94	2.05
29	6	602	CLA	MG-NA	-5.50	1.93	2.06
29	5	604	CLA	MG-NB	-5.50	1.94	2.05
29	9	604	CLA	C1B-NB	5.50	1.44	1.37
29	R	202	CLA	MG-NB	-5.49	1.94	2.05
29	A	817	CLA	MG-NA	-5.49	1.93	2.06
29	a	606	CLA	MG-ND	-5.49	1.94	2.05
29	6	602	CLA	C1B-NB	5.49	1.44	1.37
29	c	604	CLA	C1B-NB	5.49	1.44	1.37
29	6	601	CLA	MG-ND	-5.49	1.94	2.05
29	2	602	CLA	C1B-NB	5.49	1.44	1.37
29	6	612	CLA	MG-ND	-5.49	1.94	2.05
29	A	824	CLA	C1B-NB	5.48	1.44	1.37
29	B	805	CLA	C1B-NB	5.48	1.44	1.37
29	F	204	CLA	MG-ND	-5.48	1.94	2.05
29	1	612	CLA	MG-ND	-5.48	1.94	2.05
29	1	601	CLA	MG-NA	-5.48	1.93	2.06
29	A	830	CLA	MG-ND	-5.48	1.94	2.05
29	A	838	CLA	MG-ND	-5.48	1.94	2.05
29	c	602	CLA	MG-ND	-5.48	1.94	2.05
29	7	602	CLA	C1B-NB	5.48	1.44	1.37
29	e	607	CLA	C1B-NB	5.48	1.44	1.37
29	a	602	CLA	MG-ND	-5.48	1.94	2.05
29	B	802	CLA	MG-NB	-5.48	1.94	2.05
29	7	603	CLA	C1B-NB	5.47	1.44	1.37
29	B	831	CLA	MG-NB	-5.47	1.94	2.05
29	Z	304	CLA	MG-ND	-5.47	1.94	2.05
29	7	609	CLA	MG-ND	-5.47	1.94	2.05
29	4	603	CLA	C1B-NB	5.47	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	7	607	CLA	MG-ND	-5.47	1.94	2.05
29	B	817	CLA	MG-ND	-5.47	1.94	2.05
29	5	602	CLA	C1B-NB	5.47	1.44	1.37
29	a	601	CLA	C1B-NB	5.47	1.44	1.37
29	8	601	CLA	C1B-NB	5.47	1.44	1.37
29	8	604	CLA	MG-ND	-5.47	1.95	2.05
29	B	833	CLA	MG-NB	-5.47	1.95	2.05
29	c	602	CLA	C1B-NB	5.47	1.44	1.37
29	d	611	CLA	MG-ND	-5.47	1.95	2.05
29	b	601	CLA	MG-ND	-5.46	1.95	2.05
29	6	609	CLA	C1B-NB	5.46	1.44	1.37
29	d	606	CLA	MG-ND	-5.46	1.95	2.05
29	6	609	CLA	MG-ND	-5.46	1.95	2.05
29	7	604	CLA	MG-ND	-5.46	1.95	2.05
29	J	102	CLA	C1B-NB	5.46	1.44	1.37
29	a	602	CLA	C1B-NB	5.46	1.44	1.37
29	b	604	CLA	C1B-NB	5.46	1.44	1.37
29	1	603	CLA	MG-ND	-5.46	1.95	2.05
29	2	606	CLA	C1B-NB	5.46	1.44	1.37
29	d	607	CLA	C1B-NB	5.46	1.44	1.37
29	c	613	CLA	C1B-NB	5.46	1.44	1.37
29	L	207	CLA	MG-NA	-5.46	1.93	2.06
29	A	838	CLA	C1B-NB	5.45	1.44	1.37
29	B	823	CLA	MG-ND	-5.45	1.95	2.05
29	K	101	CLA	MG-ND	-5.45	1.95	2.05
29	7	611	CLA	C1B-NB	5.45	1.44	1.37
29	J	102	CLA	MG-NB	-5.45	1.95	2.05
29	A	815	CLA	MG-ND	-5.45	1.95	2.05
29	5	609	CLA	C1B-NB	5.45	1.44	1.37
29	5	607	CLA	C1B-NB	5.45	1.44	1.37
29	3	601	CLA	C1B-NB	5.45	1.44	1.37
29	c	606	CLA	C1B-NB	5.45	1.44	1.37
29	8	602	CLA	C1B-NB	5.45	1.44	1.37
29	5	613	CLA	C1B-NB	5.45	1.44	1.37
29	4	604	CLA	C1B-NB	5.44	1.44	1.37
29	5	601	CLA	MG-ND	-5.44	1.95	2.05
29	1	613	CLA	MG-ND	-5.44	1.95	2.05
29	B	811	CLA	C1B-NB	5.44	1.44	1.37
29	7	601	CLA	C1B-NB	5.44	1.44	1.37
29	2	611	CLA	MG-ND	-5.44	1.95	2.05
29	A	833	CLA	MG-ND	-5.44	1.95	2.05
29	d	605	CLA	C1B-NB	5.44	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	9	603	CLA	MG-ND	-5.44	1.95	2.05
29	9	606	CLA	MG-ND	-5.44	1.95	2.05
29	c	614	CLA	C1B-NB	5.44	1.44	1.37
29	4	604	CLA	MG-ND	-5.44	1.95	2.05
29	b	603	CLA	C1B-NB	5.44	1.44	1.37
29	c	607	CLA	C1B-NB	5.44	1.44	1.37
29	A	817	CLA	MG-ND	-5.44	1.95	2.05
29	B	815	CLA	MG-ND	-5.44	1.95	2.05
29	b	602	CLA	MG-NB	-5.44	1.95	2.05
29	3	609	CLA	MG-ND	-5.44	1.95	2.05
29	1	613	CLA	C1B-NB	5.43	1.44	1.37
29	3	607	CLA	C1B-NB	5.43	1.44	1.37
29	F	202	CLA	C1B-NB	5.43	1.44	1.37
29	b	608	CLA	MG-ND	-5.43	1.95	2.05
29	L	202	CLA	C1B-NB	5.43	1.44	1.37
29	e	604	CLA	C1B-NB	5.43	1.44	1.37
30	Z	307	KC2	C4B-NB	5.43	1.44	1.37
29	A	814	CLA	MG-NB	-5.43	1.95	2.05
29	2	601	CLA	MG-ND	-5.43	1.95	2.05
29	1	607	CLA	MG-ND	-5.43	1.95	2.05
29	3	609	CLA	C1B-NB	5.43	1.44	1.37
29	e	603	CLA	MG-ND	-5.43	1.95	2.05
29	9	614	CLA	MG-NB	-5.43	1.95	2.05
29	8	607	CLA	C1B-NB	5.43	1.44	1.37
29	A	813	CLA	C1B-NB	5.43	1.44	1.37
29	B	813	CLA	MG-ND	-5.43	1.95	2.05
29	B	814	CLA	MG-NA	-5.42	1.93	2.06
29	8	615	CLA	MG-ND	-5.42	1.95	2.05
29	2	611	CLA	C1B-NB	5.42	1.44	1.37
29	5	613	CLA	MG-ND	-5.42	1.95	2.05
29	A	825	CLA	MG-ND	-5.42	1.95	2.05
29	F	202	CLA	MG-ND	-5.42	1.95	2.05
29	B	829	CLA	MG-NA	-5.42	1.93	2.06
29	9	613	CLA	MG-ND	-5.42	1.95	2.05
29	7	605	CLA	MG-ND	-5.42	1.95	2.05
29	3	605	CLA	MG-ND	-5.42	1.95	2.05
29	2	601	CLA	MG-NA	-5.42	1.93	2.06
29	A	822	CLA	MG-ND	-5.42	1.95	2.05
29	5	606	CLA	C1B-NB	5.42	1.44	1.37
29	6	606	CLA	MG-NB	-5.42	1.95	2.05
29	d	602	CLA	MG-ND	-5.42	1.95	2.05
29	B	839	CLA	C1B-NB	5.42	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	612	CLA	C1B-NB	5.42	1.44	1.37
29	c	601	CLA	MG-ND	-5.42	1.95	2.05
29	3	604	CLA	MG-ND	-5.42	1.95	2.05
29	d	604	CLA	MG-ND	-5.41	1.95	2.05
29	A	821	CLA	MG-ND	-5.41	1.95	2.05
29	B	803	CLA	MG-NB	-5.41	1.95	2.05
29	9	601	CLA	MG-ND	-5.41	1.95	2.05
29	d	603	CLA	MG-ND	-5.41	1.95	2.05
29	6	607	CLA	MG-ND	-5.41	1.95	2.05
29	5	601	CLA	MG-NB	-5.41	1.95	2.05
29	B	837	CLA	MG-NB	-5.41	1.95	2.05
29	B	838	CLA	C1B-NB	5.41	1.44	1.37
29	A	807	CLA	MG-ND	-5.41	1.95	2.05
29	B	837	CLA	MG-ND	-5.41	1.95	2.05
29	L	204	CLA	MG-ND	-5.41	1.95	2.05
29	9	614	CLA	MG-NA	-5.41	1.93	2.06
29	d	601	CLA	MG-ND	-5.41	1.95	2.05
29	5	604	CLA	MG-NA	-5.41	1.93	2.06
29	1	606	CLA	C1B-NB	5.41	1.44	1.37
29	2	609	CLA	MG-NB	-5.41	1.95	2.05
29	d	605	CLA	MG-NB	-5.41	1.95	2.05
29	B	841	CLA	C1B-NB	5.41	1.44	1.37
29	5	609	CLA	MG-ND	-5.41	1.95	2.05
29	2	612	CLA	C1B-NB	5.41	1.44	1.37
29	A	811	CLA	MG-ND	-5.41	1.95	2.05
29	3	604	CLA	C1B-NB	5.40	1.44	1.37
29	b	611	CLA	MG-ND	-5.40	1.95	2.05
29	B	835	CLA	C1B-NB	5.40	1.44	1.37
29	b	607	CLA	C1B-NB	5.40	1.44	1.37
29	3	603	CLA	MG-ND	-5.40	1.95	2.05
29	A	828	CLA	MG-ND	-5.40	1.95	2.05
29	5	611	CLA	C1B-NB	5.40	1.44	1.37
29	4	609	CLA	C1B-NB	5.40	1.44	1.37
29	5	606	CLA	MG-ND	-5.40	1.95	2.05
29	B	807	CLA	MG-ND	-5.40	1.95	2.05
29	c	604	CLA	MG-ND	-5.40	1.95	2.05
29	3	602	CLA	C1B-NB	5.40	1.44	1.37
29	6	611	CLA	C1B-NB	5.40	1.44	1.37
29	1	606	CLA	MG-ND	-5.40	1.95	2.05
29	O	203	CLA	MG-NB	-5.40	1.95	2.05
29	1	604	CLA	MG-ND	-5.39	1.95	2.05
29	B	828	CLA	MG-NB	-5.39	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	7	611	CLA	MG-ND	-5.39	1.95	2.05
29	4	606	CLA	MG-NB	-5.39	1.95	2.05
29	7	612	CLA	MG-NB	-5.39	1.95	2.05
29	1	605	CLA	MG-NB	-5.39	1.95	2.05
29	4	602	CLA	MG-ND	-5.39	1.95	2.05
29	b	608	CLA	C1B-NB	5.39	1.44	1.37
29	A	816	CLA	MG-ND	-5.39	1.95	2.05
29	a	604	CLA	MG-NB	-5.39	1.95	2.05
29	A	837	CLA	MG-ND	-5.39	1.95	2.05
29	c	605	CLA	C1B-NB	5.39	1.44	1.37
29	3	611	CLA	MG-NB	-5.39	1.95	2.05
29	4	609	CLA	MG-ND	-5.39	1.95	2.05
29	3	605	CLA	C1B-NB	5.39	1.44	1.37
29	Z	304	CLA	C1B-NB	5.39	1.44	1.37
29	8	603	CLA	MG-ND	-5.38	1.95	2.05
29	9	603	CLA	C1B-NB	5.38	1.44	1.37
29	e	606	CLA	C1B-NB	5.38	1.44	1.37
29	5	603	CLA	MG-ND	-5.38	1.95	2.05
29	B	828	CLA	MG-ND	-5.38	1.95	2.05
29	4	601	CLA	C1B-NB	5.38	1.44	1.37
29	7	608	CLA	MG-ND	-5.38	1.95	2.05
29	O	202	CLA	MG-NB	-5.38	1.95	2.05
29	8	615	CLA	C1B-NB	5.38	1.44	1.37
29	e	602	CLA	MG-ND	-5.38	1.95	2.05
29	3	607	CLA	MG-ND	-5.38	1.95	2.05
29	B	808	CLA	MG-NB	-5.37	1.95	2.05
29	B	827	CLA	MG-NB	-5.37	1.95	2.05
29	3	610	CLA	C1B-NB	5.37	1.44	1.37
29	A	802	CLA	MG-ND	-5.37	1.95	2.05
29	3	612	CLA	MG-ND	-5.37	1.95	2.05
29	3	608	CLA	MG-ND	-5.37	1.95	2.05
29	3	611	CLA	C1B-NB	5.37	1.44	1.37
29	2	609	CLA	MG-ND	-5.37	1.95	2.05
29	a	603	CLA	MG-NB	-5.37	1.95	2.05
29	A	820	CLA	MG-ND	-5.37	1.95	2.05
29	2	603	CLA	MG-ND	-5.37	1.95	2.05
29	2	603	CLA	C1B-NB	5.37	1.44	1.37
29	4	608	CLA	C1B-NB	5.37	1.44	1.37
29	3	601	CLA	MG-ND	-5.37	1.95	2.05
29	e	608	CLA	MG-ND	-5.37	1.95	2.05
29	B	812	CLA	MG-ND	-5.37	1.95	2.05
29	B	811	CLA	MG-ND	-5.37	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	819	CLA	MG-ND	-5.37	1.95	2.05
29	B	808	CLA	MG-NA	-5.37	1.93	2.06
29	2	602	CLA	MG-ND	-5.37	1.95	2.05
29	O	201	CLA	MG-ND	-5.37	1.95	2.05
29	A	818	CLA	MG-ND	-5.37	1.95	2.05
29	A	808	CLA	MG-ND	-5.36	1.95	2.05
29	a	607	CLA	C1B-NB	5.36	1.44	1.37
29	A	805	CLA	C1B-NB	5.36	1.44	1.37
29	b	601	CLA	C1B-NB	5.36	1.44	1.37
29	b	610	CLA	C1B-NB	5.36	1.44	1.37
29	B	829	CLA	MG-ND	-5.36	1.95	2.05
29	c	612	CLA	MG-ND	-5.36	1.95	2.05
29	2	609	CLA	MG-NA	-5.36	1.93	2.06
29	c	609	CLA	MG-ND	-5.36	1.95	2.05
29	c	613	CLA	MG-ND	-5.36	1.95	2.05
29	9	602	CLA	MG-ND	-5.36	1.95	2.05
29	8	608	CLA	MG-NB	-5.36	1.95	2.05
29	A	820	CLA	C1B-NB	5.36	1.44	1.37
29	A	815	CLA	MG-NB	-5.36	1.95	2.05
29	a	601	CLA	MG-ND	-5.35	1.95	2.05
29	A	815	CLA	C1B-NB	5.35	1.44	1.37
29	c	607	CLA	MG-ND	-5.35	1.95	2.05
29	B	804	CLA	C1B-NB	5.35	1.44	1.37
29	6	605	CLA	MG-NB	-5.35	1.95	2.05
29	A	813	CLA	MG-ND	-5.35	1.95	2.05
29	A	808	CLA	C1B-NB	5.35	1.44	1.37
29	A	821	CLA	C1B-NB	5.35	1.44	1.37
29	A	843	CLA	C1B-NB	5.35	1.44	1.37
29	A	822	CLA	C1B-NB	5.35	1.44	1.37
29	a	609	CLA	MG-ND	-5.35	1.95	2.05
29	1	612	CLA	C1B-NB	5.35	1.44	1.37
29	1	602	CLA	MG-ND	-5.35	1.95	2.05
29	3	602	CLA	MG-NA	-5.35	1.93	2.06
29	e	611	CLA	C1B-NB	5.35	1.44	1.37
29	d	602	CLA	MG-NB	-5.35	1.95	2.05
29	d	604	CLA	MG-NB	-5.35	1.95	2.05
29	1	609	CLA	MG-ND	-5.34	1.95	2.05
29	2	612	CLA	MG-ND	-5.34	1.95	2.05
29	9	608	CLA	MG-ND	-5.34	1.95	2.05
29	B	838	CLA	MG-ND	-5.34	1.95	2.05
29	6	603	CLA	MG-NA	-5.34	1.93	2.06
29	9	613	CLA	MG-NB	-5.34	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	602	CLA	MG-NB	-5.34	1.95	2.05
29	K	102	CLA	C1B-NB	5.34	1.44	1.37
29	6	609	CLA	MG-NA	-5.34	1.93	2.06
29	B	810	CLA	MG-ND	-5.34	1.95	2.05
29	4	610	CLA	MG-ND	-5.34	1.95	2.05
29	8	606	CLA	MG-ND	-5.34	1.95	2.05
29	A	819	CLA	MG-NB	-5.34	1.95	2.05
29	e	601	CLA	MG-ND	-5.34	1.95	2.05
29	A	829	CLA	C1B-NB	5.34	1.44	1.37
29	b	607	CLA	MG-ND	-5.34	1.95	2.05
29	3	610	CLA	MG-NB	-5.34	1.95	2.05
29	7	605	CLA	MG-NB	-5.34	1.95	2.05
29	A	824	CLA	MG-ND	-5.34	1.95	2.05
29	3	602	CLA	MG-ND	-5.33	1.95	2.05
29	3	611	CLA	MG-ND	-5.33	1.95	2.05
29	B	834	CLA	MG-ND	-5.33	1.95	2.05
29	O	202	CLA	MG-NA	-5.33	1.93	2.06
29	5	611	CLA	MG-ND	-5.33	1.95	2.05
29	1	611	CLA	MG-ND	-5.33	1.95	2.05
29	9	609	CLA	MG-NB	-5.33	1.95	2.05
29	B	830	CLA	MG-NB	-5.33	1.95	2.05
29	A	814	CLA	MG-NA	-5.33	1.93	2.06
29	5	604	CLA	MG-ND	-5.33	1.95	2.05
29	5	605	CLA	MG-NB	-5.33	1.95	2.05
29	a	604	CLA	MG-NA	-5.33	1.93	2.06
29	b	606	CLA	MG-NB	-5.33	1.95	2.05
29	8	602	CLA	MG-NB	-5.33	1.95	2.05
29	8	608	CLA	MG-ND	-5.33	1.95	2.05
29	A	835	CLA	MG-ND	-5.33	1.95	2.05
29	Z	304	CLA	MG-NB	-5.33	1.95	2.05
29	B	838	CLA	MG-NA	-5.33	1.93	2.06
29	a	603	CLA	C1B-NB	5.33	1.44	1.37
29	8	601	CLA	MG-ND	-5.33	1.95	2.05
29	7	601	CLA	MG-ND	-5.32	1.95	2.05
29	A	835	CLA	C1B-NB	5.32	1.44	1.37
29	2	607	CLA	C1B-NB	5.32	1.44	1.37
29	A	828	CLA	MG-NB	-5.32	1.95	2.05
29	B	814	CLA	C1B-NB	5.32	1.44	1.37
29	B	820	CLA	MG-ND	-5.32	1.95	2.05
29	A	836	CLA	C1B-NB	5.32	1.44	1.37
29	B	804	CLA	MG-ND	-5.32	1.95	2.05
29	7	602	CLA	MG-ND	-5.32	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	827	CLA	MG-NB	-5.32	1.95	2.05
29	1	611	CLA	MG-NB	-5.32	1.95	2.05
29	b	606	CLA	C1B-NB	5.32	1.44	1.37
29	A	832	CLA	MG-NB	-5.32	1.95	2.05
29	a	608	CLA	MG-ND	-5.32	1.95	2.05
29	1	603	CLA	MG-NB	-5.32	1.95	2.05
29	A	817	CLA	MG-NB	-5.32	1.95	2.05
29	6	601	CLA	C1B-NB	5.31	1.44	1.37
29	L	201	CLA	C1B-NB	5.31	1.44	1.37
29	F	203	CLA	C1B-NB	5.31	1.44	1.37
29	e	610	CLA	MG-ND	-5.31	1.95	2.05
29	K	102	CLA	MG-NA	-5.31	1.93	2.06
29	b	603	CLA	MG-ND	-5.31	1.95	2.05
29	c	602	CLA	MG-NB	-5.31	1.95	2.05
29	d	609	CLA	MG-ND	-5.31	1.95	2.05
29	5	605	CLA	C1B-NB	5.31	1.44	1.37
29	6	606	CLA	C1B-NB	5.31	1.44	1.37
29	5	602	CLA	MG-NB	-5.31	1.95	2.05
30	c	610	KC2	C4B-NB	5.31	1.44	1.37
29	A	824	CLA	MG-NB	-5.31	1.95	2.05
29	7	604	CLA	MG-NB	-5.31	1.95	2.05
29	A	830	CLA	C1B-NB	5.31	1.44	1.37
29	a	605	CLA	C1B-NB	5.31	1.44	1.37
29	1	601	CLA	MG-NB	-5.31	1.95	2.05
29	B	813	CLA	C1B-NB	5.30	1.44	1.37
29	B	816	CLA	MG-NB	-5.30	1.95	2.05
29	A	812	CLA	MG-NB	-5.30	1.95	2.05
29	1	603	CLA	C1B-NB	5.30	1.44	1.37
29	4	610	CLA	C1B-NB	5.30	1.44	1.37
29	d	608	CLA	MG-NA	-5.30	1.93	2.06
29	9	602	CLA	MG-NB	-5.30	1.95	2.05
29	A	824	CLA	MG-NA	-5.30	1.93	2.06
29	A	820	CLA	MG-NB	-5.30	1.95	2.05
29	6	608	CLA	MG-NA	-5.30	1.93	2.06
29	a	612	CLA	C1B-NB	5.30	1.44	1.37
29	B	805	CLA	MG-ND	-5.30	1.95	2.05
29	A	803	CLA	MG-NA	-5.30	1.93	2.06
29	A	818	CLA	C1B-NB	5.30	1.44	1.37
29	5	602	CLA	MG-NA	-5.30	1.93	2.06
29	F	204	CLA	C1B-NB	5.29	1.44	1.37
29	a	611	CLA	MG-ND	-5.29	1.95	2.05
29	a	602	CLA	MG-NA	-5.29	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	603	CLA	C1B-NB	5.29	1.44	1.37
29	5	602	CLA	MG-ND	-5.29	1.95	2.05
29	L	203	CLA	MG-ND	-5.29	1.95	2.05
29	b	610	CLA	MG-ND	-5.29	1.95	2.05
29	9	611	CLA	MG-NB	-5.29	1.95	2.05
29	5	608	CLA	MG-NB	-5.29	1.95	2.05
29	9	605	CLA	C1B-NB	5.29	1.44	1.37
29	A	839	CLA	C1B-NB	5.29	1.44	1.37
29	9	602	CLA	MG-NA	-5.29	1.93	2.06
29	e	604	CLA	MG-ND	-5.29	1.95	2.05
29	6	608	CLA	C1B-NB	5.29	1.44	1.37
29	A	841	CLA	MG-NB	-5.28	1.95	2.05
30	3	606	KC2	C4B-NB	5.28	1.44	1.37
29	B	816	CLA	C1B-NB	5.28	1.44	1.37
29	5	603	CLA	MG-NB	-5.28	1.95	2.05
29	K	102	CLA	MG-ND	-5.28	1.95	2.05
29	4	606	CLA	C1B-NB	5.28	1.44	1.37
29	4	607	CLA	MG-ND	-5.28	1.95	2.05
29	B	815	CLA	MG-NB	-5.28	1.95	2.05
29	3	612	CLA	C1B-NB	5.28	1.44	1.37
29	B	815	CLA	MG-NA	-5.28	1.93	2.06
29	9	602	CLA	C1B-NB	5.28	1.44	1.37
29	9	612	CLA	C1B-NB	5.28	1.44	1.37
29	Z	306	CLA	C1B-NB	5.28	1.44	1.37
29	c	612	CLA	MG-NA	-5.28	1.93	2.06
29	e	602	CLA	MG-NB	-5.28	1.95	2.05
29	2	603	CLA	MG-NA	-5.28	1.93	2.06
29	c	603	CLA	MG-ND	-5.27	1.95	2.05
29	6	606	CLA	MG-NA	-5.27	1.93	2.06
29	A	816	CLA	C1B-NB	5.27	1.44	1.37
29	B	820	CLA	C1B-NB	5.27	1.44	1.37
29	A	834	CLA	MG-ND	-5.27	1.95	2.05
29	9	611	CLA	C1B-NB	5.27	1.44	1.37
29	6	608	CLA	MG-ND	-5.27	1.95	2.05
29	B	841	CLA	MG-ND	-5.27	1.95	2.05
29	5	608	CLA	MG-ND	-5.27	1.95	2.05
29	B	837	CLA	C1B-NB	5.27	1.44	1.37
29	e	608	CLA	MG-NA	-5.27	1.93	2.06
29	4	602	CLA	MG-NB	-5.27	1.95	2.05
29	B	818	CLA	MG-NB	-5.27	1.95	2.05
29	A	803	CLA	C1B-NB	5.27	1.44	1.37
29	B	828	CLA	C1B-NB	5.27	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	L	204	CLA	C1B-NB	5.27	1.44	1.37
29	B	829	CLA	MG-NB	-5.27	1.95	2.05
29	A	808	CLA	MG-NA	-5.27	1.93	2.06
29	6	605	CLA	C1B-NB	5.27	1.44	1.37
29	A	806	CLA	C1B-NB	5.27	1.44	1.37
29	d	605	CLA	MG-NA	-5.26	1.93	2.06
29	2	602	CLA	MG-NB	-5.26	1.95	2.05
29	8	605	CLA	MG-ND	-5.26	1.95	2.05
29	Z	301	CLA	MG-ND	-5.26	1.95	2.05
29	L	201	CLA	MG-NB	-5.26	1.95	2.05
29	A	819	CLA	MG-NA	-5.26	1.93	2.06
29	9	603	CLA	MG-NB	-5.26	1.95	2.05
29	B	840	CLA	MG-ND	-5.26	1.95	2.05
29	B	832	CLA	MG-NB	-5.26	1.95	2.05
29	d	604	CLA	MG-NA	-5.26	1.93	2.06
29	A	825	CLA	C1B-NB	5.26	1.44	1.37
29	6	604	CLA	MG-ND	-5.26	1.95	2.05
29	e	607	CLA	MG-ND	-5.26	1.95	2.05
29	6	609	CLA	MG-NB	-5.26	1.95	2.05
29	9	609	CLA	MG-ND	-5.26	1.95	2.05
29	L	202	CLA	MG-NB	-5.26	1.95	2.05
29	d	606	CLA	C1B-NB	5.26	1.44	1.37
29	a	604	CLA	MG-ND	-5.26	1.95	2.05
29	5	603	CLA	C1B-NB	5.25	1.44	1.37
29	A	833	CLA	C1B-NB	5.25	1.44	1.37
29	A	809	CLA	C1B-NB	5.25	1.44	1.37
29	A	814	CLA	C1B-NB	5.25	1.44	1.37
29	A	807	CLA	C1B-NB	5.25	1.44	1.37
29	b	604	CLA	MG-ND	-5.25	1.95	2.05
29	2	606	CLA	MG-NB	-5.25	1.95	2.05
29	3	601	CLA	MG-NB	-5.25	1.95	2.05
29	8	606	CLA	MG-NB	-5.25	1.95	2.05
29	d	612	CLA	MG-NB	-5.25	1.95	2.05
29	A	834	CLA	MG-NA	-5.25	1.93	2.06
29	c	605	CLA	MG-NB	-5.25	1.95	2.05
29	4	603	CLA	MG-ND	-5.25	1.95	2.05
29	c	601	CLA	MG-NA	-5.25	1.93	2.06
29	7	612	CLA	C1B-NB	5.24	1.44	1.37
29	2	601	CLA	MG-NB	-5.24	1.95	2.05
29	B	835	CLA	MG-NB	-5.24	1.95	2.05
29	2	602	CLA	MG-NA	-5.24	1.93	2.06
29	6	612	CLA	C1B-NB	5.24	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	819	CLA	C1B-NB	5.24	1.44	1.37
29	c	601	CLA	MG-NB	-5.24	1.95	2.05
29	3	602	CLA	MG-NB	-5.24	1.95	2.05
29	O	201	CLA	MG-NA	-5.24	1.93	2.06
29	O	201	CLA	C1B-NB	5.24	1.44	1.37
29	A	815	CLA	MG-NA	-5.24	1.93	2.06
29	B	834	CLA	C1B-NB	5.24	1.44	1.37
29	B	836	CLA	C1B-NB	5.24	1.44	1.37
29	A	842	CLA	MG-ND	-5.24	1.95	2.05
29	3	610	CLA	MG-NA	-5.24	1.93	2.06
29	A	831	CLA	MG-NB	-5.24	1.95	2.05
29	9	613	CLA	C1B-NB	5.24	1.44	1.37
29	2	605	CLA	MG-NB	-5.23	1.95	2.05
29	7	612	CLA	MG-NA	-5.23	1.93	2.06
29	2	603	CLA	MG-NB	-5.23	1.95	2.05
29	5	609	CLA	MG-NB	-5.23	1.95	2.05
29	A	805	CLA	MG-ND	-5.23	1.95	2.05
29	8	603	CLA	MG-NA	-5.23	1.93	2.06
29	A	822	CLA	MG-NA	-5.23	1.93	2.06
29	8	607	CLA	MG-NB	-5.23	1.95	2.05
29	B	824	CLA	MG-NB	-5.23	1.95	2.05
29	A	804	CLA	C1B-NB	5.23	1.44	1.37
29	d	603	CLA	MG-NB	-5.23	1.95	2.05
29	A	806	CLA	MG-NB	-5.23	1.95	2.05
29	c	603	CLA	MG-NB	-5.23	1.95	2.05
29	B	806	CLA	C1B-NB	5.23	1.44	1.37
29	c	608	CLA	MG-ND	-5.22	1.95	2.05
29	A	839	CLA	MG-NB	-5.22	1.95	2.05
29	B	821	CLA	MG-NB	-5.22	1.95	2.05
29	4	611	CLA	MG-NB	-5.22	1.95	2.05
29	4	604	CLA	MG-NB	-5.22	1.95	2.05
29	9	605	CLA	MG-NB	-5.22	1.95	2.05
29	7	609	CLA	MG-NA	-5.22	1.93	2.06
29	e	604	CLA	MG-NB	-5.22	1.95	2.05
29	e	608	CLA	MG-NB	-5.22	1.95	2.05
29	5	601	CLA	MG-NA	-5.22	1.93	2.06
29	A	836	CLA	MG-ND	-5.21	1.95	2.05
29	A	826	CLA	MG-NB	-5.21	1.95	2.05
29	B	825	CLA	C1B-NB	5.21	1.44	1.37
29	1	609	CLA	MG-NB	-5.21	1.95	2.05
29	A	802	CLA	C1B-NB	5.21	1.44	1.37
29	b	611	CLA	C1B-NB	5.21	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	814	CLA	MG-ND	-5.21	1.95	2.05
29	e	611	CLA	MG-NB	-5.21	1.95	2.05
29	B	823	CLA	C1B-NB	5.21	1.44	1.37
29	B	814	CLA	MG-NB	-5.20	1.95	2.05
29	7	609	CLA	MG-NB	-5.20	1.95	2.05
29	b	610	CLA	MG-NB	-5.20	1.95	2.05
29	B	832	CLA	C1B-NB	5.20	1.44	1.37
29	A	803	CLA	MG-ND	-5.20	1.95	2.05
29	B	819	CLA	MG-NA	-5.20	1.93	2.06
29	K	101	CLA	C1B-NB	5.20	1.44	1.37
29	A	818	CLA	MG-NA	-5.20	1.93	2.06
29	A	843	CLA	MG-NB	-5.20	1.95	2.05
29	5	613	CLA	MG-NB	-5.20	1.95	2.05
29	F	203	CLA	MG-NB	-5.20	1.95	2.05
29	A	837	CLA	C1B-NB	5.20	1.44	1.37
29	7	603	CLA	MG-ND	-5.19	1.95	2.05
29	B	811	CLA	MG-NB	-5.19	1.95	2.05
29	d	608	CLA	MG-ND	-5.19	1.95	2.05
29	B	804	CLA	MG-NA	-5.19	1.93	2.06
29	8	605	CLA	MG-NB	-5.19	1.95	2.05
29	1	604	CLA	MG-NA	-5.19	1.93	2.06
29	e	606	CLA	MG-NB	-5.19	1.95	2.05
29	Z	305	CLA	C1B-NB	5.19	1.44	1.37
29	B	822	CLA	MG-NB	-5.19	1.95	2.05
29	A	804	CLA	MG-NB	-5.19	1.95	2.05
29	B	836	CLA	MG-NB	-5.19	1.95	2.05
29	B	818	CLA	C1B-NB	5.18	1.44	1.37
29	9	607	CLA	C1B-NB	5.18	1.44	1.37
29	B	822	CLA	MG-NA	-5.18	1.94	2.06
29	8	603	CLA	MG-NB	-5.18	1.95	2.05
29	a	611	CLA	MG-NB	-5.18	1.95	2.05
29	1	605	CLA	C1B-NB	5.18	1.44	1.37
29	8	602	CLA	MG-NA	-5.18	1.94	2.06
29	3	610	CLA	MG-ND	-5.18	1.95	2.05
29	b	607	CLA	MG-NB	-5.18	1.95	2.05
29	F	202	CLA	MG-NB	-5.18	1.95	2.05
29	e	610	CLA	MG-NB	-5.18	1.95	2.05
29	d	603	CLA	C1B-NB	5.18	1.44	1.37
29	c	613	CLA	MG-NB	-5.18	1.95	2.05
29	3	611	CLA	MG-NA	-5.18	1.94	2.06
29	A	822	CLA	MG-NB	-5.18	1.95	2.05
29	8	607	CLA	MG-ND	-5.18	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	611	CLA	MG-NA	-5.18	1.94	2.06
29	b	604	CLA	MG-NB	-5.18	1.95	2.05
29	1	613	CLA	MG-NA	-5.18	1.94	2.06
29	b	610	CLA	MG-NA	-5.18	1.94	2.06
29	B	823	CLA	MG-NB	-5.17	1.95	2.05
29	B	812	CLA	MG-NB	-5.17	1.95	2.05
29	a	611	CLA	MG-NA	-5.17	1.94	2.06
29	A	810	CLA	MG-NB	-5.17	1.95	2.05
29	b	604	CLA	MG-NA	-5.17	1.94	2.06
29	2	604	CLA	MG-ND	-5.17	1.95	2.05
29	8	604	CLA	C1B-NB	5.17	1.44	1.37
29	b	602	CLA	MG-NA	-5.17	1.94	2.06
29	7	603	CLA	MG-NB	-5.16	1.95	2.05
29	B	827	CLA	MG-NA	-5.16	1.94	2.06
29	A	821	CLA	MG-NB	-5.16	1.95	2.05
29	3	603	CLA	MG-NB	-5.16	1.95	2.05
29	B	809	CLA	MG-NB	-5.16	1.95	2.05
29	A	821	CLA	MG-NA	-5.16	1.94	2.06
29	9	604	CLA	MG-ND	-5.16	1.95	2.05
29	2	607	CLA	MG-NB	-5.16	1.95	2.05
29	3	604	CLA	MG-NB	-5.16	1.95	2.05
29	7	603	CLA	MG-NA	-5.16	1.94	2.06
29	9	603	CLA	MG-NA	-5.16	1.94	2.06
29	B	826	CLA	C1B-NB	5.16	1.44	1.37
29	9	608	CLA	MG-NB	-5.16	1.95	2.05
29	c	614	CLA	MG-NB	-5.16	1.95	2.05
29	8	615	CLA	MG-NB	-5.15	1.95	2.05
29	9	604	CLA	MG-NA	-5.15	1.94	2.06
29	B	828	CLA	MG-NA	-5.15	1.94	2.06
29	a	606	CLA	MG-NB	-5.15	1.95	2.05
29	a	607	CLA	MG-NB	-5.15	1.95	2.05
29	B	803	CLA	MG-NA	-5.15	1.94	2.06
29	2	604	CLA	MG-NB	-5.15	1.95	2.05
29	A	834	CLA	MG-NB	-5.15	1.95	2.05
29	e	603	CLA	MG-NB	-5.15	1.95	2.05
29	1	608	CLA	MG-ND	-5.15	1.95	2.05
29	e	607	CLA	MG-NA	-5.15	1.94	2.06
29	6	608	CLA	MG-NB	-5.14	1.95	2.05
29	5	603	CLA	MG-NA	-5.14	1.94	2.06
29	A	818	CLA	MG-NB	-5.14	1.95	2.05
29	B	830	CLA	MG-NA	-5.14	1.94	2.06
29	B	832	CLA	MG-NA	-5.14	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	831	CLA	MG-ND	-5.14	1.95	2.05
29	A	830	CLA	MG-NB	-5.14	1.95	2.05
29	B	830	CLA	C1B-NB	5.14	1.44	1.37
29	A	811	CLA	MG-NB	-5.14	1.95	2.05
29	B	818	CLA	MG-NA	-5.14	1.94	2.06
29	b	607	CLA	MG-NA	-5.14	1.94	2.06
29	3	608	CLA	MG-NB	-5.14	1.95	2.05
29	Z	306	CLA	MG-NB	-5.14	1.95	2.05
29	B	807	CLA	MG-NA	-5.14	1.94	2.06
29	A	828	CLA	MG-NA	-5.14	1.94	2.06
29	A	825	CLA	MG-NA	-5.13	1.94	2.06
29	9	606	CLA	C1B-NB	5.13	1.44	1.37
29	c	602	CLA	MG-NA	-5.13	1.94	2.06
29	B	833	CLA	C1B-NB	5.13	1.44	1.37
29	a	606	CLA	C1B-NB	5.13	1.44	1.37
29	2	611	CLA	MG-NB	-5.13	1.95	2.05
29	A	834	CLA	C1B-NB	5.13	1.44	1.37
29	7	602	CLA	MG-NB	-5.12	1.95	2.05
29	c	612	CLA	C1B-NB	5.12	1.44	1.37
29	A	813	CLA	MG-NA	-5.12	1.94	2.06
29	B	821	CLA	C1B-NB	5.12	1.44	1.37
29	2	605	CLA	MG-NA	-5.12	1.94	2.06
29	O	202	CLA	MG-ND	-5.12	1.95	2.05
29	1	607	CLA	MG-NB	-5.12	1.95	2.05
29	6	604	CLA	MG-NB	-5.12	1.95	2.05
29	B	809	CLA	C1B-NB	5.12	1.44	1.37
29	e	607	CLA	MG-NB	-5.12	1.95	2.05
29	b	603	CLA	MG-NA	-5.12	1.94	2.06
29	8	608	CLA	MG-NA	-5.12	1.94	2.06
29	A	810	CLA	C1B-NB	5.12	1.44	1.37
29	7	607	CLA	MG-NA	-5.12	1.94	2.06
29	3	601	CLA	MG-NA	-5.12	1.94	2.06
29	4	603	CLA	MG-NA	-5.12	1.94	2.06
29	Z	305	CLA	MG-NB	-5.12	1.95	2.05
29	9	609	CLA	MG-NA	-5.11	1.94	2.06
29	A	832	CLA	C1B-NB	5.11	1.44	1.37
29	5	606	CLA	MG-NB	-5.11	1.95	2.05
29	5	606	CLA	MG-NA	-5.11	1.94	2.06
29	5	609	CLA	MG-NA	-5.11	1.94	2.06
29	2	604	CLA	MG-NA	-5.11	1.94	2.06
29	7	602	CLA	MG-NA	-5.11	1.94	2.06
29	A	806	CLA	MG-NA	-5.11	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	602	CLA	MG-NA	-5.11	1.94	2.06
29	8	601	CLA	MG-NB	-5.10	1.95	2.05
29	A	836	CLA	MG-NA	-5.10	1.94	2.06
29	1	603	CLA	MG-NA	-5.10	1.94	2.06
29	1	609	CLA	MG-NA	-5.10	1.94	2.06
29	2	608	CLA	MG-ND	-5.10	1.95	2.05
29	3	605	CLA	MG-NB	-5.10	1.95	2.05
29	9	607	CLA	MG-NB	-5.10	1.95	2.05
29	L	201	CLA	MG-NA	-5.10	1.94	2.06
29	c	608	CLA	MG-NB	-5.10	1.95	2.05
29	A	823	CLA	MG-NB	-5.10	1.95	2.05
29	8	615	CLA	MG-NA	-5.10	1.94	2.06
29	a	601	CLA	MG-NB	-5.10	1.95	2.05
29	B	805	CLA	MG-NA	-5.10	1.94	2.06
29	B	806	CLA	MG-NB	-5.10	1.95	2.05
29	1	606	CLA	MG-NB	-5.10	1.95	2.05
29	B	820	CLA	MG-NB	-5.09	1.95	2.05
29	6	604	CLA	MG-NA	-5.09	1.94	2.06
29	K	101	CLA	MG-NB	-5.09	1.95	2.05
29	B	817	CLA	MG-NB	-5.09	1.95	2.05
29	1	606	CLA	MG-NA	-5.09	1.94	2.06
29	6	612	CLA	MG-NB	-5.09	1.95	2.05
29	c	609	CLA	MG-NB	-5.09	1.95	2.05
29	6	603	CLA	C1B-NB	5.09	1.44	1.37
29	B	838	CLA	MG-NB	-5.09	1.95	2.05
29	c	604	CLA	MG-NA	-5.09	1.94	2.06
29	4	603	CLA	MG-NB	-5.09	1.95	2.05
29	1	602	CLA	MG-NB	-5.09	1.95	2.05
29	7	611	CLA	MG-NB	-5.09	1.95	2.05
29	B	811	CLA	MG-NA	-5.09	1.94	2.06
29	A	817	CLA	C1B-NB	5.09	1.44	1.37
29	B	837	CLA	MG-NA	-5.09	1.94	2.06
29	a	607	CLA	MG-NA	-5.09	1.94	2.06
29	A	823	CLA	C1B-NB	5.09	1.44	1.37
29	c	606	CLA	MG-NA	-5.09	1.94	2.06
29	9	606	CLA	MG-NB	-5.08	1.95	2.05
29	3	609	CLA	MG-NB	-5.08	1.95	2.05
29	4	601	CLA	MG-NB	-5.08	1.95	2.05
29	B	819	CLA	MG-NB	-5.08	1.95	2.05
29	A	820	CLA	MG-NA	-5.08	1.94	2.06
29	F	204	CLA	MG-NB	-5.08	1.95	2.05
29	c	606	CLA	MG-NB	-5.08	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	611	CLA	C1B-NB	5.08	1.44	1.37
29	8	606	CLA	C1B-NB	5.08	1.44	1.37
29	A	841	CLA	C1B-NB	5.08	1.44	1.37
29	d	609	CLA	MG-NA	-5.07	1.94	2.06
29	3	607	CLA	MG-NA	-5.07	1.94	2.06
29	a	605	CLA	MG-NB	-5.07	1.95	2.05
29	A	839	CLA	MG-NA	-5.07	1.94	2.06
29	1	607	CLA	MG-NA	-5.07	1.94	2.06
29	b	601	CLA	MG-NB	-5.07	1.95	2.05
29	B	824	CLA	C1B-NB	5.07	1.44	1.37
29	3	605	CLA	MG-NA	-5.07	1.94	2.06
29	A	816	CLA	MG-NA	-5.07	1.94	2.06
29	B	805	CLA	MG-NB	-5.07	1.95	2.05
29	e	601	CLA	MG-NB	-5.07	1.95	2.05
29	A	833	CLA	MG-NB	-5.06	1.95	2.05
29	8	605	CLA	C1B-NB	5.06	1.44	1.37
29	A	833	CLA	MG-NA	-5.06	1.94	2.06
29	A	836	CLA	MG-NB	-5.06	1.95	2.05
29	b	601	CLA	MG-NA	-5.06	1.94	2.06
29	R	202	CLA	C1B-NB	5.06	1.44	1.37
29	B	840	CLA	C1B-NB	5.06	1.44	1.37
29	8	606	CLA	MG-NA	-5.06	1.94	2.06
29	a	609	CLA	MG-NB	-5.06	1.95	2.05
29	d	609	CLA	MG-NB	-5.06	1.95	2.05
29	L	203	CLA	C1B-NB	5.06	1.44	1.37
29	b	608	CLA	MG-NB	-5.06	1.95	2.05
29	7	608	CLA	MG-NA	-5.06	1.94	2.06
29	A	829	CLA	MG-NB	-5.06	1.95	2.05
29	A	812	CLA	C1B-NB	5.06	1.44	1.37
29	d	611	CLA	MG-NB	-5.05	1.95	2.05
29	B	821	CLA	MG-NA	-5.05	1.94	2.06
29	B	834	CLA	MG-NA	-5.05	1.94	2.06
29	3	608	CLA	MG-NA	-5.05	1.94	2.06
29	2	606	CLA	MG-NA	-5.05	1.94	2.06
29	A	831	CLA	C1B-NB	5.05	1.44	1.37
29	J	102	CLA	MG-NA	-5.05	1.94	2.06
29	L	202	CLA	MG-NA	-5.05	1.94	2.06
29	Z	306	CLA	MG-NA	-5.05	1.94	2.06
29	F	202	CLA	MG-NA	-5.05	1.94	2.06
29	5	612	CLA	MG-NA	-5.05	1.94	2.06
29	A	813	CLA	MG-NB	-5.05	1.95	2.05
29	K	102	CLA	MG-NB	-5.05	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	838	CLA	MG-NB	-5.05	1.95	2.05
29	a	601	CLA	MG-NA	-5.04	1.94	2.06
29	5	611	CLA	MG-NB	-5.04	1.95	2.05
29	B	817	CLA	C1B-NB	5.04	1.44	1.37
29	4	609	CLA	MG-NB	-5.04	1.95	2.05
29	2	605	CLA	C1B-NB	5.04	1.44	1.37
29	9	611	CLA	MG-NA	-5.04	1.94	2.06
29	4	608	CLA	MG-NB	-5.04	1.95	2.05
29	d	606	CLA	MG-NB	-5.04	1.95	2.05
29	d	602	CLA	MG-NA	-5.04	1.94	2.06
29	9	601	CLA	MG-NB	-5.04	1.95	2.05
29	A	803	CLA	MG-NB	-5.04	1.95	2.05
29	A	808	CLA	MG-NB	-5.04	1.95	2.05
29	9	604	CLA	MG-NB	-5.04	1.95	2.05
29	d	607	CLA	MG-NB	-5.04	1.95	2.05
29	6	611	CLA	MG-NB	-5.03	1.95	2.05
29	B	839	CLA	MG-NA	-5.03	1.94	2.06
29	a	606	CLA	MG-NA	-5.03	1.94	2.06
29	A	837	CLA	MG-NB	-5.03	1.95	2.05
29	1	602	CLA	MG-NA	-5.03	1.94	2.06
29	A	812	CLA	MG-NA	-5.03	1.94	2.06
29	a	612	CLA	MG-NB	-5.03	1.95	2.05
29	5	608	CLA	MG-NA	-5.03	1.94	2.06
29	A	802	CLA	MG-NB	-5.03	1.95	2.05
29	A	828	CLA	C1B-NB	5.02	1.44	1.37
29	b	611	CLA	MG-NA	-5.02	1.94	2.06
29	e	601	CLA	MG-NA	-5.02	1.94	2.06
29	B	804	CLA	MG-NB	-5.02	1.95	2.05
29	B	833	CLA	MG-NA	-5.02	1.94	2.06
29	d	606	CLA	MG-NA	-5.02	1.94	2.06
29	c	612	CLA	MG-NB	-5.02	1.95	2.05
29	3	607	CLA	MG-NB	-5.02	1.95	2.05
29	b	611	CLA	MG-NB	-5.02	1.95	2.05
29	B	826	CLA	MG-NB	-5.02	1.95	2.05
29	A	838	CLA	MG-NA	-5.02	1.94	2.06
29	5	612	CLA	MG-NB	-5.02	1.95	2.05
29	e	602	CLA	MG-NA	-5.01	1.94	2.06
29	B	834	CLA	MG-NB	-5.01	1.95	2.05
29	6	601	CLA	MG-NB	-5.01	1.95	2.05
29	4	604	CLA	MG-NA	-5.01	1.94	2.06
29	e	604	CLA	MG-NA	-5.01	1.94	2.06
29	B	803	CLA	C1B-NB	5.01	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	7	611	CLA	MG-NA	-5.01	1.94	2.06
29	A	842	CLA	MG-NA	-5.01	1.94	2.06
29	2	611	CLA	MG-NA	-5.01	1.94	2.06
29	c	609	CLA	MG-NA	-5.01	1.94	2.06
29	4	606	CLA	MG-NA	-5.00	1.94	2.06
29	d	601	CLA	MG-NA	-5.00	1.94	2.06
29	4	607	CLA	MG-NA	-5.00	1.94	2.06
29	9	605	CLA	MG-NA	-5.00	1.94	2.06
29	e	610	CLA	MG-NA	-5.00	1.94	2.06
29	B	807	CLA	MG-NB	-5.00	1.95	2.05
29	2	612	CLA	MG-NA	-5.00	1.94	2.06
29	7	605	CLA	MG-NA	-4.99	1.94	2.06
29	4	607	CLA	MG-NB	-4.99	1.95	2.05
29	5	605	CLA	MG-NA	-4.99	1.94	2.06
29	7	604	CLA	MG-NA	-4.99	1.94	2.06
29	A	811	CLA	MG-NA	-4.99	1.94	2.06
29	b	606	CLA	MG-NA	-4.99	1.94	2.06
29	d	601	CLA	MG-NB	-4.99	1.95	2.05
29	A	805	CLA	MG-NB	-4.99	1.95	2.05
29	A	816	CLA	MG-NB	-4.99	1.95	2.05
29	B	822	CLA	C1B-NB	4.99	1.43	1.37
29	7	608	CLA	MG-NB	-4.99	1.95	2.05
29	B	840	CLA	MG-NA	-4.99	1.94	2.06
29	6	605	CLA	MG-NA	-4.99	1.94	2.06
29	B	836	CLA	MG-NA	-4.99	1.94	2.06
29	A	807	CLA	MG-NB	-4.99	1.95	2.05
29	2	608	CLA	MG-NA	-4.98	1.94	2.06
29	3	604	CLA	MG-NA	-4.98	1.94	2.06
29	3	603	CLA	MG-NA	-4.98	1.94	2.06
29	B	825	CLA	MG-NB	-4.98	1.95	2.05
29	Z	301	CLA	MG-NB	-4.98	1.95	2.05
29	A	807	CLA	MG-NA	-4.98	1.94	2.06
29	2	608	CLA	MG-NB	-4.98	1.95	2.05
29	6	611	CLA	MG-NA	-4.98	1.94	2.06
29	Z	304	CLA	MG-NA	-4.98	1.94	2.06
29	4	610	CLA	MG-NB	-4.97	1.95	2.05
29	a	608	CLA	MG-NA	-4.97	1.94	2.06
29	A	832	CLA	MG-NA	-4.97	1.94	2.06
29	6	612	CLA	MG-NA	-4.97	1.94	2.06
29	A	805	CLA	MG-NA	-4.97	1.94	2.06
29	B	806	CLA	MG-NA	-4.97	1.94	2.06
29	8	604	CLA	MG-NB	-4.97	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	9	612	CLA	MG-NA	-4.97	1.94	2.06
29	a	608	CLA	MG-NB	-4.97	1.95	2.05
29	d	603	CLA	MG-NA	-4.97	1.94	2.06
29	A	804	CLA	MG-NA	-4.97	1.94	2.06
29	B	810	CLA	MG-NA	-4.96	1.94	2.06
29	3	612	CLA	MG-NB	-4.96	1.95	2.05
29	9	608	CLA	MG-NA	-4.96	1.94	2.06
29	5	607	CLA	MG-NB	-4.96	1.96	2.05
29	A	825	CLA	MG-NB	-4.96	1.96	2.05
29	L	204	CLA	MG-NB	-4.96	1.96	2.05
29	7	607	CLA	MG-NB	-4.96	1.96	2.05
29	d	611	CLA	MG-NA	-4.96	1.94	2.06
29	B	816	CLA	MG-NA	-4.96	1.94	2.06
29	a	605	CLA	MG-NA	-4.95	1.94	2.06
29	b	603	CLA	MG-NB	-4.95	1.96	2.05
29	A	829	CLA	MG-NA	-4.95	1.94	2.06
29	4	601	CLA	MG-NA	-4.95	1.94	2.06
29	A	831	CLA	MG-NA	-4.95	1.94	2.06
29	2	607	CLA	MG-NA	-4.95	1.94	2.06
29	O	201	CLA	MG-NB	-4.95	1.96	2.05
29	3	609	CLA	MG-NA	-4.94	1.94	2.06
29	9	606	CLA	MG-NA	-4.94	1.94	2.06
29	3	612	CLA	MG-NA	-4.94	1.94	2.06
29	A	840	CLA	MG-NA	-4.94	1.94	2.06
29	a	612	CLA	MG-NA	-4.94	1.94	2.06
29	B	810	CLA	MG-NB	-4.94	1.96	2.05
29	4	610	CLA	MG-NA	-4.94	1.94	2.06
29	1	608	CLA	MG-NB	-4.93	1.96	2.05
29	B	841	CLA	MG-NB	-4.93	1.96	2.05
29	c	605	CLA	MG-NA	-4.93	1.94	2.06
29	6	607	CLA	MG-NB	-4.93	1.96	2.05
29	B	825	CLA	MG-NA	-4.93	1.94	2.06
29	A	802	CLA	MG-NA	-4.93	1.94	2.06
29	B	817	CLA	MG-NA	-4.93	1.94	2.06
29	8	604	CLA	MG-NA	-4.93	1.94	2.06
29	6	601	CLA	MG-NA	-4.92	1.94	2.06
29	B	840	CLA	MG-NB	-4.92	1.96	2.05
29	9	612	CLA	MG-NB	-4.92	1.96	2.05
29	B	841	CLA	MG-NA	-4.92	1.94	2.06
29	1	612	CLA	MG-NB	-4.92	1.96	2.05
29	e	603	CLA	MG-NA	-4.91	1.94	2.06
29	B	812	CLA	MG-NA	-4.91	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	608	CLA	MG-NA	-4.91	1.94	2.06
29	7	601	CLA	MG-NB	-4.91	1.96	2.05
29	4	608	CLA	MG-NA	-4.90	1.94	2.06
29	9	601	CLA	MG-NA	-4.90	1.94	2.06
29	7	601	CLA	MG-NA	-4.89	1.94	2.06
29	B	807	CLA	C1B-NB	4.89	1.43	1.37
29	F	203	CLA	MG-NA	-4.89	1.94	2.06
29	Z	301	CLA	MG-NA	-4.89	1.94	2.06
29	2	612	CLA	MG-NB	-4.89	1.96	2.05
29	a	603	CLA	MG-NA	-4.89	1.94	2.06
29	B	826	CLA	MG-NA	-4.88	1.94	2.06
29	L	204	CLA	MG-NA	-4.88	1.94	2.06
29	9	607	CLA	MG-NA	-4.88	1.94	2.06
29	4	609	CLA	MG-NA	-4.88	1.94	2.06
29	4	611	CLA	MG-NA	-4.88	1.94	2.06
29	A	826	CLA	MG-NA	-4.87	1.94	2.06
29	e	606	CLA	MG-NA	-4.87	1.94	2.06
29	8	607	CLA	MG-NA	-4.87	1.94	2.06
29	1	608	CLA	MG-NA	-4.87	1.94	2.06
29	d	608	CLA	MG-NB	-4.87	1.96	2.05
29	B	809	CLA	MG-NA	-4.87	1.94	2.06
29	B	820	CLA	MG-NA	-4.87	1.94	2.06
29	c	607	CLA	MG-NB	-4.86	1.96	2.05
29	B	802	CLA	MG-NA	-4.86	1.94	2.06
29	e	611	CLA	MG-NA	-4.86	1.94	2.06
29	a	609	CLA	MG-NA	-4.86	1.94	2.06
29	A	835	CLA	MG-NB	-4.86	1.96	2.05
29	A	835	CLA	MG-NA	-4.85	1.94	2.06
29	5	613	CLA	MG-NA	-4.85	1.94	2.06
29	K	101	CLA	MG-NA	-4.85	1.94	2.06
29	5	611	CLA	MG-NA	-4.84	1.94	2.06
29	A	830	CLA	MG-NA	-4.84	1.94	2.06
29	B	808	CLA	C1B-NB	4.83	1.43	1.37
29	8	601	CLA	MG-NA	-4.83	1.94	2.06
29	B	810	CLA	C1B-NB	4.83	1.43	1.37
29	6	607	CLA	MG-NA	-4.83	1.94	2.06
29	A	837	CLA	MG-NA	-4.83	1.94	2.06
29	A	827	CLA	MG-NA	-4.83	1.94	2.06
29	d	612	CLA	MG-NA	-4.82	1.94	2.06
29	A	826	CLA	C1B-NB	4.82	1.43	1.37
29	c	607	CLA	MG-NA	-4.82	1.94	2.06
29	B	813	CLA	MG-NA	-4.82	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	842	CLA	MG-NB	-4.81	1.96	2.05
29	O	203	CLA	MG-NA	-4.81	1.94	2.06
29	c	614	CLA	MG-NA	-4.81	1.94	2.06
29	9	613	CLA	MG-NA	-4.80	1.94	2.06
29	5	607	CLA	MG-NA	-4.80	1.94	2.06
29	A	840	CLA	C1B-NB	4.78	1.43	1.37
29	B	813	CLA	MG-NB	-4.78	1.96	2.05
29	B	827	CLA	C1B-NB	4.78	1.43	1.37
29	d	607	CLA	MG-NA	-4.78	1.94	2.06
29	1	612	CLA	MG-NA	-4.77	1.94	2.06
29	B	823	CLA	MG-NA	-4.77	1.94	2.06
29	A	823	CLA	MG-NA	-4.75	1.95	2.06
29	Z	305	CLA	MG-NA	-4.75	1.95	2.06
29	L	207	CLA	C3A-C2A	-4.74	1.50	1.54
29	A	827	CLA	C1B-NB	4.73	1.43	1.37
29	L	207	CLA	C1B-NB	4.72	1.43	1.37
29	A	801	CLA	MG-NA	-4.71	1.95	2.06
29	c	613	CLA	MG-NA	-4.71	1.95	2.06
29	b	608	CLA	MG-NA	-4.70	1.95	2.06
29	c	603	CLA	MG-NA	-4.70	1.95	2.06
29	1	605	CLA	MG-NA	-4.69	1.95	2.06
29	F	204	CLA	MG-NA	-4.69	1.95	2.06
29	A	801	CLA	C1B-NB	4.68	1.43	1.37
36	O	206	SQD	O8-S	4.64	1.64	1.47
36	3	621	SQD	O8-S	4.64	1.64	1.47
29	A	844	CLA	MG-NA	-4.63	1.95	2.06
29	A	810	CLA	MG-NA	-4.61	1.95	2.06
29	O	203	CLA	C1B-NB	4.52	1.43	1.37
29	B	802	CLA	C1B-NB	4.51	1.43	1.37
29	A	844	CLA	C1B-NB	4.48	1.43	1.37
29	O	202	CLA	MG-NC	-4.47	1.95	2.06
29	c	608	CLA	C4B-NB	4.37	1.43	1.37
29	1	608	CLA	C4B-NB	4.37	1.43	1.37
29	2	608	CLA	C4B-NB	4.34	1.43	1.37
29	Z	301	CLA	C4B-NB	4.32	1.43	1.37
29	J	102	CLA	C3A-C2A	-4.30	1.50	1.54
29	9	608	CLA	C4B-NB	4.30	1.43	1.37
29	5	613	CLA	C4B-NB	4.29	1.43	1.37
36	O	206	SQD	O48-C23	4.28	1.45	1.33
29	1	607	CLA	C4B-NB	4.27	1.43	1.37
29	c	613	CLA	C4B-NB	4.27	1.43	1.37
29	2	611	CLA	C4B-NB	4.27	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	604	CLA	C4B-NB	4.27	1.43	1.37
29	7	607	CLA	C4B-NB	4.26	1.43	1.37
29	A	842	CLA	C4B-NB	4.26	1.43	1.37
29	A	838	CLA	C4B-NB	4.26	1.43	1.37
29	4	607	CLA	C4B-NB	4.24	1.43	1.37
36	3	621	SQD	O48-C23	4.24	1.45	1.33
29	2	609	CLA	C4B-NB	4.24	1.43	1.37
29	1	601	CLA	C4B-NB	4.23	1.43	1.37
29	1	611	CLA	C4B-NB	4.21	1.43	1.37
29	A	839	CLA	C4B-NB	4.21	1.43	1.37
29	8	607	CLA	C4B-NB	4.21	1.43	1.37
29	1	602	CLA	C4B-NB	4.20	1.43	1.37
29	c	607	CLA	C4B-NB	4.20	1.43	1.37
29	c	609	CLA	C4B-NB	4.20	1.42	1.37
29	e	607	CLA	C4B-NB	4.20	1.42	1.37
29	B	819	CLA	C4B-NB	4.20	1.42	1.37
29	6	607	CLA	C4B-NB	4.19	1.42	1.37
29	7	602	CLA	C4B-NB	4.19	1.42	1.37
29	8	601	CLA	C4B-NB	4.18	1.42	1.37
29	b	610	CLA	C4B-NB	4.18	1.42	1.37
29	3	607	CLA	C4B-NB	4.17	1.42	1.37
29	2	604	CLA	C4B-NB	4.17	1.42	1.37
29	e	602	CLA	C4B-NB	4.17	1.42	1.37
29	A	815	CLA	C4B-NB	4.17	1.42	1.37
29	e	610	CLA	C4B-NB	4.17	1.42	1.37
29	A	830	CLA	C4B-NB	4.16	1.42	1.37
29	5	607	CLA	C4B-NB	4.16	1.42	1.37
29	c	614	CLA	C4B-NB	4.16	1.42	1.37
29	9	613	CLA	C4B-NB	4.15	1.42	1.37
29	A	805	CLA	C4B-NB	4.15	1.42	1.37
29	e	608	CLA	C4B-NB	4.15	1.42	1.37
29	3	608	CLA	C4B-NB	4.15	1.42	1.37
29	d	607	CLA	C4B-NB	4.15	1.42	1.37
29	1	612	CLA	C4B-NB	4.15	1.42	1.37
29	3	605	CLA	C4B-NB	4.14	1.42	1.37
29	B	841	CLA	C4B-NB	4.14	1.42	1.37
29	a	608	CLA	C4B-NB	4.14	1.42	1.37
29	e	604	CLA	C4B-NB	4.14	1.42	1.37
29	A	810	CLA	C4B-NB	4.14	1.42	1.37
29	5	611	CLA	C4B-NB	4.13	1.42	1.37
29	b	608	CLA	C4B-NB	4.13	1.42	1.37
29	d	604	CLA	C4B-NB	4.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	2	612	CLA	C4B-NB	4.13	1.42	1.37
29	9	609	CLA	C4B-NB	4.13	1.42	1.37
29	c	601	CLA	C4B-NB	4.13	1.42	1.37
29	b	607	CLA	C4B-NB	4.13	1.42	1.37
29	7	601	CLA	C4B-NB	4.12	1.42	1.37
29	9	612	CLA	C4B-NB	4.12	1.42	1.37
29	4	604	CLA	C4B-NB	4.11	1.42	1.37
29	e	611	CLA	C4B-NB	4.11	1.42	1.37
29	9	604	CLA	C4B-NB	4.11	1.42	1.37
29	d	608	CLA	C4B-NB	4.11	1.42	1.37
29	b	604	CLA	C4B-NB	4.11	1.42	1.37
29	5	601	CLA	C4B-NB	4.11	1.42	1.37
29	a	602	CLA	C4B-NB	4.11	1.42	1.37
29	B	804	CLA	C4B-NB	4.11	1.42	1.37
29	9	601	CLA	C4B-NB	4.10	1.42	1.37
29	3	604	CLA	C4B-NB	4.10	1.42	1.37
29	3	602	CLA	C4B-NB	4.10	1.42	1.37
29	a	609	CLA	C4B-NB	4.10	1.42	1.37
29	B	820	CLA	C4B-NB	4.10	1.42	1.37
29	K	101	CLA	C4B-NB	4.10	1.42	1.37
29	O	201	CLA	C4B-NB	4.10	1.42	1.37
29	A	820	CLA	C4B-NB	4.10	1.42	1.37
29	d	602	CLA	C4B-NB	4.10	1.42	1.37
29	d	611	CLA	C4B-NB	4.09	1.42	1.37
29	d	609	CLA	C4B-NB	4.09	1.42	1.37
29	8	602	CLA	C4B-NB	4.09	1.42	1.37
29	1	606	CLA	C4B-NB	4.09	1.42	1.37
29	a	604	CLA	C4B-NB	4.09	1.42	1.37
29	4	609	CLA	C4B-NB	4.09	1.42	1.37
29	6	611	CLA	C4B-NB	4.08	1.42	1.37
29	B	823	CLA	C4B-NB	4.08	1.42	1.37
29	e	601	CLA	C4B-NB	4.08	1.42	1.37
29	B	831	CLA	C4B-NB	4.08	1.42	1.37
29	b	603	CLA	C4B-NB	4.08	1.42	1.37
29	5	608	CLA	C4B-NB	4.08	1.42	1.37
29	A	811	CLA	C4B-NB	4.08	1.42	1.37
29	7	608	CLA	C4B-NB	4.08	1.42	1.37
29	B	815	CLA	C4B-NB	4.08	1.42	1.37
29	1	609	CLA	C4B-NB	4.08	1.42	1.37
29	A	833	CLA	C4B-NB	4.08	1.42	1.37
29	A	843	CLA	C4B-NB	4.08	1.42	1.37
29	b	602	CLA	C4B-NB	4.08	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	5	609	CLA	C4B-NB	4.07	1.42	1.37
29	7	603	CLA	C4B-NB	4.07	1.42	1.37
29	8	615	CLA	C4B-NB	4.06	1.42	1.37
29	F	202	CLA	C4B-NB	4.06	1.42	1.37
29	2	607	CLA	C4B-NB	4.06	1.42	1.37
36	3	621	SQD	O47-C7	4.06	1.45	1.34
29	A	807	CLA	C4B-NB	4.06	1.42	1.37
29	9	605	CLA	C4B-NB	4.05	1.42	1.37
29	3	609	CLA	C4B-NB	4.05	1.42	1.37
29	B	813	CLA	C4B-NB	4.05	1.42	1.37
29	F	204	CLA	C4B-NB	4.05	1.42	1.37
29	8	604	CLA	C4B-NB	4.05	1.42	1.37
29	6	602	CLA	C4B-NB	4.05	1.42	1.37
29	1	604	CLA	C4B-NB	4.04	1.42	1.37
29	A	813	CLA	C4B-NB	4.04	1.42	1.37
29	A	823	CLA	C4B-NB	4.04	1.42	1.37
29	d	603	CLA	C4B-NB	4.04	1.42	1.37
29	2	601	CLA	C4B-NB	4.04	1.42	1.37
29	A	802	CLA	C4B-NB	4.04	1.42	1.37
29	B	810	CLA	C4B-NB	4.04	1.42	1.37
29	e	603	CLA	C4B-NB	4.04	1.42	1.37
29	3	601	CLA	C4B-NB	4.03	1.42	1.37
29	A	806	CLA	C4B-NB	4.03	1.42	1.37
29	A	835	CLA	C4B-NB	4.03	1.42	1.37
29	c	603	CLA	C4B-NB	4.03	1.42	1.37
29	O	202	CLA	C1B-NB	4.03	1.42	1.37
29	7	605	CLA	C4B-NB	4.03	1.42	1.37
29	9	611	CLA	C4B-NB	4.02	1.42	1.37
29	c	602	CLA	C4B-NB	4.02	1.42	1.37
29	d	601	CLA	C4B-NB	4.02	1.42	1.37
29	4	603	CLA	C4B-NB	4.02	1.42	1.37
36	O	206	SQD	O47-C7	4.02	1.45	1.34
29	3	612	CLA	C4B-NB	4.02	1.42	1.37
29	B	838	CLA	C4B-NB	4.02	1.42	1.37
29	8	603	CLA	C4B-NB	4.01	1.42	1.37
29	6	603	CLA	MG-NC	-4.01	1.96	2.06
29	2	603	CLA	C4B-NB	4.01	1.42	1.37
29	9	614	CLA	C4B-NB	4.01	1.42	1.37
29	A	825	CLA	C4B-NB	4.01	1.42	1.37
29	a	601	CLA	C4B-NB	4.01	1.42	1.37
29	d	606	CLA	C4B-NB	4.01	1.42	1.37
29	8	608	CLA	C4B-NB	4.01	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	3	611	CLA	C4B-NB	4.00	1.42	1.37
29	7	609	CLA	C4B-NB	4.00	1.42	1.37
29	A	836	CLA	C4B-NB	4.00	1.42	1.37
29	B	831	CLA	MG-NC	-4.00	1.96	2.06
29	7	611	CLA	C4B-NB	3.99	1.42	1.37
29	9	603	CLA	C4B-NB	3.99	1.42	1.37
29	7	604	CLA	C4B-NB	3.99	1.42	1.37
29	c	604	CLA	C4B-NB	3.99	1.42	1.37
29	4	606	CLA	C4B-NB	3.99	1.42	1.37
29	e	606	CLA	C4B-NB	3.99	1.42	1.37
29	4	608	CLA	C4B-NB	3.99	1.42	1.37
29	5	602	CLA	C4B-NB	3.99	1.42	1.37
29	B	834	CLA	C4B-NB	3.97	1.42	1.37
29	d	605	CLA	C4B-NB	3.97	1.42	1.37
29	1	603	CLA	C4B-NB	3.97	1.42	1.37
29	9	606	CLA	C4B-NB	3.96	1.42	1.37
29	b	601	CLA	C4B-NB	3.96	1.42	1.37
29	b	606	CLA	C4B-NB	3.96	1.42	1.37
29	a	611	CLA	C4B-NB	3.96	1.42	1.37
29	c	605	CLA	C4B-NB	3.96	1.42	1.37
29	a	603	CLA	C4B-NB	3.96	1.42	1.37
29	A	817	CLA	C4B-NB	3.95	1.42	1.37
29	4	602	CLA	C4B-NB	3.95	1.42	1.37
29	A	828	CLA	C4B-NB	3.95	1.42	1.37
29	2	602	CLA	C4B-NB	3.95	1.42	1.37
29	A	804	CLA	C4B-NB	3.95	1.42	1.37
29	A	814	CLA	C4B-NB	3.95	1.42	1.37
29	Z	305	CLA	C4B-NB	3.95	1.42	1.37
29	8	605	CLA	MG-NC	-3.94	1.96	2.06
29	c	606	CLA	C4B-NB	3.94	1.42	1.37
29	9	602	CLA	C4B-NB	3.94	1.42	1.37
29	B	832	CLA	C4B-NB	3.94	1.42	1.37
29	3	603	CLA	C4B-NB	3.94	1.42	1.37
29	5	606	CLA	C4B-NB	3.94	1.42	1.37
29	L	202	CLA	C4B-NB	3.94	1.42	1.37
29	8	606	CLA	C4B-NB	3.93	1.42	1.37
29	6	608	CLA	C4B-NB	3.93	1.42	1.37
29	A	808	CLA	C4B-NB	3.93	1.42	1.37
29	A	841	CLA	MG-NC	-3.93	1.96	2.06
29	A	822	CLA	C4B-NB	3.93	1.42	1.37
29	K	102	CLA	C4B-NB	3.93	1.42	1.37
29	5	604	CLA	C4B-NB	3.93	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	807	CLA	C4B-NB	3.92	1.42	1.37
29	B	814	CLA	C4B-NB	3.92	1.42	1.37
29	B	811	CLA	C4B-NB	3.92	1.42	1.37
29	B	826	CLA	C4B-NB	3.92	1.42	1.37
29	a	605	CLA	C4B-NB	3.92	1.42	1.37
29	A	824	CLA	C4B-NB	3.91	1.42	1.37
29	6	612	CLA	C4B-NB	3.91	1.42	1.37
29	L	204	CLA	C4B-NB	3.91	1.42	1.37
29	4	610	CLA	C4B-NB	3.91	1.42	1.37
29	Z	304	CLA	C4B-NB	3.91	1.42	1.37
29	A	809	CLA	C4B-NB	3.91	1.42	1.37
29	B	818	CLA	C4B-NB	3.91	1.42	1.37
29	B	817	CLA	C4B-NB	3.91	1.42	1.37
29	3	610	CLA	C4B-NB	3.91	1.42	1.37
29	A	812	CLA	C4B-NB	3.91	1.42	1.37
29	5	605	CLA	C4B-NB	3.90	1.42	1.37
29	K	102	CLA	MG-NC	-3.90	1.97	2.06
29	b	611	CLA	C4B-NB	3.90	1.42	1.37
29	B	812	CLA	C4B-NB	3.89	1.42	1.37
29	B	835	CLA	C4B-NB	3.89	1.42	1.37
29	a	606	CLA	C4B-NB	3.88	1.42	1.37
29	B	837	CLA	C4B-NB	3.87	1.42	1.37
29	6	609	CLA	C4B-NB	3.87	1.42	1.37
29	A	809	CLA	MG-NC	-3.87	1.97	2.06
29	1	613	CLA	C4B-NB	3.86	1.42	1.37
29	4	601	CLA	C4B-NB	3.86	1.42	1.37
29	B	830	CLA	C4B-NB	3.86	1.42	1.37
29	A	829	CLA	C4B-NB	3.86	1.42	1.37
29	A	843	CLA	MG-NC	-3.86	1.97	2.06
29	L	203	CLA	MG-NC	-3.85	1.97	2.06
29	A	826	CLA	C4B-NB	3.85	1.42	1.37
30	5	610	KC2	C4C-NC	3.85	1.43	1.37
29	c	612	CLA	C4B-NB	3.85	1.42	1.37
29	4	611	CLA	C4B-NB	3.85	1.42	1.37
29	A	803	CLA	C4B-NB	3.84	1.42	1.37
29	B	840	CLA	C4B-NB	3.84	1.42	1.37
29	7	612	CLA	C4B-NB	3.84	1.42	1.37
29	B	806	CLA	C4B-NB	3.84	1.42	1.37
29	2	606	CLA	C4B-NB	3.84	1.42	1.37
29	5	603	CLA	C4B-NB	3.84	1.42	1.37
29	A	816	CLA	C4B-NB	3.84	1.42	1.37
29	B	825	CLA	C4B-NB	3.84	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R	202	CLA	MG-NC	-3.83	1.97	2.06
29	5	612	CLA	C4B-NB	3.83	1.42	1.37
29	6	606	CLA	C4B-NB	3.83	1.42	1.37
29	B	824	CLA	C4B-NB	3.83	1.42	1.37
29	B	829	CLA	C4B-NB	3.83	1.42	1.37
29	A	814	CLA	MG-NC	-3.83	1.97	2.06
29	a	607	CLA	C4B-NB	3.83	1.42	1.37
29	B	803	CLA	MG-NC	-3.82	1.97	2.06
30	7	610	KC2	C4C-NC	3.82	1.43	1.37
29	5	604	CLA	MG-NC	-3.81	1.97	2.06
29	A	819	CLA	C4B-NB	3.81	1.42	1.37
29	6	605	CLA	C4B-NB	3.81	1.42	1.37
29	a	612	CLA	C4B-NB	3.81	1.42	1.37
29	B	839	CLA	C4B-NB	3.81	1.42	1.37
29	Z	306	CLA	C4B-NB	3.80	1.42	1.37
29	A	834	CLA	C4B-NB	3.80	1.42	1.37
29	A	818	CLA	C4B-NB	3.80	1.42	1.37
29	A	837	CLA	C4B-NB	3.80	1.42	1.37
30	d	610	KC2	C4C-NC	3.80	1.43	1.37
29	6	608	CLA	MG-NC	-3.79	1.97	2.06
29	J	102	CLA	C4B-NB	3.79	1.42	1.37
29	6	602	CLA	MG-NC	-3.79	1.97	2.06
29	9	602	CLA	MG-NC	-3.79	1.97	2.06
29	6	601	CLA	C4B-NB	3.78	1.42	1.37
29	B	809	CLA	C4B-NB	3.78	1.42	1.37
29	L	203	CLA	C4B-NB	3.78	1.42	1.37
29	B	814	CLA	MG-NC	-3.78	1.97	2.06
29	8	605	CLA	C4B-NB	3.77	1.42	1.37
29	A	827	CLA	C4B-NB	3.77	1.42	1.37
30	4	605	KC2	C1B-NB	3.77	1.42	1.37
29	2	609	CLA	MG-NC	-3.76	1.97	2.06
29	B	827	CLA	C4B-NB	3.76	1.42	1.37
29	A	832	CLA	C4B-NB	3.76	1.42	1.37
30	c	615	KC2	C1B-NB	3.76	1.42	1.37
29	L	201	CLA	C4B-NB	3.75	1.42	1.37
29	1	613	CLA	MG-NC	-3.75	1.97	2.06
29	F	203	CLA	C4B-NB	3.75	1.42	1.37
29	B	829	CLA	MG-NC	-3.75	1.97	2.06
29	B	808	CLA	C4B-NB	3.75	1.42	1.37
30	1	610	KC2	C4C-NC	3.74	1.43	1.37
29	d	612	CLA	C4B-NB	3.74	1.42	1.37
29	6	609	CLA	MG-NC	-3.74	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	601	CLA	MG-NC	-3.74	1.97	2.06
29	A	817	CLA	MG-NC	-3.73	1.97	2.06
30	2	610	KC2	C4C-NC	3.73	1.43	1.37
29	1	605	CLA	C4B-NB	3.73	1.42	1.37
29	B	836	CLA	C4B-NB	3.73	1.42	1.37
29	B	835	CLA	MG-NC	-3.73	1.97	2.06
29	a	604	CLA	MG-NC	-3.72	1.97	2.06
29	5	602	CLA	MG-NC	-3.72	1.97	2.06
29	9	607	CLA	C4B-NB	3.71	1.42	1.37
29	A	803	CLA	MG-NC	-3.70	1.97	2.06
29	B	805	CLA	C4B-NB	3.70	1.42	1.37
29	7	603	CLA	MG-NC	-3.70	1.97	2.06
29	O	201	CLA	MG-NC	-3.70	1.97	2.06
29	c	612	CLA	MG-NC	-3.69	1.97	2.06
29	6	603	CLA	C4B-NB	3.69	1.42	1.37
29	d	608	CLA	MG-NC	-3.69	1.97	2.06
29	c	601	CLA	MG-NC	-3.69	1.97	2.06
30	1	610	KC2	C1B-NB	3.69	1.42	1.37
29	b	602	CLA	MG-NC	-3.69	1.97	2.06
29	5	601	CLA	MG-NC	-3.68	1.97	2.06
29	B	828	CLA	C4B-NB	3.68	1.42	1.37
29	6	606	CLA	MG-NC	-3.68	1.97	2.06
29	A	842	CLA	MG-NC	-3.68	1.97	2.06
29	B	815	CLA	MG-NC	-3.68	1.97	2.06
29	A	819	CLA	MG-NC	-3.68	1.97	2.06
29	3	602	CLA	MG-NC	-3.68	1.97	2.06
29	B	816	CLA	C4B-NB	3.67	1.42	1.37
29	A	834	CLA	MG-NC	-3.67	1.97	2.06
29	A	821	CLA	C4B-NB	3.67	1.42	1.37
29	B	803	CLA	C4B-NB	3.67	1.42	1.37
29	2	601	CLA	MG-NC	-3.67	1.97	2.06
29	A	831	CLA	C4B-NB	3.67	1.42	1.37
29	2	603	CLA	MG-NC	-3.66	1.97	2.06
29	9	603	CLA	MG-NC	-3.66	1.97	2.06
29	2	602	CLA	MG-NC	-3.66	1.97	2.06
29	9	614	CLA	MG-NC	-3.66	1.97	2.06
29	B	834	CLA	MG-NC	-3.66	1.97	2.06
29	B	824	CLA	MG-NC	-3.65	1.97	2.06
30	7	606	KC2	C4C-NC	3.65	1.43	1.37
29	1	611	CLA	MG-NC	-3.65	1.97	2.06
29	e	607	CLA	MG-NC	-3.65	1.97	2.06
30	b	609	KC2	C4C-NC	3.64	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	603	CLA	MG-NC	-3.64	1.97	2.06
30	e	609	KC2	C4C-NC	3.64	1.43	1.37
30	9	610	KC2	C4C-NC	3.63	1.43	1.37
29	B	808	CLA	MG-NC	-3.63	1.97	2.06
29	A	808	CLA	MG-NC	-3.63	1.97	2.06
29	3	610	CLA	MG-NC	-3.63	1.97	2.06
29	b	607	CLA	MG-NC	-3.63	1.97	2.06
29	e	608	CLA	MG-NC	-3.63	1.97	2.06
29	5	608	CLA	MG-NC	-3.63	1.97	2.06
29	A	841	CLA	C4B-NB	3.62	1.42	1.37
29	5	603	CLA	MG-NC	-3.62	1.97	2.06
29	A	815	CLA	MG-NC	-3.62	1.97	2.06
30	6	613	KC2	C4C-NC	3.61	1.43	1.37
29	d	604	CLA	MG-NC	-3.61	1.97	2.06
29	c	604	CLA	MG-NC	-3.61	1.97	2.06
29	A	828	CLA	MG-NC	-3.61	1.97	2.06
29	B	838	CLA	MG-NC	-3.61	1.97	2.06
29	B	802	CLA	C4B-NB	3.61	1.42	1.37
29	3	611	CLA	MG-NC	-3.61	1.97	2.06
29	5	601	CLA	C3A-C2A	-3.61	1.51	1.54
29	1	604	CLA	MG-NC	-3.61	1.97	2.06
29	A	824	CLA	MG-NC	-3.61	1.97	2.06
29	B	804	CLA	MG-NC	-3.61	1.97	2.06
29	B	833	CLA	C4B-NB	3.61	1.42	1.37
29	A	811	CLA	MG-NC	-3.60	1.97	2.06
29	L	207	CLA	MG-NC	-3.59	1.97	2.06
29	a	602	CLA	MG-NC	-3.59	1.97	2.06
29	B	819	CLA	MG-NC	-3.59	1.97	2.06
29	8	603	CLA	MG-NC	-3.59	1.97	2.06
29	b	610	CLA	MG-NC	-3.59	1.97	2.06
30	c	611	KC2	C4C-NC	3.59	1.43	1.37
30	e	605	KC2	C1B-NB	3.59	1.42	1.37
29	9	604	CLA	MG-NC	-3.58	1.97	2.06
29	B	821	CLA	C4B-NB	3.58	1.42	1.37
29	B	822	CLA	MG-NC	-3.58	1.97	2.06
29	B	827	CLA	MG-NC	-3.58	1.97	2.06
29	R	202	CLA	C4B-NB	3.58	1.42	1.37
29	B	805	CLA	MG-NC	-3.58	1.97	2.06
29	L	201	CLA	MG-NC	-3.58	1.97	2.06
29	2	605	CLA	C4B-NB	3.58	1.42	1.37
29	5	609	CLA	MG-NC	-3.58	1.97	2.06
29	7	602	CLA	MG-NC	-3.58	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	9	609	CLA	MG-NC	-3.58	1.97	2.06
29	9	611	CLA	MG-NC	-3.58	1.97	2.06
29	B	837	CLA	MG-NC	-3.58	1.97	2.06
29	e	602	CLA	MG-NC	-3.58	1.97	2.06
29	8	602	CLA	MG-NC	-3.58	1.97	2.06
29	3	603	CLA	MG-NC	-3.57	1.97	2.06
30	a	610	KC2	C4C-NC	3.57	1.43	1.37
29	6	604	CLA	MG-NC	-3.57	1.97	2.06
29	A	818	CLA	MG-NC	-3.57	1.97	2.06
29	1	603	CLA	MG-NC	-3.57	1.97	2.06
29	1	606	CLA	MG-NC	-3.57	1.97	2.06
29	2	604	CLA	MG-NC	-3.57	1.97	2.06
29	3	605	CLA	MG-NC	-3.57	1.97	2.06
29	B	822	CLA	C4B-NB	3.57	1.42	1.37
29	d	602	CLA	MG-NC	-3.57	1.97	2.06
29	A	813	CLA	MG-NC	-3.56	1.97	2.06
29	d	606	CLA	C3A-C2A	-3.56	1.51	1.54
29	B	807	CLA	MG-NC	-3.56	1.97	2.06
30	Z	307	KC2	C4C-NC	3.56	1.43	1.37
29	B	818	CLA	MG-NC	-3.56	1.97	2.06
30	7	606	KC2	C1B-NB	3.56	1.42	1.37
29	7	607	CLA	MG-NC	-3.55	1.97	2.06
29	b	611	CLA	MG-NC	-3.55	1.97	2.06
29	B	830	CLA	MG-NC	-3.55	1.97	2.06
29	7	605	CLA	MG-NC	-3.55	1.97	2.06
29	A	820	CLA	MG-NC	-3.55	1.97	2.06
30	4	605	KC2	C4C-NC	3.55	1.43	1.37
29	7	609	CLA	MG-NC	-3.55	1.97	2.06
29	5	606	CLA	MG-NC	-3.55	1.97	2.06
29	d	603	CLA	MG-NC	-3.55	1.97	2.06
29	7	604	CLA	MG-NC	-3.54	1.97	2.06
29	8	606	CLA	MG-NC	-3.54	1.97	2.06
29	A	801	CLA	MG-NC	-3.54	1.97	2.06
29	A	822	CLA	MG-NC	-3.54	1.97	2.06
29	e	603	CLA	MG-NC	-3.54	1.97	2.06
29	6	609	CLA	C3A-C2A	-3.53	1.51	1.54
29	B	839	CLA	MG-NC	-3.53	1.97	2.06
29	2	609	CLA	C3A-C2A	-3.53	1.51	1.54
29	B	828	CLA	MG-NC	-3.53	1.97	2.06
29	A	807	CLA	MG-NC	-3.53	1.97	2.06
29	1	609	CLA	MG-NC	-3.53	1.97	2.06
29	b	604	CLA	MG-NC	-3.52	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	2	611	CLA	MG-NC	-3.52	1.97	2.06
29	A	816	CLA	MG-NC	-3.52	1.97	2.06
30	6	610	KC2	C1B-NB	3.52	1.42	1.37
30	b	605	KC2	C1B-NB	3.51	1.42	1.37
29	d	605	CLA	MG-NC	-3.51	1.97	2.06
29	c	602	CLA	MG-NC	-3.51	1.97	2.06
30	9	610	KC2	C1B-NB	3.51	1.42	1.37
29	B	810	CLA	MG-NC	-3.51	1.97	2.06
29	5	612	CLA	MG-NC	-3.51	1.97	2.06
29	B	806	CLA	MG-NC	-3.51	1.97	2.06
29	A	825	CLA	MG-NC	-3.51	1.97	2.06
30	e	605	KC2	C4C-NC	3.51	1.43	1.37
29	4	607	CLA	MG-NC	-3.51	1.97	2.06
29	9	613	CLA	MG-NC	-3.50	1.97	2.06
29	L	202	CLA	MG-NC	-3.50	1.97	2.06
29	A	829	CLA	MG-NC	-3.50	1.97	2.06
29	Z	304	CLA	MG-NC	-3.50	1.97	2.06
29	A	821	CLA	MG-NC	-3.50	1.98	2.06
29	a	611	CLA	MG-NC	-3.50	1.98	2.06
29	4	606	CLA	MG-NC	-3.50	1.98	2.06
29	a	608	CLA	MG-NC	-3.50	1.98	2.06
29	3	601	CLA	MG-NC	-3.50	1.98	2.06
29	A	812	CLA	MG-NC	-3.49	1.98	2.06
29	d	609	CLA	MG-NC	-3.49	1.98	2.06
29	7	608	CLA	MG-NC	-3.49	1.98	2.06
29	A	833	CLA	MG-NC	-3.49	1.98	2.06
30	3	606	KC2	C4C-NC	3.49	1.43	1.37
29	B	840	CLA	MG-NC	-3.49	1.98	2.06
29	b	601	CLA	MG-NC	-3.49	1.98	2.06
29	8	604	CLA	MG-NC	-3.49	1.98	2.06
29	8	615	CLA	MG-NC	-3.49	1.98	2.06
29	F	202	CLA	MG-NC	-3.48	1.98	2.06
29	e	610	CLA	MG-NC	-3.48	1.98	2.06
29	8	608	CLA	MG-NC	-3.47	1.98	2.06
29	a	601	CLA	MG-NC	-3.47	1.98	2.06
30	5	610	KC2	C1B-NB	3.47	1.42	1.37
29	a	603	CLA	MG-NC	-3.47	1.98	2.06
29	a	606	CLA	MG-NC	-3.47	1.98	2.06
30	c	615	KC2	C4C-NC	3.47	1.43	1.37
29	J	102	CLA	MG-NC	-3.47	1.98	2.06
29	e	604	CLA	MG-NC	-3.46	1.98	2.06
29	2	608	CLA	MG-NC	-3.46	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	606	CLA	MG-NC	-3.46	1.98	2.06
29	A	840	CLA	MG-NC	-3.46	1.98	2.06
29	Z	301	CLA	MG-NC	-3.46	1.98	2.06
29	b	603	CLA	MG-NC	-3.46	1.98	2.06
29	8	607	CLA	MG-NC	-3.46	1.98	2.06
30	6	610	KC2	C4C-NC	3.45	1.43	1.37
29	A	839	CLA	MG-NC	-3.45	1.98	2.06
29	6	611	CLA	MG-NC	-3.45	1.98	2.06
29	B	823	CLA	MG-NC	-3.45	1.98	2.06
29	B	841	CLA	MG-NC	-3.45	1.98	2.06
29	Z	306	CLA	MG-NC	-3.44	1.98	2.06
29	2	606	CLA	MG-NC	-3.44	1.98	2.06
30	Z	307	KC2	C1B-NB	3.44	1.42	1.37
29	9	612	CLA	MG-NC	-3.44	1.98	2.06
29	1	607	CLA	MG-NC	-3.44	1.98	2.06
29	7	612	CLA	MG-NC	-3.44	1.98	2.06
29	4	609	CLA	MG-NC	-3.44	1.98	2.06
29	5	605	CLA	MG-NC	-3.44	1.98	2.06
29	5	613	CLA	MG-NC	-3.44	1.98	2.06
29	A	805	CLA	MG-NC	-3.43	1.98	2.06
29	4	602	CLA	MG-NC	-3.43	1.98	2.06
29	A	804	CLA	MG-NC	-3.43	1.98	2.06
29	A	801	CLA	C4B-NB	3.43	1.42	1.37
29	7	601	CLA	MG-NC	-3.43	1.98	2.06
29	e	611	CLA	MG-NC	-3.42	1.98	2.06
29	3	604	CLA	MG-NC	-3.42	1.98	2.06
29	1	602	CLA	MG-NC	-3.42	1.98	2.06
29	c	606	CLA	MG-NC	-3.42	1.98	2.06
29	2	612	CLA	MG-NC	-3.42	1.98	2.06
29	A	835	CLA	MG-NC	-3.42	1.98	2.06
29	B	820	CLA	MG-NC	-3.41	1.98	2.06
29	e	601	CLA	MG-NC	-3.41	1.98	2.06
29	d	611	CLA	MG-NC	-3.41	1.98	2.06
29	A	826	CLA	MG-NC	-3.41	1.98	2.06
29	4	604	CLA	MG-NC	-3.41	1.98	2.06
30	7	610	KC2	C1B-NB	3.41	1.42	1.37
29	A	836	CLA	MG-NC	-3.40	1.98	2.06
29	B	812	CLA	MG-NC	-3.40	1.98	2.06
29	3	607	CLA	MG-NC	-3.40	1.98	2.06
29	b	606	CLA	MG-NC	-3.40	1.98	2.06
29	3	608	CLA	MG-NC	-3.40	1.98	2.06
30	b	609	KC2	C1B-NB	3.40	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	7	611	CLA	MG-NC	-3.40	1.98	2.06
29	a	607	CLA	MG-NC	-3.39	1.98	2.06
29	A	823	CLA	MG-NC	-3.39	1.98	2.06
29	9	605	CLA	MG-NC	-3.39	1.98	2.06
30	e	609	KC2	C1B-NB	3.39	1.42	1.37
29	B	821	CLA	MG-NC	-3.39	1.98	2.06
29	d	601	CLA	MG-NC	-3.38	1.98	2.06
29	9	606	CLA	MG-NC	-3.38	1.98	2.06
29	5	609	CLA	C3A-C2A	-3.38	1.51	1.54
29	8	601	CLA	MG-NC	-3.38	1.98	2.06
30	a	610	KC2	C1B-NB	3.38	1.41	1.37
29	B	811	CLA	MG-NC	-3.38	1.98	2.06
29	L	204	CLA	MG-NC	-3.37	1.98	2.06
30	2	610	KC2	C1B-NB	3.37	1.41	1.37
30	6	613	KC2	C1B-NB	3.37	1.41	1.37
29	c	607	CLA	MG-NC	-3.37	1.98	2.06
29	3	609	CLA	MG-NC	-3.37	1.98	2.06
29	9	608	CLA	MG-NC	-3.37	1.98	2.06
29	c	608	CLA	MG-NC	-3.36	1.98	2.06
29	A	838	CLA	MG-NC	-3.36	1.98	2.06
29	4	610	CLA	MG-NC	-3.36	1.98	2.06
29	5	611	CLA	MG-NC	-3.35	1.98	2.06
29	6	601	CLA	MG-NC	-3.35	1.98	2.06
29	B	825	CLA	MG-NC	-3.35	1.98	2.06
29	a	609	CLA	MG-NC	-3.35	1.98	2.06
29	c	609	CLA	MG-NC	-3.35	1.98	2.06
29	A	806	CLA	MG-NC	-3.35	1.98	2.06
29	B	817	CLA	MG-NC	-3.35	1.98	2.06
29	c	613	CLA	MG-NC	-3.34	1.98	2.06
29	6	612	CLA	MG-NC	-3.34	1.98	2.06
29	a	605	CLA	MG-NC	-3.34	1.98	2.06
30	c	610	KC2	C1B-NB	3.34	1.41	1.37
29	B	832	CLA	MG-NC	-3.34	1.98	2.06
29	A	837	CLA	MG-NC	-3.34	1.98	2.06
29	d	607	CLA	MG-NC	-3.34	1.98	2.06
29	2	607	CLA	MG-NC	-3.34	1.98	2.06
29	2	605	CLA	MG-NC	-3.34	1.98	2.06
30	c	610	KC2	C4C-NC	3.34	1.42	1.37
29	e	608	CLA	C3A-C2A	-3.33	1.51	1.54
29	K	101	CLA	MG-NC	-3.33	1.98	2.06
29	B	836	CLA	MG-NC	-3.32	1.98	2.06
29	4	611	CLA	MG-NC	-3.32	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	611	KC2	C1B-NB	3.32	1.41	1.37
29	a	612	CLA	MG-NC	-3.32	1.98	2.06
29	e	606	CLA	MG-NC	-3.32	1.98	2.06
29	A	802	CLA	MG-NC	-3.32	1.98	2.06
29	A	830	CLA	MG-NC	-3.31	1.98	2.06
29	c	605	CLA	MG-NC	-3.31	1.98	2.06
29	c	603	CLA	MG-NC	-3.31	1.98	2.06
29	1	608	CLA	MG-NC	-3.31	1.98	2.06
29	9	601	CLA	MG-NC	-3.30	1.98	2.06
29	B	816	CLA	MG-NC	-3.30	1.98	2.06
29	F	203	CLA	MG-NC	-3.30	1.98	2.06
29	4	608	CLA	MG-NC	-3.29	1.98	2.06
29	6	607	CLA	MG-NC	-3.29	1.98	2.06
29	F	204	CLA	MG-NC	-3.29	1.98	2.06
29	c	609	CLA	C3A-C2A	-3.29	1.51	1.54
29	7	609	CLA	C3A-C2A	-3.29	1.51	1.54
29	3	612	CLA	MG-NC	-3.29	1.98	2.06
29	B	802	CLA	MG-NC	-3.29	1.98	2.06
29	5	607	CLA	MG-NC	-3.28	1.98	2.06
29	A	832	CLA	MG-NC	-3.28	1.98	2.06
29	B	826	CLA	MG-NC	-3.28	1.98	2.06
29	L	207	CLA	C4B-NB	3.28	1.41	1.37
29	A	810	CLA	MG-NC	-3.27	1.98	2.06
29	d	609	CLA	C3A-C2A	-3.27	1.51	1.54
29	O	203	CLA	C4B-NB	3.26	1.41	1.37
29	A	840	CLA	C4B-NB	3.26	1.41	1.37
30	d	610	KC2	C1B-NB	3.26	1.41	1.37
29	B	813	CLA	MG-NC	-3.25	1.98	2.06
29	6	605	CLA	MG-NC	-3.25	1.98	2.06
29	A	827	CLA	MG-NC	-3.24	1.98	2.06
29	9	614	CLA	C3A-C2A	-3.24	1.51	1.54
29	c	614	CLA	MG-NC	-3.23	1.98	2.06
29	1	612	CLA	MG-NC	-3.22	1.98	2.06
29	9	609	CLA	C3A-C2A	-3.21	1.51	1.54
29	O	203	CLA	MG-NC	-3.21	1.98	2.06
29	B	809	CLA	MG-NC	-3.21	1.98	2.06
29	d	612	CLA	MG-NC	-3.21	1.98	2.06
29	A	844	CLA	MG-NC	-3.20	1.98	2.06
29	B	833	CLA	MG-NC	-3.19	1.98	2.06
29	9	607	CLA	MG-NC	-3.19	1.98	2.06
29	A	831	CLA	MG-NC	-3.18	1.98	2.06
30	b	605	KC2	C4C-NC	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	608	CLA	MG-NC	-3.17	1.98	2.06
29	1	609	CLA	C3A-C2A	-3.16	1.51	1.54
29	5	613	CLA	C3A-C2A	-3.15	1.51	1.54
29	4	601	CLA	MG-NC	-3.15	1.98	2.06
30	3	606	KC2	C1B-NB	3.14	1.41	1.37
29	8	607	CLA	C3A-C2A	-3.14	1.51	1.54
29	Z	305	CLA	MG-NC	-3.14	1.98	2.06
29	A	844	CLA	C4B-NB	3.12	1.41	1.37
29	9	611	CLA	C3A-C2A	-3.04	1.51	1.54
29	1	605	CLA	MG-NC	-3.00	1.99	2.06
36	3	621	SQD	C6-S	-2.86	1.66	1.77
36	O	206	SQD	C6-S	-2.65	1.67	1.77
37	F	201	8CT	C35-C30	2.60	1.63	1.56
29	O	202	CLA	C3D-C4D	-2.56	1.38	1.44
41	Z	303	DGD	O2G-C2G	-2.51	1.40	1.46
32	b	613	II3	C05-C03	-2.50	1.51	1.54
29	O	202	CLA	C4B-NB	2.49	1.40	1.37
29	L	207	CLA	C1D-C2D	-2.47	1.40	1.45
29	O	203	CLA	C3D-C4D	-2.47	1.38	1.44
34	6	619	LMG	C4-C5	2.45	1.58	1.53
29	1	605	CLA	C1D-C2D	-2.45	1.40	1.45
29	A	844	CLA	C3D-C4D	-2.45	1.38	1.44
29	R	202	CLA	C1D-C2D	-2.43	1.40	1.45
29	A	840	CLA	C3D-C4D	-2.41	1.38	1.44
29	L	207	CLA	C3D-C4D	-2.40	1.38	1.44
29	A	823	CLA	C1D-C2D	-2.37	1.40	1.45
29	O	202	CLA	C1D-C2D	-2.36	1.40	1.45
29	K	101	CLA	C1D-C2D	-2.35	1.40	1.45
29	8	604	CLA	C1D-C2D	-2.35	1.40	1.45
29	b	602	CLA	C1D-C2D	-2.35	1.40	1.45
29	O	203	CLA	C1D-C2D	-2.34	1.40	1.45
36	O	206	SQD	O6-C1	2.34	1.44	1.40
29	8	602	CLA	C1D-C2D	-2.34	1.40	1.45
29	B	839	CLA	C1D-C2D	-2.34	1.40	1.45
41	Z	303	DGD	O1G-C1G	-2.34	1.39	1.45
29	B	825	CLA	C1D-C2D	-2.33	1.40	1.45
29	A	819	CLA	C3D-C4D	-2.32	1.38	1.44
29	A	801	CLA	C1D-C2D	-2.32	1.40	1.45
29	6	602	CLA	C1D-C2D	-2.32	1.40	1.45
29	9	608	CLA	C1D-C2D	-2.32	1.40	1.45
29	F	204	CLA	C1D-C2D	-2.32	1.40	1.45
29	a	603	CLA	C1D-C2D	-2.32	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	605	CLA	C1D-C2D	-2.32	1.40	1.45
29	5	605	CLA	C1D-C2D	-2.31	1.40	1.45
29	A	810	CLA	C1D-C2D	-2.31	1.40	1.45
29	A	825	CLA	C1D-C2D	-2.30	1.40	1.45
29	c	605	CLA	C1D-C2D	-2.30	1.40	1.45
29	B	803	CLA	C1D-C2D	-2.30	1.40	1.45
29	c	614	CLA	C1D-C2D	-2.30	1.40	1.45
29	A	804	CLA	C1D-C2D	-2.30	1.40	1.45
29	A	826	CLA	C1D-C2D	-2.30	1.40	1.45
29	a	602	CLA	C1D-C2D	-2.30	1.40	1.45
29	3	609	CLA	C1D-C2D	-2.29	1.40	1.45
35	6	618	LHG	O7-C5	-2.29	1.40	1.46
29	9	611	CLA	C1D-C2D	-2.29	1.40	1.45
29	B	813	CLA	C1D-C2D	-2.29	1.40	1.45
29	d	609	CLA	C1D-C2D	-2.29	1.40	1.45
29	B	820	CLA	C1D-C2D	-2.29	1.40	1.45
29	A	806	CLA	C1D-C2D	-2.29	1.40	1.45
29	B	823	CLA	C1D-C2D	-2.29	1.40	1.45
34	8	614	LMG	O6-C5	-2.29	1.38	1.44
29	A	812	CLA	C1D-C2D	-2.29	1.40	1.45
29	1	602	CLA	C1D-C2D	-2.28	1.40	1.45
29	B	822	CLA	C1D-C2D	-2.28	1.40	1.45
29	B	815	CLA	C1D-C2D	-2.28	1.40	1.45
29	A	815	CLA	C1D-C2D	-2.28	1.40	1.45
29	A	839	CLA	C1D-C2D	-2.28	1.40	1.45
35	B	849	LHG	O7-C5	-2.28	1.40	1.46
29	A	827	CLA	C1D-C2D	-2.28	1.40	1.45
29	B	809	CLA	C1D-C2D	-2.28	1.40	1.45
29	2	602	CLA	C1D-C2D	-2.28	1.40	1.45
29	9	613	CLA	C1D-C2D	-2.27	1.40	1.45
29	B	808	CLA	C1D-C2D	-2.27	1.40	1.45
29	B	826	CLA	C1D-C2D	-2.27	1.40	1.45
29	L	202	CLA	C1D-C2D	-2.27	1.40	1.45
29	5	603	CLA	C1D-C2D	-2.27	1.40	1.45
29	Z	305	CLA	C1D-C2D	-2.27	1.40	1.45
29	B	833	CLA	C1D-C2D	-2.27	1.40	1.45
29	B	824	CLA	C1D-C2D	-2.27	1.40	1.45
29	A	828	CLA	C1D-C2D	-2.27	1.40	1.45
29	4	610	CLA	C1D-C2D	-2.27	1.40	1.45
29	A	838	CLA	C1D-C2D	-2.27	1.40	1.45
32	1	615	II3	C05-C03	-2.27	1.51	1.54
29	6	605	CLA	C1D-C2D	-2.27	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	611	CLA	C1D-C2D	-2.27	1.40	1.45
29	c	613	CLA	C1D-C2D	-2.26	1.40	1.45
29	d	602	CLA	C1D-C2D	-2.26	1.40	1.45
29	4	604	CLA	C1D-C2D	-2.26	1.40	1.45
29	9	612	CLA	C1D-C2D	-2.26	1.40	1.45
29	B	839	CLA	C3D-C4D	-2.26	1.39	1.44
29	3	612	CLA	C1D-C2D	-2.26	1.40	1.45
29	c	602	CLA	C1D-C2D	-2.26	1.40	1.45
29	e	606	CLA	C1D-C2D	-2.26	1.40	1.45
29	6	608	CLA	C1D-C2D	-2.26	1.40	1.45
29	B	821	CLA	C1D-C2D	-2.26	1.40	1.45
29	1	604	CLA	C1D-C2D	-2.26	1.40	1.45
29	B	806	CLA	C1D-C2D	-2.26	1.40	1.45
29	B	827	CLA	C1D-C2D	-2.26	1.40	1.45
29	A	824	CLA	C3D-C4D	-2.26	1.39	1.44
29	L	201	CLA	C1D-C2D	-2.25	1.40	1.45
29	7	608	CLA	C1D-C2D	-2.25	1.40	1.45
29	A	811	CLA	C1D-C2D	-2.25	1.40	1.45
29	B	830	CLA	C3D-C4D	-2.25	1.39	1.44
29	b	607	CLA	C1D-C2D	-2.25	1.40	1.45
29	6	603	CLA	C1D-C2D	-2.25	1.40	1.45
29	4	602	CLA	C1D-C2D	-2.25	1.40	1.45
37	7	617	8CT	C35-C30	2.25	1.62	1.56
29	B	821	CLA	C3D-C4D	-2.25	1.39	1.44
29	A	841	CLA	C1D-C2D	-2.25	1.40	1.45
29	b	606	CLA	C1D-C2D	-2.25	1.40	1.45
29	B	832	CLA	C1D-C2D	-2.25	1.40	1.45
29	c	603	CLA	C1D-C2D	-2.25	1.40	1.45
29	A	834	CLA	C1D-C2D	-2.25	1.40	1.45
29	A	809	CLA	C3D-C4D	-2.24	1.39	1.44
29	B	829	CLA	C3D-C4D	-2.24	1.39	1.44
29	4	608	CLA	C1D-C2D	-2.24	1.40	1.45
29	7	609	CLA	C1D-C2D	-2.24	1.40	1.45
29	c	607	CLA	C1D-C2D	-2.24	1.40	1.45
29	3	602	CLA	C1D-C2D	-2.24	1.40	1.45
29	B	838	CLA	C1D-C2D	-2.24	1.40	1.45
41	Z	303	DGD	O6D-C5D	-2.24	1.38	1.44
29	A	824	CLA	C1D-C2D	-2.24	1.40	1.45
29	d	612	CLA	C1D-C2D	-2.24	1.40	1.45
29	A	838	CLA	C3D-C4D	-2.24	1.39	1.44
29	B	836	CLA	C1D-C2D	-2.24	1.40	1.45
29	A	821	CLA	C3D-C4D	-2.24	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	605	CLA	C3D-C4D	-2.24	1.39	1.44
29	5	612	CLA	C3D-C4D	-2.24	1.39	1.44
29	3	604	CLA	C1D-C2D	-2.24	1.40	1.45
29	B	817	CLA	C1D-C2D	-2.24	1.40	1.45
29	A	815	CLA	C3D-C4D	-2.24	1.39	1.44
29	B	804	CLA	C1D-C2D	-2.24	1.40	1.45
29	Z	301	CLA	C1D-C2D	-2.24	1.40	1.45
29	3	608	CLA	C1D-C2D	-2.24	1.40	1.45
29	B	834	CLA	C3D-C4D	-2.24	1.39	1.44
29	2	606	CLA	C1D-C2D	-2.24	1.40	1.45
29	F	203	CLA	C1D-C2D	-2.24	1.40	1.45
29	8	606	CLA	C1D-C2D	-2.24	1.40	1.45
29	A	830	CLA	C1D-C2D	-2.24	1.40	1.45
29	A	820	CLA	C1D-C2D	-2.24	1.40	1.45
29	5	609	CLA	C1D-C2D	-2.24	1.40	1.45
29	a	612	CLA	C1D-C2D	-2.24	1.40	1.45
29	4	609	CLA	C1D-C2D	-2.24	1.40	1.45
29	B	802	CLA	C1D-C2D	-2.24	1.40	1.45
29	c	609	CLA	C1D-C2D	-2.24	1.40	1.45
29	A	839	CLA	C3D-C4D	-2.24	1.39	1.44
29	A	831	CLA	C1D-C2D	-2.23	1.40	1.45
29	A	836	CLA	C1D-C2D	-2.23	1.40	1.45
29	c	606	CLA	C1D-C2D	-2.23	1.40	1.45
29	a	603	CLA	C3D-C4D	-2.23	1.39	1.44
29	B	816	CLA	C1D-C2D	-2.23	1.40	1.45
29	4	601	CLA	C1D-C2D	-2.23	1.40	1.45
29	B	835	CLA	C1D-C2D	-2.23	1.40	1.45
29	7	602	CLA	C3D-C4D	-2.23	1.39	1.44
29	3	605	CLA	C3D-C4D	-2.23	1.39	1.44
29	A	803	CLA	C3D-C4D	-2.23	1.39	1.44
29	8	603	CLA	C3D-C4D	-2.23	1.39	1.44
29	Z	304	CLA	C1D-C2D	-2.23	1.40	1.45
29	e	611	CLA	C1D-C2D	-2.23	1.40	1.45
29	A	832	CLA	C1D-C2D	-2.23	1.40	1.45
29	8	615	CLA	C1D-C2D	-2.23	1.40	1.45
29	9	603	CLA	C1D-C2D	-2.23	1.40	1.45
29	B	841	CLA	C1D-C2D	-2.23	1.40	1.45
29	5	611	CLA	C1D-C2D	-2.23	1.40	1.45
29	c	608	CLA	C1D-C2D	-2.23	1.40	1.45
29	A	822	CLA	C3D-C4D	-2.23	1.39	1.44
29	B	822	CLA	C3D-C4D	-2.23	1.39	1.44
29	A	835	CLA	C1D-C2D	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	818	CLA	C3D-C4D	-2.23	1.39	1.44
29	e	603	CLA	C1D-C2D	-2.23	1.40	1.45
29	a	609	CLA	C1D-C2D	-2.22	1.40	1.45
29	6	607	CLA	C1D-C2D	-2.22	1.40	1.45
29	A	842	CLA	C1D-C2D	-2.22	1.40	1.45
29	7	603	CLA	C1D-C2D	-2.22	1.40	1.45
29	L	204	CLA	C1D-C2D	-2.22	1.40	1.45
29	b	604	CLA	C1D-C2D	-2.22	1.40	1.45
29	7	601	CLA	C1D-C2D	-2.22	1.40	1.45
29	e	602	CLA	C1D-C2D	-2.22	1.40	1.45
29	e	604	CLA	C1D-C2D	-2.22	1.40	1.45
29	A	829	CLA	C1D-C2D	-2.22	1.40	1.45
29	L	203	CLA	C1D-C2D	-2.22	1.40	1.45
29	A	817	CLA	C3D-C4D	-2.22	1.39	1.44
29	B	817	CLA	C3D-C4D	-2.22	1.39	1.44
29	A	837	CLA	C1D-C2D	-2.22	1.40	1.45
29	5	607	CLA	C1D-C2D	-2.22	1.40	1.45
29	B	819	CLA	C1D-C2D	-2.22	1.40	1.45
29	3	601	CLA	C1D-C2D	-2.22	1.40	1.45
29	6	603	CLA	C3D-C4D	-2.22	1.39	1.44
29	1	606	CLA	C1D-C2D	-2.22	1.40	1.45
29	B	838	CLA	C3D-C4D	-2.22	1.39	1.44
29	8	601	CLA	C1D-C2D	-2.22	1.40	1.45
29	a	608	CLA	C1D-C2D	-2.22	1.40	1.45
29	b	608	CLA	C1D-C2D	-2.22	1.40	1.45
29	B	833	CLA	C3D-C4D	-2.22	1.39	1.44
29	B	840	CLA	C1D-C2D	-2.22	1.41	1.45
29	e	608	CLA	C1D-C2D	-2.22	1.41	1.45
29	A	829	CLA	C3D-C4D	-2.22	1.39	1.44
29	B	807	CLA	C1D-C2D	-2.22	1.41	1.45
29	B	837	CLA	C3D-C4D	-2.22	1.39	1.44
29	9	605	CLA	C1D-C2D	-2.22	1.41	1.45
29	1	612	CLA	C1D-C2D	-2.21	1.41	1.45
29	B	813	CLA	C3D-C4D	-2.21	1.39	1.44
29	b	601	CLA	C1D-C2D	-2.21	1.41	1.45
29	d	608	CLA	C1D-C2D	-2.21	1.41	1.45
29	3	603	CLA	C3D-C4D	-2.21	1.39	1.44
29	B	837	CLA	C1D-C2D	-2.21	1.41	1.45
29	B	834	CLA	C1D-C2D	-2.21	1.41	1.45
29	2	603	CLA	C3D-C4D	-2.21	1.39	1.44
29	4	607	CLA	C1D-C2D	-2.21	1.41	1.45
29	K	102	CLA	C1D-C2D	-2.21	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	811	CLA	C3D-C4D	-2.21	1.39	1.44
29	1	603	CLA	C1D-C2D	-2.21	1.41	1.45
29	3	607	CLA	C1D-C2D	-2.21	1.41	1.45
29	B	812	CLA	C1D-C2D	-2.21	1.41	1.45
29	B	806	CLA	C3D-C4D	-2.21	1.39	1.44
29	7	602	CLA	C1D-C2D	-2.21	1.41	1.45
29	7	612	CLA	C1D-C2D	-2.21	1.41	1.45
29	A	833	CLA	C1D-C2D	-2.21	1.41	1.45
29	a	604	CLA	C3D-C4D	-2.20	1.39	1.44
29	b	602	CLA	C3D-C4D	-2.20	1.39	1.44
29	c	606	CLA	C3D-C4D	-2.20	1.39	1.44
29	b	603	CLA	C1D-C2D	-2.20	1.41	1.45
29	1	603	CLA	C3D-C4D	-2.20	1.39	1.44
29	A	835	CLA	C3D-C4D	-2.20	1.39	1.44
29	a	601	CLA	C1D-C2D	-2.20	1.41	1.45
29	9	611	CLA	C3D-C4D	-2.20	1.39	1.44
29	F	203	CLA	C3D-C4D	-2.20	1.39	1.44
29	9	605	CLA	C3D-C4D	-2.20	1.39	1.44
29	2	607	CLA	C1D-C2D	-2.20	1.41	1.45
29	b	610	CLA	C1D-C2D	-2.20	1.41	1.45
29	d	611	CLA	C1D-C2D	-2.20	1.41	1.45
29	2	606	CLA	C3D-C4D	-2.20	1.39	1.44
29	A	818	CLA	C1D-C2D	-2.20	1.41	1.45
32	e	613	II3	C05-C03	-2.20	1.52	1.54
29	7	604	CLA	C1D-C2D	-2.20	1.41	1.45
37	B	845	8CT	C35-C30	2.20	1.62	1.56
29	B	828	CLA	C1D-C2D	-2.20	1.41	1.45
29	1	605	CLA	C3D-C4D	-2.20	1.39	1.44
29	B	810	CLA	C3D-C4D	-2.20	1.39	1.44
29	B	815	CLA	C3D-C4D	-2.20	1.39	1.44
29	d	611	CLA	C3D-C4D	-2.20	1.39	1.44
29	A	805	CLA	C3D-C4D	-2.20	1.39	1.44
35	8	613	LHG	P-O6	2.20	1.68	1.59
29	d	605	CLA	C3D-C4D	-2.20	1.39	1.44
29	L	203	CLA	C3D-C4D	-2.20	1.39	1.44
29	3	602	CLA	C3D-C4D	-2.20	1.39	1.44
29	A	826	CLA	C3D-C4D	-2.20	1.39	1.44
29	O	201	CLA	C1D-C2D	-2.20	1.41	1.45
29	6	608	CLA	C3D-C4D	-2.20	1.39	1.44
29	A	816	CLA	C3D-C4D	-2.20	1.39	1.44
29	A	843	CLA	C1D-C2D	-2.20	1.41	1.45
29	9	601	CLA	C1D-C2D	-2.20	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Z	306	CLA	C1D-C2D	-2.20	1.41	1.45
29	8	605	CLA	C3D-C4D	-2.20	1.39	1.44
29	B	831	CLA	C3D-C4D	-2.20	1.39	1.44
29	a	606	CLA	C3D-C4D	-2.20	1.39	1.44
29	c	604	CLA	C3D-C4D	-2.20	1.39	1.44
29	2	602	CLA	C3D-C4D	-2.19	1.39	1.44
29	7	605	CLA	C1D-C2D	-2.19	1.41	1.45
29	A	822	CLA	C1D-C2D	-2.19	1.41	1.45
29	A	836	CLA	C3D-C4D	-2.19	1.39	1.44
29	B	831	CLA	C1D-C2D	-2.19	1.41	1.45
29	4	602	CLA	C3D-C4D	-2.19	1.39	1.44
29	R	202	CLA	C3D-C4D	-2.19	1.39	1.44
29	5	606	CLA	C1D-C2D	-2.19	1.41	1.45
29	3	611	CLA	C1D-C2D	-2.19	1.41	1.45
29	a	606	CLA	C1D-C2D	-2.19	1.41	1.45
29	A	827	CLA	C3D-C4D	-2.19	1.39	1.44
29	L	204	CLA	C3D-C4D	-2.19	1.39	1.44
29	B	805	CLA	C1D-C2D	-2.19	1.41	1.45
29	e	607	CLA	C1D-C2D	-2.19	1.41	1.45
29	6	609	CLA	C1D-C2D	-2.19	1.41	1.45
29	A	808	CLA	C3D-C4D	-2.19	1.39	1.44
29	6	601	CLA	C1D-C2D	-2.19	1.41	1.45
29	6	612	CLA	C1D-C2D	-2.19	1.41	1.45
29	A	807	CLA	C1D-C2D	-2.19	1.41	1.45
29	a	611	CLA	C1D-C2D	-2.19	1.41	1.45
29	c	612	CLA	C1D-C2D	-2.19	1.41	1.45
29	6	611	CLA	C3D-C4D	-2.19	1.39	1.44
29	B	818	CLA	C1D-C2D	-2.19	1.41	1.45
29	A	843	CLA	C3D-C4D	-2.19	1.39	1.44
29	2	603	CLA	C1D-C2D	-2.19	1.41	1.45
29	A	807	CLA	C3D-C4D	-2.19	1.39	1.44
29	4	611	CLA	C1D-C2D	-2.19	1.41	1.45
29	9	606	CLA	C1D-C2D	-2.19	1.41	1.45
29	a	607	CLA	C1D-C2D	-2.19	1.41	1.45
29	4	611	CLA	C3D-C4D	-2.19	1.39	1.44
29	A	804	CLA	C3D-C4D	-2.19	1.39	1.44
29	Z	305	CLA	C3D-C4D	-2.19	1.39	1.44
29	2	608	CLA	C1D-C2D	-2.19	1.41	1.45
29	5	601	CLA	C3D-C4D	-2.19	1.39	1.44
29	6	606	CLA	C3D-C4D	-2.19	1.39	1.44
29	2	605	CLA	C1D-C2D	-2.19	1.41	1.45
29	2	609	CLA	C1D-C2D	-2.19	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	604	CLA	C1D-C2D	-2.19	1.41	1.45
29	e	601	CLA	C1D-C2D	-2.19	1.41	1.45
29	1	609	CLA	C1D-C2D	-2.19	1.41	1.45
29	F	202	CLA	C1D-C2D	-2.19	1.41	1.45
29	A	816	CLA	C1D-C2D	-2.19	1.41	1.45
29	7	611	CLA	C3D-C4D	-2.18	1.39	1.44
29	B	826	CLA	C3D-C4D	-2.18	1.39	1.44
29	d	607	CLA	C3D-C4D	-2.18	1.39	1.44
29	1	606	CLA	C3D-C4D	-2.18	1.39	1.44
29	9	606	CLA	C3D-C4D	-2.18	1.39	1.44
29	1	607	CLA	C1D-C2D	-2.18	1.41	1.45
29	9	607	CLA	C1D-C2D	-2.18	1.41	1.45
29	B	814	CLA	C1D-C2D	-2.18	1.41	1.45
29	B	827	CLA	C3D-C4D	-2.18	1.39	1.44
29	K	102	CLA	C3D-C4D	-2.18	1.39	1.44
29	1	608	CLA	C1D-C2D	-2.18	1.41	1.45
29	7	611	CLA	C1D-C2D	-2.18	1.41	1.45
29	A	812	CLA	C3D-C4D	-2.18	1.39	1.44
29	5	608	CLA	C3D-C4D	-2.18	1.39	1.44
29	B	840	CLA	C3D-C4D	-2.18	1.39	1.44
35	L	208	LHG	P-O6	2.18	1.68	1.59
29	B	824	CLA	C3D-C4D	-2.18	1.39	1.44
29	2	611	CLA	C1D-C2D	-2.18	1.41	1.45
29	3	603	CLA	C1D-C2D	-2.18	1.41	1.45
29	A	817	CLA	C1D-C2D	-2.18	1.41	1.45
29	3	601	CLA	C3D-C4D	-2.18	1.39	1.44
29	2	604	CLA	C1D-C2D	-2.18	1.41	1.45
29	A	808	CLA	C1D-C2D	-2.18	1.41	1.45
29	d	603	CLA	C1D-C2D	-2.18	1.41	1.45
29	5	602	CLA	C1D-C2D	-2.18	1.41	1.45
29	B	808	CLA	C3D-C4D	-2.18	1.39	1.44
29	d	608	CLA	C3D-C4D	-2.18	1.39	1.44
29	5	613	CLA	C1D-C2D	-2.18	1.41	1.45
29	B	811	CLA	C3D-C4D	-2.18	1.39	1.44
29	5	604	CLA	C1D-C2D	-2.18	1.41	1.45
29	B	811	CLA	C1D-C2D	-2.18	1.41	1.45
29	6	604	CLA	C3D-C4D	-2.17	1.39	1.44
29	e	603	CLA	C3D-C4D	-2.17	1.39	1.44
29	5	602	CLA	C3D-C4D	-2.17	1.39	1.44
29	b	601	CLA	C3D-C4D	-2.17	1.39	1.44
29	b	603	CLA	C3D-C4D	-2.17	1.39	1.44
29	A	802	CLA	C1D-C2D	-2.17	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	841	CLA	C3D-C4D	-2.17	1.39	1.44
29	A	813	CLA	C1D-C2D	-2.17	1.41	1.45
29	4	609	CLA	C3D-C4D	-2.17	1.39	1.44
29	8	608	CLA	C3D-C4D	-2.17	1.39	1.44
29	7	607	CLA	C1D-C2D	-2.17	1.41	1.45
29	9	614	CLA	C1D-C2D	-2.17	1.41	1.45
29	e	610	CLA	C1D-C2D	-2.17	1.41	1.45
29	A	830	CLA	C3D-C4D	-2.17	1.39	1.44
29	c	605	CLA	C3D-C4D	-2.17	1.39	1.44
29	B	835	CLA	C3D-C4D	-2.17	1.39	1.44
29	B	836	CLA	C3D-C4D	-2.17	1.39	1.44
29	8	608	CLA	C1D-C2D	-2.17	1.41	1.45
29	b	611	CLA	C1D-C2D	-2.17	1.41	1.45
29	5	608	CLA	C1D-C2D	-2.17	1.41	1.45
29	3	610	CLA	C3D-C4D	-2.17	1.39	1.44
29	3	611	CLA	C3D-C4D	-2.17	1.39	1.44
29	3	607	CLA	C3D-C4D	-2.17	1.39	1.44
29	a	607	CLA	C3D-C4D	-2.17	1.39	1.44
29	b	606	CLA	C3D-C4D	-2.17	1.39	1.44
29	c	612	CLA	C3D-C4D	-2.17	1.39	1.44
29	3	612	CLA	C3D-C4D	-2.17	1.39	1.44
29	2	605	CLA	C3D-C4D	-2.17	1.39	1.44
29	B	812	CLA	C3D-C4D	-2.17	1.39	1.44
29	3	605	CLA	C1D-C2D	-2.17	1.41	1.45
29	3	610	CLA	C1D-C2D	-2.17	1.41	1.45
29	9	609	CLA	C1D-C2D	-2.17	1.41	1.45
29	d	604	CLA	C3D-C4D	-2.17	1.39	1.44
29	d	606	CLA	C3D-C4D	-2.17	1.39	1.44
29	7	609	CLA	C3D-C4D	-2.17	1.39	1.44
29	e	610	CLA	C3D-C4D	-2.17	1.39	1.44
29	4	604	CLA	C3D-C4D	-2.17	1.39	1.44
29	A	818	CLA	C3D-C4D	-2.17	1.39	1.44
29	4	610	CLA	C3D-C4D	-2.17	1.39	1.44
29	A	805	CLA	C1D-C2D	-2.17	1.41	1.45
29	3	608	CLA	C3D-C4D	-2.17	1.39	1.44
29	A	831	CLA	C3D-C4D	-2.17	1.39	1.44
29	a	602	CLA	C3D-C4D	-2.16	1.39	1.44
29	1	611	CLA	C3D-C4D	-2.16	1.39	1.44
29	5	606	CLA	C3D-C4D	-2.16	1.39	1.44
29	9	602	CLA	C3D-C4D	-2.16	1.39	1.44
29	2	601	CLA	C1D-C2D	-2.16	1.41	1.45
29	A	809	CLA	C1D-C2D	-2.16	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	837	CLA	C3D-C4D	-2.16	1.39	1.44
29	B	828	CLA	C3D-C4D	-2.16	1.39	1.44
29	J	102	CLA	C3D-C4D	-2.16	1.39	1.44
29	e	602	CLA	C3D-C4D	-2.16	1.39	1.44
29	1	611	CLA	C1D-C2D	-2.16	1.41	1.45
29	B	809	CLA	C3D-C4D	-2.16	1.39	1.44
29	1	613	CLA	C1D-C2D	-2.16	1.41	1.45
29	4	606	CLA	C1D-C2D	-2.16	1.41	1.45
35	d	618	LHG	P-O6	2.16	1.68	1.59
29	4	606	CLA	C3D-C4D	-2.16	1.39	1.44
29	A	832	CLA	C3D-C4D	-2.16	1.39	1.44
29	L	202	CLA	C3D-C4D	-2.16	1.39	1.44
29	A	806	CLA	C3D-C4D	-2.16	1.39	1.44
29	b	611	CLA	C3D-C4D	-2.16	1.39	1.44
29	5	607	CLA	C3D-C4D	-2.16	1.39	1.44
29	2	609	CLA	C3D-C4D	-2.16	1.39	1.44
29	9	614	CLA	C3D-C4D	-2.16	1.39	1.44
29	b	610	CLA	C3D-C4D	-2.16	1.39	1.44
29	6	602	CLA	C3D-C4D	-2.16	1.39	1.44
29	A	802	CLA	C3D-C4D	-2.16	1.39	1.44
29	9	607	CLA	C3D-C4D	-2.16	1.39	1.44
29	A	825	CLA	C3D-C4D	-2.16	1.39	1.44
29	A	813	CLA	C3D-C4D	-2.16	1.39	1.44
29	B	820	CLA	C3D-C4D	-2.16	1.39	1.44
29	9	612	CLA	C3D-C4D	-2.16	1.39	1.44
29	c	601	CLA	C3D-C4D	-2.16	1.39	1.44
29	4	603	CLA	C1D-C2D	-2.16	1.41	1.45
29	A	840	CLA	C1D-C2D	-2.16	1.41	1.45
29	5	604	CLA	C3D-C4D	-2.16	1.39	1.44
29	Z	306	CLA	C3D-C4D	-2.16	1.39	1.44
29	5	603	CLA	C3D-C4D	-2.16	1.39	1.44
29	6	609	CLA	C3D-C4D	-2.16	1.39	1.44
29	a	612	CLA	C3D-C4D	-2.16	1.39	1.44
29	2	607	CLA	C3D-C4D	-2.16	1.39	1.44
29	6	605	CLA	C3D-C4D	-2.16	1.39	1.44
29	B	832	CLA	C3D-C4D	-2.16	1.39	1.44
29	c	608	CLA	C3D-C4D	-2.15	1.39	1.44
29	7	604	CLA	C3D-C4D	-2.15	1.39	1.44
29	8	607	CLA	C3D-C4D	-2.15	1.39	1.44
29	a	611	CLA	C3D-C4D	-2.15	1.39	1.44
29	2	604	CLA	C3D-C4D	-2.15	1.39	1.44
29	c	604	CLA	C1D-C2D	-2.15	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	607	CLA	C1D-C2D	-2.15	1.41	1.45
29	a	605	CLA	C1D-C2D	-2.15	1.41	1.45
29	2	612	CLA	C3D-C4D	-2.15	1.39	1.44
29	4	603	CLA	C3D-C4D	-2.15	1.39	1.44
29	c	609	CLA	C3D-C4D	-2.15	1.39	1.44
29	7	607	CLA	C3D-C4D	-2.15	1.39	1.44
29	7	603	CLA	C3D-C4D	-2.15	1.39	1.44
29	a	604	CLA	C1D-C2D	-2.15	1.41	1.45
29	1	601	CLA	C3D-C4D	-2.15	1.39	1.44
29	d	601	CLA	C3D-C4D	-2.15	1.39	1.44
35	5	619	LHG	O7-C5	-2.15	1.41	1.46
29	d	607	CLA	C1D-C2D	-2.15	1.41	1.45
29	5	612	CLA	C1D-C2D	-2.15	1.41	1.45
29	6	606	CLA	C1D-C2D	-2.15	1.41	1.45
29	b	604	CLA	C3D-C4D	-2.15	1.39	1.44
29	B	825	CLA	C3D-C4D	-2.15	1.39	1.44
29	8	603	CLA	C1D-C2D	-2.15	1.41	1.45
29	B	814	CLA	C3D-C4D	-2.15	1.39	1.44
29	a	608	CLA	C3D-C4D	-2.15	1.39	1.44
29	e	607	CLA	C3D-C4D	-2.15	1.39	1.44
29	4	607	CLA	C3D-C4D	-2.15	1.39	1.44
29	8	604	CLA	C3D-C4D	-2.15	1.39	1.44
29	d	606	CLA	C1D-C2D	-2.15	1.41	1.45
29	d	602	CLA	C3D-C4D	-2.15	1.39	1.44
29	B	830	CLA	C1D-C2D	-2.15	1.41	1.45
29	7	608	CLA	C3D-C4D	-2.14	1.39	1.44
29	9	603	CLA	C3D-C4D	-2.14	1.39	1.44
29	A	834	CLA	C3D-C4D	-2.14	1.39	1.44
29	c	602	CLA	C3D-C4D	-2.14	1.39	1.44
29	B	810	CLA	C1D-C2D	-2.14	1.41	1.45
29	2	612	CLA	C1D-C2D	-2.14	1.41	1.45
29	6	607	CLA	C3D-C4D	-2.14	1.39	1.44
29	B	816	CLA	C3D-C4D	-2.14	1.39	1.44
29	e	604	CLA	C3D-C4D	-2.14	1.39	1.44
29	J	102	CLA	C1D-C2D	-2.14	1.41	1.45
29	B	807	CLA	C3D-C4D	-2.14	1.39	1.44
29	6	604	CLA	C1D-C2D	-2.14	1.41	1.45
29	A	844	CLA	C1D-C2D	-2.14	1.41	1.45
29	A	814	CLA	C3D-C4D	-2.14	1.39	1.44
29	B	804	CLA	C3D-C4D	-2.14	1.39	1.44
29	A	833	CLA	C3D-C4D	-2.14	1.39	1.44
29	8	606	CLA	C3D-C4D	-2.14	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	8	614	LMG	C3-C2	2.14	1.57	1.52
29	1	604	CLA	C3D-C4D	-2.14	1.39	1.44
29	L	201	CLA	C3D-C4D	-2.14	1.39	1.44
29	A	819	CLA	C1D-C2D	-2.14	1.41	1.45
29	8	601	CLA	C3D-C4D	-2.14	1.39	1.44
29	9	608	CLA	C3D-C4D	-2.14	1.39	1.44
29	1	602	CLA	C3D-C4D	-2.13	1.39	1.44
29	F	202	CLA	C3D-C4D	-2.13	1.39	1.44
29	9	609	CLA	C3D-C4D	-2.13	1.39	1.44
29	O	201	CLA	C3D-C4D	-2.13	1.39	1.44
29	e	608	CLA	C3D-C4D	-2.13	1.39	1.44
41	B	848	DGD	O2G-C2G	-2.13	1.41	1.46
29	9	601	CLA	C3D-C4D	-2.13	1.39	1.44
29	9	604	CLA	C1D-C2D	-2.13	1.41	1.45
29	3	604	CLA	C3D-C4D	-2.13	1.39	1.44
29	3	609	CLA	C3D-C4D	-2.13	1.39	1.44
29	A	842	CLA	C3D-C4D	-2.13	1.39	1.44
29	6	601	CLA	C3D-C4D	-2.13	1.39	1.44
29	5	609	CLA	C3D-C4D	-2.13	1.39	1.44
29	B	805	CLA	C3D-C4D	-2.13	1.39	1.44
29	A	828	CLA	C3D-C4D	-2.13	1.39	1.44
29	A	814	CLA	C1D-C2D	-2.13	1.41	1.45
29	A	820	CLA	C3D-C4D	-2.13	1.39	1.44
29	B	802	CLA	C3D-C4D	-2.13	1.39	1.44
29	4	601	CLA	C3D-C4D	-2.13	1.39	1.44
29	d	601	CLA	C1D-C2D	-2.13	1.41	1.45
29	4	608	CLA	C3D-C4D	-2.12	1.39	1.44
29	8	605	CLA	C1D-C2D	-2.12	1.41	1.45
29	a	601	CLA	C3D-C4D	-2.12	1.39	1.44
29	1	608	CLA	C3D-C4D	-2.12	1.39	1.44
29	Z	301	CLA	C3D-C4D	-2.12	1.39	1.44
29	2	601	CLA	C3D-C4D	-2.12	1.39	1.44
29	A	803	CLA	C1D-C2D	-2.12	1.41	1.45
29	c	601	CLA	C1D-C2D	-2.12	1.41	1.45
29	A	810	CLA	C3D-C4D	-2.12	1.39	1.44
29	8	615	CLA	C3D-C4D	-2.12	1.39	1.44
29	1	601	CLA	C1D-C2D	-2.12	1.41	1.45
29	5	613	CLA	C3D-C4D	-2.12	1.39	1.44
29	7	605	CLA	C3D-C4D	-2.12	1.39	1.44
29	1	607	CLA	C3D-C4D	-2.12	1.39	1.44
29	5	605	CLA	C3D-C4D	-2.12	1.39	1.44
29	6	612	CLA	C3D-C4D	-2.12	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	819	CLA	C3D-C4D	-2.12	1.39	1.44
29	d	609	CLA	C3D-C4D	-2.11	1.39	1.44
35	d	619	LHG	P-O6	2.11	1.67	1.59
29	2	608	CLA	C3D-C4D	-2.11	1.39	1.44
29	e	601	CLA	C3D-C4D	-2.11	1.39	1.44
29	c	607	CLA	C3D-C4D	-2.11	1.39	1.44
29	8	602	CLA	C3D-C4D	-2.11	1.39	1.44
29	b	607	CLA	C3D-C4D	-2.11	1.39	1.44
29	c	603	CLA	C3D-C4D	-2.11	1.39	1.44
38	O	207	LMU	O1'-C1'	2.11	1.43	1.40
29	5	601	CLA	C1D-C2D	-2.11	1.41	1.45
33	5	618	IHT	C18-C07	2.11	1.52	1.45
29	Z	304	CLA	C3D-C4D	-2.11	1.39	1.44
35	4	619	LHG	O7-C5	-2.11	1.41	1.46
29	F	204	CLA	C3D-C4D	-2.10	1.39	1.44
29	c	614	CLA	C3D-C4D	-2.10	1.39	1.44
29	9	602	CLA	C1D-C2D	-2.10	1.41	1.45
29	a	609	CLA	C3D-C4D	-2.10	1.39	1.44
29	7	601	CLA	C3D-C4D	-2.09	1.39	1.44
29	d	603	CLA	C3D-C4D	-2.09	1.39	1.44
35	4	619	LHG	P-O6	2.09	1.67	1.59
29	2	611	CLA	C3D-C4D	-2.09	1.39	1.44
29	9	604	CLA	C3D-C4D	-2.09	1.39	1.44
29	B	803	CLA	C3D-C4D	-2.09	1.39	1.44
29	K	101	CLA	C3D-C4D	-2.09	1.39	1.44
29	A	821	CLA	C1D-C2D	-2.08	1.41	1.45
29	7	612	CLA	C3D-C4D	-2.08	1.39	1.44
29	e	606	CLA	C3D-C4D	-2.08	1.39	1.44
29	B	829	CLA	C1D-C2D	-2.08	1.41	1.45
34	3	618	LMG	O7-C8	-2.07	1.41	1.46
29	1	609	CLA	C3D-C4D	-2.07	1.39	1.44
29	1	613	CLA	C3D-C4D	-2.07	1.39	1.44
38	4	618	LMU	O1'-C1'	2.07	1.43	1.40
29	9	613	CLA	C3D-C4D	-2.07	1.39	1.44
29	B	841	CLA	C3D-C4D	-2.06	1.39	1.44
29	1	612	CLA	C3D-C4D	-2.06	1.39	1.44
29	A	823	CLA	C3D-C4D	-2.06	1.39	1.44
29	e	611	CLA	C3D-C4D	-2.06	1.39	1.44
29	c	613	CLA	C3D-C4D	-2.06	1.39	1.44
29	B	823	CLA	C3D-C4D	-2.06	1.39	1.44
29	5	611	CLA	C3D-C4D	-2.06	1.39	1.44
33	K	104	IHT	C18-C07	2.05	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	612	CLA	C3D-C4D	-2.04	1.39	1.44
35	A	851	LHG	O7-C5	-2.04	1.41	1.46
29	b	608	CLA	C3D-C4D	-2.04	1.39	1.44
35	6	618	LHG	P-O6	2.04	1.67	1.59
35	3	623	LHG	O7-C5	-2.03	1.41	1.46
35	b	616	LHG	P-O6	2.02	1.67	1.59
34	8	614	LMG	C4-C3	2.01	1.57	1.52
37	B	850	8CT	C35-C30	2.01	1.62	1.56

All (3286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	609	IHT	C02-C07-C10	-10.25	108.18	122.61
33	9	619	IHT	C02-C07-C10	-10.19	108.27	122.61
33	d	617	IHT	C02-C07-C10	-9.38	109.40	122.61
33	5	618	IHT	C02-C07-C10	-8.97	109.98	122.61
33	L	205	IHT	C02-C07-C10	-8.87	110.12	122.61
33	6	617	IHT	C02-C07-C10	-8.13	111.16	122.61
33	a	617	IHT	C02-C07-C10	-7.88	111.51	122.61
33	2	616	IHT	C02-C07-C10	-7.74	111.70	122.61
33	Z	302	IHT	C18-C07-C10	-7.06	104.36	121.46
29	B	835	CLA	C4A-NA-C1A	-6.95	103.58	106.71
33	1	618	IHT	C02-C07-C10	-6.90	112.89	122.61
29	6	602	CLA	C4A-NA-C1A	-6.84	103.63	106.71
29	L	207	CLA	C4A-NA-C1A	-6.74	103.68	106.71
33	c	620	IHT	C02-C07-C10	-6.68	113.20	122.61
29	A	809	CLA	C4A-NA-C1A	-6.62	103.73	106.71
29	B	829	CLA	C4A-NA-C1A	-6.56	103.76	106.71
29	B	824	CLA	C4A-NA-C1A	-6.56	103.76	106.71
29	A	817	CLA	C4A-NA-C1A	-6.51	103.78	106.71
29	1	601	CLA	C4A-NA-C1A	-6.49	103.79	106.71
29	6	606	CLA	C4A-NA-C1A	-6.48	103.79	106.71
29	R	202	CLA	C4A-NA-C1A	-6.47	103.80	106.71
29	a	604	CLA	C1D-ND-C4D	-6.43	101.77	106.33
29	9	614	CLA	C4A-NA-C1A	-6.37	103.84	106.71
29	5	608	CLA	C1D-ND-C4D	-6.34	101.83	106.33
29	B	829	CLA	C1D-ND-C4D	-6.33	101.84	106.33
29	4	609	CLA	C1D-ND-C4D	-6.32	101.85	106.33
29	B	834	CLA	C1D-ND-C4D	-6.32	101.85	106.33
29	A	812	CLA	C4A-NA-C1A	-6.31	103.87	106.71
29	2	601	CLA	C4A-NA-C1A	-6.30	103.87	106.71
29	3	610	CLA	C1D-ND-C4D	-6.30	101.86	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	840	CLA	C4A-NA-C1A	-6.29	103.88	106.71
29	c	604	CLA	C1D-ND-C4D	-6.29	101.87	106.33
29	5	604	CLA	C1D-ND-C4D	-6.29	101.87	106.33
29	A	814	CLA	C1D-ND-C4D	-6.28	101.88	106.33
29	5	601	CLA	C4A-NA-C1A	-6.27	103.89	106.71
29	7	602	CLA	C1D-ND-C4D	-6.27	101.88	106.33
29	e	602	CLA	C1D-ND-C4D	-6.26	101.89	106.33
29	B	839	CLA	C1D-ND-C4D	-6.26	101.89	106.33
29	e	610	CLA	C1D-ND-C4D	-6.25	101.89	106.33
29	1	611	CLA	C1D-ND-C4D	-6.24	101.90	106.33
29	5	612	CLA	C1D-ND-C4D	-6.24	101.90	106.33
29	L	203	CLA	C1D-ND-C4D	-6.24	101.90	106.33
29	A	843	CLA	C4A-NA-C1A	-6.24	103.90	106.71
29	5	601	CLA	C1D-ND-C4D	-6.24	101.90	106.33
29	3	608	CLA	C1D-ND-C4D	-6.24	101.90	106.33
29	6	608	CLA	C1D-ND-C4D	-6.23	101.91	106.33
29	B	838	CLA	C1D-ND-C4D	-6.23	101.91	106.33
29	d	608	CLA	C1D-ND-C4D	-6.23	101.91	106.33
29	d	611	CLA	C1D-ND-C4D	-6.22	101.92	106.33
29	A	811	CLA	C1D-ND-C4D	-6.21	101.92	106.33
29	c	601	CLA	C1D-ND-C4D	-6.21	101.92	106.33
29	7	605	CLA	C1D-ND-C4D	-6.21	101.93	106.33
29	6	604	CLA	C1D-ND-C4D	-6.21	101.93	106.33
29	1	608	CLA	C1D-ND-C4D	-6.20	101.93	106.33
29	7	603	CLA	C1D-ND-C4D	-6.19	101.94	106.33
29	8	603	CLA	C1D-ND-C4D	-6.19	101.94	106.33
29	d	605	CLA	C4A-NA-C1A	-6.19	103.92	106.71
29	9	609	CLA	C1D-ND-C4D	-6.19	101.94	106.33
29	A	805	CLA	C1D-ND-C4D	-6.19	101.94	106.33
29	8	607	CLA	C1D-ND-C4D	-6.19	101.94	106.33
29	9	602	CLA	C1D-ND-C4D	-6.19	101.94	106.33
29	2	608	CLA	C1D-ND-C4D	-6.18	101.94	106.33
29	3	604	CLA	C1D-ND-C4D	-6.18	101.94	106.33
29	Z	301	CLA	C1D-ND-C4D	-6.18	101.95	106.33
29	O	203	CLA	C4A-NA-C1A	-6.18	103.93	106.71
29	b	610	CLA	C1D-ND-C4D	-6.17	101.95	106.33
29	5	602	CLA	C1D-ND-C4D	-6.17	101.95	106.33
29	A	807	CLA	C1D-ND-C4D	-6.17	101.95	106.33
29	4	607	CLA	C1D-ND-C4D	-6.17	101.95	106.33
29	A	813	CLA	C1D-ND-C4D	-6.17	101.95	106.33
29	3	603	CLA	C1D-ND-C4D	-6.17	101.95	106.33
29	e	607	CLA	C1D-ND-C4D	-6.17	101.95	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	K	102	CLA	C1D-ND-C4D	-6.16	101.96	106.33
29	2	602	CLA	C1D-ND-C4D	-6.16	101.96	106.33
29	3	601	CLA	C1D-ND-C4D	-6.16	101.96	106.33
29	c	608	CLA	C1D-ND-C4D	-6.16	101.96	106.33
29	3	605	CLA	C4A-NA-C1A	-6.16	103.94	106.71
29	O	202	CLA	C1D-ND-C4D	-6.16	101.96	106.33
29	2	612	CLA	C1D-ND-C4D	-6.15	101.96	106.33
29	a	611	CLA	C1D-ND-C4D	-6.15	101.96	106.33
29	A	803	CLA	C1D-ND-C4D	-6.15	101.96	106.33
29	A	821	CLA	C1D-ND-C4D	-6.15	101.96	106.33
29	7	604	CLA	C1D-ND-C4D	-6.15	101.97	106.33
29	9	604	CLA	C1D-ND-C4D	-6.15	101.97	106.33
29	d	604	CLA	C1D-ND-C4D	-6.15	101.97	106.33
29	Z	304	CLA	C1D-ND-C4D	-6.15	101.97	106.33
29	A	842	CLA	C1D-ND-C4D	-6.14	101.97	106.33
29	b	601	CLA	C1D-ND-C4D	-6.14	101.97	106.33
29	9	611	CLA	C1D-ND-C4D	-6.14	101.97	106.33
29	9	608	CLA	C1D-ND-C4D	-6.14	101.97	106.33
29	d	601	CLA	C1D-ND-C4D	-6.14	101.97	106.33
29	d	602	CLA	C1D-ND-C4D	-6.14	101.97	106.33
29	1	604	CLA	C1D-ND-C4D	-6.14	101.97	106.33
29	L	204	CLA	C1D-ND-C4D	-6.14	101.98	106.33
29	B	812	CLA	C1D-ND-C4D	-6.13	101.98	106.33
29	4	603	CLA	C1D-ND-C4D	-6.13	101.98	106.33
29	8	608	CLA	C1D-ND-C4D	-6.13	101.98	106.33
29	1	606	CLA	C1D-ND-C4D	-6.12	101.98	106.33
29	B	811	CLA	C1D-ND-C4D	-6.11	101.99	106.33
29	A	819	CLA	C1D-ND-C4D	-6.11	102.00	106.33
29	c	609	CLA	C1D-ND-C4D	-6.11	102.00	106.33
29	a	605	CLA	C1D-ND-C4D	-6.11	102.00	106.33
29	a	606	CLA	C1D-ND-C4D	-6.10	102.00	106.33
29	4	602	CLA	C1D-ND-C4D	-6.10	102.00	106.33
29	8	601	CLA	C1D-ND-C4D	-6.10	102.00	106.33
29	2	604	CLA	C1D-ND-C4D	-6.10	102.00	106.33
29	6	611	CLA	C1D-ND-C4D	-6.10	102.00	106.33
29	b	607	CLA	C1D-ND-C4D	-6.10	102.00	106.33
29	3	605	CLA	C1D-ND-C4D	-6.09	102.01	106.33
29	6	601	CLA	C1D-ND-C4D	-6.09	102.01	106.33
29	A	835	CLA	C1D-ND-C4D	-6.09	102.01	106.33
29	e	603	CLA	C1D-ND-C4D	-6.09	102.01	106.33
29	4	604	CLA	C1D-ND-C4D	-6.09	102.01	106.33
29	3	611	CLA	C1D-ND-C4D	-6.09	102.01	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	609	CLA	C1D-ND-C4D	-6.09	102.01	106.33
29	d	606	CLA	C1D-ND-C4D	-6.08	102.01	106.33
29	b	602	CLA	C1D-ND-C4D	-6.08	102.01	106.33
29	1	601	CLA	C1D-ND-C4D	-6.08	102.02	106.33
29	7	608	CLA	C1D-ND-C4D	-6.08	102.02	106.33
29	A	822	CLA	C1D-ND-C4D	-6.08	102.02	106.33
29	L	201	CLA	C4A-NA-C1A	-6.08	103.97	106.71
29	9	601	CLA	C1D-ND-C4D	-6.08	102.02	106.33
29	9	614	CLA	C1D-ND-C4D	-6.08	102.02	106.33
29	9	603	CLA	C1D-ND-C4D	-6.07	102.02	106.33
29	a	608	CLA	C4A-NA-C1A	-6.07	103.98	106.71
29	A	818	CLA	C1D-ND-C4D	-6.07	102.02	106.33
29	5	613	CLA	C1D-ND-C4D	-6.07	102.03	106.33
29	e	604	CLA	C1D-ND-C4D	-6.07	102.03	106.33
29	7	611	CLA	C1D-ND-C4D	-6.07	102.03	106.33
29	A	836	CLA	C1D-ND-C4D	-6.07	102.03	106.33
29	a	601	CLA	C1D-ND-C4D	-6.07	102.03	106.33
29	c	613	CLA	C1D-ND-C4D	-6.07	102.03	106.33
29	O	203	CLA	C1D-ND-C4D	-6.06	102.03	106.33
29	1	602	CLA	C1D-ND-C4D	-6.06	102.03	106.33
29	d	609	CLA	C1D-ND-C4D	-6.06	102.03	106.33
29	3	602	CLA	C1D-ND-C4D	-6.06	102.03	106.33
29	7	601	CLA	C1D-ND-C4D	-6.05	102.03	106.33
29	a	608	CLA	C1D-ND-C4D	-6.05	102.03	106.33
29	A	825	CLA	C1D-ND-C4D	-6.05	102.04	106.33
29	A	829	CLA	C1D-ND-C4D	-6.05	102.04	106.33
29	4	610	CLA	C1D-ND-C4D	-6.05	102.04	106.33
29	B	821	CLA	C1D-ND-C4D	-6.05	102.04	106.33
29	b	604	CLA	C1D-ND-C4D	-6.04	102.04	106.33
29	B	815	CLA	C1D-ND-C4D	-6.04	102.04	106.33
29	2	603	CLA	C1D-ND-C4D	-6.04	102.04	106.33
29	a	609	CLA	C1D-ND-C4D	-6.04	102.05	106.33
29	6	603	CLA	C1D-ND-C4D	-6.04	102.05	106.33
29	c	612	CLA	C1D-ND-C4D	-6.04	102.05	106.33
29	A	821	CLA	C4A-NA-C1A	-6.03	103.99	106.71
29	e	601	CLA	C1D-ND-C4D	-6.03	102.05	106.33
29	A	808	CLA	C1D-ND-C4D	-6.03	102.05	106.33
29	J	102	CLA	C4A-NA-C1A	-6.03	104.00	106.71
29	b	603	CLA	C1D-ND-C4D	-6.03	102.05	106.33
29	3	612	CLA	C1D-ND-C4D	-6.02	102.06	106.33
29	c	602	CLA	C4A-NA-C1A	-6.02	104.00	106.71
29	5	611	CLA	C1D-ND-C4D	-6.02	102.06	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	837	CLA	C1D-ND-C4D	-6.02	102.06	106.33
29	B	818	CLA	C4A-NA-C1A	-6.02	104.00	106.71
29	A	824	CLA	C1D-ND-C4D	-6.02	102.06	106.33
29	B	841	CLA	C1D-ND-C4D	-6.02	102.06	106.33
29	a	602	CLA	C1D-ND-C4D	-6.02	102.06	106.33
29	c	602	CLA	C1D-ND-C4D	-6.02	102.06	106.33
29	8	606	CLA	C1D-ND-C4D	-6.02	102.06	106.33
29	9	606	CLA	C1D-ND-C4D	-6.02	102.06	106.33
29	5	603	CLA	C1D-ND-C4D	-6.01	102.06	106.33
29	6	609	CLA	C1D-ND-C4D	-6.01	102.06	106.33
29	c	607	CLA	C1D-ND-C4D	-6.01	102.06	106.33
29	2	609	CLA	C1D-ND-C4D	-6.01	102.06	106.33
29	1	603	CLA	C1D-ND-C4D	-6.01	102.06	106.33
29	7	609	CLA	C1D-ND-C4D	-6.01	102.06	106.33
29	Z	306	CLA	C1D-ND-C4D	-6.01	102.07	106.33
29	B	813	CLA	C1D-ND-C4D	-6.01	102.07	106.33
29	1	613	CLA	C1D-ND-C4D	-6.00	102.07	106.33
29	A	815	CLA	C1D-ND-C4D	-6.00	102.07	106.33
29	2	609	CLA	C4A-NA-C1A	-6.00	104.01	106.71
29	7	607	CLA	C1D-ND-C4D	-6.00	102.07	106.33
29	c	614	CLA	C1D-ND-C4D	-6.00	102.07	106.33
29	6	606	CLA	C1D-ND-C4D	-5.99	102.08	106.33
29	B	840	CLA	C1D-ND-C4D	-5.99	102.08	106.33
29	A	830	CLA	C1D-ND-C4D	-5.99	102.08	106.33
29	B	810	CLA	C1D-ND-C4D	-5.99	102.08	106.33
29	B	831	CLA	C1D-ND-C4D	-5.99	102.08	106.33
29	e	608	CLA	C1D-ND-C4D	-5.99	102.08	106.33
29	d	604	CLA	C4A-NA-C1A	-5.98	104.02	106.71
29	2	601	CLA	C1D-ND-C4D	-5.98	102.09	106.33
29	A	816	CLA	C1D-ND-C4D	-5.98	102.09	106.33
29	A	838	CLA	C1D-ND-C4D	-5.98	102.09	106.33
29	4	611	CLA	C1D-ND-C4D	-5.97	102.09	106.33
29	c	601	CLA	C4A-NA-C1A	-5.97	104.02	106.71
29	3	609	CLA	C1D-ND-C4D	-5.97	102.09	106.33
29	B	805	CLA	C1D-ND-C4D	-5.97	102.09	106.33
29	5	609	CLA	C1D-ND-C4D	-5.97	102.10	106.33
29	B	819	CLA	C1D-ND-C4D	-5.97	102.10	106.33
29	F	203	CLA	C1D-ND-C4D	-5.96	102.10	106.33
29	c	606	CLA	C1D-ND-C4D	-5.96	102.10	106.33
29	A	834	CLA	C1D-ND-C4D	-5.96	102.10	106.33
29	5	606	CLA	C1D-ND-C4D	-5.96	102.10	106.33
29	J	102	CLA	C1D-ND-C4D	-5.96	102.10	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	837	CLA	C1D-ND-C4D	-5.96	102.10	106.33
29	B	820	CLA	C1D-ND-C4D	-5.95	102.11	106.33
29	d	607	CLA	C1D-ND-C4D	-5.95	102.11	106.33
29	9	612	CLA	C1D-ND-C4D	-5.95	102.11	106.33
29	A	820	CLA	C1D-ND-C4D	-5.95	102.11	106.33
29	B	830	CLA	C1D-ND-C4D	-5.95	102.11	106.33
29	A	833	CLA	C1D-ND-C4D	-5.95	102.11	106.33
29	B	814	CLA	C1D-ND-C4D	-5.95	102.11	106.33
29	B	807	CLA	C1D-ND-C4D	-5.95	102.11	106.33
29	K	101	CLA	C1D-ND-C4D	-5.94	102.11	106.33
29	a	612	CLA	C1D-ND-C4D	-5.94	102.12	106.33
29	B	823	CLA	C1D-ND-C4D	-5.94	102.12	106.33
29	1	607	CLA	C1D-ND-C4D	-5.93	102.12	106.33
29	d	603	CLA	C1D-ND-C4D	-5.93	102.12	106.33
29	8	615	CLA	C1D-ND-C4D	-5.93	102.12	106.33
29	F	204	CLA	C1D-ND-C4D	-5.93	102.12	106.33
29	3	607	CLA	C1D-ND-C4D	-5.92	102.13	106.33
29	B	817	CLA	C1D-ND-C4D	-5.92	102.13	106.33
29	6	607	CLA	C1D-ND-C4D	-5.92	102.13	106.33
29	B	818	CLA	C1D-ND-C4D	-5.92	102.13	106.33
29	e	611	CLA	C1D-ND-C4D	-5.92	102.13	106.33
29	B	830	CLA	C4A-NA-C1A	-5.91	104.05	106.71
29	A	839	CLA	C1D-ND-C4D	-5.91	102.13	106.33
29	a	607	CLA	C1D-ND-C4D	-5.91	102.14	106.33
29	4	601	CLA	C1D-ND-C4D	-5.91	102.14	106.33
29	B	819	CLA	C4A-NA-C1A	-5.91	104.05	106.71
29	2	607	CLA	C1D-ND-C4D	-5.90	102.14	106.33
29	d	608	CLA	C4A-NA-C1A	-5.90	104.05	106.71
29	5	607	CLA	C1D-ND-C4D	-5.90	102.14	106.33
29	3	603	CLA	C4A-NA-C1A	-5.90	104.06	106.71
29	d	605	CLA	C1D-ND-C4D	-5.89	102.15	106.33
29	A	828	CLA	C1D-ND-C4D	-5.89	102.15	106.33
29	a	603	CLA	C1D-ND-C4D	-5.89	102.15	106.33
29	6	602	CLA	C1D-ND-C4D	-5.89	102.15	106.33
29	9	605	CLA	C1D-ND-C4D	-5.88	102.16	106.33
29	4	602	CLA	C4A-NA-C1A	-5.88	104.06	106.71
29	B	828	CLA	C1D-ND-C4D	-5.88	102.16	106.33
29	F	202	CLA	C1D-ND-C4D	-5.88	102.16	106.33
29	Z	305	CLA	C1D-ND-C4D	-5.88	102.16	106.33
29	A	817	CLA	C1D-ND-C4D	-5.88	102.16	106.33
29	7	612	CLA	C4A-NA-C1A	-5.87	104.06	106.71
29	2	611	CLA	C1D-ND-C4D	-5.87	102.16	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	806	CLA	C4A-NA-C1A	-5.87	104.07	106.71
29	9	613	CLA	C1D-ND-C4D	-5.87	102.17	106.33
29	B	816	CLA	C1D-ND-C4D	-5.87	102.17	106.33
29	B	827	CLA	C4A-NA-C1A	-5.87	104.07	106.71
29	1	613	CLA	C4A-NA-C1A	-5.86	104.07	106.71
29	B	833	CLA	C1D-ND-C4D	-5.86	102.17	106.33
29	b	611	CLA	C1D-ND-C4D	-5.86	102.17	106.33
29	2	606	CLA	C1D-ND-C4D	-5.85	102.18	106.33
29	B	836	CLA	C1D-ND-C4D	-5.85	102.18	106.33
29	4	608	CLA	C1D-ND-C4D	-5.84	102.18	106.33
29	A	831	CLA	C1D-ND-C4D	-5.84	102.18	106.33
29	B	804	CLA	C1D-ND-C4D	-5.84	102.18	106.33
29	A	844	CLA	C1D-ND-C4D	-5.84	102.19	106.33
29	B	835	CLA	C1D-ND-C4D	-5.83	102.19	106.33
29	9	605	CLA	C4A-NA-C1A	-5.83	104.09	106.71
31	d	616	II0	C38-C36-C40	-5.83	114.76	122.92
29	B	826	CLA	C1D-ND-C4D	-5.82	102.20	106.33
29	c	605	CLA	C1D-ND-C4D	-5.82	102.20	106.33
29	B	839	CLA	C4A-NA-C1A	-5.82	104.09	106.71
29	B	822	CLA	C1D-ND-C4D	-5.82	102.20	106.33
29	1	605	CLA	C1D-ND-C4D	-5.81	102.21	106.33
29	A	802	CLA	C1D-ND-C4D	-5.81	102.21	106.33
29	c	603	CLA	C1D-ND-C4D	-5.81	102.21	106.33
29	8	605	CLA	C1D-ND-C4D	-5.80	102.21	106.33
29	4	606	CLA	C1D-ND-C4D	-5.80	102.21	106.33
29	8	604	CLA	C1D-ND-C4D	-5.79	102.22	106.33
29	A	832	CLA	C1D-ND-C4D	-5.79	102.22	106.33
29	5	604	CLA	C4A-NA-C1A	-5.79	104.10	106.71
29	A	842	CLA	C4A-NA-C1A	-5.79	104.10	106.71
29	A	811	CLA	C4A-NA-C1A	-5.79	104.11	106.71
29	A	804	CLA	C1D-ND-C4D	-5.78	102.23	106.33
29	A	823	CLA	C1D-ND-C4D	-5.78	102.23	106.33
29	6	612	CLA	C1D-ND-C4D	-5.78	102.23	106.33
29	O	201	CLA	C1D-ND-C4D	-5.77	102.23	106.33
33	Z	302	IHT	C02-C07-C10	-5.77	114.48	122.61
29	b	603	CLA	C4A-NA-C1A	-5.77	104.11	106.71
29	2	607	CLA	C4A-NA-C1A	-5.77	104.11	106.71
29	3	602	CLA	C4A-NA-C1A	-5.77	104.11	106.71
29	Z	306	CLA	C4A-NA-C1A	-5.76	104.12	106.71
29	L	201	CLA	C1D-ND-C4D	-5.76	102.25	106.33
29	B	810	CLA	C4A-NA-C1A	-5.75	104.12	106.71
29	e	603	CLA	C4A-NA-C1A	-5.75	104.12	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	e	607	CLA	C4A-NA-C1A	-5.75	104.12	106.71
29	B	806	CLA	C1D-ND-C4D	-5.75	102.25	106.33
29	B	827	CLA	C1D-ND-C4D	-5.75	102.25	106.33
29	L	202	CLA	C1D-ND-C4D	-5.73	102.26	106.33
29	B	825	CLA	C1D-ND-C4D	-5.73	102.27	106.33
29	A	819	CLA	C4A-NA-C1A	-5.72	104.13	106.71
29	B	809	CLA	C1D-ND-C4D	-5.72	102.27	106.33
29	A	803	CLA	C4A-NA-C1A	-5.72	104.13	106.71
29	B	834	CLA	C4A-NA-C1A	-5.72	104.14	106.71
29	9	607	CLA	C1D-ND-C4D	-5.71	102.28	106.33
29	A	843	CLA	C1D-ND-C4D	-5.71	102.28	106.33
29	B	832	CLA	C1D-ND-C4D	-5.71	102.28	106.33
29	A	840	CLA	C1D-ND-C4D	-5.71	102.28	106.33
29	b	608	CLA	C1D-ND-C4D	-5.70	102.28	106.33
29	b	606	CLA	C1D-ND-C4D	-5.70	102.29	106.33
37	M	101	8CT	C30-C31-C32	-5.70	114.46	121.47
29	b	602	CLA	C4A-NA-C1A	-5.69	104.15	106.71
29	A	809	CLA	C1D-ND-C4D	-5.69	102.29	106.33
29	A	810	CLA	C1D-ND-C4D	-5.68	102.30	106.33
29	5	605	CLA	C1D-ND-C4D	-5.68	102.30	106.33
29	A	829	CLA	C4A-NA-C1A	-5.67	104.16	106.71
29	5	605	CLA	C4A-NA-C1A	-5.66	104.16	106.71
29	c	606	CLA	C4A-NA-C1A	-5.66	104.16	106.71
29	c	612	CLA	C4A-NA-C1A	-5.65	104.16	106.71
29	d	602	CLA	C4A-NA-C1A	-5.65	104.17	106.71
29	a	604	CLA	C4A-NA-C1A	-5.65	104.17	106.71
29	6	604	CLA	C4A-NA-C1A	-5.64	104.17	106.71
29	B	815	CLA	C4A-NA-C1A	-5.64	104.17	106.71
29	1	612	CLA	C1D-ND-C4D	-5.63	102.33	106.33
29	B	824	CLA	C1D-ND-C4D	-5.63	102.34	106.33
29	7	612	CLA	C1D-ND-C4D	-5.62	102.34	106.33
29	d	612	CLA	C1D-ND-C4D	-5.62	102.34	106.33
29	A	827	CLA	C1D-ND-C4D	-5.61	102.35	106.33
29	B	814	CLA	C4A-NA-C1A	-5.61	104.18	106.71
33	K	104	IHT	C02-C07-C10	-5.60	114.73	122.61
33	a	617	IHT	C41-C38-C35	-5.60	119.32	127.31
29	2	605	CLA	C1D-ND-C4D	-5.60	102.36	106.33
29	7	604	CLA	C4A-NA-C1A	-5.59	104.19	106.71
29	7	608	CLA	C4A-NA-C1A	-5.59	104.19	106.71
29	6	605	CLA	C1D-ND-C4D	-5.58	102.37	106.33
29	7	609	CLA	C4A-NA-C1A	-5.58	104.20	106.71
29	A	806	CLA	C1D-ND-C4D	-5.57	102.38	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	202	CLA	C4A-NA-C1A	-5.57	104.20	106.71
29	A	812	CLA	C1D-ND-C4D	-5.57	102.38	106.33
29	1	606	CLA	C4A-NA-C1A	-5.57	104.20	106.71
29	a	606	CLA	C4A-NA-C1A	-5.57	104.20	106.71
29	4	603	CLA	C4A-NA-C1A	-5.57	104.20	106.71
29	a	603	CLA	C4A-NA-C1A	-5.56	104.20	106.71
29	8	602	CLA	C1D-ND-C4D	-5.56	102.38	106.33
29	L	207	CLA	C1D-ND-C4D	-5.56	102.38	106.33
29	9	608	CLA	C4A-NA-C1A	-5.56	104.21	106.71
29	A	830	CLA	C4A-NA-C1A	-5.56	104.21	106.71
29	c	605	CLA	C4A-NA-C1A	-5.56	104.21	106.71
29	9	602	CLA	C4A-NA-C1A	-5.56	104.21	106.71
29	5	612	CLA	C4A-NA-C1A	-5.55	104.21	106.71
29	8	603	CLA	C4A-NA-C1A	-5.54	104.21	106.71
29	R	202	CLA	C1D-ND-C4D	-5.54	102.40	106.33
29	B	808	CLA	C1D-ND-C4D	-5.52	102.41	106.33
29	7	602	CLA	C4A-NA-C1A	-5.52	104.22	106.71
29	2	605	CLA	C4A-NA-C1A	-5.52	104.23	106.71
29	A	841	CLA	C1D-ND-C4D	-5.50	102.43	106.33
29	B	812	CLA	C4A-NA-C1A	-5.50	104.23	106.71
29	a	602	CLA	C4A-NA-C1A	-5.50	104.23	106.71
29	1	607	CLA	C4A-NA-C1A	-5.49	104.24	106.71
29	5	606	CLA	C4A-NA-C1A	-5.49	104.24	106.71
29	7	607	CLA	C4A-NA-C1A	-5.49	104.24	106.71
29	6	603	CLA	C4A-NA-C1A	-5.48	104.24	106.71
29	2	602	CLA	C4A-NA-C1A	-5.48	104.24	106.71
29	A	813	CLA	C4A-NA-C1A	-5.47	104.25	106.71
29	A	844	CLA	C4A-NA-C1A	-5.46	104.25	106.71
29	9	601	CLA	C4A-NA-C1A	-5.46	104.25	106.71
29	e	606	CLA	C1D-ND-C4D	-5.45	102.46	106.33
29	A	822	CLA	C4A-NA-C1A	-5.45	104.26	106.71
29	c	604	CLA	C4A-NA-C1A	-5.45	104.26	106.71
29	2	611	CLA	C4A-NA-C1A	-5.44	104.26	106.71
29	6	609	CLA	C4A-NA-C1A	-5.44	104.26	106.71
29	e	602	CLA	C4A-NA-C1A	-5.44	104.26	106.71
29	B	811	CLA	C4A-NA-C1A	-5.43	104.27	106.71
29	A	818	CLA	C4A-NA-C1A	-5.42	104.27	106.71
29	a	607	CLA	C4A-NA-C1A	-5.42	104.27	106.71
29	1	609	CLA	C4A-NA-C1A	-5.42	104.27	106.71
29	e	608	CLA	C4A-NA-C1A	-5.41	104.27	106.71
29	5	608	CLA	C4A-NA-C1A	-5.41	104.27	106.71
29	2	608	CLA	C4A-NA-C1A	-5.40	104.28	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	608	CLA	C4A-NA-C1A	-5.39	104.28	106.71
29	9	606	CLA	C4A-NA-C1A	-5.38	104.29	106.71
29	8	605	CLA	CHD-C1D-ND	-5.37	119.52	124.45
29	5	602	CLA	C4A-NA-C1A	-5.36	104.30	106.71
29	e	610	CLA	C4A-NA-C1A	-5.36	104.30	106.71
29	A	801	CLA	CHD-C1D-ND	-5.36	119.53	124.45
29	B	802	CLA	C4A-NA-C1A	-5.36	104.30	106.71
29	6	608	CLA	C4A-NA-C1A	-5.35	104.30	106.71
29	b	611	CLA	C4A-NA-C1A	-5.34	104.30	106.71
29	B	821	CLA	C4A-NA-C1A	-5.34	104.31	106.71
29	B	817	CLA	C4A-NA-C1A	-5.33	104.31	106.71
29	B	829	CLA	CHD-C1D-ND	-5.33	119.56	124.45
29	A	804	CLA	C4A-NA-C1A	-5.33	104.31	106.71
29	b	607	CLA	C4A-NA-C1A	-5.33	104.31	106.71
29	B	816	CLA	C4A-NA-C1A	-5.32	104.31	106.71
29	A	827	CLA	C4A-NA-C1A	-5.32	104.31	106.71
29	A	826	CLA	C1D-ND-C4D	-5.32	102.56	106.33
33	9	619	IHT	C30-C27-C23	-5.31	119.74	127.31
29	4	611	CLA	C4A-NA-C1A	-5.29	104.33	106.71
29	d	606	CLA	C4A-NA-C1A	-5.29	104.33	106.71
29	8	608	CLA	C4A-NA-C1A	-5.28	104.33	106.71
29	A	833	CLA	C4A-NA-C1A	-5.28	104.33	106.71
33	c	620	IHT	C19-C10-C07	-5.28	118.60	124.53
29	B	831	CLA	CHD-C1D-ND	-5.28	119.60	124.45
29	8	605	CLA	C4A-NA-C1A	-5.28	104.33	106.71
29	A	841	CLA	C4A-NA-C1A	-5.28	104.33	106.71
29	c	603	CLA	C4A-NA-C1A	-5.27	104.33	106.71
29	3	607	CLA	C4A-NA-C1A	-5.27	104.34	106.71
29	B	836	CLA	C4A-NA-C1A	-5.26	104.34	106.71
29	A	821	CLA	CHD-C1D-ND	-5.26	119.62	124.45
29	1	611	CLA	C4A-NA-C1A	-5.26	104.34	106.71
29	d	607	CLA	C4A-NA-C1A	-5.25	104.34	106.71
29	3	608	CLA	C4A-NA-C1A	-5.24	104.35	106.71
29	7	605	CLA	C4A-NA-C1A	-5.24	104.35	106.71
29	B	806	CLA	C4A-NA-C1A	-5.24	104.35	106.71
29	L	204	CLA	C4A-NA-C1A	-5.24	104.35	106.71
29	2	604	CLA	C4A-NA-C1A	-5.23	104.35	106.71
29	3	610	CLA	C4A-NA-C1A	-5.23	104.35	106.71
29	6	605	CLA	C4A-NA-C1A	-5.22	104.36	106.71
29	9	611	CLA	C4A-NA-C1A	-5.22	104.36	106.71
29	O	201	CLA	C4A-NA-C1A	-5.21	104.36	106.71
29	9	602	CLA	CHD-C1D-ND	-5.21	119.67	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	838	CLA	C4A-NA-C1A	-5.21	104.36	106.71
29	A	803	CLA	CHD-C1D-ND	-5.20	119.67	124.45
29	A	808	CLA	C4A-NA-C1A	-5.20	104.37	106.71
29	1	602	CLA	C4A-NA-C1A	-5.20	104.37	106.71
29	2	612	CLA	C4A-NA-C1A	-5.19	104.37	106.71
29	4	601	CLA	C4A-NA-C1A	-5.19	104.37	106.71
29	c	609	CLA	C4A-NA-C1A	-5.19	104.37	106.71
29	O	202	CLA	CHD-C1D-ND	-5.19	119.69	124.45
29	A	805	CLA	CHD-C1D-ND	-5.18	119.70	124.45
29	8	615	CLA	C4A-NA-C1A	-5.17	104.38	106.71
29	9	603	CLA	C4A-NA-C1A	-5.17	104.38	106.71
29	4	609	CLA	C4A-NA-C1A	-5.17	104.38	106.71
29	5	612	CLA	CHD-C1D-ND	-5.17	119.70	124.45
29	A	814	CLA	CHD-C1D-ND	-5.17	119.71	124.45
29	4	606	CLA	C4A-NA-C1A	-5.16	104.39	106.71
29	B	820	CLA	C4A-NA-C1A	-5.16	104.39	106.71
29	b	608	CLA	C4A-NA-C1A	-5.16	104.39	106.71
29	e	601	CLA	C4A-NA-C1A	-5.15	104.39	106.71
29	B	814	CLA	CHD-C1D-ND	-5.15	119.72	124.45
29	3	601	CLA	C4A-NA-C1A	-5.14	104.39	106.71
29	A	839	CLA	C4A-NA-C1A	-5.14	104.39	106.71
29	a	605	CLA	C4A-NA-C1A	-5.14	104.39	106.71
29	2	606	CLA	C4A-NA-C1A	-5.14	104.40	106.71
29	B	807	CLA	C4A-NA-C1A	-5.14	104.40	106.71
29	1	601	CLA	CHD-C1D-ND	-5.13	119.74	124.45
29	F	202	CLA	CHD-C1D-ND	-5.13	119.74	124.45
29	9	607	CLA	C4A-NA-C1A	-5.13	104.40	106.71
29	A	820	CLA	C4A-NA-C1A	-5.13	104.40	106.71
29	5	601	CLA	CHD-C1D-ND	-5.13	119.74	124.45
29	A	809	CLA	CHD-C1D-ND	-5.13	119.74	124.45
29	A	835	CLA	C4A-NA-C1A	-5.12	104.40	106.71
29	A	802	CLA	C4A-NA-C1A	-5.12	104.41	106.71
33	5	618	IHT	C06-C09-C10	5.11	123.20	114.08
29	B	832	CLA	C4A-NA-C1A	-5.11	104.41	106.71
29	A	805	CLA	C4A-NA-C1A	-5.10	104.41	106.71
29	L	203	CLA	CHD-C1D-ND	-5.10	119.77	124.45
29	A	824	CLA	C4A-NA-C1A	-5.09	104.42	106.71
29	O	202	CLA	C4A-NA-C1A	-5.09	104.42	106.71
29	B	803	CLA	C1D-ND-C4D	-5.08	102.73	106.33
29	5	608	CLA	CHD-C1D-ND	-5.07	119.79	124.45
29	b	601	CLA	C4A-NA-C1A	-5.07	104.43	106.71
29	K	101	CLA	C4A-NA-C1A	-5.07	104.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	844	CLA	CHD-C1D-ND	-5.06	119.80	124.45
29	O	201	CLA	CHD-C1D-ND	-5.06	119.80	124.45
29	9	604	CLA	C4A-NA-C1A	-5.06	104.43	106.71
29	B	803	CLA	CHD-C1D-ND	-5.06	119.80	124.45
29	B	802	CLA	C1D-ND-C4D	-5.06	102.74	106.33
29	B	828	CLA	C4A-NA-C1A	-5.06	104.43	106.71
29	3	610	CLA	CHD-C1D-ND	-5.05	119.81	124.45
29	c	604	CLA	CHD-C1D-ND	-5.04	119.82	124.45
29	B	804	CLA	CHD-C1D-ND	-5.04	119.82	124.45
29	B	830	CLA	CHD-C1D-ND	-5.04	119.83	124.45
33	Z	302	IHT	C19-C10-C07	-5.04	118.87	124.53
29	A	825	CLA	C4A-NA-C1A	-5.04	104.44	106.71
29	F	202	CLA	C4A-NA-C1A	-5.04	104.44	106.71
29	6	606	CLA	CHD-C1D-ND	-5.03	119.83	124.45
29	1	608	CLA	C4A-NA-C1A	-5.03	104.44	106.71
29	a	612	CLA	C4A-NA-C1A	-5.03	104.44	106.71
33	a	617	IHT	C18-C07-C10	-5.03	109.27	121.46
29	A	819	CLA	CHD-C1D-ND	-5.03	119.83	124.45
29	8	606	CLA	CHD-C1D-ND	-5.03	119.83	124.45
29	B	840	CLA	CHD-C1D-ND	-5.03	119.83	124.45
29	b	601	CLA	CHD-C1D-ND	-5.03	119.84	124.45
29	B	805	CLA	C4A-NA-C1A	-5.02	104.45	106.71
29	4	603	CLA	CHD-C1D-ND	-5.02	119.84	124.45
29	6	607	CLA	C4A-NA-C1A	-5.02	104.45	106.71
29	F	204	CLA	C4A-NA-C1A	-5.02	104.45	106.71
29	A	841	CLA	CHD-C1D-ND	-5.02	119.84	124.45
29	A	813	CLA	CHD-C1D-ND	-5.02	119.84	124.45
29	c	601	CLA	CHD-C1D-ND	-5.02	119.84	124.45
29	5	607	CLA	C4A-NA-C1A	-5.02	104.45	106.71
29	A	808	CLA	CHD-C1D-ND	-5.02	119.84	124.45
29	B	805	CLA	CHD-C1D-ND	-5.02	119.84	124.45
29	8	604	CLA	C4A-NA-C1A	-5.01	104.45	106.71
29	6	604	CLA	CHD-C1D-ND	-5.01	119.85	124.45
29	8	608	CLA	CHD-C1D-ND	-5.01	119.85	124.45
29	B	827	CLA	CHD-C1D-ND	-5.01	119.85	124.45
29	a	601	CLA	C4A-NA-C1A	-5.01	104.45	106.71
29	c	612	CLA	CHD-C1D-ND	-5.01	119.85	124.45
29	4	607	CLA	C4A-NA-C1A	-5.00	104.46	106.71
29	6	603	CLA	CHD-C1D-ND	-5.00	119.86	124.45
29	b	610	CLA	CHD-C1D-ND	-5.00	119.86	124.45
29	2	607	CLA	CHD-C1D-ND	-5.00	119.86	124.45
29	b	610	CLA	C4A-NA-C1A	-5.00	104.46	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	9	606	CLA	CHD-C1D-ND	-5.00	119.86	124.45
29	7	607	CLA	CHD-C1D-ND	-4.99	119.86	124.45
29	b	611	CLA	CHD-C1D-ND	-4.99	119.86	124.45
29	7	603	CLA	C4A-NA-C1A	-4.99	104.46	106.71
29	2	612	CLA	CHD-C1D-ND	-4.99	119.87	124.45
29	d	608	CLA	CHD-C1D-ND	-4.99	119.87	124.45
29	B	817	CLA	CHD-C1D-ND	-4.99	119.87	124.45
29	A	842	CLA	CHD-C1D-ND	-4.99	119.87	124.45
29	a	606	CLA	CHD-C1D-ND	-4.99	119.87	124.45
29	d	607	CLA	CHD-C1D-ND	-4.99	119.87	124.45
29	B	831	CLA	C4A-NA-C1A	-4.99	104.46	106.71
29	2	608	CLA	CHD-C1D-ND	-4.99	119.87	124.45
29	5	602	CLA	CHD-C1D-ND	-4.99	119.87	124.45
29	8	603	CLA	CHD-C1D-ND	-4.99	119.87	124.45
29	A	818	CLA	CHD-C1D-ND	-4.98	119.87	124.45
29	B	828	CLA	CHD-C1D-ND	-4.98	119.88	124.45
29	9	609	CLA	C4A-NA-C1A	-4.98	104.47	106.71
29	a	611	CLA	C4A-NA-C1A	-4.98	104.47	106.71
29	a	605	CLA	CHD-C1D-ND	-4.98	119.88	124.45
29	B	838	CLA	CHD-C1D-ND	-4.98	119.88	124.45
29	1	603	CLA	C4A-NA-C1A	-4.97	104.47	106.71
29	A	807	CLA	CHD-C1D-ND	-4.97	119.89	124.45
29	B	841	CLA	CHD-C1D-ND	-4.97	119.89	124.45
29	A	840	CLA	CHD-C1D-ND	-4.97	119.89	124.45
29	1	613	CLA	CHD-C1D-ND	-4.97	119.89	124.45
29	3	603	CLA	CHD-C1D-ND	-4.97	119.89	124.45
29	a	609	CLA	C4A-NA-C1A	-4.96	104.47	106.71
33	6	617	IHT	C06-C09-C10	4.96	122.94	114.08
29	2	604	CLA	CHD-C1D-ND	-4.96	119.89	124.45
33	9	619	IHT	C18-C07-C10	-4.96	109.44	121.46
29	B	808	CLA	C4A-NA-C1A	-4.96	104.47	106.71
29	B	809	CLA	C4A-NA-C1A	-4.96	104.48	106.71
29	e	606	CLA	C4A-NA-C1A	-4.96	104.48	106.71
29	e	610	CLA	CHD-C1D-ND	-4.96	119.90	124.45
29	B	837	CLA	CHD-C1D-ND	-4.96	119.90	124.45
29	9	614	CLA	CHD-C1D-ND	-4.95	119.90	124.45
29	A	817	CLA	CHD-C1D-ND	-4.95	119.90	124.45
29	b	607	CLA	CHD-C1D-ND	-4.95	119.90	124.45
29	3	604	CLA	C4A-NA-C1A	-4.95	104.48	106.71
29	8	615	CLA	CHD-C1D-ND	-4.95	119.90	124.45
29	B	826	CLA	CHD-C1D-ND	-4.95	119.91	124.45
29	2	603	CLA	CHD-C1D-ND	-4.95	119.91	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	601	CLA	CHD-C1D-ND	-4.95	119.91	124.45
29	3	605	CLA	CHD-C1D-ND	-4.94	119.91	124.45
29	B	811	CLA	CHD-C1D-ND	-4.94	119.91	124.45
33	1	618	IHT	C06-C09-C10	4.94	122.90	114.08
29	B	810	CLA	CHD-C1D-ND	-4.94	119.91	124.45
33	L	205	IHT	C06-C09-C10	4.94	122.90	114.08
30	7	606	KC2	C4D-C3D-CAD	4.94	110.75	107.42
29	A	833	CLA	CHD-C1D-ND	-4.94	119.91	124.45
29	e	607	CLA	CHD-C1D-ND	-4.94	119.92	124.45
29	2	611	CLA	CHD-C1D-ND	-4.94	119.92	124.45
29	4	606	CLA	CHD-C1D-ND	-4.94	119.92	124.45
29	7	605	CLA	CHD-C1D-ND	-4.94	119.92	124.45
29	A	843	CLA	CHD-C1D-ND	-4.94	119.92	124.45
29	4	607	CLA	CHD-C1D-ND	-4.93	119.92	124.45
29	A	829	CLA	CHD-C1D-ND	-4.93	119.92	124.45
29	a	611	CLA	CHD-C1D-ND	-4.93	119.92	124.45
29	a	607	CLA	CHD-C1D-ND	-4.93	119.92	124.45
33	d	617	IHT	C06-C09-C10	4.93	122.88	114.08
29	4	611	CLA	CHD-C1D-ND	-4.93	119.92	124.45
29	B	807	CLA	CHD-C1D-ND	-4.93	119.92	124.45
29	5	604	CLA	CHD-C1D-ND	-4.93	119.92	124.45
29	d	611	CLA	CHD-C1D-ND	-4.93	119.92	124.45
29	B	818	CLA	CHD-C1D-ND	-4.93	119.92	124.45
29	e	601	CLA	CHD-C1D-ND	-4.93	119.92	124.45
29	A	826	CLA	C4A-NA-C1A	-4.93	104.49	106.71
29	B	824	CLA	CHD-C1D-ND	-4.93	119.93	124.45
29	B	832	CLA	CHD-C1D-ND	-4.93	119.93	124.45
29	A	810	CLA	C4A-NA-C1A	-4.93	104.49	106.71
29	2	601	CLA	CHD-C1D-ND	-4.93	119.93	124.45
29	L	201	CLA	CHD-C1D-ND	-4.93	119.93	124.45
29	3	607	CLA	CHD-C1D-ND	-4.92	119.93	124.45
29	O	203	CLA	CHD-C1D-ND	-4.92	119.93	124.45
29	A	834	CLA	CHD-C1D-ND	-4.92	119.93	124.45
29	2	603	CLA	C4A-NA-C1A	-4.92	104.49	106.71
29	d	601	CLA	CHD-C1D-ND	-4.92	119.93	124.45
29	B	834	CLA	CHD-C1D-ND	-4.92	119.93	124.45
29	A	827	CLA	CHD-C1D-ND	-4.92	119.93	124.45
29	b	603	CLA	CHD-C1D-ND	-4.92	119.93	124.45
29	A	838	CLA	C4A-NA-C1A	-4.92	104.50	106.71
29	F	203	CLA	CHD-C1D-ND	-4.92	119.94	124.45
29	6	609	CLA	CHD-C1D-ND	-4.92	119.94	124.45
29	7	604	CLA	CHD-C1D-ND	-4.91	119.94	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	6	612	CLA	C4A-NA-C1A	-4.91	104.50	106.71
29	9	612	CLA	CHD-C1D-ND	-4.91	119.94	124.45
29	A	816	CLA	CHD-C1D-ND	-4.91	119.94	124.45
29	B	825	CLA	C4A-NA-C1A	-4.91	104.50	106.71
29	7	603	CLA	CHD-C1D-ND	-4.91	119.94	124.45
29	2	609	CLA	CHD-C1D-ND	-4.91	119.95	124.45
29	K	102	CLA	C4A-NA-C1A	-4.90	104.50	106.71
29	A	837	CLA	CHD-C1D-ND	-4.90	119.95	124.45
29	8	607	CLA	CHD-C1D-ND	-4.90	119.95	124.45
29	7	601	CLA	CHD-C1D-ND	-4.89	119.96	124.45
29	e	603	CLA	CHD-C1D-ND	-4.89	119.96	124.45
29	a	604	CLA	CHD-C1D-ND	-4.89	119.96	124.45
29	3	601	CLA	CHD-C1D-ND	-4.89	119.96	124.45
33	c	620	IHT	C18-C07-C10	-4.89	109.62	121.46
29	6	601	CLA	C4A-NA-C1A	-4.89	104.51	106.71
29	B	835	CLA	CHD-C1D-ND	-4.89	119.96	124.45
29	J	102	CLA	CHD-C1D-ND	-4.89	119.96	124.45
37	A	847	8CT	C30-C31-C32	-4.89	115.46	121.47
29	6	611	CLA	CHD-C1D-ND	-4.88	119.97	124.45
29	d	606	CLA	CHD-C1D-ND	-4.88	119.97	124.45
29	A	826	CLA	CHD-C1D-ND	-4.88	119.97	124.45
29	1	608	CLA	CHD-C1D-ND	-4.88	119.97	124.45
29	B	836	CLA	CHD-C1D-ND	-4.88	119.97	124.45
29	4	608	CLA	C4A-NA-C1A	-4.88	104.51	106.71
29	6	611	CLA	C4A-NA-C1A	-4.88	104.51	106.71
29	Z	306	CLA	CHD-C1D-ND	-4.88	119.97	124.45
29	B	819	CLA	CHD-C1D-ND	-4.88	119.97	124.45
29	A	824	CLA	CHD-C1D-ND	-4.88	119.97	124.45
29	9	604	CLA	CHD-C1D-ND	-4.87	119.97	124.45
29	A	823	CLA	C4A-NA-C1A	-4.87	104.52	106.71
29	8	601	CLA	CHD-C1D-ND	-4.87	119.98	124.45
29	Z	301	CLA	CHD-C1D-ND	-4.87	119.98	124.45
29	5	611	CLA	C4A-NA-C1A	-4.87	104.52	106.71
29	3	608	CLA	CHD-C1D-ND	-4.87	119.98	124.45
29	c	606	CLA	CHD-C1D-ND	-4.86	119.98	124.45
31	8	616	II0	C20-C14-C10	-4.86	117.75	124.35
29	9	603	CLA	CHD-C1D-ND	-4.85	120.00	124.45
29	c	608	CLA	CHD-C1D-ND	-4.85	120.00	124.45
29	1	603	CLA	CHD-C1D-ND	-4.85	120.00	124.45
29	e	602	CLA	CHD-C1D-ND	-4.85	120.00	124.45
29	A	832	CLA	C4A-NA-C1A	-4.85	104.53	106.71
29	7	611	CLA	C4A-NA-C1A	-4.84	104.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	606	CLA	C4A-NA-C1A	-4.84	104.53	106.71
29	1	611	CLA	CHD-C1D-ND	-4.84	120.00	124.45
29	9	609	CLA	CHD-C1D-ND	-4.84	120.00	124.45
29	7	608	CLA	CHD-C1D-ND	-4.84	120.01	124.45
29	B	802	CLA	CHD-C1D-ND	-4.84	120.01	124.45
29	B	825	CLA	CHD-C1D-ND	-4.84	120.01	124.45
29	5	603	CLA	CHD-C1D-ND	-4.84	120.01	124.45
29	d	604	CLA	CHD-C1D-ND	-4.84	120.01	124.45
29	A	822	CLA	CHD-C1D-ND	-4.83	120.01	124.45
29	a	603	CLA	CHD-C1D-ND	-4.83	120.01	124.45
29	7	602	CLA	CHD-C1D-ND	-4.83	120.01	124.45
29	A	825	CLA	CHD-C1D-ND	-4.83	120.02	124.45
29	1	606	CLA	CHD-C1D-ND	-4.83	120.02	124.45
29	F	203	CLA	C4A-NA-C1A	-4.83	104.53	106.71
29	A	835	CLA	CHD-C1D-ND	-4.83	120.02	124.45
29	6	608	CLA	CHD-C1D-ND	-4.83	120.02	124.45
29	B	816	CLA	CHD-C1D-ND	-4.82	120.02	124.45
29	9	605	CLA	CHD-C1D-ND	-4.82	120.02	124.45
29	A	820	CLA	CHD-C1D-ND	-4.82	120.02	124.45
29	4	604	CLA	CHD-C1D-ND	-4.82	120.03	124.45
29	7	612	CLA	CHD-C1D-ND	-4.82	120.03	124.45
29	L	202	CLA	CHD-C1D-ND	-4.82	120.03	124.45
29	3	611	CLA	CHD-C1D-ND	-4.82	120.03	124.45
29	c	607	CLA	CHD-C1D-ND	-4.81	120.03	124.45
29	e	608	CLA	CHD-C1D-ND	-4.81	120.03	124.45
29	2	602	CLA	CHD-C1D-ND	-4.81	120.03	124.45
29	A	832	CLA	CHD-C1D-ND	-4.81	120.03	124.45
29	d	603	CLA	C4A-NA-C1A	-4.81	104.54	106.71
29	4	609	CLA	CHD-C1D-ND	-4.81	120.03	124.45
29	5	609	CLA	CHD-C1D-ND	-4.81	120.04	124.45
29	b	606	CLA	CHD-C1D-ND	-4.81	120.04	124.45
29	B	809	CLA	CHD-C1D-ND	-4.80	120.04	124.45
29	L	204	CLA	CHD-C1D-ND	-4.80	120.04	124.45
29	d	603	CLA	CHD-C1D-ND	-4.80	120.04	124.45
29	9	613	CLA	C4A-NA-C1A	-4.80	104.55	106.71
29	d	601	CLA	C4A-NA-C1A	-4.80	104.55	106.71
29	a	612	CLA	CHD-C1D-ND	-4.80	120.04	124.45
29	c	603	CLA	CHD-C1D-ND	-4.80	120.05	124.45
29	A	811	CLA	CHD-C1D-ND	-4.80	120.05	124.45
29	3	604	CLA	CHD-C1D-ND	-4.79	120.05	124.45
29	9	607	CLA	CHD-C1D-ND	-4.79	120.05	124.45
29	1	609	CLA	CHD-C1D-ND	-4.79	120.06	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	4	602	CLA	CHD-C1D-ND	-4.79	120.06	124.45
29	B	820	CLA	CHD-C1D-ND	-4.79	120.06	124.45
29	3	611	CLA	C4A-NA-C1A	-4.78	104.56	106.71
29	Z	304	CLA	C4A-NA-C1A	-4.78	104.56	106.71
29	2	605	CLA	CHD-C1D-ND	-4.78	120.06	124.45
29	5	609	CLA	C4A-NA-C1A	-4.78	104.56	106.71
29	1	607	CLA	CHD-C1D-ND	-4.78	120.06	124.45
29	3	602	CLA	CHD-C1D-ND	-4.78	120.06	124.45
29	4	610	CLA	C4A-NA-C1A	-4.78	104.56	106.71
29	K	102	CLA	CHD-C1D-ND	-4.78	120.06	124.45
29	5	607	CLA	CHD-C1D-ND	-4.77	120.07	124.45
33	8	609	IHT	C18-C07-C10	-4.77	109.90	121.46
29	A	836	CLA	CHD-C1D-ND	-4.77	120.07	124.45
29	a	608	CLA	CHD-C1D-ND	-4.77	120.07	124.45
29	5	606	CLA	CHD-C1D-ND	-4.77	120.07	124.45
29	A	802	CLA	CHD-C1D-ND	-4.77	120.07	124.45
29	2	606	CLA	CHD-C1D-ND	-4.77	120.07	124.45
29	6	612	CLA	CHD-C1D-ND	-4.77	120.07	124.45
33	c	620	IHT	C06-C09-C10	4.76	122.58	114.08
29	d	612	CLA	CHD-C1D-ND	-4.76	120.08	124.45
29	7	611	CLA	CHD-C1D-ND	-4.76	120.08	124.45
29	e	606	CLA	CHD-C1D-ND	-4.76	120.08	124.45
29	c	607	CLA	C4A-NA-C1A	-4.76	104.57	106.71
29	e	604	CLA	CHD-C1D-ND	-4.76	120.08	124.45
29	e	611	CLA	CHD-C1D-ND	-4.76	120.08	124.45
29	9	613	CLA	CHD-C1D-ND	-4.75	120.08	124.45
29	9	612	CLA	C4A-NA-C1A	-4.75	104.57	106.71
29	9	601	CLA	CHD-C1D-ND	-4.75	120.09	124.45
29	9	611	CLA	CHD-C1D-ND	-4.75	120.09	124.45
29	B	839	CLA	CHD-C1D-ND	-4.75	120.09	124.45
29	Z	301	CLA	C4A-NA-C1A	-4.75	104.57	106.71
29	5	603	CLA	C4A-NA-C1A	-4.75	104.57	106.71
29	3	612	CLA	CHD-C1D-ND	-4.75	120.09	124.45
29	d	612	CLA	C4A-NA-C1A	-4.74	104.57	106.71
29	A	830	CLA	CHD-C1D-ND	-4.74	120.10	124.45
29	c	613	CLA	CHD-C1D-ND	-4.74	120.10	124.45
29	A	815	CLA	C4A-NA-C1A	-4.74	104.58	106.71
29	c	602	CLA	CHD-C1D-ND	-4.74	120.10	124.45
29	5	613	CLA	C4A-NA-C1A	-4.74	104.58	106.71
29	A	815	CLA	CHD-C1D-ND	-4.73	120.10	124.45
29	B	815	CLA	CHD-C1D-ND	-4.73	120.10	124.45
30	4	605	KC2	C4D-C3D-CAD	4.73	110.61	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	833	CLA	C4A-NA-C1A	-4.73	104.58	106.71
29	d	609	CLA	CHD-C1D-ND	-4.73	120.11	124.45
29	6	601	CLA	CHD-C1D-ND	-4.73	120.11	124.45
29	8	607	CLA	C4A-NA-C1A	-4.73	104.58	106.71
29	B	822	CLA	CHD-C1D-ND	-4.73	120.11	124.45
29	3	609	CLA	C4A-NA-C1A	-4.73	104.58	106.71
29	8	601	CLA	C4A-NA-C1A	-4.73	104.58	106.71
29	B	841	CLA	C4A-NA-C1A	-4.73	104.58	106.71
29	6	607	CLA	CHD-C1D-ND	-4.72	120.11	124.45
29	B	837	CLA	C4A-NA-C1A	-4.72	104.58	106.71
29	5	605	CLA	CHD-C1D-ND	-4.72	120.12	124.45
29	5	611	CLA	CHD-C1D-ND	-4.72	120.12	124.45
29	4	608	CLA	CHD-C1D-ND	-4.72	120.12	124.45
29	A	812	CLA	CHD-C1D-ND	-4.72	120.12	124.45
29	d	609	CLA	C4A-NA-C1A	-4.72	104.59	106.71
29	A	828	CLA	CHD-C1D-ND	-4.71	120.12	124.45
29	B	806	CLA	CHD-C1D-ND	-4.71	120.12	124.45
29	7	609	CLA	CHD-C1D-ND	-4.71	120.13	124.45
29	A	831	CLA	CHD-C1D-ND	-4.71	120.13	124.45
29	A	806	CLA	CHD-C1D-ND	-4.71	120.13	124.45
29	L	203	CLA	C4A-NA-C1A	-4.70	104.59	106.71
30	6	610	KC2	C4D-C3D-CAD	4.70	110.59	107.42
29	A	810	CLA	CHD-C1D-ND	-4.69	120.14	124.45
29	Z	305	CLA	CHD-C1D-ND	-4.69	120.14	124.45
29	b	608	CLA	CHD-C1D-ND	-4.69	120.14	124.45
29	1	605	CLA	C4A-NA-C1A	-4.69	104.60	106.71
29	4	610	CLA	CHD-C1D-ND	-4.69	120.15	124.45
29	c	609	CLA	CHD-C1D-ND	-4.69	120.15	124.45
29	1	604	CLA	CHD-C1D-ND	-4.68	120.15	124.45
29	1	612	CLA	CHD-C1D-ND	-4.68	120.16	124.45
29	5	613	CLA	CHD-C1D-ND	-4.67	120.16	124.45
29	A	807	CLA	C4A-NA-C1A	-4.67	104.61	106.71
29	Z	304	CLA	CHD-C1D-ND	-4.67	120.16	124.45
29	a	602	CLA	CHD-C1D-ND	-4.67	120.16	124.45
29	1	604	CLA	C4A-NA-C1A	-4.67	104.61	106.71
29	B	812	CLA	CHD-C1D-ND	-4.66	120.17	124.45
29	L	207	CLA	CHD-C1D-ND	-4.66	120.17	124.45
29	A	838	CLA	CHD-C1D-ND	-4.66	120.18	124.45
29	1	602	CLA	CHD-C1D-ND	-4.65	120.18	124.45
29	b	602	CLA	CHD-C1D-ND	-4.65	120.18	124.45
29	9	608	CLA	CHD-C1D-ND	-4.65	120.18	124.45
29	B	826	CLA	C4A-NA-C1A	-4.65	104.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	F	204	CLA	CHD-C1D-ND	-4.65	120.18	124.45
29	8	604	CLA	CHD-C1D-ND	-4.65	120.18	124.45
29	B	821	CLA	CHD-C1D-ND	-4.65	120.19	124.45
29	A	839	CLA	CHD-C1D-ND	-4.64	120.19	124.45
29	B	823	CLA	C4A-NA-C1A	-4.64	104.62	106.71
29	a	609	CLA	CHD-C1D-ND	-4.64	120.19	124.45
29	B	808	CLA	CHD-C1D-ND	-4.63	120.20	124.45
29	d	602	CLA	CHD-C1D-ND	-4.63	120.20	124.45
29	e	611	CLA	C4A-NA-C1A	-4.63	104.63	106.71
29	b	604	CLA	CHD-C1D-ND	-4.62	120.21	124.45
29	d	605	CLA	CHD-C1D-ND	-4.62	120.21	124.45
30	6	613	KC2	C4D-C3D-CAD	4.61	110.53	107.42
29	B	823	CLA	CHD-C1D-ND	-4.61	120.22	124.45
29	c	605	CLA	CHD-C1D-ND	-4.61	120.22	124.45
29	A	804	CLA	CHD-C1D-ND	-4.61	120.22	124.45
29	4	601	CLA	CHD-C1D-ND	-4.60	120.23	124.45
30	d	610	KC2	C4D-C3D-CAD	4.60	110.52	107.42
29	A	831	CLA	C4A-NA-C1A	-4.59	104.64	106.71
33	2	616	IHT	C18-C07-C10	-4.59	110.34	121.46
29	B	833	CLA	CHD-C1D-ND	-4.59	120.23	124.45
29	5	608	CLA	C1-C2-C3	-4.58	118.12	126.04
29	A	816	CLA	C4A-NA-C1A	-4.58	104.65	106.71
30	b	605	KC2	C4D-C3D-CAD	4.58	110.51	107.42
29	e	604	CLA	C4A-NA-C1A	-4.57	104.65	106.71
29	c	614	CLA	C4A-NA-C1A	-4.57	104.65	106.71
30	e	605	KC2	C4D-C3D-CAD	4.56	110.49	107.42
29	7	601	CLA	C4A-NA-C1A	-4.56	104.66	106.71
29	6	602	CLA	CHD-C1D-ND	-4.56	120.27	124.45
29	K	101	CLA	CHD-C1D-ND	-4.56	120.27	124.45
29	b	604	CLA	C4A-NA-C1A	-4.54	104.66	106.71
29	8	602	CLA	CHD-C1D-ND	-4.54	120.28	124.45
29	B	822	CLA	C4A-NA-C1A	-4.54	104.67	106.71
30	c	615	KC2	C4D-C3D-CAD	4.53	110.47	107.42
29	4	604	CLA	C4A-NA-C1A	-4.53	104.67	106.71
30	7	610	KC2	C4D-C3D-CAD	4.53	110.47	107.42
29	8	602	CLA	C4A-NA-C1A	-4.52	104.67	106.71
29	B	813	CLA	CHD-C1D-ND	-4.50	120.32	124.45
29	3	609	CLA	CHD-C1D-ND	-4.50	120.32	124.45
29	A	823	CLA	CHD-C1D-ND	-4.49	120.32	124.45
29	6	605	CLA	CHD-C1D-ND	-4.49	120.33	124.45
29	Z	305	CLA	C4A-NA-C1A	-4.49	104.69	106.71
33	6	617	IHT	C19-C10-C07	-4.49	119.49	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	606	KC2	C4D-C3D-CAD	4.48	110.44	107.42
29	B	803	CLA	C4A-NA-C1A	-4.48	104.69	106.71
31	8	616	II0	C41-C39-C35	-4.48	120.91	127.31
33	a	617	IHT	C19-C10-C07	-4.48	119.50	124.53
29	R	202	CLA	CHD-C1D-ND	-4.47	120.35	124.45
29	c	614	CLA	CHD-C1D-ND	-4.47	120.35	124.45
29	d	611	CLA	C4A-NA-C1A	-4.46	104.70	106.71
33	6	617	IHT	C18-C07-C10	-4.44	110.72	121.46
30	Z	307	KC2	C4D-C3D-CAD	4.43	110.41	107.42
30	c	611	KC2	C4D-C3D-CAD	4.42	110.40	107.42
33	K	104	IHT	C30-C27-C23	-4.38	121.06	127.31
30	5	610	KC2	C4D-C3D-CAD	4.36	110.36	107.42
29	A	814	CLA	C4A-NA-C1A	-4.36	104.75	106.71
29	A	834	CLA	C4A-NA-C1A	-4.36	104.75	106.71
30	e	609	KC2	C4D-C3D-CAD	4.35	110.36	107.42
33	9	619	IHT	C19-C10-C09	4.35	121.97	113.62
29	A	828	CLA	C4A-NA-C1A	-4.34	104.75	106.71
30	7	606	KC2	C1D-ND-C4D	4.32	109.40	106.33
31	d	613	II0	C42-C40-C36	-4.31	121.16	127.31
29	A	836	CLA	CHB-C1B-NB	-4.30	119.70	124.26
29	B	804	CLA	C4A-NA-C1A	-4.30	104.77	106.71
30	1	610	KC2	C4D-C3D-CAD	4.28	110.31	107.42
29	A	801	CLA	C4A-NA-C1A	-4.27	104.79	106.71
30	c	610	KC2	C4D-C3D-CAD	4.27	110.30	107.42
33	1	618	IHT	C19-C10-C07	-4.26	119.74	124.53
30	3	606	KC2	C1D-ND-C4D	4.26	109.36	106.33
29	A	801	CLA	CHB-C1B-NB	-4.26	119.75	124.26
37	Z	309	8CT	C30-C31-C32	-4.25	116.24	121.47
36	O	206	SQD	O8-S-C6	4.24	112.50	105.74
30	2	610	KC2	C4D-C3D-CAD	4.24	110.28	107.42
35	5	619	LHG	O4-P-O5	4.23	133.18	112.24
30	d	610	KC2	C1D-ND-C4D	4.23	109.34	106.33
29	B	840	CLA	C4A-NA-C1A	-4.22	104.81	106.71
30	b	609	KC2	C4D-C3D-CAD	4.21	110.26	107.42
35	3	619	LHG	O4-P-O5	4.20	133.03	112.24
33	d	617	IHT	C18-C07-C10	-4.20	111.28	121.46
30	a	610	KC2	C4D-C3D-CAD	4.20	110.25	107.42
35	c	621	LHG	O4-P-O5	4.20	133.01	112.24
29	B	831	CLA	C1-C2-C3	-4.20	118.78	126.04
35	4	617	LHG	O4-P-O5	4.20	133.00	112.24
35	7	618	LHG	O4-P-O5	4.19	132.98	112.24
35	2	619	LHG	O4-P-O5	4.19	132.97	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	618	LHG	O4-P-O5	4.19	132.96	112.24
35	2	620	LHG	O4-P-O5	4.19	132.94	112.24
35	a	618	LHG	O4-P-O5	4.18	132.89	112.24
35	7	619	LHG	O4-P-O5	4.17	132.87	112.24
30	2	610	KC2	C1D-ND-C4D	4.17	109.30	106.33
35	A	851	LHG	O4-P-O5	4.17	132.85	112.24
30	e	609	KC2	C1D-ND-C4D	4.17	109.29	106.33
35	d	619	LHG	O4-P-O5	4.16	132.83	112.24
29	c	613	CLA	C4A-NA-C1A	-4.16	104.84	106.71
35	A	850	LHG	O4-P-O5	4.16	132.80	112.24
35	3	623	LHG	O4-P-O5	4.16	132.80	112.24
35	Z	310	LHG	O4-P-O5	4.16	132.80	112.24
35	6	618	LHG	O4-P-O5	4.16	132.78	112.24
35	4	619	LHG	O4-P-O5	4.15	132.77	112.24
35	b	616	LHG	O4-P-O5	4.15	132.77	112.24
31	1	616	II0	C42-C40-C36	-4.15	121.39	127.31
29	1	605	CLA	CHD-C1D-ND	-4.15	120.64	124.45
30	Z	307	KC2	C1D-ND-C4D	4.15	109.28	106.33
29	B	813	CLA	C4A-NA-C1A	-4.15	104.84	106.71
31	4	613	II0	C42-C40-C36	-4.15	121.39	127.31
30	9	610	KC2	C4D-C3D-CAD	4.15	110.22	107.42
35	3	622	LHG	O4-P-O5	4.14	132.70	112.24
35	L	208	LHG	O4-P-O5	4.14	132.69	112.24
30	9	610	KC2	C1D-ND-C4D	4.13	109.27	106.33
35	B	849	LHG	O4-P-O5	4.13	132.67	112.24
33	K	104	IHT	C40-C37-C33	-4.13	121.42	127.31
35	8	613	LHG	O4-P-O5	4.12	132.63	112.24
29	A	801	CLA	C1D-ND-C4D	-4.11	103.41	106.33
29	B	802	CLA	CHB-C1B-NB	-4.11	119.90	124.26
29	1	612	CLA	C4A-NA-C1A	-4.11	104.86	106.71
35	d	618	LHG	O4-P-O5	4.11	132.54	112.24
31	3	614	II0	C42-C40-C36	-4.10	121.45	127.31
29	8	606	CLA	CHB-C1B-NB	-4.10	119.92	124.26
30	c	610	KC2	C1D-ND-C4D	4.09	109.24	106.33
29	R	202	CLA	C1-C2-C3	-4.09	118.97	126.04
29	a	609	CLA	C1-C2-C3	-4.09	118.97	126.04
33	8	609	IHT	C09-C10-C07	-4.08	116.81	122.73
31	7	616	II0	C42-C40-C36	-4.08	121.49	127.31
30	7	610	KC2	C1D-ND-C4D	4.07	109.23	106.33
33	8	609	IHT	C19-C10-C09	4.07	121.44	113.62
30	b	609	KC2	C1D-ND-C4D	4.07	109.22	106.33
29	3	612	CLA	CHB-C1B-NB	-4.07	119.95	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	843	II0	C42-C40-C36	-4.07	121.51	127.31
30	b	605	KC2	C1D-ND-C4D	4.06	109.22	106.33
30	5	610	KC2	C1D-ND-C4D	4.06	109.22	106.33
31	8	612	II0	C20-C14-C10	-4.06	118.83	124.35
29	3	612	CLA	C4A-NA-C1A	-4.05	104.88	106.71
31	b	614	II0	C20-C14-C10	-4.05	118.85	124.35
33	c	620	IHT	C25-C23-C22	4.04	124.44	118.08
29	B	822	CLA	CHB-C1B-NB	-4.04	119.98	124.26
29	8	605	CLA	CHB-C1B-NB	-4.04	119.98	124.26
29	c	612	CLA	CHB-C1B-NB	-4.04	119.98	124.26
33	5	618	IHT	C18-C07-C10	-4.03	111.69	121.46
31	5	615	II0	C42-C40-C36	-4.03	121.55	127.31
30	6	610	KC2	C1D-ND-C4D	4.03	109.20	106.33
30	a	610	KC2	C1D-ND-C4D	4.03	109.19	106.33
32	e	613	II3	C25-C24-C21	4.02	124.41	118.08
32	b	613	II3	C25-C24-C21	4.02	124.40	118.08
29	B	832	CLA	CHB-C1B-NB	-4.01	120.01	124.26
33	9	619	IHT	C09-C10-C07	-4.01	116.91	122.73
33	9	619	IHT	C36-C33-C37	-4.01	117.31	122.92
29	A	837	CLA	C4A-NA-C1A	-4.00	104.91	106.71
29	A	831	CLA	CHB-C1B-NB	-4.00	120.02	124.26
30	e	605	KC2	C1D-ND-C4D	4.00	109.18	106.33
33	L	205	IHT	C25-C23-C22	3.99	124.37	118.08
33	2	616	IHT	C09-C10-C07	-3.98	116.95	122.73
33	2	616	IHT	C19-C10-C09	3.98	121.25	113.62
31	9	617	II0	C42-C40-C36	-3.96	121.65	127.31
29	A	824	CLA	CHB-C1B-NB	-3.95	120.07	124.26
30	1	610	KC2	C1D-ND-C4D	3.95	109.14	106.33
31	a	613	II0	C42-C40-C36	-3.95	121.67	127.31
41	Z	303	DGD	O3G-C3G-C2G	-3.95	101.37	110.90
31	1	614	II0	C20-C14-C10	-3.94	118.99	124.35
29	1	612	CLA	CHB-C1B-NB	-3.93	120.10	124.26
29	B	826	CLA	CHB-C1B-NB	-3.93	120.10	124.26
29	A	816	CLA	CHB-C1B-NB	-3.91	120.12	124.26
31	7	613	II0	C42-C40-C36	-3.90	121.74	127.31
29	7	608	CLA	C1-C2-C3	-3.90	119.29	126.04
29	8	606	CLA	C4A-NA-C1A	-3.90	104.95	106.71
29	1	605	CLA	CHB-C1B-NB	-3.90	120.13	124.26
29	A	843	CLA	CHB-C1B-NB	-3.89	120.13	124.26
30	4	605	KC2	C1D-ND-C4D	3.89	109.10	106.33
31	2	614	II0	C42-C40-C36	-3.89	121.76	127.31
30	6	613	KC2	C1D-ND-C4D	3.88	109.09	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	609	IHT	C36-C33-C32	3.88	124.20	118.08
29	6	612	CLA	CHB-C1B-NB	-3.87	120.16	124.26
29	A	838	CLA	CHB-C1B-NB	-3.87	120.16	124.26
30	c	611	KC2	C1D-ND-C4D	3.86	109.08	106.33
29	A	809	CLA	CHB-C1B-NB	-3.86	120.17	124.26
29	B	807	CLA	CHB-C1B-NB	-3.86	120.17	124.26
33	d	617	IHT	C19-C10-C07	-3.86	120.20	124.53
31	4	612	II0	C20-C14-C10	-3.85	119.11	124.35
31	5	617	II0	C20-C14-C10	-3.85	119.11	124.35
29	B	813	CLA	CHB-C1B-NB	-3.85	120.18	124.26
29	B	824	CLA	CHB-C1B-NB	-3.84	120.19	124.26
33	2	616	IHT	C36-C33-C32	3.83	124.11	118.08
29	d	611	CLA	CHB-C1B-NB	-3.82	120.21	124.26
29	B	833	CLA	CHB-C1B-NB	-3.82	120.21	124.26
31	e	614	II0	C42-C40-C36	-3.82	121.85	127.31
30	c	615	KC2	CHD-C1D-ND	-3.82	120.21	124.26
29	R	202	CLA	CHB-C1B-NB	-3.82	120.22	124.26
31	5	617	II0	C03-C09-C13	-3.81	117.25	122.63
29	A	837	CLA	CHB-C1B-NB	-3.81	120.22	124.26
31	8	610	II0	C20-C14-C10	-3.81	119.17	124.35
33	1	618	IHT	C30-C27-C23	-3.81	121.88	127.31
37	B	850	8CT	C30-C31-C32	-3.81	116.78	121.47
29	1	601	CLA	CHB-C1B-NB	-3.80	120.23	124.26
29	B	810	CLA	CHB-C1B-NB	-3.80	120.23	124.26
29	B	814	CLA	CHB-C1B-NB	-3.80	120.23	124.26
33	a	617	IHT	C20-C15-C11	-3.80	119.19	124.35
33	Z	302	IHT	C30-C27-C23	-3.79	121.90	127.31
29	A	815	CLA	CHB-C1B-NB	-3.79	120.25	124.26
29	B	808	CLA	CHB-C1B-NB	-3.79	120.25	124.26
29	B	836	CLA	CHB-C1B-NB	-3.78	120.25	124.26
33	2	616	IHT	C30-C27-C23	-3.78	121.91	127.31
29	L	203	CLA	CHB-C1B-NB	-3.78	120.25	124.26
29	A	844	CLA	CHB-C1B-NB	-3.78	120.25	124.26
29	7	607	CLA	CHB-C1B-NB	-3.78	120.25	124.26
29	d	601	CLA	CHB-C1B-NB	-3.78	120.25	124.26
29	c	613	CLA	CHB-C1B-NB	-3.78	120.26	124.26
30	c	615	KC2	C1D-ND-C4D	3.78	109.02	106.33
33	2	616	IHT	C25-C23-C22	3.78	124.03	118.08
29	Z	305	CLA	CHB-C1B-NB	-3.78	120.26	124.26
29	9	607	CLA	CHB-C1B-NB	-3.77	120.26	124.26
29	B	831	CLA	CHB-C1B-NB	-3.77	120.27	124.26
29	2	607	CLA	CHB-C1B-NB	-3.76	120.28	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	601	CLA	CHB-C1B-NB	-3.76	120.28	124.26
31	8	612	II0	C38-C36-C34	3.75	123.98	118.08
33	L	205	IHT	C36-C33-C32	3.75	123.98	118.08
29	A	804	CLA	CHB-C1B-NB	-3.75	120.29	124.26
29	A	814	CLA	CHB-C1B-NB	-3.75	120.29	124.26
29	3	611	CLA	CHB-C1B-NB	-3.74	120.29	124.26
31	1	617	II0	C20-C14-C10	-3.74	119.26	124.35
29	B	809	CLA	CHB-C1B-NB	-3.74	120.29	124.26
30	a	610	KC2	CHD-C1D-ND	-3.74	120.29	124.26
29	8	615	CLA	CHB-C1B-NB	-3.74	120.30	124.26
30	4	605	KC2	CHD-C1D-ND	-3.74	120.30	124.26
33	2	616	IHT	C41-C40-C37	-3.74	115.81	123.47
29	5	607	CLA	CHB-C1B-NB	-3.74	120.30	124.26
29	A	833	CLA	CHB-C1B-NB	-3.74	120.30	124.26
29	A	822	CLA	CHB-C1B-NB	-3.74	120.30	124.26
29	4	601	CLA	CHB-C1B-NB	-3.73	120.30	124.26
29	b	601	CLA	CHB-C1B-NB	-3.73	120.30	124.26
30	c	610	KC2	CHD-C1D-ND	-3.73	120.30	124.26
31	5	616	II0	C38-C36-C34	3.73	123.96	118.08
29	A	806	CLA	CHB-C1B-NB	-3.73	120.31	124.26
29	5	609	CLA	CHB-C1B-NB	-3.73	120.31	124.26
31	4	615	II0	C20-C14-C10	-3.73	119.28	124.35
30	1	610	KC2	CHD-C1D-ND	-3.73	120.31	124.26
29	L	204	CLA	C1-C2-C3	-3.73	120.72	126.75
29	B	819	CLA	CHB-C1B-NB	-3.73	120.31	124.26
29	9	612	CLA	CHB-C1B-NB	-3.73	120.31	124.26
29	2	612	CLA	CHB-C1B-NB	-3.72	120.31	124.26
29	A	828	CLA	CHB-C1B-NB	-3.72	120.32	124.26
33	9	619	IHT	C40-C37-C33	-3.72	122.00	127.31
29	A	802	CLA	CHB-C1B-NB	-3.72	120.32	124.26
32	b	613	II3	C39-C36-C33	-3.72	122.00	127.31
33	Z	302	IHT	C40-C37-C33	-3.72	122.00	127.31
31	c	618	II0	C38-C36-C34	3.72	123.94	118.08
29	5	613	CLA	CHB-C1B-NB	-3.72	120.32	124.26
29	9	601	CLA	CHB-C1B-NB	-3.72	120.32	124.26
29	B	825	CLA	CHB-C1B-NB	-3.72	120.32	124.26
31	O	204	II0	C42-C40-C36	-3.71	122.01	127.31
31	b	612	II0	C42-C40-C36	-3.71	122.01	127.31
29	4	610	CLA	CHB-C1B-NB	-3.71	120.33	124.26
29	6	609	CLA	CHB-C1B-NB	-3.71	120.33	124.26
29	e	602	CLA	C1-C2-C3	-3.71	119.62	126.04
31	1	619	II0	C42-C40-C36	-3.71	122.02	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	9	619	IHT	C22-C23-C27	3.71	124.63	118.94
29	7	612	CLA	CHB-C1B-NB	-3.71	120.33	124.26
31	9	618	II0	C38-C36-C34	3.71	123.92	118.08
29	6	605	CLA	CHB-C1B-NB	-3.71	120.33	124.26
29	B	816	CLA	CHB-C1B-NB	-3.71	120.33	124.26
29	A	841	CLA	CHB-C1B-NB	-3.70	120.33	124.26
29	2	606	CLA	CHB-C1B-NB	-3.70	120.34	124.26
29	B	804	CLA	CHB-C1B-NB	-3.70	120.34	124.26
31	9	615	II0	C42-C40-C36	-3.70	122.03	127.31
29	a	605	CLA	CHB-C1B-NB	-3.70	120.34	124.26
29	a	607	CLA	CHB-C1B-NB	-3.70	120.34	124.26
29	A	803	CLA	CHB-C1B-NB	-3.70	120.34	124.26
29	A	839	CLA	CHB-C1B-NB	-3.70	120.34	124.26
31	2	615	II0	C38-C36-C34	3.70	123.90	118.08
29	B	838	CLA	CHB-C1B-NB	-3.70	120.34	124.26
29	c	608	CLA	CHB-C1B-NB	-3.69	120.35	124.26
29	2	602	CLA	C1-C2-C3	-3.69	119.66	126.04
29	F	204	CLA	CHB-C1B-NB	-3.69	120.35	124.26
30	c	611	KC2	CHD-C1D-ND	-3.69	120.35	124.26
32	1	615	II3	C25-C24-C21	3.69	123.89	118.08
29	6	607	CLA	CHB-C1B-NB	-3.69	120.35	124.26
29	d	609	CLA	CHB-C1B-NB	-3.69	120.35	124.26
29	A	836	CLA	C4A-NA-C1A	-3.69	105.05	106.71
29	Z	306	CLA	CHB-C1B-NB	-3.69	120.35	124.26
29	b	611	CLA	CHB-C1B-NB	-3.69	120.36	124.26
29	3	601	CLA	CHB-C1B-NB	-3.68	120.36	124.26
29	e	608	CLA	CHB-C1B-NB	-3.68	120.36	124.26
29	4	603	CLA	CHB-C1B-NB	-3.68	120.36	124.26
29	O	203	CLA	CHB-C1B-NB	-3.68	120.36	124.26
31	5	620	II0	C19-C13-C11	3.67	121.16	114.36
29	e	611	CLA	CHB-C1B-NB	-3.67	120.37	124.26
30	Z	307	KC2	CHD-C1D-ND	-3.67	120.37	124.26
30	7	606	KC2	CHD-C1D-ND	-3.67	120.37	124.26
29	3	607	CLA	CHB-C1B-NB	-3.67	120.37	124.26
29	6	601	CLA	CHB-C1B-NB	-3.67	120.37	124.26
29	O	202	CLA	CHB-C1B-NB	-3.67	120.37	124.26
29	L	204	CLA	CHB-C1B-NB	-3.67	120.38	124.26
29	a	601	CLA	CHB-C1B-NB	-3.67	120.38	124.26
30	6	613	KC2	CHD-C1D-ND	-3.66	120.38	124.26
29	A	808	CLA	CHB-C1B-NB	-3.66	120.38	124.26
29	B	803	CLA	CHB-C1B-NB	-3.66	120.38	124.26
29	2	601	CLA	CHB-C1B-NB	-3.66	120.38	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	3	608	CLA	CHB-C1B-NB	-3.66	120.38	124.26
29	1	609	CLA	CHB-C1B-NB	-3.66	120.38	124.26
29	1	604	CLA	CHB-C1B-NB	-3.66	120.38	124.26
29	2	605	CLA	CHB-C1B-NB	-3.66	120.38	124.26
29	4	608	CLA	CHB-C1B-NB	-3.66	120.39	124.26
33	9	619	IHT	C22-C18-C07	-3.66	116.93	127.20
29	A	832	CLA	CHB-C1B-NB	-3.66	120.39	124.26
29	e	601	CLA	CHB-C1B-NB	-3.65	120.39	124.26
29	e	604	CLA	CHB-C1B-NB	-3.65	120.39	124.26
29	a	612	CLA	CHB-C1B-NB	-3.65	120.39	124.26
29	1	607	CLA	CHB-C1B-NB	-3.65	120.39	124.26
29	B	821	CLA	CHB-C1B-NB	-3.65	120.39	124.26
29	b	608	CLA	CHB-C1B-NB	-3.65	120.39	124.26
31	7	615	II0	C20-C14-C10	-3.65	119.39	124.35
29	1	611	CLA	CHB-C1B-NB	-3.65	120.39	124.26
29	A	825	CLA	CHB-C1B-NB	-3.65	120.40	124.26
29	3	609	CLA	CHB-C1B-NB	-3.64	120.40	124.26
29	5	603	CLA	CHB-C1B-NB	-3.64	120.40	124.26
29	6	608	CLA	CHB-C1B-NB	-3.64	120.40	124.26
29	A	818	CLA	CHB-C1B-NB	-3.64	120.40	124.26
33	K	104	IHT	C36-C33-C32	3.64	123.81	118.08
30	9	610	KC2	CHD-C1D-ND	-3.64	120.41	124.26
29	c	609	CLA	CHB-C1B-NB	-3.64	120.41	124.26
29	B	817	CLA	CHB-C1B-NB	-3.64	120.41	124.26
31	e	615	II0	C20-C14-C10	-3.64	119.41	124.35
29	4	604	CLA	CHB-C1B-NB	-3.63	120.41	124.26
29	A	805	CLA	CHB-C1B-NB	-3.63	120.41	124.26
31	6	615	II0	C42-C40-C36	-3.63	122.12	127.31
29	4	609	CLA	CHB-C1B-NB	-3.63	120.41	124.26
29	b	603	CLA	CHB-C1B-NB	-3.63	120.41	124.26
29	1	602	CLA	CHB-C1B-NB	-3.63	120.41	124.26
29	9	604	CLA	CHB-C1B-NB	-3.63	120.41	124.26
29	b	610	CLA	CHB-C1B-NB	-3.63	120.41	124.26
30	b	605	KC2	CHD-C1D-ND	-3.63	120.41	124.26
31	6	616	II0	C42-C40-C36	-3.63	122.13	127.31
30	2	610	KC2	CHD-C1D-ND	-3.63	120.42	124.26
29	B	840	CLA	CHB-C1B-NB	-3.62	120.42	124.26
29	8	602	CLA	CHB-C1B-NB	-3.62	120.42	124.26
29	9	603	CLA	CHB-C1B-NB	-3.62	120.42	124.26
31	5	617	II0	C42-C40-C36	-3.62	122.14	127.31
31	c	617	II0	C42-C40-C36	-3.62	122.14	127.31
29	B	811	CLA	CHB-C1B-NB	-3.62	120.42	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	810	CLA	CHB-C1B-NB	-3.62	120.42	124.26
31	7	613	II0	C20-C14-C10	-3.62	119.43	124.35
31	3	615	II0	C38-C36-C34	3.62	123.78	118.08
31	R	204	II0	C41-C42-C40	-3.62	116.06	123.47
29	7	603	CLA	CHB-C1B-NB	-3.62	120.43	124.26
29	b	606	CLA	CHB-C1B-NB	-3.62	120.43	124.26
29	7	609	CLA	CHB-C1B-NB	-3.62	120.43	124.26
30	6	610	KC2	CHD-C1D-ND	-3.62	120.43	124.26
29	B	806	CLA	CHB-C1B-NB	-3.61	120.43	124.26
29	c	605	CLA	CHB-C1B-NB	-3.61	120.43	124.26
31	6	614	II0	C38-C36-C34	3.61	123.77	118.08
29	9	614	CLA	CHB-C1B-NB	-3.61	120.43	124.26
29	A	813	CLA	CHB-C1B-NB	-3.61	120.43	124.26
29	4	607	CLA	CHB-C1B-NB	-3.61	120.44	124.26
31	a	616	II0	C42-C40-C36	-3.61	122.16	127.31
29	A	840	CLA	CHB-C1B-NB	-3.61	120.44	124.26
29	1	603	CLA	CHB-C1B-NB	-3.61	120.44	124.26
29	A	826	CLA	CHB-C1B-NB	-3.61	120.44	124.26
29	d	605	CLA	CHB-C1B-NB	-3.60	120.44	124.26
31	6	616	II0	C38-C36-C34	3.60	123.75	118.08
31	a	614	II0	C38-C36-C34	3.60	123.75	118.08
29	Z	301	CLA	CHB-C1B-NB	-3.60	120.44	124.26
30	5	610	KC2	CHD-C1D-ND	-3.60	120.44	124.26
29	e	606	CLA	CHB-C1B-NB	-3.60	120.44	124.26
29	5	611	CLA	CHB-C1B-NB	-3.60	120.44	124.26
29	9	609	CLA	CHB-C1B-NB	-3.60	120.44	124.26
31	2	613	II0	C38-C36-C34	3.60	123.75	118.08
29	2	611	CLA	CHB-C1B-NB	-3.60	120.45	124.26
31	a	615	II0	C38-C36-C34	3.60	123.75	118.08
29	K	101	CLA	CHB-C1B-NB	-3.60	120.45	124.26
29	9	608	CLA	CHB-C1B-NB	-3.60	120.45	124.26
29	K	102	CLA	CHB-C1B-NB	-3.60	120.45	124.26
29	3	604	CLA	CHB-C1B-NB	-3.60	120.45	124.26
33	5	618	IHT	C36-C33-C32	3.59	123.74	118.08
33	a	617	IHT	C06-C09-C10	3.59	120.48	114.08
29	2	603	CLA	CHB-C1B-NB	-3.58	120.46	124.26
29	8	607	CLA	CHB-C1B-NB	-3.58	120.46	124.26
29	8	608	CLA	CHB-C1B-NB	-3.58	120.46	124.26
29	c	603	CLA	CHB-C1B-NB	-3.58	120.46	124.26
29	9	602	CLA	CHB-C1B-NB	-3.58	120.47	124.26
29	B	829	CLA	CHB-C1B-NB	-3.58	120.47	124.26
29	3	610	CLA	CHB-C1B-NB	-3.58	120.47	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	604	CLA	CHB-C1B-NB	-3.58	120.47	124.26
29	A	821	CLA	CHB-C1B-NB	-3.58	120.47	124.26
33	5	618	IHT	C30-C27-C23	-3.58	122.20	127.31
29	3	602	CLA	CHB-C1B-NB	-3.58	120.47	124.26
29	b	602	CLA	CHB-C1B-NB	-3.58	120.47	124.26
30	7	610	KC2	CHD-C1D-ND	-3.58	120.47	124.26
29	2	609	CLA	CHB-C1B-NB	-3.58	120.47	124.26
31	7	616	II0	C20-C14-C10	-3.58	119.49	124.35
31	B	843	II0	C20-C14-C10	-3.58	119.49	124.35
31	e	615	II0	C42-C40-C36	-3.58	122.20	127.31
29	b	604	CLA	CHB-C1B-NB	-3.58	120.47	124.26
31	c	619	II0	C38-C36-C34	3.58	123.71	118.08
29	5	602	CLA	CHB-C1B-NB	-3.58	120.47	124.26
29	B	805	CLA	CHB-C1B-NB	-3.58	120.47	124.26
29	6	604	CLA	CHB-C1B-NB	-3.57	120.47	124.26
29	a	611	CLA	CHB-C1B-NB	-3.57	120.47	124.26
29	B	841	CLA	CHB-C1B-NB	-3.57	120.47	124.26
31	1	617	II0	C42-C40-C36	-3.57	122.21	127.31
29	7	611	CLA	CHB-C1B-NB	-3.57	120.48	124.26
31	2	615	II0	C42-C40-C36	-3.57	122.22	127.31
29	9	605	CLA	CHB-C1B-NB	-3.57	120.48	124.26
29	a	609	CLA	CHB-C1B-NB	-3.57	120.48	124.26
31	4	614	II0	C20-C14-C10	-3.56	119.50	124.35
31	d	615	II0	C42-C40-C36	-3.56	122.22	127.31
29	c	614	CLA	CHB-C1B-NB	-3.56	120.48	124.26
30	e	605	KC2	CHD-C1D-ND	-3.56	120.48	124.26
31	J	101	II0	C38-C36-C34	3.56	123.69	118.08
29	5	605	CLA	CHB-C1B-NB	-3.56	120.49	124.26
29	8	601	CLA	CHB-C1B-NB	-3.56	120.49	124.26
29	A	823	CLA	CHB-C1B-NB	-3.56	120.49	124.26
33	1	618	IHT	C40-C37-C33	-3.56	122.23	127.31
31	b	614	II0	C38-C36-C34	3.56	123.68	118.08
31	e	615	II0	C38-C36-C34	3.56	123.68	118.08
29	c	607	CLA	CHB-C1B-NB	-3.55	120.50	124.26
29	A	827	CLA	CHB-C1B-NB	-3.55	120.50	124.26
29	d	612	CLA	CHB-C1B-NB	-3.55	120.50	124.26
29	e	607	CLA	CHB-C1B-NB	-3.55	120.50	124.26
29	4	611	CLA	CHB-C1B-NB	-3.55	120.50	124.26
29	A	820	CLA	CHB-C1B-NB	-3.55	120.50	124.26
29	e	603	CLA	CHB-C1B-NB	-3.55	120.50	124.26
33	1	618	IHT	C18-C07-C10	-3.55	112.86	121.46
29	B	835	CLA	CHB-C1B-NB	-3.55	120.50	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Z	304	CLA	CHB-C1B-NB	-3.55	120.50	124.26
29	7	602	CLA	CHB-C1B-NB	-3.55	120.50	124.26
29	A	807	CLA	CHB-C1B-NB	-3.55	120.50	124.26
29	2	602	CLA	CHB-C1B-NB	-3.54	120.50	124.26
31	8	610	II0	C38-C36-C34	3.54	123.66	118.08
31	e	614	II0	C38-C36-C34	3.54	123.66	118.08
29	6	611	CLA	CHB-C1B-NB	-3.54	120.51	124.26
29	7	605	CLA	CHB-C1B-NB	-3.54	120.51	124.26
32	e	613	II3	C39-C36-C33	-3.54	122.26	127.31
29	d	607	CLA	CHB-C1B-NB	-3.54	120.51	124.26
31	a	616	II0	C20-C14-C10	-3.54	119.55	124.35
31	8	611	II0	C42-C40-C36	-3.53	122.27	127.31
29	7	608	CLA	CHB-C1B-NB	-3.53	120.52	124.26
31	5	620	II0	C03-C09-C13	-3.53	117.65	122.63
29	A	829	CLA	CHB-C1B-NB	-3.53	120.52	124.26
29	d	608	CLA	CHB-C1B-NB	-3.53	120.52	124.26
29	5	606	CLA	CHB-C1B-NB	-3.53	120.52	124.26
29	F	202	CLA	CHB-C1B-NB	-3.53	120.53	124.26
29	A	835	CLA	CHB-C1B-NB	-3.52	120.53	124.26
29	B	815	CLA	CHB-C1B-NB	-3.52	120.53	124.26
29	a	602	CLA	CHB-C1B-NB	-3.52	120.53	124.26
31	5	614	II0	C42-C40-C36	-3.52	122.29	127.31
29	b	607	CLA	CHB-C1B-NB	-3.52	120.53	124.26
36	O	206	SQD	O48-C23-C24	3.52	120.61	111.38
29	5	612	CLA	CHB-C1B-NB	-3.52	120.53	124.26
29	9	606	CLA	CHB-C1B-NB	-3.52	120.53	124.26
31	2	615	II0	C03-C09-C13	-3.52	117.67	122.63
30	3	606	KC2	CHD-C1D-ND	-3.52	120.53	124.26
31	c	616	II0	C38-C36-C34	3.51	123.61	118.08
29	1	606	CLA	CHB-C1B-NB	-3.51	120.54	124.26
29	A	842	CLA	CHB-C1B-NB	-3.51	120.54	124.26
29	B	823	CLA	CHB-C1B-NB	-3.51	120.54	124.26
29	L	201	CLA	CHB-C1B-NB	-3.51	120.54	124.26
29	d	611	CLA	C1-C2-C3	-3.51	121.08	126.75
29	6	602	CLA	CHB-C1B-NB	-3.51	120.55	124.26
29	d	602	CLA	CHB-C1B-NB	-3.51	120.55	124.26
29	a	603	CLA	CHB-C1B-NB	-3.50	120.55	124.26
31	3	613	II0	C20-C14-C10	-3.50	119.59	124.35
31	3	613	II0	C38-C36-C34	3.50	123.60	118.08
29	L	207	CLA	CHB-C1B-NB	-3.50	120.55	124.26
36	3	621	SQD	O8-S-C6	3.50	111.32	105.74
31	3	616	II0	C20-C14-C10	-3.50	119.59	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	606	CLA	CHB-C1B-NB	-3.50	120.55	124.26
33	8	609	IHT	C25-C23-C22	3.50	123.59	118.08
29	4	602	CLA	CHB-C1B-NB	-3.50	120.55	124.26
29	5	601	CLA	CHB-C1B-NB	-3.50	120.55	124.26
29	B	837	CLA	CHB-C1B-NB	-3.50	120.55	124.26
31	d	614	II0	C20-C14-C10	-3.50	119.59	124.35
33	d	617	IHT	C36-C33-C32	3.50	123.59	118.08
29	c	602	CLA	CHB-C1B-NB	-3.50	120.55	124.26
29	e	602	CLA	CHB-C1B-NB	-3.50	120.55	124.26
29	1	613	CLA	CHB-C1B-NB	-3.50	120.56	124.26
29	a	608	CLA	CHB-C1B-NB	-3.49	120.56	124.26
31	3	616	II0	C42-C40-C36	-3.49	122.32	127.31
33	d	617	IHT	C41-C40-C37	-3.49	116.32	123.47
29	6	603	CLA	CHB-C1B-NB	-3.49	120.56	124.26
29	d	603	CLA	CHB-C1B-NB	-3.49	120.56	124.26
29	c	601	CLA	CHB-C1B-NB	-3.49	120.56	124.26
32	1	615	II3	C39-C36-C33	-3.48	122.34	127.31
30	d	610	KC2	CHD-C1D-ND	-3.48	120.57	124.26
31	4	614	II0	C38-C36-C34	3.48	123.56	118.08
31	4	615	II0	C38-C36-C34	3.48	123.56	118.08
29	1	608	CLA	CHB-C1B-NB	-3.48	120.57	124.26
29	2	608	CLA	CHB-C1B-NB	-3.48	120.58	124.26
29	8	604	CLA	CHB-C1B-NB	-3.48	120.58	124.26
31	a	619	II0	C38-C36-C34	3.48	123.55	118.08
29	d	606	CLA	CHB-C1B-NB	-3.47	120.58	124.26
33	6	617	IHT	C25-C23-C22	3.47	123.55	118.08
30	e	609	KC2	CHD-C1D-ND	-3.47	120.59	124.26
33	d	617	IHT	C25-C23-C22	3.47	123.54	118.08
33	5	618	IHT	C25-C23-C22	3.46	123.53	118.08
33	c	620	IHT	C41-C40-C37	-3.46	116.38	123.47
29	9	611	CLA	CHB-C1B-NB	-3.46	120.60	124.26
29	B	812	CLA	CHB-C1B-NB	-3.46	120.60	124.26
29	9	613	CLA	CHB-C1B-NB	-3.46	120.60	124.26
29	O	203	CLA	C2C-C1C-NC	3.45	113.21	109.97
31	4	612	II0	C38-C36-C34	3.45	123.52	118.08
31	1	619	II0	C38-C36-C34	3.45	123.52	118.08
29	A	812	CLA	CHB-C1B-NB	-3.45	120.60	124.26
29	2	604	CLA	CHB-C1B-NB	-3.45	120.61	124.26
29	4	606	CLA	CHB-C1B-NB	-3.45	120.61	124.26
29	d	604	CLA	CHB-C1B-NB	-3.45	120.61	124.26
29	6	606	CLA	CHB-C1B-NB	-3.45	120.61	124.26
36	O	206	SQD	O47-C7-C8	3.44	118.92	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	9	616	II0	C38-C36-C34	3.44	123.50	118.08
31	a	613	II0	C20-C14-C10	-3.44	119.67	124.35
29	B	839	CLA	CHB-C1B-NB	-3.44	120.61	124.26
31	5	620	II0	C20-C14-C10	-3.44	119.68	124.35
31	1	614	II0	C38-C36-C34	3.44	123.50	118.08
31	2	615	II0	C20-C14-C10	-3.44	119.68	124.35
33	1	618	IHT	C36-C33-C32	3.43	123.49	118.08
33	c	620	IHT	C22-C18-C07	-3.43	117.57	127.20
31	d	614	II0	C42-C40-C36	-3.43	122.42	127.31
29	7	604	CLA	CHB-C1B-NB	-3.43	120.63	124.26
29	a	606	CLA	CHB-C1B-NB	-3.43	120.63	124.26
31	8	611	II0	C20-C14-C10	-3.43	119.69	124.35
31	J	101	II0	C20-C14-C10	-3.43	119.69	124.35
31	a	619	II0	C20-C14-C10	-3.43	119.69	124.35
29	O	201	CLA	CHB-C1B-NB	-3.43	120.63	124.26
31	7	614	II0	C42-C40-C36	-3.42	122.42	127.31
32	1	615	II3	C35-C33-C32	3.42	123.47	118.08
29	F	203	CLA	CHB-C1B-NB	-3.42	120.63	124.26
31	O	205	II0	C20-C14-C10	-3.42	119.70	124.35
29	a	604	CLA	CHB-C1B-NB	-3.41	120.64	124.26
30	b	609	KC2	CHD-C1D-ND	-3.41	120.64	124.26
29	B	828	CLA	CHB-C1B-NB	-3.41	120.64	124.26
29	L	202	CLA	CHB-C1B-NB	-3.41	120.64	124.26
33	K	104	IHT	C25-C23-C22	3.41	123.45	118.08
31	d	614	II0	C38-C36-C34	3.41	123.45	118.08
33	L	205	IHT	C18-C07-C10	-3.41	113.21	121.46
29	e	610	CLA	CHB-C1B-NB	-3.41	120.65	124.26
31	8	611	II0	C38-C36-C34	3.41	123.44	118.08
31	5	620	II0	C38-C36-C34	3.40	123.44	118.08
31	7	614	II0	C20-C14-C10	-3.40	119.73	124.35
32	e	613	II3	C35-C33-C32	3.40	123.43	118.08
31	6	616	II0	C20-C14-C10	-3.40	119.73	124.35
29	c	604	CLA	CHB-C1B-NB	-3.39	120.66	124.26
31	3	617	II0	C20-C14-C10	-3.39	119.74	124.35
31	R	204	II0	C20-C14-C10	-3.39	119.74	124.35
31	5	620	II0	C42-C40-C36	-3.39	122.47	127.31
29	A	830	CLA	CHB-C1B-NB	-3.39	120.67	124.26
31	7	615	II0	C38-C36-C34	3.39	123.42	118.08
31	e	612	II0	C20-C14-C10	-3.39	119.75	124.35
29	B	827	CLA	CHB-C1B-NB	-3.38	120.68	124.26
32	b	613	II3	C35-C33-C32	3.38	123.41	118.08
31	c	618	II0	C42-C40-C36	-3.38	122.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	O	205	II0	C42-C40-C36	-3.38	122.49	127.31
29	A	817	CLA	CHB-C1B-NB	-3.37	120.69	124.26
33	1	618	IHT	C25-C23-C22	3.37	123.38	118.08
29	A	834	CLA	CHB-C1B-NB	-3.37	120.69	124.26
31	2	613	II0	C20-C14-C10	-3.36	119.78	124.35
31	5	616	II0	C42-C40-C36	-3.36	122.52	127.31
29	3	605	CLA	CHB-C1B-NB	-3.35	120.71	124.26
31	8	612	II0	C41-C42-C40	-3.35	116.61	123.47
36	3	621	SQD	O47-C7-C8	3.35	118.72	111.50
29	8	603	CLA	CHB-C1B-NB	-3.34	120.72	124.26
31	O	205	II0	C38-C36-C34	3.34	123.34	118.08
31	O	204	II0	C20-C14-C10	-3.34	119.81	124.35
29	5	608	CLA	CHB-C1B-NB	-3.34	120.72	124.26
29	3	603	CLA	CHB-C1B-NB	-3.34	120.72	124.26
34	I	102	LMG	O6-C1-O1	-3.33	102.09	109.97
29	B	820	CLA	CHB-C1B-NB	-3.32	120.74	124.26
31	5	617	II0	C19-C13-C11	3.32	120.50	114.36
33	8	609	IHT	C41-C40-C37	-3.32	116.68	123.47
29	B	830	CLA	CHB-C1B-NB	-3.31	120.75	124.26
33	L	205	IHT	C40-C37-C33	-3.31	122.58	127.31
29	A	819	CLA	CHB-C1B-NB	-3.30	120.76	124.26
29	A	844	CLA	C3D-C4D-ND	3.30	115.58	110.24
29	B	818	CLA	CHB-C1B-NB	-3.29	120.78	124.26
31	9	618	II0	C42-C40-C36	-3.28	122.62	127.31
31	c	619	II0	C41-C42-C40	-3.28	116.75	123.47
31	8	616	II0	C19-C13-C09	-3.28	119.90	124.35
33	6	617	IHT	C22-C18-C07	-3.27	118.01	127.20
31	3	614	II0	C20-C14-C10	-3.27	119.90	124.35
33	a	617	IHT	C22-C18-C07	-3.27	118.01	127.20
31	a	615	II0	C20-C14-C10	-3.27	119.90	124.35
31	9	616	II0	C20-C14-C10	-3.27	119.91	124.35
33	L	205	IHT	C30-C27-C23	-3.26	122.65	127.31
31	9	616	II0	C42-C40-C36	-3.26	122.65	127.31
31	5	617	II0	C38-C36-C34	3.26	123.21	118.08
31	5	615	II0	C20-C14-C12	3.25	120.38	114.36
29	B	834	CLA	CHB-C1B-NB	-3.25	120.82	124.26
31	e	612	II0	C38-C36-C34	3.25	123.19	118.08
31	a	613	II0	C38-C36-C34	3.25	123.19	118.08
31	R	204	II0	C38-C36-C34	3.25	123.19	118.08
33	Z	302	IHT	C25-C23-C22	3.24	123.18	118.08
31	e	612	II0	C42-C40-C36	-3.24	122.69	127.31
29	A	811	CLA	CHB-C1B-NB	-3.24	120.83	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	Z	303	DGD	O6D-C1D-O3G	-3.24	102.31	109.97
31	3	616	II0	C38-C36-C34	3.23	123.17	118.08
29	b	602	CLA	C1-C2-C3	-3.23	120.45	126.04
31	5	614	II0	C20-C14-C10	-3.23	119.96	124.35
31	d	615	II0	C20-C14-C10	-3.23	119.96	124.35
31	b	612	II0	C20-C14-C10	-3.23	119.96	124.35
31	d	615	II0	C03-C09-C13	-3.23	118.08	122.63
31	d	616	II0	C04-C10-C14	-3.22	118.08	122.63
31	4	613	II0	C20-C14-C10	-3.22	119.97	124.35
32	1	615	II3	C29-C26-C24	-3.22	122.72	127.31
31	2	614	II0	C38-C36-C40	-3.22	118.42	122.92
29	A	840	CLA	C3D-C4D-ND	3.22	115.44	110.24
29	1	602	CLA	C1-C2-C3	-3.22	120.48	126.04
32	b	613	II3	C21-C24-C26	-3.21	114.01	118.94
33	2	616	IHT	C41-C38-C35	-3.21	122.73	127.31
31	d	616	II0	C41-C39-C35	-3.21	122.73	127.31
31	4	615	II0	C42-C40-C36	-3.20	122.74	127.31
33	L	205	IHT	C41-C40-C37	-3.20	116.92	123.47
31	B	843	II0	C38-C36-C34	3.20	123.12	118.08
31	7	614	II0	C38-C36-C34	3.20	123.11	118.08
29	J	102	CLA	CHB-C1B-NB	-3.20	120.87	124.26
33	c	620	IHT	C36-C33-C32	3.19	123.11	118.08
31	d	615	II0	C38-C36-C34	3.19	123.10	118.08
31	9	617	II0	C20-C14-C10	-3.19	120.02	124.35
31	3	613	II0	C42-C40-C36	-3.18	122.77	127.31
31	9	615	II0	C20-C14-C12	3.18	120.25	114.36
29	A	811	CLA	CHC-C4B-NB	-3.18	120.89	124.26
31	7	616	II0	C38-C36-C34	3.18	123.08	118.08
31	8	610	II0	C41-C42-C40	-3.17	116.97	123.47
31	1	616	II0	C20-C14-C10	-3.17	120.04	124.35
33	8	609	IHT	C22-C18-C07	-3.17	118.30	127.20
29	a	604	CLA	C3D-C4D-ND	3.17	115.36	110.24
33	2	616	IHT	C22-C18-C07	-3.17	118.30	127.20
31	c	618	II0	C20-C14-C10	-3.16	120.05	124.35
31	8	610	II0	C42-C40-C36	-3.16	122.80	127.31
31	c	617	II0	C20-C14-C10	-3.15	120.07	124.35
31	d	616	II0	C20-C14-C10	-3.15	120.07	124.35
32	e	613	II3	C21-C24-C26	-3.15	114.11	118.94
33	9	619	IHT	C36-C33-C32	3.15	123.04	118.08
29	5	608	CLA	C3D-C4D-ND	3.14	115.33	110.24
31	5	615	II0	C38-C36-C40	-3.14	118.52	122.92
31	d	613	II0	C42-C41-C39	-3.14	117.03	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	616	II0	C07-C11-C13	-3.14	105.59	111.85
31	b	614	II0	C42-C40-C36	-3.14	122.83	127.31
33	d	617	IHT	C22-C18-C07	-3.13	118.42	127.20
31	7	616	II0	C42-C41-C39	-3.12	117.07	123.47
31	d	616	II0	C03-C09-C13	-3.12	118.22	122.63
31	7	615	II0	C42-C40-C36	-3.12	122.86	127.31
31	c	619	II0	C42-C40-C36	-3.12	122.86	127.31
33	a	617	IHT	C41-C40-C37	-3.12	117.09	123.47
31	9	617	II0	C38-C36-C40	-3.11	118.57	122.92
29	8	606	CLA	C2C-C1C-NC	3.10	112.88	109.97
29	4	602	CLA	C3D-C4D-ND	3.10	115.25	110.24
31	a	616	II0	C38-C36-C34	3.10	122.96	118.08
29	A	819	CLA	C3D-C4D-ND	3.10	115.25	110.24
38	O	207	LMU	O5'-C5'-C6'	3.10	114.14	106.44
31	4	612	II0	C03-C09-C13	-3.09	118.27	122.63
31	a	613	II0	C42-C41-C39	-3.09	117.14	123.47
31	9	615	II0	C38-C36-C34	3.09	122.94	118.08
31	1	619	II0	C20-C14-C10	-3.09	120.15	124.35
33	6	617	IHT	C36-C33-C32	3.09	122.94	118.08
29	6	608	CLA	C3D-C4D-ND	3.09	115.23	110.24
31	9	617	II0	C38-C36-C34	3.09	122.94	118.08
31	e	614	II0	C20-C14-C12	3.09	120.07	114.36
31	b	612	II0	C38-C36-C40	-3.09	118.60	122.92
29	A	811	CLA	C3D-C4D-ND	3.08	115.22	110.24
29	c	604	CLA	C3D-C4D-ND	3.08	115.22	110.24
33	L	205	IHT	C22-C18-C07	-3.08	118.55	127.20
33	5	618	IHT	C19-C10-C07	-3.08	121.07	124.53
33	K	104	IHT	C09-C10-C07	-3.08	118.26	122.73
31	J	101	II0	C42-C40-C36	-3.08	122.92	127.31
33	5	618	IHT	C13-C02-C07	3.08	115.29	110.30
31	a	614	II0	C42-C40-C36	-3.08	122.92	127.31
31	b	612	II0	C38-C36-C34	3.08	122.92	118.08
31	c	619	II0	C04-C10-C14	-3.08	118.29	122.63
31	3	614	II0	C42-C41-C39	-3.08	117.17	123.47
31	c	617	II0	C38-C36-C34	3.07	122.92	118.08
31	1	619	II0	C03-C09-C13	-3.07	118.29	122.63
29	e	602	CLA	C3D-C4D-ND	3.07	115.21	110.24
31	7	613	II0	C38-C36-C34	3.07	122.92	118.08
31	5	617	II0	C38-C36-C40	-3.07	118.62	122.92
29	O	203	CLA	C3D-C4D-ND	3.06	115.19	110.24
29	A	801	CLA	CHA-C1A-NA	-3.06	119.38	126.40
31	6	615	II0	C38-C36-C34	3.06	122.90	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	614	II0	C41-C42-C40	-3.06	117.20	123.47
29	5	604	CLA	C3D-C4D-ND	3.06	115.19	110.24
29	c	601	CLA	C3D-C4D-ND	3.06	115.19	110.24
31	5	617	II0	C19-C13-C09	-3.06	120.19	124.35
31	9	617	II0	C20-C14-C12	3.06	120.03	114.36
31	5	614	II0	C38-C36-C34	3.06	122.90	118.08
29	3	610	CLA	C3D-C4D-ND	3.06	115.19	110.24
39	B	842	PQN	C11-C3-C4	-3.06	115.23	118.50
29	A	814	CLA	C3D-C4D-ND	3.06	115.19	110.24
29	8	603	CLA	C3D-C4D-ND	3.06	115.18	110.24
29	5	601	CLA	C3D-C4D-ND	3.05	115.17	110.24
33	K	104	IHT	C02-C07-C18	-3.05	107.14	115.78
29	7	602	CLA	C3D-C4D-ND	3.05	115.17	110.24
29	d	608	CLA	C3D-C4D-ND	3.05	115.17	110.24
29	B	829	CLA	C3D-C4D-ND	3.05	115.17	110.24
34	8	614	LMG	O6-C1-O1	-3.05	102.75	109.97
31	2	613	II0	C41-C42-C40	-3.05	117.23	123.47
29	A	807	CLA	C1-C2-C3	-3.05	121.82	126.75
31	3	614	II0	C38-C36-C34	3.05	122.88	118.08
29	A	836	CLA	C2C-C1C-NC	3.04	112.82	109.97
31	a	619	II0	C42-C40-C36	-3.04	122.98	127.31
33	9	619	IHT	C19-C10-C07	-3.04	121.12	124.53
29	Z	305	CLA	C1-C2-C3	-3.04	121.84	126.75
29	a	611	CLA	C3D-C4D-ND	3.03	115.15	110.24
29	d	602	CLA	C3D-C4D-ND	3.03	115.15	110.24
31	6	614	II0	C20-C14-C12	3.03	119.98	114.36
31	3	617	II0	C38-C36-C34	3.03	122.86	118.08
29	A	821	CLA	C3D-C4D-ND	3.03	115.14	110.24
31	4	613	II0	C38-C36-C34	3.03	122.85	118.08
31	1	616	II0	C38-C36-C40	-3.03	118.68	122.92
29	L	203	CLA	C3D-C4D-ND	3.02	115.13	110.24
31	6	614	II0	C20-C14-C10	-3.02	120.24	124.35
29	5	602	CLA	C3D-C4D-ND	3.02	115.13	110.24
29	8	608	CLA	C3D-C4D-ND	3.02	115.13	110.24
29	3	612	CLA	C2C-C1C-NC	3.02	112.80	109.97
29	a	605	CLA	C3D-C4D-ND	3.02	115.13	110.24
31	O	204	II0	C38-C36-C34	3.02	122.84	118.08
29	3	602	CLA	C3D-C4D-ND	3.02	115.12	110.24
38	7	620	LMU	C2'-C3'-C4'	3.02	116.58	109.68
29	A	840	CLA	CHC-C4B-NB	-3.02	121.06	124.26
33	a	617	IHT	C19-C10-C09	3.01	119.41	113.62
29	3	608	CLA	C3D-C4D-ND	3.01	115.11	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	614	II0	C38-C36-C40	-3.01	118.71	122.92
29	2	602	CLA	C3D-C4D-ND	3.01	115.11	110.24
29	B	812	CLA	C3D-C4D-ND	3.01	115.10	110.24
29	e	610	CLA	C3D-C4D-ND	3.01	115.10	110.24
33	2	616	IHT	C40-C37-C33	-3.00	123.02	127.31
29	1	611	CLA	C3D-C4D-ND	3.00	115.10	110.24
31	c	619	II0	C20-C14-C12	3.00	119.92	114.36
29	B	838	CLA	C3D-C4D-ND	3.00	115.09	110.24
31	1	619	II0	C20-C14-C12	3.00	119.92	114.36
29	2	612	CLA	C3D-C4D-ND	3.00	115.09	110.24
29	1	608	CLA	C3D-C4D-ND	3.00	115.09	110.24
31	a	614	II0	C20-C14-C10	-3.00	120.27	124.35
29	A	813	CLA	C3D-C4D-ND	3.00	115.09	110.24
31	d	616	II0	C20-C14-C12	2.99	119.90	114.36
29	B	811	CLA	C3D-C4D-ND	2.99	115.08	110.24
34	6	619	LMG	O6-C1-O1	-2.99	102.89	109.97
29	B	834	CLA	C3D-C4D-ND	2.99	115.07	110.24
29	b	601	CLA	C3D-C4D-ND	2.99	115.07	110.24
29	d	605	CLA	C3D-C4D-ND	2.99	115.07	110.24
29	2	608	CLA	C3D-C4D-ND	2.99	115.07	110.24
29	a	601	CLA	C3D-C4D-ND	2.99	115.07	110.24
31	a	615	II0	C42-C40-C36	-2.99	123.05	127.31
33	5	618	IHT	C40-C37-C33	-2.99	123.05	127.31
29	A	803	CLA	C3D-C4D-ND	2.99	115.07	110.24
29	9	608	CLA	C3D-C4D-ND	2.98	115.07	110.24
29	6	604	CLA	C3D-C4D-ND	2.98	115.06	110.24
29	7	608	CLA	C3D-C4D-ND	2.98	115.06	110.24
29	A	822	CLA	C3D-C4D-ND	2.98	115.06	110.24
33	c	620	IHT	C30-C27-C23	-2.98	123.05	127.31
31	d	613	II0	C38-C36-C34	2.98	122.78	118.08
29	Z	306	CLA	C3D-C4D-ND	2.98	115.06	110.24
31	4	614	II0	C42-C40-C36	-2.98	123.06	127.31
29	A	818	CLA	C3D-C4D-ND	2.98	115.06	110.24
37	R	203	8CT	C30-C31-C32	-2.98	117.80	121.47
29	B	822	CLA	C2C-C1C-NC	2.98	112.76	109.97
31	9	618	II0	C41-C42-C40	-2.97	117.38	123.47
31	3	615	II0	C20-C14-C12	2.97	119.86	114.36
33	2	616	IHT	C03-C11-C15	-2.97	118.44	122.63
29	9	609	CLA	C3D-C4D-ND	2.97	115.04	110.24
31	2	613	II0	C42-C40-C36	-2.97	123.07	127.31
29	4	607	CLA	C3D-C4D-ND	2.97	115.04	110.24
29	O	202	CLA	C3D-C4D-ND	2.97	115.04	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	839	CLA	C3D-C4D-ND	2.97	115.04	110.24
29	9	602	CLA	C3D-C4D-ND	2.97	115.04	110.24
33	d	617	IHT	C19-C10-C09	2.97	119.32	113.62
29	a	608	CLA	C3D-C4D-ND	2.97	115.04	110.24
31	2	614	II0	C20-C14-C10	-2.97	120.32	124.35
31	5	616	II0	C20-C14-C10	-2.97	120.32	124.35
29	O	201	CLA	CHC-C4B-NB	-2.97	121.12	124.26
29	1	601	CLA	C3D-C4D-ND	2.97	115.04	110.24
29	3	601	CLA	C3D-C4D-ND	2.97	115.04	110.24
29	4	603	CLA	C3D-C4D-ND	2.97	115.03	110.24
29	9	604	CLA	C3D-C4D-ND	2.96	115.03	110.24
29	B	810	CLA	C3D-C4D-ND	2.96	115.03	110.24
29	c	608	CLA	C3D-C4D-ND	2.96	115.03	110.24
33	Z	302	IHT	C06-C09-C10	2.96	119.37	114.08
29	A	817	CLA	C3D-C4D-ND	2.96	115.03	110.24
29	2	601	CLA	C3D-C4D-ND	2.96	115.03	110.24
29	d	604	CLA	C3D-C4D-ND	2.96	115.03	110.24
29	A	842	CLA	CHC-C4B-NB	-2.96	121.12	124.26
29	b	602	CLA	C3D-C4D-ND	2.96	115.03	110.24
31	c	618	II0	C38-C36-C40	-2.96	118.78	122.92
31	4	613	II0	C42-C41-C39	-2.96	117.41	123.47
29	Z	304	CLA	C3D-C4D-ND	2.96	115.02	110.24
29	c	612	CLA	C3D-C4D-ND	2.96	115.02	110.24
29	e	607	CLA	C3D-C4D-ND	2.96	115.02	110.24
29	A	808	CLA	C3D-C4D-ND	2.96	115.02	110.24
29	9	611	CLA	C3D-C4D-ND	2.96	115.02	110.24
29	A	839	CLA	C3D-C4D-ND	2.96	115.02	110.24
29	B	833	CLA	C2C-C1C-NC	2.96	112.74	109.97
32	b	613	II3	C03-C04-C12	-2.96	108.97	112.70
31	3	615	II0	C04-C10-C14	-2.96	118.46	122.63
31	4	612	II0	C42-C40-C36	-2.95	123.09	127.31
29	d	611	CLA	C3D-C4D-ND	2.95	115.02	110.24
29	3	603	CLA	C3D-C4D-ND	2.95	115.01	110.24
31	a	616	II0	C41-C42-C40	-2.95	117.43	123.47
29	5	612	CLA	C3D-C4D-ND	2.95	115.01	110.24
29	a	602	CLA	C3D-C4D-ND	2.95	115.01	110.24
31	R	204	II0	C41-C39-C35	-2.95	123.10	127.31
31	6	616	II0	C19-C13-C11	2.95	119.82	114.36
29	B	831	CLA	C3D-C4D-ND	2.95	115.01	110.24
29	K	102	CLA	C3D-C4D-ND	2.95	115.01	110.24
31	2	615	II0	C20-C14-C12	2.95	119.82	114.36
31	1	617	II0	C41-C42-C40	-2.95	117.43	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	608	CLA	C1-C2-C3	-2.95	120.95	126.04
29	B	830	CLA	C3D-C4D-ND	2.94	115.00	110.24
29	B	821	CLA	C3D-C4D-ND	2.94	115.00	110.24
33	K	104	IHT	C06-C09-C10	2.94	119.33	114.08
29	7	603	CLA	C3D-C4D-ND	2.94	114.99	110.24
31	8	616	II0	C41-C42-C40	-2.94	117.46	123.47
29	d	601	CLA	C3D-C4D-ND	2.94	114.99	110.24
29	A	805	CLA	C3D-C4D-ND	2.93	114.98	110.24
29	A	816	CLA	C3D-C4D-ND	2.93	114.98	110.24
29	7	604	CLA	C3D-C4D-ND	2.93	114.98	110.24
31	1	617	II0	C38-C36-C34	2.93	122.70	118.08
29	9	606	CLA	C3D-C4D-ND	2.93	114.98	110.24
29	c	612	CLA	C2C-C1C-NC	2.93	112.72	109.97
29	2	609	CLA	C3D-C4D-ND	2.93	114.97	110.24
29	b	607	CLA	C3D-C4D-ND	2.93	114.97	110.24
31	2	614	II0	C38-C36-C34	2.93	122.69	118.08
29	L	204	CLA	C3D-C4D-ND	2.93	114.97	110.24
29	A	842	CLA	C3D-C4D-ND	2.92	114.97	110.24
29	9	614	CLA	C3D-C4D-ND	2.92	114.97	110.24
29	A	815	CLA	C3D-C4D-ND	2.92	114.97	110.24
29	B	807	CLA	C3D-C4D-ND	2.92	114.96	110.24
29	2	603	CLA	C3D-C4D-ND	2.92	114.96	110.24
29	9	603	CLA	C3D-C4D-ND	2.92	114.96	110.24
29	1	602	CLA	C3D-C4D-ND	2.92	114.95	110.24
29	c	606	CLA	C3D-C4D-ND	2.92	114.95	110.24
29	a	606	CLA	C3D-C4D-ND	2.91	114.95	110.24
29	4	606	CLA	C2C-C1C-NC	2.91	112.70	109.97
29	3	604	CLA	C3D-C4D-ND	2.91	114.95	110.24
29	c	609	CLA	C3D-C4D-ND	2.91	114.95	110.24
29	B	822	CLA	C3D-C4D-ND	2.91	114.94	110.24
31	8	610	II0	C41-C39-C35	-2.91	123.16	127.31
29	F	204	CLA	C2C-C1C-NC	2.91	112.70	109.97
31	3	617	II0	C42-C40-C36	-2.91	123.16	127.31
31	6	615	II0	C20-C14-C10	-2.91	120.40	124.35
29	B	818	CLA	C3D-C4D-ND	2.91	114.94	110.24
29	6	606	CLA	C3D-C4D-ND	2.91	114.94	110.24
31	7	615	II0	C03-C09-C13	-2.90	118.53	122.63
29	1	609	CLA	C3D-C4D-ND	2.90	114.94	110.24
29	b	610	CLA	C3D-C4D-ND	2.90	114.94	110.24
31	5	615	II0	C38-C36-C34	2.90	122.65	118.08
30	a	610	KC2	CHB-C1B-NB	2.90	127.12	124.45
29	B	817	CLA	C3D-C4D-ND	2.90	114.93	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	6	602	CLA	C3D-C4D-ND	2.90	114.93	110.24
29	3	611	CLA	C3D-C4D-ND	2.90	114.93	110.24
35	a	618	LHG	O8-C23-C24	2.90	121.01	111.91
29	4	609	CLA	C3D-C4D-ND	2.90	114.93	110.24
35	3	622	LHG	O8-C23-C24	2.90	121.01	111.91
29	e	603	CLA	C3D-C4D-ND	2.90	114.93	110.24
31	J	101	II0	C38-C36-C40	-2.90	118.86	122.92
29	1	613	CLA	C3D-C4D-ND	2.90	114.92	110.24
33	5	618	IHT	C41-C40-C37	-2.90	117.54	123.47
29	c	602	CLA	C3D-C4D-ND	2.90	114.92	110.24
29	6	609	CLA	C3D-C4D-ND	2.90	114.92	110.24
29	b	603	CLA	C3D-C4D-ND	2.90	114.92	110.24
29	a	612	CLA	C3D-C4D-ND	2.89	114.92	110.24
29	7	605	CLA	C3D-C4D-ND	2.89	114.92	110.24
29	a	607	CLA	C3D-C4D-ND	2.89	114.92	110.24
31	1	619	II0	C04-C10-C14	-2.89	118.55	122.63
29	1	606	CLA	C3D-C4D-ND	2.89	114.92	110.24
29	6	601	CLA	C3D-C4D-ND	2.89	114.92	110.24
29	B	815	CLA	C3D-C4D-ND	2.89	114.92	110.24
33	5	618	IHT	C04-C02-C07	-2.89	106.03	110.48
29	A	837	CLA	C3D-C4D-ND	2.89	114.91	110.24
29	1	605	CLA	C2C-C1C-NC	2.89	112.68	109.97
29	B	835	CLA	C1-C2-C3	-2.89	121.05	126.04
29	e	608	CLA	C3D-C4D-ND	2.89	114.91	110.24
31	1	614	II0	C42-C40-C36	-2.88	123.19	127.31
29	A	838	CLA	C3D-C4D-ND	2.88	114.90	110.24
29	B	836	CLA	C2C-C1C-NC	2.88	112.67	109.97
29	A	829	CLA	C3D-C4D-ND	2.88	114.90	110.24
29	e	601	CLA	C3D-C4D-ND	2.88	114.90	110.24
30	3	606	KC2	CHB-C1B-NB	2.88	127.10	124.45
29	3	605	CLA	C3D-C4D-ND	2.88	114.89	110.24
29	7	607	CLA	C3D-C4D-ND	2.88	114.89	110.24
29	9	601	CLA	C3D-C4D-ND	2.88	114.89	110.24
31	c	616	II0	C41-C42-C40	-2.87	117.58	123.47
29	A	836	CLA	C3D-C4D-ND	2.87	114.89	110.24
29	A	824	CLA	C3D-C4D-ND	2.87	114.89	110.24
29	d	607	CLA	C3D-C4D-ND	2.87	114.89	110.24
31	1	616	II0	C38-C36-C34	2.87	122.60	118.08
29	5	606	CLA	C3D-C4D-ND	2.87	114.88	110.24
29	2	607	CLA	C3D-C4D-ND	2.87	114.88	110.24
29	8	607	CLA	C3D-C4D-ND	2.87	114.88	110.24
29	4	611	CLA	C3D-C4D-ND	2.87	114.88	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	2	604	CLA	C3D-C4D-ND	2.87	114.88	110.24
29	6	603	CLA	C3D-C4D-ND	2.87	114.88	110.24
31	d	613	II0	C20-C14-C10	-2.87	120.45	124.35
29	A	835	CLA	C3D-C4D-ND	2.87	114.87	110.24
29	d	606	CLA	C3D-C4D-ND	2.87	114.87	110.24
29	6	611	CLA	C3D-C4D-ND	2.86	114.87	110.24
29	b	611	CLA	C3D-C4D-ND	2.86	114.87	110.24
29	d	609	CLA	C3D-C4D-ND	2.86	114.87	110.24
29	A	802	CLA	C3D-C4D-ND	2.86	114.87	110.24
29	6	601	CLA	C2C-C1C-NC	2.86	112.65	109.97
33	K	104	IHT	C04-C02-C07	2.86	114.88	110.48
29	B	814	CLA	C3D-C4D-ND	2.86	114.86	110.24
29	4	604	CLA	C3D-C4D-ND	2.86	114.86	110.24
29	7	609	CLA	C3D-C4D-ND	2.86	114.86	110.24
29	A	833	CLA	C3D-C4D-ND	2.86	114.86	110.24
31	d	616	II0	C42-C40-C36	-2.86	123.23	127.31
29	1	603	CLA	C3D-C4D-ND	2.86	114.86	110.24
29	A	834	CLA	C3D-C4D-ND	2.86	114.86	110.24
29	2	606	CLA	C3D-C4D-ND	2.85	114.86	110.24
29	6	607	CLA	C3D-C4D-ND	2.85	114.86	110.24
29	B	819	CLA	C3D-C4D-ND	2.85	114.85	110.24
35	B	849	LHG	O8-C23-C24	2.85	120.86	111.91
29	a	609	CLA	C3D-C4D-ND	2.85	114.85	110.24
29	8	605	CLA	C3D-C4D-ND	2.85	114.85	110.24
29	9	605	CLA	C3D-C4D-ND	2.85	114.85	110.24
29	5	607	CLA	C3D-C4D-ND	2.85	114.84	110.24
29	B	828	CLA	C3D-C4D-ND	2.85	114.84	110.24
29	1	607	CLA	C3D-C4D-ND	2.85	114.84	110.24
29	8	601	CLA	C3D-C4D-ND	2.85	114.84	110.24
33	1	618	IHT	C36-C33-C37	-2.85	118.94	122.92
29	Z	301	CLA	C3D-C4D-ND	2.85	114.84	110.24
29	B	840	CLA	C3D-C4D-ND	2.84	114.84	110.24
29	B	805	CLA	C3D-C4D-ND	2.84	114.83	110.24
35	6	618	LHG	O8-C23-C24	2.84	120.82	111.91
33	K	104	IHT	C36-C33-C37	-2.84	118.95	122.92
29	1	604	CLA	C3D-C4D-ND	2.84	114.83	110.24
29	3	612	CLA	C3D-C4D-ND	2.84	114.83	110.24
29	7	611	CLA	C3D-C4D-ND	2.84	114.83	110.24
29	B	827	CLA	C3D-C4D-ND	2.84	114.83	110.24
31	1	617	II0	C41-C39-C35	-2.84	123.26	127.31
29	A	820	CLA	C3D-C4D-ND	2.84	114.83	110.24
29	B	809	CLA	C3D-C4D-ND	2.84	114.83	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	e	613	II3	C39-C41-C40	-2.84	117.66	123.47
41	Z	303	DGD	O5D-C6D-C5D	-2.84	103.80	109.05
29	1	605	CLA	C3D-C4D-ND	2.83	114.82	110.24
29	c	613	CLA	C2C-C1C-NC	2.83	112.63	109.97
31	d	616	II0	C34-C36-C40	2.83	123.29	118.94
29	B	837	CLA	C3D-C4D-ND	2.83	114.82	110.24
29	b	604	CLA	C3D-C4D-ND	2.83	114.81	110.24
31	c	619	II0	C41-C39-C35	-2.83	123.28	127.31
29	B	833	CLA	C3D-C4D-ND	2.82	114.81	110.24
29	d	603	CLA	C3D-C4D-ND	2.82	114.81	110.24
29	B	813	CLA	C3D-C4D-ND	2.82	114.80	110.24
31	d	615	II0	C19-C13-C11	2.82	119.58	114.36
29	A	809	CLA	C3D-C4D-ND	2.82	114.80	110.24
31	5	615	II0	C20-C14-C10	-2.82	120.52	124.35
36	3	621	SQD	O48-C23-C24	2.82	120.75	111.91
29	d	603	CLA	C1-C2-C3	-2.82	122.19	126.75
29	B	841	CLA	C3D-C4D-ND	2.82	114.79	110.24
29	J	102	CLA	C3D-C4D-ND	2.82	114.79	110.24
29	F	202	CLA	C3D-C4D-ND	2.82	114.79	110.24
31	d	613	II0	C38-C36-C40	-2.82	118.98	122.92
29	3	609	CLA	C3D-C4D-ND	2.82	114.79	110.24
29	4	601	CLA	C3D-C4D-ND	2.82	114.79	110.24
30	2	610	KC2	CHB-C1B-NB	2.81	127.04	124.45
33	a	617	IHT	C31-C34-C35	-2.81	118.51	126.42
29	A	807	CLA	C3D-C4D-ND	2.81	114.79	110.24
29	9	612	CLA	C3D-C4D-ND	2.81	114.79	110.24
29	c	605	CLA	C3D-C4D-ND	2.81	114.78	110.24
29	A	830	CLA	C3D-C4D-ND	2.81	114.78	110.24
29	c	614	CLA	C3D-C4D-ND	2.81	114.78	110.24
29	B	836	CLA	C3D-C4D-ND	2.81	114.78	110.24
29	5	609	CLA	C3D-C4D-ND	2.81	114.78	110.24
29	B	804	CLA	C3D-C4D-ND	2.81	114.78	110.24
29	O	201	CLA	C3D-C4D-ND	2.81	114.78	110.24
41	B	848	DGD	O3G-C3G-C2G	-2.81	104.13	110.90
29	7	601	CLA	C2C-C1C-NC	2.81	112.60	109.97
29	4	606	CLA	C3D-C4D-ND	2.80	114.78	110.24
29	A	825	CLA	C3D-C4D-ND	2.80	114.77	110.24
34	2	617	LMG	O6-C1-O1	-2.80	103.34	109.97
29	A	828	CLA	C3D-C4D-ND	2.80	114.77	110.24
29	B	820	CLA	C3D-C4D-ND	2.80	114.77	110.24
29	3	607	CLA	C3D-C4D-ND	2.80	114.77	110.24
29	c	607	CLA	C3D-C4D-ND	2.80	114.77	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	2	606	CLA	C2C-C1C-NC	2.80	112.59	109.97
29	e	601	CLA	C2C-C1C-NC	2.80	112.59	109.97
33	d	617	IHT	C41-C38-C35	-2.80	123.32	127.31
29	F	203	CLA	C3D-C4D-ND	2.80	114.76	110.24
29	L	202	CLA	C3D-C4D-ND	2.80	114.76	110.24
29	Z	305	CLA	C2C-C1C-NC	2.79	112.59	109.97
29	B	816	CLA	C3D-C4D-ND	2.79	114.75	110.24
29	4	610	CLA	C3D-C4D-ND	2.79	114.75	110.24
29	5	613	CLA	C3D-C4D-ND	2.79	114.75	110.24
29	5	603	CLA	C3D-C4D-ND	2.79	114.75	110.24
29	e	604	CLA	C3D-C4D-ND	2.79	114.75	110.24
29	4	608	CLA	C3D-C4D-ND	2.79	114.75	110.24
29	A	841	CLA	C3D-C4D-ND	2.79	114.75	110.24
31	3	616	II0	C05-C07-C11	-2.79	106.49	110.30
29	A	810	CLA	O2A-C1-C2	2.78	115.95	108.64
29	2	611	CLA	C3D-C4D-ND	2.78	114.74	110.24
29	8	615	CLA	C3D-C4D-ND	2.78	114.74	110.24
30	4	605	KC2	CHB-C1B-NB	2.78	127.01	124.45
31	1	616	II0	C42-C41-C39	-2.78	117.78	123.47
31	a	616	II0	C20-C14-C12	2.78	119.51	114.36
29	L	202	CLA	C2C-C1C-NC	2.78	112.58	109.97
29	B	826	CLA	C3D-C4D-ND	2.78	114.74	110.24
31	3	614	II0	C38-C36-C40	-2.78	119.03	122.92
29	4	609	CLA	C2C-C1C-NC	2.78	112.58	109.97
29	B	816	CLA	C2C-C1C-NC	2.78	112.58	109.97
29	d	611	CLA	C2C-C1C-NC	2.78	112.58	109.97
35	3	619	LHG	O8-C23-C24	2.78	120.62	111.91
35	7	619	LHG	O8-C23-C24	2.77	120.62	111.91
29	a	603	CLA	C3D-C4D-ND	2.77	114.72	110.24
29	A	828	CLA	C2C-C1C-NC	2.77	112.57	109.97
29	9	601	CLA	C2C-C1C-NC	2.77	112.57	109.97
29	B	835	CLA	C3D-C4D-ND	2.77	114.72	110.24
31	c	617	II0	C38-C36-C40	-2.77	119.05	122.92
29	7	601	CLA	C3D-C4D-ND	2.77	114.72	110.24
29	6	605	CLA	C3D-C4D-ND	2.77	114.71	110.24
33	6	617	IHT	C41-C40-C37	-2.77	117.81	123.47
29	9	607	CLA	C3D-C4D-ND	2.77	114.71	110.24
33	5	618	IHT	C25-C23-C27	-2.77	119.05	122.92
29	2	605	CLA	C3D-C4D-ND	2.77	114.71	110.24
33	c	620	IHT	C19-C10-C09	2.76	118.93	113.62
29	B	825	CLA	C2C-C1C-NC	2.76	112.56	109.97
31	3	615	II0	C41-C42-C40	-2.76	117.82	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	609	IHT	C32-C33-C37	-2.76	114.70	118.94
33	c	620	IHT	C41-C38-C35	-2.76	123.37	127.31
29	7	612	CLA	C3D-C4D-ND	2.76	114.69	110.24
29	A	843	CLA	C3D-C4D-ND	2.76	114.69	110.24
31	8	611	II0	C38-C36-C40	-2.75	119.06	122.92
29	A	837	CLA	C2C-C1C-NC	2.75	112.55	109.97
33	6	617	IHT	C40-C37-C33	-2.75	123.38	127.31
41	B	848	DGD	O6D-C1D-O3G	-2.75	103.46	109.97
29	b	606	CLA	C3D-C4D-ND	2.75	114.69	110.24
29	A	831	CLA	C2C-C1C-NC	2.75	112.55	109.97
29	B	808	CLA	C3D-C4D-ND	2.75	114.68	110.24
29	A	831	CLA	C3D-C4D-ND	2.75	114.68	110.24
31	3	615	II0	C20-C14-C10	-2.75	120.61	124.35
29	5	605	CLA	C3D-C4D-ND	2.75	114.68	110.24
31	6	616	II0	C38-C36-C40	-2.74	119.08	122.92
30	d	610	KC2	CHB-C1B-NB	2.74	126.97	124.45
30	5	610	KC2	CHB-C1B-NB	2.74	126.97	124.45
29	5	611	CLA	C3D-C4D-ND	2.74	114.67	110.24
31	2	613	II0	C19-C13-C09	-2.74	120.63	124.35
33	Z	302	IHT	C22-C18-C07	-2.74	119.51	127.20
29	8	606	CLA	C3D-C4D-ND	2.74	114.67	110.24
29	6	603	CLA	C2C-C1C-NC	2.74	112.54	109.97
29	5	609	CLA	C2C-C1C-NC	2.74	112.54	109.97
29	d	607	CLA	C1-C2-C3	-2.74	121.31	126.04
29	6	612	CLA	C3D-C4D-ND	2.74	114.66	110.24
38	7	620	LMU	C1'-C2'-C3'	2.73	115.69	110.00
33	Z	302	IHT	C19-C10-C09	2.73	118.87	113.62
29	L	207	CLA	C3D-C4D-ND	2.73	114.66	110.24
33	a	617	IHT	C40-C37-C33	-2.73	123.42	127.31
29	A	814	CLA	C2C-C1C-NC	2.73	112.53	109.97
29	c	613	CLA	C3D-C4D-ND	2.73	114.65	110.24
29	A	806	CLA	C3D-C4D-ND	2.72	114.64	110.24
31	9	617	II0	C04-C10-C14	-2.72	118.79	122.63
35	2	619	LHG	O8-C23-C24	2.72	120.45	111.91
31	4	615	II0	C03-C09-C13	-2.72	118.79	122.63
31	8	612	II0	C41-C39-C35	-2.72	123.42	127.31
31	7	613	II0	C38-C36-C40	-2.72	119.11	122.92
29	A	833	CLA	C2C-C1C-NC	2.72	112.52	109.97
31	B	843	II0	C42-C41-C39	-2.72	117.91	123.47
31	7	614	II0	C16-C03-C09	-2.72	106.15	110.47
29	A	826	CLA	CHC-C4B-NB	-2.72	121.38	124.26
29	b	608	CLA	C2C-C1C-NC	2.71	112.52	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	F	203	CLA	C2C-C1C-NC	2.71	112.51	109.97
29	Z	305	CLA	C3D-C4D-ND	2.71	114.63	110.24
29	B	811	CLA	C2C-C1C-NC	2.71	112.51	109.97
29	K	101	CLA	C2C-C1C-NC	2.71	112.51	109.97
31	b	614	II0	C03-C09-C13	-2.71	118.81	122.63
29	c	606	CLA	C1-C2-C3	-2.71	121.36	126.04
33	Z	302	IHT	C36-C33-C32	2.71	122.34	118.08
29	A	812	CLA	C3D-C4D-ND	2.71	114.62	110.24
29	5	606	CLA	C2C-C1C-NC	2.70	112.51	109.97
31	d	615	II0	C20-C14-C12	2.70	119.37	114.36
29	b	601	CLA	C2C-C1C-NC	2.70	112.50	109.97
29	a	603	CLA	C2C-C1C-NC	2.70	112.50	109.97
29	A	832	CLA	C3D-C4D-ND	2.70	114.61	110.24
33	K	104	IHT	C13-C02-C07	-2.70	105.92	110.30
29	R	202	CLA	C3D-C4D-ND	2.70	114.60	110.24
29	L	204	CLA	C2C-C1C-NC	2.70	112.50	109.97
29	B	824	CLA	C3D-C4D-ND	2.69	114.60	110.24
31	a	615	II0	C41-C42-C40	-2.69	117.96	123.47
34	F	205	LMG	O6-C1-O1	-2.69	103.60	109.97
29	B	823	CLA	C1-C2-C3	-2.69	121.39	126.04
31	9	615	II0	C38-C36-C40	-2.69	119.15	122.92
29	K	101	CLA	C3D-C4D-ND	2.69	114.59	110.24
29	B	803	CLA	CHC-C4B-NB	-2.69	121.41	124.26
29	6	606	CLA	C2C-C1C-NC	2.69	112.49	109.97
29	d	601	CLA	C2C-C1C-NC	2.69	112.49	109.97
29	1	612	CLA	C2C-C1C-NC	2.69	112.49	109.97
31	J	101	II0	C20-C14-C12	2.69	119.33	114.36
29	A	827	CLA	C2C-C1C-NC	2.68	112.49	109.97
30	e	609	KC2	CHB-C1B-NB	2.68	126.92	124.45
29	A	823	CLA	C2C-C1C-NC	2.68	112.48	109.97
29	B	809	CLA	C2C-C1C-NC	2.68	112.48	109.97
31	8	610	II0	C19-C13-C11	2.68	119.32	114.36
35	A	850	LHG	O8-C23-C24	2.68	120.32	111.91
29	A	801	CLA	C2C-C1C-NC	2.68	112.48	109.97
29	A	804	CLA	C1-C2-C3	-2.68	121.41	126.04
30	1	610	KC2	CHB-C1B-NB	2.68	126.91	124.45
29	A	839	CLA	O2A-C1-C2	-2.68	101.60	108.64
29	a	609	CLA	C2C-C1C-NC	2.68	112.48	109.97
29	B	827	CLA	C2C-C1C-NC	2.68	112.48	109.97
32	b	613	II3	C39-C41-C40	-2.67	118.00	123.47
31	a	614	II0	C41-C42-C40	-2.67	118.00	123.47
30	e	605	KC2	CHB-C1B-NB	2.67	126.91	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	613	II0	C38-C36-C40	-2.67	119.18	122.92
30	6	613	KC2	CHB-C1B-NB	2.67	126.91	124.45
29	F	204	CLA	C3D-C4D-ND	2.67	114.55	110.24
33	5	618	IHT	C36-C33-C37	-2.67	119.19	122.92
29	7	611	CLA	C2C-C1C-NC	2.67	112.47	109.97
29	A	804	CLA	C3D-C4D-ND	2.67	114.55	110.24
31	3	613	II0	C38-C36-C40	-2.67	119.19	122.92
29	4	607	CLA	C1-C2-C3	-2.67	121.43	126.04
29	B	832	CLA	C3D-C4D-ND	2.66	114.55	110.24
30	b	609	KC2	CHB-C1B-NB	2.66	126.90	124.45
29	8	601	CLA	C2C-C1C-NC	2.66	112.47	109.97
29	7	612	CLA	C2C-C1C-NC	2.66	112.47	109.97
29	d	612	CLA	C2C-C1C-NC	2.66	112.47	109.97
29	B	806	CLA	C3D-C4D-ND	2.66	114.54	110.24
29	b	608	CLA	C3D-C4D-ND	2.66	114.54	110.24
30	6	610	KC2	CHB-C1B-NB	2.66	126.90	124.45
29	B	821	CLA	C1-C2-C3	-2.66	121.45	126.04
29	a	602	CLA	CAA-C2A-C1A	-2.66	103.27	111.97
33	c	620	IHT	C22-C23-C27	-2.66	114.86	118.94
29	a	611	CLA	C2C-C1C-NC	2.66	112.46	109.97
29	9	613	CLA	C3D-C4D-ND	2.66	114.53	110.24
29	3	607	CLA	CHC-C4B-NB	-2.66	121.45	124.26
29	c	603	CLA	C3D-C4D-ND	2.65	114.53	110.24
30	9	610	KC2	CHB-C1B-NB	2.65	126.89	124.45
30	Z	307	KC2	CHB-C1B-NB	2.65	126.89	124.45
29	B	823	CLA	C3D-C4D-ND	2.65	114.53	110.24
29	O	203	CLA	CHC-C1C-C2C	-2.65	119.37	126.73
33	L	205	IHT	C19-C10-C09	2.65	118.70	113.62
31	2	615	II0	C04-C10-C14	-2.65	118.89	122.63
29	A	816	CLA	C2C-C1C-NC	2.65	112.45	109.97
33	K	104	IHT	C25-C23-C27	-2.65	119.22	122.92
31	O	204	II0	C38-C36-C40	-2.65	119.22	122.92
35	a	618	LHG	C11-C10-C9	-2.64	101.00	114.42
29	A	835	CLA	C2C-C1C-NC	2.64	112.45	109.97
31	9	617	II0	C42-C41-C39	-2.64	118.06	123.47
33	6	617	IHT	C30-C27-C23	-2.64	123.54	127.31
35	8	613	LHG	O8-C23-C24	2.64	120.20	111.91
30	c	611	KC2	CHB-C1B-NB	2.64	126.88	124.45
29	A	817	CLA	CAA-C2A-C1A	-2.64	103.33	111.97
31	9	618	II0	C41-C39-C35	-2.64	123.55	127.31
31	5	614	II0	C06-C08-C12	-2.64	106.69	110.30
35	5	619	LHG	O8-C23-C24	2.63	120.18	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	201	CLA	C3D-C4D-ND	2.63	114.50	110.24
35	2	620	LHG	C11-C10-C9	-2.63	101.06	114.42
29	B	825	CLA	C3D-C4D-ND	2.63	114.50	110.24
29	5	601	CLA	C2C-C1C-NC	2.63	112.44	109.97
29	A	827	CLA	C3D-C4D-ND	2.63	114.49	110.24
31	7	615	II0	C19-C13-C11	2.63	119.23	114.36
36	O	206	SQD	C45-O47-C7	-2.63	111.32	117.79
29	4	610	CLA	C2C-C1C-NC	2.63	112.43	109.97
29	c	607	CLA	C2C-C1C-NC	2.63	112.43	109.97
29	A	804	CLA	C2C-C1C-NC	2.62	112.43	109.97
29	A	820	CLA	C2C-C1C-NC	2.62	112.43	109.97
29	e	606	CLA	C3D-C4D-ND	2.62	114.48	110.24
30	7	610	KC2	CHB-C1B-NB	2.62	126.86	124.45
31	8	616	II0	C29-C31-C33	-2.62	115.04	123.22
31	7	614	II0	C38-C36-C40	-2.62	119.25	122.92
29	5	611	CLA	C2C-C1C-NC	2.62	112.42	109.97
29	d	603	CLA	C2C-C1C-NC	2.62	112.42	109.97
31	2	615	II0	C41-C42-C40	-2.61	118.12	123.47
30	3	606	KC2	C4C-C3C-C2C	2.61	109.19	107.11
33	5	618	IHT	C41-C38-C35	-2.61	123.58	127.31
39	A	849	PQN	C11-C3-C4	-2.61	115.71	118.50
29	B	821	CLA	C2C-C1C-NC	2.61	112.42	109.97
32	e	613	II3	C26-C29-C32	-2.61	115.07	123.22
29	6	611	CLA	C1-C2-C3	-2.61	121.53	126.04
29	5	603	CLA	C2C-C1C-NC	2.61	112.42	109.97
31	8	610	II0	C19-C13-C09	-2.61	120.80	124.35
35	c	621	LHG	O8-C23-C24	2.61	120.09	111.91
29	A	829	CLA	C2C-C1C-NC	2.61	112.41	109.97
29	d	609	CLA	C2C-C1C-NC	2.60	112.41	109.97
30	c	615	KC2	CHB-C1B-NB	2.60	126.85	124.45
29	A	844	CLA	CHC-C4B-NB	-2.60	121.50	124.26
29	d	612	CLA	C3D-C4D-ND	2.60	114.45	110.24
29	e	611	CLA	C3D-C4D-ND	2.60	114.45	110.24
31	5	615	II0	C42-C41-C39	-2.60	118.14	123.47
29	3	610	CLA	C2C-C1C-NC	2.60	112.41	109.97
29	9	612	CLA	C2C-C1C-NC	2.60	112.41	109.97
29	A	826	CLA	C3D-C4D-ND	2.60	114.44	110.24
29	2	605	CLA	C2C-C1C-NC	2.59	112.40	109.97
29	2	608	CLA	CHC-C4B-NB	-2.59	121.51	124.26
29	4	608	CLA	C2C-C1C-NC	2.59	112.40	109.97
30	3	606	KC2	CHC-C4B-NB	2.59	126.84	124.45
29	4	604	CLA	C2C-C1C-NC	2.59	112.40	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	3	623	LHG	O8-C23-C24	2.59	120.04	111.91
35	Z	310	LHG	O8-C23-C24	2.59	120.04	111.91
29	d	604	CLA	CHC-C4B-NB	-2.59	121.52	124.26
29	e	604	CLA	C2C-C1C-NC	2.59	112.40	109.97
29	6	611	CLA	C2C-C1C-NC	2.59	112.40	109.97
29	9	613	CLA	C2C-C1C-NC	2.59	112.39	109.97
29	A	818	CLA	C2C-C1C-NC	2.59	112.39	109.97
31	5	616	II0	C41-C42-C40	-2.59	118.18	123.47
29	A	810	CLA	C2C-C1C-NC	2.59	112.39	109.97
31	3	615	II0	C42-C40-C36	-2.58	123.62	127.31
29	6	612	CLA	C2C-C1C-NC	2.58	112.39	109.97
31	7	613	II0	C42-C41-C39	-2.58	118.18	123.47
29	B	807	CLA	C1-C2-C3	-2.58	121.58	126.04
29	4	601	CLA	C2C-C1C-NC	2.58	112.39	109.97
29	9	606	CLA	C2C-C1C-NC	2.58	112.39	109.97
29	B	840	CLA	C2C-C1C-NC	2.58	112.39	109.97
29	8	602	CLA	C3D-C4D-ND	2.58	114.41	110.24
31	a	619	II0	C41-C42-C40	-2.58	118.19	123.47
29	a	601	CLA	C2C-C1C-NC	2.58	112.39	109.97
29	A	807	CLA	C2C-C1C-NC	2.58	112.39	109.97
29	A	843	CLA	CHC-C4B-NB	-2.58	121.53	124.26
29	9	605	CLA	C2C-C1C-NC	2.58	112.39	109.97
30	7	606	KC2	CHB-C1B-NB	2.57	126.82	124.45
31	O	205	II0	C38-C36-C40	-2.57	119.32	122.92
31	e	614	II0	C20-C14-C10	-2.57	120.85	124.35
29	2	611	CLA	C2C-C1C-NC	2.57	112.38	109.97
31	6	616	II0	C03-C09-C13	-2.57	119.01	122.63
29	9	602	CLA	CHC-C4B-NB	-2.57	121.54	124.26
29	B	807	CLA	C2C-C1C-NC	2.57	112.38	109.97
29	c	609	CLA	C2C-C1C-NC	2.57	112.38	109.97
31	c	619	II0	C20-C14-C10	-2.57	120.86	124.35
31	4	612	II0	C41-C42-C40	-2.56	118.22	123.47
29	A	838	CLA	C2C-C1C-NC	2.56	112.37	109.97
31	a	619	II0	C20-C14-C12	2.56	119.10	114.36
31	6	615	II0	C20-C14-C12	2.56	119.10	114.36
29	6	609	CLA	C2C-C1C-NC	2.56	112.37	109.97
33	L	205	IHT	C22-C23-C27	-2.56	115.01	118.94
29	1	612	CLA	C3D-C4D-ND	2.56	114.38	110.24
29	A	805	CLA	C2C-C1C-NC	2.56	112.37	109.97
29	c	606	CLA	C2C-C1C-NC	2.56	112.37	109.97
29	1	609	CLA	C2C-C1C-NC	2.56	112.37	109.97
29	7	605	CLA	C2C-C1C-NC	2.56	112.37	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	834	CLA	C2C-C1C-NC	2.56	112.37	109.97
29	8	607	CLA	C2C-C1C-NC	2.56	112.37	109.97
29	d	608	CLA	CHC-C4B-NB	-2.55	121.55	124.26
32	e	613	II3	C37-C38-C40	-2.55	115.03	118.94
29	a	604	CLA	CHC-C4B-NB	-2.55	121.56	124.26
29	A	823	CLA	C3D-C4D-ND	2.55	114.36	110.24
31	c	616	II0	C20-C14-C10	-2.55	120.89	124.35
30	b	605	KC2	CHB-C1B-NB	2.55	126.80	124.45
31	d	614	II0	C41-C42-C40	-2.55	118.26	123.47
33	1	618	IHT	C41-C40-C37	-2.55	118.26	123.47
33	2	616	IHT	C20-C15-C12	2.54	119.06	114.36
29	A	808	CLA	C2C-C1C-NC	2.54	112.35	109.97
29	A	839	CLA	CHC-C4B-NB	-2.54	121.57	124.26
29	d	606	CLA	C2C-C1C-NC	2.54	112.35	109.97
31	8	612	II0	C42-C40-C36	-2.53	123.69	127.31
33	Z	302	IHT	C36-C33-C37	-2.53	119.37	122.92
29	c	614	CLA	C2C-C1C-NC	2.53	112.34	109.97
33	Z	302	IHT	C04-C06-C09	-2.53	105.72	111.38
29	8	602	CLA	CHC-C4B-NB	-2.53	121.58	124.26
29	B	805	CLA	C2C-C1C-NC	2.53	112.34	109.97
29	c	605	CLA	C2C-C1C-NC	2.53	112.34	109.97
31	7	613	II0	C20-C14-C12	2.53	119.04	114.36
29	9	603	CLA	C2C-C1C-NC	2.53	112.34	109.97
29	8	605	CLA	C1-C2-C3	-2.53	122.66	126.75
29	a	608	CLA	CHC-C4B-NB	-2.53	121.58	124.26
29	5	607	CLA	C2C-C1C-NC	2.53	112.34	109.97
33	8	609	IHT	C30-C27-C23	-2.53	123.70	127.31
33	5	618	IHT	C19-C10-C09	2.52	118.47	113.62
29	8	604	CLA	C3D-C4D-ND	2.52	114.32	110.24
31	5	616	II0	C19-C13-C11	2.52	119.03	114.36
29	2	609	CLA	C2C-C1C-NC	2.52	112.33	109.97
31	J	101	II0	C06-C08-C12	-2.52	106.85	110.30
29	e	603	CLA	C2C-C1C-NC	2.52	112.33	109.97
29	4	603	CLA	C2C-C1C-NC	2.52	112.33	109.97
29	2	604	CLA	CHC-C4B-NB	-2.52	121.59	124.26
31	6	614	II0	C41-C39-C35	-2.52	123.72	127.31
31	O	205	II0	C03-C09-C13	-2.52	119.08	122.63
29	2	612	CLA	C2C-C1C-NC	2.52	112.33	109.97
29	B	841	CLA	C2C-C1C-NC	2.52	112.33	109.97
29	A	810	CLA	C3D-C4D-ND	2.51	114.30	110.24
29	8	604	CLA	C2C-C1C-NC	2.51	112.33	109.97
29	Z	306	CLA	C2C-C1C-NC	2.51	112.33	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	J	101	II0	C41-C42-C40	-2.51	118.33	123.47
33	L	205	IHT	C41-C38-C35	-2.51	123.73	127.31
29	5	613	CLA	C2C-C1C-NC	2.51	112.32	109.97
29	A	842	CLA	C2C-C1C-NC	2.51	112.32	109.97
29	b	606	CLA	C2C-C1C-NC	2.51	112.32	109.97
35	2	620	LHG	O8-C23-C24	2.51	119.77	111.91
31	O	205	II0	C05-C07-C11	2.51	113.73	110.30
33	9	619	IHT	C41-C38-C35	-2.51	123.73	127.31
35	d	618	LHG	O8-C6-C5	-2.51	105.14	111.78
29	1	613	CLA	C2C-C1C-NC	2.51	112.32	109.97
29	B	813	CLA	C2C-C1C-NC	2.51	112.32	109.97
31	9	616	II0	C41-C42-C40	-2.50	118.34	123.47
31	6	615	II0	C42-C41-C39	-2.50	118.35	123.47
31	6	615	II0	C38-C36-C40	-2.50	119.42	122.92
31	2	614	II0	C42-C41-C39	-2.50	118.35	123.47
29	9	614	CLA	C2C-C1C-NC	2.50	112.31	109.97
29	B	818	CLA	C2C-C1C-NC	2.50	112.31	109.97
29	A	812	CLA	C1-C2-C3	-2.50	121.72	126.04
29	B	802	CLA	C3D-C4D-ND	2.50	114.28	110.24
29	6	605	CLA	C2C-C1C-NC	2.50	112.31	109.97
29	L	203	CLA	C2C-C1C-NC	2.50	112.31	109.97
29	a	605	CLA	C2C-C1C-NC	2.50	112.31	109.97
32	b	613	II3	C29-C26-C24	-2.50	123.75	127.31
29	B	826	CLA	C2C-C1C-NC	2.49	112.31	109.97
35	L	208	LHG	O8-C23-C24	2.49	119.72	111.91
31	1	616	II0	C06-C08-C12	-2.49	106.89	110.30
29	B	802	CLA	C2C-C1C-NC	2.49	112.30	109.97
35	d	619	LHG	O8-C23-C24	2.49	119.72	111.91
31	2	615	II0	C41-C39-C35	-2.49	123.76	127.31
31	a	616	II0	C08-C12-C14	-2.49	106.90	111.85
29	b	610	CLA	C1-C2-C3	-2.48	121.75	126.04
31	7	613	II0	C05-C07-C11	-2.48	106.90	110.30
31	b	614	II0	C41-C42-C40	-2.48	118.39	123.47
31	d	614	II0	C38-C36-C40	-2.48	119.45	122.92
31	5	615	II0	C04-C10-C14	-2.48	119.13	122.63
31	a	616	II0	C41-C39-C35	-2.48	123.77	127.31
31	1	614	II0	C41-C42-C40	-2.48	118.40	123.47
29	A	832	CLA	C2C-C1C-NC	2.48	112.29	109.97
31	9	616	II0	C38-C36-C40	-2.48	119.45	122.92
29	A	815	CLA	C2C-C1C-NC	2.48	112.29	109.97
29	b	611	CLA	C2C-C1C-NC	2.47	112.29	109.97
29	4	606	CLA	C1-C2-C3	-2.47	121.77	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	8	615	CLA	C2C-C1C-NC	2.47	112.29	109.97
29	9	609	CLA	CHC-C4B-NB	-2.47	121.64	124.26
35	7	618	LHG	O8-C23-C24	2.47	119.66	111.91
41	B	848	DGD	O5D-C6D-C5D	-2.47	104.47	109.05
29	B	820	CLA	C2C-C1C-NC	2.47	112.29	109.97
31	a	614	II0	C41-C39-C35	-2.47	123.78	127.31
33	8	609	IHT	C19-C10-C07	-2.47	121.75	124.53
29	7	607	CLA	CHC-C4B-NB	-2.47	121.64	124.26
29	A	819	CLA	C2C-C1C-NC	2.47	112.28	109.97
35	d	618	LHG	C11-C10-C9	-2.47	101.91	114.42
29	Z	304	CLA	C2C-C1C-NC	2.47	112.28	109.97
31	a	613	II0	C38-C36-C40	-2.46	119.47	122.92
37	B	845	8CT	C30-C31-C32	-2.46	118.44	121.47
29	B	837	CLA	C2C-C1C-NC	2.46	112.28	109.97
31	6	614	II0	C42-C40-C36	-2.46	123.79	127.31
30	c	610	KC2	CHB-C1B-NB	2.46	126.72	124.45
29	5	606	CLA	CHC-C4B-NB	-2.46	121.65	124.26
29	b	603	CLA	C2C-C1C-NC	2.46	112.28	109.97
33	a	617	IHT	C30-C27-C23	-2.46	123.80	127.31
29	B	831	CLA	CHC-C4B-NB	-2.46	121.66	124.26
30	c	611	KC2	CHD-C4C-NC	2.45	127.93	124.20
31	a	615	II0	C05-C07-C11	-2.45	106.94	110.30
29	3	609	CLA	C2C-C1C-NC	2.45	112.27	109.97
29	d	605	CLA	C2C-C1C-NC	2.45	112.27	109.97
29	d	606	CLA	CHC-C4B-NB	-2.45	121.66	124.26
33	c	620	IHT	C40-C37-C33	-2.45	123.81	127.31
31	7	616	II0	C38-C36-C40	-2.45	119.49	122.92
31	c	616	II0	C42-C40-C36	-2.45	123.81	127.31
33	6	617	IHT	C19-C10-C09	2.45	118.32	113.62
29	A	802	CLA	C2C-C1C-NC	2.45	112.27	109.97
31	6	616	II0	C41-C42-C40	-2.45	118.46	123.47
33	1	618	IHT	C41-C38-C35	-2.45	123.82	127.31
32	b	613	II3	C26-C29-C32	-2.45	115.58	123.22
29	6	601	CLA	CHC-C1C-C2C	-2.45	119.94	126.73
29	1	603	CLA	C2C-C1C-NC	2.44	112.26	109.97
29	B	819	CLA	C2C-C1C-NC	2.44	112.26	109.97
31	7	616	II0	C33-C35-C39	-2.44	115.19	118.94
29	a	607	CLA	C2C-C1C-NC	2.44	112.26	109.97
29	B	834	CLA	CHC-C4B-NB	-2.44	121.67	124.26
31	4	614	II0	C38-C36-C40	-2.44	119.50	122.92
29	A	830	CLA	C2C-C1C-NC	2.44	112.26	109.97
31	B	843	II0	C38-C36-C40	-2.44	119.50	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	602	CLA	CAA-C2A-C3A	2.44	119.46	112.78
29	B	802	CLA	CHA-C1A-NA	-2.44	120.81	126.40
33	2	616	IHT	C19-C10-C07	-2.44	121.79	124.53
29	B	808	CLA	C2C-C1C-NC	2.44	112.26	109.97
29	b	610	CLA	C2C-C1C-NC	2.44	112.26	109.97
29	B	803	CLA	CHA-C1A-NA	-2.44	120.81	126.40
31	1	619	II0	C38-C36-C40	-2.44	119.51	122.92
31	9	615	II0	C42-C41-C39	-2.44	118.48	123.47
29	B	819	CLA	CHC-C4B-NB	-2.44	121.68	124.26
29	B	830	CLA	C2C-C1C-NC	2.44	112.25	109.97
31	3	615	II0	C41-C39-C35	-2.43	123.84	127.31
29	7	609	CLA	C2C-C1C-NC	2.43	112.25	109.97
29	9	611	CLA	C2C-C1C-NC	2.43	112.25	109.97
29	K	102	CLA	CHC-C4B-NB	-2.43	121.68	124.26
29	e	607	CLA	CHC-C4B-NB	-2.43	121.68	124.26
41	Z	303	DGD	C3G-C2G-C1G	-2.43	106.04	111.79
31	c	616	II0	C41-C39-C35	-2.43	123.84	127.31
29	A	813	CLA	C2C-C1C-NC	2.43	112.25	109.97
33	K	104	IHT	C18-C22-C23	-2.43	122.56	126.23
33	a	617	IHT	C18-C22-C23	-2.43	122.56	126.23
29	3	605	CLA	CHC-C4B-NB	-2.43	121.69	124.26
29	1	611	CLA	C2C-C1C-NC	2.43	112.25	109.97
29	B	806	CLA	C2C-C1C-NC	2.43	112.25	109.97
31	3	617	II0	C41-C42-C40	-2.43	118.50	123.47
29	2	603	CLA	C2C-C1C-NC	2.43	112.25	109.97
29	4	611	CLA	C2C-C1C-NC	2.43	112.25	109.97
30	6	610	KC2	CHD-C4C-NC	2.43	127.88	124.20
29	7	603	CLA	C2C-C1C-NC	2.43	112.24	109.97
29	B	803	CLA	C3D-C4D-ND	2.42	114.16	110.24
29	9	609	CLA	C2C-C1C-NC	2.42	112.24	109.97
31	d	616	II0	C38-C36-C34	2.42	121.89	118.08
29	B	838	CLA	C2C-C1C-NC	2.42	112.24	109.97
34	8	614	LMG	O2-C2-C1	-2.42	104.17	110.05
29	7	607	CLA	C2C-C1C-NC	2.42	112.24	109.97
35	5	619	LHG	C5-O7-C7	-2.42	113.39	117.90
29	L	202	CLA	CHC-C4B-NB	-2.42	121.70	124.26
31	b	612	II0	C42-C41-C39	-2.42	118.52	123.47
29	A	810	CLA	CHA-C1A-NA	-2.42	120.86	126.40
31	5	616	II0	C20-C14-C12	2.42	118.83	114.36
29	3	611	CLA	C2C-C1C-NC	2.42	112.23	109.97
29	L	201	CLA	C2C-C1C-NC	2.42	112.23	109.97
29	B	832	CLA	C2C-C1C-NC	2.41	112.23	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	b	616	LHG	O8-C23-C24	2.41	119.48	111.91
31	9	615	II0	C20-C14-C10	-2.41	121.07	124.35
31	a	615	II0	C28-C26-C24	2.41	121.61	116.84
29	3	604	CLA	C2C-C1C-NC	2.41	112.23	109.97
29	6	607	CLA	C2C-C1C-NC	2.41	112.23	109.97
31	c	617	II0	C42-C41-C39	-2.41	118.53	123.47
38	J	104	LMU	O5B-C5B-C4B	2.41	114.07	109.69
31	1	616	II0	C05-C07-C11	-2.41	107.01	110.30
31	b	612	II0	C05-C07-C11	-2.41	107.01	110.30
31	d	614	II0	C41-C39-C35	-2.41	123.88	127.31
29	3	603	CLA	CHC-C4B-NB	-2.40	121.71	124.26
29	B	817	CLA	C2C-C1C-NC	2.40	112.22	109.97
31	d	616	II0	C19-C13-C11	2.40	118.81	114.36
29	A	808	CLA	CHC-C4B-NB	-2.40	121.71	124.26
33	d	617	IHT	C22-C23-C27	-2.40	115.25	118.94
31	1	617	II0	C06-C08-C12	-2.40	107.02	110.30
29	4	607	CLA	C2C-C1C-NC	2.40	112.22	109.97
30	c	610	KC2	CHB-C4A-NA	2.40	127.98	124.20
29	B	828	CLA	C2C-C1C-NC	2.40	112.22	109.97
31	5	614	II0	C05-C07-C11	-2.40	107.02	110.30
29	1	612	CLA	C1-C2-C3	-2.40	121.90	126.04
29	9	601	CLA	CHC-C1C-C2C	-2.40	120.08	126.73
29	c	603	CLA	C2C-C1C-NC	2.40	112.22	109.97
38	4	618	LMU	C6B-C5B-C4B	-2.40	107.39	113.00
31	7	613	II0	C04-C10-C14	-2.39	119.25	122.63
33	8	609	IHT	C06-C09-C10	2.39	118.35	114.08
29	8	608	CLA	C2C-C1C-NC	2.39	112.22	109.97
29	B	810	CLA	C2C-C1C-NC	2.39	112.22	109.97
29	J	102	CLA	C2C-C1C-NC	2.39	112.22	109.97
30	e	605	KC2	CHC-C4B-NB	2.39	126.65	124.45
29	7	602	CLA	C1-C2-C3	-2.39	121.90	126.04
33	L	205	IHT	C19-C10-C07	-2.39	121.84	124.53
29	e	602	CLA	C2C-C1C-NC	2.39	112.21	109.97
29	5	604	CLA	CHC-C4B-NB	-2.39	121.72	124.26
29	9	604	CLA	C2C-C1C-NC	2.39	112.21	109.97
29	2	601	CLA	C2C-C1C-NC	2.39	112.21	109.97
29	5	605	CLA	C2C-C1C-NC	2.39	112.21	109.97
29	3	601	CLA	C2C-C1C-NC	2.39	112.21	109.97
29	A	803	CLA	C2C-C1C-NC	2.39	112.21	109.97
29	c	604	CLA	CHC-C4B-NB	-2.39	121.73	124.26
30	4	605	KC2	CHD-C4C-NC	2.39	127.82	124.20
29	1	606	CLA	CHC-C4B-NB	-2.39	121.73	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	F	204	CLA	CHC-C1C-C2C	-2.38	120.11	126.73
29	O	201	CLA	C1-C2-C3	-2.38	121.92	126.04
29	5	606	CLA	CHC-C1C-C2C	-2.38	120.11	126.73
29	B	805	CLA	CAA-C2A-C1A	-2.38	104.16	111.97
35	3	619	LHG	C11-C10-C9	-2.38	102.32	114.42
29	O	202	CLA	CHC-C4B-NB	-2.38	121.73	124.26
34	3	620	LMG	O6-C1-O1	-2.38	104.33	109.97
29	c	612	CLA	CHC-C1C-C2C	-2.38	120.11	126.73
38	4	618	LMU	C1B-O5B-C5B	2.38	118.36	113.69
29	3	612	CLA	CHC-C1C-C2C	-2.38	120.12	126.73
29	A	806	CLA	C2C-C1C-NC	2.38	112.20	109.97
29	A	841	CLA	CHC-C4B-NB	-2.38	121.74	124.26
31	8	611	II0	C41-C42-C40	-2.38	118.60	123.47
31	e	612	II0	C41-C42-C40	-2.38	118.60	123.47
33	Z	302	IHT	C40-C41-C38	-2.38	118.60	123.47
31	4	615	II0	C41-C42-C40	-2.38	118.60	123.47
31	a	615	II0	C41-C39-C35	-2.38	123.92	127.31
31	6	616	II0	C41-C39-C35	-2.38	123.92	127.31
29	6	605	CLA	C1-C2-C3	-2.37	121.94	126.04
29	2	606	CLA	CHC-C1C-C2C	-2.37	120.14	126.73
29	B	812	CLA	C1-C2-C3	-2.37	121.94	126.04
29	e	608	CLA	C2C-C1C-NC	2.37	112.19	109.97
31	O	204	II0	C42-C41-C39	-2.37	118.62	123.47
29	8	606	CLA	CHC-C1C-C2C	-2.37	120.15	126.73
29	1	601	CLA	C2C-C1C-NC	2.37	112.19	109.97
29	B	814	CLA	C2C-C1C-NC	2.37	112.19	109.97
29	A	822	CLA	C2C-C1C-NC	2.37	112.19	109.97
29	1	606	CLA	C2C-C1C-NC	2.37	112.19	109.97
29	9	607	CLA	C2C-C1C-NC	2.36	112.19	109.97
31	e	614	II0	C06-C08-C12	2.36	113.54	110.30
31	5	614	II0	C42-C41-C39	-2.36	118.64	123.47
37	A	852	8CT	C07-C02-C03	-2.36	119.30	122.73
32	1	615	II3	C41-C39-C36	-2.36	118.64	123.47
30	a	610	KC2	CHD-C4C-NC	2.36	127.78	124.20
31	a	616	II0	C05-C07-C11	-2.36	107.07	110.30
29	8	605	CLA	CHD-C1D-C2D	2.36	130.43	125.48
29	4	609	CLA	CHC-C1C-C2C	-2.36	120.17	126.73
31	9	615	II0	C08-C12-C14	-2.36	107.15	111.85
29	A	836	CLA	CHC-C1C-C2C	-2.36	120.18	126.73
29	L	204	CLA	CHC-C1C-C2C	-2.36	120.18	126.73
29	5	608	CLA	CHC-C4B-NB	-2.36	121.76	124.26
31	8	612	II0	C38-C36-C40	-2.36	119.62	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	6	603	CLA	CHC-C1C-C2C	-2.36	120.19	126.73
29	A	807	CLA	CHC-C1C-C2C	-2.35	120.19	126.73
33	8	609	IHT	C40-C37-C33	-2.35	123.95	127.31
29	e	611	CLA	C2C-C1C-NC	2.35	112.18	109.97
30	c	610	KC2	C4C-C3C-C2C	2.35	108.98	107.11
32	1	615	II3	C08-C03-C04	2.35	113.11	109.55
31	b	614	II0	C38-C36-C40	-2.35	119.63	122.92
29	A	821	CLA	CHD-C1D-C2D	2.35	130.41	125.48
29	B	822	CLA	CHC-C1C-C2C	-2.35	120.20	126.73
31	d	615	II0	C42-C41-C39	-2.35	118.67	123.47
30	d	610	KC2	CHB-C4A-NA	2.35	127.90	124.20
35	4	619	LHG	O8-C23-C24	2.35	119.27	111.91
29	9	605	CLA	CHC-C4B-NB	-2.35	121.77	124.26
29	B	829	CLA	CHD-C1D-C2D	2.35	130.40	125.48
31	4	614	II0	C41-C42-C40	-2.35	118.67	123.47
29	c	613	CLA	CHC-C1C-C2C	-2.34	120.22	126.73
30	c	611	KC2	C4C-C3C-C2C	2.34	108.98	107.11
29	B	822	CLA	O2A-C1-C2	-2.34	102.47	108.64
29	9	608	CLA	C1-C2-C3	-2.34	121.99	126.04
31	2	614	II0	C06-C08-C12	-2.34	107.10	110.30
31	c	617	II0	C06-C08-C12	-2.34	107.10	110.30
29	7	608	CLA	CHC-C4B-NB	-2.34	121.78	124.26
31	2	613	II0	C41-C39-C35	-2.34	123.97	127.31
29	A	825	CLA	C2C-C1C-NC	2.34	112.17	109.97
31	8	610	II0	C38-C36-C40	-2.34	119.65	122.92
34	I	102	LMG	O3-C3-C2	-2.34	104.94	110.35
29	K	102	CLA	CHC-C1C-C2C	-2.34	120.24	126.73
33	8	609	IHT	C27-C30-C32	-2.34	115.92	123.22
31	9	618	II0	C20-C14-C10	-2.34	121.17	124.35
29	A	839	CLA	C2C-C1C-NC	2.34	112.16	109.97
35	4	617	LHG	O8-C23-C24	2.34	119.24	111.91
30	b	605	KC2	CHC-C4B-NB	2.34	126.60	124.45
33	Z	302	IHT	C25-C23-C27	-2.34	119.65	122.92
34	F	205	LMG	C3-C4-C5	-2.33	106.07	110.24
29	A	842	CLA	CHC-C1C-C2C	-2.33	120.25	126.73
29	1	604	CLA	C2C-C1C-NC	2.33	112.16	109.97
29	7	601	CLA	CHC-C1C-C2C	-2.33	120.25	126.73
29	4	606	CLA	CHC-C1C-C2C	-2.33	120.25	126.73
30	4	605	KC2	CHC-C4B-NB	2.33	126.60	124.45
29	A	801	CLA	CHD-C1D-C2D	2.33	130.37	125.48
34	3	618	LMG	O6-C1-O1	-2.33	104.45	109.97
33	2	616	IHT	C31-C34-C35	-2.33	119.86	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	613	II0	C19-C13-C09	-2.33	121.18	124.35
29	1	607	CLA	C2C-C1C-NC	2.33	112.16	109.97
31	5	620	II0	C19-C13-C09	-2.33	121.18	124.35
29	6	609	CLA	CHC-C1C-C2C	-2.33	120.26	126.73
31	e	615	II0	C41-C42-C40	-2.33	118.70	123.47
31	O	205	II0	C41-C42-C40	-2.33	118.70	123.47
31	e	615	II0	C38-C36-C40	-2.33	119.66	122.92
29	A	817	CLA	CHC-C4B-NB	-2.33	121.79	124.26
29	a	602	CLA	CHC-C4B-NB	-2.33	121.79	124.26
29	B	839	CLA	C2C-C1C-NC	2.33	112.15	109.97
31	2	615	II0	C38-C36-C40	-2.33	119.66	122.92
29	A	828	CLA	CHC-C1C-C2C	-2.33	120.27	126.73
29	5	612	CLA	C2C-C1C-NC	2.32	112.15	109.97
29	b	607	CLA	C2C-C1C-NC	2.32	112.15	109.97
34	I	102	LMG	O1-C7-C8	-2.32	105.29	110.90
33	d	617	IHT	C27-C30-C32	-2.32	115.97	123.22
29	L	202	CLA	CHC-C1C-C2C	-2.32	120.28	126.73
30	b	605	KC2	CHB-C4A-NA	2.32	127.86	124.20
29	A	821	CLA	C2C-C1C-NC	2.32	112.15	109.97
29	d	601	CLA	CHC-C1C-C2C	-2.32	120.28	126.73
31	1	619	II0	C41-C42-C40	-2.32	118.72	123.47
30	6	613	KC2	CHC-C4B-NB	2.32	126.58	124.45
31	e	612	II0	C20-C14-C12	2.32	118.65	114.36
29	B	823	CLA	C2C-C1C-NC	2.32	112.14	109.97
31	R	204	II0	C19-C13-C09	-2.32	121.20	124.35
33	6	617	IHT	C41-C38-C35	-2.32	124.00	127.31
35	2	619	LHG	C11-C10-C9	-2.31	102.67	114.42
29	1	602	CLA	C2C-C1C-NC	2.31	112.14	109.97
29	a	609	CLA	CHC-C1C-C2C	-2.31	120.30	126.73
33	L	205	IHT	C32-C33-C37	-2.31	115.39	118.94
29	B	835	CLA	CHC-C4B-NB	-2.31	121.81	124.26
31	6	614	II0	C04-C10-C14	-2.31	119.37	122.63
29	A	812	CLA	C2C-C1C-NC	2.31	112.14	109.97
29	F	202	CLA	C2C-C1C-NC	2.31	112.14	109.97
29	4	601	CLA	CHC-C1C-C2C	-2.31	120.31	126.73
31	a	614	II0	C05-C07-C11	-2.31	107.14	110.30
29	7	604	CLA	C2C-C1C-NC	2.31	112.13	109.97
29	8	603	CLA	C2C-C1C-NC	2.31	112.13	109.97
29	B	824	CLA	C2C-C1C-NC	2.31	112.13	109.97
29	d	611	CLA	CHC-C1C-C2C	-2.31	120.32	126.73
33	c	620	IHT	C27-C30-C32	-2.31	116.02	123.22
29	O	201	CLA	C2C-C1C-NC	2.31	112.13	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	d	617	IHT	C04-C02-C07	-2.31	106.93	110.48
31	d	613	II0	C20-C14-C12	2.31	118.63	114.36
29	6	604	CLA	C2C-C1C-NC	2.30	112.13	109.97
32	1	615	II3	C22-C18-C16	-2.30	121.22	124.35
29	5	601	CLA	CHD-C1D-C2D	2.30	130.31	125.48
29	5	609	CLA	CHC-C1C-C2C	-2.30	120.33	126.73
29	a	606	CLA	C2C-C1C-NC	2.30	112.13	109.97
31	4	615	II0	C38-C36-C40	-2.30	119.70	122.92
31	3	617	II0	C20-C14-C12	2.30	118.62	114.36
31	b	612	II0	C06-C08-C12	-2.30	107.15	110.30
31	e	614	II0	C41-C39-C35	-2.30	124.03	127.31
34	F	205	LMG	O1-C7-C8	-2.30	105.35	110.90
29	4	608	CLA	CHC-C1C-C2C	-2.30	120.34	126.73
31	J	101	II0	C41-C39-C35	-2.30	124.03	127.31
29	2	607	CLA	C2C-C1C-NC	2.30	112.13	109.97
29	6	608	CLA	CHC-C4B-NB	-2.30	121.82	124.26
31	5	620	II0	C20-C14-C12	2.30	118.62	114.36
31	8	616	II0	C20-C14-C12	2.30	118.61	114.36
33	8	609	IHT	C41-C38-C35	-2.30	124.03	127.31
29	B	811	CLA	CHC-C1C-C2C	-2.30	120.35	126.73
29	A	821	CLA	CHC-C4B-NB	-2.30	121.83	124.26
29	A	835	CLA	CHC-C1C-C2C	-2.29	120.36	126.73
29	1	609	CLA	CHC-C1C-C2C	-2.29	120.36	126.73
31	c	618	II0	C41-C42-C40	-2.29	118.78	123.47
29	9	606	CLA	CHC-C1C-C2C	-2.29	120.37	126.73
33	K	104	IHT	C41-C38-C35	-2.29	124.04	127.31
29	1	612	CLA	CHC-C1C-C2C	-2.29	120.37	126.73
29	d	609	CLA	CHC-C1C-C2C	-2.29	120.37	126.73
32	b	613	II3	C31-C34-C37	-2.29	116.07	123.22
29	3	607	CLA	C2C-C1C-NC	2.29	112.12	109.97
30	9	610	KC2	CHD-C4C-NC	2.29	127.67	124.20
33	a	617	IHT	C20-C15-C12	2.29	118.59	114.36
29	a	611	CLA	C1-C2-C3	-2.29	122.09	126.04
29	d	606	CLA	CHC-C1C-C2C	-2.29	120.38	126.73
31	c	618	II0	C20-C14-C12	2.29	118.59	114.36
33	K	104	IHT	C14-C02-C07	2.29	114.01	110.30
29	K	102	CLA	CHC-C1C-NC	2.29	127.67	124.20
35	A	851	LHG	O8-C23-C24	2.29	119.08	111.91
30	c	615	KC2	CHD-C4C-NC	2.29	127.67	124.20
29	4	610	CLA	CHC-C1C-C2C	-2.29	120.38	126.73
29	B	833	CLA	CHC-C1C-C2C	-2.28	120.38	126.73
30	c	610	KC2	CHD-C4C-NC	2.28	127.67	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	8	606	CLA	O2A-C1-C2	2.28	114.64	108.64
29	7	602	CLA	C2C-C1C-NC	2.28	112.11	109.97
29	9	602	CLA	CHD-C1D-C2D	2.28	130.27	125.48
29	A	814	CLA	CHC-C1C-C2C	-2.28	120.39	126.73
41	B	848	DGD	CDB-CCB-CBB	-2.28	102.83	114.42
41	Z	303	DGD	C1D-O6D-C5D	-2.28	109.20	113.69
29	1	603	CLA	CHC-C1C-C2C	-2.28	120.39	126.73
29	6	606	CLA	CHC-C1C-C2C	-2.28	120.39	126.73
35	2	618	LHG	O8-C23-C24	2.28	119.07	111.91
31	5	614	II0	C20-C14-C12	2.28	118.58	114.36
31	7	616	II0	C20-C14-C12	2.28	118.58	114.36
29	A	803	CLA	CHD-C1D-C2D	2.28	130.26	125.48
33	6	617	IHT	C22-C23-C27	-2.28	115.44	118.94
29	2	605	CLA	CHC-C1C-C2C	-2.28	120.40	126.73
30	6	610	KC2	CHC-C4B-NB	2.28	126.55	124.45
31	e	612	II0	C28-C26-C24	2.28	121.35	116.84
29	5	612	CLA	CHD-C1D-C2D	2.28	130.26	125.48
30	Z	307	KC2	CHD-C4C-NC	2.28	127.66	124.20
34	3	618	LMG	O2-C2-C1	-2.28	104.51	110.05
29	9	609	CLA	CHC-C1C-C2C	-2.28	120.41	126.73
29	e	601	CLA	CHC-C1C-C2C	-2.28	120.41	126.73
29	B	810	CLA	CHC-C4B-NB	-2.28	121.85	124.26
29	2	603	CLA	CHC-C1C-C2C	-2.28	120.41	126.73
29	L	207	CLA	CAA-C2A-C1A	-2.28	106.19	111.81
29	A	816	CLA	CHC-C1C-C2C	-2.28	120.41	126.73
29	c	609	CLA	CHC-C1C-C2C	-2.27	120.41	126.73
29	5	602	CLA	C2C-C1C-NC	2.27	112.10	109.97
29	A	809	CLA	C2C-C1C-NC	2.27	112.10	109.97
29	A	805	CLA	CHD-C1D-C2D	2.27	130.25	125.48
29	5	611	CLA	CHC-C1C-C2C	-2.27	120.41	126.73
29	6	612	CLA	CHC-C1C-C2C	-2.27	120.41	126.73
31	d	614	II0	C05-C07-C11	-2.27	107.19	110.30
33	1	618	IHT	C19-C10-C09	2.27	117.98	113.62
29	a	601	CLA	CHC-C1C-C2C	-2.27	120.42	126.73
29	1	605	CLA	CHC-C1C-C2C	-2.27	120.42	126.73
29	O	202	CLA	C2C-C1C-NC	2.27	112.10	109.97
31	4	612	II0	C41-C39-C35	-2.27	124.07	127.31
29	b	608	CLA	CHC-C1C-C2C	-2.27	120.42	126.73
29	Z	305	CLA	CHC-C1C-C2C	-2.27	120.42	126.73
29	A	812	CLA	CHC-C4B-NB	-2.27	121.85	124.26
29	F	203	CLA	CHC-C1C-C2C	-2.27	120.42	126.73
29	a	609	CLA	O2A-C1-C2	2.27	114.60	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	837	CLA	CHC-C1C-C2C	-2.27	120.42	126.73
30	2	610	KC2	CHC-C4B-NB	2.27	126.54	124.45
29	b	601	CLA	CHC-C1C-C2C	-2.27	120.43	126.73
29	K	101	CLA	CHC-C1C-C2C	-2.27	120.43	126.73
29	2	602	CLA	CHC-C4B-NB	-2.27	121.86	124.26
31	O	205	II0	C41-C39-C35	-2.27	124.07	127.31
31	1	616	II0	C20-C14-C12	2.27	118.56	114.36
29	A	812	CLA	CHA-C1A-NA	-2.27	121.20	126.40
29	B	804	CLA	CHC-C4B-NB	-2.27	121.86	124.26
29	B	807	CLA	CHC-C1C-C2C	-2.27	120.43	126.73
31	3	616	II0	C42-C41-C39	-2.27	118.83	123.47
29	4	602	CLA	C2C-C1C-NC	2.27	112.10	109.97
29	1	613	CLA	CHC-C1C-C2C	-2.27	120.43	126.73
29	1	604	CLA	CHC-C4B-NB	-2.27	121.86	124.26
29	A	809	CLA	CHD-C1D-C2D	2.27	130.23	125.48
29	5	601	CLA	CHC-C1C-C2C	-2.27	120.44	126.73
33	K	104	IHT	C40-C41-C38	-2.27	118.83	123.47
29	9	603	CLA	CHC-C1C-C2C	-2.27	120.44	126.73
29	c	607	CLA	CHC-C1C-C2C	-2.27	120.44	126.73
29	B	831	CLA	CHD-C1D-C2D	2.27	130.23	125.48
29	A	844	CLA	CBA-CAA-C2A	2.26	120.55	113.86
35	c	621	LHG	C11-C10-C9	-2.26	102.93	114.42
31	2	613	II0	C06-C08-C12	-2.26	107.20	110.30
31	e	614	II0	C42-C41-C39	-2.26	118.84	123.47
29	b	611	CLA	CHC-C4B-NB	-2.26	121.86	124.26
29	B	825	CLA	CHC-C1C-C2C	-2.26	120.44	126.73
29	A	809	CLA	C3A-C2A-C1A	-2.26	97.95	101.34
29	7	609	CLA	CHC-C1C-C2C	-2.26	120.44	126.73
29	Z	306	CLA	CHC-C1C-C2C	-2.26	120.44	126.73
29	c	601	CLA	C2C-C1C-NC	2.26	112.09	109.97
29	1	608	CLA	CHD-C4C-C3C	-2.26	121.52	124.84
29	9	607	CLA	CHC-C4B-NB	-2.26	121.86	124.26
29	A	844	CLA	CHD-C1D-C2D	2.26	130.22	125.48
29	A	824	CLA	C2C-C1C-NC	2.26	112.09	109.97
33	L	205	IHT	C09-C10-C07	-2.26	119.45	122.73
29	B	827	CLA	CHC-C1C-C2C	-2.26	120.45	126.73
34	3	618	LMG	O3-C3-C2	-2.26	105.13	110.35
29	L	203	CLA	C1-C2-C3	-2.26	122.14	126.04
29	8	605	CLA	CHC-C4B-NB	-2.26	121.87	124.26
29	d	607	CLA	CHC-C4B-NB	-2.26	121.87	124.26
30	6	613	KC2	CHD-C4C-NC	2.26	127.63	124.20
29	6	602	CLA	CHC-C4B-NB	-2.26	121.87	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	829	CLA	CHC-C4B-NB	-2.26	121.87	124.26
30	7	606	KC2	CHB-C4A-NA	2.26	127.76	124.20
29	Z	301	CLA	C2C-C1C-NC	2.26	112.08	109.97
29	d	602	CLA	C2C-C1C-NC	2.26	112.08	109.97
29	d	607	CLA	C2C-C1C-NC	2.26	112.08	109.97
29	e	606	CLA	C2C-C1C-NC	2.26	112.08	109.97
29	a	603	CLA	CHC-C1C-C2C	-2.26	120.47	126.73
30	9	610	KC2	CHB-C4A-NA	2.25	127.76	124.20
29	9	612	CLA	CHC-C1C-C2C	-2.25	120.47	126.73
29	B	836	CLA	CHC-C1C-C2C	-2.25	120.47	126.73
29	A	844	CLA	CHA-C1A-NA	-2.25	121.24	126.40
32	1	615	II3	C21-C24-C26	-2.25	115.48	118.94
29	7	605	CLA	CHC-C1C-C2C	-2.25	120.47	126.73
29	B	838	CLA	CHC-C4B-NB	-2.25	121.87	124.26
30	1	610	KC2	C4C-C3C-C2C	2.25	108.90	107.11
29	6	606	CLA	CHD-C1D-C2D	2.25	130.20	125.48
31	e	614	II0	C04-C10-C14	-2.25	119.46	122.63
31	1	617	II0	C20-C14-C12	2.25	118.52	114.36
29	e	611	CLA	CHA-C1A-NA	-2.25	121.25	126.40
29	B	834	CLA	CHC-C1C-C2C	-2.25	120.48	126.73
29	6	608	CLA	C1-C2-C3	-2.25	122.15	126.04
33	6	617	IHT	C04-C02-C07	-2.25	107.02	110.48
31	4	614	II0	C20-C14-C12	2.25	118.52	114.36
29	A	833	CLA	CHC-C1C-C2C	-2.25	120.49	126.73
35	3	619	LHG	C18-C17-C16	-2.25	103.02	114.42
29	3	610	CLA	CHC-C1C-C2C	-2.25	120.49	126.73
31	5	616	II0	C38-C36-C40	-2.25	119.78	122.92
29	e	603	CLA	CHC-C1C-C2C	-2.25	120.49	126.73
31	9	618	II0	C38-C36-C40	-2.25	119.78	122.92
29	B	825	CLA	C1-C2-C3	-2.25	122.16	126.04
29	A	810	CLA	CHC-C1C-C2C	-2.24	120.50	126.73
31	e	614	II0	C38-C36-C40	-2.24	119.78	122.92
32	b	613	II3	C37-C38-C40	-2.24	115.50	118.94
29	c	614	CLA	CHC-C1C-C2C	-2.24	120.50	126.73
29	a	607	CLA	CHC-C1C-C2C	-2.24	120.50	126.73
32	e	613	II3	C32-C33-C36	-2.24	115.50	118.94
29	a	611	CLA	CHC-C1C-C2C	-2.24	120.50	126.73
29	c	606	CLA	CHC-C1C-C2C	-2.24	120.50	126.73
31	8	611	II0	C41-C39-C35	-2.24	124.11	127.31
29	B	809	CLA	CHC-C1C-C2C	-2.24	120.51	126.73
29	B	838	CLA	CHC-C1C-C2C	-2.24	120.51	126.73
30	b	609	KC2	CHC-C4B-NB	2.24	126.51	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	613	CLA	CHC-C1C-C2C	-2.24	120.51	126.73
29	d	612	CLA	C1-C2-C3	-2.24	122.17	126.04
29	O	202	CLA	CHD-C1D-C2D	2.24	130.18	125.48
29	8	604	CLA	CHC-C1C-C2C	-2.24	120.51	126.73
32	e	613	II3	C31-C34-C37	-2.24	116.23	123.22
29	A	818	CLA	CHC-C1C-C2C	-2.24	120.51	126.73
30	c	615	KC2	CHC-C4B-NB	2.24	126.51	124.45
29	e	610	CLA	C1-C2-C3	-2.24	122.17	126.04
30	1	610	KC2	CHD-C4C-NC	2.24	127.60	124.20
33	1	618	IHT	C25-C23-C27	-2.24	119.79	122.92
34	8	614	LMG	O3-C3-C2	-2.24	105.18	110.35
29	A	822	CLA	CHC-C1C-C2C	-2.24	120.52	126.73
29	A	823	CLA	CHC-C1C-C2C	-2.24	120.52	126.73
29	7	611	CLA	CHC-C1C-C2C	-2.24	120.52	126.73
29	9	614	CLA	CHC-C1C-C2C	-2.24	120.52	126.73
29	B	819	CLA	CHC-C1C-C2C	-2.24	120.52	126.73
29	A	819	CLA	CHC-C1C-C2C	-2.23	120.53	126.73
29	d	603	CLA	CHC-C1C-C2C	-2.23	120.53	126.73
29	1	601	CLA	CHD-C1D-C2D	2.23	130.16	125.48
29	4	603	CLA	CHC-C1C-C2C	-2.23	120.53	126.73
31	a	615	II0	C34-C36-C40	-2.23	115.52	118.94
29	8	615	CLA	CHC-C1C-C2C	-2.23	120.53	126.73
29	e	608	CLA	CHC-C1C-C2C	-2.23	120.53	126.73
31	a	619	II0	C41-C39-C35	-2.23	124.12	127.31
29	9	606	CLA	CHD-C1D-C2D	2.23	130.16	125.48
31	O	205	II0	C06-C08-C12	-2.23	107.25	110.30
34	3	620	LMG	O1-C7-C8	-2.23	105.52	110.90
31	O	205	II0	C20-C14-C12	2.23	118.49	114.36
29	8	601	CLA	CHC-C1C-C2C	-2.23	120.54	126.73
29	B	815	CLA	CHC-C4B-NB	-2.23	121.90	124.26
29	A	829	CLA	CHC-C1C-C2C	-2.23	120.54	126.73
31	7	615	II0	C41-C42-C40	-2.23	118.91	123.47
29	A	803	CLA	CHC-C1C-C2C	-2.23	120.54	126.73
29	B	840	CLA	CHC-C1C-C2C	-2.23	120.54	126.73
32	1	615	II3	C39-C41-C40	-2.23	118.91	123.47
34	6	619	LMG	O2-C2-C1	-2.23	104.64	110.05
29	2	611	CLA	CHC-C1C-C2C	-2.23	120.55	126.73
29	A	819	CLA	CHD-C1D-C2D	2.23	130.15	125.48
29	Z	301	CLA	O2A-C1-C2	2.23	114.48	108.64
29	5	608	CLA	CHD-C4C-C3C	-2.22	121.57	124.84
29	B	803	CLA	CHD-C1D-C2D	2.22	130.15	125.48
30	3	606	KC2	CHD-C4C-NC	2.22	127.58	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	814	CLA	CHD-C1D-C2D	2.22	130.15	125.48
29	B	821	CLA	CHC-C1C-C2C	-2.22	120.55	126.73
29	B	819	CLA	CBA-CAA-C2A	2.22	120.43	113.86
29	A	804	CLA	CHC-C1C-C2C	-2.22	120.55	126.73
29	d	602	CLA	CHD-C4C-C3C	-2.22	121.57	124.84
29	1	606	CLA	CHC-C1C-C2C	-2.22	120.56	126.73
29	1	607	CLA	CHC-C4B-NB	-2.22	121.91	124.26
31	c	619	II0	C38-C36-C40	-2.22	119.81	122.92
29	2	608	CLA	CHD-C4C-C3C	-2.22	121.58	124.84
30	7	606	KC2	CHC-C4B-NB	2.22	126.50	124.45
29	A	838	CLA	CHC-C1C-C2C	-2.22	120.56	126.73
29	3	602	CLA	C2C-C1C-NC	2.22	112.05	109.97
29	c	606	CLA	CHC-C4B-NB	-2.22	121.91	124.26
29	c	602	CLA	C2C-C1C-NC	2.22	112.05	109.97
29	9	607	CLA	C1-C2-C3	-2.22	122.20	126.04
29	F	202	CLA	CHC-C4B-NB	-2.22	121.91	124.26
35	3	619	LHG	C20-C19-C18	-2.22	103.16	114.42
29	9	613	CLA	CHC-C1C-C2C	-2.22	120.57	126.73
33	K	104	IHT	C41-C40-C37	-2.22	118.93	123.47
29	B	827	CLA	CHD-C1D-C2D	2.22	130.13	125.48
29	d	612	CLA	CHC-C1C-C2C	-2.22	120.57	126.73
29	B	805	CLA	CHC-C1C-C2C	-2.22	120.58	126.73
31	4	613	II0	C06-C08-C12	-2.22	107.27	110.30
31	9	616	II0	C41-C39-C35	-2.21	124.15	127.31
29	B	834	CLA	C2C-C1C-NC	2.21	112.05	109.97
29	R	202	CLA	C2C-C1C-NC	2.21	112.05	109.97
29	8	608	CLA	CHD-C1D-C2D	2.21	130.12	125.48
29	5	603	CLA	CHC-C1C-C2C	-2.21	120.58	126.73
29	A	831	CLA	CHC-C1C-C2C	-2.21	120.58	126.73
29	1	601	CLA	CHC-C1C-C2C	-2.21	120.59	126.73
29	6	607	CLA	CHC-C1C-C2C	-2.21	120.59	126.73
29	B	804	CLA	CHD-C1D-C2D	2.21	130.12	125.48
29	A	815	CLA	CHC-C1C-C2C	-2.21	120.59	126.73
31	3	614	II0	C33-C35-C39	-2.21	115.55	118.94
29	B	814	CLA	CHD-C1D-C2D	2.21	130.12	125.48
29	B	841	CLA	CHC-C1C-C2C	-2.21	120.59	126.73
31	c	616	II0	C38-C36-C40	-2.21	119.83	122.92
29	a	606	CLA	CHD-C1D-C2D	2.21	130.11	125.48
29	B	824	CLA	CHC-C4B-NB	-2.21	121.92	124.26
31	4	612	II0	C38-C36-C40	-2.21	119.83	122.92
29	5	607	CLA	CHC-C1C-C2C	-2.21	120.60	126.73
29	b	611	CLA	CHC-C1C-C2C	-2.21	120.60	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	6	611	CLA	CHC-C1C-C2C	-2.21	120.60	126.73
29	A	834	CLA	CHC-C4B-NB	-2.21	121.92	124.26
29	c	605	CLA	CHC-C1C-C2C	-2.21	120.60	126.73
41	Z	303	DGD	C4E-C3E-C2E	-2.21	106.97	110.82
29	B	813	CLA	CHC-C1C-C2C	-2.21	120.60	126.73
29	3	610	CLA	CHD-C1D-C2D	2.21	130.10	125.48
41	B	848	DGD	C1D-C2D-C3D	-2.20	105.40	110.00
29	B	816	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
31	c	618	II0	C19-C13-C09	-2.20	121.35	124.35
29	1	613	CLA	CHD-C1D-C2D	2.20	130.10	125.48
29	7	603	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
29	7	607	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
29	B	823	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
29	A	829	CLA	CHC-C4B-NB	-2.20	121.92	124.26
29	b	602	CLA	CHD-C4C-C3C	-2.20	121.60	124.84
29	a	605	CLA	CHD-C1D-C2D	2.20	130.10	125.48
29	8	607	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
33	1	618	IHT	C02-C07-C18	-2.20	109.55	115.78
29	B	806	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
29	b	603	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
33	Z	302	IHT	C05-C08-C12	-2.20	107.29	110.30
33	a	617	IHT	C05-C08-C12	-2.20	107.29	110.30
29	2	612	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
29	A	805	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
29	B	808	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
29	c	601	CLA	CHD-C1D-C2D	2.20	130.10	125.48
29	A	827	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
31	7	615	II0	C20-C14-C12	2.20	118.43	114.36
34	2	617	LMG	O3-C3-C2	-2.20	105.26	110.35
29	e	611	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
30	e	605	KC2	CHD-C4C-NC	2.20	127.54	124.20
31	5	616	II0	C41-C39-C35	-2.20	124.17	127.31
30	9	610	KC2	C4C-C3C-C2C	2.20	108.86	107.11
29	b	611	CLA	CHD-C1D-C2D	2.20	130.09	125.48
29	A	834	CLA	CHC-C1C-C2C	-2.20	120.62	126.73
29	B	810	CLA	CHC-C1C-C2C	-2.20	120.62	126.73
29	2	612	CLA	CHD-C1D-C2D	2.20	130.09	125.48
29	7	607	CLA	CHD-C1D-C2D	2.20	130.09	125.48
29	a	605	CLA	CHC-C1C-C2C	-2.20	120.62	126.73
29	9	614	CLA	CHD-C1D-C2D	2.20	130.09	125.48
30	4	605	KC2	C4C-C3C-C2C	2.20	108.86	107.11
41	Z	303	DGD	CAB-C9B-C8B	-2.20	103.26	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	604	CLA	CHD-C1D-C2D	2.20	130.09	125.48
29	9	607	CLA	CHC-C1C-C2C	-2.20	120.62	126.73
29	Z	301	CLA	CHC-C4B-NB	-2.20	121.93	124.26
29	d	602	CLA	O2A-C1-C2	2.20	114.41	108.64
30	Z	307	KC2	CHC-C4B-NB	2.20	126.47	124.45
29	A	840	CLA	CHD-C1D-C2D	2.20	130.09	125.48
29	A	808	CLA	CHC-C1C-C2C	-2.20	120.63	126.73
29	8	605	CLA	CHB-C4A-NA	2.20	127.55	124.51
35	3	623	LHG	C11-C10-C9	-2.20	103.27	114.42
29	c	604	CLA	C2C-C1C-NC	2.20	112.03	109.97
29	3	611	CLA	CHC-C1C-C2C	-2.20	120.63	126.73
30	e	609	KC2	CHD-C4C-NC	2.20	127.53	124.20
29	c	612	CLA	CHD-C1D-C2D	2.20	130.09	125.48
29	b	610	CLA	CHC-C1C-C2C	-2.19	120.63	126.73
29	K	102	CLA	C2C-C1C-NC	2.19	112.03	109.97
29	4	603	CLA	CHD-C1D-C2D	2.19	130.08	125.48
29	B	830	CLA	CHD-C1D-C2D	2.19	130.08	125.48
31	c	617	II0	C05-C07-C11	-2.19	107.30	110.30
31	2	614	II0	C20-C14-C12	2.19	118.42	114.36
29	A	808	CLA	CHD-C1D-C2D	2.19	130.08	125.48
29	d	607	CLA	CHD-C1D-C2D	2.19	130.08	125.48
29	2	609	CLA	CHC-C1C-C2C	-2.19	120.64	126.73
29	B	805	CLA	CHD-C1D-C2D	2.19	130.08	125.48
29	A	802	CLA	CHC-C1C-C2C	-2.19	120.64	126.73
29	B	818	CLA	CHD-C1D-C2D	2.19	130.08	125.48
29	c	608	CLA	CHD-C4C-C3C	-2.19	121.62	124.84
29	b	604	CLA	C2C-C1C-NC	2.19	112.03	109.97
29	c	612	CLA	O2A-C1-C2	2.19	114.40	108.64
29	5	608	CLA	CHD-C1D-C2D	2.19	130.08	125.48
29	1	611	CLA	CHC-C1C-C2C	-2.19	120.64	126.73
29	3	605	CLA	CHD-C1D-C2D	2.19	130.08	125.48
29	e	604	CLA	CHC-C1C-C2C	-2.19	120.64	126.73
29	4	606	CLA	CHD-C1D-C2D	2.19	130.08	125.48
29	a	607	CLA	CHD-C1D-C2D	2.19	130.08	125.48
29	3	609	CLA	CHC-C1C-C2C	-2.19	120.64	126.73
29	9	605	CLA	CHC-C1C-C2C	-2.19	120.64	126.73
29	B	803	CLA	CHB-C4A-NA	2.19	127.54	124.51
29	B	826	CLA	CHD-C1D-C2D	2.19	130.07	125.48
29	B	837	CLA	CHD-C1D-C2D	2.19	130.07	125.48
31	3	616	II0	C38-C36-C40	-2.19	119.86	122.92
29	2	601	CLA	CHC-C1C-C2C	-2.19	120.65	126.73
35	A	851	LHG	C11-C10-C9	-2.19	103.31	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	9	604	CLA	CHC-C1C-C2C	-2.19	120.65	126.73
29	B	812	CLA	C2C-C1C-NC	2.19	112.02	109.97
29	A	818	CLA	CHD-C1D-C2D	2.19	130.07	125.48
29	F	202	CLA	CHD-C1D-C2D	2.19	130.07	125.48
29	7	612	CLA	CHC-C1C-C2C	-2.19	120.66	126.73
30	b	605	KC2	CHD-C4C-NC	2.19	127.52	124.20
29	b	606	CLA	CHC-C1C-C2C	-2.19	120.66	126.73
38	e	617	LMU	C6B-C5B-C4B	-2.19	107.89	113.00
29	B	810	CLA	CHD-C1D-C2D	2.19	130.06	125.48
29	9	608	CLA	CHC-C4B-NB	-2.18	121.94	124.26
29	3	607	CLA	CHD-C1D-C2D	2.18	130.06	125.48
29	B	829	CLA	CHC-C1C-C2C	-2.18	120.66	126.73
29	B	838	CLA	C1-C2-C3	-2.18	122.27	126.04
29	A	817	CLA	CHD-C1D-C2D	2.18	130.06	125.48
29	O	201	CLA	CHD-C1D-C2D	2.18	130.06	125.48
29	5	612	CLA	CHC-C4B-NB	-2.18	121.95	124.26
29	B	815	CLA	C1-C2-C3	-2.18	122.27	126.04
29	B	837	CLA	CHC-C1C-C2C	-2.18	120.67	126.73
29	8	603	CLA	CHD-C1D-C2D	2.18	130.06	125.48
29	B	817	CLA	CHD-C1D-C2D	2.18	130.06	125.48
29	A	829	CLA	CHD-C1D-C2D	2.18	130.06	125.48
29	J	102	CLA	CHD-C1D-C2D	2.18	130.06	125.48
29	3	601	CLA	CHC-C1C-C2C	-2.18	120.67	126.73
29	B	818	CLA	CHC-C1C-C2C	-2.18	120.67	126.73
29	a	612	CLA	C2C-C1C-NC	2.18	112.01	109.97
35	4	619	LHG	C27-C26-C25	-2.18	103.36	114.42
29	A	813	CLA	CHD-C1D-C2D	2.18	130.05	125.48
29	5	612	CLA	CHC-C1C-C2C	-2.18	120.68	126.73
29	9	611	CLA	CHC-C1C-C2C	-2.18	120.68	126.73
38	4	618	LMU	O5B-C5B-C4B	2.18	113.65	109.69
29	O	203	CLA	CHD-C1D-C2D	2.18	130.05	125.48
29	e	610	CLA	CHC-C4B-NB	-2.18	121.95	124.26
29	L	201	CLA	O2A-C1-C2	2.18	114.36	108.64
29	6	603	CLA	CHD-C1D-C2D	2.18	130.05	125.48
29	A	820	CLA	CHC-C1C-C2C	-2.18	120.68	126.73
29	2	607	CLA	CHC-C1C-C2C	-2.18	120.68	126.73
29	2	607	CLA	CHD-C1D-C2D	2.18	130.05	125.48
29	6	605	CLA	CHC-C1C-C2C	-2.18	120.68	126.73
29	O	201	CLA	CHC-C1C-C2C	-2.18	120.68	126.73
33	d	617	IHT	C30-C27-C23	-2.18	124.20	127.31
32	b	613	II3	C32-C33-C36	-2.18	115.60	118.94
29	6	604	CLA	CHD-C1D-C2D	2.18	130.04	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	842	CLA	CHD-C1D-C2D	2.18	130.04	125.48
29	b	610	CLA	CHD-C1D-C2D	2.18	130.04	125.48
29	1	607	CLA	CHC-C1C-C2C	-2.18	120.69	126.73
30	e	609	KC2	CHB-C4A-NA	2.18	127.63	124.20
29	a	612	CLA	CHC-C4B-NB	-2.18	121.95	124.26
29	3	604	CLA	CHC-C1C-C2C	-2.18	120.69	126.73
31	9	618	II0	C19-C13-C09	-2.18	121.39	124.35
29	8	615	CLA	C1-C2-C3	-2.18	122.28	126.04
29	O	202	CLA	CHC-C1C-C2C	-2.17	120.69	126.73
29	2	611	CLA	CHD-C1D-C2D	2.17	130.04	125.48
29	1	604	CLA	CHC-C1C-C2C	-2.17	120.69	126.73
29	c	603	CLA	CHA-C1A-NA	-2.17	121.42	126.40
29	2	604	CLA	CHD-C1D-C2D	2.17	130.03	125.48
29	6	602	CLA	CHA-C1A-NA	-2.17	121.42	126.40
29	J	102	CLA	CHC-C1C-C2C	-2.17	120.70	126.73
29	B	839	CLA	CHC-C1C-C2C	-2.17	120.70	126.73
31	a	619	II0	C38-C36-C40	-2.17	119.88	122.92
30	c	615	KC2	C4C-C3C-C2C	2.17	108.84	107.11
31	b	614	II0	C41-C39-C35	-2.17	124.21	127.31
29	a	606	CLA	CHC-C1C-C2C	-2.17	120.70	126.73
29	3	608	CLA	C2C-C1C-NC	2.17	112.00	109.97
29	A	807	CLA	CHD-C1D-C2D	2.17	130.03	125.48
34	3	620	LMG	O3-C3-C2	-2.17	105.34	110.35
31	a	614	II0	C38-C36-C40	-2.17	119.89	122.92
29	A	841	CLA	CHD-C1D-C2D	2.17	130.03	125.48
29	9	602	CLA	CAA-C2A-C1A	-2.17	104.87	111.97
34	3	618	LMG	C1-O6-C5	-2.17	109.43	113.69
33	K	104	IHT	C31-C34-C35	-2.17	120.33	126.42
29	4	611	CLA	CHD-C1D-C2D	2.17	130.03	125.48
29	L	203	CLA	CHD-C1D-C2D	2.17	130.03	125.48
33	L	205	IHT	C27-C30-C32	-2.17	116.45	123.22
38	J	104	LMU	C6B-C5B-C4B	-2.17	107.93	113.00
29	5	602	CLA	CHD-C1D-C2D	2.17	130.02	125.48
29	B	824	CLA	CHD-C1D-C2D	2.17	130.02	125.48
35	4	619	LHG	C11-C10-C9	-2.17	103.43	114.42
29	b	603	CLA	CHD-C1D-C2D	2.17	130.02	125.48
29	d	601	CLA	CHD-C1D-C2D	2.17	130.02	125.48
29	3	602	CLA	CHC-C4B-NB	-2.17	121.96	124.26
29	e	601	CLA	CHD-C1D-C2D	2.17	130.02	125.48
29	A	813	CLA	CHC-C1C-C2C	-2.16	120.72	126.73
29	B	840	CLA	CHD-C1D-C2D	2.16	130.02	125.48
29	8	615	CLA	CHD-C1D-C2D	2.16	130.02	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	821	CLA	CHC-C1C-C2C	-2.16	120.72	126.73
29	7	605	CLA	CHD-C1D-C2D	2.16	130.02	125.48
29	8	606	CLA	CHD-C1D-C2D	2.16	130.02	125.48
29	9	605	CLA	CHD-C1D-C2D	2.16	130.01	125.48
29	a	602	CLA	CBA-CAA-C2A	2.16	120.25	113.86
29	e	607	CLA	CHD-C1D-C2D	2.16	130.01	125.48
29	B	830	CLA	CHC-C1C-C2C	-2.16	120.72	126.73
31	e	615	II0	C42-C41-C39	-2.16	119.05	123.47
29	A	827	CLA	CHD-C1D-C2D	2.16	130.01	125.48
29	a	601	CLA	CHD-C1D-C2D	2.16	130.01	125.48
29	a	611	CLA	CHD-C1D-C2D	2.16	130.01	125.48
31	7	615	II0	C31-C33-C35	-2.16	120.34	126.42
31	1	614	II0	C41-C39-C35	-2.16	124.23	127.31
35	Z	310	LHG	C11-C10-C9	-2.16	103.45	114.42
29	R	202	CLA	CHC-C4B-NB	-2.16	121.97	124.26
29	A	816	CLA	CHD-C1D-C2D	2.16	130.01	125.48
31	1	619	II0	C41-C39-C35	-2.16	124.23	127.31
29	A	843	CLA	CHD-C1D-C2D	2.16	130.01	125.48
35	b	616	LHG	C20-C19-C18	-2.16	103.46	114.42
29	A	825	CLA	CHD-C4C-C3C	-2.16	121.67	124.84
30	5	610	KC2	CHD-C4C-NC	2.16	127.48	124.20
29	L	201	CLA	CHD-C1D-C2D	2.16	130.01	125.48
29	1	608	CLA	CHC-C4B-NB	-2.16	121.97	124.26
29	d	611	CLA	CHD-C1D-C2D	2.16	130.01	125.48
29	F	203	CLA	CHD-C1D-C2D	2.16	130.00	125.48
29	4	604	CLA	CHC-C1C-C2C	-2.16	120.74	126.73
30	2	610	KC2	CHD-C4C-NC	2.16	127.47	124.20
29	2	603	CLA	CHD-C1D-C2D	2.16	130.00	125.48
29	d	608	CLA	CHD-C1D-C2D	2.16	130.00	125.48
29	A	825	CLA	CHC-C4B-NB	-2.16	121.97	124.26
29	b	602	CLA	CHC-C4B-NB	-2.16	121.97	124.26
29	d	607	CLA	CHC-C1C-C2C	-2.16	120.74	126.73
29	e	610	CLA	CHD-C1D-C2D	2.16	130.00	125.48
30	7	606	KC2	CHD-C4C-NC	2.16	127.47	124.20
29	8	605	CLA	C2C-C1C-NC	2.16	111.99	109.97
29	A	826	CLA	CHD-C1D-C2D	2.16	130.00	125.48
29	2	602	CLA	CAA-C2A-C3A	2.15	118.68	112.78
29	1	613	CLA	CHC-C4B-NB	-2.15	121.98	124.26
29	B	811	CLA	CHD-C1D-C2D	2.15	130.00	125.48
29	c	601	CLA	CHC-C4B-NB	-2.15	121.98	124.26
29	B	841	CLA	CHD-C1D-C2D	2.15	130.00	125.48
29	B	814	CLA	CHC-C1C-C2C	-2.15	120.75	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	601	CLA	CHC-C1C-C2C	-2.15	120.75	126.73
30	e	605	KC2	CHB-C4A-NA	2.15	127.60	124.20
29	B	826	CLA	CHC-C1C-C2C	-2.15	120.75	126.73
29	2	601	CLA	CHD-C1D-C2D	2.15	129.99	125.48
29	R	202	CLA	CHB-C4A-NA	2.15	127.49	124.51
29	6	609	CLA	CHD-C1D-C2D	2.15	129.99	125.48
29	B	835	CLA	CHD-C1D-C2D	2.15	129.99	125.48
41	B	848	DGD	O6E-C1E-O5D	-2.15	104.88	109.97
29	L	203	CLA	CHC-C1C-C2C	-2.15	120.75	126.73
30	a	610	KC2	C4C-C3C-C2C	2.15	108.82	107.11
29	b	601	CLA	CHD-C1D-C2D	2.15	129.99	125.48
29	2	609	CLA	CHD-C1D-C2D	2.15	129.99	125.48
29	5	604	CLA	CHD-C1D-C2D	2.15	129.99	125.48
29	B	802	CLA	CHD-C1D-C2D	2.15	129.99	125.48
33	2	616	IHT	C25-C23-C27	-2.15	119.91	122.92
29	B	832	CLA	CHD-C1D-C2D	2.15	129.99	125.48
29	B	807	CLA	CHD-C1D-C2D	2.15	129.99	125.48
29	6	608	CLA	CHD-C4C-C3C	-2.15	121.68	124.84
29	A	839	CLA	CHC-C1C-C2C	-2.15	120.77	126.73
29	c	606	CLA	CHD-C1D-C2D	2.15	129.98	125.48
29	B	803	CLA	C2C-C1C-NC	2.15	111.98	109.97
29	9	612	CLA	CHD-C1D-C2D	2.15	129.98	125.48
29	B	817	CLA	CHC-C1C-C2C	-2.15	120.77	126.73
29	Z	304	CLA	CHC-C1C-C2C	-2.15	120.77	126.73
29	A	819	CLA	C1-C2-C3	-2.15	122.33	126.04
29	8	607	CLA	CHD-C1D-C2D	2.14	129.98	125.48
29	4	611	CLA	CHC-C1C-C2C	-2.14	120.77	126.73
29	B	820	CLA	CHC-C1C-C2C	-2.14	120.77	126.73
29	B	828	CLA	CHC-C1C-C2C	-2.14	120.77	126.73
29	L	201	CLA	CHC-C1C-C2C	-2.14	120.78	126.73
29	7	604	CLA	CHC-C1C-C2C	-2.14	120.78	126.73
29	3	603	CLA	CHD-C1D-C2D	2.14	129.97	125.48
34	I	102	LMG	C42-C41-C40	-2.14	103.55	114.42
29	1	601	CLA	CHC-C4B-NB	-2.14	121.99	124.26
29	a	606	CLA	CHC-C4B-NB	-2.14	121.99	124.26
31	7	615	II0	C41-C39-C35	-2.14	124.25	127.31
29	B	812	CLA	CHC-C1C-C2C	-2.14	120.78	126.73
29	9	604	CLA	CHD-C1D-C2D	2.14	129.97	125.48
34	2	617	LMG	O2-C2-C1	-2.14	104.85	110.05
29	Z	306	CLA	CHD-C1D-C2D	2.14	129.97	125.48
29	8	605	CLA	CHC-C1C-C2C	-2.14	120.79	126.73
29	e	606	CLA	O2A-C1-C2	2.14	114.26	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	603	CLA	CHC-C1C-C2C	-2.14	120.79	126.73
31	7	614	II0	C05-C07-C11	-2.14	107.38	110.30
35	B	849	LHG	C18-C17-C16	-2.14	103.57	114.42
29	B	828	CLA	CHD-C1D-C2D	2.14	129.97	125.48
29	B	836	CLA	CHD-C1D-C2D	2.14	129.97	125.48
34	6	619	LMG	O3-C3-C2	-2.14	105.41	110.35
29	B	834	CLA	CHD-C1D-C2D	2.14	129.96	125.48
29	1	613	CLA	CHA-C1A-NA	-2.14	121.50	126.40
29	9	607	CLA	CHD-C1D-C2D	2.14	129.96	125.48
29	e	603	CLA	CHD-C1D-C2D	2.14	129.96	125.48
29	4	607	CLA	CHC-C1C-C2C	-2.14	120.79	126.73
30	e	609	KC2	CHC-C4B-NB	2.14	126.42	124.45
29	B	838	CLA	CHD-C1D-C2D	2.14	129.96	125.48
29	A	822	CLA	CHC-C4B-NB	-2.14	122.00	124.26
29	9	609	CLA	CAA-C2A-C1A	-2.14	106.53	111.81
29	3	601	CLA	CHD-C1D-C2D	2.14	129.96	125.48
29	A	837	CLA	CHD-C1D-C2D	2.14	129.96	125.48
29	J	102	CLA	CAA-C2A-C1A	-2.14	106.53	111.81
29	7	601	CLA	CHD-C1D-C2D	2.13	129.96	125.48
29	9	612	CLA	CHC-C4B-NB	-2.13	122.00	124.26
29	A	832	CLA	CHC-C1C-C2C	-2.13	120.80	126.73
29	B	829	CLA	C2C-C1C-NC	2.13	111.97	109.97
29	A	830	CLA	CHC-C1C-C2C	-2.13	120.80	126.73
31	9	616	II0	C20-C14-C12	2.13	118.31	114.36
30	c	610	KC2	C1A-NA-C4A	2.13	107.67	106.71
30	b	609	KC2	CHB-C4A-NA	2.13	127.56	124.20
29	2	608	CLA	CHD-C1D-C2D	2.13	129.95	125.48
29	B	832	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	e	602	CLA	CHC-C1C-C2C	-2.13	120.81	126.73
29	7	612	CLA	CHD-C1D-C2D	2.13	129.95	125.48
29	B	822	CLA	CHB-C4A-NA	2.13	127.46	124.51
29	d	605	CLA	CHC-C1C-C2C	-2.13	120.81	126.73
34	6	619	LMG	O1-C7-C8	-2.13	105.76	110.90
29	A	803	CLA	CHC-C4B-NB	-2.13	122.00	124.26
31	9	618	II0	C06-C08-C12	-2.13	107.39	110.30
29	A	823	CLA	CHD-C4C-C3C	-2.13	121.71	124.84
29	7	604	CLA	CHD-C1D-C2D	2.13	129.95	125.48
29	A	835	CLA	CHD-C1D-C2D	2.13	129.95	125.48
29	A	823	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	A	834	CLA	CHD-C1D-C2D	2.13	129.95	125.48
30	9	610	KC2	CHC-C4B-NB	2.13	126.41	124.45
29	e	602	CLA	CHD-C1D-C2D	2.13	129.94	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	e	614	II0	C41-C42-C40	-2.13	119.12	123.47
29	B	816	CLA	CHD-C1D-C2D	2.13	129.94	125.48
29	B	806	CLA	CHC-C4B-NB	-2.13	122.00	124.26
29	A	825	CLA	CHC-C1C-C2C	-2.13	120.82	126.73
29	B	825	CLA	CHD-C1D-C2D	2.13	129.94	125.48
29	d	606	CLA	CHD-C1D-C2D	2.13	129.94	125.48
29	7	603	CLA	CHD-C1D-C2D	2.13	129.94	125.48
32	e	613	II3	C08-C03-C04	2.13	112.77	109.55
29	8	603	CLA	CHC-C1C-C2C	-2.13	120.83	126.73
29	2	605	CLA	CHD-C1D-C2D	2.13	129.94	125.48
35	b	616	LHG	C11-C10-C9	-2.13	103.64	114.42
29	d	609	CLA	CAA-C2A-C1A	-2.13	106.56	111.81
29	1	611	CLA	CHD-C1D-C2D	2.12	129.94	125.48
29	3	611	CLA	CHD-C1D-C2D	2.12	129.94	125.48
29	4	607	CLA	CHD-C1D-C2D	2.12	129.94	125.48
29	d	604	CLA	CHD-C1D-C2D	2.12	129.94	125.48
29	9	613	CLA	CHC-C4B-NB	-2.12	122.01	124.26
29	6	611	CLA	CHD-C1D-C2D	2.12	129.94	125.48
29	A	806	CLA	CHC-C1C-C2C	-2.12	120.83	126.73
29	A	803	CLA	CAA-C2A-C1A	-2.12	105.02	111.97
29	e	610	CLA	C2C-C1C-NC	2.12	111.96	109.97
29	a	603	CLA	CHD-C1D-C2D	2.12	129.93	125.48
30	7	610	KC2	CHD-C4C-NC	2.12	127.42	124.20
29	2	608	CLA	C1-C2-C3	-2.12	122.37	126.04
29	A	833	CLA	CHD-C1D-C2D	2.12	129.93	125.48
32	b	613	II3	C41-C39-C36	-2.12	119.13	123.47
29	B	819	CLA	CHD-C1D-C2D	2.12	129.93	125.48
30	7	610	KC2	CHB-C4A-NA	2.12	127.55	124.20
33	a	617	IHT	C39-C35-C38	-2.12	119.95	122.92
29	b	607	CLA	CHD-C1D-C2D	2.12	129.93	125.48
29	2	609	CLA	CHC-C4B-NB	-2.12	122.01	124.26
29	A	824	CLA	CHD-C1D-C2D	2.12	129.93	125.48
29	6	604	CLA	CHC-C1C-C2C	-2.12	120.84	126.73
29	Z	301	CLA	CHC-C1C-C2C	-2.12	120.84	126.73
34	3	620	LMG	O1-C1-C2	-2.12	105.00	108.30
29	2	604	CLA	C2C-C1C-NC	2.12	111.96	109.97
29	6	612	CLA	CHD-C1D-C2D	2.12	129.92	125.48
29	d	608	CLA	CHD-C4C-C3C	-2.12	121.73	124.84
29	B	806	CLA	C6-C7-C8	2.12	122.76	115.92
29	A	822	CLA	CHD-C1D-C2D	2.12	129.92	125.48
29	B	823	CLA	CHC-C4B-NB	-2.12	122.02	124.26
29	d	608	CLA	C2C-C1C-NC	2.12	111.95	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	613	II0	C20-C14-C12	2.12	118.27	114.36
30	Z	307	KC2	CHB-C4A-NA	2.12	127.54	124.20
29	A	801	CLA	CHC-C1C-C2C	-2.12	120.85	126.73
29	A	826	CLA	C2C-C1C-NC	2.11	111.95	109.97
29	6	601	CLA	CHD-C1D-C2D	2.11	129.91	125.48
29	b	606	CLA	CHD-C1D-C2D	2.11	129.91	125.48
29	B	824	CLA	CHC-C1C-C2C	-2.11	120.86	126.73
29	A	802	CLA	CHD-C1D-C2D	2.11	129.91	125.48
34	I	102	LMG	O2-C2-C1	-2.11	104.91	110.05
35	A	850	LHG	C11-C10-C9	-2.11	103.70	114.42
31	a	615	II0	C30-C32-C34	-2.11	116.62	123.22
29	3	607	CLA	CHC-C1C-C2C	-2.11	120.86	126.73
29	B	813	CLA	CBA-CAA-C2A	2.11	120.10	113.86
29	9	603	CLA	CHD-C1D-C2D	2.11	129.91	125.48
29	B	809	CLA	CHD-C1D-C2D	2.11	129.91	125.48
29	b	604	CLA	CHC-C1C-C2C	-2.11	120.86	126.73
29	2	606	CLA	CHD-C1D-C2D	2.11	129.91	125.48
29	B	822	CLA	CHD-C1D-C2D	2.11	129.91	125.48
29	L	202	CLA	CHD-C1D-C2D	2.11	129.91	125.48
29	e	610	CLA	CHC-C1C-C2C	-2.11	120.87	126.73
29	1	603	CLA	CHD-C1D-C2D	2.11	129.91	125.48
29	1	609	CLA	CHD-C1D-C2D	2.11	129.91	125.48
32	e	613	II3	C29-C26-C24	-2.11	124.30	127.31
29	B	806	CLA	C1-C2-C3	-2.11	122.39	126.04
29	A	827	CLA	CHA-C1A-NA	-2.11	121.56	126.40
29	b	603	CLA	CHC-C4B-NB	-2.11	122.02	124.26
29	3	608	CLA	CHD-C1D-C2D	2.11	129.91	125.48
29	1	601	CLA	CHA-C1A-NA	-2.11	121.57	126.40
29	b	602	CLA	CHA-C1A-NA	-2.11	121.57	126.40
29	e	602	CLA	CHD-C4C-C3C	-2.11	121.74	124.84
34	I	102	LMG	C38-C37-C36	-2.11	103.72	114.42
29	A	805	CLA	CHC-C4B-NB	-2.11	122.02	124.26
29	2	602	CLA	C2C-C1C-NC	2.11	111.95	109.97
29	a	604	CLA	CHD-C1D-C2D	2.11	129.90	125.48
29	3	605	CLA	CHC-C1C-C2C	-2.11	120.87	126.73
29	B	802	CLA	CHC-C1C-C2C	-2.11	120.87	126.73
29	B	804	CLA	C2C-C1C-NC	2.11	111.95	109.97
29	1	606	CLA	CHD-C1D-C2D	2.11	129.90	125.48
29	A	832	CLA	CHD-C1D-C2D	2.11	129.90	125.48
29	9	609	CLA	CHD-C1D-C2D	2.11	129.90	125.48
35	4	617	LHG	C11-C10-C9	-2.11	103.73	114.42
29	8	601	CLA	CHD-C1D-C2D	2.11	129.90	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	820	CLA	CHD-C1D-C2D	2.11	129.90	125.48
33	2	616	IHT	C36-C33-C37	-2.11	119.97	122.92
29	Z	301	CLA	CHD-C1D-C2D	2.11	129.90	125.48
29	A	810	CLA	CHC-C4B-NB	-2.10	122.03	124.26
29	O	202	CLA	CHD-C4C-C3C	-2.10	121.75	124.84
31	6	616	II0	C32-C30-C26	-2.10	120.47	126.58
30	c	610	KC2	CHC-C4B-NB	2.10	126.39	124.45
29	5	606	CLA	CHD-C1D-C2D	2.10	129.89	125.48
29	c	607	CLA	CHD-C1D-C2D	2.10	129.89	125.48
29	F	202	CLA	CHC-C1C-C2C	-2.10	120.89	126.73
31	e	615	II0	C41-C39-C35	-2.10	124.31	127.31
29	b	604	CLA	CHC-C4B-NB	-2.10	122.03	124.26
29	7	602	CLA	CHD-C1D-C2D	2.10	129.89	125.48
29	d	603	CLA	CHD-C1D-C2D	2.10	129.89	125.48
29	5	607	CLA	CHD-C1D-C2D	2.10	129.89	125.48
29	7	608	CLA	CHD-C1D-C2D	2.10	129.89	125.48
29	3	610	CLA	C1-C2-C3	-2.10	122.41	126.04
31	3	613	II0	C42-C41-C39	-2.10	119.17	123.47
35	2	619	LHG	C27-C26-C25	-2.10	103.76	114.42
29	c	608	CLA	C2C-C1C-NC	2.10	111.94	109.97
29	5	605	CLA	CHC-C1C-C2C	-2.10	120.89	126.73
29	9	602	CLA	CHC-C1C-C2C	-2.10	120.89	126.73
29	A	841	CLA	CHC-C1C-C2C	-2.10	120.90	126.73
29	2	611	CLA	CHC-C4B-NB	-2.10	122.03	124.26
29	5	605	CLA	CHA-C1A-NA	-2.10	121.59	126.40
29	c	612	CLA	CHA-C1A-NA	-2.10	121.59	126.40
29	9	601	CLA	CHD-C1D-C2D	2.10	129.88	125.48
29	L	204	CLA	CHD-C1D-C2D	2.10	129.88	125.48
29	B	825	CLA	CHB-C4A-NA	2.10	127.42	124.51
29	a	612	CLA	CHD-C1D-C2D	2.10	129.88	125.48
33	6	617	IHT	C27-C30-C32	-2.10	116.67	123.22
29	B	820	CLA	CHD-C4C-C3C	-2.10	121.75	124.84
30	2	610	KC2	C4C-C3C-C2C	2.10	108.78	107.11
30	6	610	KC2	C4C-C3C-C2C	2.10	108.78	107.11
29	1	607	CLA	CHD-C1D-C2D	2.10	129.88	125.48
29	e	606	CLA	CHD-C1D-C2D	2.10	129.88	125.48
29	2	602	CLA	CHD-C1D-C2D	2.10	129.88	125.48
29	B	820	CLA	CHD-C1D-C2D	2.10	129.88	125.48
29	e	607	CLA	C2C-C1C-NC	2.10	111.94	109.97
29	A	801	CLA	C4D-CHA-C1A	-2.10	118.70	121.25
29	5	604	CLA	CHC-C1C-C2C	-2.10	120.91	126.73
29	A	806	CLA	CHD-C1D-C2D	2.10	129.88	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	603	CLA	CHD-C1D-C2D	2.10	129.88	125.48
29	A	812	CLA	CHC-C1C-C2C	-2.10	120.91	126.73
31	5	620	II0	C38-C36-C40	-2.10	119.99	122.92
29	O	203	CLA	CHA-C1A-NA	-2.10	121.60	126.40
29	3	608	CLA	C1-C2-C3	-2.09	122.42	126.04
29	R	202	CLA	CHA-C1A-NA	-2.09	121.60	126.40
29	A	801	CLA	C3D-C4D-ND	2.09	113.62	110.24
29	A	841	CLA	CAA-C2A-C1A	-2.09	105.11	111.97
30	5	610	KC2	C4C-C3C-C2C	2.09	108.78	107.11
31	1	617	II0	C38-C36-C40	-2.09	119.99	122.92
29	B	803	CLA	CHC-C1C-C2C	-2.09	120.92	126.73
29	A	836	CLA	CHD-C1D-C2D	2.09	129.87	125.48
29	b	608	CLA	CHD-C1D-C2D	2.09	129.87	125.48
29	c	603	CLA	CHD-C4C-C3C	-2.09	121.77	124.84
29	b	602	CLA	C2C-C1C-NC	2.09	111.93	109.97
30	d	610	KC2	CHD-C4C-NC	2.09	127.38	124.20
35	3	622	LHG	C11-C10-C9	-2.09	103.81	114.42
29	1	608	CLA	CHD-C1D-C2D	2.09	129.87	125.48
29	A	808	CLA	CAA-C2A-C1A	-2.09	105.12	111.97
29	5	609	CLA	CHD-C1D-C2D	2.09	129.86	125.48
29	4	602	CLA	CHD-C1D-C2D	2.09	129.86	125.48
29	a	612	CLA	CHC-C1C-C2C	-2.09	120.92	126.73
29	5	603	CLA	CAA-C2A-C1A	-2.09	105.13	111.97
29	6	604	CLA	CHC-C4B-NB	-2.09	122.05	124.26
33	c	620	IHT	C32-C33-C37	-2.09	115.74	118.94
29	d	612	CLA	CHD-C1D-C2D	2.09	129.86	125.48
30	7	606	KC2	C4C-C3C-C2C	2.09	108.77	107.11
30	Z	307	KC2	C4C-C3C-C2C	2.09	108.77	107.11
29	A	825	CLA	CHD-C1D-C2D	2.09	129.86	125.48
31	a	619	II0	C06-C08-C12	-2.09	107.45	110.30
29	F	204	CLA	CHA-C1A-NA	-2.09	121.62	126.40
33	6	617	IHT	C02-C07-C18	-2.09	109.88	115.78
31	c	618	II0	C41-C39-C35	-2.09	124.33	127.31
29	3	612	CLA	CHD-C1D-C2D	2.09	129.85	125.48
29	c	608	CLA	CHD-C1D-C2D	2.09	129.85	125.48
29	B	813	CLA	CHB-C4A-NA	2.09	127.40	124.51
30	c	611	KC2	CHB-C4A-NA	2.09	127.49	124.20
29	7	611	CLA	CHD-C1D-C2D	2.08	129.85	125.48
29	B	841	CLA	CHC-C4B-NB	-2.08	122.05	124.26
29	3	603	CLA	C2C-C1C-NC	2.08	111.92	109.97
31	1	619	II0	C19-C13-C11	2.08	118.22	114.36
29	A	815	CLA	CHD-C1D-C2D	2.08	129.85	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	606	CLA	CHC-C1C-NC	2.08	127.36	124.20
29	3	604	CLA	CHD-C1D-C2D	2.08	129.85	125.48
29	A	811	CLA	CHD-C1D-C2D	2.08	129.85	125.48
31	9	615	II0	C06-C04-C10	2.08	113.84	109.62
29	3	603	CLA	CHC-C1C-C2C	-2.08	120.94	126.73
29	1	612	CLA	CHD-C1D-C2D	2.08	129.85	125.48
31	b	612	II0	C20-C14-C12	2.08	118.21	114.36
29	A	826	CLA	CHA-C1A-NA	-2.08	121.63	126.40
29	c	608	CLA	CHC-C4B-NB	-2.08	122.05	124.26
29	7	602	CLA	CHC-C1C-C2C	-2.08	120.95	126.73
35	7	619	LHG	C27-C26-C25	-2.08	103.86	114.42
29	A	840	CLA	CHA-C1A-NA	-2.08	121.63	126.40
30	a	610	KC2	CHB-C4A-NA	2.08	127.48	124.20
29	1	602	CLA	CHC-C1C-C2C	-2.08	120.95	126.73
29	R	202	CLA	CHC-C1C-C2C	-2.08	120.95	126.73
29	B	832	CLA	CHC-C1C-C2C	-2.08	120.95	126.73
29	4	609	CLA	CHD-C1D-C2D	2.08	129.84	125.48
29	5	605	CLA	CHD-C1D-C2D	2.08	129.84	125.48
29	7	603	CLA	CHC-C4B-NB	-2.08	122.06	124.26
32	b	613	II3	C08-C03-C04	2.08	112.69	109.55
29	A	831	CLA	CHD-C1D-C2D	2.08	129.84	125.48
29	e	604	CLA	CHD-C1D-C2D	2.08	129.84	125.48
29	5	602	CLA	CHC-C4B-NB	-2.08	122.06	124.26
29	8	608	CLA	CHC-C1C-C2C	-2.08	120.96	126.73
29	c	609	CLA	CAA-C2A-C1A	-2.08	106.68	111.81
29	4	604	CLA	CHD-C1D-C2D	2.08	129.84	125.48
29	5	603	CLA	CHD-C1D-C2D	2.08	129.84	125.48
30	c	615	KC2	CHB-C4A-NA	2.08	127.48	124.20
29	2	606	CLA	CHC-C4B-NB	-2.08	122.06	124.26
29	7	602	CLA	CHC-C4B-NB	-2.08	122.06	124.26
29	B	839	CLA	CHC-C4B-NB	-2.08	122.06	124.26
29	K	102	CLA	CHD-C1D-C2D	2.08	129.83	125.48
30	6	613	KC2	C4C-C3C-C2C	2.08	108.76	107.11
29	B	815	CLA	CHD-C1D-C2D	2.08	129.83	125.48
29	Z	305	CLA	CHD-C1D-C2D	2.08	129.83	125.48
29	c	613	CLA	CHD-C1D-C2D	2.08	129.83	125.48
29	2	607	CLA	CHC-C4B-NB	-2.08	122.06	124.26
31	2	613	II0	C34-C36-C40	-2.07	115.76	118.94
29	B	823	CLA	CHA-C1A-NA	-2.07	121.65	126.40
29	L	203	CLA	CHC-C4B-NB	-2.07	122.06	124.26
29	6	601	CLA	CHC-C1C-NC	2.07	127.35	124.20
36	O	206	SQD	C4-C3-C2	-2.07	107.20	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	4	602	CLA	CHC-C4B-NB	-2.07	122.06	124.26
29	L	201	CLA	CHA-C1A-NA	-2.07	121.65	126.40
35	B	849	LHG	C11-C10-C9	-2.07	103.90	114.42
29	A	842	CLA	CHC-C1C-NC	2.07	127.35	124.20
29	c	602	CLA	CHD-C1D-C2D	2.07	129.83	125.48
29	d	602	CLA	CHC-C4B-NB	-2.07	122.06	124.26
29	B	839	CLA	CHD-C1D-C2D	2.07	129.83	125.48
31	9	615	II0	C05-C07-C11	-2.07	107.47	110.30
32	e	613	II3	C15-C07-C10	-2.07	119.13	123.56
34	F	205	LMG	O3-C3-C2	-2.07	105.56	110.35
29	c	602	CLA	CHC-C1C-C2C	-2.07	120.98	126.73
29	5	608	CLA	C2C-C1C-NC	2.07	111.91	109.97
29	b	608	CLA	CHA-C1A-NA	-2.07	121.66	126.40
29	A	834	CLA	C1-C2-C3	-2.07	122.46	126.04
29	A	830	CLA	CHD-C1D-C2D	2.07	129.82	125.48
29	e	608	CLA	CHD-C1D-C2D	2.07	129.82	125.48
29	9	613	CLA	CHD-C1D-C2D	2.07	129.82	125.48
32	1	615	II3	C15-C07-C10	-2.07	119.13	123.56
29	5	613	CLA	CHD-C1D-C2D	2.07	129.82	125.48
29	A	810	CLA	CHD-C1D-C2D	2.07	129.82	125.48
29	3	602	CLA	CHD-C1D-C2D	2.07	129.82	125.48
29	3	610	CLA	CAA-C2A-C1A	-2.07	105.20	111.97
34	F	205	LMG	O2-C2-C1	-2.07	105.03	110.05
29	B	835	CLA	CHC-C1C-C2C	-2.07	120.99	126.73
29	e	611	CLA	CHD-C1D-C2D	2.07	129.81	125.48
29	A	809	CLA	CHC-C4B-NB	-2.07	122.07	124.26
29	a	608	CLA	CHD-C1D-C2D	2.07	129.81	125.48
29	3	602	CLA	CHC-C1C-C2C	-2.06	120.99	126.73
29	A	817	CLA	CHC-C1C-C2C	-2.06	120.99	126.73
31	7	616	II0	C06-C08-C12	-2.06	107.48	110.30
35	B	849	LHG	C27-C26-C25	-2.06	103.95	114.42
29	J	102	CLA	CHC-C4B-NB	-2.06	122.07	124.26
29	4	608	CLA	CHD-C1D-C2D	2.06	129.81	125.48
35	Z	310	LHG	C27-C26-C25	-2.06	103.95	114.42
29	d	611	CLA	CHB-C4A-NA	2.06	127.36	124.51
29	8	615	CLA	CHC-C4B-NB	-2.06	122.07	124.26
29	1	604	CLA	CHD-C1D-C2D	2.06	129.81	125.48
29	4	610	CLA	CHD-C1D-C2D	2.06	129.81	125.48
29	c	605	CLA	CHD-C1D-C2D	2.06	129.81	125.48
35	3	619	LHG	C27-C26-C25	-2.06	103.95	114.42
31	5	617	II0	C32-C30-C26	-2.06	120.59	126.58
29	6	607	CLA	CHC-C4B-NB	-2.06	122.07	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	8	604	CLA	CHA-C1A-NA	-2.06	121.68	126.40
29	B	829	CLA	CHC-C1C-NC	2.06	127.33	124.20
41	Z	303	DGD	O2D-C2D-C1D	-2.06	105.04	110.05
29	6	607	CLA	CHD-C1D-C2D	2.06	129.80	125.48
29	Z	304	CLA	CHD-C1D-C2D	2.06	129.80	125.48
29	c	609	CLA	CHD-C1D-C2D	2.06	129.80	125.48
29	B	814	CLA	CHA-C1A-NA	-2.06	121.68	126.40
29	A	839	CLA	CHD-C1D-C2D	2.06	129.80	125.48
29	b	607	CLA	CHC-C1C-C2C	-2.06	121.01	126.73
29	5	611	CLA	CHD-C1D-C2D	2.06	129.80	125.48
29	A	838	CLA	CHD-C1D-C2D	2.06	129.80	125.48
29	B	806	CLA	CHD-C1D-C2D	2.06	129.80	125.48
29	B	833	CLA	CHD-C1D-C2D	2.06	129.80	125.48
29	A	812	CLA	CHD-C1D-C2D	2.06	129.80	125.48
31	J	101	II0	C31-C33-C35	-2.06	120.63	126.42
29	9	602	CLA	C2C-C1C-NC	2.06	111.90	109.97
38	e	617	LMU	C4B-C3B-C2B	2.06	114.42	110.82
29	B	837	CLA	CHC-C4B-NB	-2.06	122.08	124.26
29	5	602	CLA	CHC-C1C-C2C	-2.06	121.02	126.73
29	6	608	CLA	CHC-C1C-C2C	-2.06	121.02	126.73
29	B	804	CLA	CHC-C1C-C2C	-2.06	121.02	126.73
33	d	617	IHT	C40-C37-C33	-2.06	124.38	127.31
34	3	618	LMG	O7-C10-O9	-2.06	118.73	123.70
29	6	608	CLA	CHD-C1D-C2D	2.06	129.79	125.48
29	O	203	CLA	CHC-C1C-NC	2.06	127.32	124.20
29	7	604	CLA	C1-C2-C3	-2.06	122.49	126.04
29	9	611	CLA	CHD-C1D-C2D	2.05	129.79	125.48
29	8	604	CLA	CHC-C4B-NB	-2.05	122.08	124.26
29	B	812	CLA	CHC-C4B-NB	-2.05	122.08	124.26
35	3	623	LHG	C27-C26-C25	-2.05	104.00	114.42
29	4	601	CLA	CHD-C1D-C2D	2.05	129.79	125.48
29	B	831	CLA	CHC-C1C-C2C	-2.05	121.03	126.73
29	B	831	CLA	C2C-C1C-NC	2.05	111.89	109.97
29	A	809	CLA	CHC-C1C-C2C	-2.05	121.03	126.73
29	B	819	CLA	CHA-C1A-NA	-2.05	121.70	126.40
29	9	603	CLA	CHC-C4B-NB	-2.05	122.08	124.26
31	R	204	II0	C20-C14-C12	2.05	118.16	114.36
35	6	618	LHG	C5-O7-C7	-2.05	112.74	117.79
32	1	615	II3	C03-C04-C12	-2.05	110.11	112.70
33	9	619	IHT	C25-C23-C22	-2.05	114.85	118.08
29	B	812	CLA	CHD-C1D-C2D	2.05	129.78	125.48
34	3	620	LMG	O7-C10-O9	-2.05	118.75	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	602	CLA	CHD-C4C-C3C	-2.05	121.83	124.84
30	1	610	KC2	CHC-C1C-NC	2.05	127.43	124.20
29	9	601	CLA	CHC-C1C-NC	2.05	127.31	124.20
29	A	828	CLA	CHD-C1D-C2D	2.05	129.78	125.48
29	7	609	CLA	CHD-C1D-C2D	2.05	129.77	125.48
30	b	605	KC2	CHC-C1C-C2C	-2.05	121.78	124.98
29	A	806	CLA	CHA-C1A-NA	-2.05	121.71	126.40
29	e	607	CLA	CHC-C1C-C2C	-2.05	121.04	126.73
29	d	609	CLA	CHD-C1D-C2D	2.05	129.77	125.48
29	2	602	CLA	CAA-C2A-C1A	-2.05	105.27	111.97
29	c	607	CLA	CHC-C4B-NB	-2.05	122.09	124.26
29	9	606	CLA	CAA-C2A-C1A	-2.05	105.27	111.97
29	a	605	CLA	CAA-C2A-C1A	-2.05	105.27	111.97
34	8	614	LMG	C1-O6-C5	-2.05	109.67	113.69
29	c	604	CLA	CHC-C1C-C2C	-2.05	121.05	126.73
31	8	611	II0	C20-C14-C12	2.05	118.14	114.36
29	4	602	CLA	C1-C2-C3	-2.05	122.51	126.04
29	7	612	CLA	CHA-C1A-NA	-2.04	121.72	126.40
30	5	610	KC2	CHC-C4B-NB	2.04	126.33	124.45
29	9	609	CLA	CHC-C1C-NC	2.04	127.31	124.20
29	d	612	CLA	CHA-C1A-NA	-2.04	121.72	126.40
29	8	604	CLA	CHD-C4C-C3C	-2.04	121.83	124.84
29	e	611	CLA	CHC-C4B-NB	-2.04	122.09	124.26
31	1	617	II0	C31-C33-C35	-2.04	120.68	126.42
34	3	620	LMG	O2-C2-C1	-2.04	105.08	110.05
33	a	617	IHT	C27-C30-C32	-2.04	116.84	123.22
31	O	205	II0	C07-C11-C13	2.04	115.92	111.85
31	7	614	II0	C07-C11-C13	-2.04	107.79	111.85
29	2	603	CLA	CHC-C4B-NB	-2.04	122.10	124.26
31	e	612	II0	C41-C39-C35	-2.04	124.40	127.31
29	2	604	CLA	CHC-C1C-C2C	-2.04	121.06	126.73
29	4	602	CLA	CHC-C1C-C2C	-2.04	121.06	126.73
29	2	603	CLA	C1-C2-C3	-2.04	123.45	126.75
29	A	802	CLA	CHC-C4B-NB	-2.04	122.10	124.26
29	c	602	CLA	CHC-C4B-NB	-2.04	122.10	124.26
29	A	804	CLA	CHD-C1D-C2D	2.04	129.75	125.48
34	F	205	LMG	O1-C1-C2	-2.04	105.12	108.30
29	B	834	CLA	CHC-C1C-NC	2.04	127.30	124.20
35	A	850	LHG	C20-C19-C18	-2.04	104.08	114.42
29	e	606	CLA	CHA-C1A-NA	-2.04	121.73	126.40
29	7	602	CLA	CHD-C4C-C3C	-2.04	121.84	124.84
29	a	608	CLA	CHD-C4C-C3C	-2.04	121.84	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	612	CLA	CHC-C4B-NB	-2.04	122.10	124.26
29	A	807	CLA	CHC-C1C-NC	2.04	127.29	124.20
31	6	616	II0	C20-C14-C12	2.04	118.13	114.36
29	B	821	CLA	CHD-C1D-C2D	2.04	129.75	125.48
29	A	834	CLA	CBA-CAA-C2A	2.04	119.87	113.86
29	L	207	CLA	CHD-C1D-C2D	2.04	129.75	125.48
29	2	602	CLA	CHC-C1C-C2C	-2.04	121.07	126.73
33	5	618	IHT	C31-C34-C35	-2.04	120.70	126.42
29	Z	304	CLA	CHC-C4B-NB	-2.03	122.10	124.26
35	3	623	LHG	C20-C19-C18	-2.03	104.10	114.42
29	4	602	CLA	CHD-C4C-C3C	-2.03	121.85	124.84
29	b	607	CLA	CHD-C4C-C3C	-2.03	121.85	124.84
31	4	614	II0	C42-C41-C39	-2.03	119.31	123.47
29	B	820	CLA	CHC-C4B-NB	-2.03	122.11	124.26
29	d	608	CLA	CHC-C1C-C2C	-2.03	121.08	126.73
31	6	614	II0	C38-C36-C40	-2.03	120.08	122.92
29	e	606	CLA	CHC-C1C-C2C	-2.03	121.08	126.73
29	8	607	CLA	CAA-C2A-C1A	-2.03	106.79	111.81
31	2	615	II0	C19-C13-C11	2.03	118.12	114.36
29	F	202	CLA	C1-C2-C3	-2.03	122.53	126.04
31	8	616	II0	C38-C36-C34	2.03	121.28	118.08
29	3	611	CLA	CHC-C4B-NB	-2.03	122.11	124.26
30	3	606	KC2	CHB-C4A-NA	2.03	127.40	124.20
38	7	620	LMU	O2'-C2'-C3'	-2.03	105.65	110.35
31	R	204	II0	C42-C40-C36	-2.03	124.41	127.31
32	e	613	II3	C41-C39-C36	-2.03	119.31	123.47
29	3	608	CLA	CHC-C1C-C2C	-2.03	121.09	126.73
31	1	619	II0	C31-C33-C35	-2.03	120.71	126.42
31	1	614	II0	C05-C07-C11	-2.03	107.53	110.30
29	9	608	CLA	C2C-C1C-NC	2.03	111.87	109.97
30	b	605	KC2	C4C-C3C-C2C	2.03	108.73	107.11
31	d	616	II0	C19-C13-C09	-2.03	121.59	124.35
31	e	612	II0	C42-C41-C39	-2.03	119.32	123.47
29	5	612	CLA	CHB-C4A-NA	2.03	127.32	124.51
29	2	601	CLA	CHA-C1A-NA	-2.03	121.75	126.40
29	d	605	CLA	CHD-C1D-C2D	2.03	129.73	125.48
33	9	619	IHT	C31-C34-C35	-2.03	120.72	126.42
29	5	601	CLA	CHC-C4B-NB	-2.03	122.11	124.26
29	A	819	CLA	CHC-C4B-NB	-2.03	122.11	124.26
29	L	207	CLA	CHC-C4B-NB	-2.03	122.11	124.26
29	A	804	CLA	CHA-C1A-NA	-2.03	121.76	126.40
32	b	613	II3	C15-C07-C10	-2.03	119.22	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	204	CLA	CHC-C1C-NC	2.03	127.28	124.20
29	L	201	CLA	CHC-C4B-NB	-2.03	122.11	124.26
29	d	602	CLA	CHD-C1D-C2D	2.02	129.73	125.48
29	1	602	CLA	CHD-C1D-C2D	2.02	129.72	125.48
29	B	815	CLA	CHC-C1C-C2C	-2.02	121.11	126.73
31	R	204	II0	C31-C33-C35	-2.02	120.73	126.42
31	7	616	II0	C29-C31-C33	-2.02	116.90	123.22
29	d	606	CLA	CHC-C1C-NC	2.02	127.27	124.20
29	d	602	CLA	CHC-C1C-C2C	-2.02	121.11	126.73
29	B	808	CLA	CHD-C1D-C2D	2.02	129.72	125.48
29	9	611	CLA	CHC-C4B-NB	-2.02	122.12	124.26
29	F	204	CLA	CHD-C1D-C2D	2.02	129.72	125.48
29	b	602	CLA	CHD-C1D-C2D	2.02	129.72	125.48
32	1	615	II3	C41-C40-C38	-2.02	124.42	127.31
30	c	611	KC2	CHC-C1C-NC	2.02	127.39	124.20
30	3	606	KC2	C4B-CHC-C1C	-2.02	121.70	126.06
31	7	615	II0	C38-C36-C40	-2.02	120.09	122.92
29	4	611	CLA	CHA-C1A-NA	-2.02	121.77	126.40
31	e	612	II0	C05-C07-C11	-2.02	107.54	110.30
31	8	610	II0	C31-C33-C35	-2.02	120.74	126.42
30	b	609	KC2	CHD-C4C-NC	2.02	127.27	124.20
29	A	811	CLA	CHD-C4C-C3C	-2.02	121.88	124.84
31	5	616	II0	C19-C13-C09	-2.02	121.61	124.35
29	2	611	CLA	CHA-C1A-NA	-2.01	121.78	126.40
29	A	824	CLA	CHC-C1C-C2C	-2.01	121.14	126.73
29	8	604	CLA	CHD-C1D-C2D	2.01	129.70	125.48
29	B	807	CLA	CHC-C4B-NB	-2.01	122.12	124.26
29	6	611	CLA	CHD-C4C-C3C	-2.01	121.88	124.84
31	a	613	II0	C33-C35-C39	-2.01	115.85	118.94
29	9	614	CLA	CHA-C1A-NA	-2.01	121.79	126.40
38	O	207	LMU	C3'-C4'-C5'	-2.01	106.31	110.93
29	1	603	CLA	CHC-C1C-NC	2.01	127.26	124.20
29	9	608	CLA	CHD-C4C-C3C	-2.01	121.88	124.84
34	8	614	LMG	C38-C37-C36	-2.01	104.21	114.42
29	d	606	CLA	CAA-C2A-C1A	-2.01	106.84	111.81
29	b	604	CLA	CHD-C1D-C2D	2.01	129.70	125.48
29	B	838	CLA	CHC-C1C-NC	2.01	127.25	124.20
35	4	617	LHG	C15-C14-C13	-2.01	104.22	114.42
31	4	612	II0	C19-C13-C11	2.01	118.08	114.36
30	e	605	KC2	C4C-C3C-C2C	2.01	108.71	107.11
29	4	601	CLA	CHC-C1C-NC	2.01	127.25	124.20
29	6	605	CLA	CHD-C1D-C2D	2.01	129.69	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	7	618	LHG	C27-C26-C25	-2.01	104.24	114.42
33	8	609	IHT	C22-C23-C27	-2.01	115.86	118.94
31	9	616	II0	C19-C13-C09	-2.01	121.62	124.35
31	2	613	II0	C30-C32-C34	-2.00	116.96	123.22
30	9	610	KC2	CHC-C1C-NC	2.00	127.36	124.20
31	3	613	II0	C32-C30-C26	-2.00	120.76	126.58
31	a	613	II0	C20-C14-C12	2.00	118.07	114.36
29	a	603	CLA	CHA-C1A-NA	-2.00	121.81	126.40
34	8	614	LMG	O1-C7-C8	-2.00	106.06	110.90
29	4	607	CLA	CHD-C4C-C3C	-2.00	121.89	124.84
30	b	609	KC2	C4C-C3C-C2C	2.00	108.70	107.11
29	9	606	CLA	CHC-C1C-NC	2.00	127.24	124.20
31	9	616	II0	C06-C08-C12	-2.00	107.56	110.30
29	A	834	CLA	CHD-C4C-C3C	-2.00	121.90	124.84
29	d	604	CLA	CHC-C1C-C2C	-2.00	121.17	126.73
29	2	607	CLA	CHA-C1A-NA	-2.00	121.81	126.40
31	e	612	II0	C06-C08-C12	-2.00	107.56	110.30
29	e	608	CLA	CAA-C2A-C1A	-2.00	106.86	111.81
29	B	816	CLA	CHA-C1A-NA	-2.00	121.81	126.40
29	A	843	CLA	CHC-C1C-C2C	-2.00	121.17	126.73
29	9	608	CLA	CHD-C1D-C2D	2.00	129.68	125.48
29	B	839	CLA	CHA-C1A-NA	-2.00	121.82	126.40

There are no chirality outliers.

All (2649) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	1	603	CLA	C1A-C2A-CAA-CBA
29	1	605	CLA	C2B-C3B-CAB-CBB
29	1	605	CLA	C4B-C3B-CAB-CBB
29	2	601	CLA	C3A-C2A-CAA-CBA
29	2	601	CLA	CHA-CBD-CGD-O1D
29	2	601	CLA	CHA-CBD-CGD-O2D
29	2	602	CLA	C3A-C2A-CAA-CBA
29	2	602	CLA	CHA-CBD-CGD-O1D
29	2	602	CLA	CHA-CBD-CGD-O2D
29	2	603	CLA	C1A-C2A-CAA-CBA
29	2	605	CLA	C2B-C3B-CAB-CBB
29	2	605	CLA	C4B-C3B-CAB-CBB
29	2	607	CLA	C2B-C3B-CAB-CBB
29	2	607	CLA	C4B-C3B-CAB-CBB
29	2	608	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	2	608	CLA	C4B-C3B-CAB-CBB
29	2	611	CLA	CHA-CBD-CGD-O1D
29	2	611	CLA	CHA-CBD-CGD-O2D
29	2	612	CLA	C2B-C3B-CAB-CBB
29	2	612	CLA	C4B-C3B-CAB-CBB
29	3	601	CLA	C2B-C3B-CAB-CBB
29	3	601	CLA	C4B-C3B-CAB-CBB
29	3	602	CLA	CHA-CBD-CGD-O1D
29	3	602	CLA	CHA-CBD-CGD-O2D
29	3	604	CLA	CHA-CBD-CGD-O1D
29	3	604	CLA	CAD-CBD-CGD-O1D
29	3	608	CLA	C2B-C3B-CAB-CBB
29	3	608	CLA	C4B-C3B-CAB-CBB
29	3	612	CLA	CHA-CBD-CGD-O1D
29	4	604	CLA	CHA-CBD-CGD-O1D
29	4	604	CLA	CHA-CBD-CGD-O2D
29	4	604	CLA	CAD-CBD-CGD-O1D
29	4	608	CLA	O2A-C1-C2-C3
29	5	605	CLA	CHA-CBD-CGD-O1D
29	5	605	CLA	CHA-CBD-CGD-O2D
29	5	606	CLA	C1A-C2A-CAA-CBA
29	5	606	CLA	C3A-C2A-CAA-CBA
29	5	608	CLA	C3A-C2A-CAA-CBA
29	5	608	CLA	C2B-C3B-CAB-CBB
29	5	608	CLA	C4B-C3B-CAB-CBB
29	5	611	CLA	CAD-CBD-CGD-O1D
29	5	611	CLA	CAD-CBD-CGD-O2D
29	5	612	CLA	C2B-C3B-CAB-CBB
29	5	612	CLA	C4B-C3B-CAB-CBB
29	6	601	CLA	C2B-C3B-CAB-CBB
29	6	601	CLA	C4B-C3B-CAB-CBB
29	6	602	CLA	CHA-CBD-CGD-O1D
29	6	602	CLA	CHA-CBD-CGD-O2D
29	6	606	CLA	C1A-C2A-CAA-CBA
29	6	606	CLA	CHA-CBD-CGD-O1D
29	6	606	CLA	CHA-CBD-CGD-O2D
29	6	606	CLA	O2A-C1-C2-C3
29	6	608	CLA	C2B-C3B-CAB-CBB
29	6	608	CLA	C4B-C3B-CAB-CBB
29	6	609	CLA	C2B-C3B-CAB-CBB
29	6	609	CLA	C4B-C3B-CAB-CBB
29	6	612	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	6	612	CLA	C3A-C2A-CAA-CBA
29	6	612	CLA	C2B-C3B-CAB-CBB
29	6	612	CLA	C4B-C3B-CAB-CBB
29	7	601	CLA	C2B-C3B-CAB-CBB
29	7	601	CLA	C4B-C3B-CAB-CBB
29	7	602	CLA	CHA-CBD-CGD-O1D
29	7	602	CLA	CHA-CBD-CGD-O2D
29	7	605	CLA	C2B-C3B-CAB-CBB
29	7	605	CLA	C4B-C3B-CAB-CBB
29	7	608	CLA	C3A-C2A-CAA-CBA
29	7	612	CLA	C1A-C2A-CAA-CBA
29	7	612	CLA	CHA-CBD-CGD-O1D
29	8	603	CLA	C4B-C3B-CAB-CBB
29	8	604	CLA	C2B-C3B-CAB-CBB
29	8	604	CLA	C4B-C3B-CAB-CBB
29	9	602	CLA	C3A-C2A-CAA-CBA
29	9	602	CLA	C2B-C3B-CAB-CBB
29	9	602	CLA	C4B-C3B-CAB-CBB
29	9	608	CLA	C1A-C2A-CAA-CBA
29	9	608	CLA	C3A-C2A-CAA-CBA
29	9	608	CLA	C2B-C3B-CAB-CBB
29	9	608	CLA	C4-C3-C5-C6
29	A	801	CLA	C2B-C3B-CAB-CBB
29	A	801	CLA	C4B-C3B-CAB-CBB
29	A	802	CLA	C1A-C2A-CAA-CBA
29	A	802	CLA	C3A-C2A-CAA-CBA
29	A	803	CLA	CHA-CBD-CGD-O1D
29	A	803	CLA	CHA-CBD-CGD-O2D
29	A	803	CLA	CAD-CBD-CGD-O1D
29	A	803	CLA	CAD-CBD-CGD-O2D
29	A	804	CLA	C3A-C2A-CAA-CBA
29	A	809	CLA	C2B-C3B-CAB-CBB
29	A	809	CLA	C4B-C3B-CAB-CBB
29	A	810	CLA	C1A-C2A-CAA-CBA
29	A	810	CLA	C3A-C2A-CAA-CBA
29	A	810	CLA	CHA-CBD-CGD-O1D
29	A	810	CLA	CHA-CBD-CGD-O2D
29	A	810	CLA	CAD-CBD-CGD-O1D
29	A	810	CLA	CAD-CBD-CGD-O2D
29	A	814	CLA	CHA-CBD-CGD-O1D
29	A	814	CLA	CHA-CBD-CGD-O2D
29	A	816	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	A	817	CLA	C3A-C2A-CAA-CBA
29	A	817	CLA	CHA-CBD-CGD-O1D
29	A	817	CLA	CHA-CBD-CGD-O2D
29	A	818	CLA	C2B-C3B-CAB-CBB
29	A	818	CLA	C4B-C3B-CAB-CBB
29	A	821	CLA	C1A-C2A-CAA-CBA
29	A	822	CLA	CHA-CBD-CGD-O1D
29	A	822	CLA	CHA-CBD-CGD-O2D
29	A	824	CLA	C2B-C3B-CAB-CBB
29	A	824	CLA	C4B-C3B-CAB-CBB
29	A	825	CLA	CHA-CBD-CGD-O1D
29	A	825	CLA	CHA-CBD-CGD-O2D
29	A	829	CLA	C2B-C3B-CAB-CBB
29	A	829	CLA	C4B-C3B-CAB-CBB
29	A	831	CLA	C2B-C3B-CAB-CBB
29	A	831	CLA	C4B-C3B-CAB-CBB
29	A	832	CLA	C2B-C3B-CAB-CBB
29	A	832	CLA	C4B-C3B-CAB-CBB
29	A	832	CLA	CHA-CBD-CGD-O1D
29	A	832	CLA	CHA-CBD-CGD-O2D
29	A	834	CLA	C1A-C2A-CAA-CBA
29	A	834	CLA	CHA-CBD-CGD-O1D
29	A	834	CLA	CHA-CBD-CGD-O2D
29	A	835	CLA	C1A-C2A-CAA-CBA
29	A	835	CLA	C3A-C2A-CAA-CBA
29	A	837	CLA	C1A-C2A-CAA-CBA
29	A	837	CLA	C3A-C2A-CAA-CBA
29	A	837	CLA	CHA-CBD-CGD-O1D
29	A	837	CLA	CHA-CBD-CGD-O2D
29	A	840	CLA	C2B-C3B-CAB-CBB
29	A	840	CLA	C4B-C3B-CAB-CBB
29	A	843	CLA	CHA-CBD-CGD-O1D
29	A	843	CLA	CHA-CBD-CGD-O2D
29	A	844	CLA	C3A-C2A-CAA-CBA
29	B	805	CLA	C1A-C2A-CAA-CBA
29	B	807	CLA	C2B-C3B-CAB-CBB
29	B	807	CLA	C4B-C3B-CAB-CBB
29	B	809	CLA	C1A-C2A-CAA-CBA
29	B	813	CLA	C1A-C2A-CAA-CBA
29	B	813	CLA	C3A-C2A-CAA-CBA
29	B	813	CLA	C2-C3-C5-C6
29	B	813	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	B	814	CLA	C1A-C2A-CAA-CBA
29	B	814	CLA	C3A-C2A-CAA-CBA
29	B	816	CLA	O2A-C1-C2-C3
29	B	818	CLA	CHA-CBD-CGD-O1D
29	B	819	CLA	C1A-C2A-CAA-CBA
29	B	819	CLA	C3A-C2A-CAA-CBA
29	B	821	CLA	C2B-C3B-CAB-CBB
29	B	821	CLA	C4B-C3B-CAB-CBB
29	B	822	CLA	CHA-CBD-CGD-O1D
29	B	822	CLA	CHA-CBD-CGD-O2D
29	B	824	CLA	CHA-CBD-CGD-O2D
29	B	831	CLA	C2B-C3B-CAB-CBB
29	B	831	CLA	C4B-C3B-CAB-CBB
29	B	832	CLA	C1A-C2A-CAA-CBA
29	F	204	CLA	C2B-C3B-CAB-CBB
29	F	204	CLA	C4B-C3B-CAB-CBB
29	F	204	CLA	CHA-CBD-CGD-O1D
29	F	204	CLA	CHA-CBD-CGD-O2D
29	K	102	CLA	O2A-C1-C2-C3
29	L	201	CLA	C1A-C2A-CAA-CBA
29	L	201	CLA	C2-C3-C5-C6
29	L	201	CLA	C4-C3-C5-C6
29	O	202	CLA	C4B-C3B-CAB-CBB
29	Z	306	CLA	C2B-C3B-CAB-CBB
29	Z	306	CLA	C4B-C3B-CAB-CBB
29	a	602	CLA	C3A-C2A-CAA-CBA
29	a	602	CLA	C4-C3-C5-C6
29	a	604	CLA	C2B-C3B-CAB-CBB
29	a	604	CLA	C4B-C3B-CAB-CBB
29	a	605	CLA	C1A-C2A-CAA-CBA
29	a	605	CLA	C3A-C2A-CAA-CBA
29	a	605	CLA	C2B-C3B-CAB-CBB
29	a	605	CLA	C4B-C3B-CAB-CBB
29	a	609	CLA	C11-C10-C8-C9
29	a	611	CLA	C2-C3-C5-C6
29	a	611	CLA	C4-C3-C5-C6
29	a	612	CLA	C2B-C3B-CAB-CBB
29	a	612	CLA	C4B-C3B-CAB-CBB
29	b	601	CLA	C2B-C3B-CAB-CBB
29	b	601	CLA	C4B-C3B-CAB-CBB
29	b	602	CLA	C1A-C2A-CAA-CBA
29	b	602	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	b	602	CLA	CHA-CBD-CGD-O1D
29	b	602	CLA	CHA-CBD-CGD-O2D
29	b	603	CLA	C6-C7-C8-C9
29	b	604	CLA	CHA-CBD-CGD-O1D
29	b	604	CLA	CHA-CBD-CGD-O2D
29	b	606	CLA	C1A-C2A-CAA-CBA
29	b	606	CLA	C3A-C2A-CAA-CBA
29	b	607	CLA	CHA-CBD-CGD-O1D
29	b	607	CLA	CHA-CBD-CGD-O2D
29	b	608	CLA	C2B-C3B-CAB-CBB
29	b	608	CLA	C4B-C3B-CAB-CBB
29	b	610	CLA	C2-C3-C5-C6
29	c	605	CLA	CHA-CBD-CGD-O1D
29	c	605	CLA	CHA-CBD-CGD-O2D
29	c	606	CLA	CHA-CBD-CGD-O2D
29	c	607	CLA	C1A-C2A-CAA-CBA
29	c	608	CLA	C2B-C3B-CAB-CBB
29	c	608	CLA	C4B-C3B-CAB-CBB
29	c	609	CLA	C2B-C3B-CAB-CBB
29	c	609	CLA	C4B-C3B-CAB-CBB
29	c	612	CLA	C2B-C3B-CAB-CBB
29	c	612	CLA	C4B-C3B-CAB-CBB
29	c	613	CLA	CHA-CBD-CGD-O1D
29	c	613	CLA	CHA-CBD-CGD-O2D
29	c	613	CLA	CAD-CBD-CGD-O1D
29	c	614	CLA	C2B-C3B-CAB-CBB
29	c	614	CLA	C4B-C3B-CAB-CBB
29	d	602	CLA	C4B-C3B-CAB-CBB
29	d	604	CLA	C2B-C3B-CAB-CBB
29	d	604	CLA	C4B-C3B-CAB-CBB
29	d	611	CLA	C1A-C2A-CAA-CBA
29	e	602	CLA	C1A-C2A-CAA-CBA
29	e	602	CLA	C3A-C2A-CAA-CBA
29	e	602	CLA	C2B-C3B-CAB-CBB
29	e	602	CLA	C4B-C3B-CAB-CBB
29	e	603	CLA	C2B-C3B-CAB-CBB
29	e	603	CLA	C4B-C3B-CAB-CBB
29	e	610	CLA	C4B-C3B-CAB-CBB
29	e	611	CLA	C2B-C3B-CAB-CBB
29	e	611	CLA	C4B-C3B-CAB-CBB
29	e	611	CLA	CBD-CGD-O2D-CED
30	1	610	KC2	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	3	606	KC2	C1A-C2A-CAA-CBA
30	3	606	KC2	C3A-C2A-CAA-CBA
30	3	606	KC2	CHA-CBD-CGD-O1D
30	3	606	KC2	CHA-CBD-CGD-O2D
30	7	606	KC2	C2B-C3B-CAB-CBB
30	7	606	KC2	C4B-C3B-CAB-CBB
30	7	606	KC2	CAA-CBA-CGA-O2A
30	7	610	KC2	C1A-C2A-CAA-CBA
30	7	610	KC2	C3A-C2A-CAA-CBA
30	7	610	KC2	CAA-CBA-CGA-O1A
30	7	610	KC2	CAA-CBA-CGA-O2A
30	9	610	KC2	CHA-CBD-CGD-O1D
30	9	610	KC2	CHA-CBD-CGD-O2D
30	a	610	KC2	CHA-CBD-CGD-O1D
30	a	610	KC2	CHA-CBD-CGD-O2D
30	b	605	KC2	C1A-C2A-CAA-CBA
30	b	605	KC2	C3A-C2A-CAA-CBA
30	c	610	KC2	CAA-CBA-CGA-O1A
30	c	610	KC2	CAA-CBA-CGA-O2A
30	c	611	KC2	C1A-C2A-CAA-CBA
30	c	611	KC2	C3A-C2A-CAA-CBA
30	c	615	KC2	C1A-C2A-CAA-CBA
30	c	615	KC2	C3A-C2A-CAA-CBA
30	c	615	KC2	C2B-C3B-CAB-CBB
30	c	615	KC2	C4B-C3B-CAB-CBB
30	d	610	KC2	C1A-C2A-CAA-CBA
30	e	605	KC2	C1A-C2A-CAA-CBA
30	e	605	KC2	C2C-C3C-CAC-CBC
30	e	605	KC2	C4C-C3C-CAC-CBC
31	3	613	II0	C10-C22-C24-C26
31	4	614	II0	C09-C21-C23-C25
31	6	615	II0	C09-C21-C23-C25
31	8	612	II0	C09-C21-C23-C25
31	9	618	II0	C09-C21-C23-C25
31	9	618	II0	C10-C22-C24-C26
31	B	843	II0	C10-C22-C24-C26
31	a	619	II0	C09-C21-C23-C25
31	c	619	II0	C10-C22-C24-C26
31	d	614	II0	C09-C21-C23-C25
31	d	616	II0	C09-C21-C23-C25
32	b	613	II3	C16-C23-C27-C28
32	e	613	II3	C03-C04-C12-C21

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Mol	Chain	Res	Type	Atoms
32	e	613	II3	C16-C23-C27-C28
33	5	618	IHT	C02-C07-C18-C22
33	6	617	IHT	C11-C21-C24-C26
33	9	619	IHT	C18-C22-C23-C25
33	9	619	IHT	C18-C22-C23-C27
33	K	104	IHT	C02-C07-C18-C22
33	L	205	IHT	C11-C21-C24-C26
33	Z	302	IHT	C10-C07-C18-C22
33	a	617	IHT	C10-C07-C18-C22
33	a	617	IHT	C31-C34-C35-C38
33	a	617	IHT	C31-C34-C35-C39
33	d	617	IHT	C10-C07-C18-C22
34	3	618	LMG	O6-C1-O1-C7
34	I	102	LMG	O6-C1-O1-C7
35	2	618	LHG	O2-C2-C3-O3
35	2	618	LHG	C4-O6-P-O5
35	2	620	LHG	C3-O3-P-O5
35	2	620	LHG	C4-O6-P-O4
35	2	620	LHG	O7-C5-C6-O8
35	3	619	LHG	C3-O3-P-O5
35	3	619	LHG	C3-O3-P-O6
35	3	619	LHG	O6-C4-C5-O7
35	3	619	LHG	C8-C7-O7-C5
35	3	622	LHG	O1-C1-C2-C3
35	3	622	LHG	C8-C7-O7-C5
35	3	623	LHG	O1-C1-C2-C3
35	3	623	LHG	C3-O3-P-O4
35	3	623	LHG	C3-O3-P-O6
35	3	623	LHG	C4-O6-P-O4
35	3	623	LHG	C4-O6-P-O5
35	3	623	LHG	C8-C7-O7-C5
35	4	617	LHG	O7-C5-C6-O8
35	4	619	LHG	C3-O3-P-O4
35	4	619	LHG	C3-O3-P-O6
35	4	619	LHG	C4-O6-P-O5
35	4	619	LHG	C8-C7-O7-C5
35	5	619	LHG	C1-C2-C3-O3
35	5	619	LHG	C3-O3-P-O5
35	5	619	LHG	C8-C7-O7-C5
35	6	618	LHG	C8-C7-O7-C5
35	7	619	LHG	C3-O3-P-O4
35	7	619	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
35	8	613	LHG	O1-C1-C2-C3
35	8	613	LHG	O2-C2-C3-O3
35	8	613	LHG	C3-O3-P-O4
35	8	613	LHG	C4-O6-P-O5
35	8	613	LHG	O7-C5-C6-O8
35	A	850	LHG	O2-C2-C3-O3
35	A	850	LHG	C3-O3-P-O4
35	A	850	LHG	C3-O3-P-O6
35	A	850	LHG	C4-O6-P-O5
35	A	851	LHG	O1-C1-C2-C3
35	A	851	LHG	C3-O3-P-O5
35	A	851	LHG	C4-O6-P-O5
35	B	849	LHG	O1-C1-C2-O2
35	B	849	LHG	O1-C1-C2-C3
35	B	849	LHG	O9-C7-O7-C5
35	B	849	LHG	C8-C7-O7-C5
35	Z	310	LHG	C1-C2-C3-O3
35	Z	310	LHG	C3-O3-P-O4
35	Z	310	LHG	C3-O3-P-O5
35	Z	310	LHG	O7-C5-C6-O8
35	Z	310	LHG	O9-C7-O7-C5
35	Z	310	LHG	C8-C7-O7-C5
35	a	618	LHG	O1-C1-C2-C3
35	a	618	LHG	C3-O3-P-O5
35	b	616	LHG	C3-O3-P-O4
35	b	616	LHG	C6-C5-O7-C7
35	c	621	LHG	O1-C1-C2-O2
35	c	621	LHG	O1-C1-C2-C3
35	c	621	LHG	C3-O3-P-O5
35	c	621	LHG	C4-O6-P-O4
35	d	618	LHG	C4-O6-P-O4
35	d	618	LHG	C8-C7-O7-C5
35	d	619	LHG	C3-O3-P-O5
35	d	619	LHG	C4-O6-P-O3
35	d	619	LHG	C4-O6-P-O4
35	d	619	LHG	C8-C7-O7-C5
36	3	621	SQD	O5-C5-C6-S
36	3	621	SQD	C5-C6-S-O7
36	O	206	SQD	O5-C5-C6-S
36	O	206	SQD	C5-C6-S-O7
36	O	206	SQD	C5-C6-S-O8
36	O	206	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
37	4	616	8CT	C02-C03-C10-C11
37	4	616	8CT	C04-C03-C10-C11
37	4	616	8CT	C28-C29-C30-C35
37	7	617	8CT	C03-C10-C11-C12
37	7	617	8CT	C13-C14-C15-C16
37	7	617	8CT	C25-C26-C28-C29
37	7	617	8CT	C27-C26-C28-C29
37	7	617	8CT	C28-C29-C30-C35
37	A	845	8CT	C21-C23-C24-C25
37	A	846	8CT	C28-C29-C30-C35
37	A	847	8CT	C03-C10-C11-C12
37	A	847	8CT	C28-C29-C30-C31
37	A	847	8CT	C28-C29-C30-C35
37	A	852	8CT	C03-C10-C11-C12
37	B	844	8CT	C28-C29-C30-C31
37	B	844	8CT	C28-C29-C30-C35
37	B	845	8CT	C28-C29-C30-C31
37	B	845	8CT	C28-C29-C30-C35
37	B	846	8CT	C28-C29-C30-C31
37	B	846	8CT	C28-C29-C30-C35
37	B	847	8CT	C28-C29-C30-C31
37	B	850	8CT	C03-C10-C11-C12
37	B	850	8CT	C28-C29-C30-C35
37	B	851	8CT	C28-C29-C30-C35
37	F	201	8CT	C28-C29-C30-C31
37	F	201	8CT	C28-C29-C30-C35
37	J	103	8CT	C28-C29-C30-C35
37	L	206	8CT	C28-C29-C30-C31
37	L	206	8CT	C28-C29-C30-C35
37	M	101	8CT	C03-C10-C11-C12
37	M	101	8CT	C28-C29-C30-C31
37	M	101	8CT	C28-C29-C30-C35
37	R	201	8CT	C10-C11-C12-C13
37	R	201	8CT	C10-C11-C12-C40
37	R	203	8CT	C03-C10-C11-C12
37	Z	309	8CT	C21-C23-C24-C25
37	Z	309	8CT	C28-C29-C30-C35
37	b	615	8CT	C28-C29-C30-C35
38	4	618	LMU	O5B-C1B-O1B-C4'
38	4	618	LMU	C2'-C1'-O1'-C1
38	4	618	LMU	O5'-C1'-O1'-C1
38	4	618	LMU	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
38	J	104	LMU	C2'-C1'-O1'-C1
38	J	104	LMU	O5'-C1'-O1'-C1
38	O	207	LMU	C2'-C1'-O1'-C1
38	O	207	LMU	O5'-C1'-O1'-C1
38	e	617	LMU	C2'-C1'-O1'-C1
39	A	849	PQN	C16-C17-C18-C19
41	B	848	DGD	O1B-C1B-O2G-C2G
29	B	841	CLA	CBD-CGD-O2D-CED
29	O	202	CLA	CBD-CGD-O2D-CED
29	d	612	CLA	CBD-CGD-O2D-CED
35	2	619	LHG	O10-C23-O8-C6
35	4	619	LHG	O10-C23-O8-C6
35	8	613	LHG	O10-C23-O8-C6
38	J	104	LMU	O5B-C1B-O1B-C4'
29	e	611	CLA	O1D-CGD-O2D-CED
35	2	619	LHG	C24-C23-O8-C6
29	B	803	CLA	CBD-CGD-O2D-CED
29	O	203	CLA	CBD-CGD-O2D-CED
35	5	619	LHG	O10-C23-O8-C6
35	a	618	LHG	O10-C23-O8-C6
30	4	605	KC2	CAA-CBA-CGA-O2A
30	9	610	KC2	CAA-CBA-CGA-O2A
30	d	610	KC2	CAA-CBA-CGA-O2A
38	O	207	LMU	O5B-C1B-O1B-C4'
35	3	619	LHG	O9-C7-O7-C5
35	3	622	LHG	O9-C7-O7-C5
35	3	623	LHG	O9-C7-O7-C5
35	6	618	LHG	O9-C7-O7-C5
35	7	619	LHG	O9-C7-O7-C5
35	8	613	LHG	O9-C7-O7-C5
35	L	208	LHG	O9-C7-O7-C5
35	a	618	LHG	O9-C7-O7-C5
35	b	616	LHG	O9-C7-O7-C5
35	d	618	LHG	O9-C7-O7-C5
35	d	619	LHG	O9-C7-O7-C5
29	4	607	CLA	C3-C5-C6-C7
29	4	611	CLA	C3-C5-C6-C7
29	A	804	CLA	C3-C5-C6-C7
29	A	806	CLA	C3-C5-C6-C7
29	A	819	CLA	C3-C5-C6-C7
29	A	823	CLA	C3-C5-C6-C7
29	A	831	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	B	811	CLA	C3-C5-C6-C7
29	B	820	CLA	C3-C5-C6-C7
29	B	832	CLA	C3-C5-C6-C7
29	O	203	CLA	C3-C5-C6-C7
29	Z	306	CLA	C3-C5-C6-C7
29	d	612	CLA	C3-C5-C6-C7
35	4	619	LHG	C24-C23-O8-C6
35	8	613	LHG	C24-C23-O8-C6
34	3	620	LMG	C4-C5-C6-O5
34	3	618	LMG	C11-C10-O7-C8
41	B	848	DGD	C2B-C1B-O2G-C2G
30	7	606	KC2	CBD-CGD-O2D-CED
30	7	606	KC2	CAA-CBA-CGA-O1A
29	4	610	CLA	C4-C3-C5-C6
29	a	605	CLA	C4-C3-C5-C6
29	b	608	CLA	C4-C3-C5-C6
34	3	618	LMG	C4-C5-C6-O5
29	9	608	CLA	C2-C3-C5-C6
29	3	610	CLA	C2A-CAA-CBA-CGA
29	A	827	CLA	C2A-CAA-CBA-CGA
29	A	834	CLA	C2A-CAA-CBA-CGA
29	B	804	CLA	C2A-CAA-CBA-CGA
29	B	809	CLA	C2A-CAA-CBA-CGA
29	B	837	CLA	C2A-CAA-CBA-CGA
29	a	602	CLA	C2A-CAA-CBA-CGA
29	c	613	CLA	C2A-CAA-CBA-CGA
29	4	604	CLA	C3-C5-C6-C7
29	5	604	CLA	C3-C5-C6-C7
29	6	611	CLA	C3-C5-C6-C7
29	A	811	CLA	C3-C5-C6-C7
29	B	808	CLA	C3-C5-C6-C7
29	F	202	CLA	C3-C5-C6-C7
29	K	102	CLA	C3-C5-C6-C7
29	d	602	CLA	C3-C5-C6-C7
35	5	619	LHG	C24-C23-O8-C6
35	a	618	LHG	C24-C23-O8-C6
35	5	619	LHG	O9-C7-O7-C5
29	O	202	CLA	O1D-CGD-O2D-CED
35	4	619	LHG	O9-C7-O7-C5
29	a	609	CLA	O1A-CGA-O2A-C1
37	J	103	8CT	C16-C17-C18-C19
37	M	101	8CT	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
38	O	207	LMU	C2B-C1B-O1B-C4'
41	Z	303	DGD	O6E-C5E-C6E-O5E
30	2	610	KC2	CAA-CBA-CGA-O1A
30	2	610	KC2	CAA-CBA-CGA-O2A
29	1	612	CLA	CBD-CGD-O2D-CED
29	c	603	CLA	CBD-CGD-O2D-CED
29	B	841	CLA	O1D-CGD-O2D-CED
35	5	619	LHG	O2-C2-C3-O3
35	7	619	LHG	O2-C2-C3-O3
35	d	618	LHG	O2-C2-C3-O3
29	A	841	CLA	C3-C5-C6-C7
29	A	810	CLA	CBA-CGA-O2A-C1
29	a	609	CLA	CBA-CGA-O2A-C1
34	I	102	LMG	C11-C10-O7-C8
35	8	613	LHG	C8-C7-O7-C5
35	a	618	LHG	C8-C7-O7-C5
30	2	610	KC2	CBD-CGD-O2D-CED
35	b	616	LHG	C11-C12-C13-C14
34	3	620	LMG	O6-C5-C6-O5
38	4	618	LMU	C4-C5-C6-C7
39	A	849	PQN	C13-C15-C16-C17
29	A	839	CLA	CBA-CGA-O2A-C1
36	O	206	SQD	C24-C23-O48-C46
34	3	618	LMG	O6-C5-C6-O5
30	4	605	KC2	CAA-CBA-CGA-O1A
30	9	610	KC2	CAA-CBA-CGA-O1A
30	d	610	KC2	CAA-CBA-CGA-O1A
30	e	609	KC2	CAA-CBA-CGA-O2A
29	4	603	CLA	C4-C3-C5-C6
29	A	834	CLA	C4-C3-C5-C6
29	B	831	CLA	C4-C3-C5-C6
29	4	603	CLA	C2-C3-C5-C6
29	A	834	CLA	C2-C3-C5-C6
29	B	831	CLA	C2-C3-C5-C6
29	a	602	CLA	C2-C3-C5-C6
29	a	605	CLA	C2-C3-C5-C6
29	6	606	CLA	C2A-CAA-CBA-CGA
29	A	839	CLA	C2A-CAA-CBA-CGA
34	F	205	LMG	O6-C5-C6-O5
36	O	206	SQD	O10-C23-O48-C46
38	e	617	LMU	O5'-C1'-O1'-C1
29	B	826	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	c	614	CLA	CBA-CGA-O2A-C1
35	Z	310	LHG	C24-C23-O8-C6
29	9	613	CLA	CBD-CGD-O2D-CED
41	Z	303	DGD	C4E-C5E-C6E-O5E
30	6	613	KC2	CAA-CBA-CGA-O2A
35	4	619	LHG	C1-C2-C3-O3
35	7	619	LHG	C1-C2-C3-O3
35	A	850	LHG	C1-C2-C3-O3
35	L	208	LHG	C1-C2-C3-O3
29	9	606	CLA	C3-C5-C6-C7
29	8	606	CLA	CBA-CGA-O2A-C1
29	L	201	CLA	CBA-CGA-O2A-C1
29	b	610	CLA	CBA-CGA-O2A-C1
29	e	606	CLA	CBA-CGA-O2A-C1
34	3	620	LMG	C29-C28-O8-C9
35	L	208	LHG	C24-C23-O8-C6
35	7	619	LHG	C23-C24-C25-C26
35	Z	310	LHG	C23-C24-C25-C26
29	B	813	CLA	C5-C6-C7-C8
30	6	613	KC2	CAA-CBA-CGA-O1A
30	b	609	KC2	CAA-CBA-CGA-O2A
30	c	611	KC2	CAA-CBA-CGA-O2A
30	e	609	KC2	CAA-CBA-CGA-O1A
29	A	839	CLA	C15-C16-C17-C18
29	B	821	CLA	C8-C10-C11-C12
29	c	607	CLA	C8-C10-C11-C12
35	4	619	LHG	O2-C2-C3-O3
35	L	208	LHG	O2-C2-C3-O3
35	Z	310	LHG	O2-C2-C3-O3
35	c	621	LHG	C7-C8-C9-C10
36	O	206	SQD	C2-C1-O6-C44
29	A	810	CLA	O1A-CGA-O2A-C1
29	4	610	CLA	C2-C3-C5-C6
29	1	612	CLA	C6-C7-C8-C9
29	9	606	CLA	C6-C7-C8-C9
29	A	806	CLA	C6-C7-C8-C9
29	A	806	CLA	C14-C13-C15-C16
29	A	822	CLA	C14-C13-C15-C16
29	A	824	CLA	C6-C7-C8-C9
29	A	833	CLA	C11-C10-C8-C9
29	A	835	CLA	C11-C10-C8-C9
29	B	816	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	B	839	CLA	C11-C10-C8-C9
29	L	203	CLA	C11-C10-C8-C9
29	b	604	CLA	C6-C7-C8-C9
29	b	604	CLA	C11-C10-C8-C9
29	c	603	CLA	C6-C7-C8-C9
29	c	607	CLA	C11-C12-C13-C14
29	c	608	CLA	C11-C10-C8-C9
29	d	612	CLA	O1D-CGD-O2D-CED
29	2	608	CLA	C8-C10-C11-C12
29	B	826	CLA	C10-C11-C12-C13
29	8	602	CLA	C2A-CAA-CBA-CGA
29	A	838	CLA	C2A-CAA-CBA-CGA
35	b	616	LHG	C8-C7-O7-C5
34	F	205	LMG	C4-C5-C6-O5
35	3	623	LHG	C23-C24-C25-C26
29	A	839	CLA	O1A-CGA-O2A-C1
29	9	606	CLA	C10-C11-C12-C13
29	B	815	CLA	C8-C10-C11-C12
29	Z	306	CLA	C10-C11-C12-C13
29	O	203	CLA	O1D-CGD-O2D-CED
38	O	207	LMU	C2-C3-C4-C5
30	b	609	KC2	CAA-CBA-CGA-O1A
30	c	611	KC2	CAA-CBA-CGA-O1A
30	c	615	KC2	CAA-CBA-CGA-O1A
30	e	605	KC2	CAA-CBA-CGA-O1A
29	4	610	CLA	C3-C5-C6-C7
29	L	204	CLA	CBA-CGA-O2A-C1
35	4	617	LHG	C24-C23-O8-C6
29	4	611	CLA	C5-C6-C7-C8
29	B	803	CLA	C5-C6-C7-C8
29	B	812	CLA	C13-C15-C16-C17
29	B	838	CLA	C13-C15-C16-C17
29	F	202	CLA	C8-C10-C11-C12
29	a	603	CLA	C5-C6-C7-C8
38	O	207	LMU	O5B-C5B-C6B-O6B
34	F	205	LMG	C10-C11-C12-C13
35	b	616	LHG	C23-C24-C25-C26
29	5	608	CLA	C5-C6-C7-C8
29	6	602	CLA	C8-C10-C11-C12
29	A	826	CLA	C8-C10-C11-C12
29	A	842	CLA	C10-C11-C12-C13
29	B	808	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	B	831	CLA	C5-C6-C7-C8
29	B	832	CLA	C13-C15-C16-C17
29	B	837	CLA	C5-C6-C7-C8
29	K	101	CLA	C5-C6-C7-C8
34	2	617	LMG	C28-C29-C30-C31
35	A	851	LHG	C23-C24-C25-C26
35	d	619	LHG	C7-C8-C9-C10
29	A	839	CLA	C13-C15-C16-C17
29	B	817	CLA	C10-C11-C12-C13
29	B	839	CLA	C10-C11-C12-C13
29	a	612	CLA	C3-C5-C6-C7
34	2	617	LMG	C29-C28-O8-C9
30	c	615	KC2	CAA-CBA-CGA-O2A
30	e	605	KC2	CAA-CBA-CGA-O2A
29	B	832	CLA	C2-C1-O2A-CGA
29	A	806	CLA	C8-C10-C11-C12
29	A	810	CLA	C5-C6-C7-C8
29	A	837	CLA	C5-C6-C7-C8
29	B	812	CLA	C5-C6-C7-C8
29	L	201	CLA	C8-C10-C11-C12
29	e	606	CLA	C5-C6-C7-C8
35	A	850	LHG	C7-C8-C9-C10
35	d	619	LHG	C23-C24-C25-C26
29	1	613	CLA	CBD-CGD-O2D-CED
35	A	851	LHG	C8-C7-O7-C5
29	A	818	CLA	C8-C10-C11-C12
29	8	615	CLA	C11-C12-C13-C15
29	A	818	CLA	C6-C7-C8-C10
29	A	825	CLA	C12-C13-C15-C16
29	A	839	CLA	C6-C7-C8-C10
29	B	806	CLA	C6-C7-C8-C10
29	B	820	CLA	C11-C10-C8-C7
29	B	832	CLA	C12-C13-C15-C16
29	8	606	CLA	O1A-CGA-O2A-C1
29	c	614	CLA	O1A-CGA-O2A-C1
37	B	845	8CT	C18-C19-C20-C21
37	R	201	8CT	C12-C13-C14-C15
29	A	809	CLA	C2A-CAA-CBA-CGA
29	A	829	CLA	C2A-CAA-CBA-CGA
29	4	608	CLA	C5-C6-C7-C8
29	e	606	CLA	O1A-CGA-O2A-C1
29	3	603	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	d	604	CLA	C10-C11-C12-C13
37	7	617	8CT	C21-C23-C24-C25
37	A	846	8CT	C21-C23-C24-C25
37	B	846	8CT	C21-C23-C24-C25
37	B	847	8CT	C21-C23-C24-C25
37	B	851	8CT	C21-C23-C24-C25
37	I	101	8CT	C21-C23-C24-C25
37	J	103	8CT	C21-C23-C24-C25
37	M	101	8CT	C21-C23-C24-C25
37	R	201	8CT	C13-C14-C15-C16
37	b	615	8CT	C21-C23-C24-C25
35	2	619	LHG	O2-C2-C3-O3
35	3	622	LHG	O2-C2-C3-O3
35	7	618	LHG	O2-C2-C3-O3
29	A	835	CLA	C3-C5-C6-C7
29	B	822	CLA	C3-C5-C6-C7
29	1	605	CLA	C2A-CAA-CBA-CGA
29	A	801	CLA	C15-C16-C17-C18
29	A	823	CLA	C15-C16-C17-C18
29	K	101	CLA	C13-C15-C16-C17
29	c	607	CLA	C10-C11-C12-C13
29	B	816	CLA	CBA-CGA-O2A-C1
29	B	832	CLA	CBA-CGA-O2A-C1
29	Z	301	CLA	CBA-CGA-O2A-C1
29	d	602	CLA	CBA-CGA-O2A-C1
29	b	610	CLA	O1A-CGA-O2A-C1
38	O	207	LMU	O1'-C1-C2-C3
29	4	610	CLA	C5-C6-C7-C8
29	A	811	CLA	C13-C15-C16-C17
29	A	831	CLA	C13-C15-C16-C17
29	B	806	CLA	C15-C16-C17-C18
29	a	608	CLA	C5-C6-C7-C8
35	L	208	LHG	C8-C7-O7-C5
29	A	825	CLA	C10-C11-C12-C13
29	A	837	CLA	C10-C11-C12-C13
29	A	841	CLA	C15-C16-C17-C18
29	B	806	CLA	C5-C6-C7-C8
35	2	618	LHG	C4-O6-P-O3
35	2	619	LHG	C4-O6-P-O3
35	3	623	LHG	C4-O6-P-O3
35	5	619	LHG	C3-O3-P-O6
35	7	619	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
35	8	613	LHG	C3-O3-P-O6
35	8	613	LHG	C4-O6-P-O3
35	A	850	LHG	C4-O6-P-O3
35	A	851	LHG	C3-O3-P-O6
35	Z	310	LHG	C3-O3-P-O6
35	a	618	LHG	C3-O3-P-O6
35	b	616	LHG	C3-O3-P-O6
35	c	621	LHG	C3-O3-P-O6
35	c	621	LHG	C4-O6-P-O3
35	d	619	LHG	C3-O3-P-O6
35	7	618	LHG	C24-C23-O8-C6
39	B	842	PQN	C25-C26-C27-C28
35	2	618	LHG	C1-C2-C3-O3
35	2	619	LHG	C1-C2-C3-O3
35	3	622	LHG	C1-C2-C3-O3
35	8	613	LHG	C1-C2-C3-O3
29	B	812	CLA	C4-C3-C5-C6
29	B	823	CLA	C4-C3-C5-C6
29	8	604	CLA	C5-C6-C7-C8
29	L	201	CLA	O1A-CGA-O2A-C1
35	3	619	LHG	C31-C32-C33-C34
29	B	819	CLA	C2A-CAA-CBA-CGA
29	a	607	CLA	C16-C17-C18-C20
29	a	611	CLA	C6-C7-C8-C9
29	c	603	CLA	C16-C17-C18-C20
38	4	618	LMU	O5'-C5'-C6'-O6'
29	1	602	CLA	C3-C5-C6-C7
30	b	605	KC2	CAA-CBA-CGA-O1A
30	b	605	KC2	CAA-CBA-CGA-O2A
29	9	606	CLA	CBA-CGA-O2A-C1
35	3	623	LHG	C24-C23-O8-C6
34	F	205	LMG	C28-C29-C30-C31
29	6	608	CLA	C8-C10-C11-C12
33	a	617	IHT	C26-C29-C31-C34
34	8	614	LMG	C31-C32-C33-C34
34	8	614	LMG	C32-C33-C34-C35
35	2	620	LHG	C32-C33-C34-C35
35	3	623	LHG	C28-C29-C30-C31
35	A	851	LHG	C15-C16-C17-C18
41	B	848	DGD	C5A-C6A-C7A-C8A
29	B	803	CLA	O1D-CGD-O2D-CED
34	3	620	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
36	3	621	SQD	C8-C7-O47-C45
36	O	206	SQD	C8-C7-O47-C45
29	A	820	CLA	C3-C5-C6-C7
34	2	617	LMG	C30-C31-C32-C33
34	8	614	LMG	C38-C39-C40-C41
35	4	619	LHG	C31-C32-C33-C34
35	7	619	LHG	C31-C32-C33-C34
35	A	850	LHG	C13-C14-C15-C16
35	L	208	LHG	C24-C25-C26-C27
35	b	616	LHG	C33-C34-C35-C36
36	3	621	SQD	C26-C27-C28-C29
38	7	620	LMU	C3-C4-C5-C6
41	B	848	DGD	C2B-C3B-C4B-C5B
41	Z	303	DGD	C3B-C4B-C5B-C6B
29	A	831	CLA	C16-C17-C18-C19
29	A	844	CLA	C16-C17-C18-C19
29	B	826	CLA	C16-C17-C18-C20
29	O	203	CLA	C6-C7-C8-C10
34	3	620	LMG	C31-C32-C33-C34
35	6	618	LHG	C24-C25-C26-C27
35	7	619	LHG	C27-C28-C29-C30
35	A	850	LHG	C31-C32-C33-C34
35	d	618	LHG	C6-C5-O7-C7
34	I	102	LMG	O9-C10-O7-C8
35	2	620	LHG	O9-C7-O7-C5
36	O	206	SQD	O49-C7-O47-C45
29	c	604	CLA	C8-C10-C11-C12
34	8	614	LMG	C34-C35-C36-C37
35	A	850	LHG	C24-C25-C26-C27
34	I	102	LMG	C19-C20-C21-C22
35	2	620	LHG	C28-C29-C30-C31
35	7	619	LHG	C29-C30-C31-C32
36	3	621	SQD	C11-C10-C9-C8
29	A	818	CLA	C13-C15-C16-C17
35	d	619	LHG	C30-C31-C32-C33
38	e	617	LMU	O5B-C5B-C6B-O6B
29	b	602	CLA	C15-C16-C17-C18
35	2	620	LHG	C34-C35-C36-C37
35	7	619	LHG	C33-C34-C35-C36
35	8	613	LHG	C27-C28-C29-C30
35	B	849	LHG	C26-C27-C28-C29
36	3	621	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	B	808	CLA	C15-C16-C17-C18
41	Z	303	DGD	O1A-C1A-O1G-C1G
29	9	608	CLA	C6-C7-C8-C9
29	Z	306	CLA	C11-C12-C13-C14
29	b	604	CLA	C16-C17-C18-C20
29	A	817	CLA	C4-C3-C5-C6
29	B	810	CLA	C4-C3-C5-C6
29	B	821	CLA	C4-C3-C5-C6
29	B	822	CLA	C4-C3-C5-C6
29	B	827	CLA	C4-C3-C5-C6
35	3	622	LHG	C11-C10-C9-C8
35	3	623	LHG	C17-C18-C19-C20
35	7	619	LHG	C24-C25-C26-C27
29	a	606	CLA	C2-C3-C5-C6
29	2	605	CLA	C11-C10-C8-C9
29	9	607	CLA	C11-C10-C8-C9
29	A	801	CLA	C14-C13-C15-C16
29	A	804	CLA	C14-C13-C15-C16
29	A	810	CLA	C11-C12-C13-C14
29	A	816	CLA	C6-C7-C8-C9
29	A	818	CLA	C6-C7-C8-C9
29	A	823	CLA	C11-C12-C13-C14
29	A	843	CLA	C11-C10-C8-C9
29	B	828	CLA	C6-C7-C8-C9
29	d	607	CLA	C14-C13-C15-C16
35	A	850	LHG	C25-C26-C27-C28
35	L	208	LHG	C28-C29-C30-C31
29	A	806	CLA	C10-C11-C12-C13
29	A	828	CLA	C5-C6-C7-C8
29	c	603	CLA	C13-C15-C16-C17
29	1	603	CLA	C2A-CAA-CBA-CGA
29	9	613	CLA	C2A-CAA-CBA-CGA
29	A	842	CLA	C2A-CAA-CBA-CGA
29	a	603	CLA	C2A-CAA-CBA-CGA
35	b	616	LHG	O1-C1-C2-C3
36	3	621	SQD	O49-C7-O47-C45
35	2	620	LHG	C8-C7-O7-C5
35	3	619	LHG	C9-C10-C11-C12
35	3	619	LHG	C18-C19-C20-C21
35	3	623	LHG	C25-C26-C27-C28
29	4	603	CLA	C5-C6-C7-C8
35	2	619	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
35	6	618	LHG	C26-C27-C28-C29
35	A	850	LHG	C14-C15-C16-C17
35	B	849	LHG	C14-C15-C16-C17
35	b	616	LHG	C11-C10-C9-C8
35	d	619	LHG	C24-C25-C26-C27
29	2	601	CLA	C4B-C3B-CAB-CBB
29	2	602	CLA	C4B-C3B-CAB-CBB
29	3	602	CLA	C4B-C3B-CAB-CBB
29	7	604	CLA	C4B-C3B-CAB-CBB
29	7	612	CLA	C4B-C3B-CAB-CBB
29	8	607	CLA	C4B-C3B-CAB-CBB
29	9	608	CLA	C4B-C3B-CAB-CBB
29	A	816	CLA	C4B-C3B-CAB-CBB
29	A	838	CLA	C4B-C3B-CAB-CBB
29	B	816	CLA	C4B-C3B-CAB-CBB
29	B	818	CLA	C4B-C3B-CAB-CBB
29	L	207	CLA	C4B-C3B-CAB-CBB
29	b	602	CLA	C4B-C3B-CAB-CBB
29	d	611	CLA	C4B-C3B-CAB-CBB
29	e	608	CLA	C4B-C3B-CAB-CBB
29	3	607	CLA	C11-C12-C13-C15
29	4	604	CLA	C6-C7-C8-C9
29	4	604	CLA	C6-C7-C8-C10
29	4	611	CLA	C16-C17-C18-C19
29	7	602	CLA	C16-C17-C18-C20
29	9	602	CLA	C6-C7-C8-C9
29	A	810	CLA	C16-C17-C18-C19
29	A	810	CLA	C16-C17-C18-C20
29	B	815	CLA	C16-C17-C18-C19
29	Z	301	CLA	C11-C12-C13-C15
29	c	606	CLA	C16-C17-C18-C20
34	I	102	LMG	C37-C38-C39-C40
35	7	618	LHG	C28-C29-C30-C31
35	8	613	LHG	C25-C26-C27-C28
35	B	849	LHG	C29-C30-C31-C32
35	b	616	LHG	C31-C32-C33-C34
35	d	619	LHG	C28-C29-C30-C31
29	7	608	CLA	C5-C6-C7-C8
34	8	614	LMG	C13-C14-C15-C16
35	2	619	LHG	C27-C28-C29-C30
30	7	606	KC2	O1D-CGD-O2D-CED
29	A	817	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
35	Z	310	LHG	C11-C12-C13-C14
41	Z	303	DGD	CAA-CBA-CCA-CDA
29	1	603	CLA	C3A-C2A-CAA-CBA
29	2	603	CLA	C3A-C2A-CAA-CBA
29	6	603	CLA	C3A-C2A-CAA-CBA
29	6	605	CLA	C3A-C2A-CAA-CBA
29	6	606	CLA	C3A-C2A-CAA-CBA
29	7	612	CLA	C3A-C2A-CAA-CBA
29	A	831	CLA	C3A-C2A-CAA-CBA
29	A	834	CLA	C3A-C2A-CAA-CBA
29	A	842	CLA	C3A-C2A-CAA-CBA
29	B	805	CLA	C3A-C2A-CAA-CBA
29	B	809	CLA	C3A-C2A-CAA-CBA
29	B	831	CLA	C3A-C2A-CAA-CBA
29	B	832	CLA	C3A-C2A-CAA-CBA
29	F	202	CLA	C3A-C2A-CAA-CBA
29	F	203	CLA	C3A-C2A-CAA-CBA
29	c	607	CLA	C3A-C2A-CAA-CBA
29	d	611	CLA	C3A-C2A-CAA-CBA
35	Z	310	LHG	C33-C34-C35-C36
35	b	616	LHG	C16-C17-C18-C19
29	4	606	CLA	C11-C12-C13-C15
29	7	602	CLA	C16-C17-C18-C19
29	A	831	CLA	C16-C17-C18-C20
29	Z	301	CLA	C11-C12-C13-C14
29	a	611	CLA	C6-C7-C8-C10
35	B	849	LHG	C31-C32-C33-C34
41	B	848	DGD	C2A-C3A-C4A-C5A
41	Z	303	DGD	C9B-CAB-CBB-CCB
35	A	851	LHG	O9-C7-O7-C5
29	8	602	CLA	CBD-CGD-O2D-CED
35	d	619	LHG	C27-C28-C29-C30
34	8	614	LMG	C10-C11-C12-C13
35	a	618	LHG	C23-C24-C25-C26
29	b	604	CLA	C15-C16-C17-C18
39	A	849	PQN	C25-C26-C27-C28
29	5	604	CLA	C4-C3-C5-C6
29	b	608	CLA	CBA-CGA-O2A-C1
29	5	604	CLA	C2-C3-C5-C6
29	B	806	CLA	C2-C3-C5-C6
29	B	821	CLA	C2-C3-C5-C6
29	B	822	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	B	823	CLA	C2-C3-C5-C6
29	B	827	CLA	C2-C3-C5-C6
29	B	834	CLA	C2-C3-C5-C6
29	b	608	CLA	C2-C3-C5-C6
35	4	617	LHG	C18-C19-C20-C21
35	3	622	LHG	O1-C1-C2-O2
35	3	623	LHG	O1-C1-C2-O2
35	8	613	LHG	O1-C1-C2-O2
35	A	851	LHG	O1-C1-C2-O2
35	a	618	LHG	O1-C1-C2-O2
29	B	823	CLA	C8-C10-C11-C12
35	6	618	LHG	C7-C8-C9-C10
29	L	204	CLA	O1A-CGA-O2A-C1
29	O	203	CLA	C6-C7-C8-C9
29	b	604	CLA	C16-C17-C18-C19
29	c	603	CLA	C16-C17-C18-C19
29	1	612	CLA	C2B-C3B-CAB-CBB
29	2	601	CLA	C2B-C3B-CAB-CBB
29	2	602	CLA	C2B-C3B-CAB-CBB
29	3	602	CLA	C2B-C3B-CAB-CBB
29	4	608	CLA	C2B-C3B-CAB-CBB
29	7	604	CLA	C2B-C3B-CAB-CBB
29	7	612	CLA	C2B-C3B-CAB-CBB
29	8	603	CLA	C2B-C3B-CAB-CBB
29	8	607	CLA	C2B-C3B-CAB-CBB
29	A	816	CLA	C2B-C3B-CAB-CBB
29	A	838	CLA	C2B-C3B-CAB-CBB
29	B	816	CLA	C2B-C3B-CAB-CBB
29	B	818	CLA	C2B-C3B-CAB-CBB
29	O	202	CLA	C2B-C3B-CAB-CBB
29	b	602	CLA	C2B-C3B-CAB-CBB
29	d	602	CLA	C2B-C3B-CAB-CBB
29	d	607	CLA	C2B-C3B-CAB-CBB
29	d	611	CLA	C2B-C3B-CAB-CBB
29	e	608	CLA	C2B-C3B-CAB-CBB
29	e	610	CLA	C2B-C3B-CAB-CBB
29	c	602	CLA	C8-C10-C11-C12
29	5	602	CLA	C3-C5-C6-C7
35	4	617	LHG	C9-C10-C11-C12
29	d	602	CLA	O1A-CGA-O2A-C1
29	A	820	CLA	C15-C16-C17-C18
38	7	620	LMU	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	3	618	LMG	O9-C10-O7-C8
34	8	614	LMG	C37-C38-C39-C40
38	e	617	LMU	O1'-C1-C2-C3
41	Z	303	DGD	C2B-C3B-C4B-C5B
29	a	603	CLA	C10-C11-C12-C13
29	B	816	CLA	O1A-CGA-O2A-C1
29	B	832	CLA	O1A-CGA-O2A-C1
34	3	620	LMG	O10-C28-O8-C9
29	c	606	CLA	C16-C17-C18-C19
33	1	618	IHT	C02-C07-C18-C22
33	2	616	IHT	C10-C07-C18-C22
33	6	617	IHT	C02-C07-C18-C22
33	8	609	IHT	C10-C07-C18-C22
33	9	619	IHT	C10-C07-C18-C22
33	L	205	IHT	C02-C07-C18-C22
33	c	620	IHT	C10-C07-C18-C22
37	7	617	8CT	C02-C03-C10-C11
37	7	617	8CT	C04-C03-C10-C11
37	A	847	8CT	C02-C03-C10-C11
37	A	847	8CT	C04-C03-C10-C11
37	B	846	8CT	C02-C03-C10-C11
37	B	846	8CT	C04-C03-C10-C11
37	B	851	8CT	C02-C03-C10-C11
37	B	851	8CT	C04-C03-C10-C11
37	J	103	8CT	C02-C03-C10-C11
37	J	103	8CT	C04-C03-C10-C11
37	Z	309	8CT	C02-C03-C10-C11
37	Z	309	8CT	C04-C03-C10-C11
29	B	816	CLA	C10-C11-C12-C13
34	2	617	LMG	C13-C14-C15-C16
34	I	102	LMG	C11-C12-C13-C14
29	B	822	CLA	CBA-CGA-O2A-C1
29	B	828	CLA	CBA-CGA-O2A-C1
29	O	202	CLA	C5-C6-C7-C8
34	I	102	LMG	C10-C11-C12-C13
35	2	620	LHG	C23-C24-C25-C26
35	4	617	LHG	C7-C8-C9-C10
35	A	851	LHG	C7-C8-C9-C10
35	3	623	LHG	C13-C14-C15-C16
35	4	619	LHG	C9-C10-C11-C12
29	B	823	CLA	C15-C16-C17-C18
29	B	827	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	9	607	CLA	C4-C3-C5-C6
29	B	806	CLA	C4-C3-C5-C6
29	B	834	CLA	C4-C3-C5-C6
29	4	604	CLA	C2-C3-C5-C6
29	7	604	CLA	C2-C3-C5-C6
29	9	606	CLA	C6-C7-C8-C10
29	9	607	CLA	C2-C3-C5-C6
29	9	607	CLA	C11-C10-C8-C7
29	A	801	CLA	C12-C13-C15-C16
29	A	810	CLA	C2-C3-C5-C6
29	A	816	CLA	C6-C7-C8-C10
29	A	817	CLA	C2-C3-C5-C6
29	A	839	CLA	C11-C12-C13-C15
29	A	843	CLA	C11-C10-C8-C7
29	B	802	CLA	C6-C7-C8-C10
29	B	806	CLA	C11-C12-C13-C15
29	B	812	CLA	C2-C3-C5-C6
29	Z	306	CLA	C6-C7-C8-C10
29	b	603	CLA	C6-C7-C8-C10
29	d	602	CLA	C11-C10-C8-C7
29	e	606	CLA	C6-C7-C8-C10
29	b	604	CLA	C3-C5-C6-C7
29	9	606	CLA	O1A-CGA-O2A-C1
29	4	601	CLA	C5-C6-C7-C8
29	7	611	CLA	C5-C6-C7-C8
29	A	817	CLA	C5-C6-C7-C8
29	A	820	CLA	C8-C10-C11-C12
29	A	827	CLA	C5-C6-C7-C8
29	8	606	CLA	CBD-CGD-O2D-CED
29	9	608	CLA	C6-C7-C8-C10
34	3	618	LMG	C28-C29-C30-C31
29	4	611	CLA	CBA-CGA-O2A-C1
35	2	620	LHG	C24-C23-O8-C6
29	A	840	CLA	C2A-CAA-CBA-CGA
29	B	835	CLA	C2A-CAA-CBA-CGA
29	Z	301	CLA	C2A-CAA-CBA-CGA
29	A	821	CLA	C5-C6-C7-C8
29	e	611	CLA	C15-C16-C17-C18
29	B	822	CLA	C8-C10-C11-C12
29	K	101	CLA	C10-C11-C12-C13
29	a	604	CLA	C8-C10-C11-C12
34	8	614	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
35	4	619	LHG	C26-C27-C28-C29
30	1	610	KC2	C2B-C3B-CAB-CBB
30	3	606	KC2	C2C-C3C-CAC-CBC
30	4	605	KC2	C2B-C3B-CAB-CBB
30	6	610	KC2	C2C-C3C-CAC-CBC
30	6	613	KC2	C2C-C3C-CAC-CBC
30	b	605	KC2	C2B-C3B-CAB-CBB
30	d	610	KC2	C2B-C3B-CAB-CBB
30	e	609	KC2	C2B-C3B-CAB-CBB
29	c	607	CLA	C3-C5-C6-C7
34	I	102	LMG	C38-C39-C40-C41
41	Z	303	DGD	C2A-C3A-C4A-C5A
29	B	828	CLA	C10-C11-C12-C13
35	2	619	LHG	C15-C16-C17-C18
34	F	205	LMG	C11-C10-O7-C8
41	Z	303	DGD	C2B-C1B-O2G-C2G
35	7	619	LHG	O6-C4-C5-O7
35	A	851	LHG	O6-C4-C5-O7
37	F	201	8CT	C13-C14-C15-C16
37	R	203	8CT	C21-C23-C24-C25
35	B	849	LHG	C10-C11-C12-C13
41	Z	303	DGD	C6A-C7A-C8A-C9A
30	3	606	KC2	C4C-C3C-CAC-CBC
30	4	605	KC2	C4B-C3B-CAB-CBB
30	6	610	KC2	C4C-C3C-CAC-CBC
30	6	613	KC2	C4C-C3C-CAC-CBC
30	b	605	KC2	C4B-C3B-CAB-CBB
30	e	609	KC2	C4B-C3B-CAB-CBB
29	A	831	CLA	C5-C6-C7-C8
29	A	835	CLA	C5-C6-C7-C8
29	L	203	CLA	C5-C6-C7-C8
29	1	608	CLA	CBD-CGD-O2D-CED
35	A	851	LHG	C9-C10-C11-C12
29	B	816	CLA	C3-C5-C6-C7
34	I	102	LMG	C13-C14-C15-C16
35	B	849	LHG	C15-C16-C17-C18
35	5	619	LHG	O7-C5-C6-O8
35	d	619	LHG	C29-C30-C31-C32
29	Z	306	CLA	C11-C12-C13-C15
34	I	102	LMG	C32-C33-C34-C35
35	3	623	LHG	C31-C32-C33-C34
35	A	850	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	A	804	CLA	C13-C15-C16-C17
29	c	602	CLA	C10-C11-C12-C13
29	4	604	CLA	C4-C3-C5-C6
29	a	606	CLA	C4-C3-C5-C6
34	8	614	LMG	C28-C29-C30-C31
29	6	606	CLA	C2-C3-C5-C6
29	B	810	CLA	C2-C3-C5-C6
31	1	614	II0	C09-C21-C23-C25
31	1	616	II0	C09-C21-C23-C25
31	1	617	II0	C09-C21-C23-C25
31	2	613	II0	C09-C21-C23-C25
31	2	613	II0	C10-C22-C24-C26
31	2	615	II0	C10-C22-C24-C26
31	3	616	II0	C09-C21-C23-C25
31	5	614	II0	C10-C22-C24-C26
31	6	614	II0	C09-C21-C23-C25
31	7	613	II0	C10-C22-C24-C26
31	7	615	II0	C09-C21-C23-C25
31	7	615	II0	C10-C22-C24-C26
31	8	610	II0	C09-C21-C23-C25
31	8	611	II0	C09-C21-C23-C25
31	9	615	II0	C09-C21-C23-C25
31	9	615	II0	C10-C22-C24-C26
31	9	616	II0	C09-C21-C23-C25
31	9	616	II0	C10-C22-C24-C26
31	9	617	II0	C09-C21-C23-C25
31	9	617	II0	C10-C22-C24-C26
31	O	204	II0	C09-C21-C23-C25
31	a	613	II0	C10-C22-C24-C26
31	a	615	II0	C10-C22-C24-C26
31	b	612	II0	C10-C22-C24-C26
31	c	616	II0	C09-C21-C23-C25
31	c	618	II0	C10-C22-C24-C26
31	c	619	II0	C09-C21-C23-C25
31	d	613	II0	C10-C22-C24-C26
31	d	614	II0	C10-C22-C24-C26
31	d	615	II0	C09-C21-C23-C25
31	d	615	II0	C10-C22-C24-C26
31	d	616	II0	C10-C22-C24-C26
31	e	614	II0	C10-C22-C24-C26
33	1	618	IHT	C11-C21-C24-C26
33	2	616	IHT	C11-C21-C24-C26

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Mol	Chain	Res	Type	Atoms
33	9	619	IHT	C11-C21-C24-C26
38	4	618	LMU	C3'-C4'-O1B-C1B
38	7	620	LMU	C1-C2-C3-C4
29	6	604	CLA	C11-C10-C8-C9
29	8	615	CLA	C11-C12-C13-C14
29	A	839	CLA	C11-C12-C13-C14
29	B	806	CLA	C6-C7-C8-C9
29	B	809	CLA	C11-C12-C13-C14
29	B	832	CLA	C14-C13-C15-C16
29	d	602	CLA	C11-C10-C8-C9
29	e	606	CLA	C11-C10-C8-C9
29	3	605	CLA	C3-C5-C6-C7
29	9	608	CLA	C3-C5-C6-C7
38	e	617	LMU	C1-C2-C3-C4
38	4	618	LMU	C5'-C4'-O1B-C1B
35	2	619	LHG	C23-C24-C25-C26
29	8	603	CLA	C8-C10-C11-C12
29	a	609	CLA	C2C-C3C-CAC-CBC
35	d	619	LHG	C34-C35-C36-C37
29	Z	301	CLA	O1A-CGA-O2A-C1
29	2	602	CLA	C1A-C2A-CAA-CBA
29	2	612	CLA	C1A-C2A-CAA-CBA
29	3	611	CLA	C1A-C2A-CAA-CBA
29	4	601	CLA	C1A-C2A-CAA-CBA
29	5	608	CLA	C1A-C2A-CAA-CBA
29	5	612	CLA	C1A-C2A-CAA-CBA
29	6	605	CLA	C1A-C2A-CAA-CBA
29	6	611	CLA	C1A-C2A-CAA-CBA
29	7	608	CLA	C1A-C2A-CAA-CBA
29	8	603	CLA	C1A-C2A-CAA-CBA
29	9	602	CLA	C1A-C2A-CAA-CBA
29	A	804	CLA	C1A-C2A-CAA-CBA
29	A	809	CLA	C1A-C2A-CAA-CBA
29	A	812	CLA	C1A-C2A-CAA-CBA
29	A	816	CLA	C1A-C2A-CAA-CBA
29	A	817	CLA	C1A-C2A-CAA-CBA
29	A	822	CLA	C1A-C2A-CAA-CBA
29	A	828	CLA	C1A-C2A-CAA-CBA
29	A	831	CLA	C1A-C2A-CAA-CBA
29	A	842	CLA	C1A-C2A-CAA-CBA
29	A	844	CLA	C1A-C2A-CAA-CBA
29	B	811	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	B	815	CLA	C1A-C2A-CAA-CBA
29	B	827	CLA	C1A-C2A-CAA-CBA
29	B	831	CLA	C1A-C2A-CAA-CBA
29	F	202	CLA	C1A-C2A-CAA-CBA
29	F	203	CLA	C1A-C2A-CAA-CBA
29	L	204	CLA	C1A-C2A-CAA-CBA
29	O	203	CLA	C1A-C2A-CAA-CBA
29	Z	306	CLA	C1A-C2A-CAA-CBA
29	a	602	CLA	C1A-C2A-CAA-CBA
29	a	611	CLA	C1A-C2A-CAA-CBA
29	a	612	CLA	C1A-C2A-CAA-CBA
29	e	606	CLA	C1A-C2A-CAA-CBA
29	e	610	CLA	C1A-C2A-CAA-CBA
29	B	815	CLA	C16-C17-C18-C20
29	B	826	CLA	C16-C17-C18-C19
29	a	607	CLA	C16-C17-C18-C19
34	6	619	LMG	C11-C10-O7-C8
35	Z	310	LHG	C30-C31-C32-C33
37	A	847	8CT	C18-C19-C20-C21
37	B	845	8CT	C23-C24-C25-C26
37	J	103	8CT	C18-C19-C20-C21
35	A	851	LHG	C4-O6-P-O3
29	3	608	CLA	C3-C5-C6-C7
29	O	202	CLA	C3-C5-C6-C7
29	A	817	CLA	C13-C15-C16-C17
29	A	830	CLA	C5-C6-C7-C8
29	B	826	CLA	C8-C10-C11-C12
35	2	618	LHG	C24-C23-O8-C6
35	3	619	LHG	O6-C4-C5-C6
35	3	622	LHG	O6-C4-C5-C6
35	6	618	LHG	O6-C4-C5-C6
35	7	619	LHG	O6-C4-C5-C6
34	8	614	LMG	C15-C16-C17-C18
35	4	617	LHG	C24-C25-C26-C27
38	7	620	LMU	C2-C3-C4-C5
38	O	207	LMU	O5'-C5'-C6'-O6'
29	B	841	CLA	C3-C5-C6-C7
30	1	610	KC2	CAA-CBA-CGA-O1A
29	4	602	CLA	C10-C11-C12-C13
41	Z	303	DGD	C8A-C9A-CAA-CBA
29	7	612	CLA	CBA-CGA-O2A-C1
29	A	823	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
35	d	618	LHG	C1-C2-C3-O3
29	6	606	CLA	C4-C3-C5-C6
29	7	604	CLA	C4-C3-C5-C6
29	9	606	CLA	C4-C3-C5-C6
29	A	819	CLA	C4-C3-C5-C6
29	A	819	CLA	C2-C3-C5-C6
41	B	848	DGD	C3B-C4B-C5B-C6B
29	3	608	CLA	C5-C6-C7-C8
29	B	805	CLA	C10-C11-C12-C13
29	K	101	CLA	C8-C10-C11-C12
39	B	842	PQN	C15-C16-C17-C18
35	Z	310	LHG	O10-C23-O8-C6
29	9	607	CLA	C2A-CAA-CBA-CGA
29	B	820	CLA	C11-C12-C13-C14
34	3	620	LMG	C7-C8-C9-O8
34	F	205	LMG	O1-C7-C8-C9
35	2	620	LHG	C4-C5-C6-O8
35	4	617	LHG	C4-C5-C6-O8
35	B	849	LHG	C4-C5-C6-O8
35	Z	310	LHG	C4-C5-C6-O8
35	Z	310	LHG	C35-C36-C37-C38
35	a	618	LHG	C4-C5-C6-O8
29	B	818	CLA	CBD-CGD-O2D-CED
30	6	610	KC2	CAA-CBA-CGA-O1A
35	4	617	LHG	C11-C12-C13-C14
35	L	208	LHG	O10-C23-O8-C6
41	Z	303	DGD	C2G-C3G-O3G-C1D
35	2	619	LHG	C12-C13-C14-C15
29	8	615	CLA	C15-C16-C17-C18
38	J	104	LMU	C2B-C1B-O1B-C4'
29	9	606	CLA	C16-C17-C18-C19
35	c	621	LHG	C24-C25-C26-C27
34	8	614	LMG	C23-C24-C25-C26
35	7	619	LHG	C35-C36-C37-C38
35	8	613	LHG	C24-C25-C26-C27
41	B	848	DGD	CEB-CFB-CGB-CHB
29	B	802	CLA	C13-C15-C16-C17
35	L	208	LHG	C31-C32-C33-C34
36	3	621	SQD	C30-C31-C32-C33
35	3	619	LHG	C11-C12-C13-C14
38	e	617	LMU	C5-C6-C7-C8
29	A	836	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
38	7	620	LMU	O5'-C5'-C6'-O6'
38	J	104	LMU	O5B-C5B-C6B-O6B
29	6	605	CLA	C4-C3-C5-C6
29	8	604	CLA	C4-C3-C5-C6
29	A	810	CLA	C4-C3-C5-C6
29	b	604	CLA	C4-C3-C5-C6
29	c	606	CLA	C4-C3-C5-C6
29	e	604	CLA	C4-C3-C5-C6
29	c	603	CLA	O1D-CGD-O2D-CED
30	2	610	KC2	C2A-CAA-CBA-CGA
30	6	610	KC2	C2A-CAA-CBA-CGA
41	Z	303	DGD	C1B-C2B-C3B-C4B
29	4	606	CLA	C11-C12-C13-C14
29	R	202	CLA	C6-C7-C8-C9
35	3	619	LHG	C29-C30-C31-C32
29	A	810	CLA	CBD-CGD-O2D-CED
29	A	828	CLA	C15-C16-C17-C18
29	B	822	CLA	C10-C11-C12-C13
35	3	623	LHG	C35-C36-C37-C38
29	8	608	CLA	C10-C11-C12-C13
29	A	832	CLA	C2-C1-O2A-CGA
29	a	609	CLA	C2-C1-O2A-CGA
29	a	611	CLA	C2-C1-O2A-CGA
34	I	102	LMG	C18-C19-C20-C21
36	3	621	SQD	C11-C12-C13-C14
29	B	802	CLA	C3-C5-C6-C7
29	Z	306	CLA	C5-C6-C7-C8
29	c	602	CLA	C13-C15-C16-C17
34	I	102	LMG	C16-C17-C18-C19
38	7	620	LMU	C5-C6-C7-C8
29	A	829	CLA	CBA-CGA-O2A-C1
29	d	611	CLA	CBA-CGA-O2A-C1
35	3	622	LHG	O6-C4-C5-O7
35	6	618	LHG	O6-C4-C5-O7
29	1	602	CLA	C10-C11-C12-C13
34	F	205	LMG	C11-C12-C13-C14
29	A	812	CLA	C5-C6-C7-C8
29	b	611	CLA	C5-C6-C7-C8
38	4	618	LMU	O1'-C1-C2-C3
29	A	817	CLA	O1A-CGA-O2A-C1
29	B	822	CLA	O1A-CGA-O2A-C1
30	1	610	KC2	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	A	832	CLA	C15-C16-C17-C18
29	B	807	CLA	C13-C15-C16-C17
34	I	102	LMG	C2-C1-O1-C7
29	d	602	CLA	C16-C17-C18-C19
35	A	850	LHG	C34-C35-C36-C37
34	I	102	LMG	O8-C28-C29-C30
34	F	205	LMG	O1-C7-C8-O7
35	A	850	LHG	O7-C5-C6-O8
35	b	616	LHG	C26-C27-C28-C29
41	Z	303	DGD	CAB-CBB-CCB-CDB
29	B	813	CLA	C8-C10-C11-C12
29	b	608	CLA	O1A-CGA-O2A-C1
35	4	617	LHG	C15-C16-C17-C18
29	3	610	CLA	C4-C3-C5-C6
29	c	602	CLA	C4-C3-C5-C6
29	B	802	CLA	C5-C6-C7-C8
29	1	612	CLA	C6-C7-C8-C10
29	5	608	CLA	C11-C10-C8-C7
29	6	604	CLA	C11-C10-C8-C7
29	6	605	CLA	C2-C3-C5-C6
29	A	811	CLA	C12-C13-C15-C16
29	A	828	CLA	C11-C12-C13-C15
29	A	833	CLA	C11-C12-C13-C15
29	B	805	CLA	C11-C12-C13-C15
29	B	809	CLA	C11-C12-C13-C15
29	B	816	CLA	C11-C10-C8-C7
29	B	838	CLA	C6-C7-C8-C10
29	L	203	CLA	C6-C7-C8-C10
29	Z	301	CLA	C11-C10-C8-C7
29	a	604	CLA	C6-C7-C8-C10
29	b	604	CLA	C6-C7-C8-C10
29	c	606	CLA	C2-C3-C5-C6
29	c	607	CLA	C11-C12-C13-C15
29	c	608	CLA	C11-C10-C8-C7
29	e	604	CLA	C2-C3-C5-C6
29	e	606	CLA	C11-C10-C8-C7
29	A	839	CLA	C3-C5-C6-C7
34	8	614	LMG	C33-C34-C35-C36
29	5	608	CLA	C11-C10-C8-C9
29	6	608	CLA	C11-C10-C8-C9
29	A	811	CLA	C14-C13-C15-C16
29	A	826	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	A	839	CLA	C6-C7-C8-C9
29	B	802	CLA	C6-C7-C8-C9
29	B	803	CLA	C11-C10-C8-C9
29	B	812	CLA	C6-C7-C8-C9
29	B	821	CLA	C6-C7-C8-C9
29	B	835	CLA	C11-C10-C8-C9
29	B	835	CLA	C14-C13-C15-C16
29	L	203	CLA	C6-C7-C8-C9
29	Z	301	CLA	C11-C10-C8-C9
29	Z	306	CLA	C6-C7-C8-C9
29	b	604	CLA	C14-C13-C15-C16
29	c	606	CLA	C11-C10-C8-C9
29	c	606	CLA	C11-C12-C13-C14
29	e	606	CLA	C6-C7-C8-C9
35	B	849	LHG	C27-C28-C29-C30
29	B	831	CLA	CBA-CGA-O2A-C1
35	b	616	LHG	C24-C23-O8-C6
41	Z	303	DGD	C2A-C1A-O1G-C1G
30	Z	307	KC2	CAA-CBA-CGA-O2A
29	6	603	CLA	C2A-CAA-CBA-CGA
29	d	612	CLA	C15-C16-C17-C18
34	8	614	LMG	C24-C25-C26-C27
35	3	619	LHG	C34-C35-C36-C37
29	A	811	CLA	C10-C11-C12-C13
29	B	819	CLA	C5-C6-C7-C8
29	B	816	CLA	C11-C12-C13-C14
34	8	614	LMG	C29-C30-C31-C32
35	6	618	LHG	C27-C28-C29-C30
29	5	608	CLA	CBA-CGA-O2A-C1
29	A	830	CLA	CBA-CGA-O2A-C1
35	3	619	LHG	C24-C23-O8-C6
29	c	606	CLA	C15-C16-C17-C18
30	6	610	KC2	CAA-CBA-CGA-O2A
35	4	617	LHG	C31-C32-C33-C34
29	1	608	CLA	C4B-C3B-CAB-CBB
29	1	612	CLA	C4B-C3B-CAB-CBB
29	3	605	CLA	C4B-C3B-CAB-CBB
29	3	609	CLA	C4B-C3B-CAB-CBB
29	4	607	CLA	C4B-C3B-CAB-CBB
29	4	608	CLA	C4B-C3B-CAB-CBB
29	6	603	CLA	C4B-C3B-CAB-CBB
29	9	613	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	9	614	CLA	C4B-C3B-CAB-CBB
29	A	837	CLA	C4B-C3B-CAB-CBB
29	B	811	CLA	C4B-C3B-CAB-CBB
29	B	826	CLA	C4B-C3B-CAB-CBB
29	c	613	CLA	C4B-C3B-CAB-CBB
29	d	607	CLA	C4B-C3B-CAB-CBB
35	2	619	LHG	O6-C4-C5-C6
35	A	851	LHG	O6-C4-C5-C6
41	B	848	DGD	C1B-C2B-C3B-C4B
29	B	828	CLA	C8-C10-C11-C12
29	7	608	CLA	C4-C3-C5-C6
29	e	602	CLA	C4-C3-C5-C6
29	3	610	CLA	C2-C3-C5-C6
29	b	604	CLA	C2-C3-C5-C6
29	c	602	CLA	C2-C3-C5-C6
30	Z	307	KC2	CAA-CBA-CGA-O1A
29	9	601	CLA	C2C-C3C-CAC-CBC
29	2	602	CLA	CBA-CGA-O2A-C1
29	8	603	CLA	CBA-CGA-O2A-C1
35	A	851	LHG	C24-C23-O8-C6
29	7	604	CLA	C5-C6-C7-C8
35	4	619	LHG	C28-C29-C30-C31
41	Z	303	DGD	C5B-C6B-C7B-C8B
29	A	809	CLA	C3A-C2A-CAA-CBA
29	L	201	CLA	C3A-C2A-CAA-CBA
29	a	612	CLA	C3A-C2A-CAA-CBA
29	3	607	CLA	C5-C6-C7-C8
37	B	851	8CT	C16-C17-C18-C19
38	J	104	LMU	C2-C1-O1'-C1'
29	6	608	CLA	C3-C5-C6-C7
29	B	823	CLA	C3-C5-C6-C7
35	3	619	LHG	O10-C23-O8-C6
29	6	607	CLA	C6-C7-C8-C10
29	A	844	CLA	C16-C17-C18-C20
29	d	608	CLA	CBA-CGA-O2A-C1
35	B	849	LHG	C18-C19-C20-C21
29	2	605	CLA	C8-C10-C11-C12
29	A	825	CLA	C5-C6-C7-C8
29	B	839	CLA	C13-C15-C16-C17
34	2	617	LMG	O6-C5-C6-O5
35	3	619	LHG	C4-C5-C6-O8
35	5	619	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
35	6	618	LHG	C4-C5-C6-O8
35	8	613	LHG	C4-C5-C6-O8
35	d	619	LHG	C4-C5-C6-O8
36	3	621	SQD	O6-C44-C45-C46
37	K	103	8CT	C28-C29-C30-C35
41	B	848	DGD	O1G-C1G-C2G-C3G
34	3	620	LMG	O9-C10-O7-C8
41	Z	303	DGD	C8B-C9B-CAB-CBB
29	B	813	CLA	C3-C5-C6-C7
30	2	610	KC2	O1D-CGD-O2D-CED
29	F	204	CLA	C6-C7-C8-C9
29	9	606	CLA	C2-C3-C5-C6
29	1	612	CLA	O1D-CGD-O2D-CED
29	a	608	CLA	C8-C10-C11-C12
35	a	618	LHG	C4-O6-P-O3
35	8	613	LHG	C23-C24-C25-C26
29	B	828	CLA	O1A-CGA-O2A-C1
29	1	608	CLA	C3-C5-C6-C7
29	5	608	CLA	C3-C5-C6-C7
34	2	617	LMG	C4-C5-C6-O5
29	B	816	CLA	C2A-CAA-CBA-CGA
35	2	619	LHG	O6-C4-C5-O7
35	3	623	LHG	O6-C4-C5-O7
29	4	611	CLA	O1A-CGA-O2A-C1
34	2	617	LMG	O10-C28-O8-C9
35	4	617	LHG	O10-C23-O8-C6
29	A	804	CLA	C10-C11-C12-C13
29	1	608	CLA	C2B-C3B-CAB-CBB
29	3	605	CLA	C2B-C3B-CAB-CBB
29	3	609	CLA	C2B-C3B-CAB-CBB
29	6	603	CLA	C2B-C3B-CAB-CBB
29	9	614	CLA	C2B-C3B-CAB-CBB
29	c	613	CLA	C2B-C3B-CAB-CBB
35	7	618	LHG	O10-C23-O8-C6
29	A	817	CLA	C3-C5-C6-C7
29	3	603	CLA	C11-C12-C13-C14
29	3	607	CLA	C11-C12-C13-C14
29	9	602	CLA	C6-C7-C8-C10
29	A	803	CLA	C16-C17-C18-C19
29	B	818	CLA	C11-C12-C13-C14
29	B	820	CLA	C11-C12-C13-C15
29	R	202	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
34	6	619	LMG	C29-C30-C31-C32
35	b	616	LHG	C19-C20-C21-C22
29	7	608	CLA	C2-C1-O2A-CGA
29	A	807	CLA	C2-C1-O2A-CGA
29	c	602	CLA	C2-C1-O2A-CGA
29	d	602	CLA	C2-C1-O2A-CGA
29	B	805	CLA	CAA-CBA-CGA-O2A
29	6	602	CLA	C14-C13-C15-C16
29	8	603	CLA	C11-C12-C13-C14
29	A	831	CLA	C11-C12-C13-C14
29	a	604	CLA	C6-C7-C8-C9
29	a	606	CLA	C14-C13-C15-C16
29	b	606	CLA	C11-C10-C8-C9
29	c	606	CLA	C14-C13-C15-C16
29	c	607	CLA	C6-C7-C8-C9
29	A	823	CLA	C8-C10-C11-C12
29	F	202	CLA	C10-C11-C12-C13
29	b	607	CLA	C5-C6-C7-C8
29	b	610	CLA	C4-C3-C5-C6
30	6	610	KC2	C1A-C2A-CAA-CBA
35	3	622	LHG	C2-C3-O3-P
35	A	851	LHG	C10-C11-C12-C13
29	2	602	CLA	C2A-CAA-CBA-CGA
29	1	612	CLA	C11-C12-C13-C15
29	4	611	CLA	C16-C17-C18-C20
29	8	608	CLA	C16-C17-C18-C19
37	R	201	8CT	C02-C03-C10-C11
37	b	615	8CT	C04-C03-C10-C11
38	4	618	LMU	C7-C8-C9-C10
41	B	848	DGD	C8A-C9A-CAA-CBA
41	Z	303	DGD	C7A-C8A-C9A-CAA
29	4	603	CLA	C6-C7-C8-C9
35	b	616	LHG	C28-C29-C30-C31
29	F	204	CLA	C6-C7-C8-C10
35	3	623	LHG	O10-C23-O8-C6
38	7	620	LMU	C9-C10-C11-C12
38	J	104	LMU	C3-C4-C5-C6
35	b	616	LHG	O6-C4-C5-C6
36	3	621	SQD	C29-C30-C31-C32
29	2	605	CLA	C11-C10-C8-C7
29	5	608	CLA	C6-C7-C8-C10
29	6	602	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	6	608	CLA	C11-C10-C8-C7
29	7	602	CLA	C12-C13-C15-C16
29	8	608	CLA	C11-C10-C8-C7
29	A	804	CLA	C11-C12-C13-C15
29	A	822	CLA	C12-C13-C15-C16
29	A	823	CLA	C11-C10-C8-C7
29	A	826	CLA	C11-C10-C8-C7
29	B	803	CLA	C11-C12-C13-C15
29	B	815	CLA	C12-C13-C15-C16
29	B	821	CLA	C6-C7-C8-C10
29	B	826	CLA	C11-C12-C13-C15
29	B	828	CLA	C6-C7-C8-C10
29	B	835	CLA	C11-C10-C8-C7
29	B	835	CLA	C12-C13-C15-C16
29	K	101	CLA	C6-C7-C8-C10
29	Z	301	CLA	C6-C7-C8-C10
29	b	602	CLA	C6-C7-C8-C10
29	b	602	CLA	C11-C10-C8-C7
29	b	602	CLA	C11-C12-C13-C15
29	c	603	CLA	C6-C7-C8-C10
29	c	606	CLA	C11-C10-C8-C7
29	c	606	CLA	C11-C12-C13-C15
29	c	607	CLA	C6-C7-C8-C10
29	c	608	CLA	C6-C7-C8-C10
39	A	849	PQN	C16-C17-C18-C20
39	A	849	PQN	C22-C23-C25-C26
39	B	842	PQN	C21-C22-C23-C25
41	Z	303	DGD	CCA-CDA-CEA-CFA
29	A	818	CLA	C10-C11-C12-C13
37	B	845	8CT	C16-C17-C18-C19
37	B	846	8CT	C18-C19-C20-C21
35	6	618	LHG	C28-C29-C30-C31
34	3	618	LMG	C11-C12-C13-C14
29	9	606	CLA	C13-C15-C16-C17
34	I	102	LMG	C34-C35-C36-C37
29	A	816	CLA	C5-C6-C7-C8
29	2	602	CLA	C11-C12-C13-C14
35	7	619	LHG	C11-C10-C9-C8
29	B	820	CLA	C5-C6-C7-C8
29	1	601	CLA	CAD-CBD-CGD-O2D
29	1	609	CLA	CAD-CBD-CGD-O2D
29	3	608	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	5	603	CLA	CAD-CBD-CGD-O2D
29	5	608	CLA	CAD-CBD-CGD-O2D
29	7	608	CLA	CAD-CBD-CGD-O2D
29	7	611	CLA	CAD-CBD-CGD-O2D
29	8	615	CLA	CAD-CBD-CGD-O2D
29	9	601	CLA	CAD-CBD-CGD-O2D
29	A	805	CLA	CAD-CBD-CGD-O2D
29	A	807	CLA	CAD-CBD-CGD-O2D
29	A	824	CLA	CAD-CBD-CGD-O2D
29	A	829	CLA	CAD-CBD-CGD-O2D
29	B	813	CLA	CAD-CBD-CGD-O2D
29	B	815	CLA	CAD-CBD-CGD-O2D
29	B	821	CLA	CAD-CBD-CGD-O2D
29	B	836	CLA	CAD-CBD-CGD-O2D
29	B	840	CLA	CAD-CBD-CGD-O2D
29	a	604	CLA	CAD-CBD-CGD-O2D
29	a	605	CLA	CAD-CBD-CGD-O2D
29	b	610	CLA	CAD-CBD-CGD-O2D
29	c	612	CLA	CAD-CBD-CGD-O2D
29	c	613	CLA	CAD-CBD-CGD-O2D
29	d	602	CLA	CAD-CBD-CGD-O2D
29	e	601	CLA	CAD-CBD-CGD-O2D
29	e	607	CLA	CAD-CBD-CGD-O2D
29	e	610	CLA	CAD-CBD-CGD-O2D
29	e	611	CLA	CAD-CBD-CGD-O2D
30	2	610	KC2	C2C-C3C-CAC-CBC
30	3	606	KC2	C2B-C3B-CAB-CBB
30	4	605	KC2	C2C-C3C-CAC-CBC
30	7	606	KC2	C2C-C3C-CAC-CBC
30	Z	307	KC2	C2C-C3C-CAC-CBC
30	b	605	KC2	CAD-CBD-CGD-O2D
30	e	609	KC2	CAD-CBD-CGD-O2D
35	7	619	LHG	C6-C5-O7-C7
29	A	832	CLA	C13-C15-C16-C17
29	4	601	CLA	C2C-C3C-CAC-CBC
29	O	203	CLA	CBA-CGA-O2A-C1
35	6	618	LHG	C24-C23-O8-C6
29	L	203	CLA	C4-C3-C5-C6
29	B	810	CLA	C11-C12-C13-C15
34	8	614	LMG	O6-C1-O1-C7
41	Z	303	DGD	O1G-C1G-C2G-C3G
41	Z	303	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
29	A	823	CLA	O1A-CGA-O2A-C1
29	3	609	CLA	C15-C16-C17-C18
29	8	604	CLA	C15-C16-C17-C18
29	b	602	CLA	C8-C10-C11-C12
30	1	610	KC2	C4B-C3B-CAB-CBB
30	c	611	KC2	C4C-C3C-CAC-CBC
30	5	610	KC2	CAA-CBA-CGA-O1A
39	A	849	PQN	C23-C25-C26-C27
29	B	831	CLA	O1A-CGA-O2A-C1
29	B	839	CLA	C16-C17-C18-C19
39	B	842	PQN	C26-C27-C28-C30
35	7	618	LHG	C1-C2-C3-O3
29	1	602	CLA	CHA-CBD-CGD-O1D
29	1	613	CLA	CHA-CBD-CGD-O1D
29	2	612	CLA	CHA-CBD-CGD-O1D
29	2	612	CLA	CHA-CBD-CGD-O2D
29	3	604	CLA	CHA-CBD-CGD-O2D
29	3	610	CLA	CHA-CBD-CGD-O1D
29	3	612	CLA	CHA-CBD-CGD-O2D
29	5	612	CLA	CHA-CBD-CGD-O1D
29	5	612	CLA	CHA-CBD-CGD-O2D
29	7	604	CLA	CHA-CBD-CGD-O1D
29	7	612	CLA	CHA-CBD-CGD-O2D
29	9	611	CLA	CHA-CBD-CGD-O1D
29	9	611	CLA	CHA-CBD-CGD-O2D
29	A	806	CLA	CHA-CBD-CGD-O1D
29	A	806	CLA	CHA-CBD-CGD-O2D
29	A	820	CLA	CHA-CBD-CGD-O1D
29	A	820	CLA	CHA-CBD-CGD-O2D
29	B	808	CLA	CHA-CBD-CGD-O1D
29	B	808	CLA	CHA-CBD-CGD-O2D
29	B	814	CLA	CHA-CBD-CGD-O1D
29	B	814	CLA	CHA-CBD-CGD-O2D
29	B	824	CLA	CHA-CBD-CGD-O1D
29	B	828	CLA	CHA-CBD-CGD-O1D
29	B	828	CLA	CHA-CBD-CGD-O2D
29	L	207	CLA	CHA-CBD-CGD-O1D
29	L	207	CLA	CHA-CBD-CGD-O2D
29	R	202	CLA	CHA-CBD-CGD-O1D
29	R	202	CLA	CHA-CBD-CGD-O2D
29	c	606	CLA	CHA-CBD-CGD-O1D
29	d	604	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	d	604	CLA	CHA-CBD-CGD-O2D
30	5	610	KC2	CHA-CBD-CGD-O1D
30	5	610	KC2	CHA-CBD-CGD-O2D
29	B	809	CLA	C5-C6-C7-C8
29	7	612	CLA	O1A-CGA-O2A-C1
29	O	203	CLA	O1A-CGA-O2A-C1
35	3	619	LHG	O7-C5-C6-O8
35	6	618	LHG	O7-C5-C6-O8
35	B	849	LHG	O7-C5-C6-O8
35	a	618	LHG	O7-C5-C6-O8
41	Z	303	DGD	O2G-C2G-C3G-O3G
35	4	619	LHG	C10-C11-C12-C13
30	5	610	KC2	CAA-CBA-CGA-O2A
29	A	829	CLA	O1A-CGA-O2A-C1
35	4	617	LHG	C33-C34-C35-C36
35	5	619	LHG	O1-C1-C2-O2
29	4	607	CLA	C4-C3-C5-C6
29	A	804	CLA	C4-C3-C5-C6
29	B	815	CLA	C4-C3-C5-C6
29	d	611	CLA	O1A-CGA-O2A-C1
31	1	619	II0	C10-C22-C24-C26
31	2	615	II0	C09-C21-C23-C25
31	3	613	II0	C09-C21-C23-C25
31	3	615	II0	C10-C22-C24-C26
31	3	616	II0	C10-C22-C24-C26
31	3	617	II0	C09-C21-C23-C25
31	4	612	II0	C09-C21-C23-C25
31	4	612	II0	C10-C22-C24-C26
31	4	615	II0	C10-C22-C24-C26
31	5	614	II0	C09-C21-C23-C25
31	5	615	II0	C09-C21-C23-C25
31	5	615	II0	C10-C22-C24-C26
31	5	617	II0	C09-C21-C23-C25
31	5	617	II0	C10-C22-C24-C26
31	5	620	II0	C10-C22-C24-C26
31	6	616	II0	C09-C21-C23-C25
31	6	616	II0	C10-C22-C24-C26
31	7	614	II0	C09-C21-C23-C25
31	7	616	II0	C10-C22-C24-C26
31	8	610	II0	C10-C22-C24-C26
31	8	611	II0	C10-C22-C24-C26
31	B	843	II0	C09-C21-C23-C25

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Mol	Chain	Res	Type	Atoms
31	J	101	II0	C09-C21-C23-C25
31	O	204	II0	C10-C22-C24-C26
31	O	205	II0	C10-C22-C24-C26
31	R	204	II0	C10-C22-C24-C26
31	a	614	II0	C10-C22-C24-C26
31	b	614	II0	C10-C22-C24-C26
31	c	616	II0	C10-C22-C24-C26
31	c	618	II0	C09-C21-C23-C25
31	d	613	II0	C09-C21-C23-C25
32	1	615	II3	C16-C23-C27-C28
33	K	104	IHT	C11-C21-C24-C26
33	Z	302	IHT	C11-C21-C24-C26
35	3	619	LHG	C27-C28-C29-C30
29	A	804	CLA	C11-C12-C13-C14
29	B	803	CLA	C11-C12-C13-C14
29	B	805	CLA	C11-C10-C8-C9
29	B	815	CLA	C14-C13-C15-C16
39	B	842	PQN	C21-C22-C23-C24
29	9	613	CLA	O1D-CGD-O2D-CED
35	B	849	LHG	C13-C14-C15-C16
35	4	619	LHG	C23-C24-C25-C26
36	3	621	SQD	C5-C6-S-O8
35	a	618	LHG	C24-C25-C26-C27
29	A	843	CLA	C2A-CAA-CBA-CGA
29	A	816	CLA	CAA-CBA-CGA-O2A
35	L	208	LHG	C30-C31-C32-C33
29	b	602	CLA	C5-C6-C7-C8
35	A	850	LHG	C27-C28-C29-C30
35	4	617	LHG	C17-C18-C19-C20
29	6	602	CLA	C1A-C2A-CAA-CBA
29	6	603	CLA	C1A-C2A-CAA-CBA
29	7	611	CLA	C1A-C2A-CAA-CBA
29	A	814	CLA	C1A-C2A-CAA-CBA
29	a	601	CLA	C1A-C2A-CAA-CBA
29	A	843	CLA	C8-C10-C11-C12
29	4	611	CLA	C2-C1-O2A-CGA
29	8	605	CLA	C2-C1-O2A-CGA
35	3	619	LHG	C19-C20-C21-C22
35	A	850	LHG	C33-C34-C35-C36
37	A	847	8CT	C23-C24-C25-C26
35	2	618	LHG	C3-O3-P-O6
35	2	619	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
29	B	808	CLA	C4-C3-C5-C6
29	B	803	CLA	C10-C11-C12-C13
35	8	613	LHG	C2-C3-O3-P
35	3	623	LHG	C29-C30-C31-C32
35	4	619	LHG	C34-C35-C36-C37
34	3	618	LMG	O10-C28-O8-C9
29	1	601	CLA	C4B-C3B-CAB-CBB
29	1	604	CLA	C4B-C3B-CAB-CBB
29	1	609	CLA	C4B-C3B-CAB-CBB
29	3	611	CLA	C4B-C3B-CAB-CBB
29	3	612	CLA	C4B-C3B-CAB-CBB
29	5	601	CLA	C4B-C3B-CAB-CBB
29	5	605	CLA	C4B-C3B-CAB-CBB
29	5	609	CLA	C4B-C3B-CAB-CBB
29	5	613	CLA	C4B-C3B-CAB-CBB
29	8	615	CLA	C4B-C3B-CAB-CBB
29	A	805	CLA	C4B-C3B-CAB-CBB
29	A	833	CLA	C4B-C3B-CAB-CBB
29	B	806	CLA	C4B-C3B-CAB-CBB
29	B	808	CLA	C4B-C3B-CAB-CBB
29	B	837	CLA	C4B-C3B-CAB-CBB
29	L	201	CLA	C4B-C3B-CAB-CBB
29	Z	301	CLA	C4B-C3B-CAB-CBB
29	a	606	CLA	C4B-C3B-CAB-CBB
29	c	604	CLA	C4B-C3B-CAB-CBB
29	c	605	CLA	C4B-C3B-CAB-CBB
29	d	601	CLA	C4B-C3B-CAB-CBB
35	2	618	LHG	C3-O3-P-O4
35	2	618	LHG	C4-O6-P-O4
35	2	619	LHG	C3-O3-P-O4
35	2	619	LHG	C4-O6-P-O5
35	5	619	LHG	C3-O3-P-O4
35	8	613	LHG	C4-O6-P-O4
35	A	850	LHG	C4-O6-P-O4
35	A	851	LHG	C3-O3-P-O4
35	A	851	LHG	C4-O6-P-O4
35	a	618	LHG	C4-O6-P-O4
35	b	616	LHG	C3-O3-P-O5
35	c	621	LHG	C4-O6-P-O5
35	d	619	LHG	C3-O3-P-O4
35	d	619	LHG	C4-O6-P-O5
29	6	607	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	7	603	CLA	C6-C7-C8-C9
29	e	611	CLA	C16-C17-C18-C20
29	a	605	CLA	CBA-CGA-O2A-C1
29	a	609	CLA	C4C-C3C-CAC-CBC
35	4	617	LHG	C12-C13-C14-C15
38	4	618	LMU	C6-C7-C8-C9
35	A	850	LHG	C19-C20-C21-C22
29	5	608	CLA	O1A-CGA-O2A-C1
29	1	603	CLA	C3-C5-C6-C7
29	F	202	CLA	C11-C12-C13-C14
35	c	621	LHG	C11-C10-C9-C8
29	3	610	CLA	CAD-CBD-CGD-O1D
29	5	613	CLA	CAD-CBD-CGD-O1D
29	6	604	CLA	CAD-CBD-CGD-O1D
29	7	604	CLA	CAD-CBD-CGD-O1D
29	8	607	CLA	CAD-CBD-CGD-O1D
29	9	611	CLA	CAD-CBD-CGD-O1D
29	B	828	CLA	CAD-CBD-CGD-O1D
29	O	203	CLA	CAD-CBD-CGD-O1D
29	R	202	CLA	CAD-CBD-CGD-O1D
29	d	611	CLA	CAD-CBD-CGD-O1D
29	e	610	CLA	C2-C3-C5-C6
30	1	610	KC2	CAD-CBD-CGD-O1D
36	3	621	SQD	C5-C6-S-O9
29	A	833	CLA	CBD-CGD-O2D-CED
29	A	801	CLA	CAA-CBA-CGA-O2A
29	4	601	CLA	C4C-C3C-CAC-CBC
35	Z	310	LHG	C15-C16-C17-C18
29	A	830	CLA	O1A-CGA-O2A-C1
34	8	614	LMG	C18-C19-C20-C21
29	8	606	CLA	C6-C7-C8-C9
29	A	840	CLA	C6-C7-C8-C10
29	b	603	CLA	C4-C3-C5-C6
29	8	603	CLA	C11-C10-C8-C7
29	A	812	CLA	C3A-C2A-CAA-CBA
29	A	824	CLA	C6-C7-C8-C10
29	A	825	CLA	C6-C7-C8-C10
29	A	828	CLA	C11-C10-C8-C7
29	B	808	CLA	C2-C3-C5-C6
29	B	823	CLA	C6-C7-C8-C10
29	B	832	CLA	C6-C7-C8-C10
29	B	835	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	a	609	CLA	C11-C10-C8-C7
29	b	604	CLA	C11-C12-C13-C15
29	b	608	CLA	C11-C10-C8-C7
29	c	603	CLA	C12-C13-C15-C16
29	d	607	CLA	C11-C12-C13-C15
29	d	608	CLA	C11-C12-C13-C15
32	e	613	II3	C07-C04-C12-C21
35	8	613	LHG	O6-C4-C5-O7
37	4	616	8CT	C28-C29-C30-C31
37	7	617	8CT	C28-C29-C30-C31
37	A	846	8CT	C28-C29-C30-C31
37	A	852	8CT	C28-C29-C30-C31
37	B	851	8CT	C28-C29-C30-C31
37	I	101	8CT	C28-C29-C30-C31
37	J	103	8CT	C28-C29-C30-C31
37	K	103	8CT	C28-C29-C30-C31
37	R	201	8CT	C28-C29-C30-C31
37	R	203	8CT	C28-C29-C30-C31
37	Z	309	8CT	C28-C29-C30-C31
37	b	615	8CT	C28-C29-C30-C31
39	A	849	PQN	C17-C18-C20-C21
29	2	605	CLA	CAA-CBA-CGA-O2A
29	A	801	CLA	C5-C6-C7-C8
35	L	208	LHG	C7-C8-C9-C10
29	A	844	CLA	CBA-CGA-O2A-C1
34	F	205	LMG	C30-C31-C32-C33
35	4	617	LHG	C19-C20-C21-C22
34	3	620	LMG	C10-C11-C12-C13
41	B	848	DGD	C9B-CAB-CBB-CCB
34	I	102	LMG	O1-C7-C8-O7
35	3	623	LHG	O7-C5-C6-O8
35	d	619	LHG	O7-C5-C6-O8
36	3	621	SQD	O6-C44-C45-O47
41	B	848	DGD	O1G-C1G-C2G-O2G
35	b	616	LHG	C14-C15-C16-C17
38	O	207	LMU	C4B-C5B-C6B-O6B
35	7	618	LHG	C27-C28-C29-C30
29	A	833	CLA	C3-C5-C6-C7
35	d	618	LHG	C5-C4-O6-P
29	F	202	CLA	C4-C3-C5-C6
35	c	621	LHG	C24-C23-O8-C6
34	I	102	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
29	4	607	CLA	C2-C3-C5-C6
29	7	602	CLA	C14-C13-C15-C16
29	8	608	CLA	C11-C10-C8-C9
29	A	804	CLA	C6-C7-C8-C9
29	A	820	CLA	C6-C7-C8-C9
29	A	823	CLA	C11-C10-C8-C9
29	A	825	CLA	C6-C7-C8-C9
29	B	808	CLA	C6-C7-C8-C9
29	B	823	CLA	C6-C7-C8-C9
29	B	826	CLA	C11-C12-C13-C14
29	B	832	CLA	C6-C7-C8-C9
29	F	202	CLA	C11-C10-C8-C9
29	b	602	CLA	C11-C10-C8-C9
29	b	602	CLA	C11-C12-C13-C14
29	c	608	CLA	C6-C7-C8-C9
39	A	849	PQN	C24-C23-C25-C26
35	2	620	LHG	C24-C25-C26-C27
38	7	620	LMU	C6-C7-C8-C9
35	3	619	LHG	C15-C16-C17-C18
29	8	603	CLA	O1A-CGA-O2A-C1
29	B	803	CLA	C2A-CAA-CBA-CGA
29	R	202	CLA	CAA-CBA-CGA-O2A
37	A	847	8CT	C16-C17-C18-C19
29	1	612	CLA	C11-C12-C13-C14
29	3	603	CLA	C11-C12-C13-C15
29	A	803	CLA	C16-C17-C18-C20
35	2	620	LHG	C30-C31-C32-C33
35	2	618	LHG	O7-C5-C6-O8
29	1	609	CLA	C2B-C3B-CAB-CBB
29	4	604	CLA	C2B-C3B-CAB-CBB
29	4	607	CLA	C2B-C3B-CAB-CBB
29	4	611	CLA	C2B-C3B-CAB-CBB
29	5	602	CLA	C2B-C3B-CAB-CBB
29	5	605	CLA	C2B-C3B-CAB-CBB
29	5	609	CLA	C2B-C3B-CAB-CBB
29	6	605	CLA	C2B-C3B-CAB-CBB
29	7	608	CLA	C2B-C3B-CAB-CBB
29	8	608	CLA	C2B-C3B-CAB-CBB
29	8	615	CLA	C2B-C3B-CAB-CBB
29	9	613	CLA	C2B-C3B-CAB-CBB
29	A	805	CLA	C2B-C3B-CAB-CBB
29	A	837	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	B	811	CLA	C2B-C3B-CAB-CBB
29	B	823	CLA	C2B-C3B-CAB-CBB
29	B	826	CLA	C2B-C3B-CAB-CBB
29	B	836	CLA	C2B-C3B-CAB-CBB
29	L	207	CLA	C2B-C3B-CAB-CBB
29	Z	301	CLA	C2B-C3B-CAB-CBB
29	Z	304	CLA	C2B-C3B-CAB-CBB
29	c	604	CLA	C2B-C3B-CAB-CBB
29	B	823	CLA	C13-C15-C16-C17
29	L	204	CLA	C4C-C3C-CAC-CBC
35	6	618	LHG	C32-C33-C34-C35
29	2	602	CLA	O1A-CGA-O2A-C1
35	2	619	LHG	C11-C10-C9-C8
34	8	614	LMG	C30-C31-C32-C33
29	2	608	CLA	C10-C11-C12-C13
29	A	827	CLA	C13-C15-C16-C17
29	B	806	CLA	C3-C5-C6-C7
29	Z	301	CLA	C3-C5-C6-C7
29	6	605	CLA	CAA-CBA-CGA-O2A
34	F	205	LMG	C9-C8-O7-C10
35	8	613	LHG	O6-C4-C5-C6
29	b	603	CLA	C2A-CAA-CBA-CGA
29	d	603	CLA	C2A-CAA-CBA-CGA
29	L	204	CLA	C2C-C3C-CAC-CBC
29	B	841	CLA	CBA-CGA-O2A-C1
29	B	802	CLA	C2-C1-O2A-CGA
29	B	838	CLA	C2-C1-O2A-CGA
29	b	607	CLA	C2-C1-O2A-CGA
29	d	603	CLA	C2-C1-O2A-CGA
35	2	619	LHG	C7-C8-C9-C10
29	a	605	CLA	C5-C6-C7-C8
35	2	619	LHG	C2-C3-O3-P
29	B	811	CLA	CBA-CGA-O2A-C1
29	c	612	CLA	CBA-CGA-O2A-C1
29	d	608	CLA	O1A-CGA-O2A-C1
29	4	601	CLA	C4-C3-C5-C6
35	3	622	LHG	C11-C12-C13-C14
33	6	617	IHT	C10-C07-C18-C22
37	B	847	8CT	C04-C03-C10-C11
37	R	201	8CT	C04-C03-C10-C11
37	Z	308	8CT	C04-C03-C10-C11
29	A	804	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A	820	CLA	C10-C11-C12-C13
36	3	621	SQD	O47-C7-C8-C9
29	5	604	CLA	C6-C7-C8-C10
29	8	608	CLA	C16-C17-C18-C20
34	3	620	LMG	O7-C8-C9-O8
35	2	620	LHG	C3-O3-P-O6
35	B	849	LHG	C3-O3-P-O6
35	B	849	LHG	C4-O6-P-O3
35	A	851	LHG	C11-C12-C13-C14
35	L	208	LHG	C11-C10-C9-C8
29	1	613	CLA	O1D-CGD-O2D-CED
35	3	623	LHG	C4-C5-C6-O8
36	3	621	SQD	C44-C45-C46-O48
29	A	822	CLA	C4-C3-C5-C6
35	4	617	LHG	C16-C17-C18-C19
29	8	604	CLA	C2-C3-C5-C6
29	A	804	CLA	C12-C13-C15-C16
29	A	810	CLA	C11-C12-C13-C15
29	A	826	CLA	C11-C12-C13-C15
29	A	831	CLA	C11-C12-C13-C15
29	B	803	CLA	C11-C10-C8-C7
29	B	812	CLA	C6-C7-C8-C10
29	F	202	CLA	C2-C3-C5-C6
29	L	203	CLA	C2-C3-C5-C6
29	6	602	CLA	C11-C10-C8-C9
29	A	828	CLA	C11-C12-C13-C14
29	B	805	CLA	C11-C12-C13-C14
29	B	824	CLA	C11-C10-C8-C9
29	B	838	CLA	C6-C7-C8-C9
29	b	602	CLA	C6-C7-C8-C9
29	c	603	CLA	C14-C13-C15-C16
34	8	614	LMG	C11-C10-O7-C8
37	A	852	8CT	C16-C17-C18-C19
34	8	614	LMG	C36-C37-C38-C39
29	9	601	CLA	C4C-C3C-CAC-CBC
38	J	104	LMU	C5'-C4'-O1B-C1B
35	4	617	LHG	C32-C33-C34-C35
29	A	830	CLA	C3-C5-C6-C7
29	a	607	CLA	C4-C3-C5-C6
35	b	616	LHG	O1-C1-C2-O2
34	6	619	LMG	O8-C28-C29-C30
29	7	608	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	B	815	CLA	C2-C3-C5-C6
35	B	849	LHG	C17-C18-C19-C20
29	B	810	CLA	C11-C12-C13-C14
29	B	819	CLA	CBA-CGA-O2A-C1
35	6	618	LHG	C31-C32-C33-C34
29	6	603	CLA	CAA-CBA-CGA-O2A
35	3	619	LHG	C10-C11-C12-C13
29	1	602	CLA	C4B-C3B-CAB-CBB
29	4	611	CLA	C4B-C3B-CAB-CBB
29	5	602	CLA	C4B-C3B-CAB-CBB
29	5	607	CLA	C4B-C3B-CAB-CBB
29	7	608	CLA	C4B-C3B-CAB-CBB
29	7	609	CLA	C4B-C3B-CAB-CBB
29	8	608	CLA	C4B-C3B-CAB-CBB
29	A	822	CLA	C4B-C3B-CAB-CBB
29	B	815	CLA	C4B-C3B-CAB-CBB
29	B	823	CLA	C4B-C3B-CAB-CBB
29	B	836	CLA	C4B-C3B-CAB-CBB
29	Z	304	CLA	C4B-C3B-CAB-CBB
29	Z	305	CLA	C4B-C3B-CAB-CBB
29	b	606	CLA	C4B-C3B-CAB-CBB
29	c	603	CLA	C4B-C3B-CAB-CBB
29	A	844	CLA	C2A-CAA-CBA-CGA
29	e	611	CLA	C16-C17-C18-C19
29	8	601	CLA	CAA-CBA-CGA-O2A
29	5	611	CLA	CAA-CBA-CGA-O1A
29	8	602	CLA	CAA-CBA-CGA-O2A
35	b	616	LHG	O6-C4-C5-O7
37	4	616	8CT	C21-C23-C24-C25
30	4	605	KC2	C4C-C3C-CAC-CBC
30	Z	307	KC2	C4B-C3B-CAB-CBB
30	Z	307	KC2	C4C-C3C-CAC-CBC
30	d	610	KC2	C4B-C3B-CAB-CBB
29	3	607	CLA	C3-C5-C6-C7
29	6	603	CLA	CAA-CBA-CGA-O1A
29	e	601	CLA	CAA-CBA-CGA-O2A
29	4	606	CLA	C2-C3-C5-C6
35	7	619	LHG	C7-C8-C9-C10
29	4	606	CLA	C2-C1-O2A-CGA
29	A	823	CLA	C2-C1-O2A-CGA
29	B	841	CLA	C2-C1-O2A-CGA
29	a	602	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	a	605	CLA	C2-C1-O2A-CGA
29	b	604	CLA	C2-C1-O2A-CGA
29	A	822	CLA	C5-C6-C7-C8
29	B	810	CLA	C8-C10-C11-C12
29	F	202	CLA	C11-C12-C13-C15
29	5	604	CLA	CBD-CGD-O2D-CED
29	9	612	CLA	CAA-CBA-CGA-O1A
29	1	604	CLA	C2A-CAA-CBA-CGA
29	7	608	CLA	C2A-CAA-CBA-CGA
29	F	203	CLA	C2A-CAA-CBA-CGA
29	Z	306	CLA	C2A-CAA-CBA-CGA
35	Z	310	LHG	C9-C10-C11-C12
35	5	619	LHG	C5-C4-O6-P
29	A	811	CLA	C3A-C2A-CAA-CBA
29	A	843	CLA	C3A-C2A-CAA-CBA
29	5	606	CLA	CAA-CBA-CGA-O2A
34	I	102	LMG	C42-C43-C44-C45
34	I	102	LMG	C12-C13-C14-C15
35	b	616	LHG	C18-C19-C20-C21
37	A	846	8CT	C23-C24-C25-C26
37	B	846	8CT	C16-C17-C18-C19
37	I	101	8CT	C18-C19-C20-C21
37	Z	308	8CT	C16-C17-C18-C19
29	8	601	CLA	CAA-CBA-CGA-O1A
34	I	102	LMG	C31-C32-C33-C34
31	a	616	II0	C10-C22-C24-C26
29	1	602	CLA	C6-C7-C8-C9
29	4	610	CLA	C11-C12-C13-C14
29	A	810	CLA	C14-C13-C15-C16
29	A	811	CLA	C11-C10-C8-C9
29	A	819	CLA	C11-C10-C8-C9
29	A	825	CLA	C11-C10-C8-C9
29	A	832	CLA	C11-C10-C8-C9
29	A	837	CLA	C6-C7-C8-C9
29	B	805	CLA	C6-C7-C8-C9
29	B	807	CLA	C11-C12-C13-C14
31	d	616	II0	C38-C36-C40-C42
35	7	619	LHG	C4-C5-C6-O8
37	A	852	8CT	C39-C16-C17-C18
37	B	845	8CT	C40-C12-C13-C14
37	B	851	8CT	C40-C12-C13-C14
29	5	606	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	L	204	CLA	C2A-CAA-CBA-CGA
29	7	603	CLA	C6-C7-C8-C10
29	9	604	CLA	C6-C7-C8-C10
29	8	615	CLA	O2A-C1-C2-C3
29	B	823	CLA	O2A-C1-C2-C3
29	Z	305	CLA	O2A-C1-C2-C3
34	3	620	LMG	O6-C1-O1-C7
29	d	601	CLA	CAA-CBA-CGA-O1A
29	a	601	CLA	CAA-CBA-CGA-O1A
35	L	208	LHG	C4-C5-O7-C7
29	A	843	CLA	C4-C3-C5-C6
29	R	202	CLA	C4-C3-C5-C6
29	5	604	CLA	C1A-C2A-CAA-CBA
29	A	811	CLA	C1A-C2A-CAA-CBA
29	B	826	CLA	C1A-C2A-CAA-CBA
29	B	841	CLA	C1A-C2A-CAA-CBA
29	O	202	CLA	C1A-C2A-CAA-CBA
29	2	602	CLA	C6-C7-C8-C10
29	A	806	CLA	C12-C13-C15-C16
29	B	808	CLA	C6-C7-C8-C10
29	B	819	CLA	C11-C10-C8-C7
29	a	603	CLA	C6-C7-C8-C10
29	a	604	CLA	C11-C10-C8-C7
29	d	607	CLA	C12-C13-C15-C16
35	b	616	LHG	C13-C14-C15-C16
29	9	601	CLA	CAA-CBA-CGA-O2A
36	O	206	SQD	O48-C23-C24-C25
29	a	602	CLA	C5-C6-C7-C8
29	A	837	CLA	C16-C17-C18-C20
29	B	818	CLA	C11-C12-C13-C15
29	B	825	CLA	C16-C17-C18-C20
35	Z	310	LHG	C25-C26-C27-C28
29	c	603	CLA	C3-C5-C6-C7
29	a	604	CLA	C2A-CAA-CBA-CGA
29	c	604	CLA	C2A-CAA-CBA-CGA
29	4	607	CLA	C5-C6-C7-C8
29	c	602	CLA	C15-C16-C17-C18
35	b	616	LHG	C32-C33-C34-C35
35	d	619	LHG	C11-C10-C9-C8
41	Z	303	DGD	CBA-CCA-CDA-CEA
29	b	608	CLA	C8-C10-C11-C12
30	1	610	KC2	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
35	A	851	LHG	C14-C15-C16-C17
35	a	618	LHG	C5-C6-O8-C23
29	B	807	CLA	C15-C16-C17-C18
29	9	612	CLA	CAA-CBA-CGA-O2A
29	c	613	CLA	CAA-CBA-CGA-O2A
29	8	603	CLA	C4-C3-C5-C6
29	B	811	CLA	C4-C3-C5-C6
29	1	601	CLA	C2B-C3B-CAB-CBB
29	1	604	CLA	C2B-C3B-CAB-CBB
29	3	611	CLA	C2B-C3B-CAB-CBB
29	3	612	CLA	C2B-C3B-CAB-CBB
29	5	601	CLA	C2B-C3B-CAB-CBB
29	5	607	CLA	C2B-C3B-CAB-CBB
29	5	613	CLA	C2B-C3B-CAB-CBB
29	7	609	CLA	C2B-C3B-CAB-CBB
29	A	822	CLA	C2B-C3B-CAB-CBB
29	A	833	CLA	C2B-C3B-CAB-CBB
29	B	806	CLA	C2B-C3B-CAB-CBB
29	B	808	CLA	C2B-C3B-CAB-CBB
29	B	837	CLA	C2B-C3B-CAB-CBB
29	L	201	CLA	C2B-C3B-CAB-CBB
29	Z	305	CLA	C2B-C3B-CAB-CBB
29	a	606	CLA	C2B-C3B-CAB-CBB
29	b	606	CLA	C2B-C3B-CAB-CBB
29	c	603	CLA	C2B-C3B-CAB-CBB
29	c	605	CLA	C2B-C3B-CAB-CBB
29	d	601	CLA	C2B-C3B-CAB-CBB
29	d	605	CLA	C2B-C3B-CAB-CBB
29	e	601	CLA	C2B-C3B-CAB-CBB
29	A	843	CLA	CBA-CGA-O2A-C1
29	e	602	CLA	CBA-CGA-O2A-C1
29	Z	301	CLA	C8-C10-C11-C12
29	c	606	CLA	C3-C5-C6-C7
31	d	616	II0	C34-C36-C40-C42
37	A	852	8CT	C15-C16-C17-C18
37	B	845	8CT	C11-C12-C13-C14
37	B	851	8CT	C11-C12-C13-C14
29	5	611	CLA	CAA-CBA-CGA-O2A
29	B	804	CLA	CAA-CBA-CGA-O2A
29	a	601	CLA	CAA-CBA-CGA-O2A
29	c	613	CLA	CAA-CBA-CGA-O1A
41	Z	303	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
38	J	104	LMU	C3'-C4'-O1B-C1B
37	A	852	8CT	C18-C19-C20-C21
37	B	845	8CT	C12-C13-C14-C15
37	R	203	8CT	C16-C17-C18-C19
29	c	605	CLA	CAA-CBA-CGA-O2A
29	e	601	CLA	CAA-CBA-CGA-O1A
35	L	208	LHG	C27-C28-C29-C30
29	c	605	CLA	CAA-CBA-CGA-O1A
29	A	837	CLA	C3-C5-C6-C7
29	A	827	CLA	C4-C3-C5-C6
29	c	614	CLA	C4-C3-C5-C6
29	7	611	CLA	C2-C1-O2A-CGA
29	B	816	CLA	C2-C1-O2A-CGA
29	B	826	CLA	C2-C1-O2A-CGA
29	L	204	CLA	C2-C1-O2A-CGA
29	Z	304	CLA	C2-C1-O2A-CGA
29	B	811	CLA	C2-C3-C5-C6
29	a	607	CLA	C2-C3-C5-C6
34	I	102	LMG	C40-C41-C42-C43
29	a	605	CLA	O1A-CGA-O2A-C1
29	B	835	CLA	C5-C6-C7-C8
29	9	601	CLA	CAA-CBA-CGA-O1A
29	3	605	CLA	CAA-CBA-CGA-O2A
29	6	601	CLA	C2C-C3C-CAC-CBC
29	6	612	CLA	CAA-CBA-CGA-O2A
29	8	602	CLA	CAA-CBA-CGA-O1A
29	e	610	CLA	C4-C3-C5-C6
30	4	605	KC2	C1A-C2A-CAA-CBA
30	c	610	KC2	C1A-C2A-CAA-CBA
29	c	614	CLA	C2A-CAA-CBA-CGA
37	b	615	8CT	C02-C03-C10-C11
29	8	615	CLA	C10-C11-C12-C13
37	B	846	8CT	C23-C24-C25-C26
37	B	850	8CT	C12-C13-C14-C15
37	B	851	8CT	C12-C13-C14-C15
29	9	602	CLA	C4-C3-C5-C6
29	c	607	CLA	C4-C3-C5-C6
29	B	812	CLA	C8-C10-C11-C12
29	A	822	CLA	C2-C3-C5-C6
29	7	605	CLA	CAA-CBA-CGA-O2A
29	A	814	CLA	CAA-CBA-CGA-O2A
29	d	601	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	A	838	CLA	C16-C17-C18-C19
29	B	809	CLA	C16-C17-C18-C19
29	B	822	CLA	C16-C17-C18-C19
29	B	827	CLA	C16-C17-C18-C19
29	4	609	CLA	C3-C5-C6-C7
29	B	824	CLA	C10-C11-C12-C13
29	5	603	CLA	CAA-CBA-CGA-O2A
29	7	605	CLA	CAA-CBA-CGA-O1A
29	B	820	CLA	C2A-CAA-CBA-CGA
29	a	606	CLA	C2A-CAA-CBA-CGA
29	A	801	CLA	C3-C5-C6-C7
29	B	804	CLA	CAA-CBA-CGA-O1A
29	4	602	CLA	C4B-C3B-CAB-CBB
29	4	604	CLA	C4B-C3B-CAB-CBB
29	5	611	CLA	C4B-C3B-CAB-CBB
29	6	605	CLA	C4B-C3B-CAB-CBB
29	A	804	CLA	C4B-C3B-CAB-CBB
29	A	819	CLA	C4B-C3B-CAB-CBB
29	B	825	CLA	C4B-C3B-CAB-CBB
29	B	833	CLA	C4B-C3B-CAB-CBB
29	J	102	CLA	C4B-C3B-CAB-CBB
29	a	603	CLA	C4B-C3B-CAB-CBB
29	a	609	CLA	C4B-C3B-CAB-CBB
29	d	612	CLA	C4B-C3B-CAB-CBB
29	e	606	CLA	C4B-C3B-CAB-CBB
38	J	104	LMU	O1'-C1-C2-C3
35	2	620	LHG	O6-C4-C5-C6
29	6	604	CLA	C4-C3-C5-C6
29	B	837	CLA	C4-C3-C5-C6
39	A	849	PQN	C14-C13-C15-C16
29	4	609	CLA	C6-C7-C8-C10
29	A	823	CLA	C6-C7-C8-C10
29	A	843	CLA	C2-C3-C5-C6
29	B	838	CLA	C11-C12-C13-C15
29	b	606	CLA	C11-C10-C8-C7
34	6	619	LMG	C30-C31-C32-C33
34	6	619	LMG	C32-C33-C34-C35
37	Z	309	8CT	C18-C19-C20-C21
37	e	616	8CT	C23-C24-C25-C26
35	4	619	LHG	C5-C4-O6-P
29	B	805	CLA	CAA-CBA-CGA-O1A
29	4	610	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	B	826	CLA	C15-C16-C17-C18
29	b	608	CLA	C3-C5-C6-C7
29	A	814	CLA	CAA-CBA-CGA-O1A
29	B	819	CLA	CAA-CBA-CGA-O2A
29	a	605	CLA	CAA-CBA-CGA-O2A
35	Z	310	LHG	O7-C7-C8-C9
29	5	603	CLA	CAA-CBA-CGA-O1A
29	3	610	CLA	CAA-CBA-CGA-O2A
29	B	821	CLA	CAA-CBA-CGA-O2A
29	e	611	CLA	CAA-CBA-CGA-O2A
29	B	816	CLA	C4-C3-C5-C6
29	F	204	CLA	C2-C3-C5-C6
29	e	602	CLA	C2-C3-C5-C6
36	O	206	SQD	O10-C23-C24-C25
29	2	602	CLA	CAA-CBA-CGA-O2A
29	A	811	CLA	CAA-CBA-CGA-O2A
29	5	608	CLA	C6-C7-C8-C9
29	8	603	CLA	C11-C10-C8-C9
29	A	826	CLA	C14-C13-C15-C16
29	A	833	CLA	C11-C12-C13-C14
29	Z	301	CLA	C6-C7-C8-C9
29	b	608	CLA	C11-C10-C8-C9
29	d	608	CLA	C11-C12-C13-C14
35	A	851	LHG	C11-C10-C9-C8
35	Z	310	LHG	C26-C27-C28-C29
35	d	619	LHG	C35-C36-C37-C38
29	3	601	CLA	CAA-CBA-CGA-O1A
29	A	808	CLA	C3A-C2A-CAA-CBA
29	B	841	CLA	O1A-CGA-O2A-C1
29	c	612	CLA	O1A-CGA-O2A-C1
41	B	848	DGD	O1A-C1A-O1G-C1G
29	A	804	CLA	CAA-CBA-CGA-O2A
29	a	604	CLA	CAA-CBA-CGA-O2A
29	b	608	CLA	CAA-CBA-CGA-O2A
35	7	618	LHG	O7-C7-C8-C9
29	1	611	CLA	CAA-CBA-CGA-O1A
29	9	603	CLA	CAA-CBA-CGA-O2A
29	d	605	CLA	CAA-CBA-CGA-O1A
29	1	603	CLA	CAD-CBD-CGD-O2D
29	1	611	CLA	CAD-CBD-CGD-O2D
29	1	613	CLA	CAD-CBD-CGD-O2D
29	2	603	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	2	606	CLA	CAD-CBD-CGD-O2D
29	3	611	CLA	CAD-CBD-CGD-O2D
29	4	604	CLA	CAD-CBD-CGD-O2D
29	5	609	CLA	CAD-CBD-CGD-O2D
29	6	608	CLA	CAD-CBD-CGD-O2D
29	6	611	CLA	CAD-CBD-CGD-O2D
29	8	604	CLA	CAD-CBD-CGD-O2D
29	9	607	CLA	CAD-CBD-CGD-O2D
29	9	614	CLA	CAD-CBD-CGD-O2D
29	A	802	CLA	CAD-CBD-CGD-O2D
29	A	811	CLA	CAD-CBD-CGD-O2D
29	A	812	CLA	CAD-CBD-CGD-O2D
29	A	823	CLA	CAD-CBD-CGD-O2D
29	A	835	CLA	CAD-CBD-CGD-O2D
29	A	838	CLA	CAD-CBD-CGD-O2D
29	A	840	CLA	CAD-CBD-CGD-O2D
29	B	805	CLA	CAD-CBD-CGD-O2D
29	B	807	CLA	CAD-CBD-CGD-O2D
29	B	810	CLA	CAD-CBD-CGD-O2D
29	B	812	CLA	CAD-CBD-CGD-O2D
29	B	819	CLA	CAD-CBD-CGD-O2D
29	B	831	CLA	CAD-CBD-CGD-O2D
29	B	833	CLA	CAD-CBD-CGD-O2D
29	J	102	CLA	CAD-CBD-CGD-O2D
29	K	102	CLA	CAD-CBD-CGD-O2D
29	L	202	CLA	CAD-CBD-CGD-O2D
29	Z	306	CLA	CAD-CBD-CGD-O2D
29	a	602	CLA	CAD-CBD-CGD-O2D
29	b	601	CLA	CAD-CBD-CGD-O2D
29	b	603	CLA	CAD-CBD-CGD-O2D
29	c	614	CLA	CAD-CBD-CGD-O2D
29	d	601	CLA	CAD-CBD-CGD-O2D
29	d	605	CLA	CAD-CBD-CGD-O2D
29	d	606	CLA	CAD-CBD-CGD-O2D
29	e	604	CLA	CAD-CBD-CGD-O2D
30	6	613	KC2	C2B-C3B-CAB-CBB
30	7	606	KC2	CAD-CBD-CGD-O2D
30	Z	307	KC2	C2B-C3B-CAB-CBB
30	e	609	KC2	C2C-C3C-CAC-CBC
29	9	604	CLA	C6-C7-C8-C9
29	3	608	CLA	C8-C10-C11-C12
29	2	603	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	4	603	CLA	C2A-CAA-CBA-CGA
38	e	617	LMU	C2-C1-O1'-C1'
29	6	612	CLA	CAA-CBA-CGA-O1A
35	3	622	LHG	C13-C14-C15-C16
35	A	850	LHG	C11-C10-C9-C8
35	3	623	LHG	O7-C7-C8-C9
29	2	602	CLA	C4-C3-C5-C6
29	5	602	CLA	C4-C3-C5-C6
29	A	838	CLA	C16-C17-C18-C20
29	B	834	CLA	C3-C5-C6-C7
29	O	201	CLA	C3-C5-C6-C7
41	B	848	DGD	O6D-C5D-C6D-O5D
29	8	603	CLA	C2-C3-C5-C6
29	9	602	CLA	C2-C3-C5-C6
29	4	609	CLA	CAA-CBA-CGA-O2A
35	3	619	LHG	C30-C31-C32-C33
35	A	850	LHG	C4-C5-C6-O8
35	L	208	LHG	C2-C3-O3-P
29	A	844	CLA	O1A-CGA-O2A-C1
29	B	803	CLA	CAA-CBA-CGA-O2A
29	B	832	CLA	CAA-CBA-CGA-O2A
29	e	603	CLA	CAA-CBA-CGA-O2A
29	e	607	CLA	CAA-CBA-CGA-O1A
29	1	612	CLA	O2A-C1-C2-C3
29	4	606	CLA	O2A-C1-C2-C3
29	7	611	CLA	O2A-C1-C2-C3
29	8	605	CLA	O2A-C1-C2-C3
29	O	201	CLA	O2A-C1-C2-C3
29	c	606	CLA	O2A-C1-C2-C3
29	d	607	CLA	O2A-C1-C2-C3
41	Z	303	DGD	C5A-C6A-C7A-C8A
30	3	606	KC2	C4B-C3B-CAB-CBB
30	6	613	KC2	C4B-C3B-CAB-CBB
30	9	610	KC2	C4C-C3C-CAC-CBC
30	e	609	KC2	C4C-C3C-CAC-CBC
29	2	604	CLA	C2A-CAA-CBA-CGA
29	9	604	CLA	C2A-CAA-CBA-CGA
29	A	815	CLA	C2A-CAA-CBA-CGA
35	b	616	LHG	C35-C36-C37-C38
29	A	803	CLA	CAA-CBA-CGA-O2A
29	b	610	CLA	CAA-CBA-CGA-O2A
29	e	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	B	811	CLA	O1A-CGA-O2A-C1
29	e	607	CLA	CAA-CBA-CGA-O2A
29	L	203	CLA	C11-C12-C13-C15
35	3	619	LHG	C14-C15-C16-C17
35	8	613	LHG	C9-C10-C11-C12
29	1	602	CLA	CHA-CBD-CGD-O2D
29	1	613	CLA	CHA-CBD-CGD-O2D
29	2	608	CLA	CHA-CBD-CGD-O1D
29	2	608	CLA	CHA-CBD-CGD-O2D
29	3	601	CLA	CHA-CBD-CGD-O1D
29	3	610	CLA	CHA-CBD-CGD-O2D
29	4	602	CLA	CHA-CBD-CGD-O2D
29	4	603	CLA	CHA-CBD-CGD-O2D
29	4	611	CLA	CHA-CBD-CGD-O2D
29	5	602	CLA	CHA-CBD-CGD-O1D
29	5	602	CLA	CHA-CBD-CGD-O2D
29	5	611	CLA	CHA-CBD-CGD-O1D
29	5	611	CLA	CHA-CBD-CGD-O2D
29	6	604	CLA	CHA-CBD-CGD-O1D
29	7	604	CLA	CHA-CBD-CGD-O2D
29	7	605	CLA	CHA-CBD-CGD-O1D
29	7	605	CLA	CHA-CBD-CGD-O2D
29	9	602	CLA	CHA-CBD-CGD-O1D
29	9	603	CLA	CHA-CBD-CGD-O1D
29	9	603	CLA	CHA-CBD-CGD-O2D
29	9	606	CLA	CHA-CBD-CGD-O2D
29	9	608	CLA	CHA-CBD-CGD-O1D
29	9	609	CLA	CHA-CBD-CGD-O1D
29	9	609	CLA	CHA-CBD-CGD-O2D
29	9	612	CLA	CHA-CBD-CGD-O2D
29	A	819	CLA	CHA-CBD-CGD-O1D
29	A	819	CLA	CHA-CBD-CGD-O2D
29	A	842	CLA	CHA-CBD-CGD-O2D
29	B	813	CLA	CHA-CBD-CGD-O1D
29	B	818	CLA	CHA-CBD-CGD-O2D
29	B	820	CLA	CHA-CBD-CGD-O1D
29	B	820	CLA	CHA-CBD-CGD-O2D
29	O	202	CLA	CHA-CBD-CGD-O1D
29	O	202	CLA	CHA-CBD-CGD-O2D
29	O	203	CLA	CHA-CBD-CGD-O1D
29	a	601	CLA	CHA-CBD-CGD-O2D
29	a	606	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	a	608	CLA	CHA-CBD-CGD-O1D
29	a	608	CLA	CHA-CBD-CGD-O2D
29	b	611	CLA	CHA-CBD-CGD-O1D
29	b	611	CLA	CHA-CBD-CGD-O2D
29	c	601	CLA	CHA-CBD-CGD-O1D
29	c	601	CLA	CHA-CBD-CGD-O2D
29	c	602	CLA	CHA-CBD-CGD-O1D
29	c	602	CLA	CHA-CBD-CGD-O2D
29	c	608	CLA	CHA-CBD-CGD-O2D
29	e	602	CLA	CHA-CBD-CGD-O2D
29	e	603	CLA	CHA-CBD-CGD-O1D
29	e	603	CLA	CHA-CBD-CGD-O2D
30	2	610	KC2	CHA-CBD-CGD-O1D
30	7	610	KC2	CHA-CBD-CGD-O1D
30	7	610	KC2	CHA-CBD-CGD-O2D
30	c	610	KC2	CHA-CBD-CGD-O2D
29	9	603	CLA	CAA-CBA-CGA-O1A
29	A	839	CLA	CAA-CBA-CGA-O2A
29	a	602	CLA	CAA-CBA-CGA-O2A
29	B	812	CLA	C2C-C3C-CAC-CBC
29	B	816	CLA	C2-C3-C5-C6
29	R	202	CLA	C2-C3-C5-C6
29	9	607	CLA	C5-C6-C7-C8
29	B	832	CLA	C5-C6-C7-C8
35	c	621	LHG	O6-C4-C5-C6
29	5	604	CLA	C6-C7-C8-C9
29	A	823	CLA	CAA-CBA-CGA-O2A
29	B	806	CLA	CAA-CBA-CGA-O2A
34	I	102	LMG	O7-C8-C9-O8
41	B	848	DGD	O2G-C2G-C3G-O3G
35	Z	310	LHG	C7-C8-C9-C10
29	A	810	CLA	C15-C16-C17-C18
29	1	611	CLA	CAA-CBA-CGA-O2A
29	3	601	CLA	CAA-CBA-CGA-O2A
29	7	607	CLA	CAA-CBA-CGA-O1A
29	B	812	CLA	C4C-C3C-CAC-CBC
35	2	620	LHG	O10-C23-O8-C6
29	a	612	CLA	CAA-CBA-CGA-O2A
35	3	622	LHG	O7-C7-C8-C9
38	4	618	LMU	C4'-C5'-C6'-O6'
29	4	609	CLA	C2A-CAA-CBA-CGA
29	9	603	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	c	605	CLA	C2A-CAA-CBA-CGA
29	d	605	CLA	CAA-CBA-CGA-O2A
41	Z	303	DGD	CDA-CEA-CFA-CGA
29	7	608	CLA	CAA-CBA-CGA-O2A
29	B	813	CLA	CAA-CBA-CGA-O2A
35	b	616	LHG	C17-C18-C19-C20
29	4	601	CLA	C2-C3-C5-C6
29	8	615	CLA	C11-C10-C8-C7
29	A	810	CLA	C11-C10-C8-C7
29	B	805	CLA	C11-C10-C8-C7
29	B	837	CLA	C11-C10-C8-C7
29	b	603	CLA	C2-C3-C5-C6
31	1	619	II0	C09-C21-C23-C25
31	3	617	II0	C10-C22-C24-C26
31	6	615	II0	C10-C22-C24-C26
31	7	616	II0	C09-C21-C23-C25
29	A	818	CLA	C11-C12-C13-C14
29	A	825	CLA	C14-C13-C15-C16
29	A	828	CLA	C11-C10-C8-C9
29	A	833	CLA	C6-C7-C8-C9
29	B	820	CLA	C11-C10-C8-C9
29	B	822	CLA	C14-C13-C15-C16
29	K	101	CLA	C6-C7-C8-C9
29	a	603	CLA	C6-C7-C8-C9
29	a	604	CLA	C11-C10-C8-C9
29	d	607	CLA	C11-C12-C13-C14
29	5	611	CLA	C2B-C3B-CAB-CBB
29	B	825	CLA	C2B-C3B-CAB-CBB
29	L	203	CLA	C2B-C3B-CAB-CBB
29	B	820	CLA	CBA-CGA-O2A-C1
29	a	604	CLA	CBA-CGA-O2A-C1
34	8	614	LMG	O7-C10-C11-C12
29	b	602	CLA	C3-C5-C6-C7
35	4	617	LHG	C11-C10-C9-C8
29	8	605	CLA	C2A-CAA-CBA-CGA
29	6	601	CLA	C4C-C3C-CAC-CBC
41	B	848	DGD	C7A-C8A-C9A-CAA
29	B	809	CLA	CAA-CBA-CGA-O2A
29	B	812	CLA	CAA-CBA-CGA-O2A
35	3	619	LHG	O7-C7-C8-C9
29	A	811	CLA	CAA-CBA-CGA-O1A
29	b	610	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
35	7	618	LHG	O9-C7-C8-C9
29	A	817	CLA	C16-C17-C18-C19
29	3	607	CLA	C4-C3-C5-C6
29	A	821	CLA	C4-C3-C5-C6
35	5	619	LHG	O1-C1-C2-C3
29	a	604	CLA	CAA-CBA-CGA-O1A
29	e	603	CLA	CAA-CBA-CGA-O1A
29	e	611	CLA	CAA-CBA-CGA-O1A
29	6	607	CLA	CBA-CGA-O2A-C1
29	4	601	CLA	C3-C5-C6-C7
34	8	614	LMG	C12-C13-C14-C15
29	1	601	CLA	C1A-C2A-CAA-CBA
29	4	606	CLA	C1A-C2A-CAA-CBA
29	A	824	CLA	C1A-C2A-CAA-CBA
29	A	830	CLA	C1A-C2A-CAA-CBA
29	B	812	CLA	C1A-C2A-CAA-CBA
29	B	822	CLA	C1A-C2A-CAA-CBA
29	B	825	CLA	C1A-C2A-CAA-CBA
29	B	833	CLA	C1A-C2A-CAA-CBA
29	B	840	CLA	C1A-C2A-CAA-CBA
29	R	202	CLA	C1A-C2A-CAA-CBA
29	b	610	CLA	C1A-C2A-CAA-CBA
29	B	812	CLA	C16-C17-C18-C20
29	2	602	CLA	CAA-CBA-CGA-O1A
29	4	609	CLA	CAA-CBA-CGA-O1A
29	B	821	CLA	CAA-CBA-CGA-O1A
29	B	832	CLA	CAA-CBA-CGA-O1A
29	B	808	CLA	C5-C6-C7-C8
29	1	603	CLA	C2-C1-O2A-CGA
29	9	607	CLA	C2-C1-O2A-CGA
29	B	811	CLA	C2-C1-O2A-CGA
29	F	202	CLA	C2-C1-O2A-CGA
29	1	612	CLA	C8-C10-C11-C12
29	2	603	CLA	CBA-CGA-O2A-C1
29	A	839	CLA	CAA-CBA-CGA-O1A
29	B	809	CLA	CAA-CBA-CGA-O1A
35	3	623	LHG	O9-C7-C8-C9
37	B	844	8CT	C12-C13-C14-C15
34	3	618	LMG	O7-C10-C11-C12
29	A	841	CLA	C8-C10-C11-C12
35	d	618	LHG	C4-O6-P-O3
29	B	803	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	B	832	CLA	C16-C17-C18-C19
29	b	607	CLA	C11-C12-C13-C14
29	3	610	CLA	CAA-CBA-CGA-O1A
29	7	608	CLA	CAA-CBA-CGA-O1A
29	A	804	CLA	CAA-CBA-CGA-O1A
29	A	823	CLA	CAA-CBA-CGA-O1A
29	4	611	CLA	C15-C16-C17-C18
29	c	608	CLA	C5-C6-C7-C8
29	3	612	CLA	CAA-CBA-CGA-O2A
34	8	614	LMG	C8-C9-O8-C28
29	4	606	CLA	C4-C3-C5-C6
29	K	101	CLA	C4-C3-C5-C6
29	7	603	CLA	C5-C6-C7-C8
34	F	205	LMG	O9-C10-O7-C8
29	d	607	CLA	C3-C5-C6-C7
35	6	618	LHG	C33-C34-C35-C36
41	Z	303	DGD	O1B-C1B-C2B-C3B
29	1	613	CLA	C4B-C3B-CAB-CBB
29	2	604	CLA	C4B-C3B-CAB-CBB
29	2	609	CLA	C4B-C3B-CAB-CBB
29	4	606	CLA	C4B-C3B-CAB-CBB
29	6	607	CLA	C4B-C3B-CAB-CBB
29	9	601	CLA	C4B-C3B-CAB-CBB
29	A	810	CLA	C4B-C3B-CAB-CBB
29	A	836	CLA	C4B-C3B-CAB-CBB
29	B	841	CLA	C4B-C3B-CAB-CBB
29	F	202	CLA	C4B-C3B-CAB-CBB
29	K	102	CLA	C4B-C3B-CAB-CBB
29	L	203	CLA	C4B-C3B-CAB-CBB
29	c	607	CLA	C4B-C3B-CAB-CBB
29	d	605	CLA	C4B-C3B-CAB-CBB
29	e	601	CLA	C4B-C3B-CAB-CBB
35	B	849	LHG	C3-O3-P-O5
35	B	849	LHG	C4-O6-P-O5
35	a	618	LHG	C4-O6-P-O5
35	b	616	LHG	C4-O6-P-O5
35	c	621	LHG	C3-O3-P-O4
29	B	819	CLA	CAA-CBA-CGA-O1A
34	8	614	LMG	O9-C10-C11-C12
35	3	623	LHG	O6-C4-C5-C6
37	Z	308	8CT	C02-C03-C10-C11
29	e	602	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	A	803	CLA	CAA-CBA-CGA-O1A
29	B	812	CLA	CAA-CBA-CGA-O1A
29	a	605	CLA	CAA-CBA-CGA-O1A
29	a	612	CLA	CAA-CBA-CGA-O1A
29	9	607	CLA	C4C-C3C-CAC-CBC
29	7	602	CLA	C13-C15-C16-C17
29	9	609	CLA	C2C-C3C-CAC-CBC
29	A	811	CLA	C2A-CAA-CBA-CGA
29	B	803	CLA	CAA-CBA-CGA-O1A
29	B	806	CLA	CAA-CBA-CGA-O1A
29	a	602	CLA	CAA-CBA-CGA-O1A
34	3	620	LMG	C30-C31-C32-C33
29	1	601	CLA	CAA-CBA-CGA-O2A
29	L	201	CLA	CAA-CBA-CGA-O2A
29	d	608	CLA	C10-C11-C12-C13
29	2	605	CLA	CAD-CBD-CGD-O1D
29	5	606	CLA	CAD-CBD-CGD-O1D
29	9	603	CLA	CAD-CBD-CGD-O1D
29	A	811	CLA	CAD-CBD-CGD-O1D
29	A	818	CLA	CAD-CBD-CGD-O1D
29	A	819	CLA	CAD-CBD-CGD-O1D
29	B	812	CLA	CAD-CBD-CGD-O1D
29	B	839	CLA	CAD-CBD-CGD-O1D
29	c	604	CLA	CAD-CBD-CGD-O1D
30	3	606	KC2	CAD-CBD-CGD-O1D
30	6	613	KC2	CAD-CBD-CGD-O1D
34	F	205	LMG	C7-C8-O7-C10
35	Z	310	LHG	O9-C7-C8-C9
35	c	621	LHG	O10-C23-C24-C25
29	B	820	CLA	C8-C10-C11-C12
39	A	849	PQN	C18-C20-C21-C22
29	3	610	CLA	C6-C7-C8-C9
29	B	821	CLA	C11-C10-C8-C9
29	B	828	CLA	C11-C10-C8-C9
29	a	603	CLA	C11-C10-C8-C9
29	b	604	CLA	C11-C12-C13-C14
39	A	849	PQN	C19-C18-C20-C21
29	3	603	CLA	C5-C6-C7-C8
29	B	835	CLA	C13-C15-C16-C17
29	d	602	CLA	C13-C15-C16-C17
29	e	611	CLA	C8-C10-C11-C12
29	b	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	3	612	CLA	CAA-CBA-CGA-O1A
29	7	607	CLA	CAA-CBA-CGA-O2A
35	2	618	LHG	C25-C26-C27-C28
29	3	604	CLA	C2A-CAA-CBA-CGA
29	1	608	CLA	CAA-CBA-CGA-O2A
29	7	602	CLA	CAA-CBA-CGA-O2A
29	A	838	CLA	C3-C5-C6-C7
34	F	205	LMG	O10-C28-C29-C30
35	7	618	LHG	O10-C23-C24-C25
29	A	841	CLA	C4-C3-C5-C6
35	B	849	LHG	C11-C10-C9-C8
29	1	601	CLA	C3A-C2A-CAA-CBA
29	4	607	CLA	C11-C10-C8-C7
29	4	610	CLA	C11-C12-C13-C15
29	5	602	CLA	C2-C3-C5-C6
29	9	607	CLA	C6-C7-C8-C10
29	A	809	CLA	C11-C10-C8-C7
29	A	817	CLA	C6-C7-C8-C10
29	A	841	CLA	C11-C10-C8-C7
29	B	812	CLA	C3A-C2A-CAA-CBA
29	B	824	CLA	C11-C10-C8-C7
29	B	830	CLA	C11-C10-C8-C7
29	F	202	CLA	C11-C10-C8-C7
29	R	202	CLA	C3A-C2A-CAA-CBA
29	a	603	CLA	C11-C10-C8-C7
29	c	603	CLA	C11-C10-C8-C7
35	2	620	LHG	O6-C4-C5-O7
35	a	618	LHG	O6-C4-C5-O7
37	B	850	8CT	C28-C29-C30-C31
37	Z	308	8CT	C28-C29-C30-C31
29	A	816	CLA	CAA-CBA-CGA-O1A
29	A	829	CLA	CAA-CBA-CGA-O1A
35	c	621	LHG	O9-C7-C8-C9
29	2	608	CLA	CAA-CBA-CGA-O2A
29	A	829	CLA	CAA-CBA-CGA-O2A
29	b	604	CLA	CAA-CBA-CGA-O2A
29	c	603	CLA	CAA-CBA-CGA-O2A
29	d	604	CLA	CAA-CBA-CGA-O2A
35	A	850	LHG	O8-C23-C24-C25
29	2	608	CLA	CAA-CBA-CGA-O1A
29	B	813	CLA	CAA-CBA-CGA-O1A
29	b	604	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	b	608	CLA	CAA-CBA-CGA-O1A
37	B	844	8CT	C23-C24-C25-C26
37	L	206	8CT	C23-C24-C25-C26
37	b	615	8CT	C12-C13-C14-C15
29	4	603	CLA	CAA-CBA-CGA-O2A
29	Z	306	CLA	CAA-CBA-CGA-O2A
29	b	606	CLA	CAA-CBA-CGA-O2A
29	b	607	CLA	CAA-CBA-CGA-O2A
35	B	849	LHG	O8-C23-C24-C25
34	3	618	LMG	C29-C30-C31-C32
41	B	848	DGD	CDB-CEB-CFB-CGB
29	9	607	CLA	C13-C15-C16-C17
29	B	808	CLA	C10-C11-C12-C13
29	c	602	CLA	C5-C6-C7-C8
29	b	607	CLA	CAA-CBA-CGA-O1A
38	e	617	LMU	C4B-C5B-C6B-O6B
35	c	621	LHG	C10-C11-C12-C13
29	A	815	CLA	C8-C10-C11-C12
29	A	837	CLA	C15-C16-C17-C18
29	a	604	CLA	C5-C6-C7-C8
29	O	201	CLA	CAA-CBA-CGA-O2A
29	A	802	CLA	C5-C6-C7-C8
29	K	101	CLA	C15-C16-C17-C18
29	c	608	CLA	C8-C10-C11-C12
29	A	803	CLA	C2A-CAA-CBA-CGA
29	A	824	CLA	C2A-CAA-CBA-CGA
29	B	807	CLA	C2A-CAA-CBA-CGA
29	A	802	CLA	C6-C7-C8-C10
29	b	601	CLA	CAA-CBA-CGA-O2A
34	2	617	LMG	C29-C30-C31-C32

There are no ring outliers.

90 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	3	614	II0	1	0
29	5	612	CLA	1	0
29	B	823	CLA	1	0
31	5	614	II0	2	0
29	Z	304	CLA	1	0
29	B	834	CLA	1	0
29	7	609	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	c	611	KC2	3	0
29	4	611	CLA	2	0
29	9	611	CLA	2	0
29	B	816	CLA	2	0
29	L	202	CLA	1	0
29	d	612	CLA	1	0
38	O	207	LMU	4	0
31	2	614	II0	1	0
29	c	601	CLA	2	0
40	C	102	SF4	1	0
30	b	609	KC2	1	0
31	4	614	II0	1	0
37	4	616	8CT	1	0
29	O	203	CLA	2	0
31	a	615	II0	1	0
29	A	834	CLA	1	0
33	6	617	IHT	1	0
29	Z	306	CLA	1	0
29	e	610	CLA	1	0
29	c	614	CLA	2	0
38	4	618	LMU	1	0
29	c	609	CLA	1	0
29	1	601	CLA	1	0
29	L	201	CLA	1	0
33	a	617	IHT	1	0
29	1	605	CLA	1	0
29	9	606	CLA	1	0
29	B	815	CLA	1	0
31	a	616	II0	1	0
29	8	603	CLA	1	0
29	9	604	CLA	2	0
33	9	619	IHT	1	0
29	1	611	CLA	2	0
29	B	835	CLA	1	0
29	B	826	CLA	1	0
31	4	613	II0	1	0
29	b	604	CLA	1	0
33	c	620	IHT	1	0
29	A	810	CLA	2	0
29	7	612	CLA	1	0
29	1	613	CLA	1	0
31	5	620	II0	1	0

Continued on next page...

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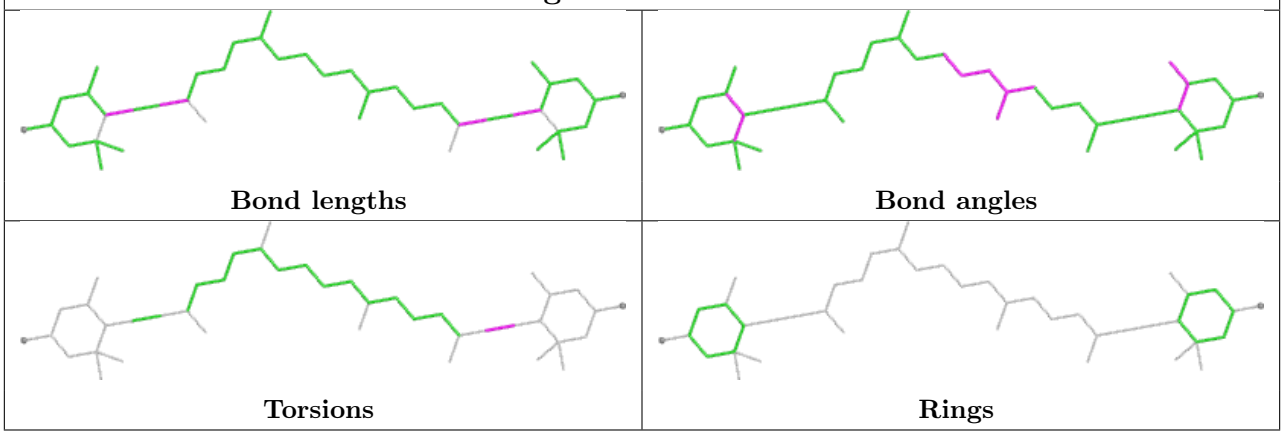
Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	Z	303	DGD	1	0
33	d	617	IHT	1	0
29	7	611	CLA	2	0
29	8	605	CLA	1	0
29	A	824	CLA	1	0
29	B	808	CLA	1	0
33	2	616	IHT	1	0
29	A	836	CLA	2	0
29	A	821	CLA	1	0
37	F	201	8CT	1	0
29	e	611	CLA	2	0
29	A	842	CLA	1	0
38	7	620	LMU	1	0
31	8	610	II0	1	0
29	5	609	CLA	2	0
29	O	201	CLA	2	0
37	7	617	8CT	1	0
29	A	823	CLA	1	0
29	B	803	CLA	1	0
35	L	208	LHG	1	0
29	A	844	CLA	1	0
29	8	608	CLA	1	0
29	B	809	CLA	1	0
29	5	604	CLA	2	0
29	5	608	CLA	1	0
29	9	608	CLA	1	0
29	c	612	CLA	1	0
29	2	612	CLA	1	0
29	8	615	CLA	1	0
31	1	614	II0	2	0
29	a	603	CLA	1	0
29	1	609	CLA	1	0
29	6	612	CLA	1	0
29	c	602	CLA	1	0
29	B	818	CLA	3	0
29	1	604	CLA	1	0
29	b	610	CLA	1	0
38	J	104	LMU	1	0
29	B	832	CLA	1	0
29	A	826	CLA	2	0
32	b	613	II3	1	0

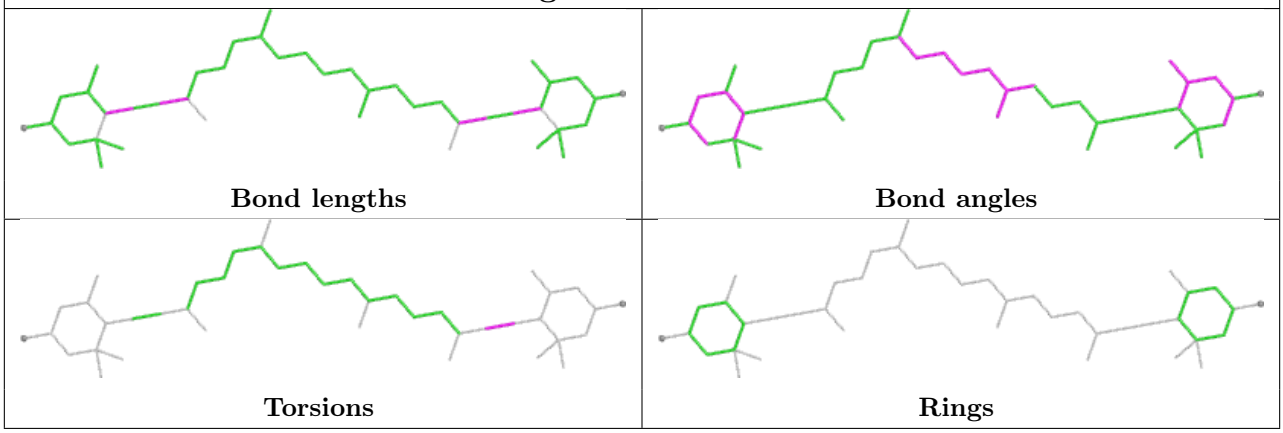
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

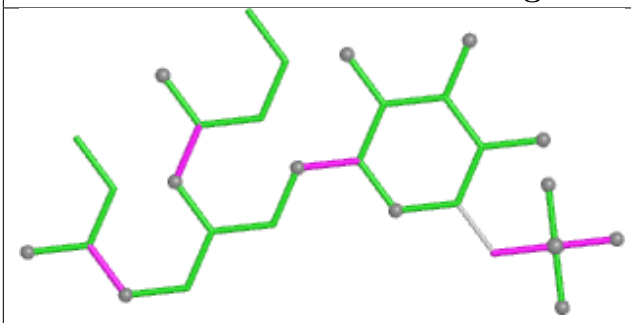
Ligand II0 4 615



Ligand II0 O 205



Ligand SQD O 206



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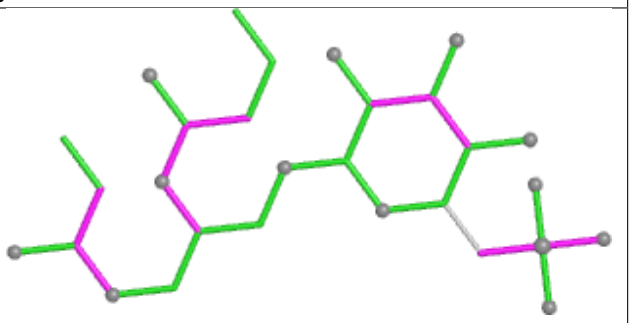
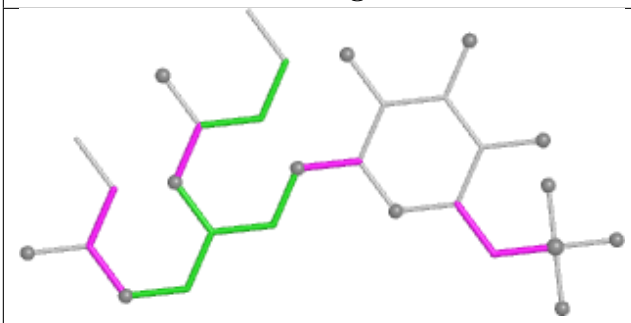
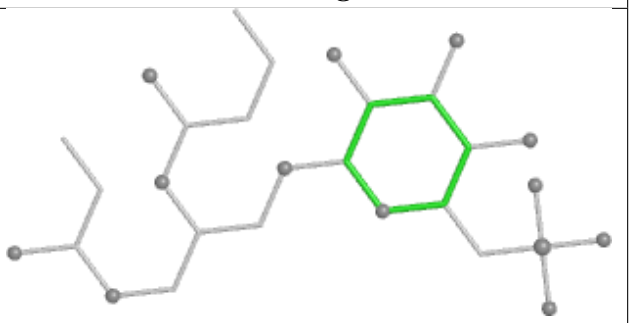


Bond angles

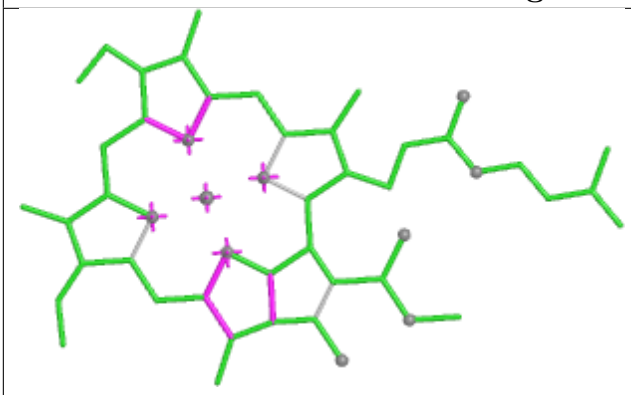


Torsions

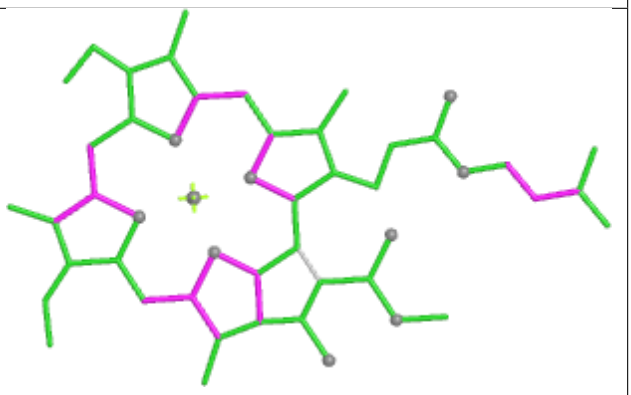


Rings

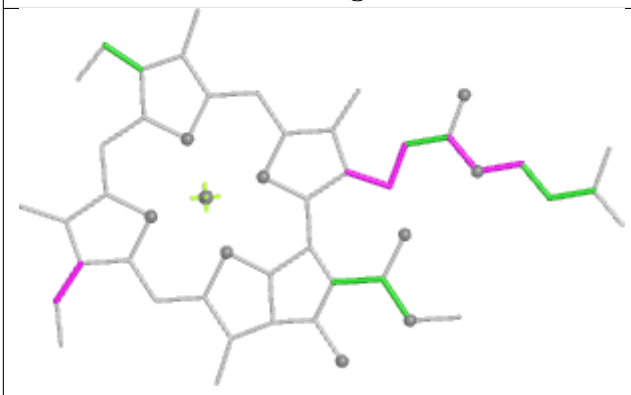
Ligand CLA L 204



Bond lengths



Bond angles



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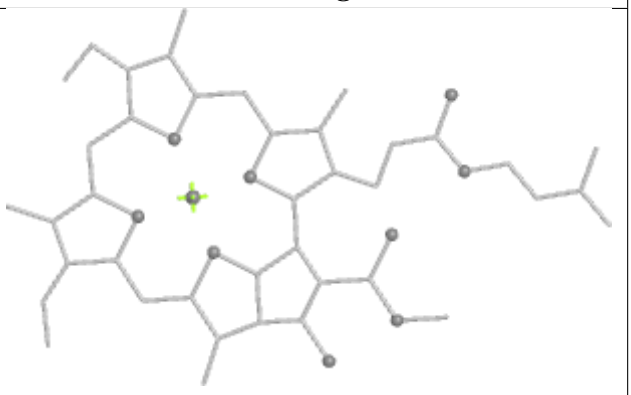
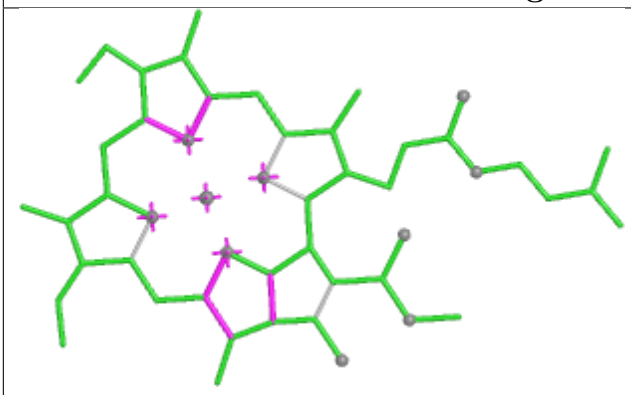
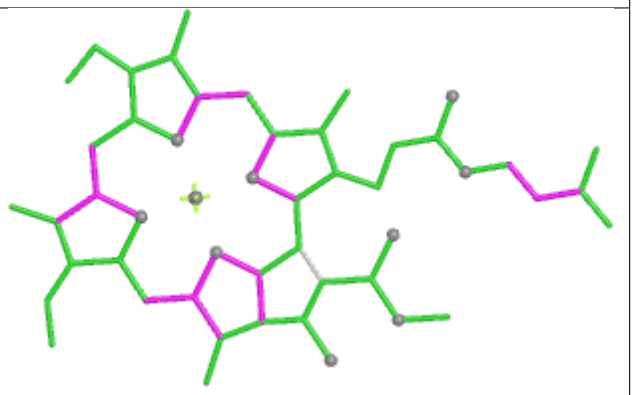


Rings

Ligand CLA Z 305



Bond lengths



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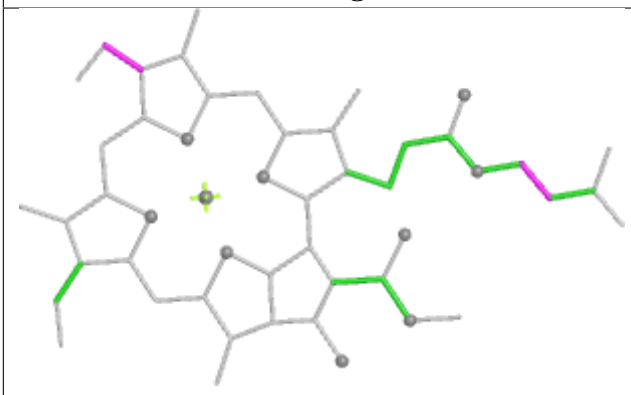

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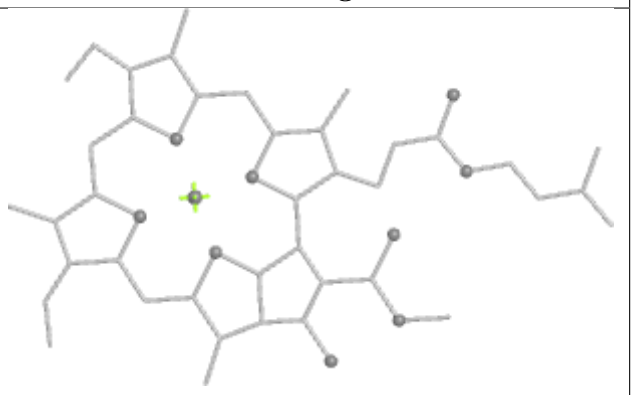
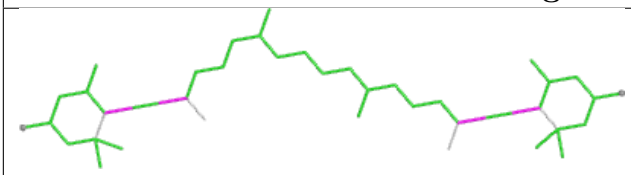


Rings

Ligand II0 3 614



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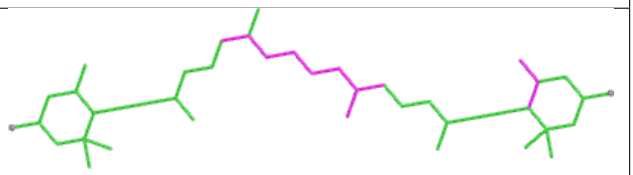
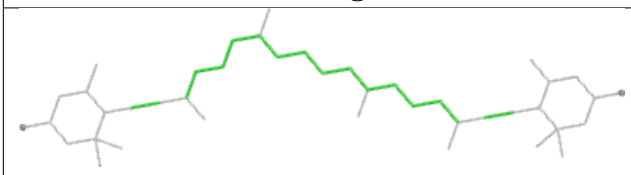


Bond angles



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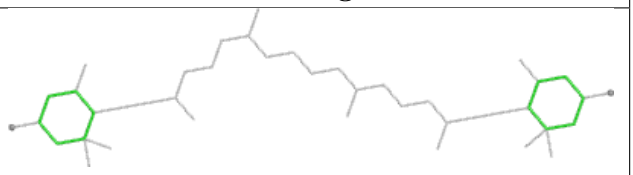
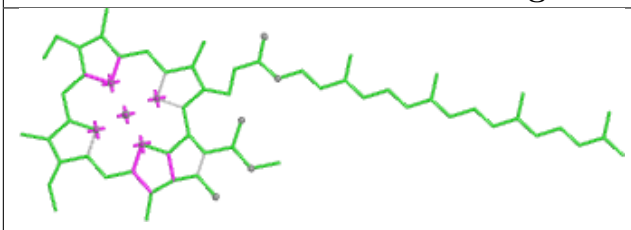


Rings

Ligand CLA 4 608



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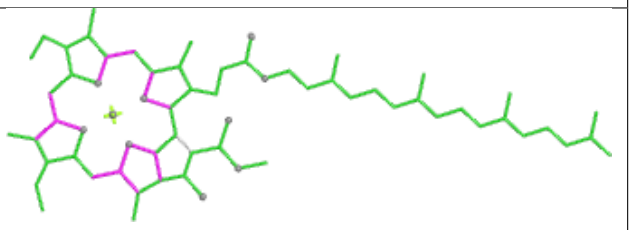

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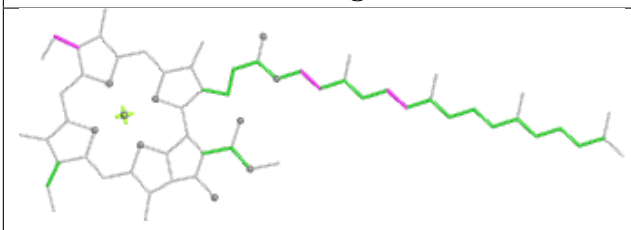

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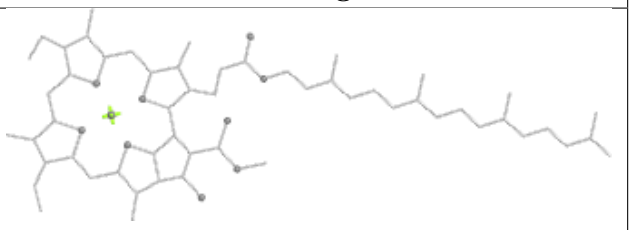
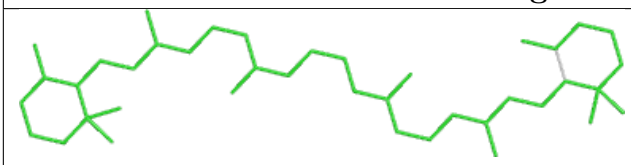


Rings

Ligand 8CT b 615



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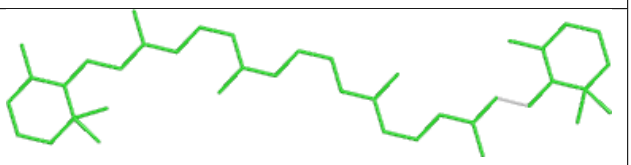

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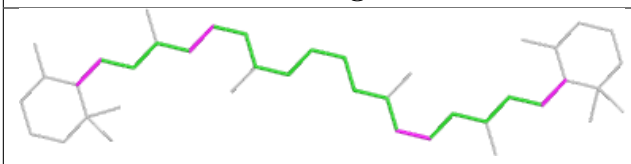

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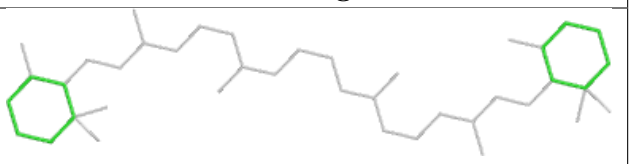
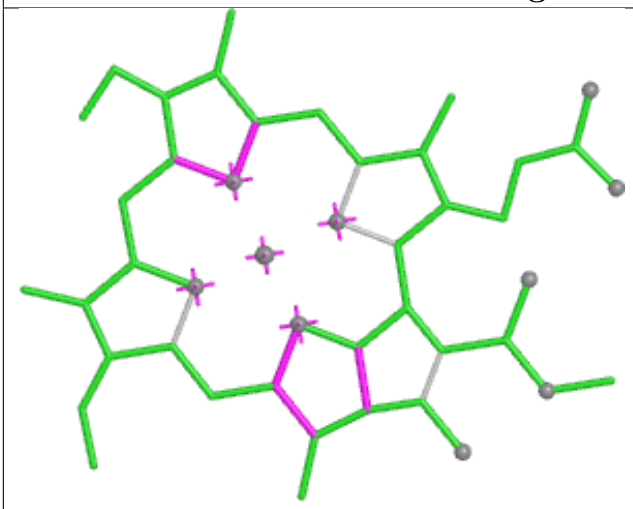


Rings

Ligand CLA 5 612



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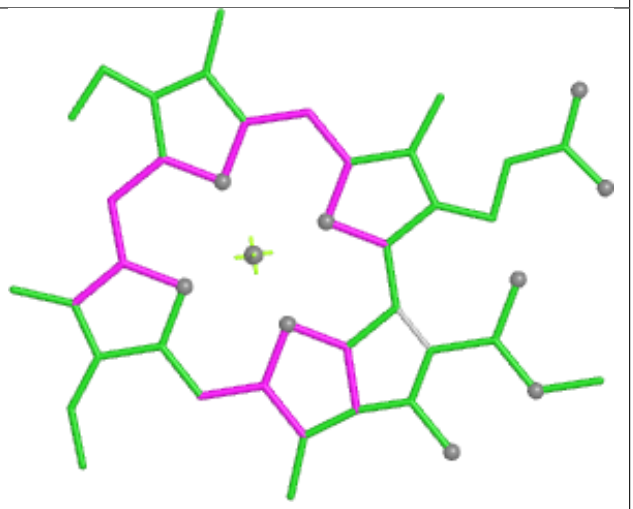

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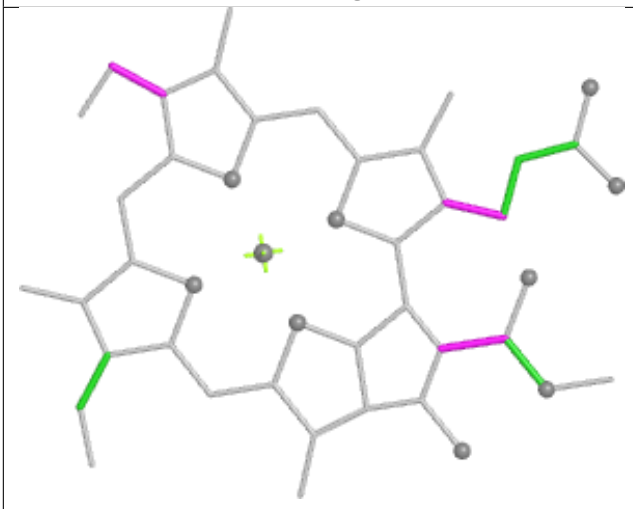
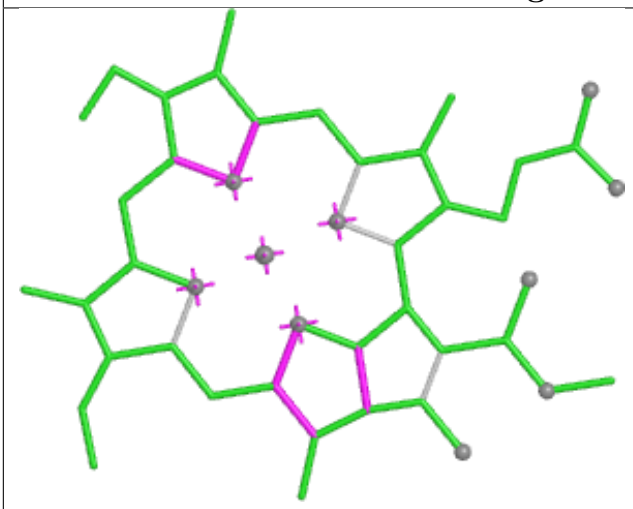


Torsions



Rings

Ligand CLA d 605



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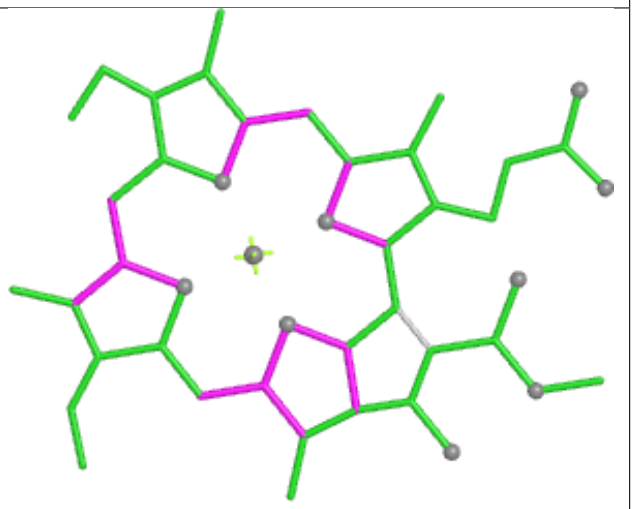

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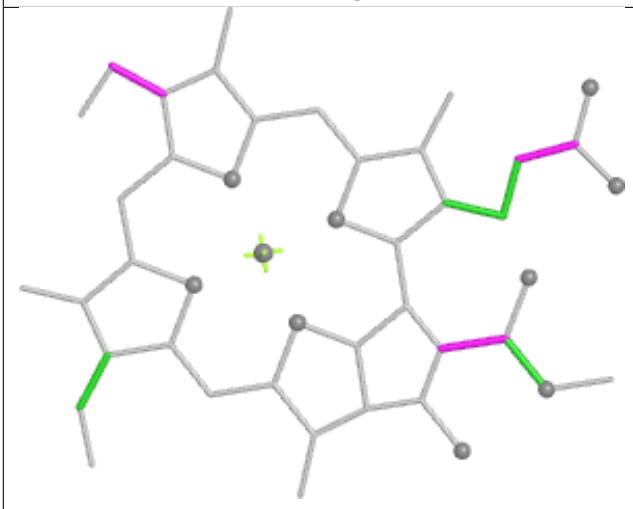
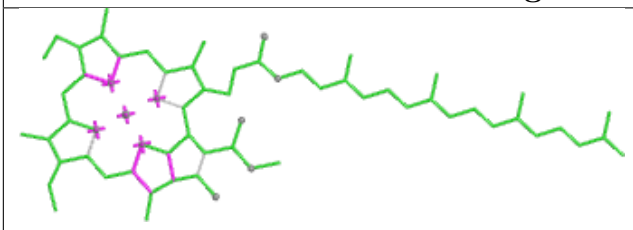


Torsions



Rings

Ligand CLA B 823



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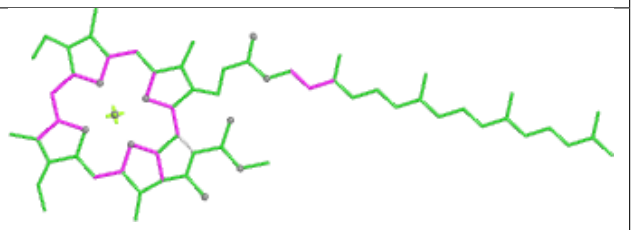

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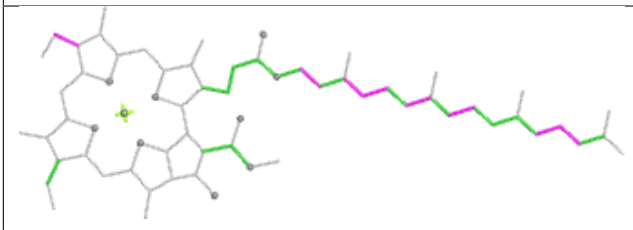

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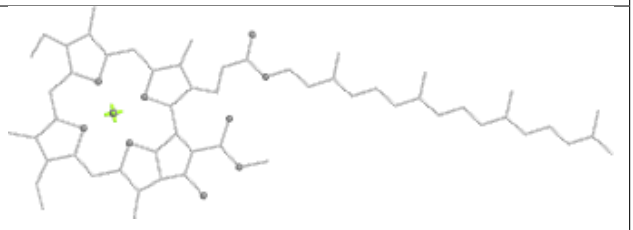
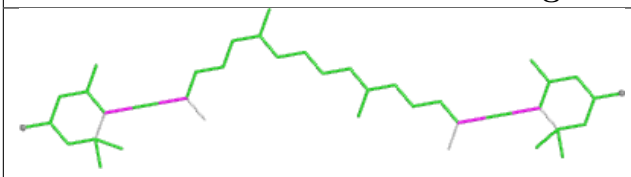
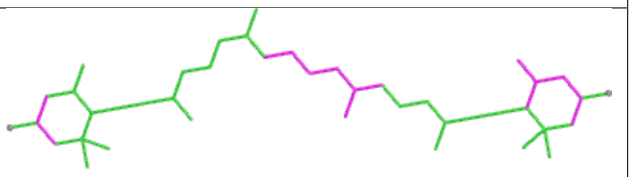
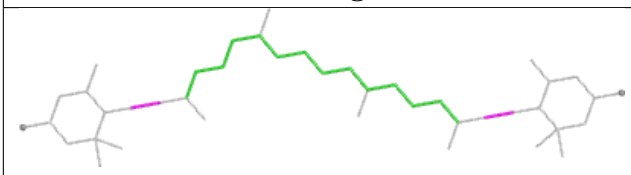
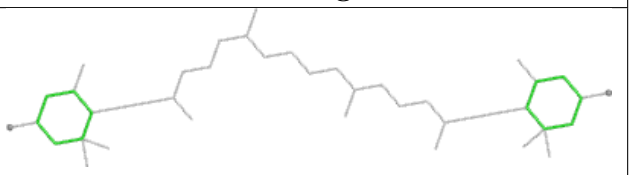


Rings

Ligand II0 5 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

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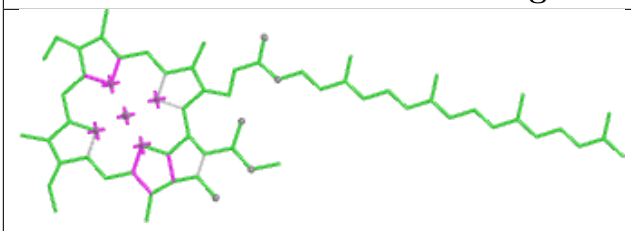
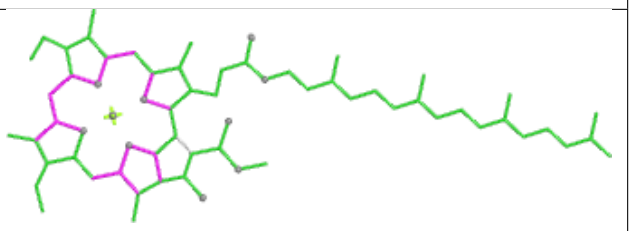
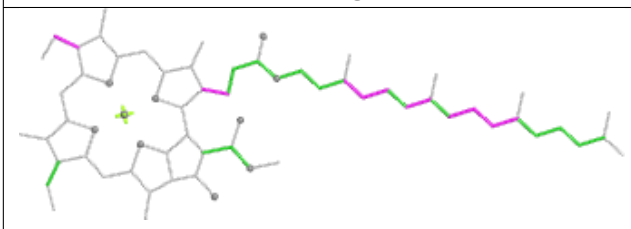
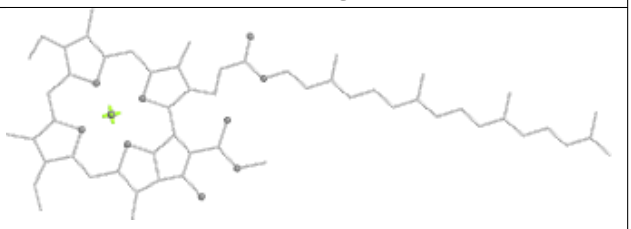
 Bond lengths	 Bond angles
 Torsions	 Rings

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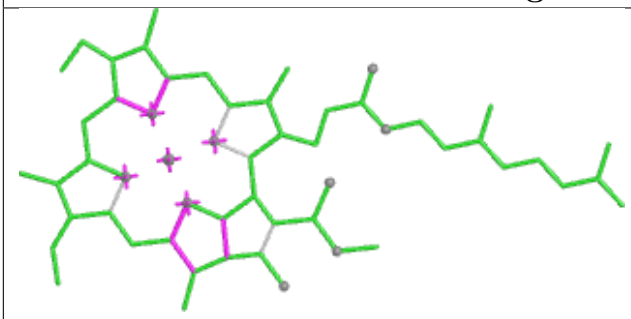
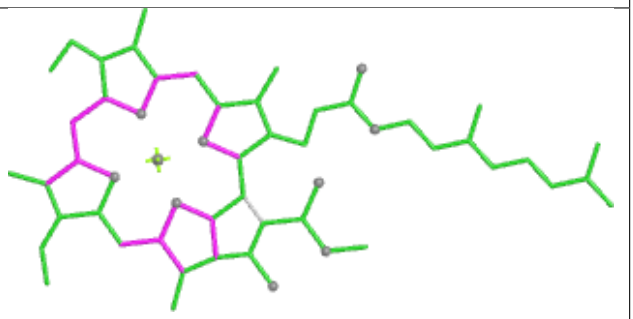
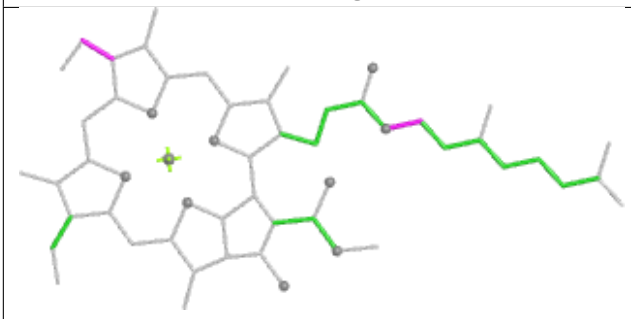


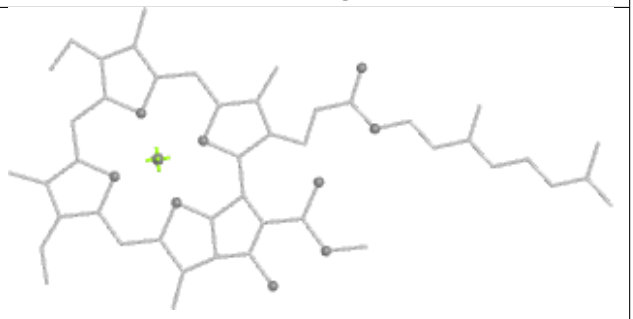
Bond lengths



Bond angles

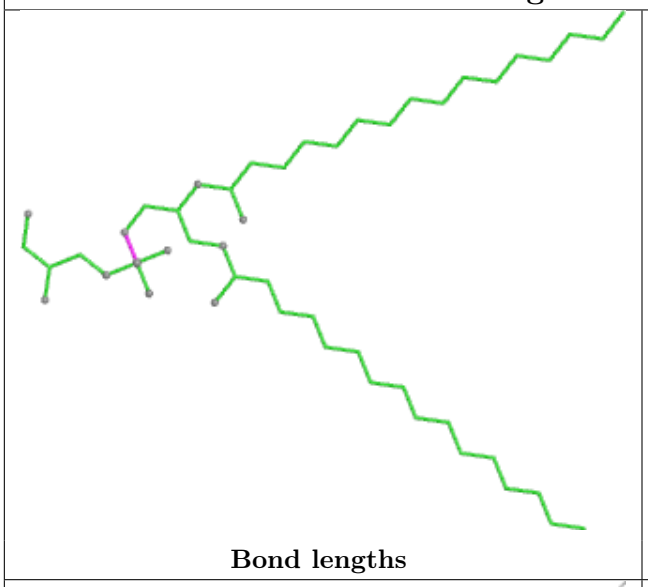


Torsions

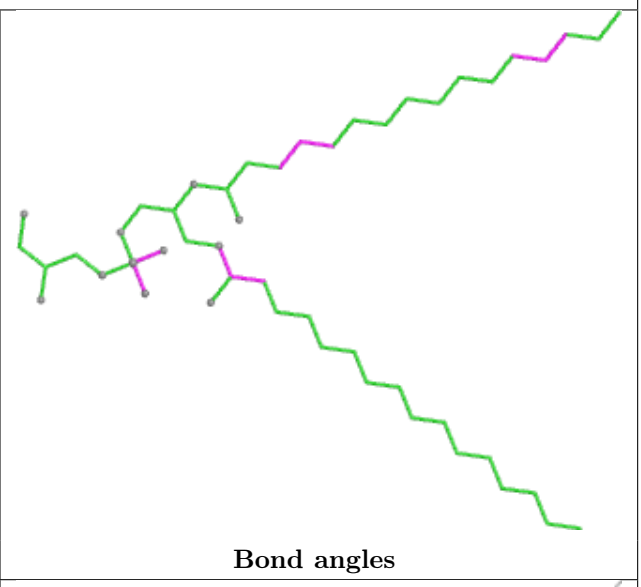


Rings

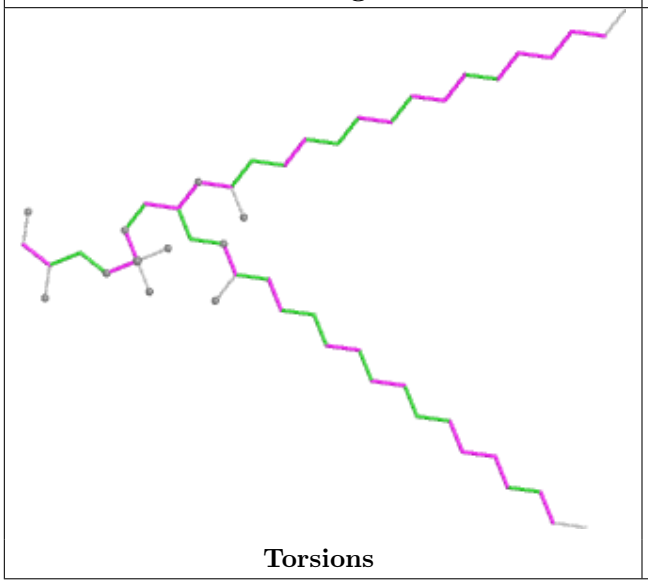
Ligand LHG b 616



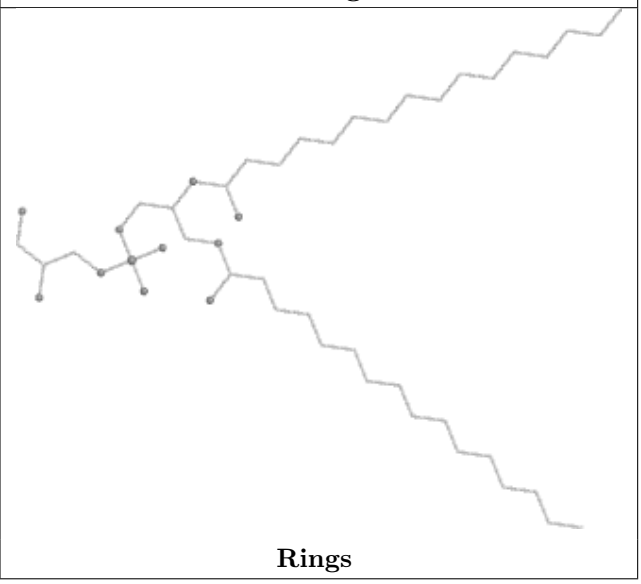
Bond lengths



Bond angles

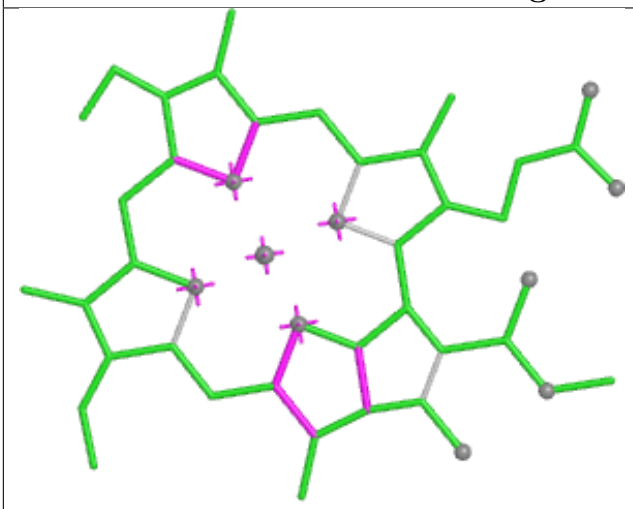


Torsions



Rings

Ligand CLA c 605



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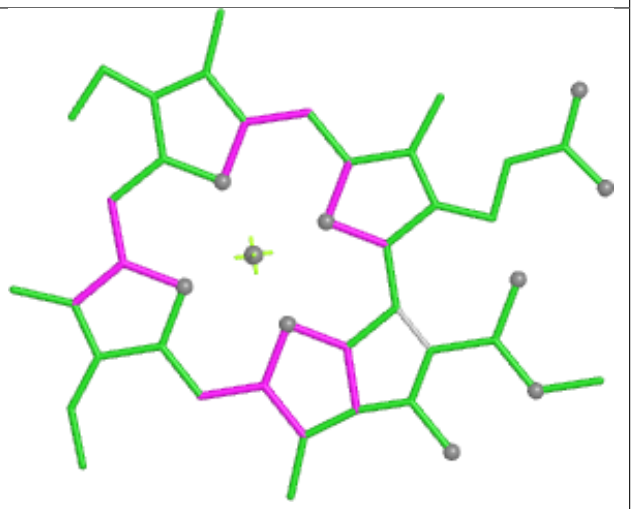
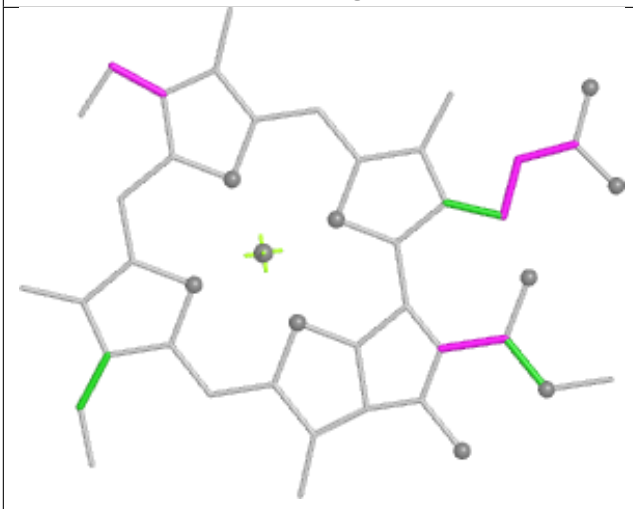


Bond angles

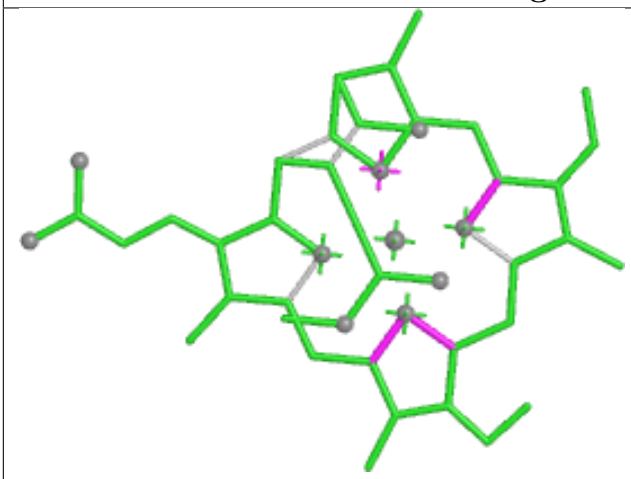


Torsions



Rings

Ligand KC2 7 610



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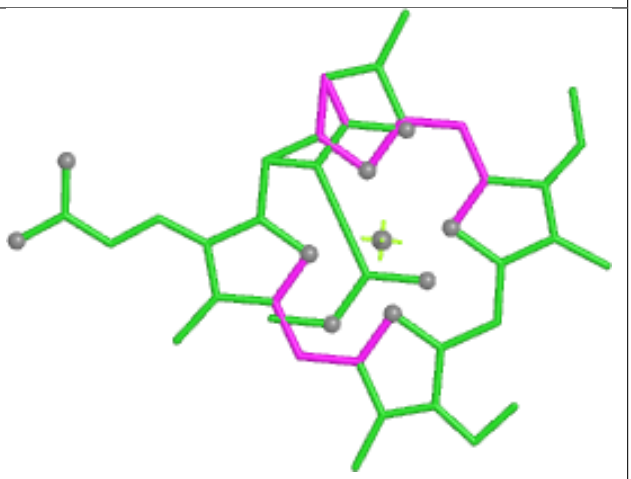

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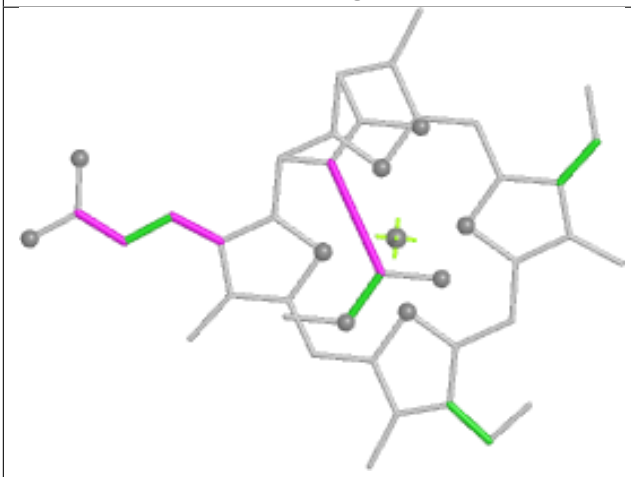

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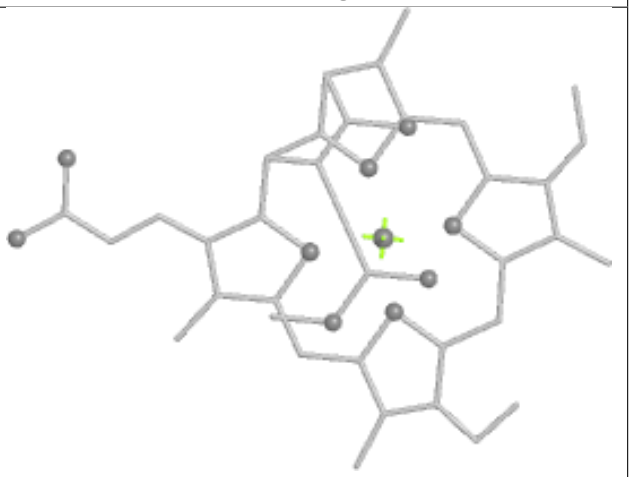
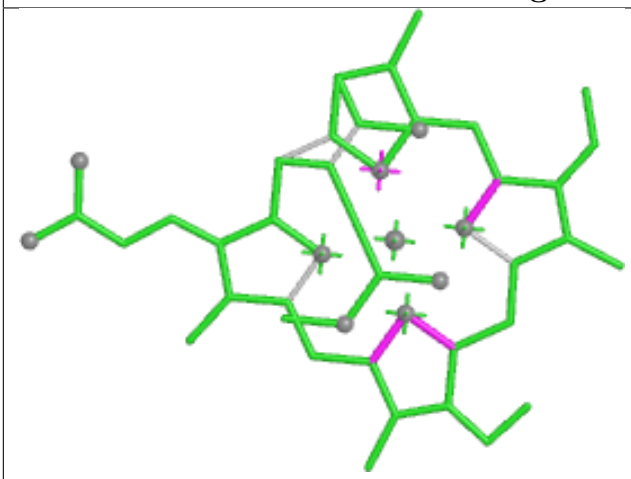


Rings

Ligand KC2 6 610



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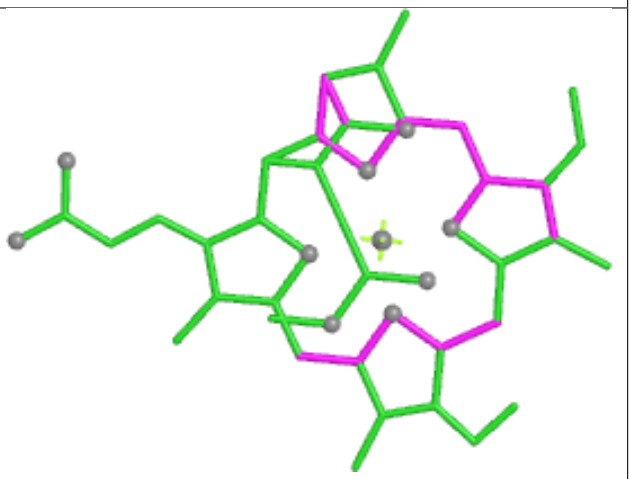
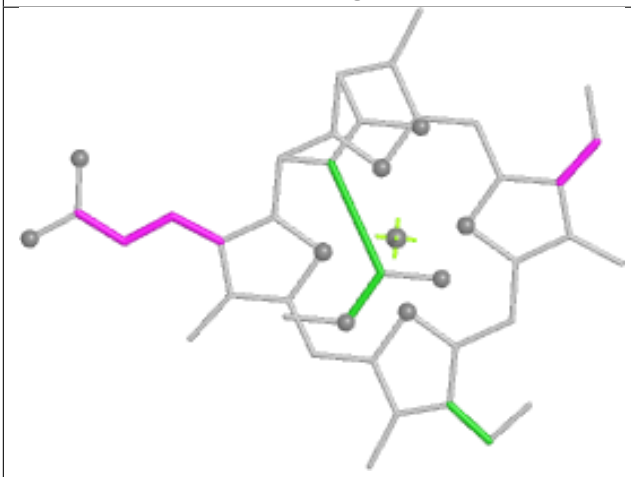


Bond angles



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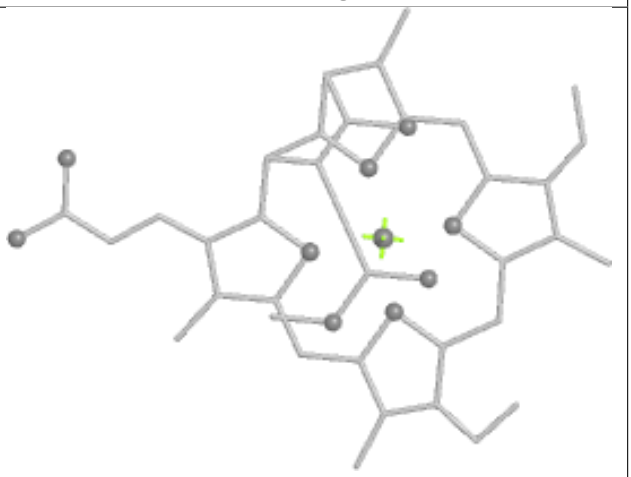
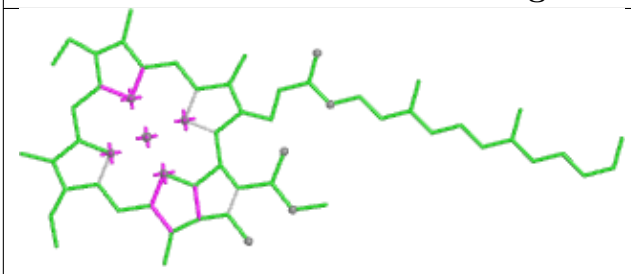


Rings

Ligand CLA 4 602



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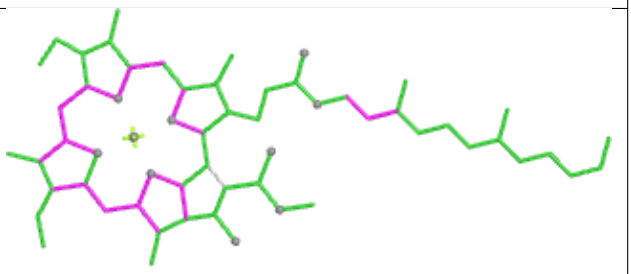

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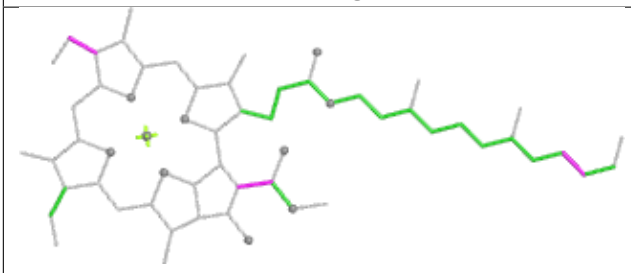

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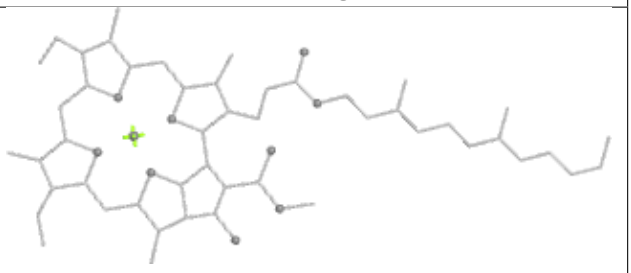
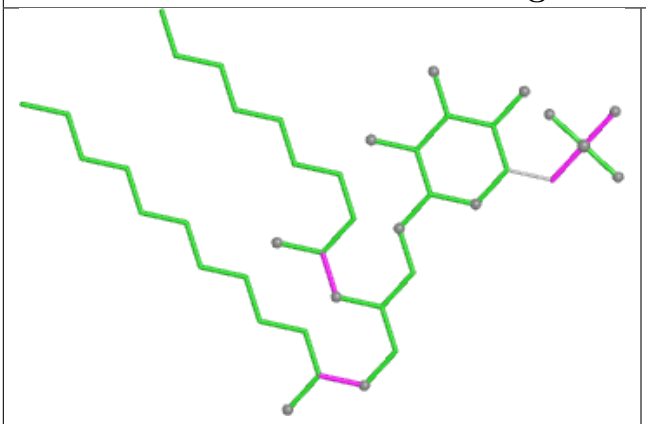


Rings

Ligand SQD 3 621



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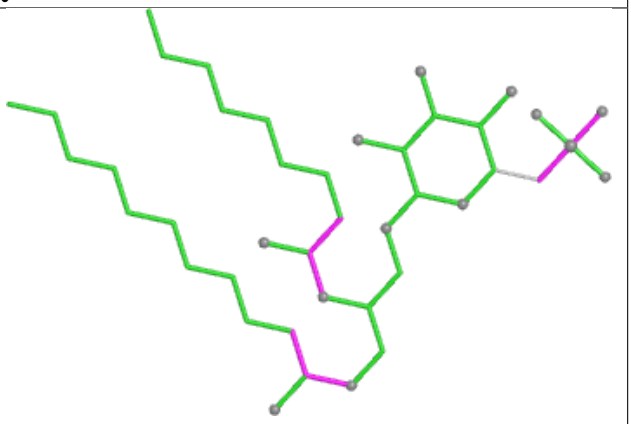
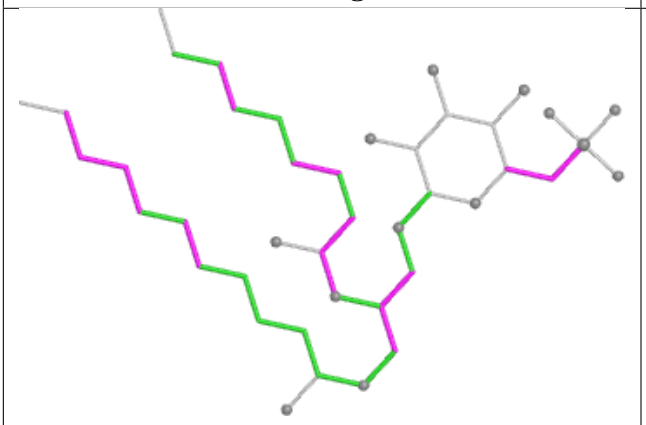


Bond angles



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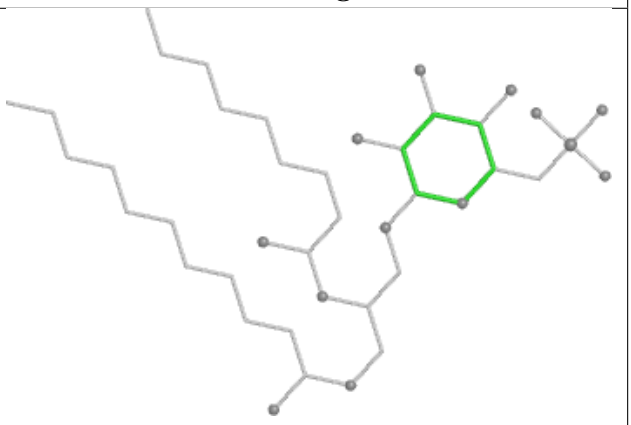
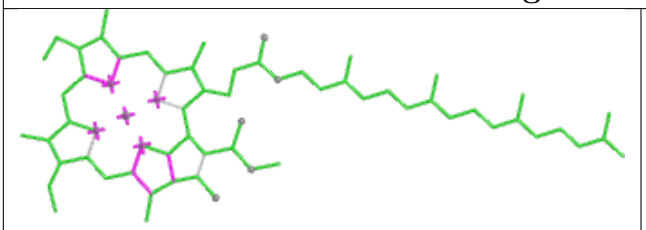


Rings

Ligand CLA K 101



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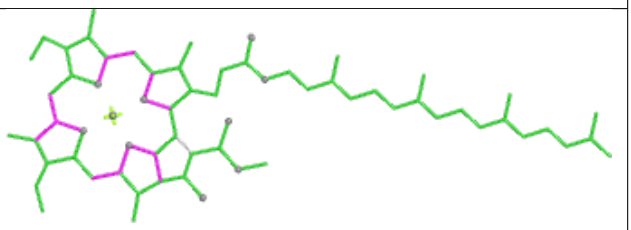

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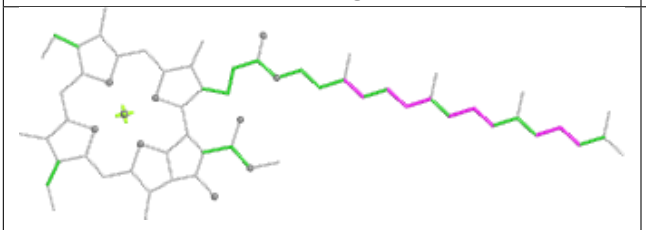

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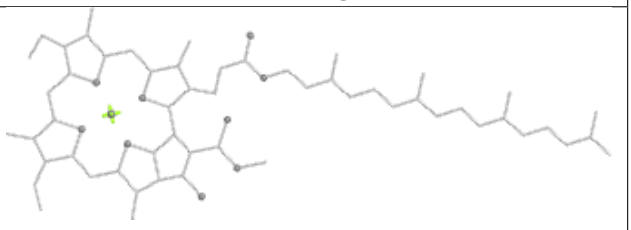
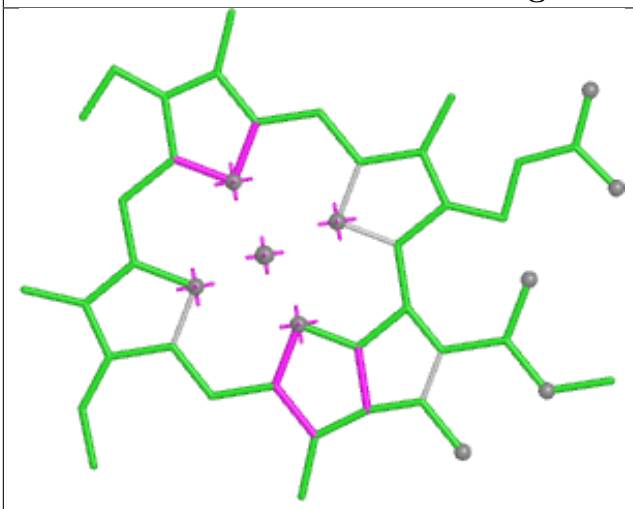


Rings

Ligand CLA 1 607



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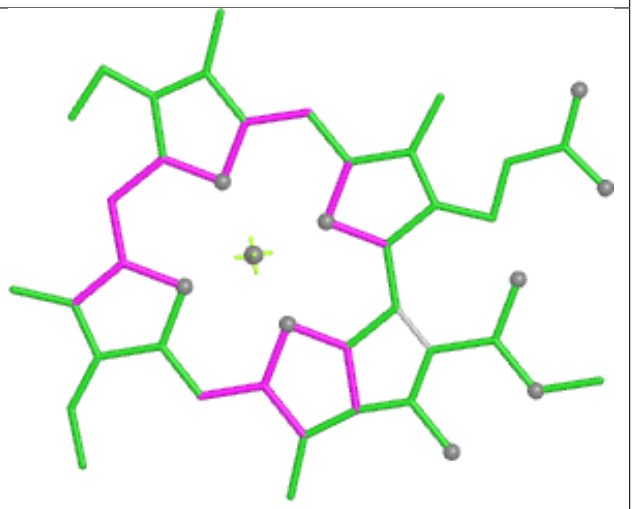

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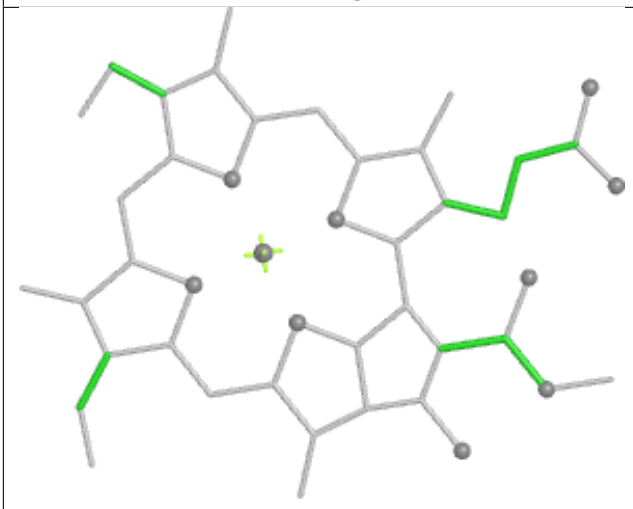
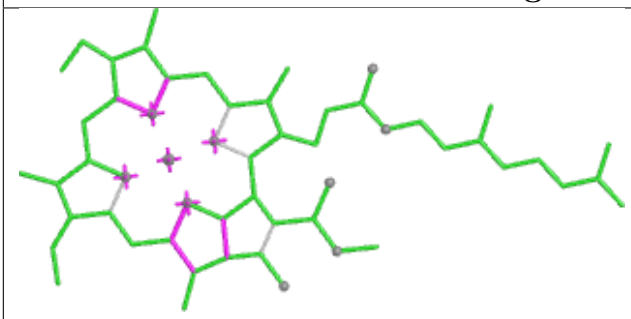


Torsions



Rings

Ligand CLA B 834



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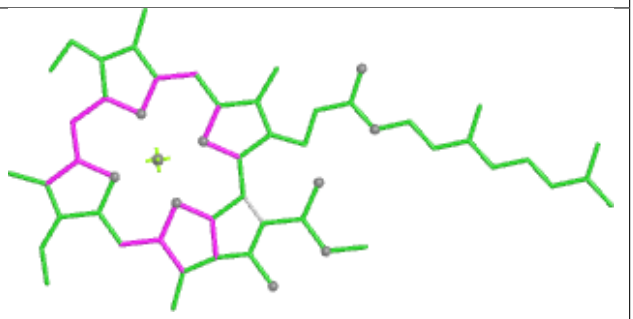

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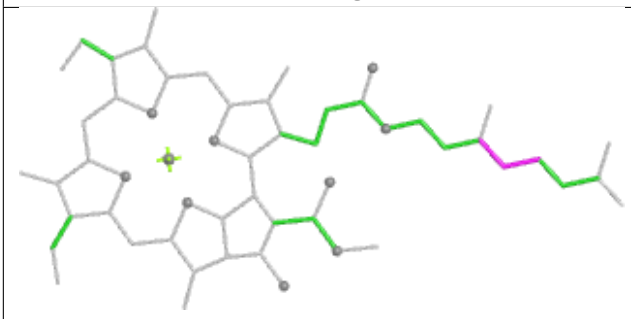

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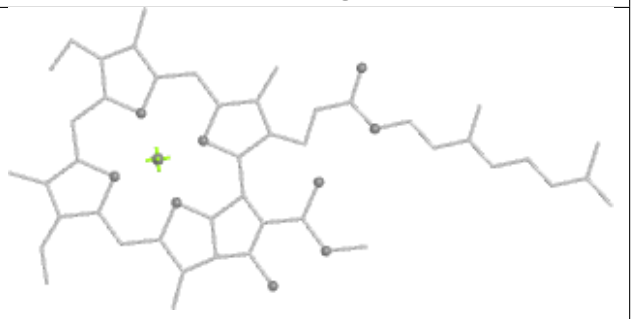
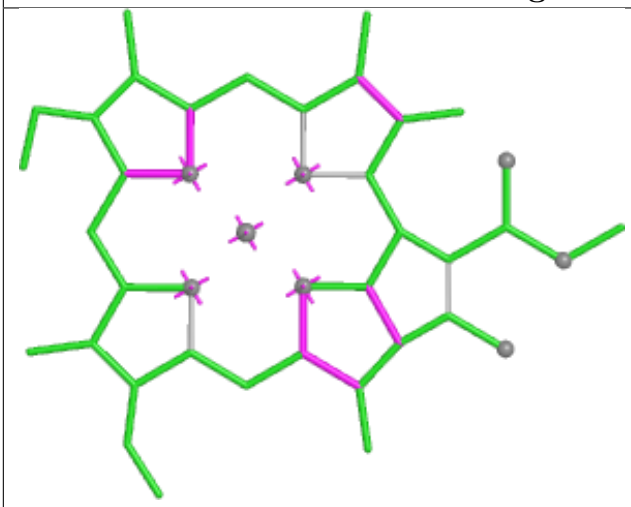


Rings

Ligand CLA 7 609



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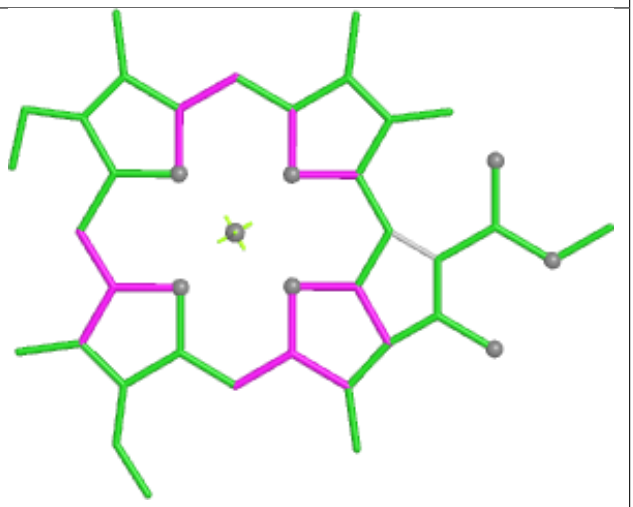
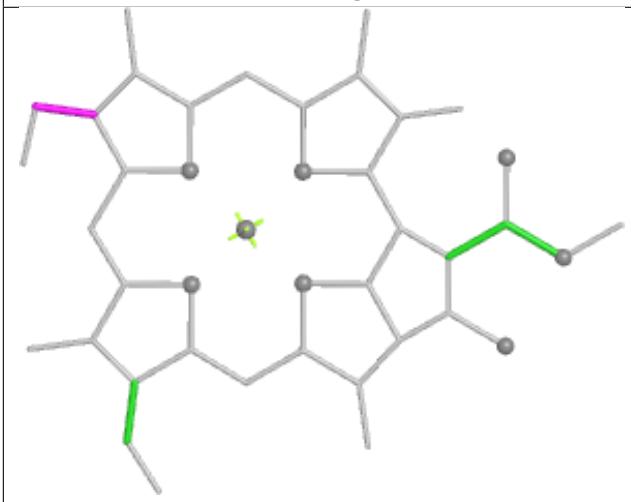


Bond angles



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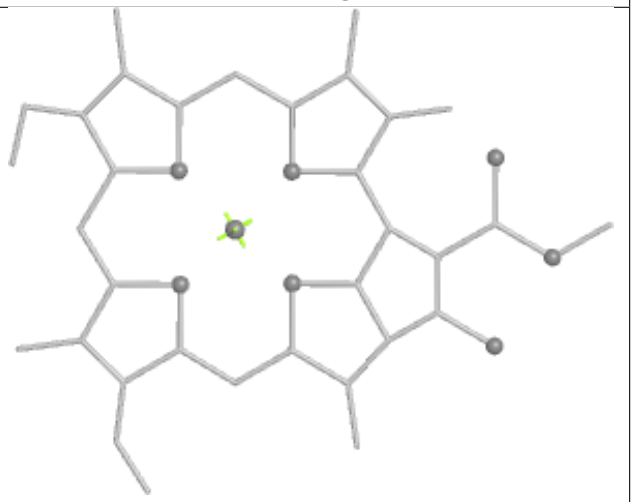
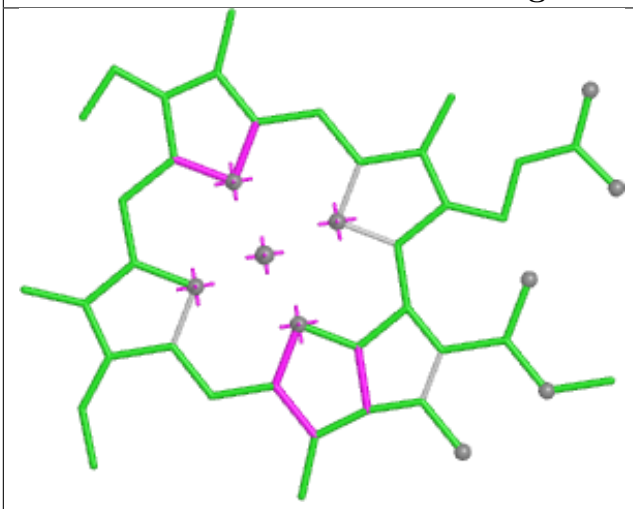


Rings

Ligand CLA 9 612



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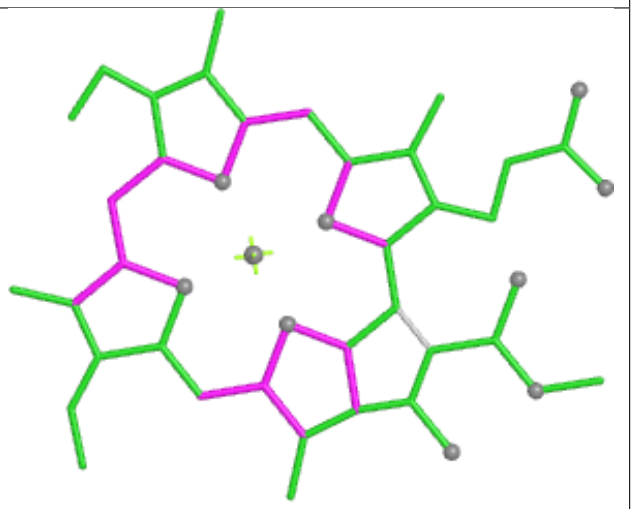

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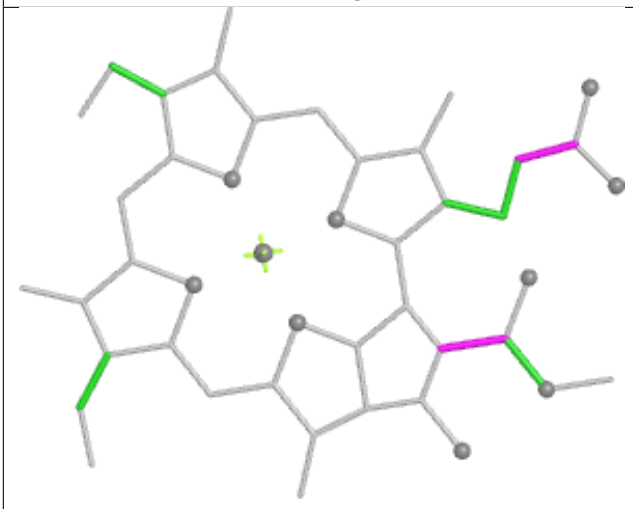
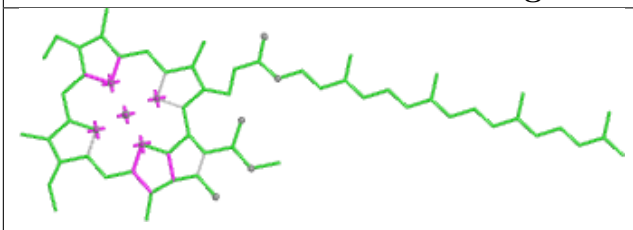


Torsions



Rings

Ligand CLA B 802



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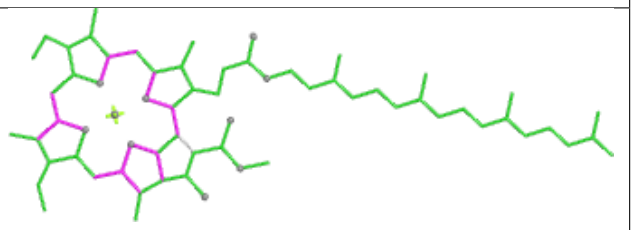

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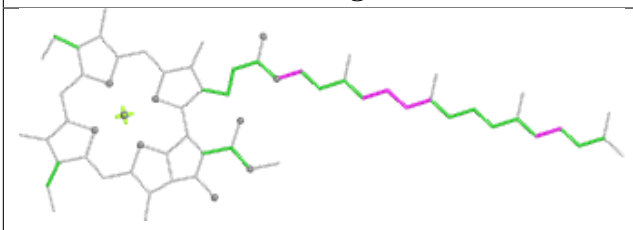

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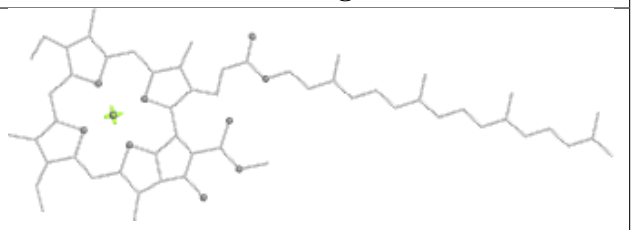
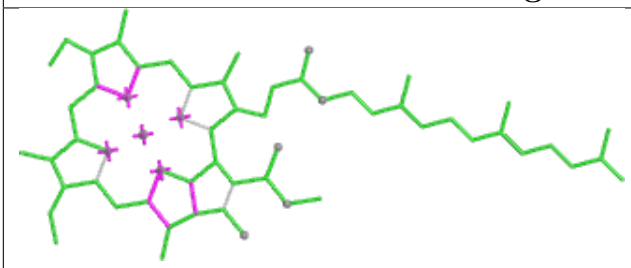


Rings

Ligand CLA B 820



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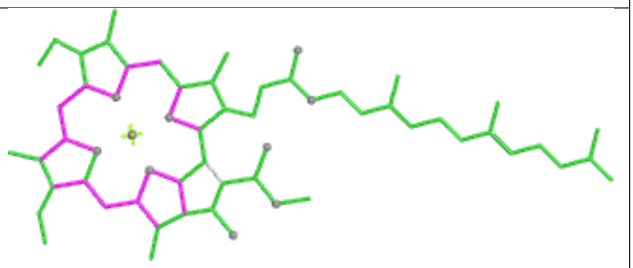

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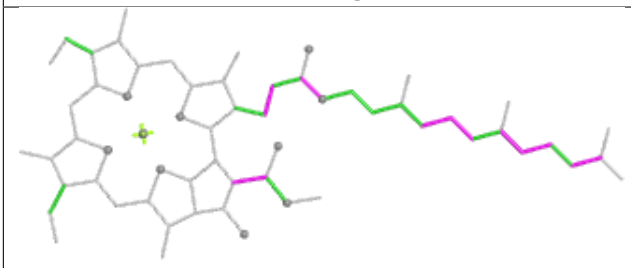

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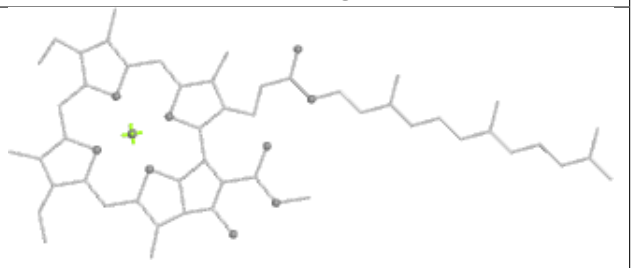
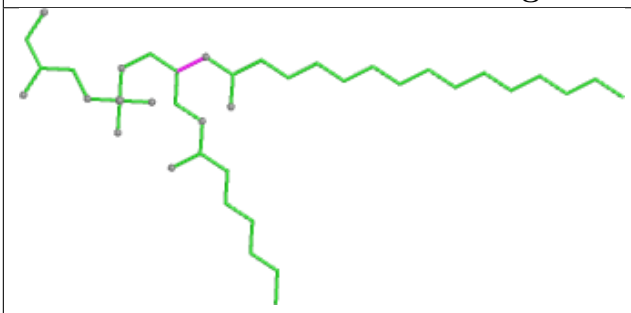


Rings

Ligand LHG A 851



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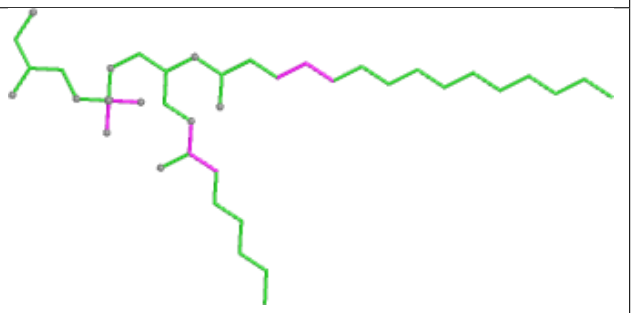
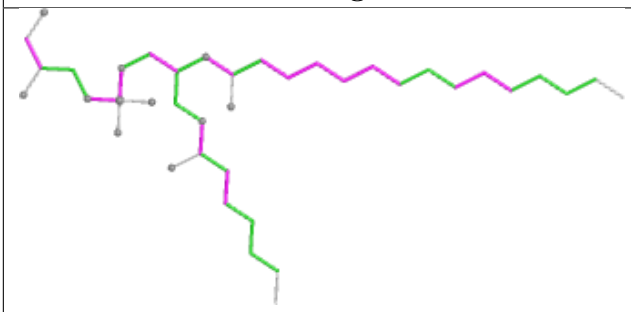


Bond angles



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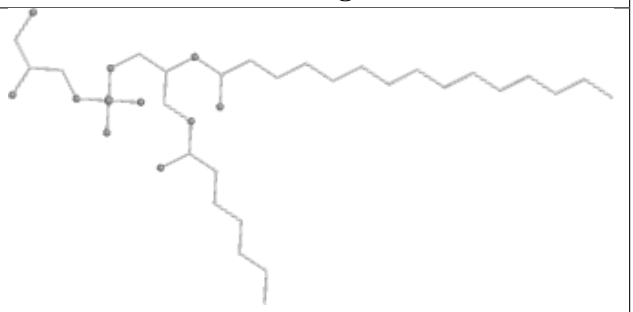
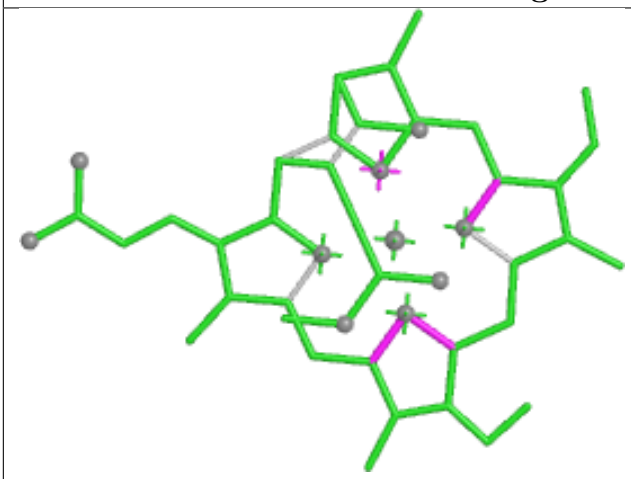


Rings

Ligand KC2 c 611



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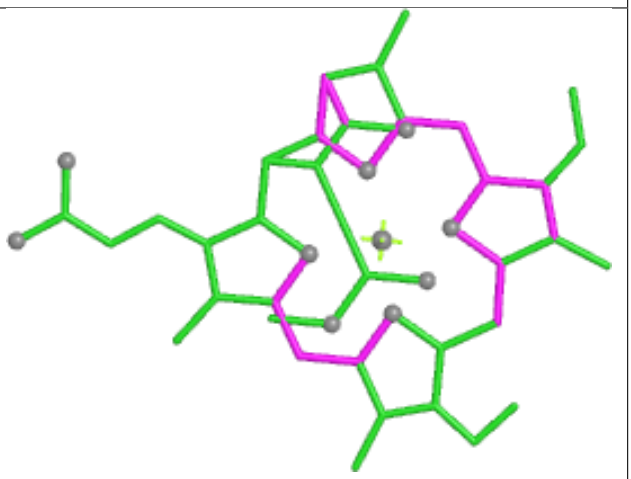
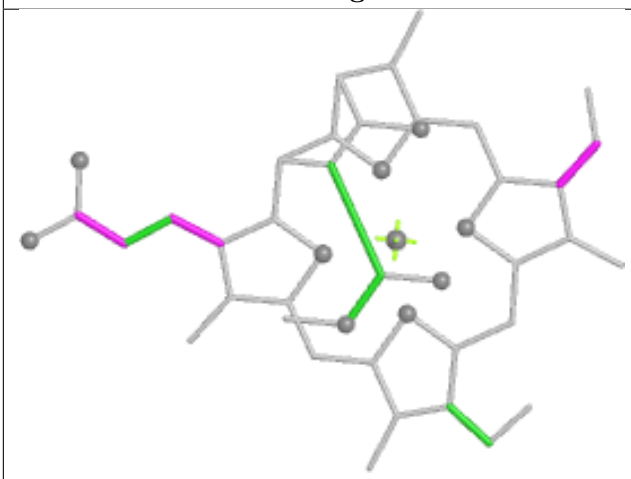


Bond angles



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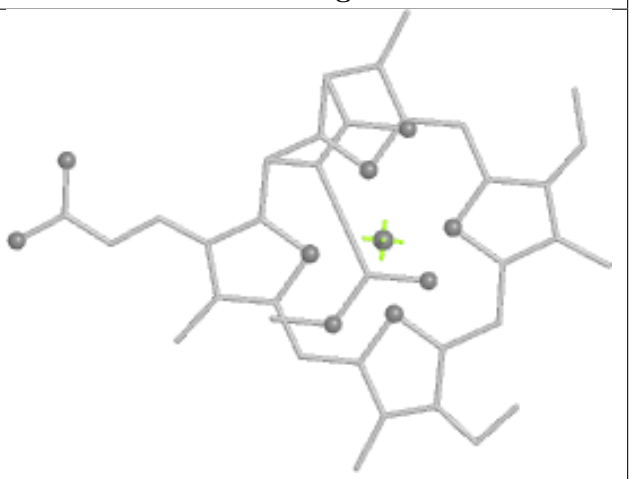


Rings

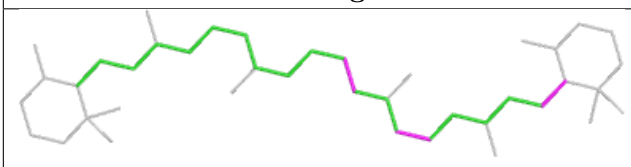
Ligand 8CT I 101



Bond lengths



Bond angles



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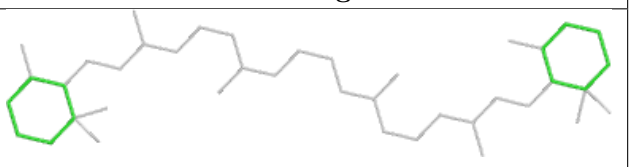
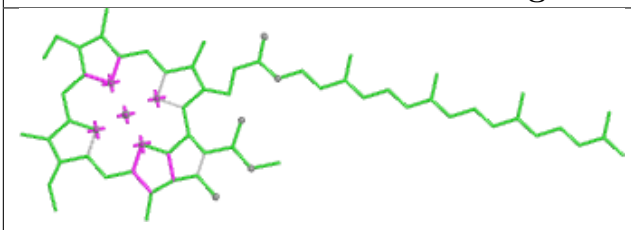


Rings

Ligand CLA 4 611



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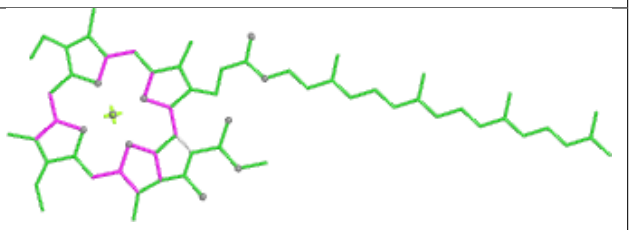
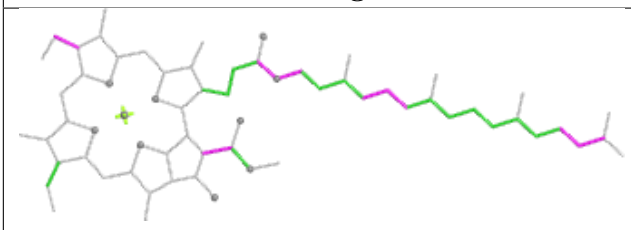
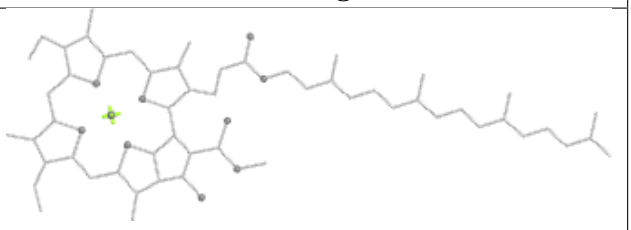


Bond angles

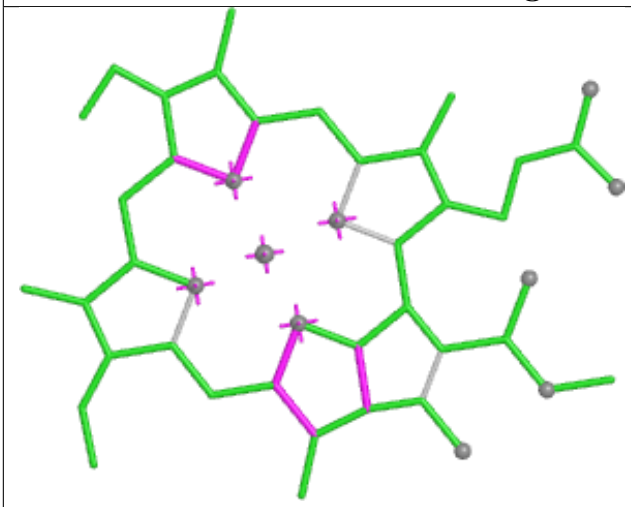


Torsions



Rings

Ligand CLA A 814



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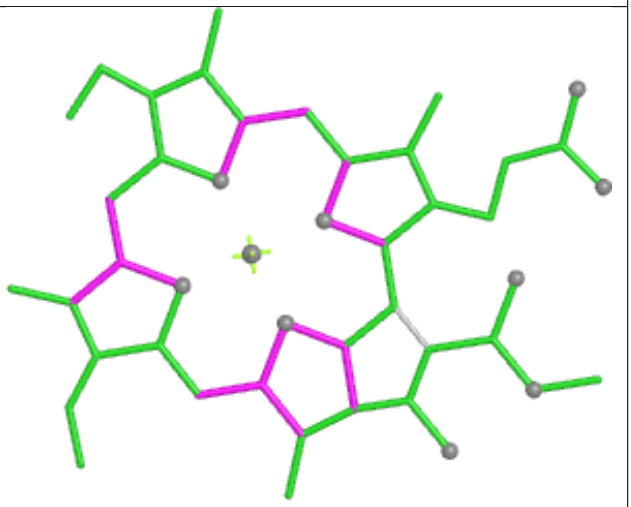

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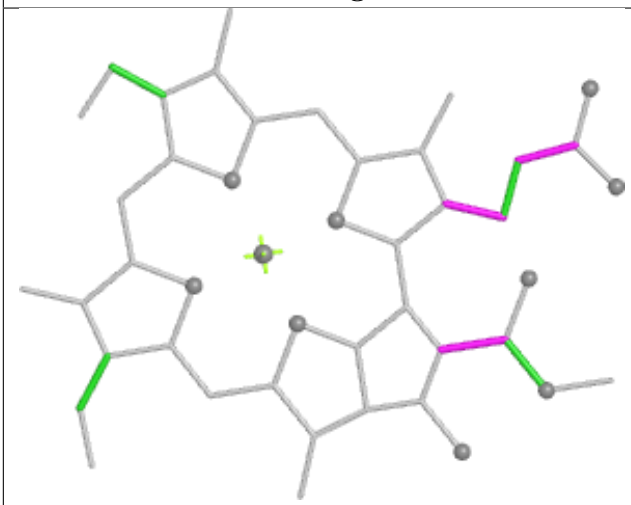

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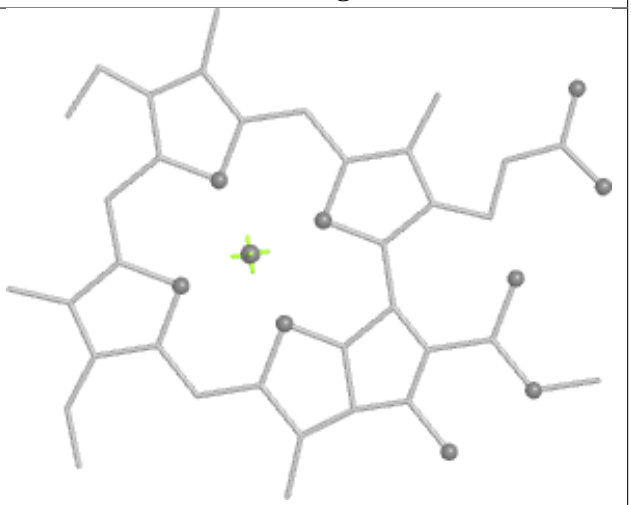
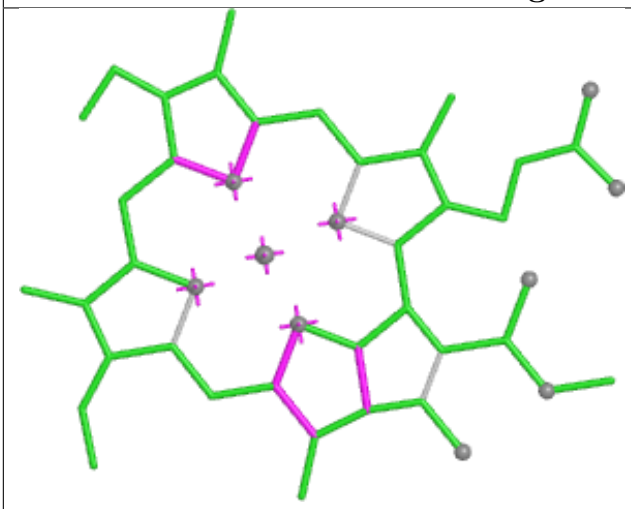


Rings

Ligand CLA 9 605



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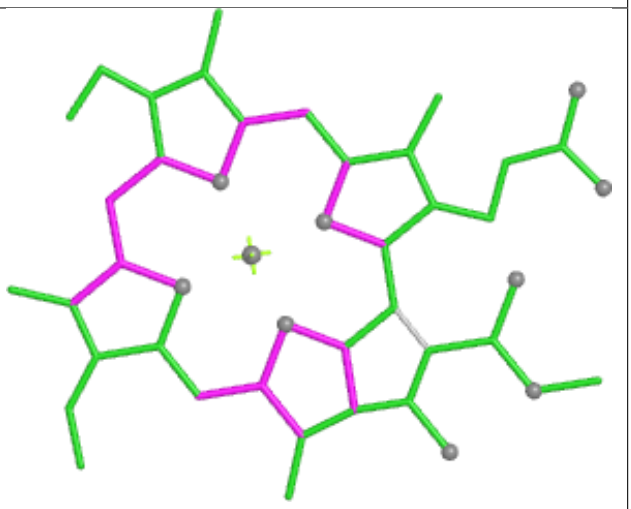

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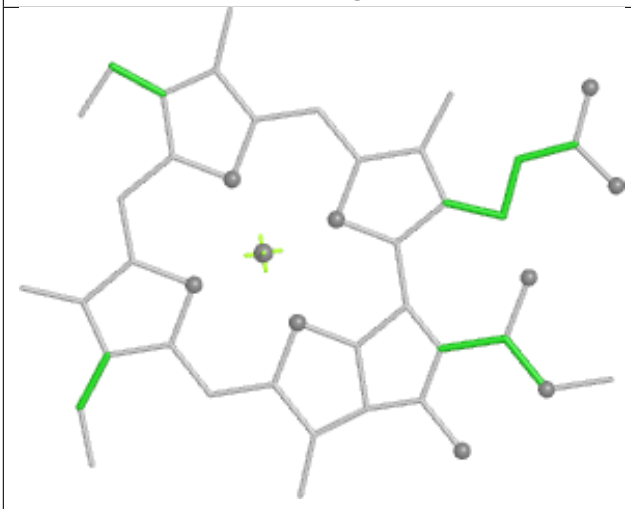
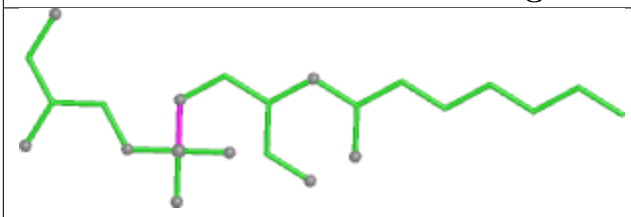


Torsions



Rings

Ligand LHG d 618



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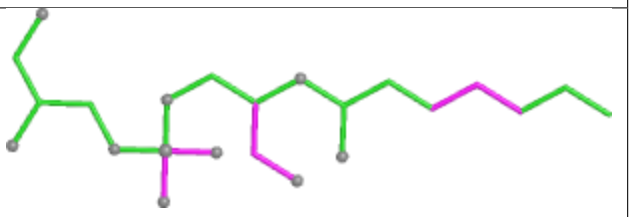

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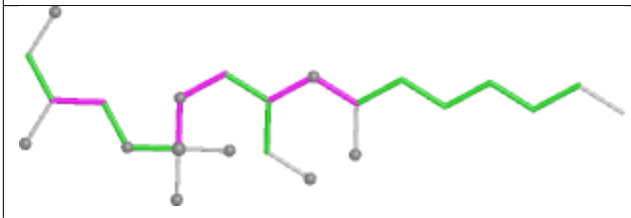

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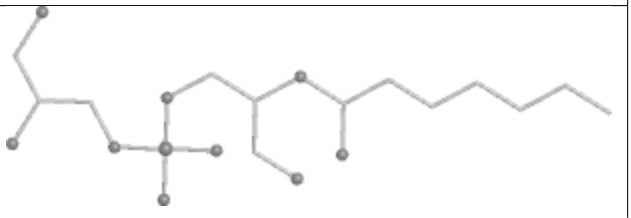
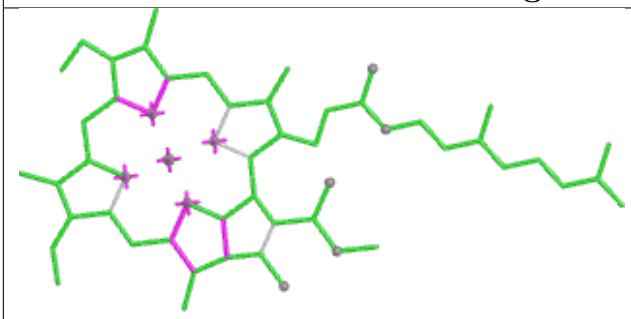


Rings

Ligand CLA O 202



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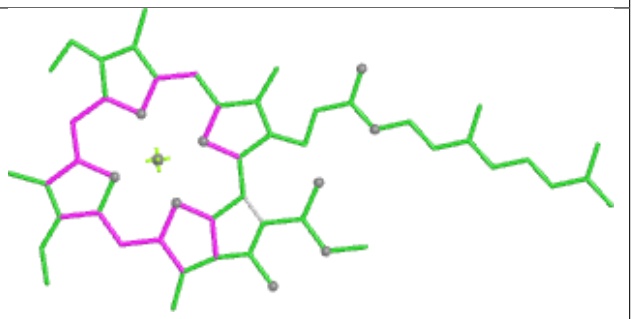

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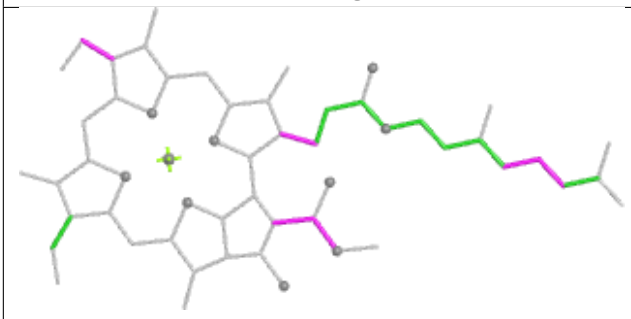

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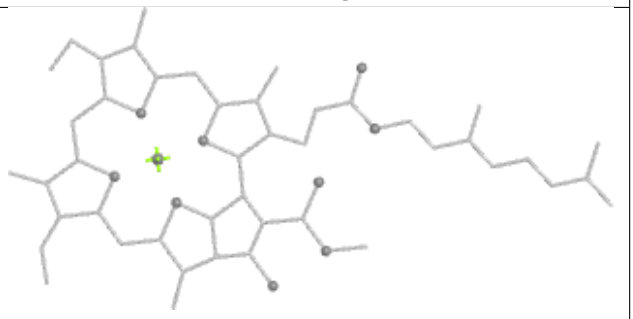
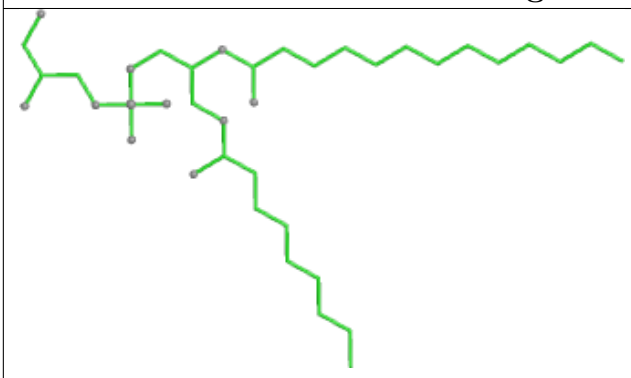


Rings

Ligand LHG 2 619



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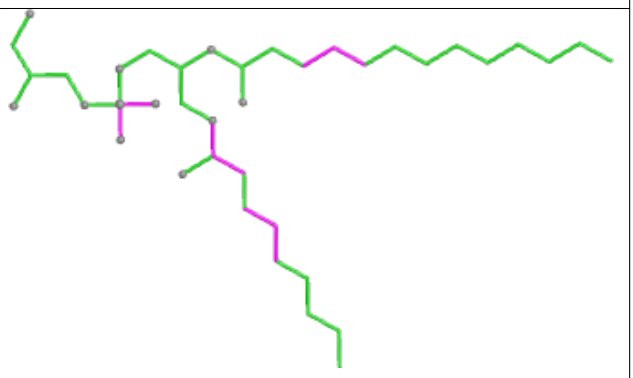

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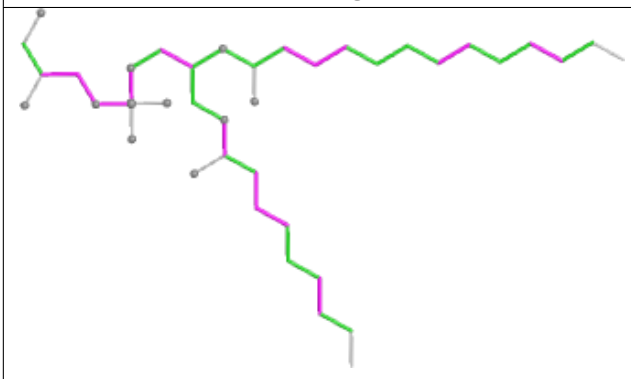

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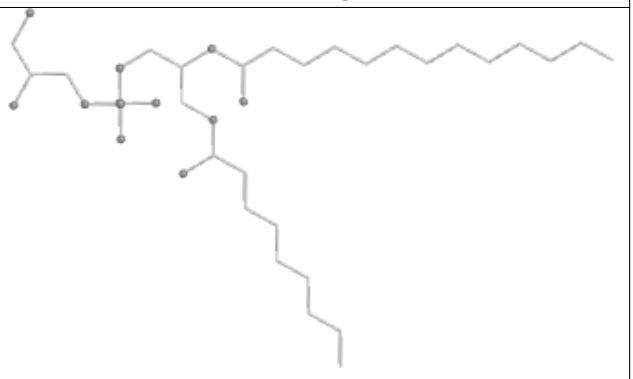
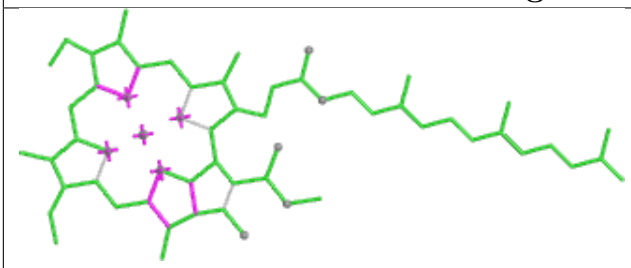


Rings

Ligand CLA Z 301



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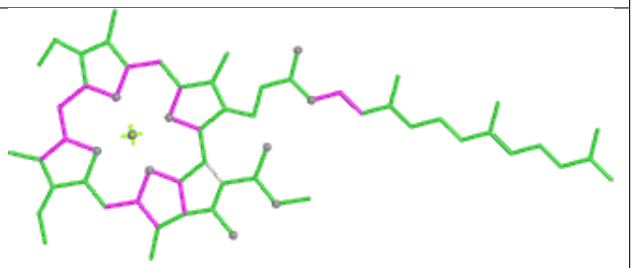

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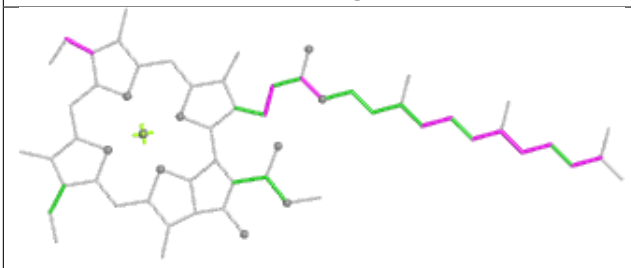

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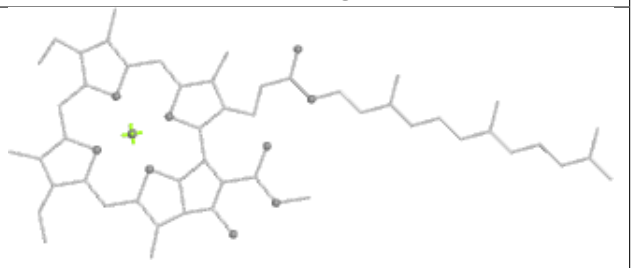
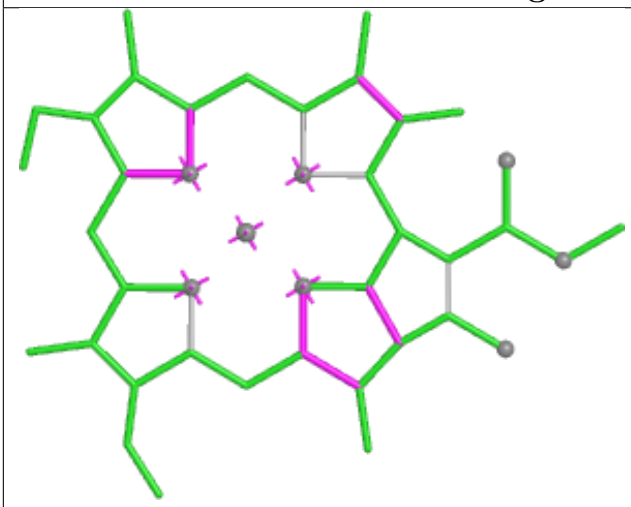


Rings

Ligand CLA 9 611



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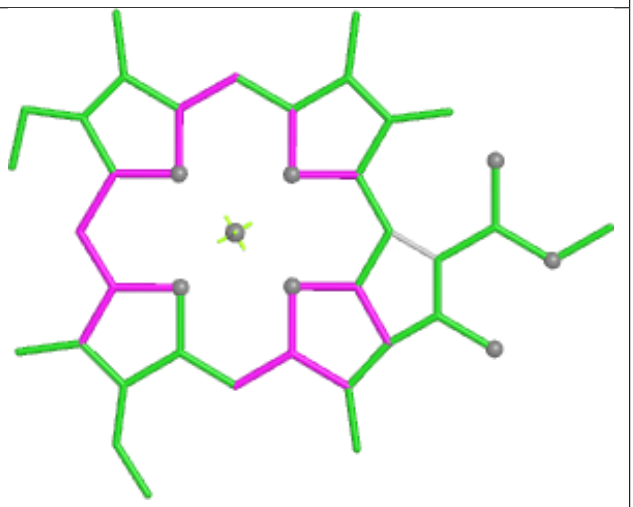

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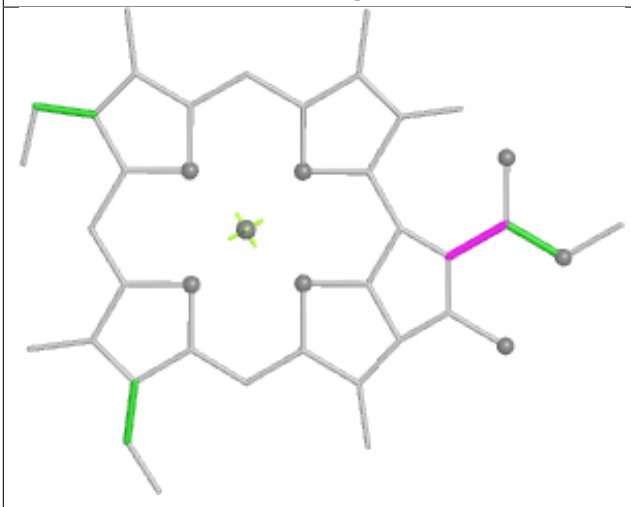

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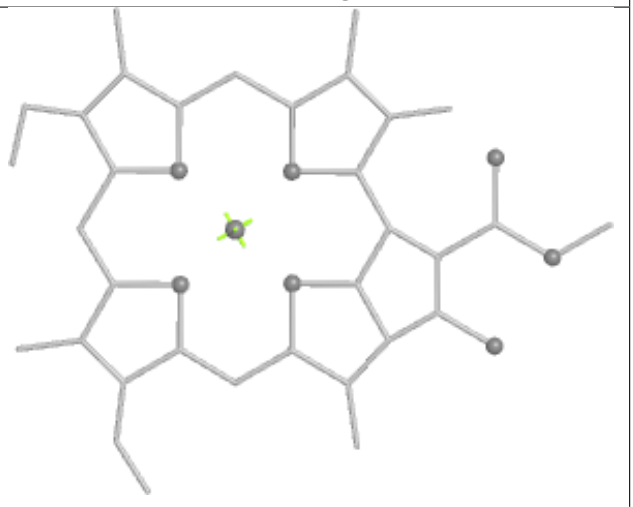
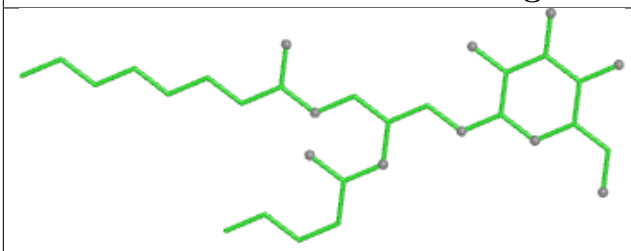


Rings

Ligand LMG 3 620



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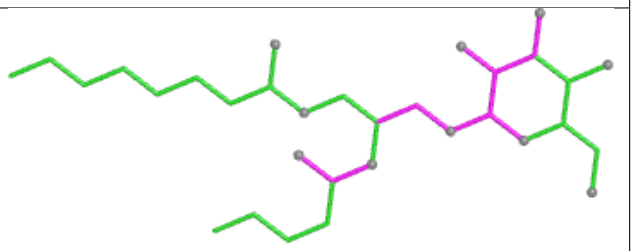

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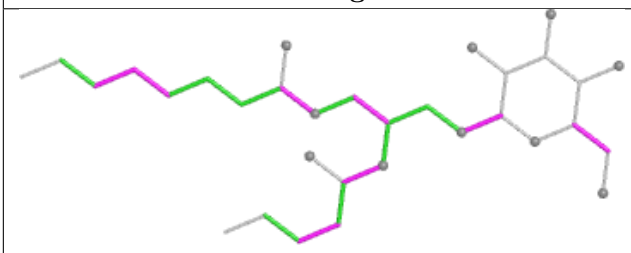

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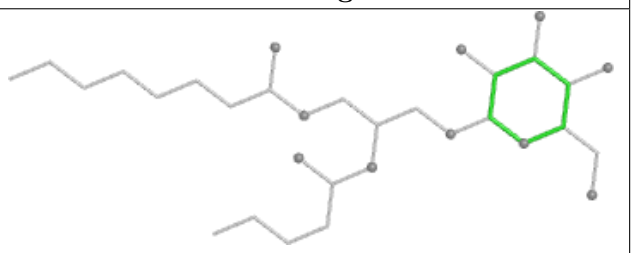
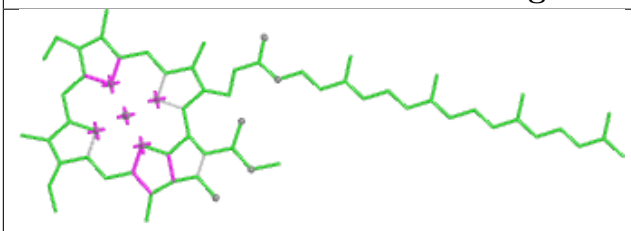


Rings

Ligand CLA 8 604



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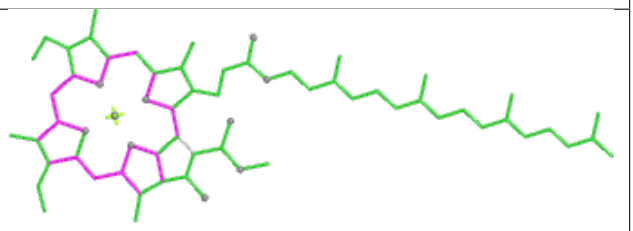

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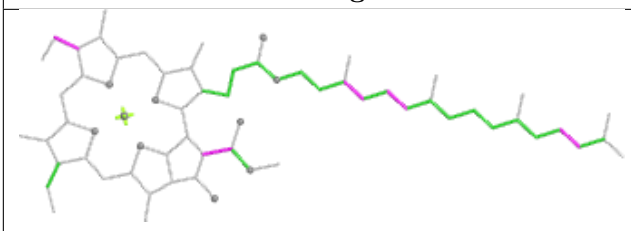

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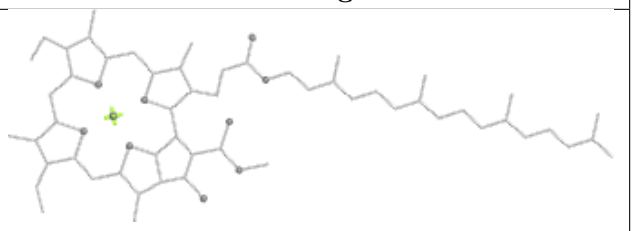
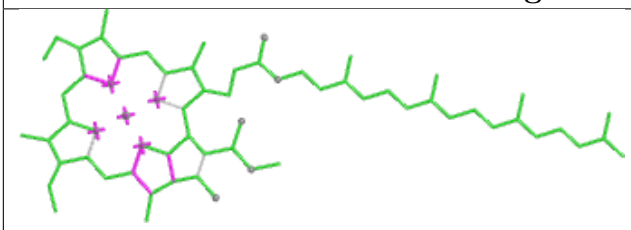


Rings

Ligand CLA B 839



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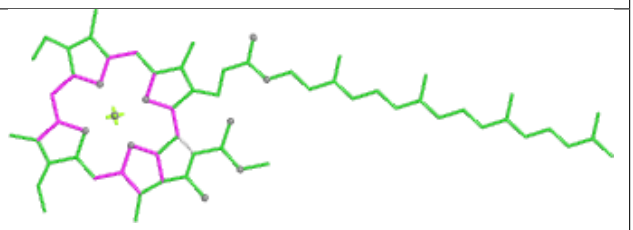

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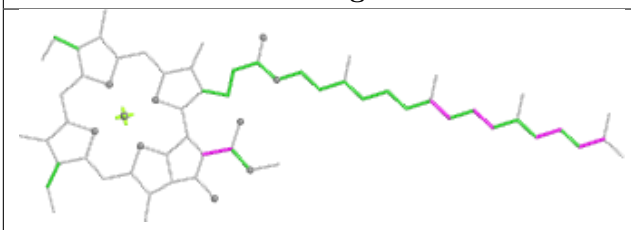

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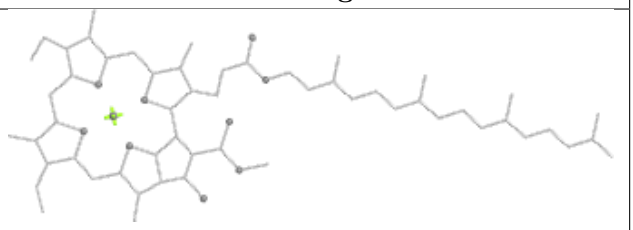
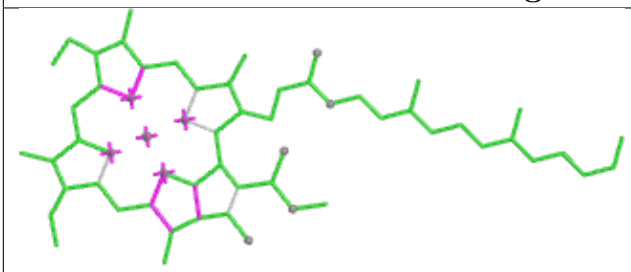


Rings

Ligand CLA B 816



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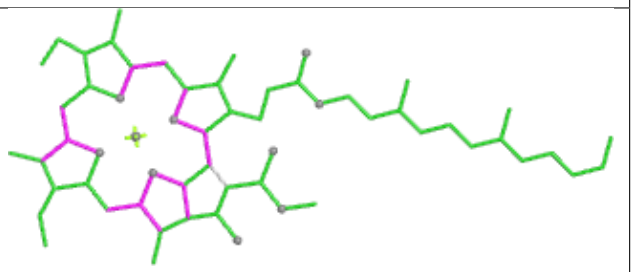

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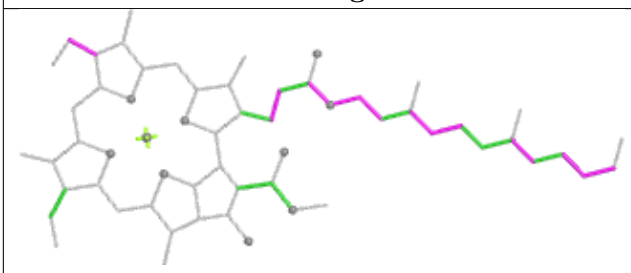

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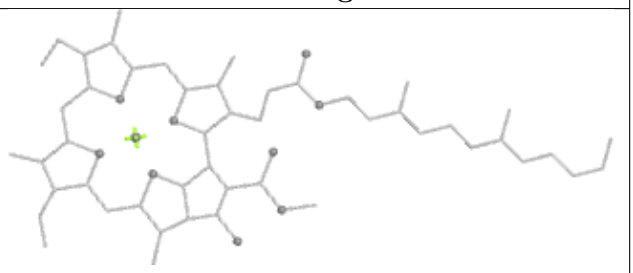
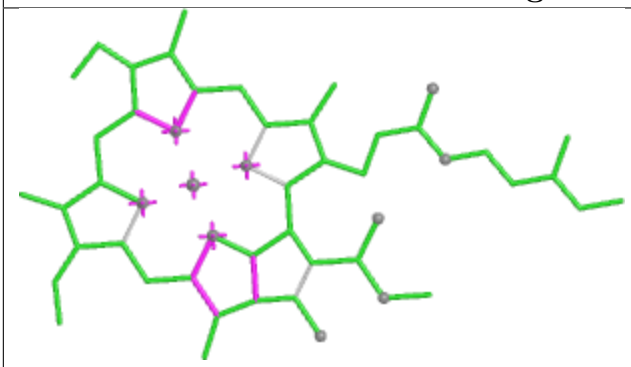


Rings

Ligand CLA L 202



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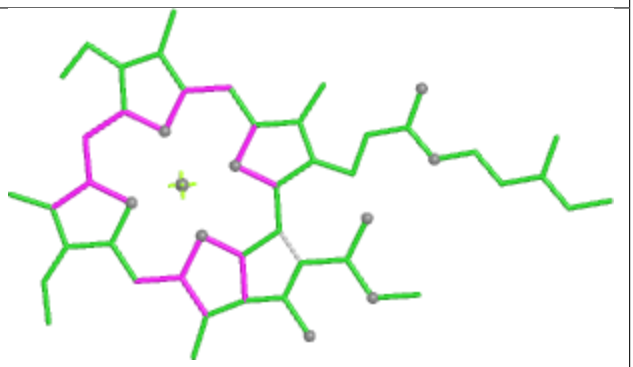
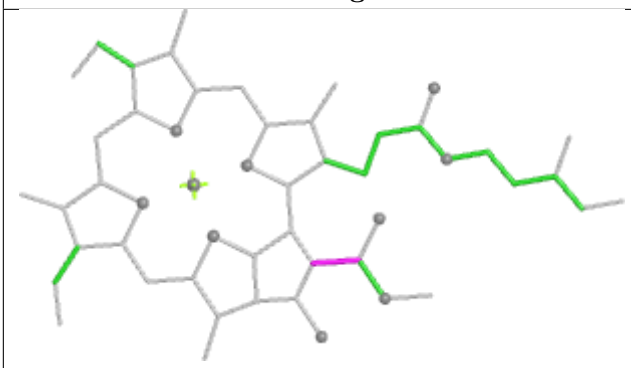


Bond angles



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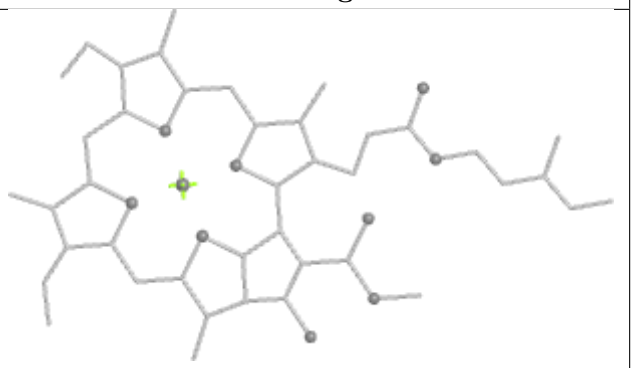
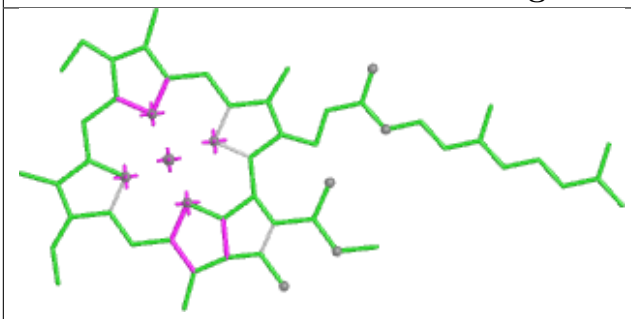


Rings

Ligand CLA 3 602



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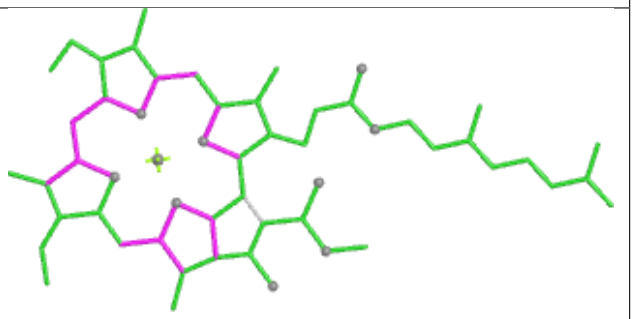
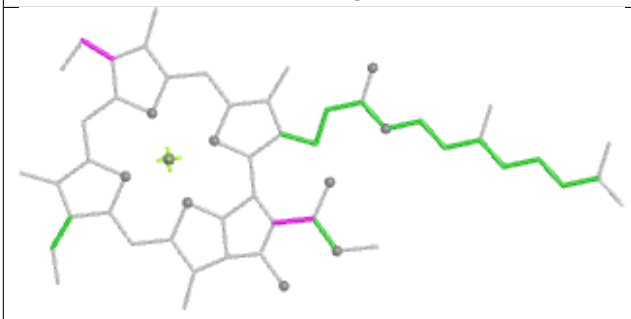


Bond angles



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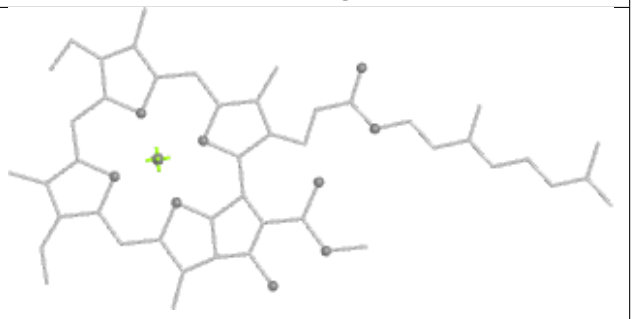
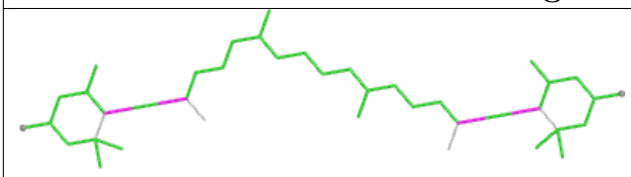


Rings

Ligand II0 c 617



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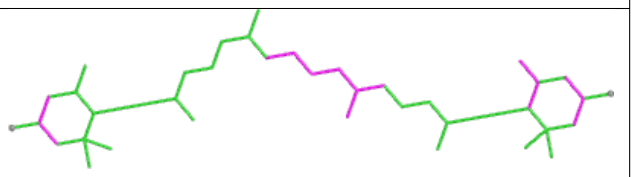
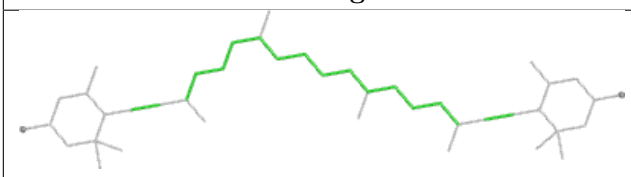


Bond angles



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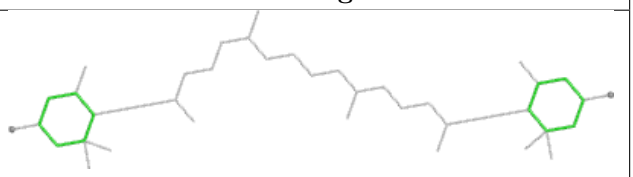
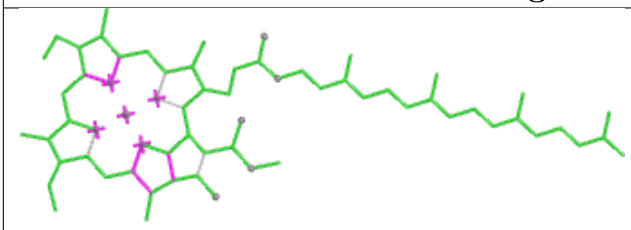
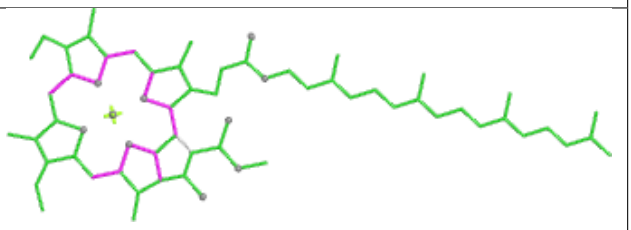


Rings

Ligand CLA 6 602	
	
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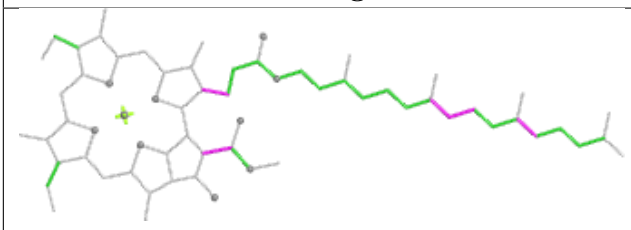	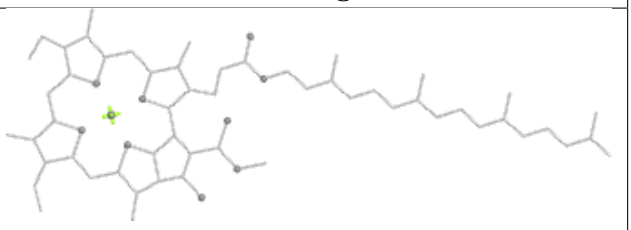
Torsions	Rings

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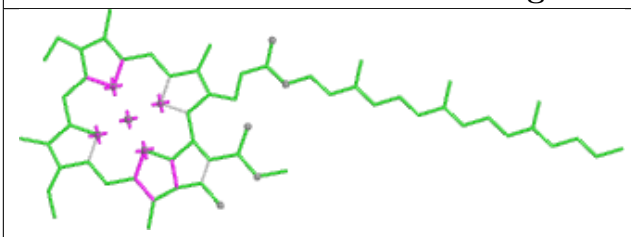	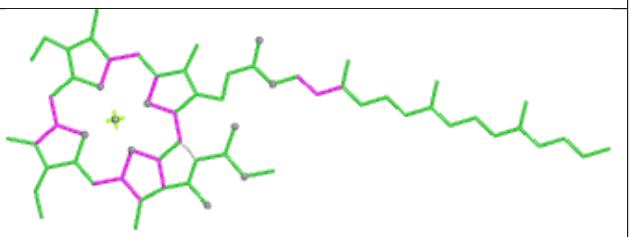
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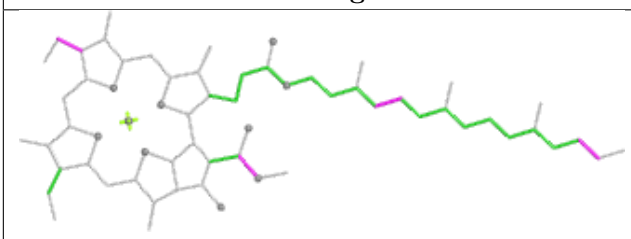
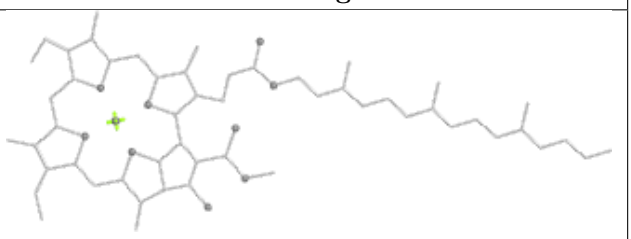
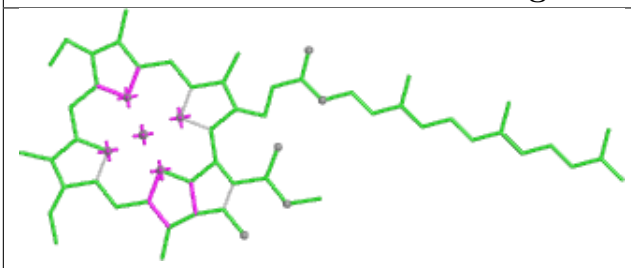
	
Torsions	Rings

Ligand CLA e 604



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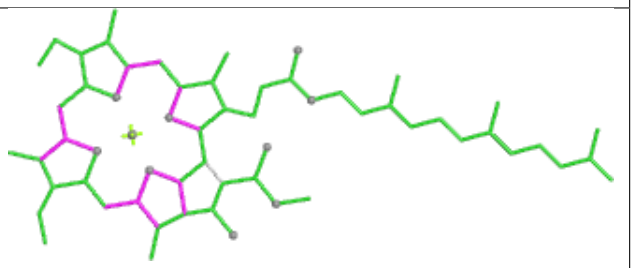

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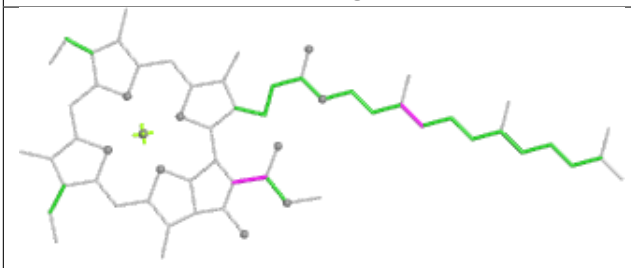

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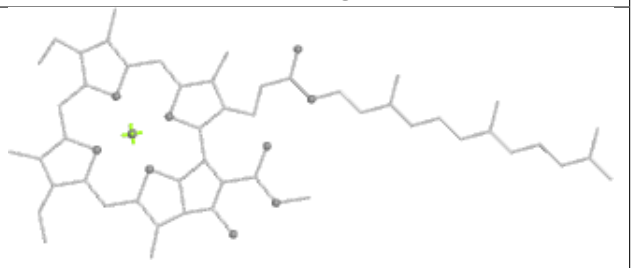
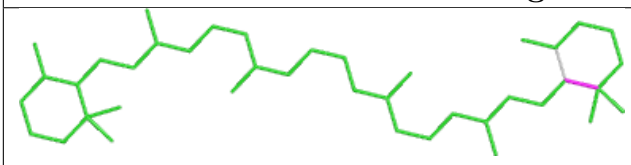


Rings

Ligand 8CT B 845



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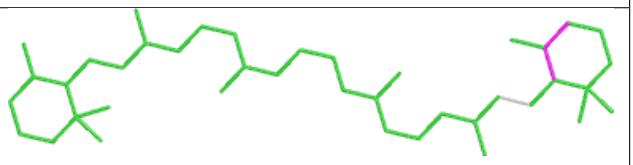

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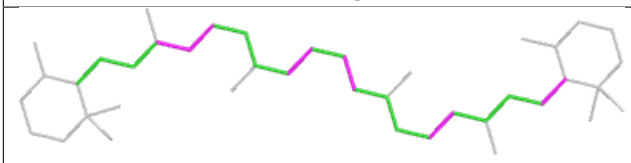

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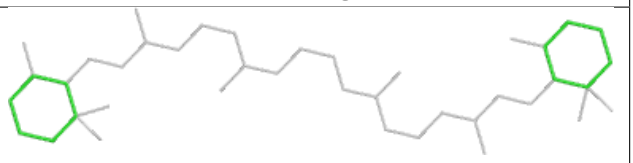
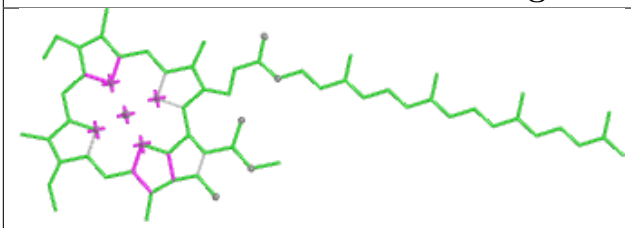


Rings

Ligand CLA 3 610



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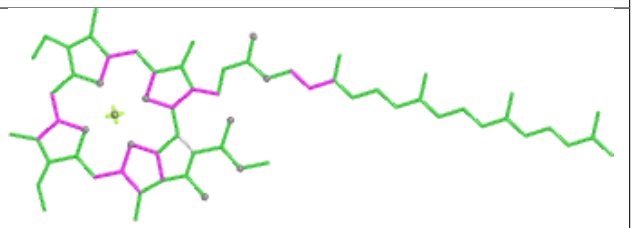
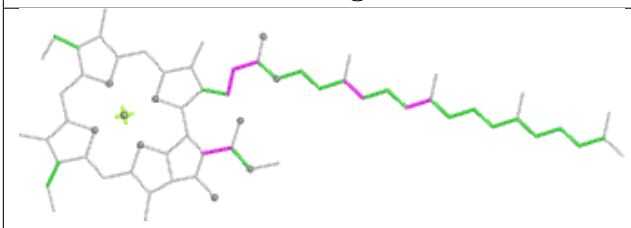


Bond angles



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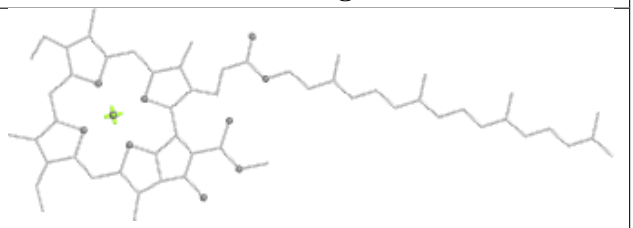
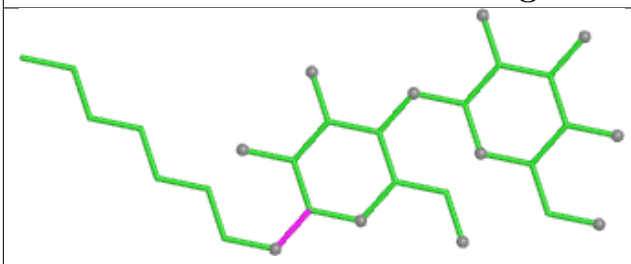
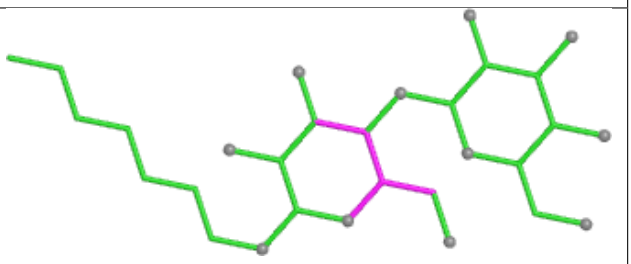
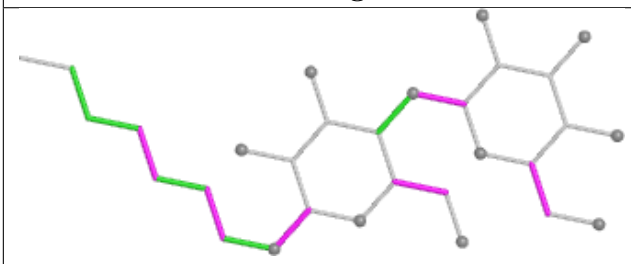
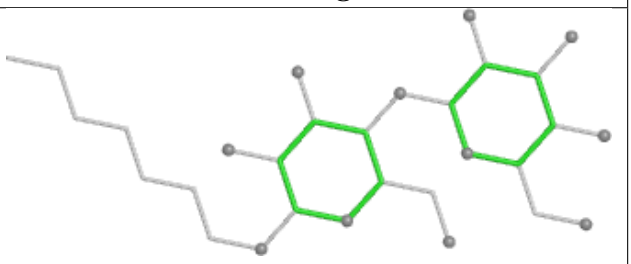


Rings

Ligand LMU O 207	
 Bond lengths	 Bond angles
 Torsions	 Rings

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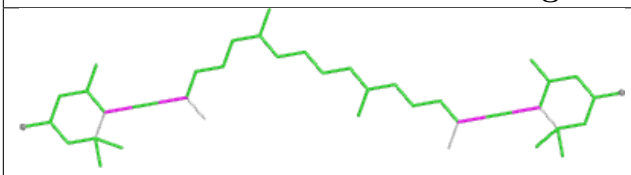
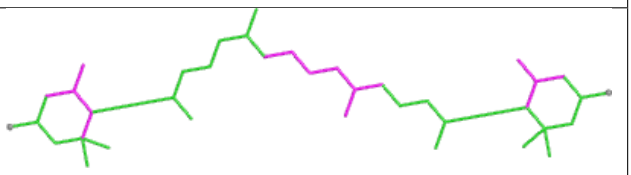
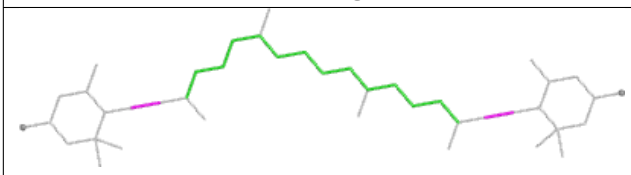
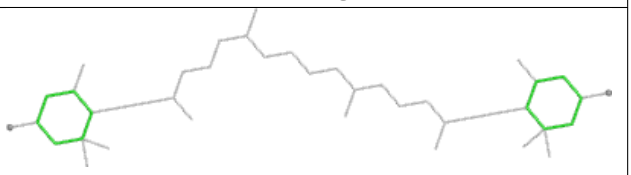
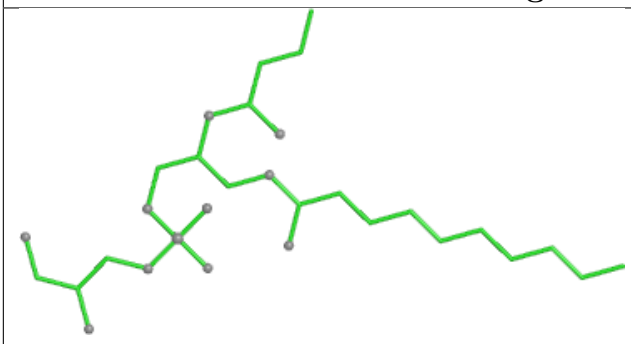
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 7 618



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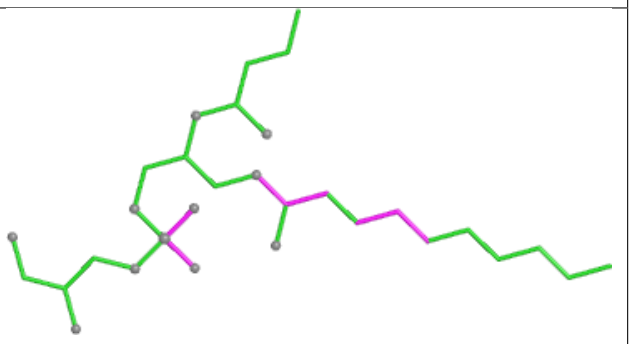
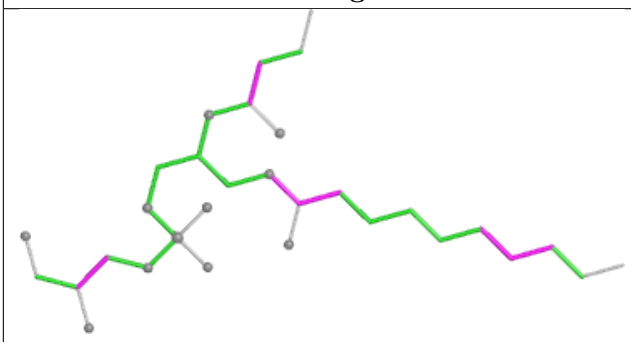


Bond angles



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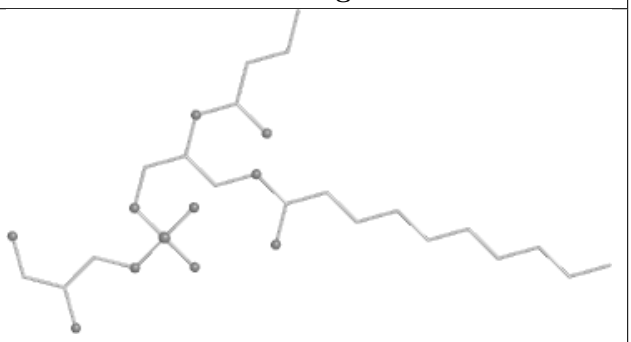
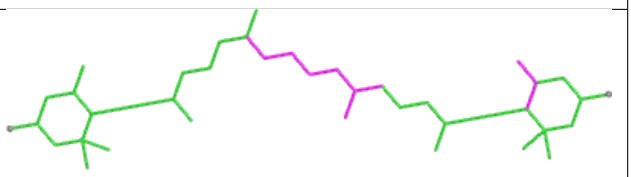


Rings

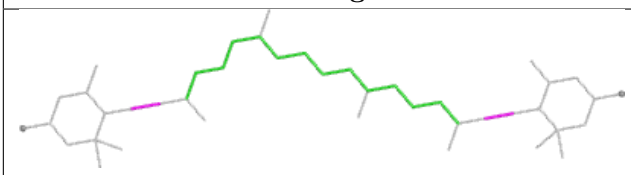
Ligand II0 c 616



Bond lengths



Bond angles



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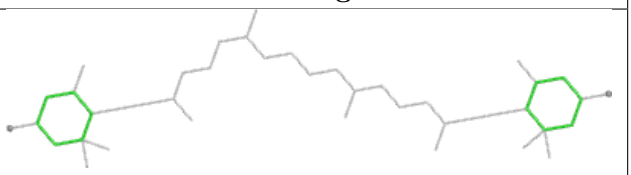
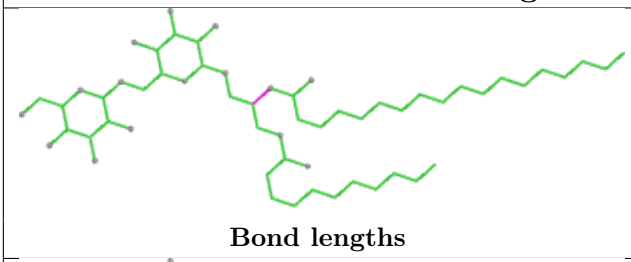


Rings

Ligand DGD B 848



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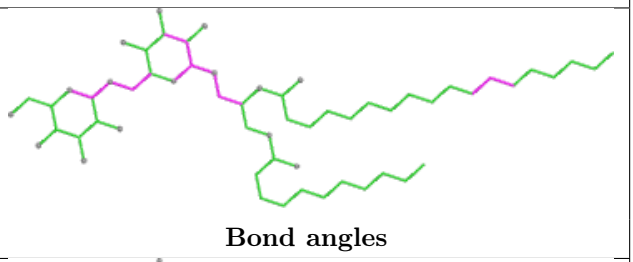

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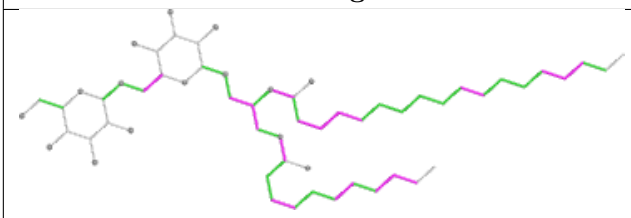

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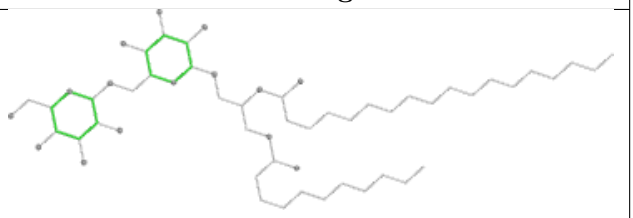
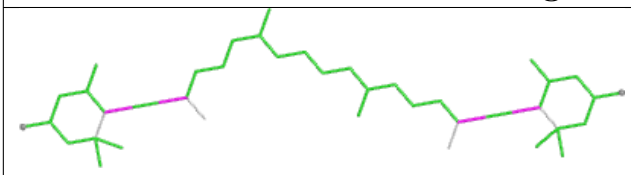


Rings

Ligand II0 5 615



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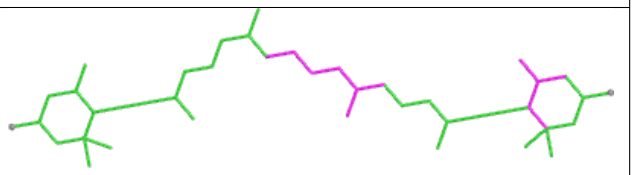

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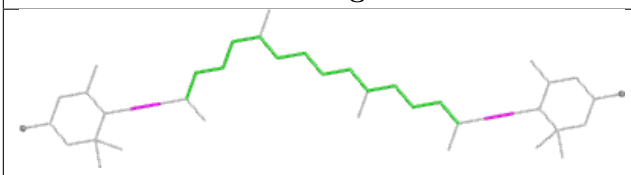

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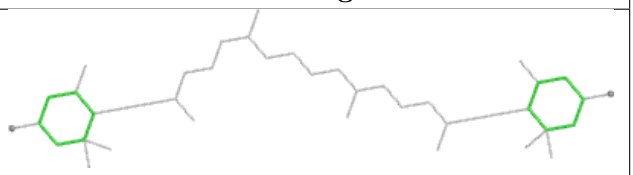
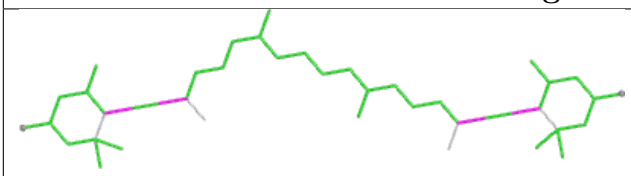


Rings

Ligand II0 2 614



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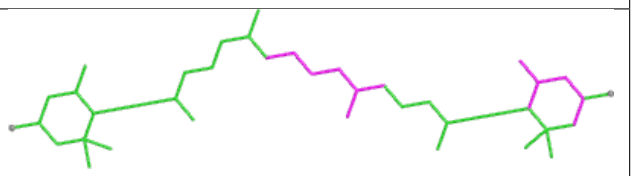
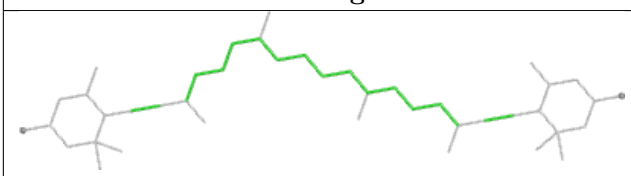


Bond angles



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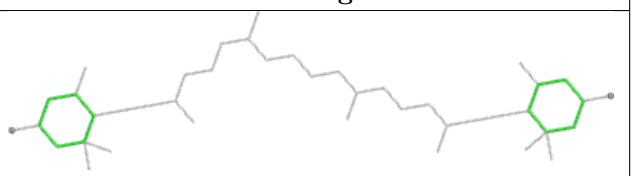
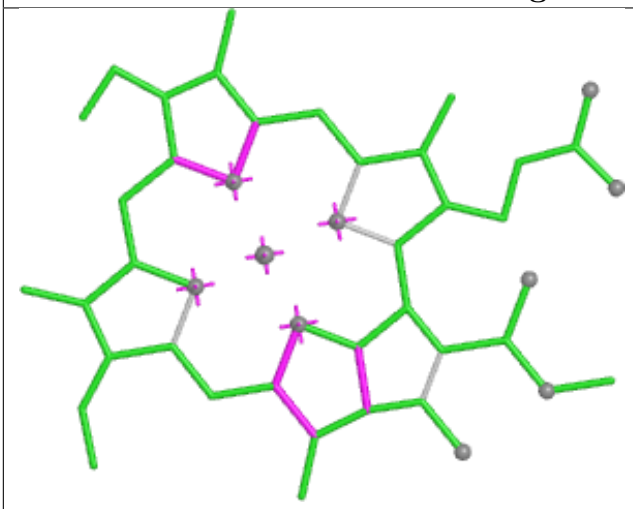


Rings

Ligand CLA c 601



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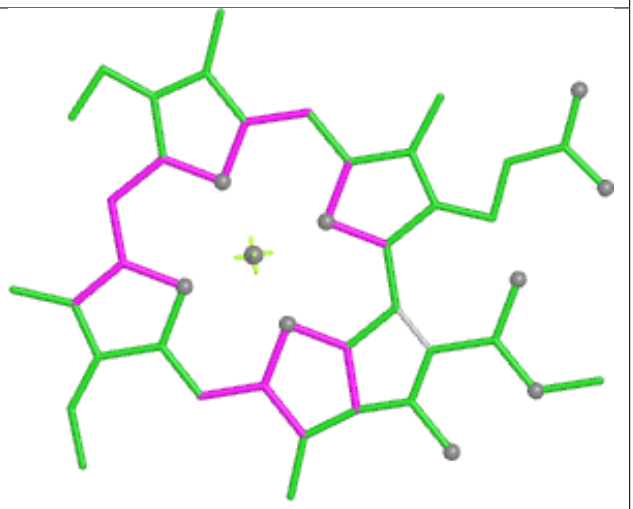
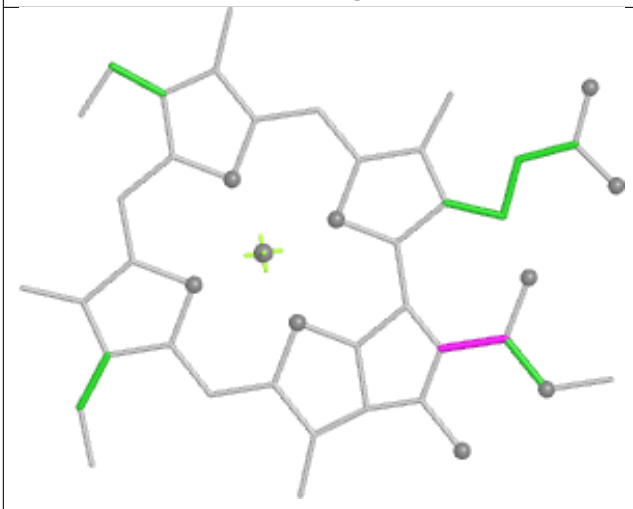


Bond angles

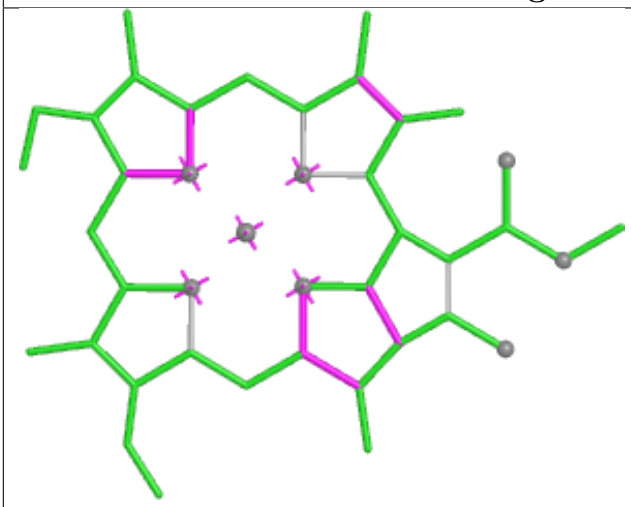


Torsions



Rings

Ligand CLA 2 609



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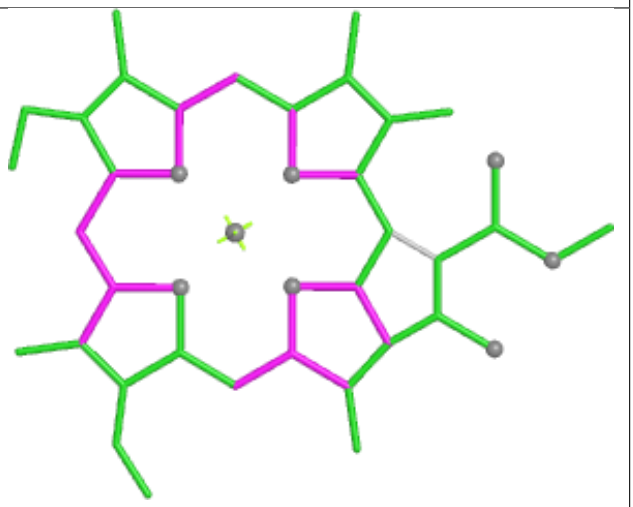
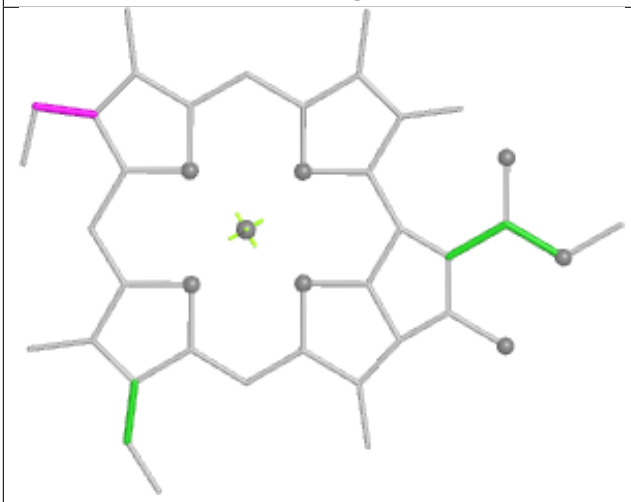


Bond angles



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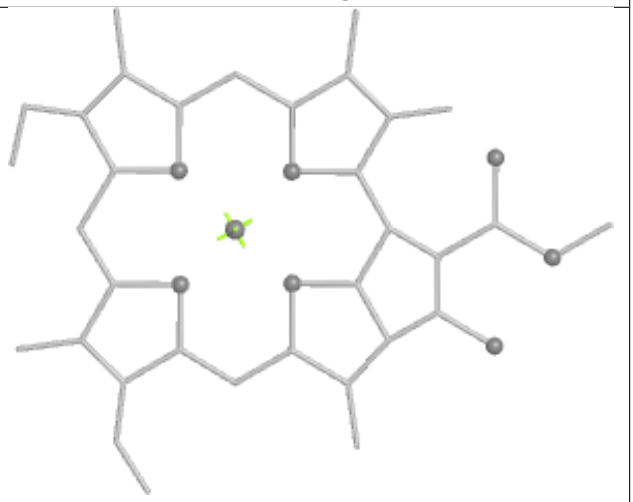
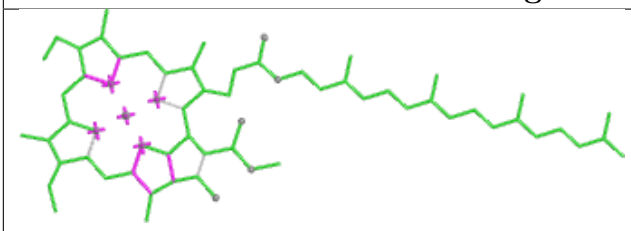


Rings

Ligand CLA B 807



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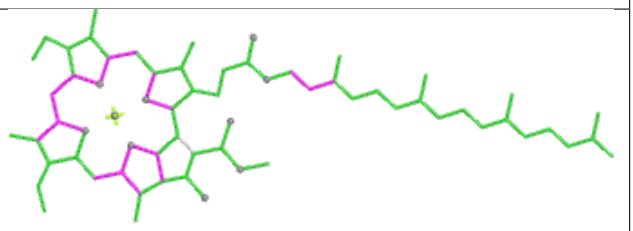
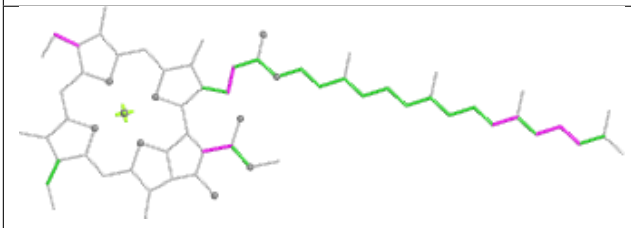


Bond angles



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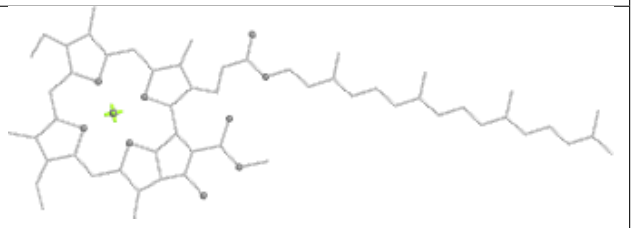
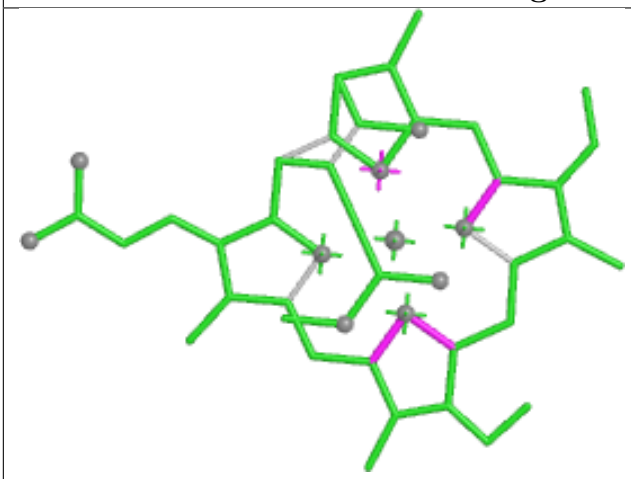


Rings

Ligand KC2 5 610



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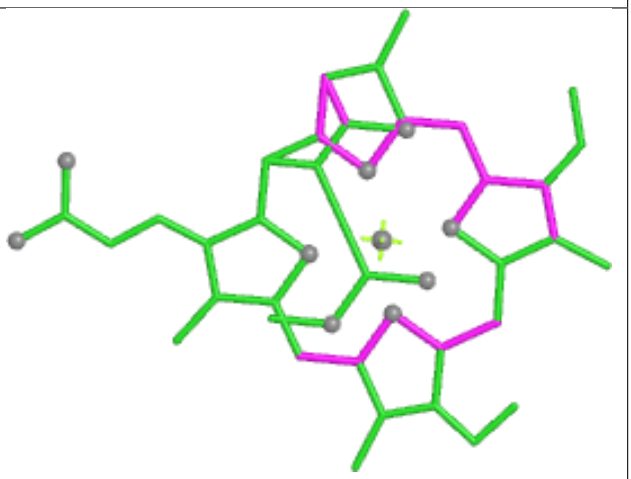
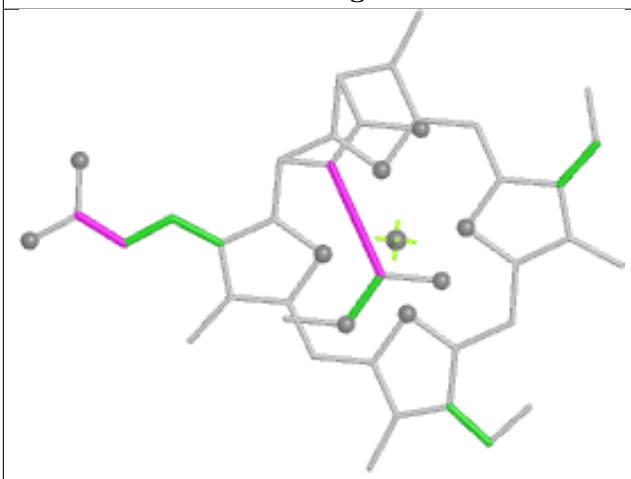
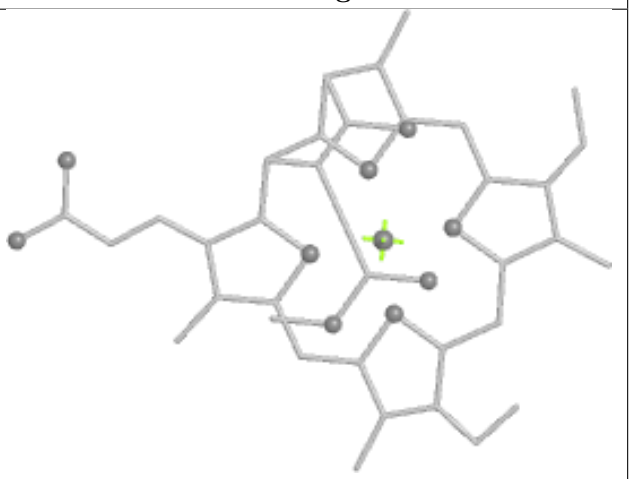


Bond angles

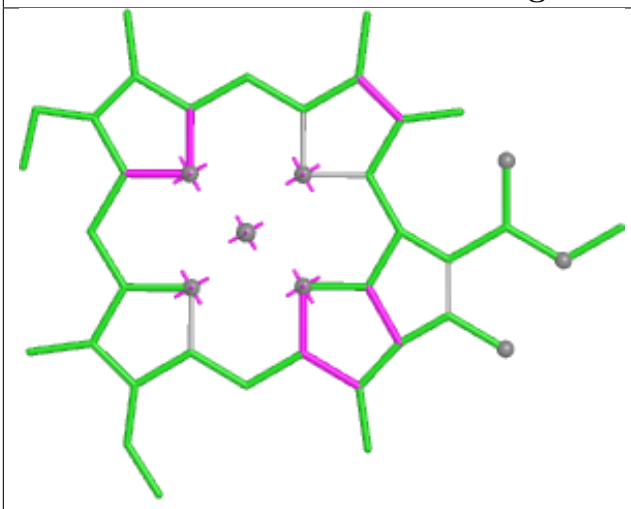


Torsions

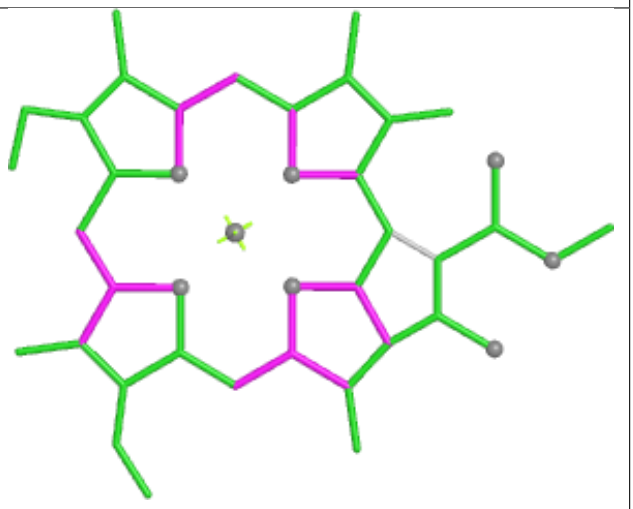


Rings

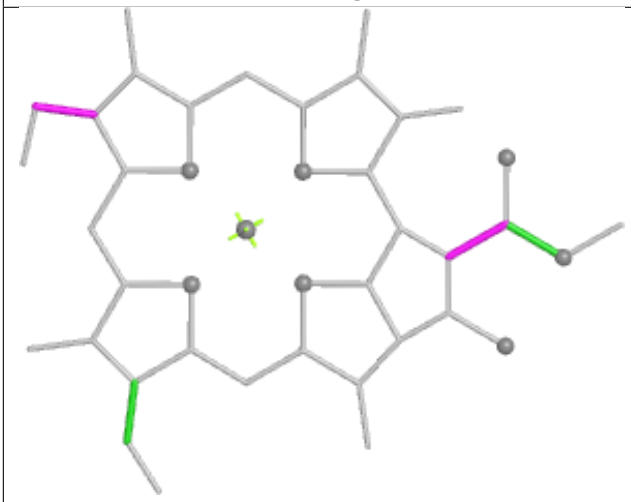
Ligand CLA 5 613



Bond lengths



Bond angles



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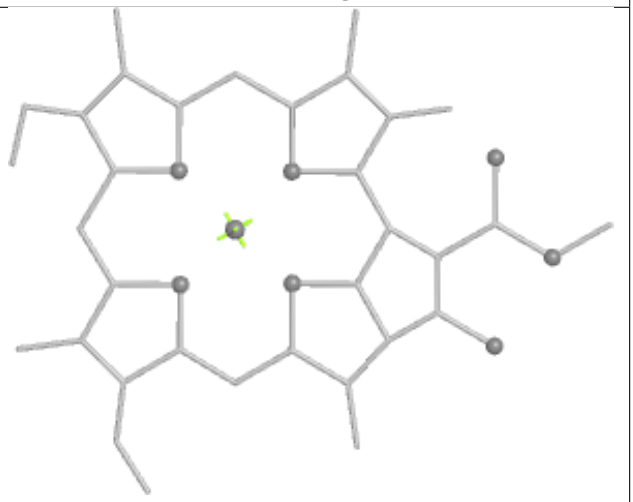
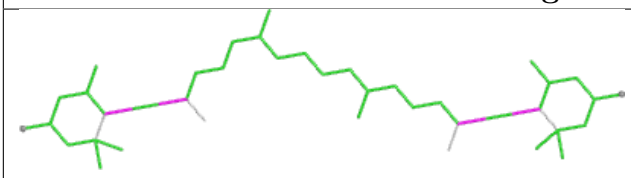


Rings

Ligand II0 b 614



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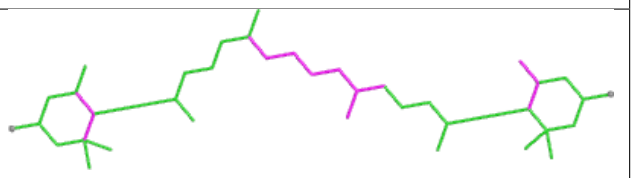
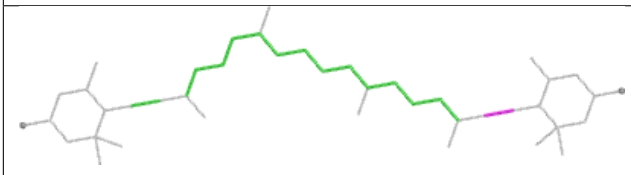


Bond angles



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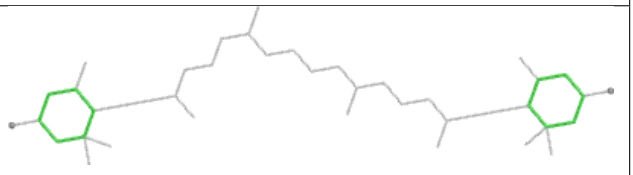
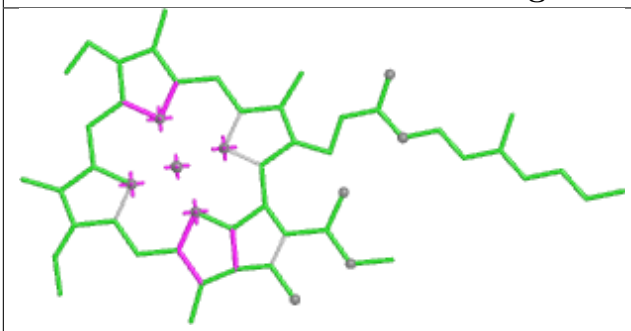


Rings

Ligand CLA 7 604



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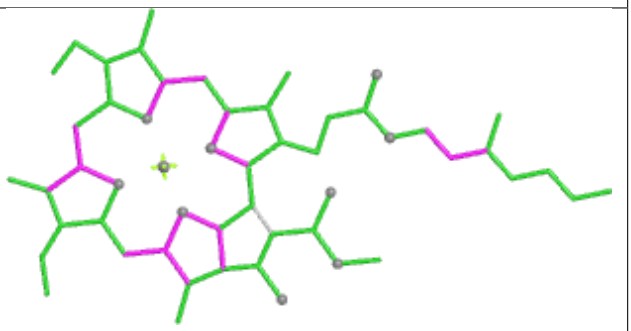
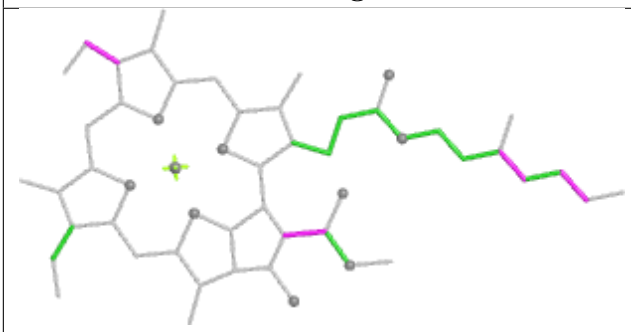


Bond angles



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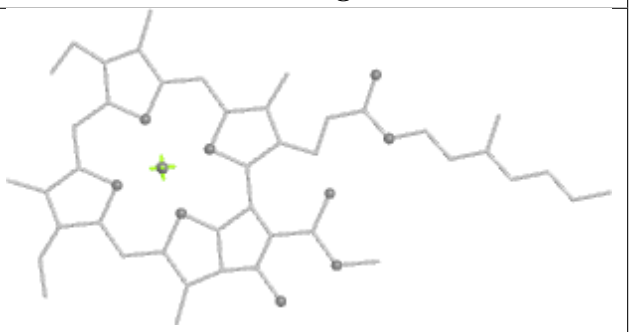
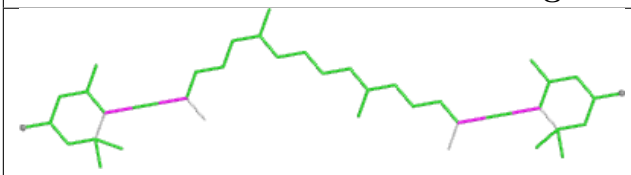


Rings

Ligand II0 c 618



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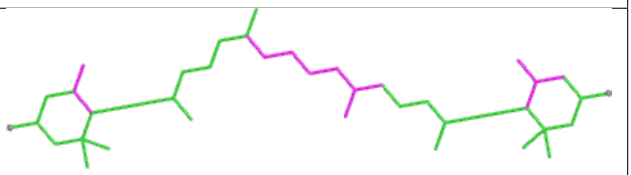
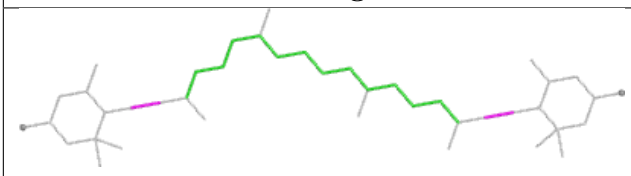


Bond angles



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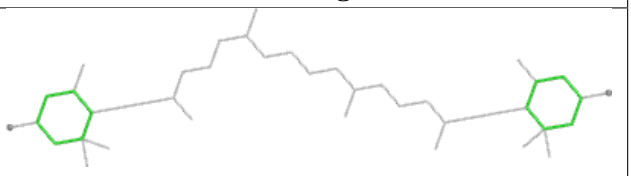
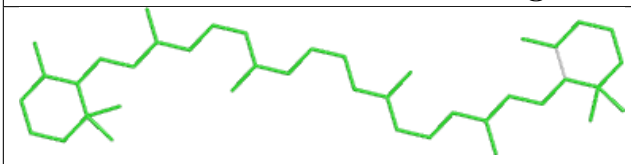


Rings

Ligand 8CT B 851



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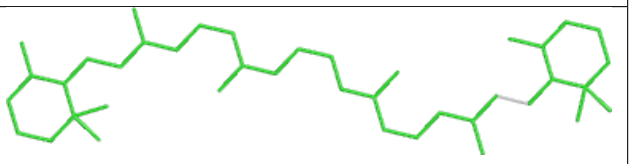
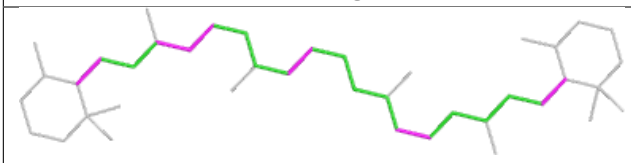


Bond angles



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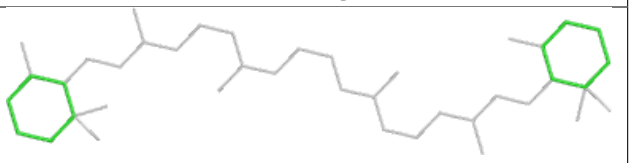
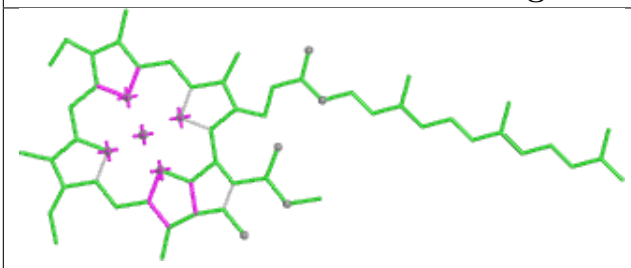


Rings

Ligand CLA b 607



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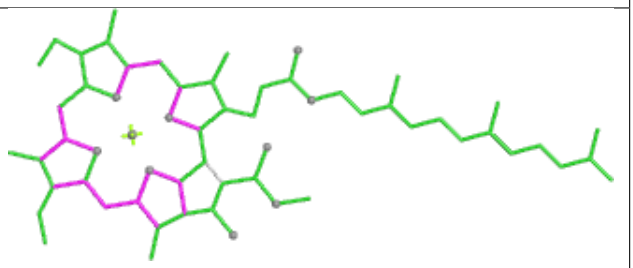
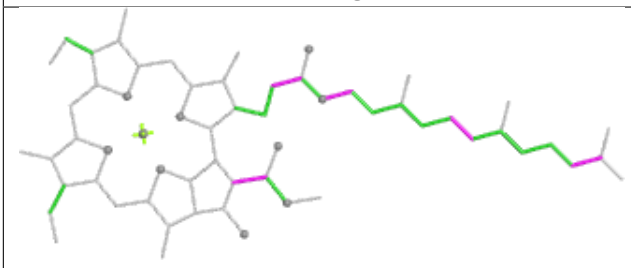


Bond angles



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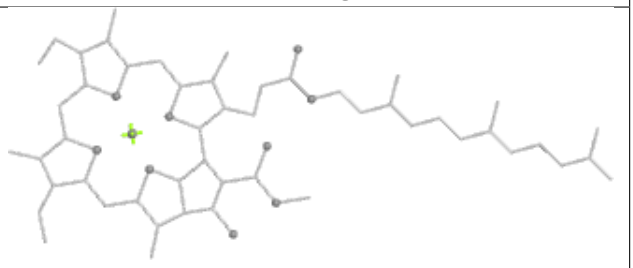
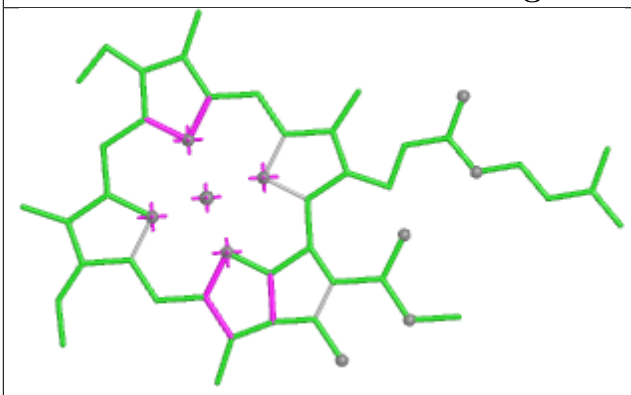


Rings

Ligand CLA A 807



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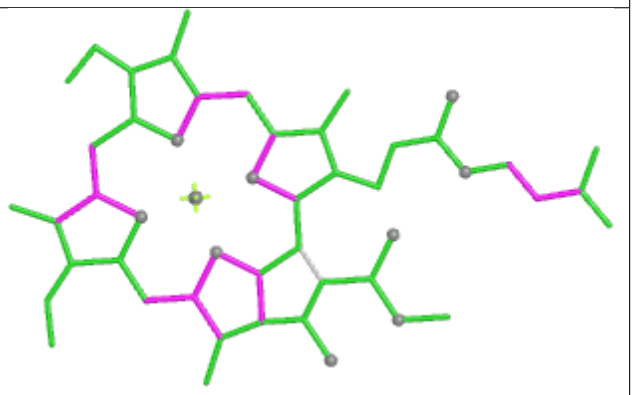
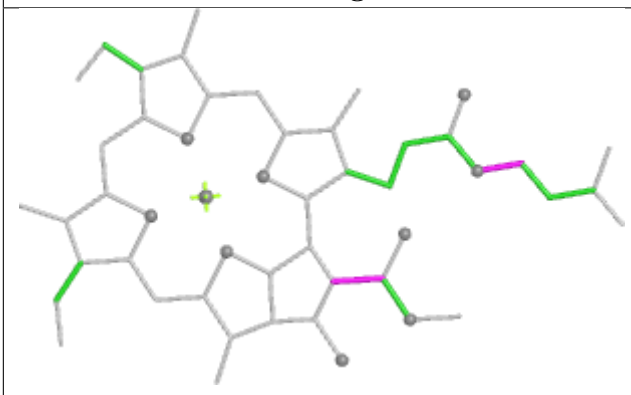


Bond angles



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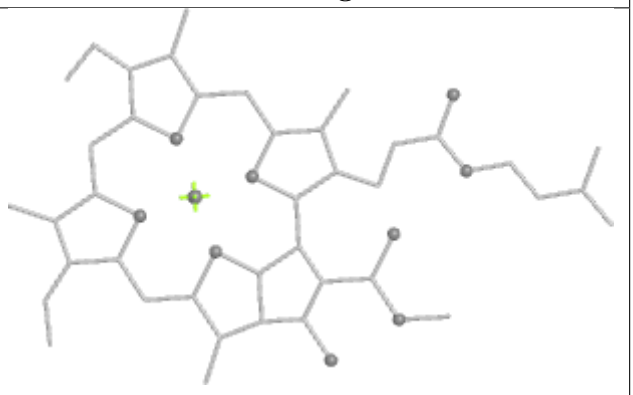
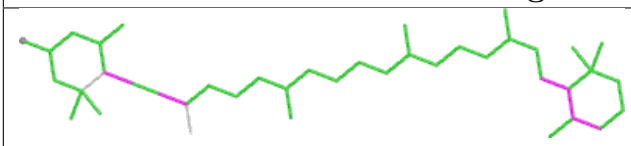


Rings

Ligand IHT K 104



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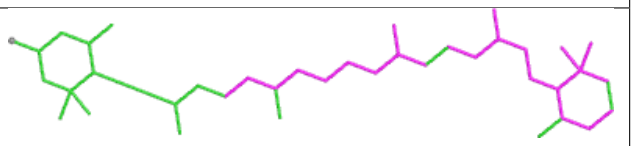


Bond angles

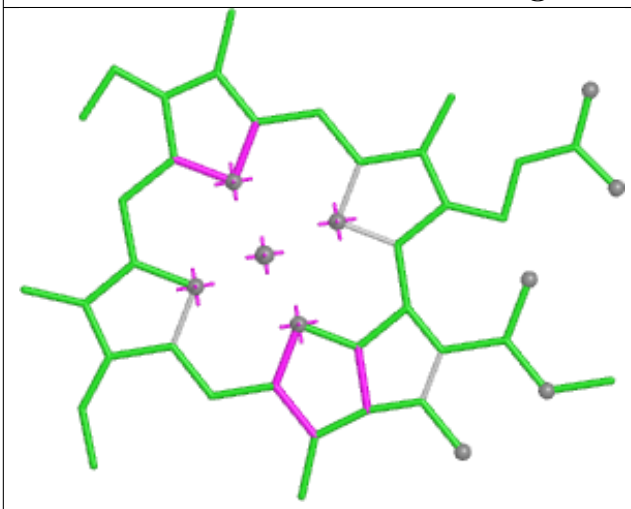


Torsions

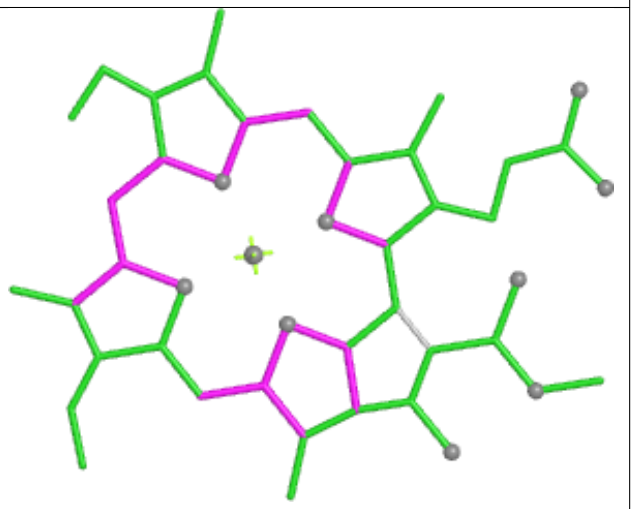


Rings

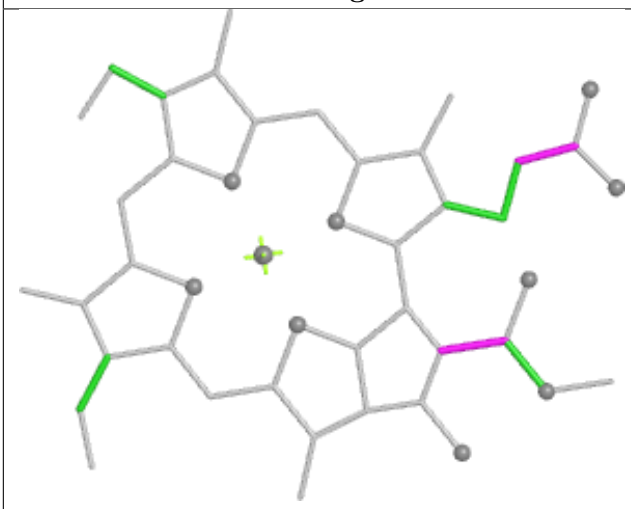
Ligand CLA e 607



Bond lengths



Bond angles



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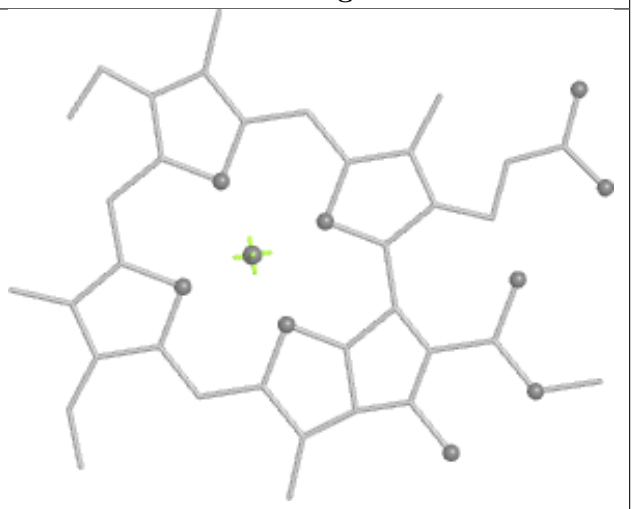
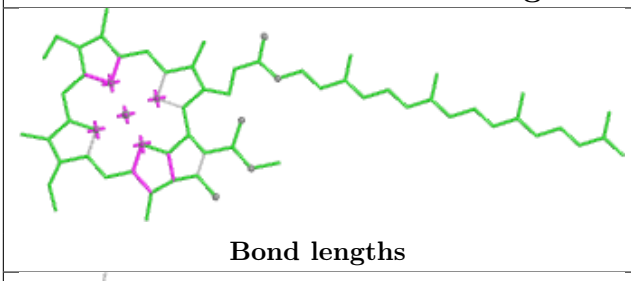


Rings

Ligand CLA A 839



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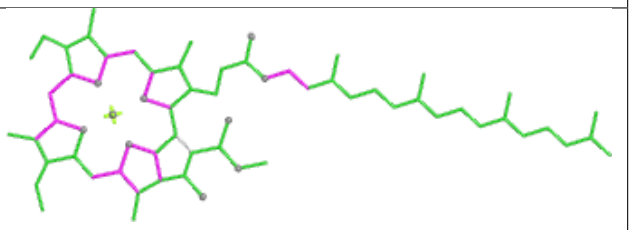
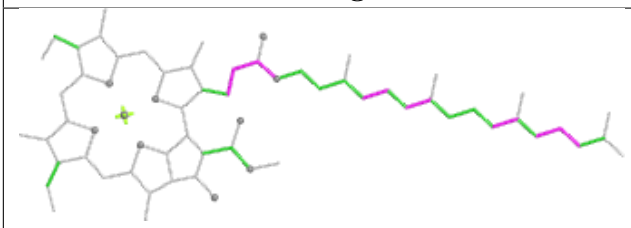


Bond angles



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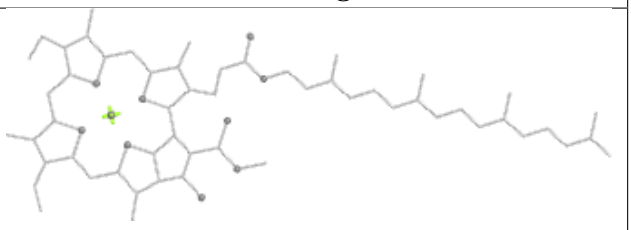
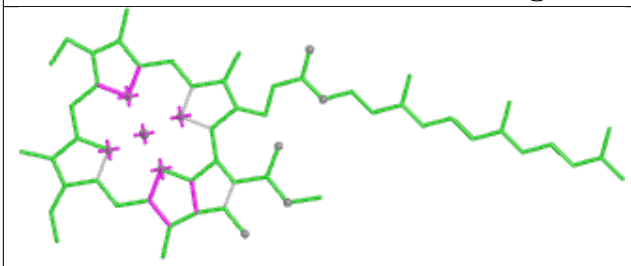


Rings

Ligand CLA a 604



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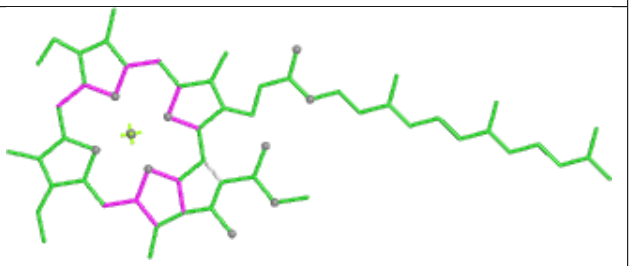
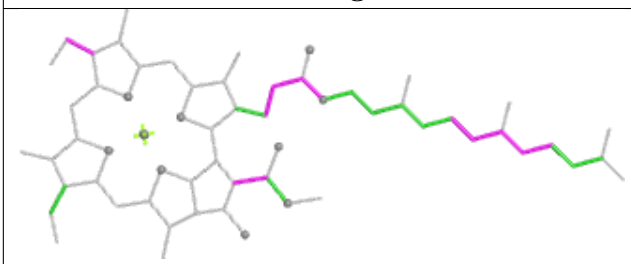


Bond angles



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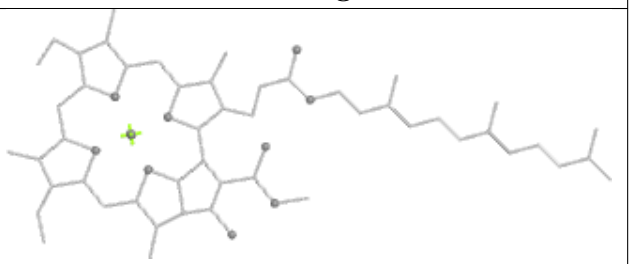
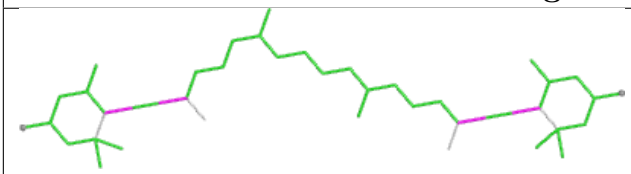


Rings

Ligand II0 e 614



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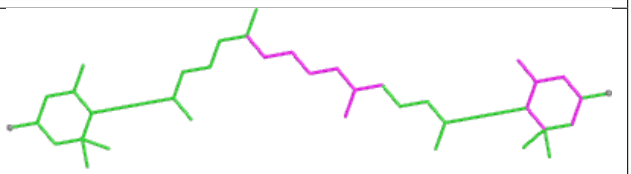
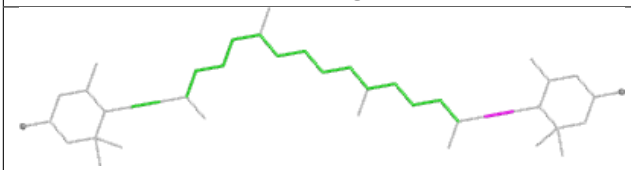


Bond angles



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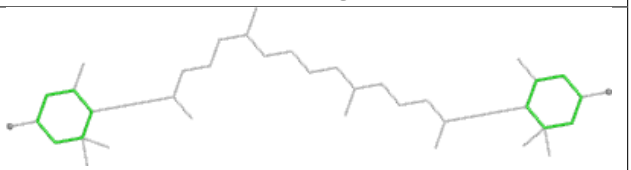
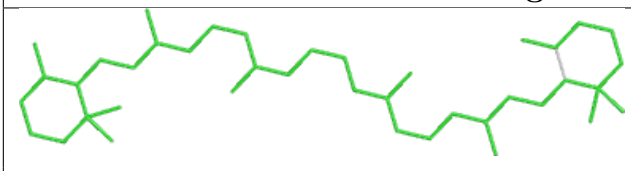


Rings

Ligand 8CT K 103



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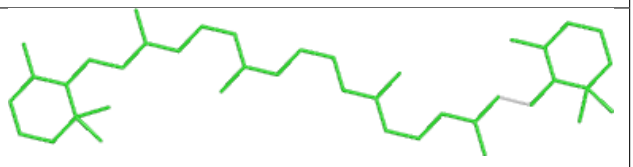
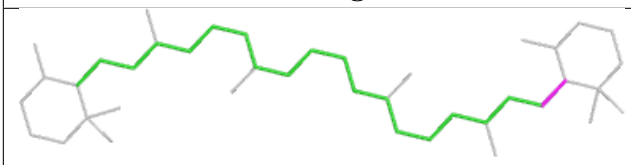


Bond angles



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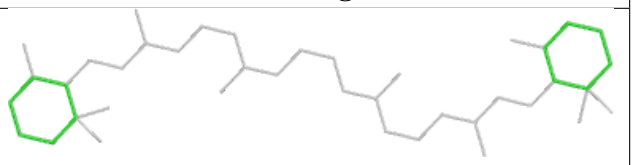
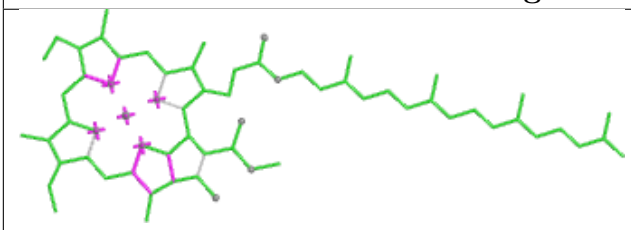


Rings

Ligand CLA A 843



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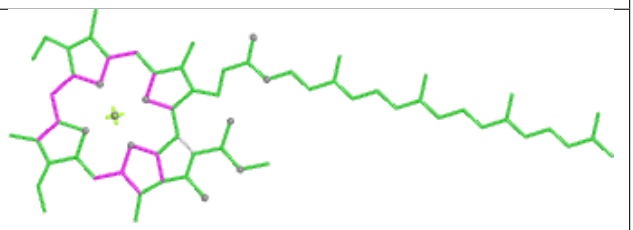
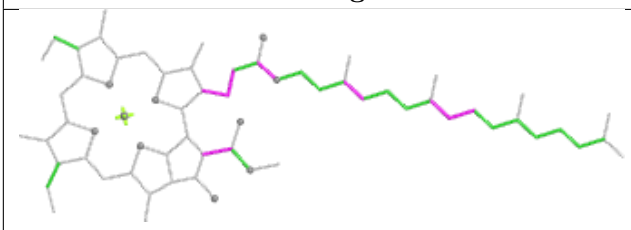


Bond angles



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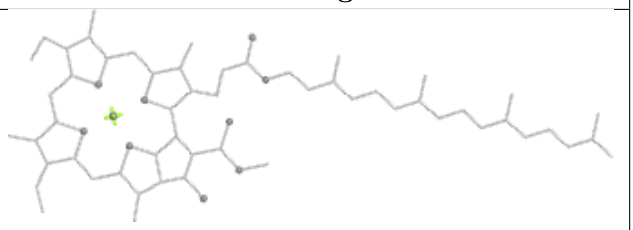
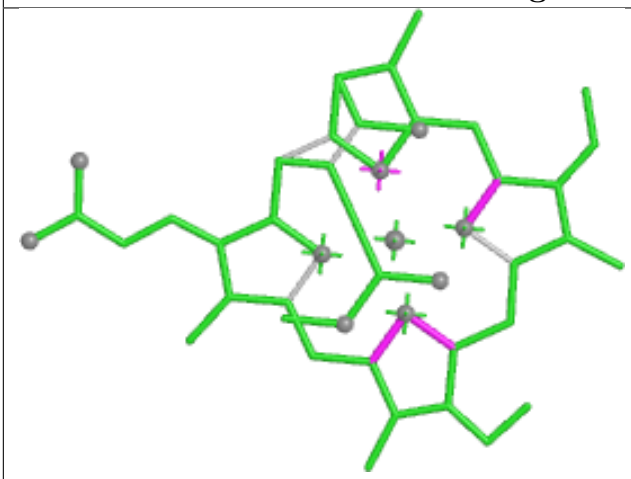
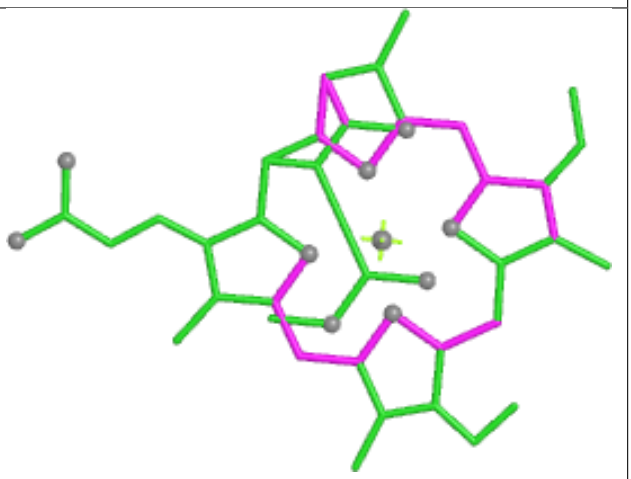


Rings

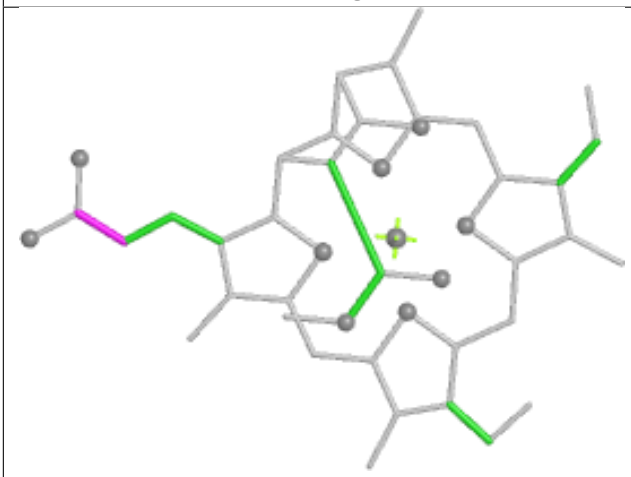
Ligand KC2 b 609



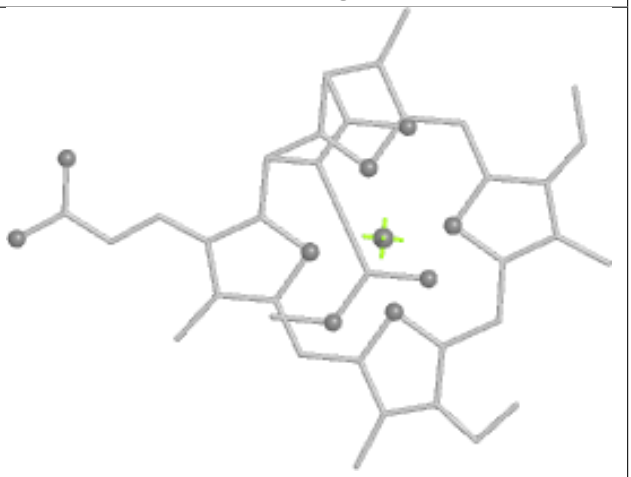
Bond lengths



Bond angles

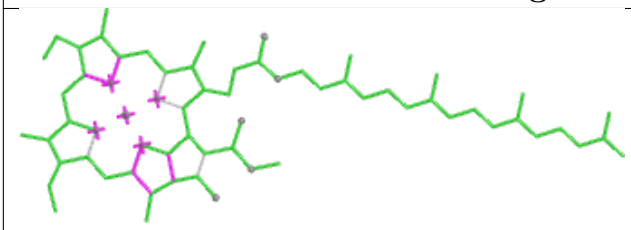


Torsions

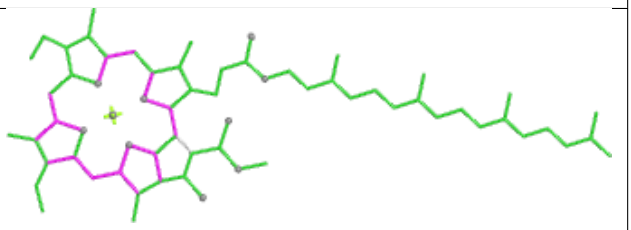


Rings

Ligand CLA c 603



Bond lengths



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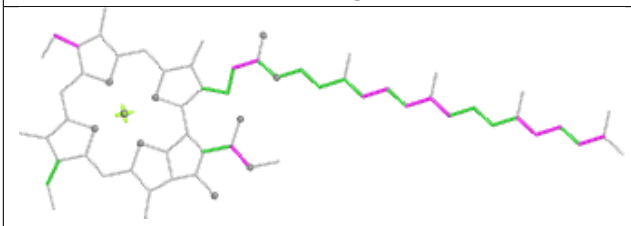

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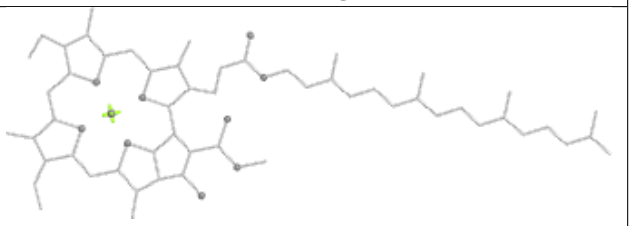
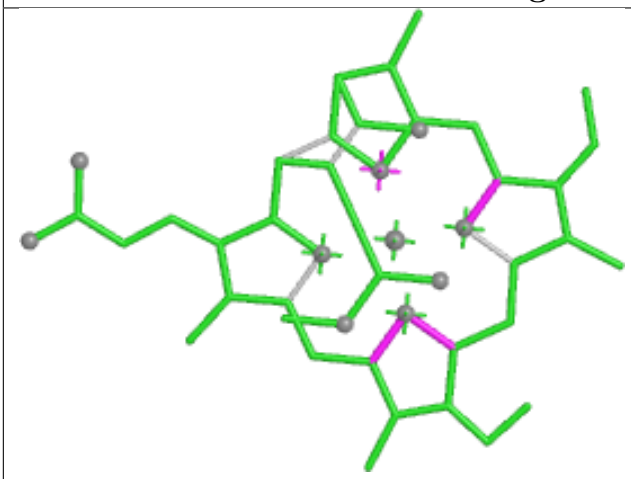


Rings

Ligand KC2 b 605



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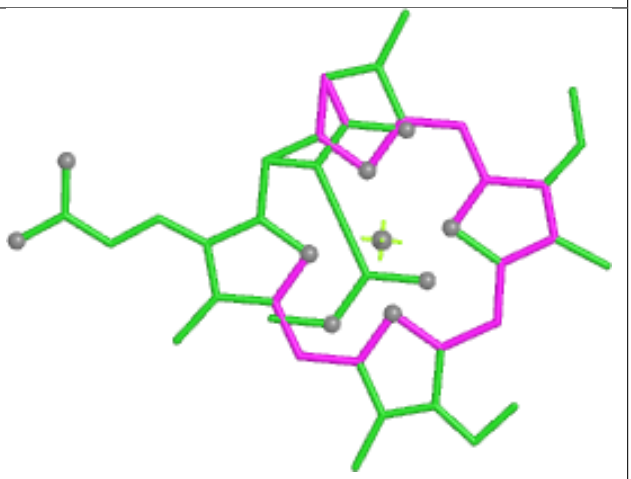

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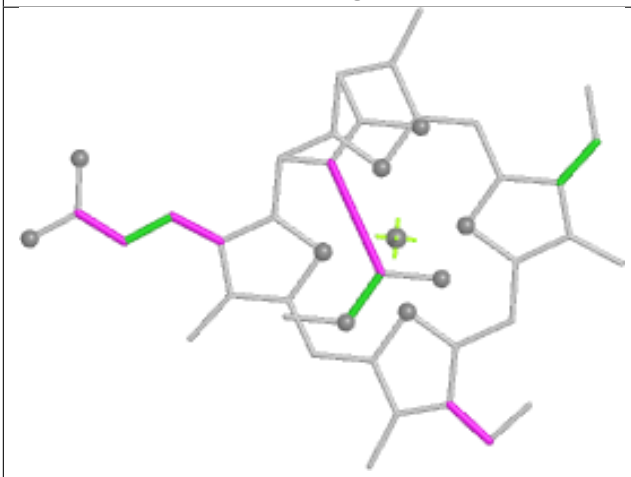

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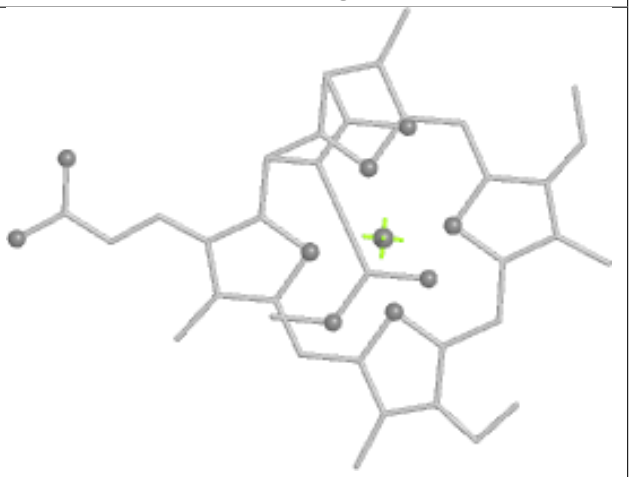
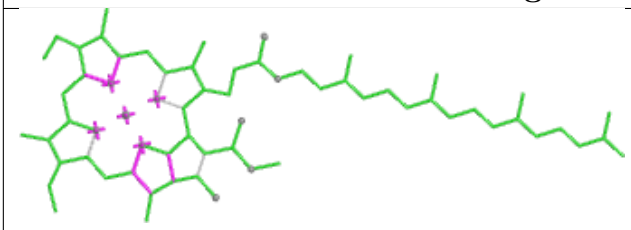


Rings

Ligand CLA B 840



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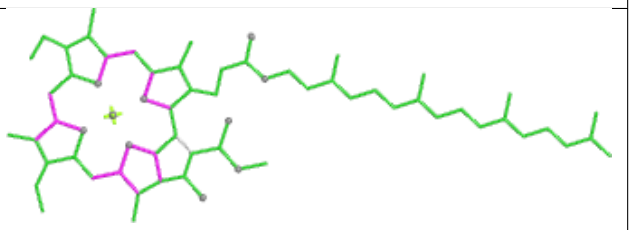
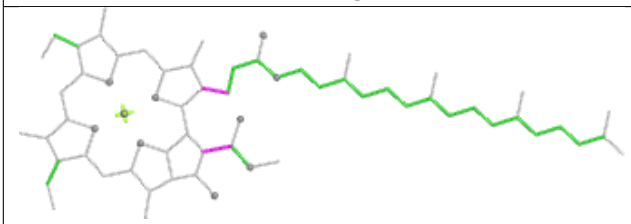


Bond angles



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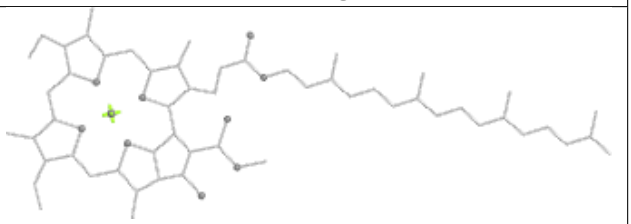
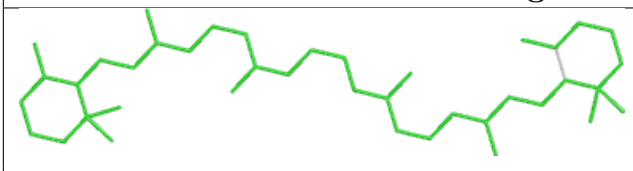


Rings

Ligand 8CT B 846



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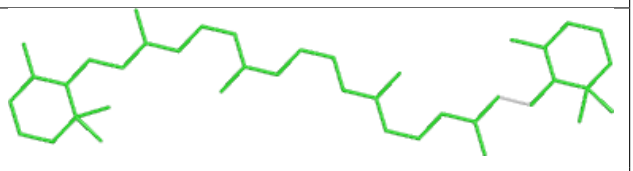
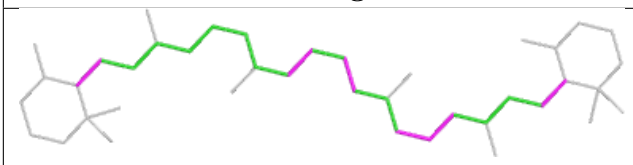


Bond angles



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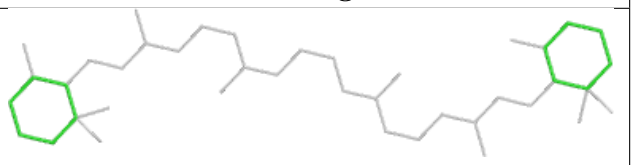
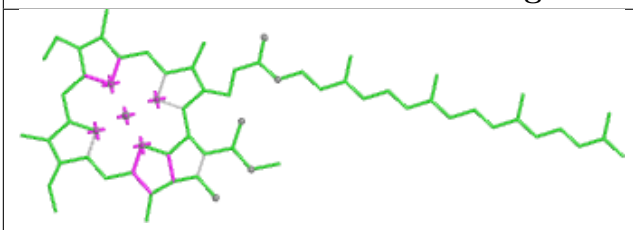


Rings

Ligand CLA B 825



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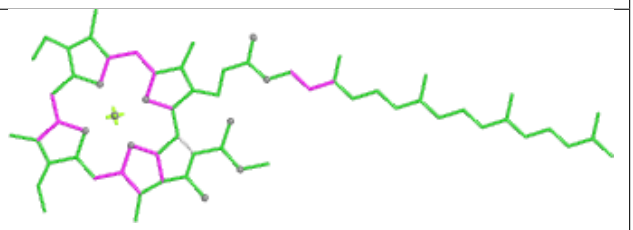

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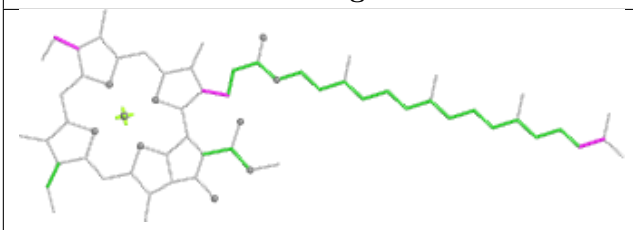

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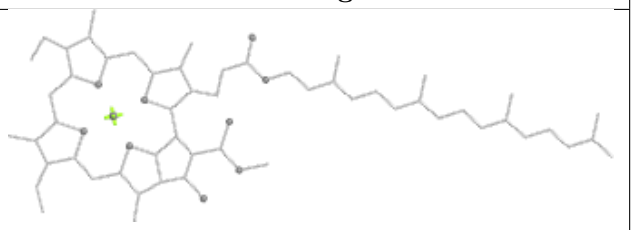
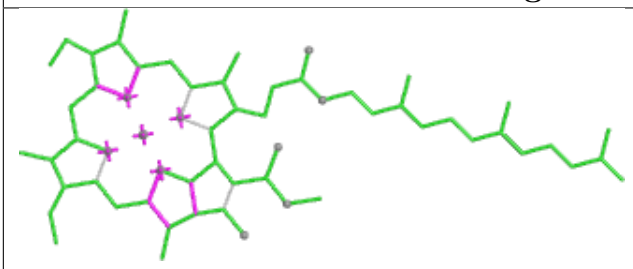


Rings

Ligand CLA B 817



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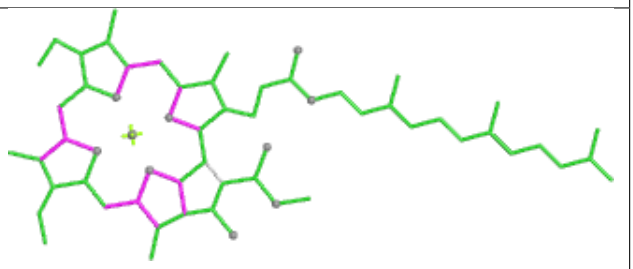
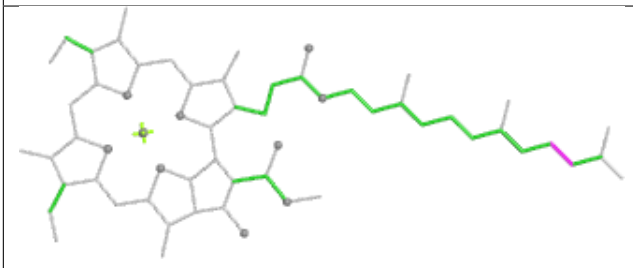


Bond angles



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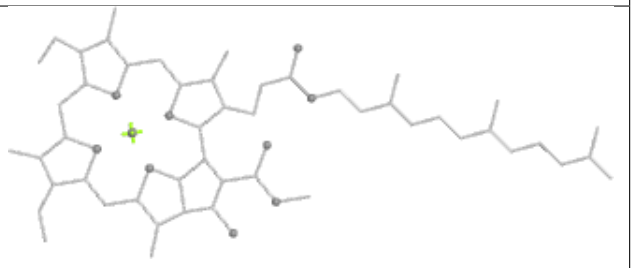
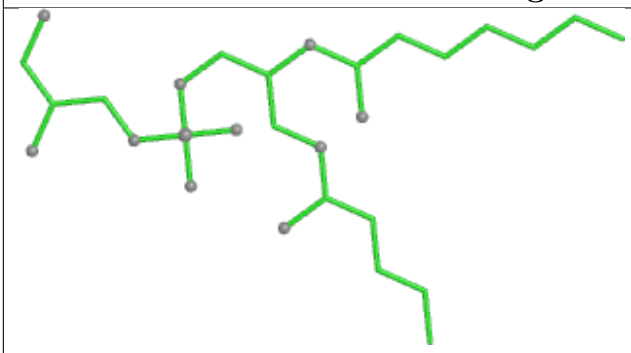


Rings

Ligand LHG a 618



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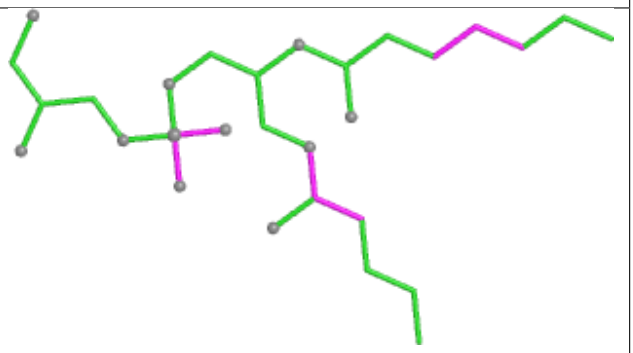

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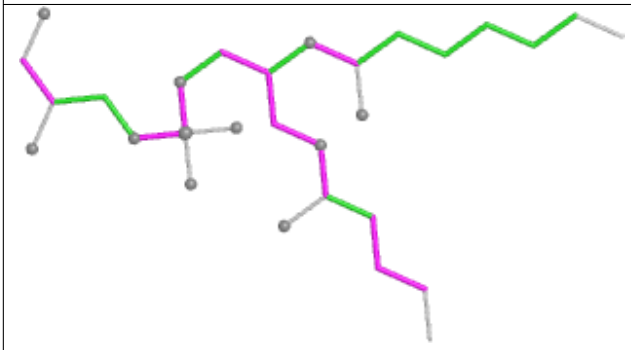

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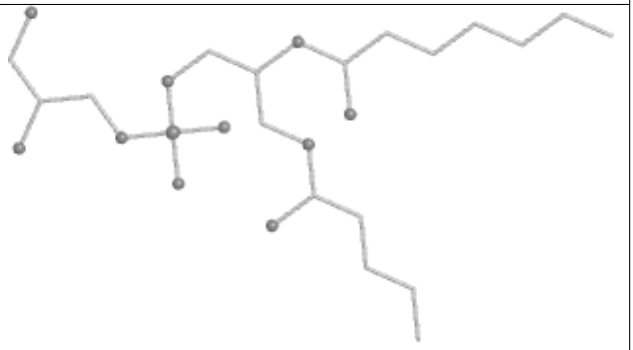
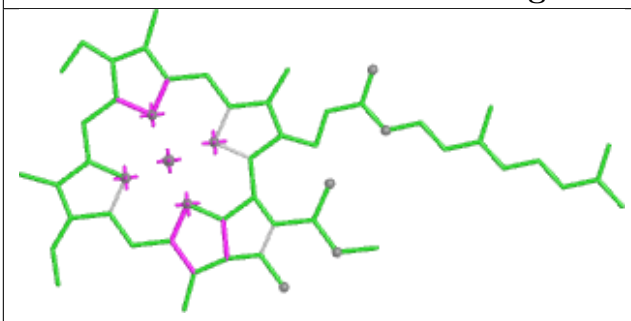


Rings

Ligand CLA a 605



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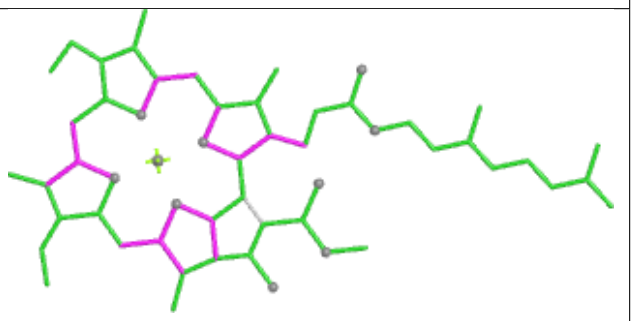
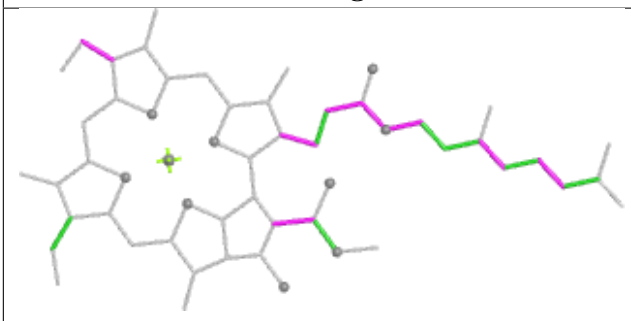


Bond angles



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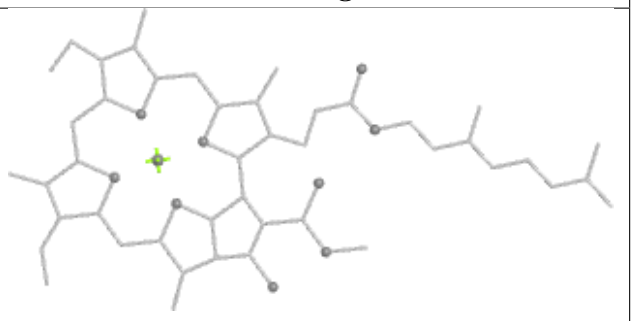
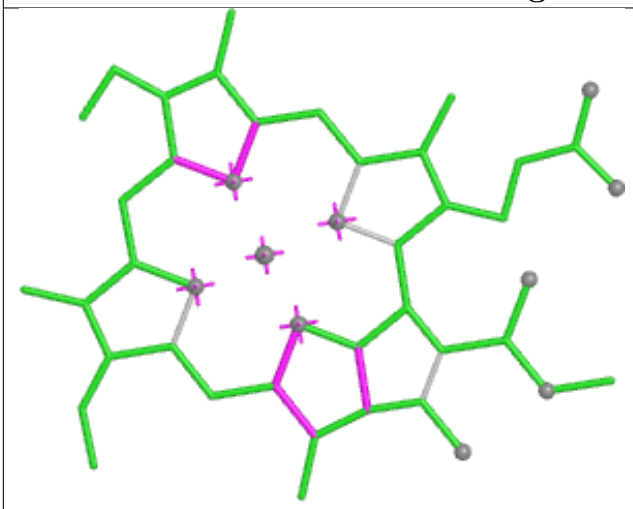


Rings

Ligand CLA 9 601



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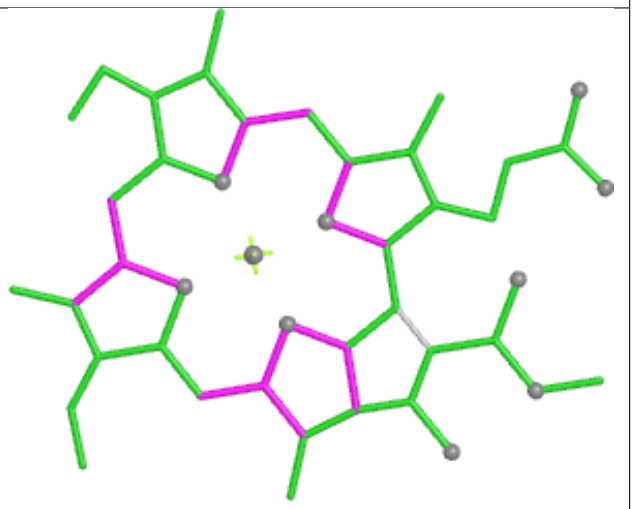

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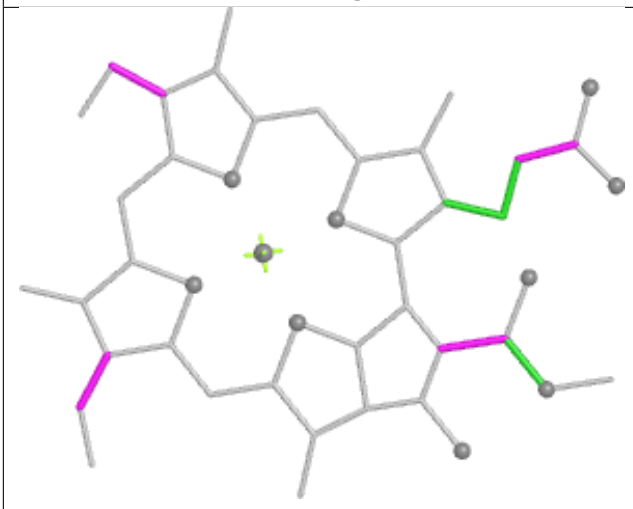
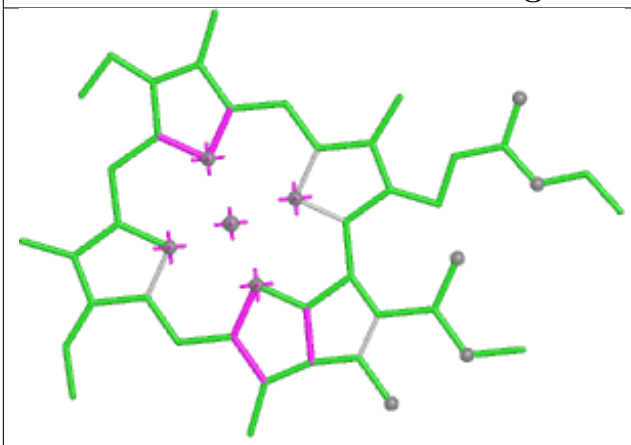


Torsions



Rings

Ligand CLA B 836



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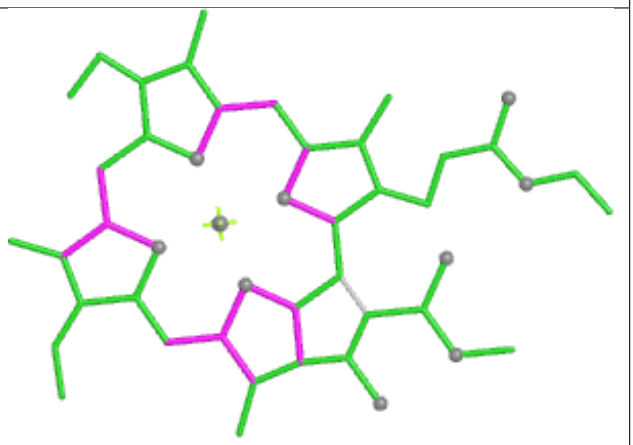

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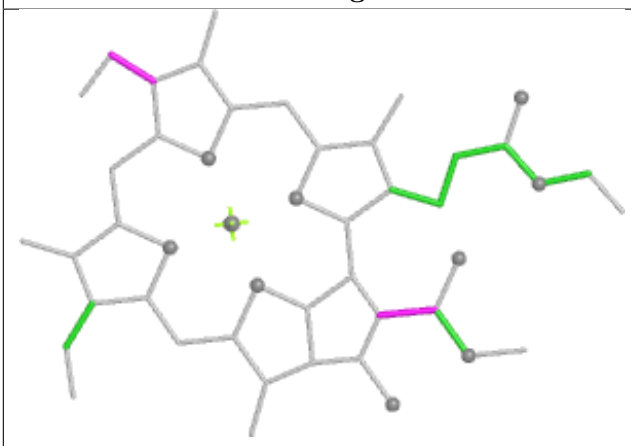

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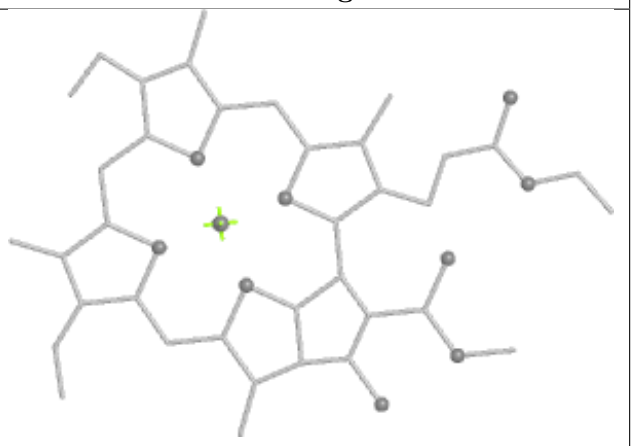
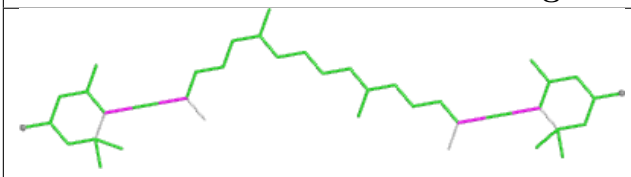


Rings

Ligand II0 4 614



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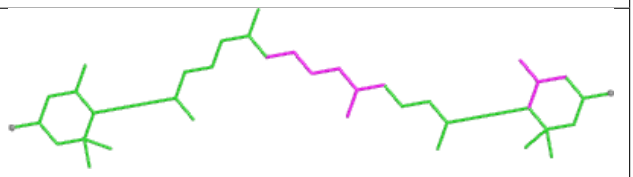

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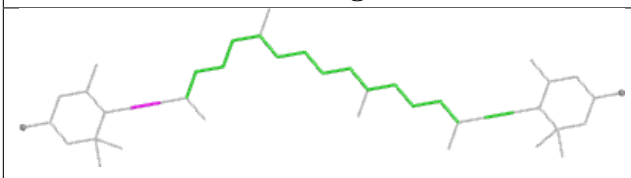

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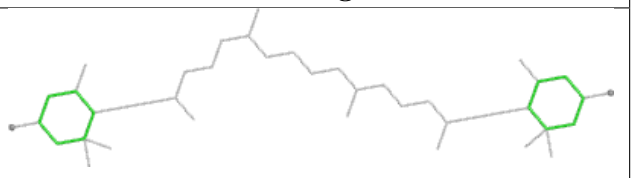
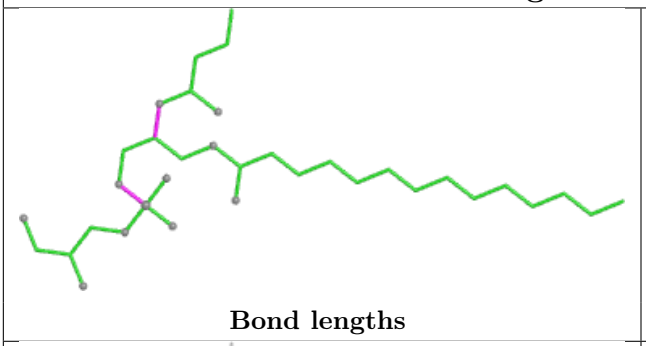


Rings

Ligand LHG 6 618



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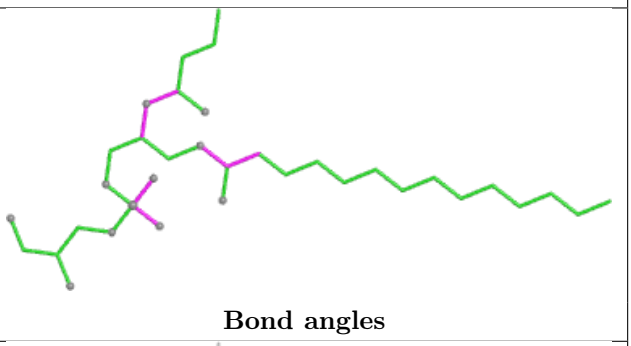
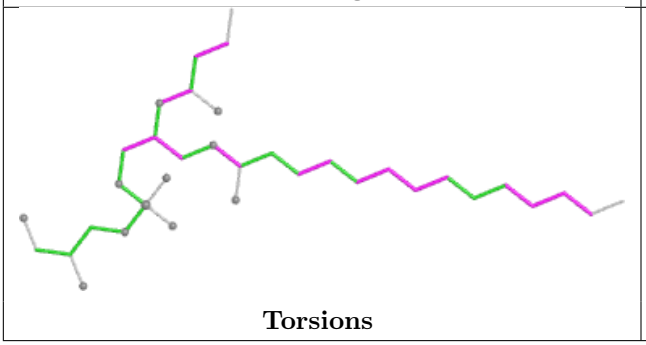


Bond angles



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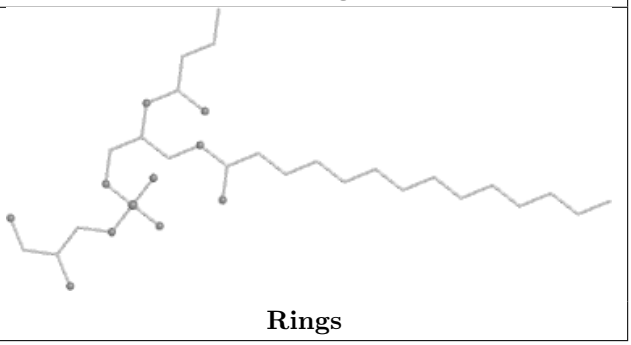
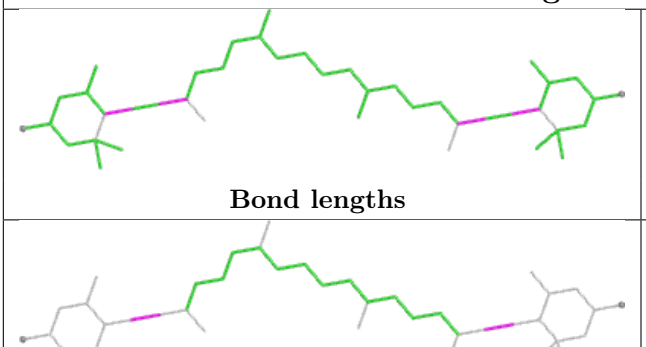


Rings

Ligand II0 2 613



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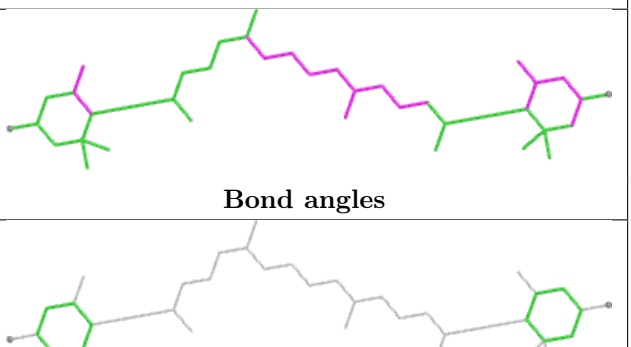
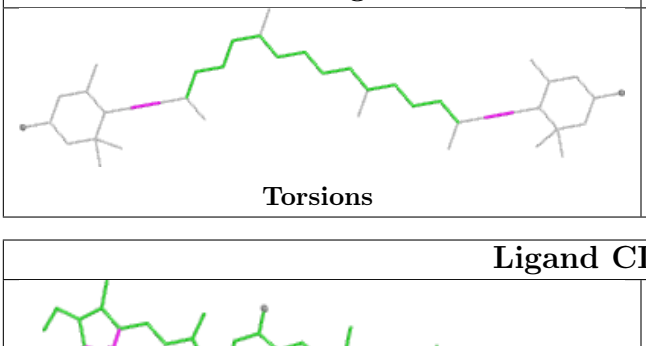


Bond angles



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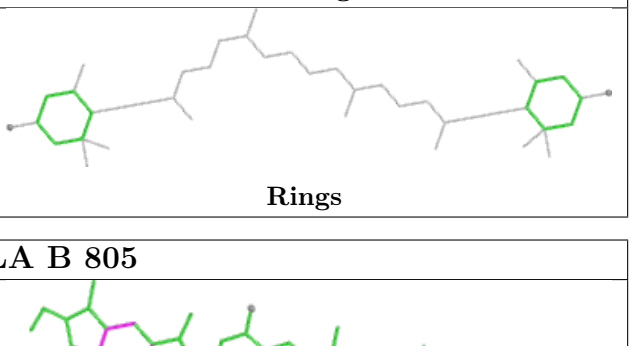
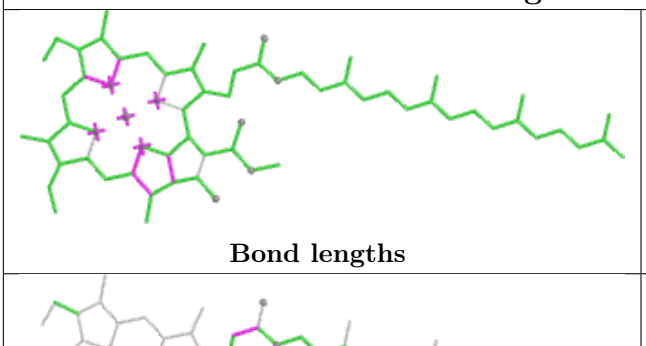


Rings

Ligand CLA B 805



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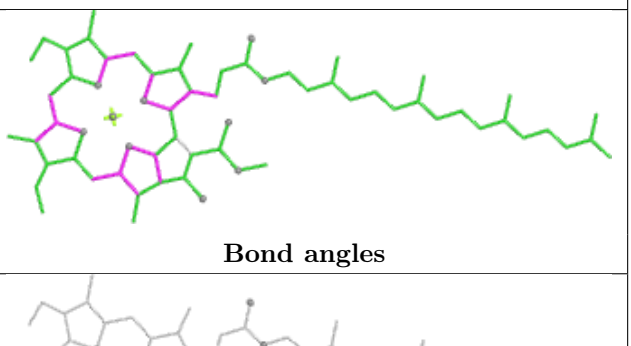
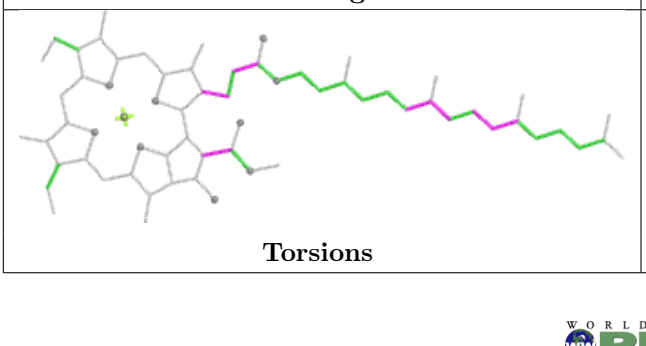


Bond angles



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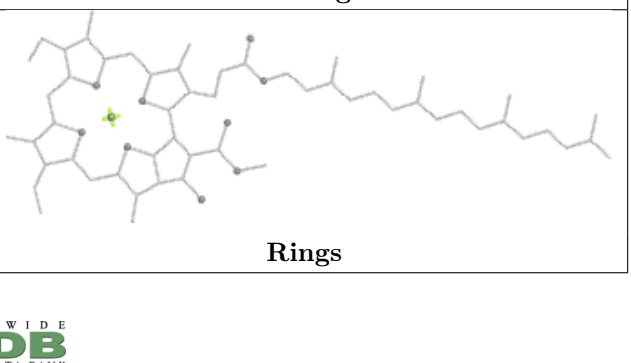
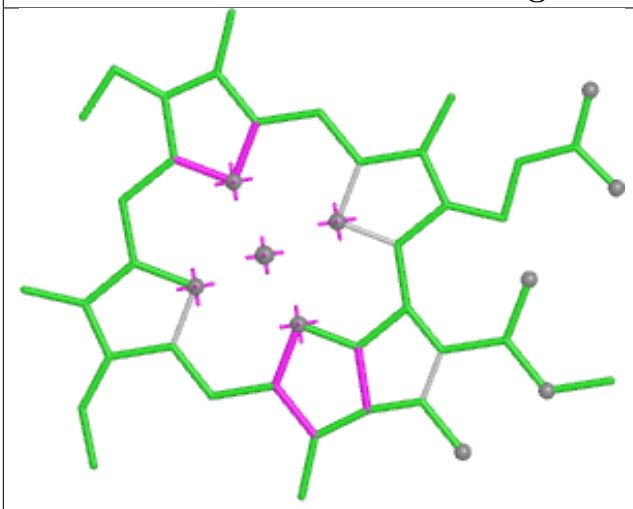
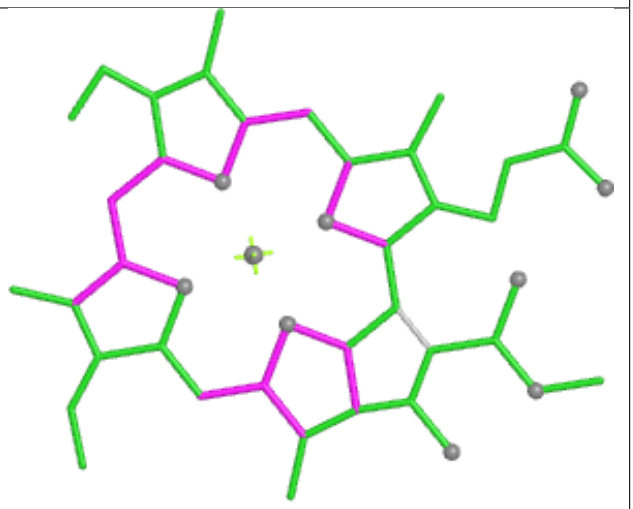


Rings

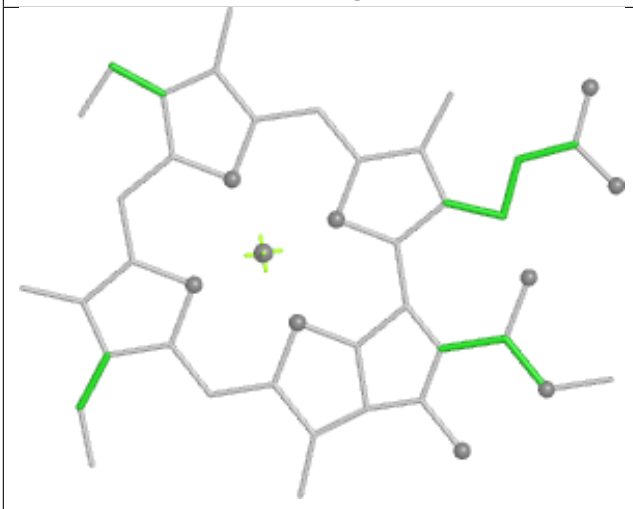
Ligand CLA 1 606



Bond lengths



Bond angles

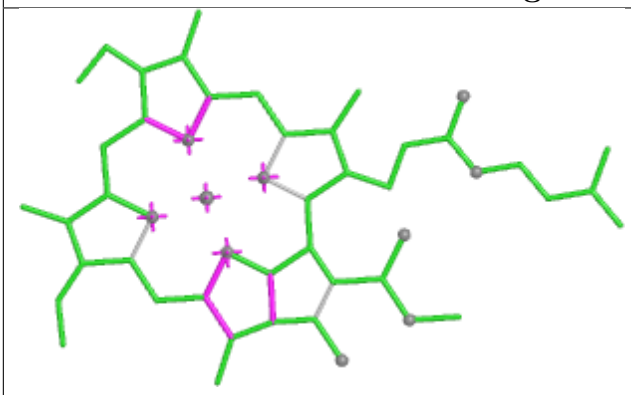


Torsions



Rings

Ligand CLA A 829



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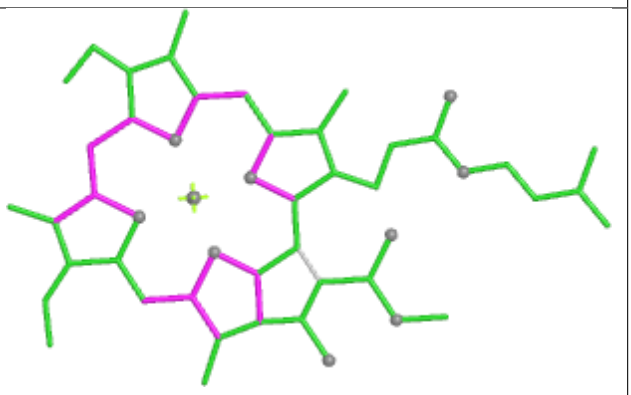
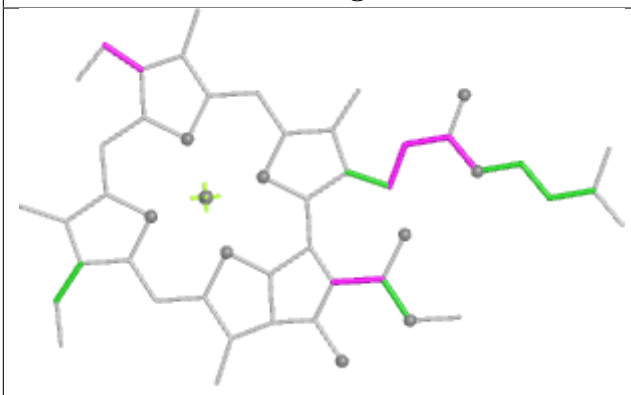


Bond angles



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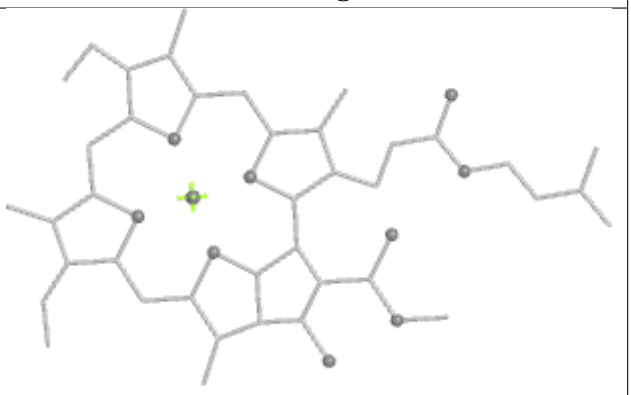
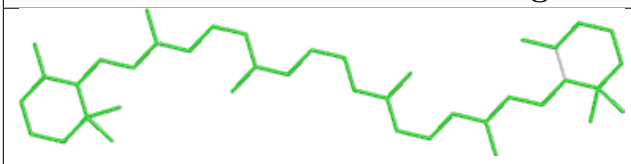


Rings

Ligand 8CT 4 616



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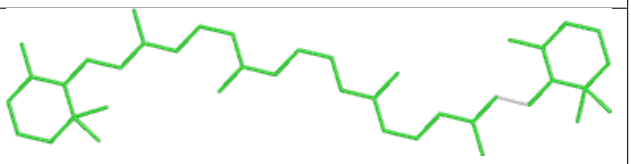
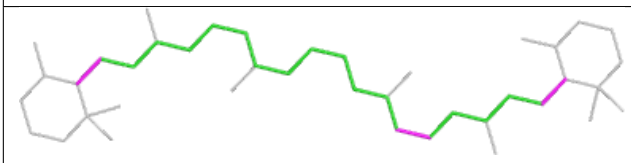


Bond angles



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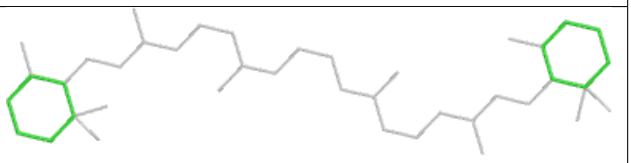
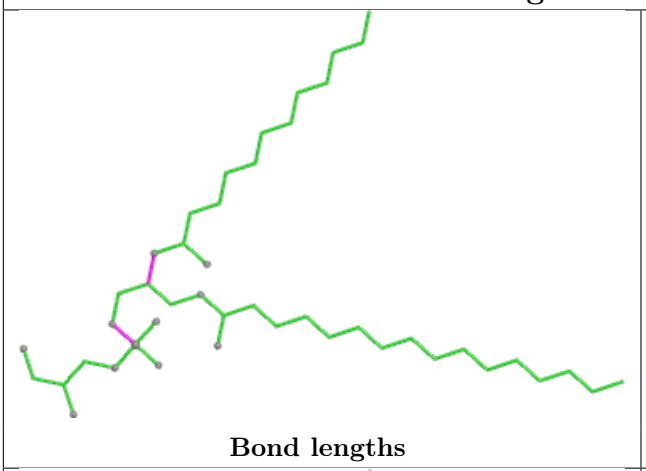


Rings

Ligand LHG 4 619



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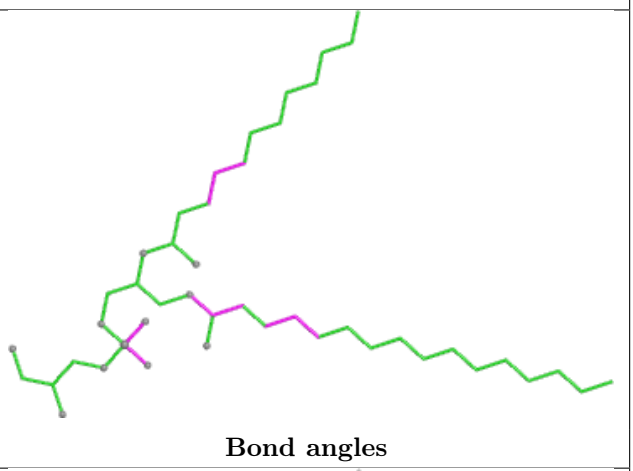

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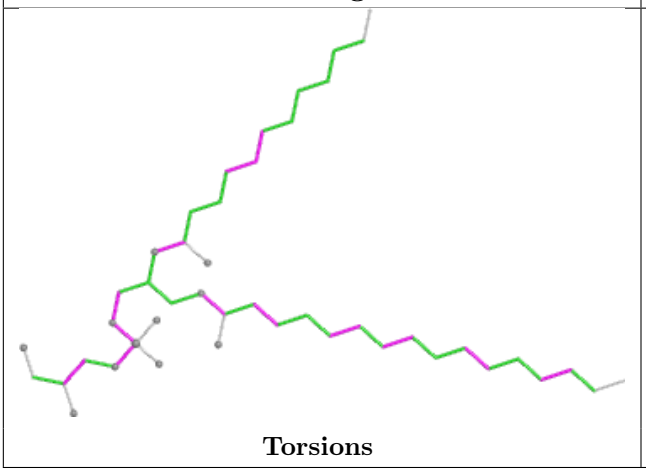

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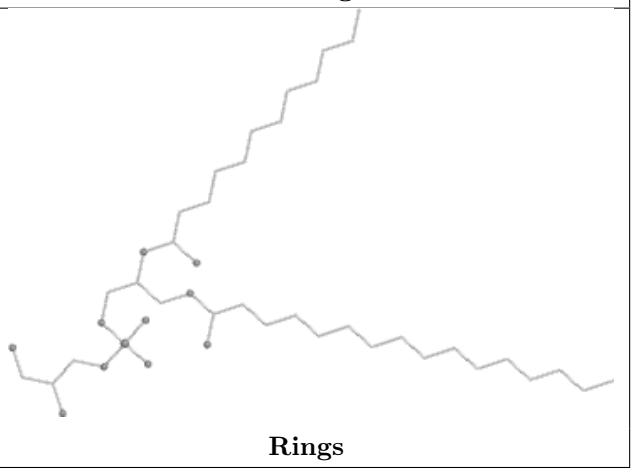
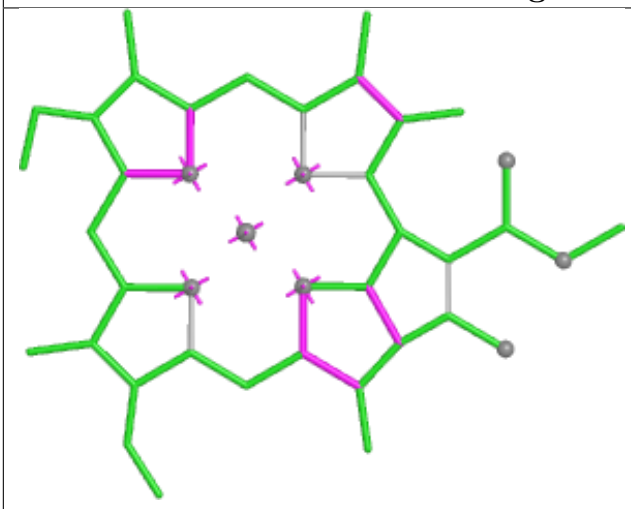


Rings

Ligand CLA 8 607



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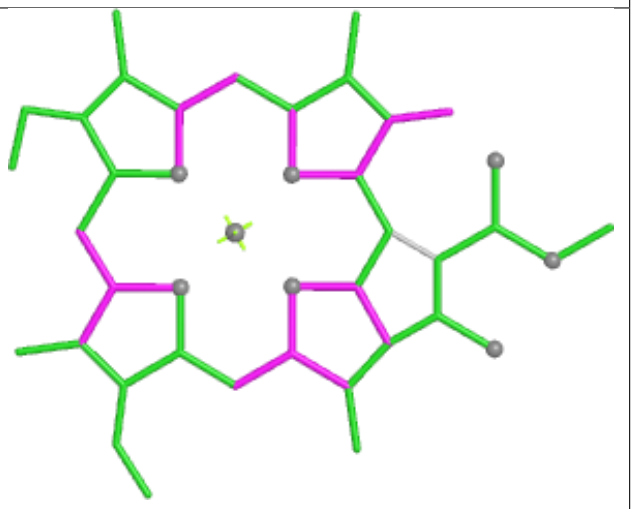
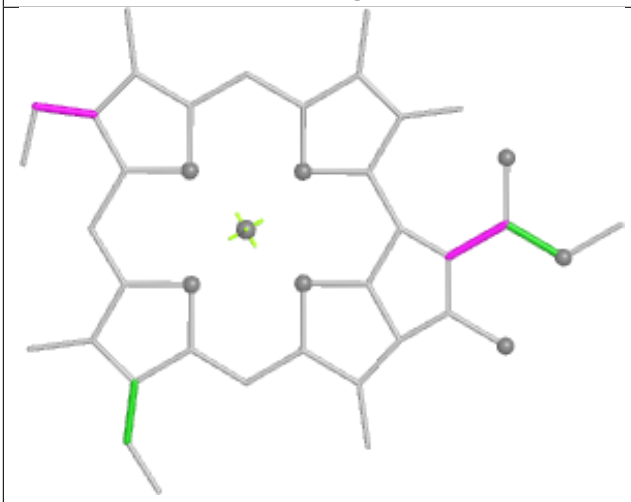


Bond angles



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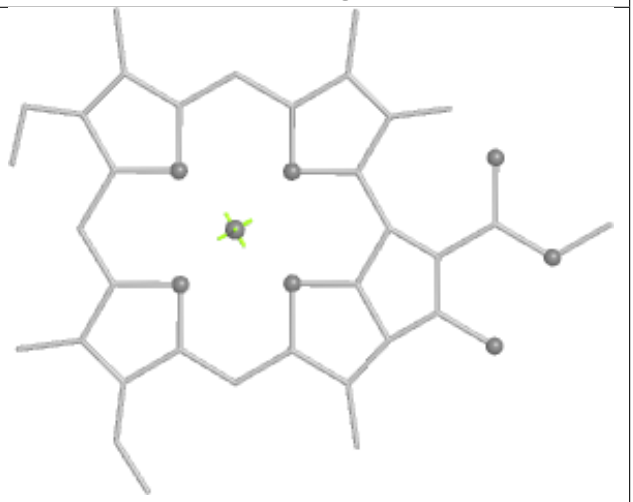
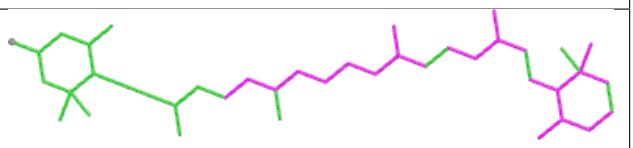


Rings

Ligand IHT 5 618



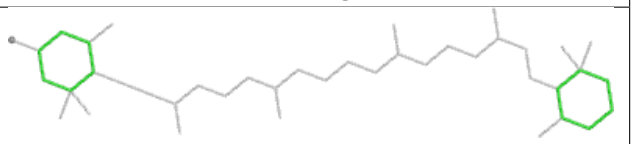
Bond lengths



Bond angles

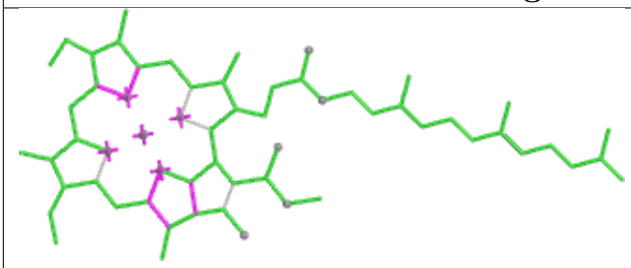


Torsions



Rings

Ligand CLA A 809



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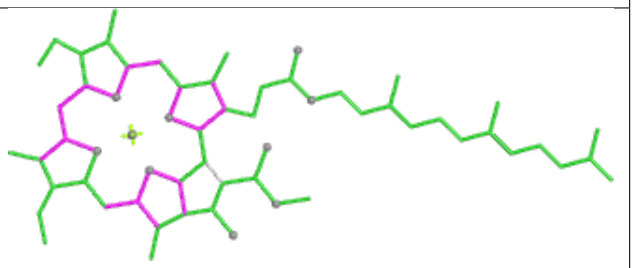
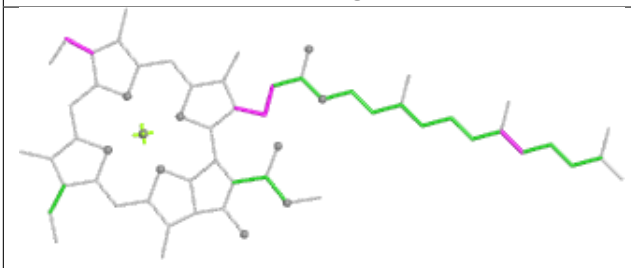


Bond angles



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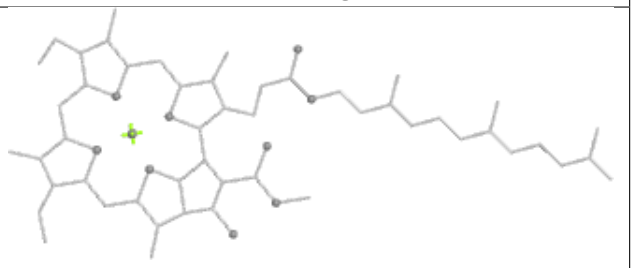
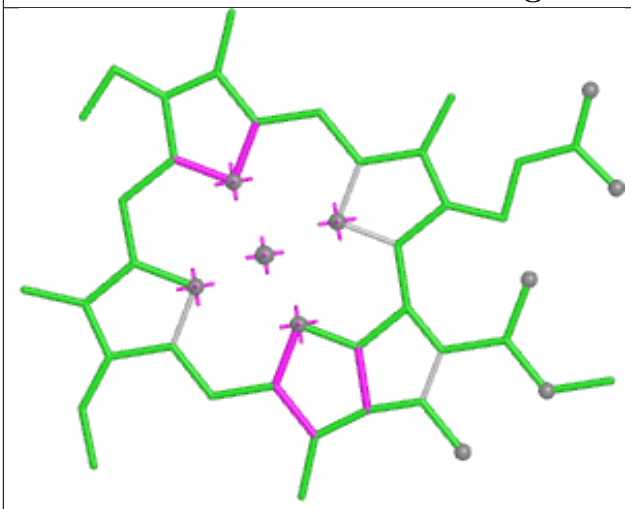


Rings

Ligand CLA B 833



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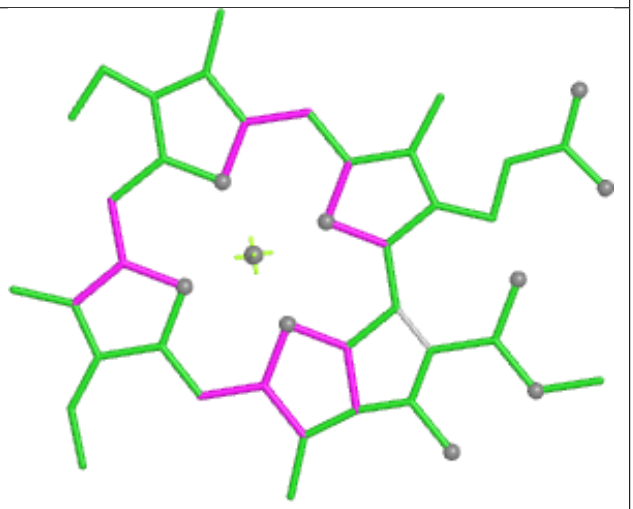

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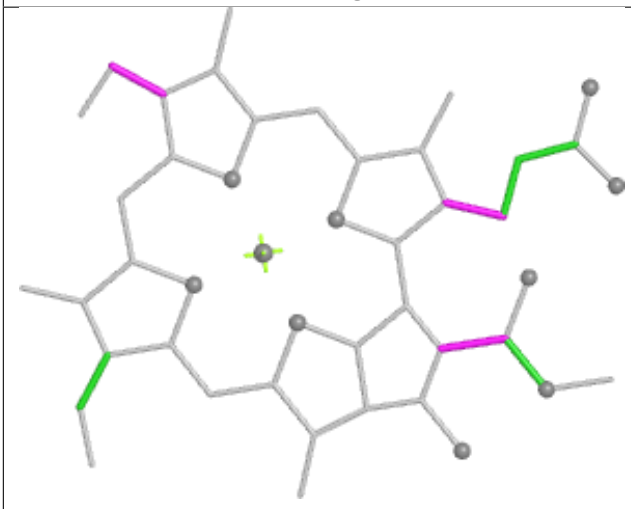
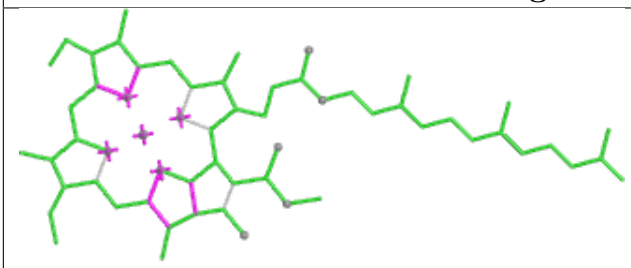


Torsions



Rings

Ligand CLA c 608



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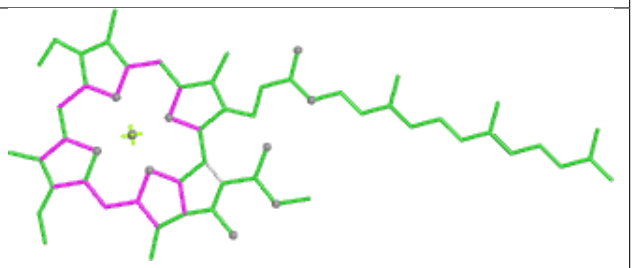
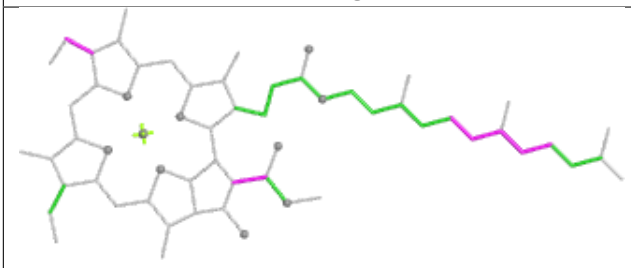


Bond angles



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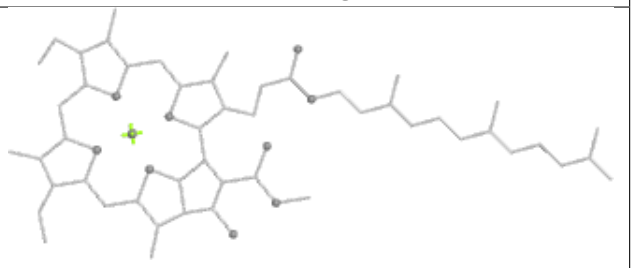
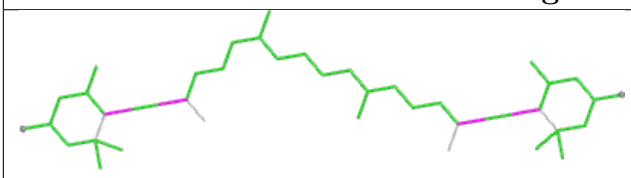


Rings

Ligand II0 b 612



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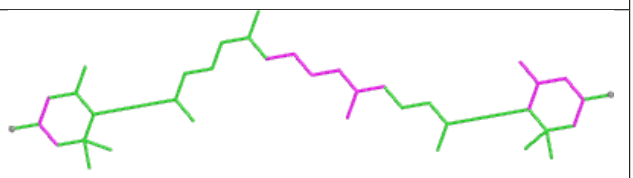
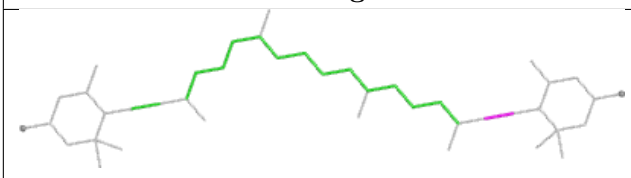


Bond angles



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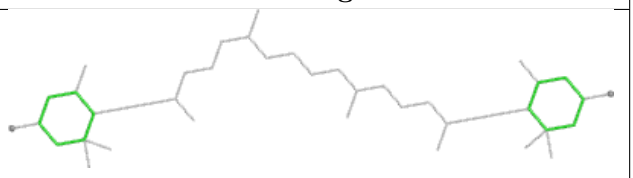
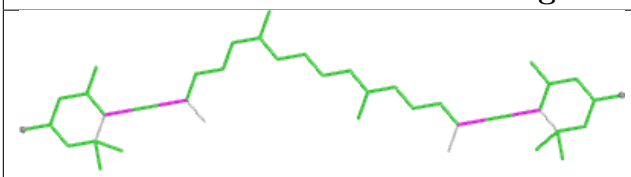


Rings

Ligand II0 O 204



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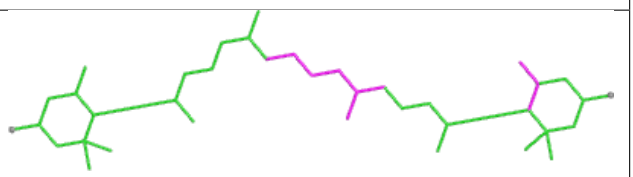
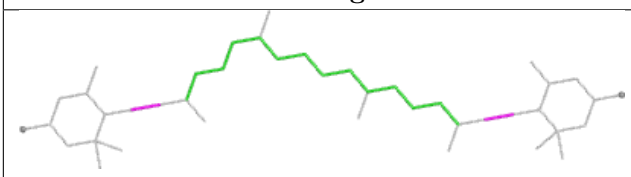


Bond angles



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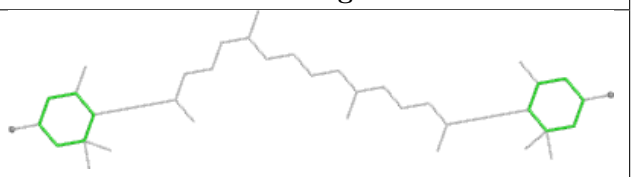
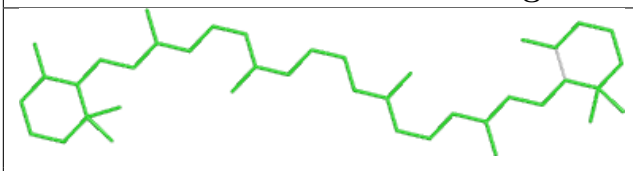


Rings

Ligand 8CT M 101



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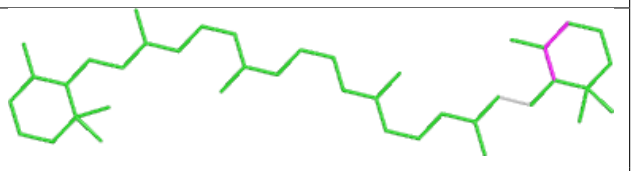
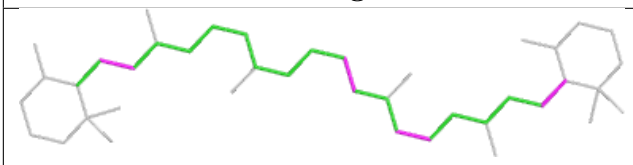


Bond angles



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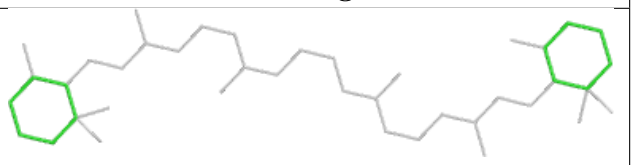
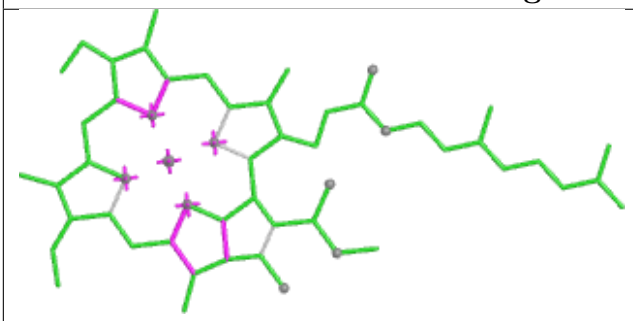


Rings

Ligand CLA O 203



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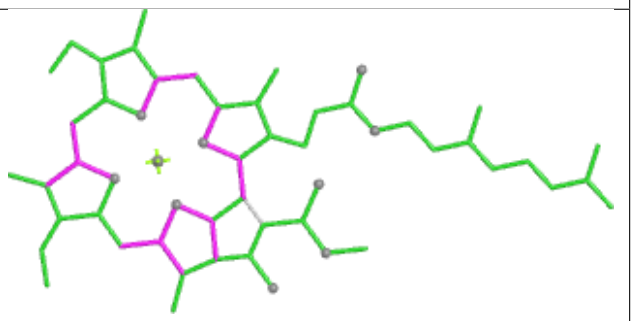
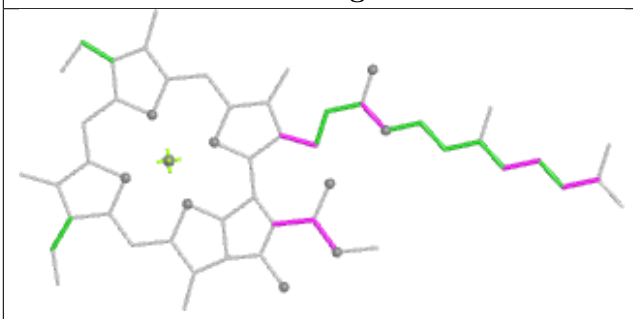


Bond angles



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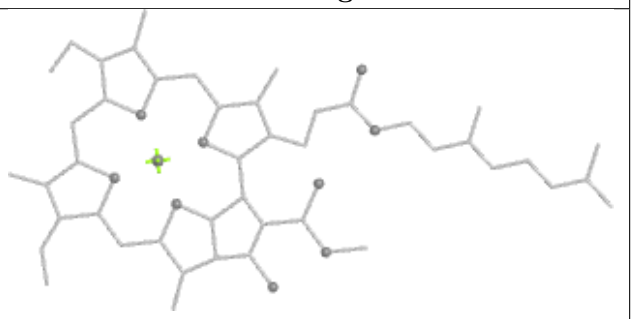
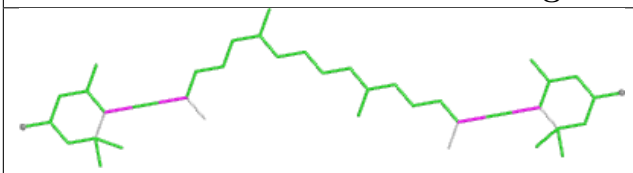


Rings

Ligand II0 a 615



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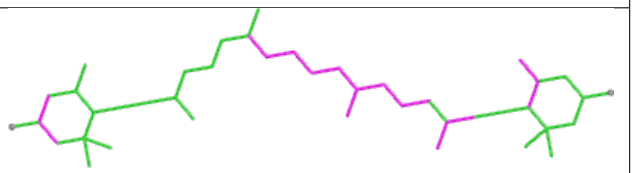
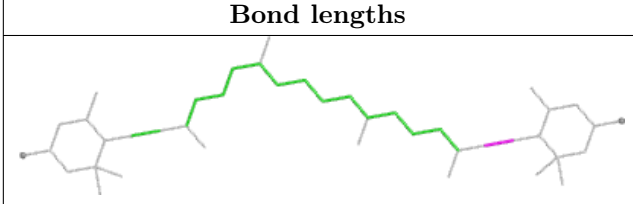


Bond angles



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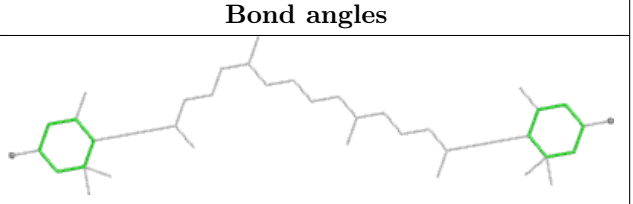
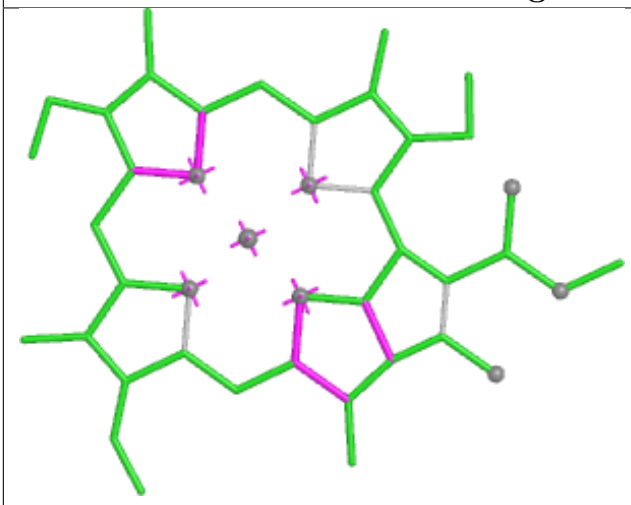


Rings

Ligand CLA 2 601



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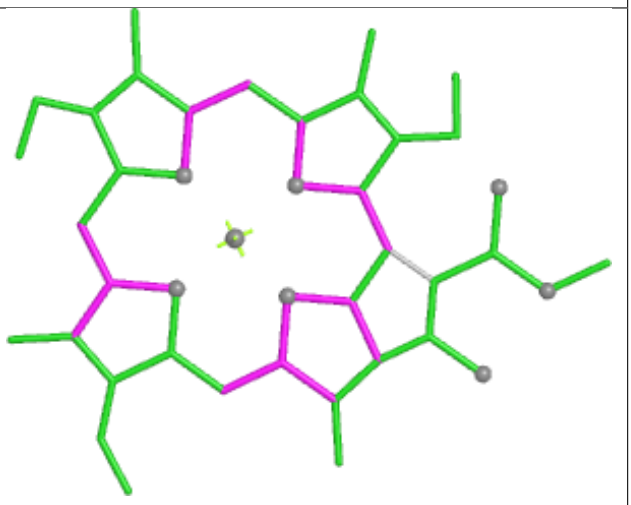
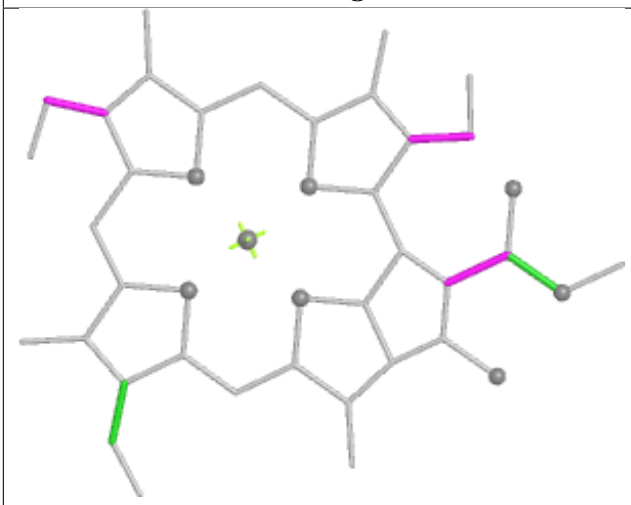


Bond angles

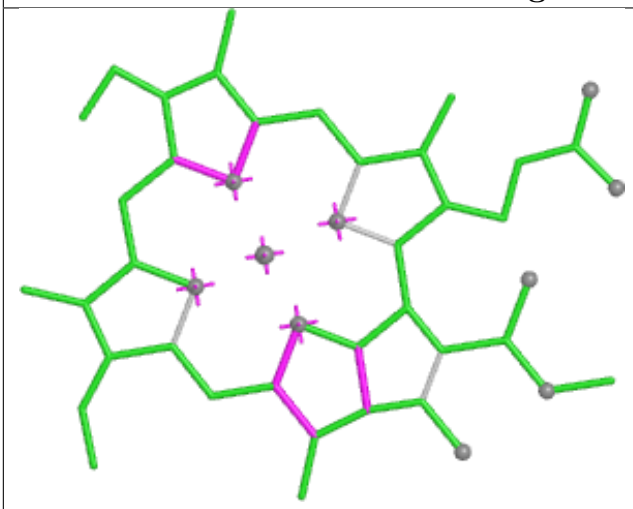


Torsions



Rings

Ligand CLA 2 611



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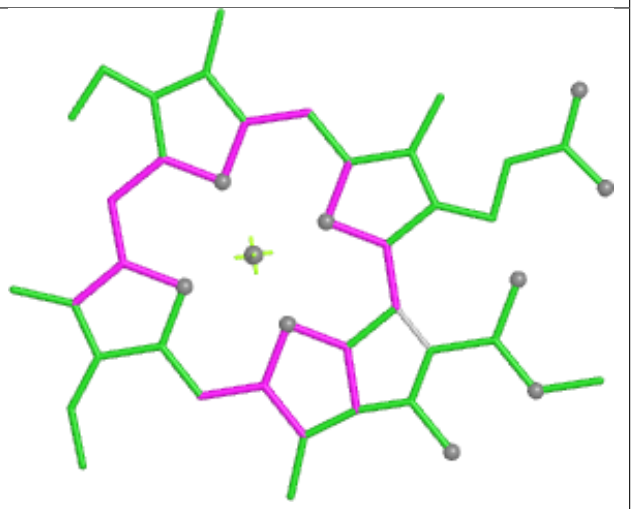
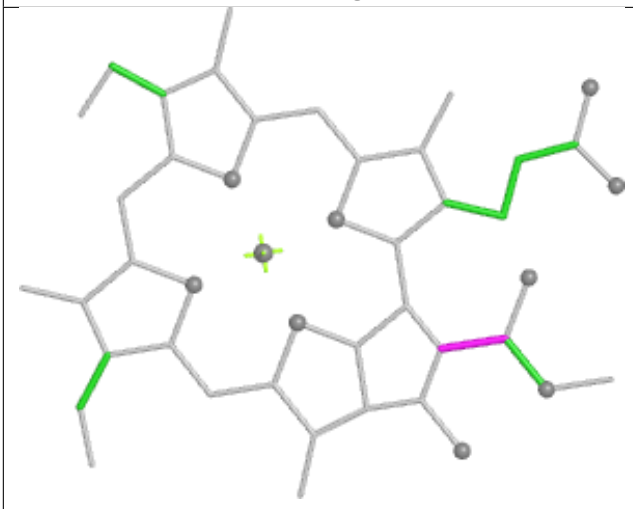


Bond angles

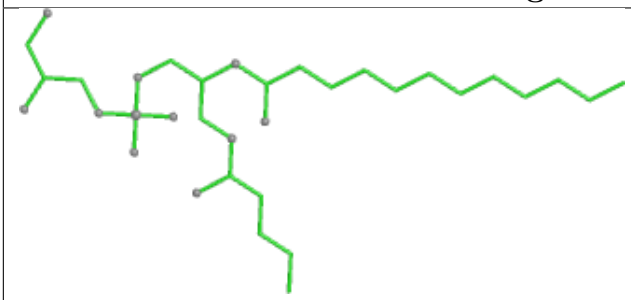


Torsions

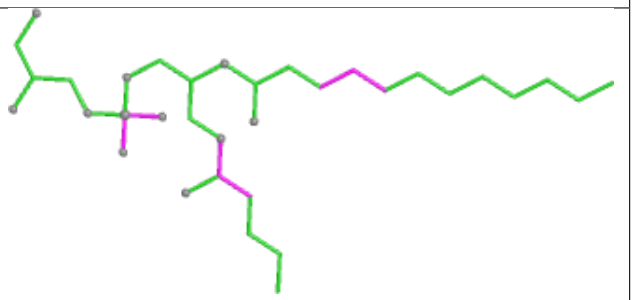


Rings

Ligand LHG 3 622



Bond lengths



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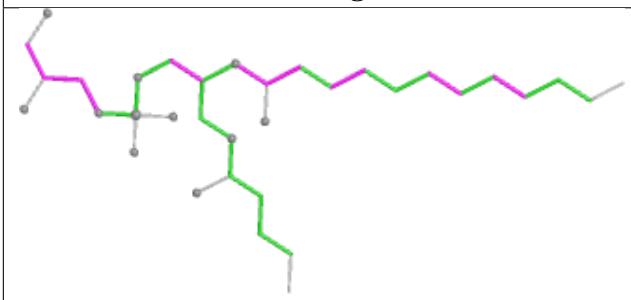

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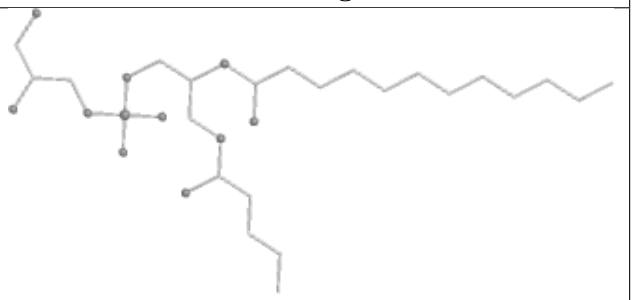
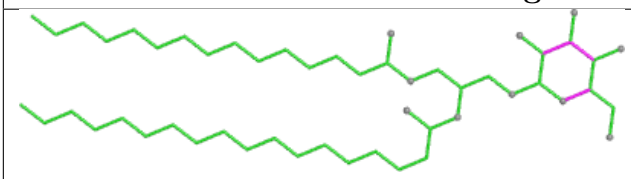


Rings

Ligand LMG 8 614



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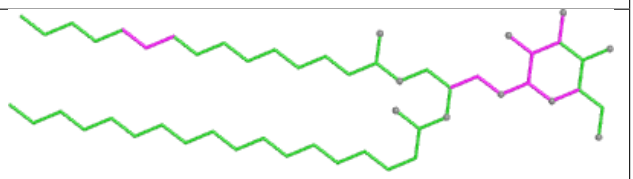

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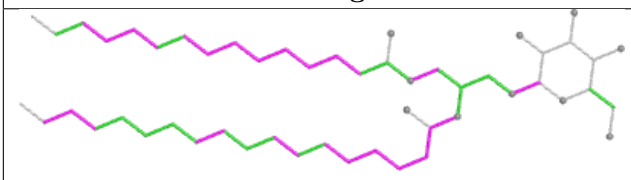

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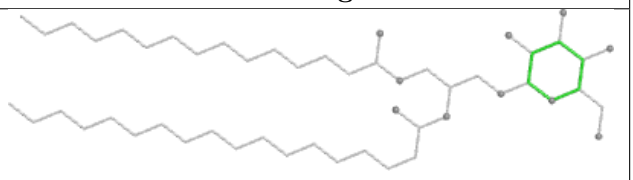

Rings

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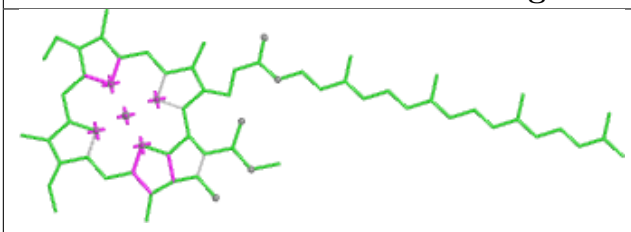

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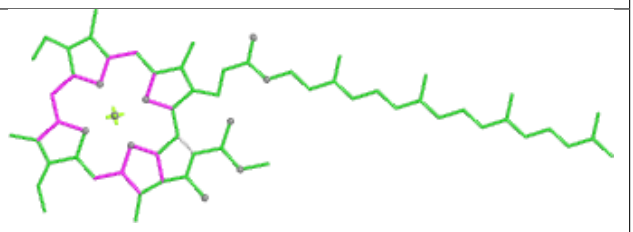

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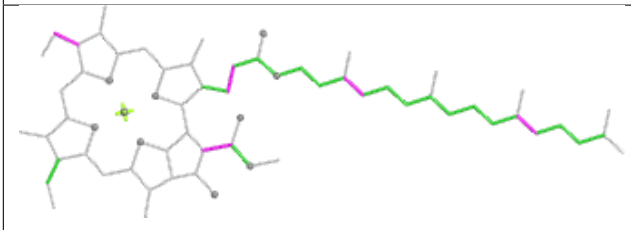

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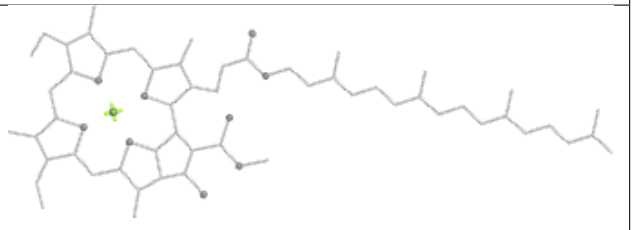
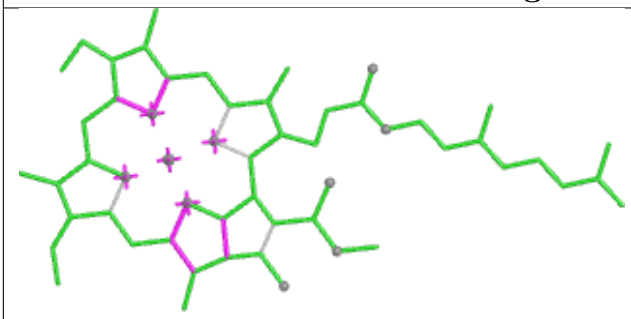


Rings

Ligand CLA A 834



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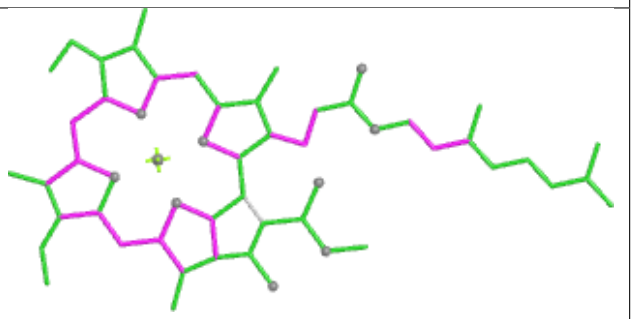

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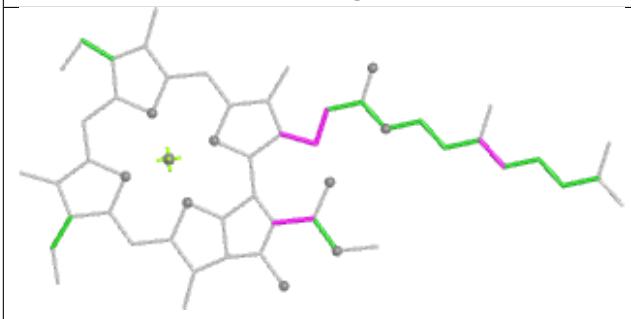

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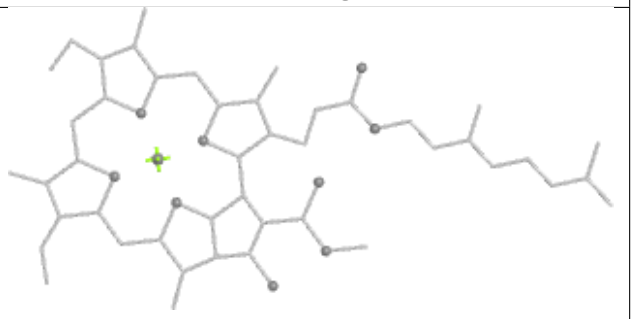
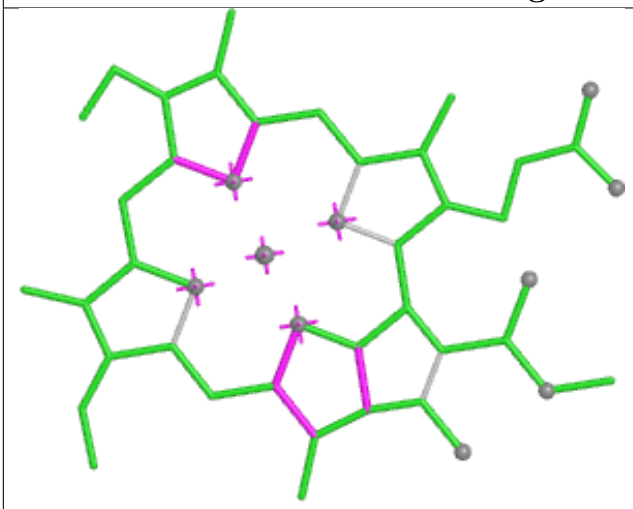


Rings

Ligand CLA 5 607



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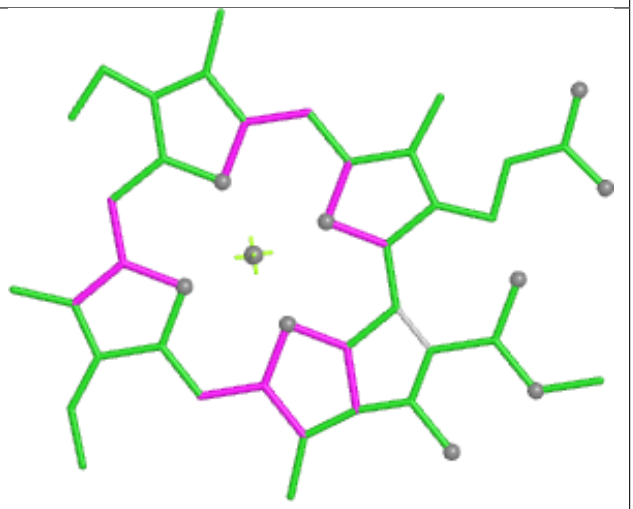

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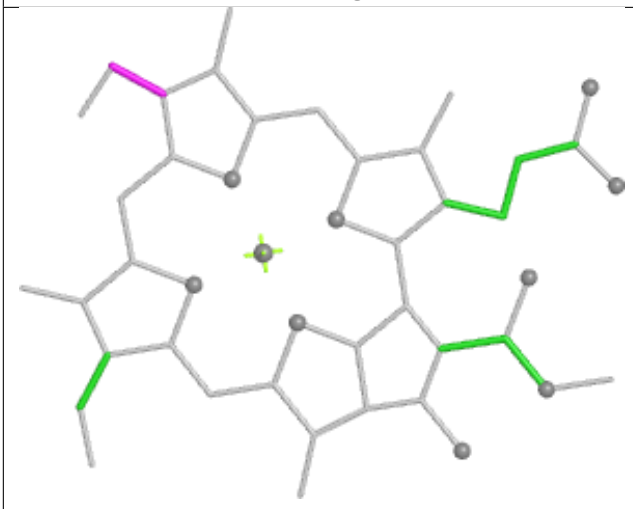
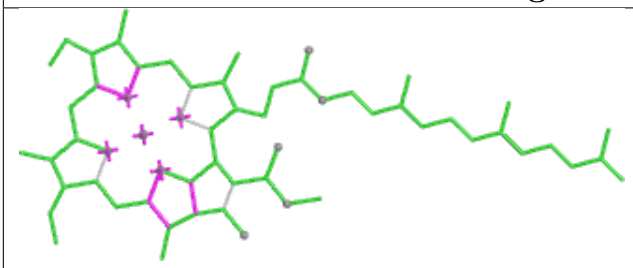


Torsions



Rings

Ligand CLA 4 609



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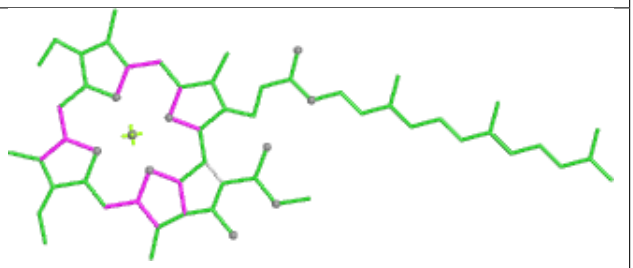

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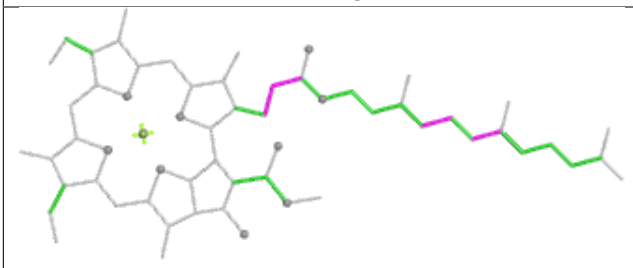

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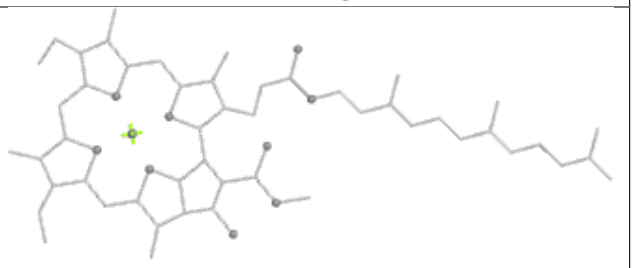
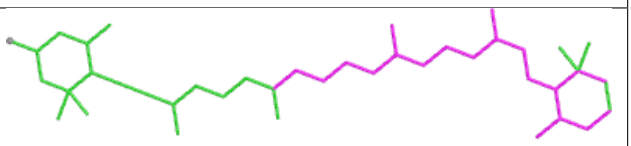
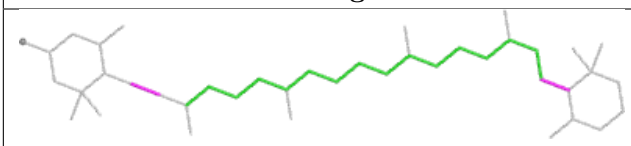
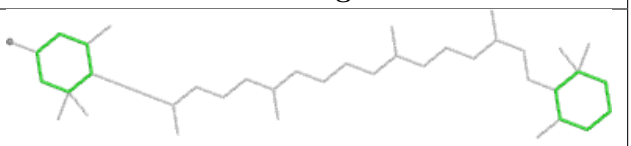


Rings

Ligand IHT 6 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

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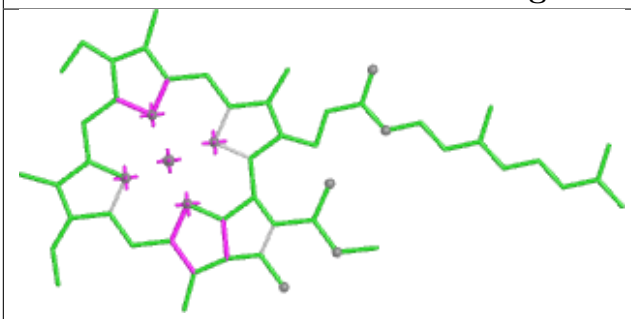
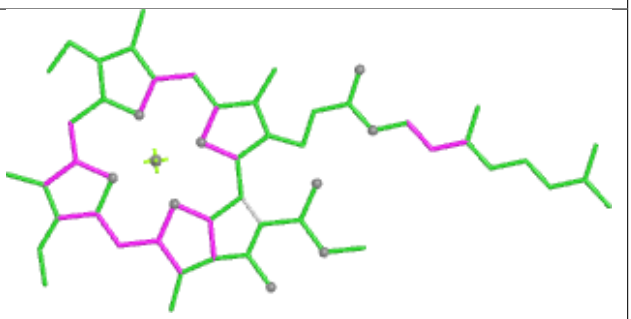
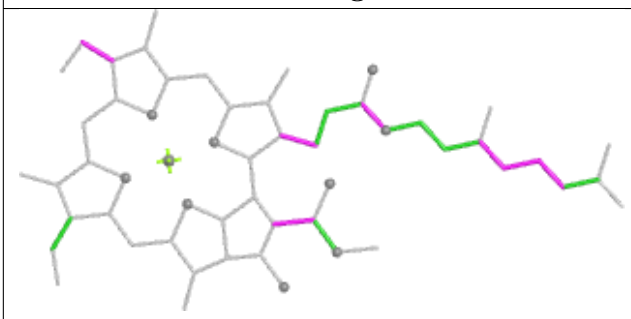
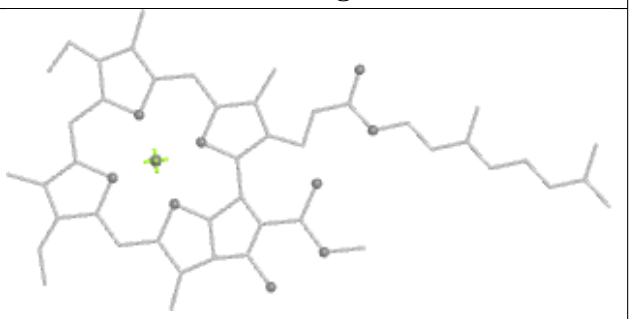
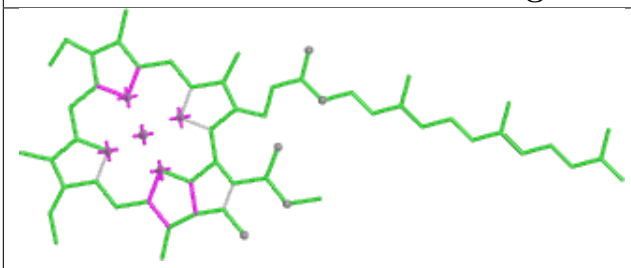
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 306



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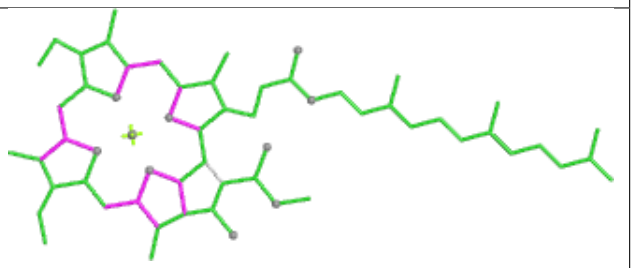

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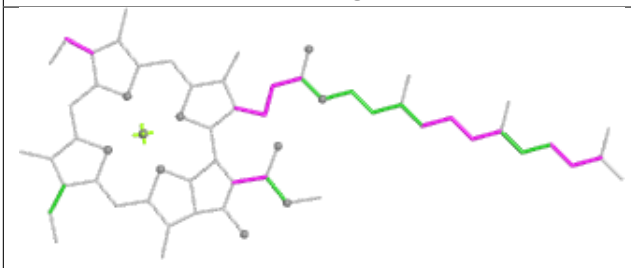

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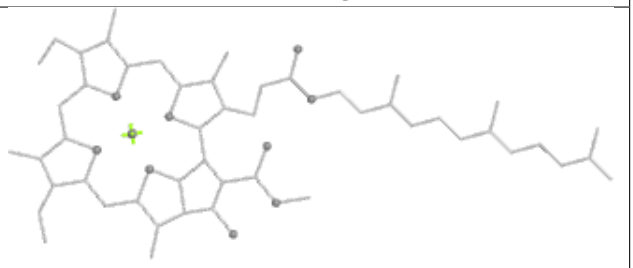
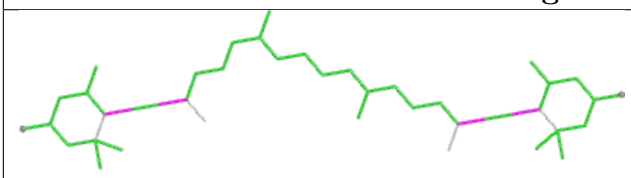


Rings

Ligand II0 d 614



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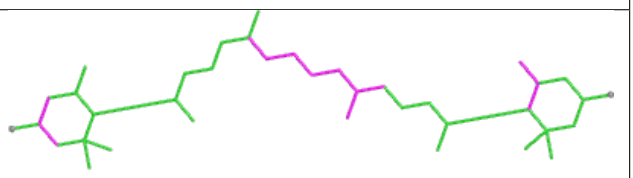

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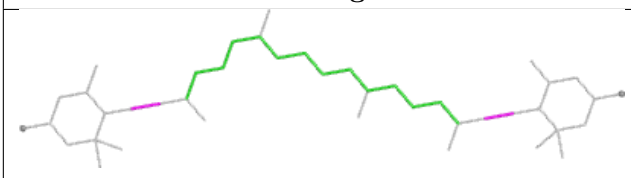

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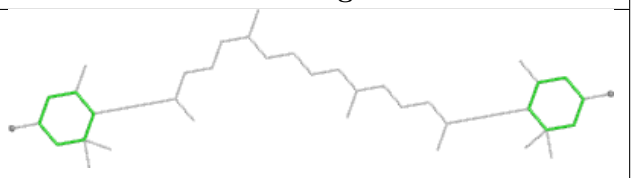
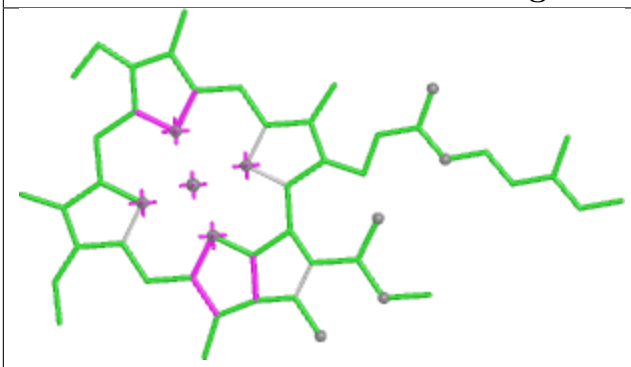


Rings

Ligand CLA e 610



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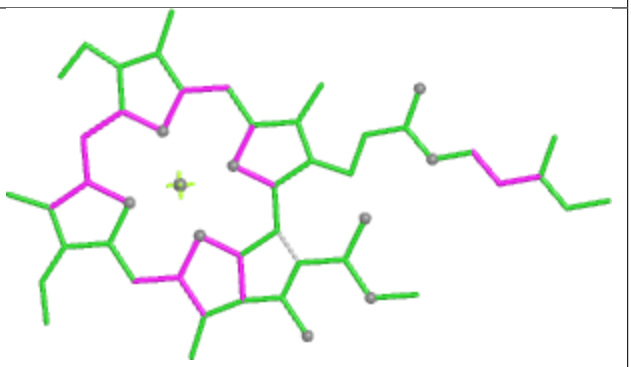

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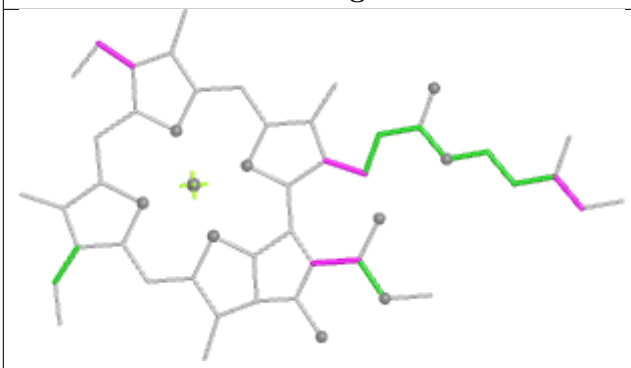

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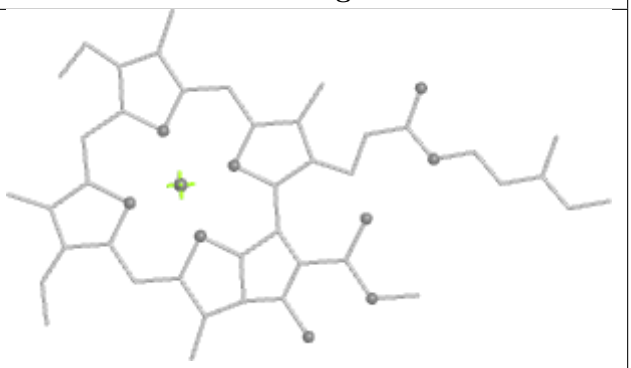

Rings

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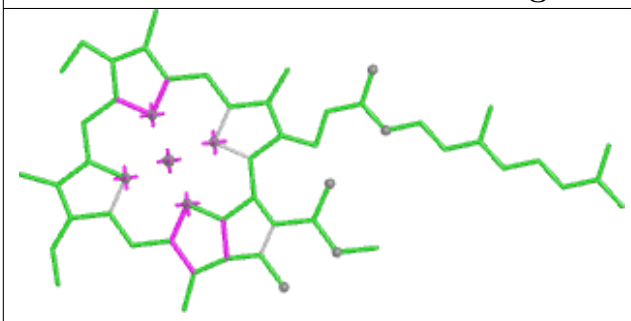

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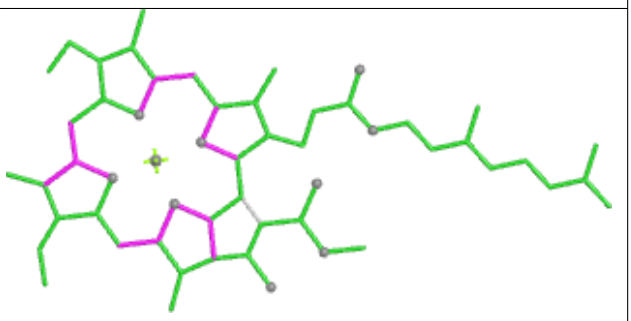

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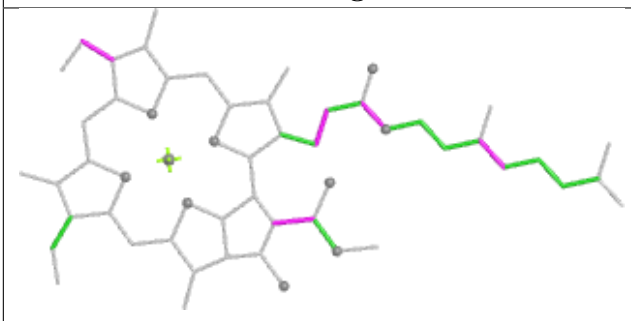

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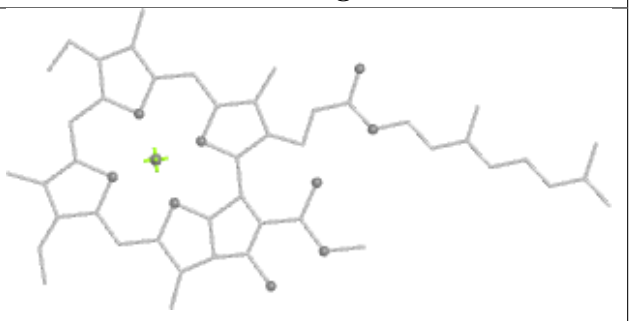
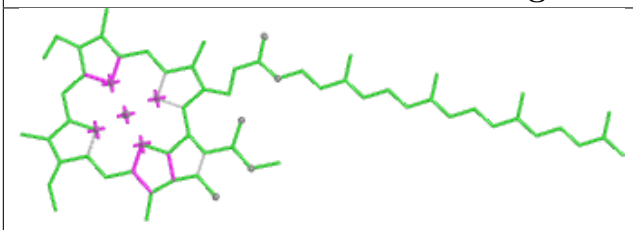


Rings

Ligand CLA a 607



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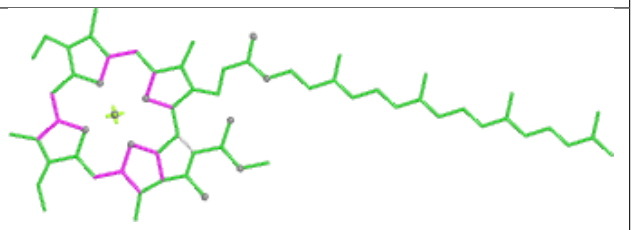
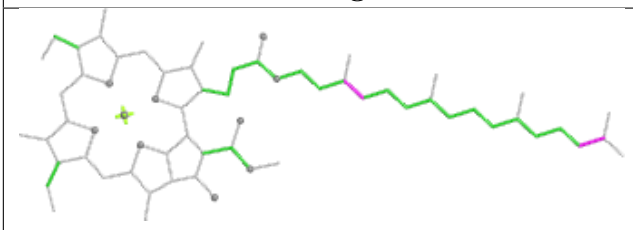


Bond angles



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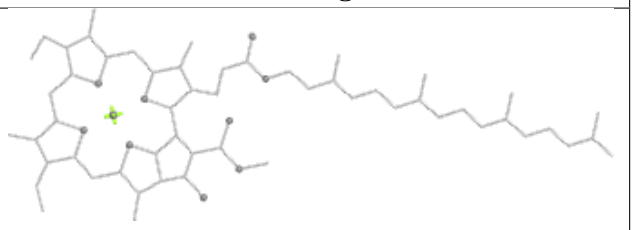

Rings

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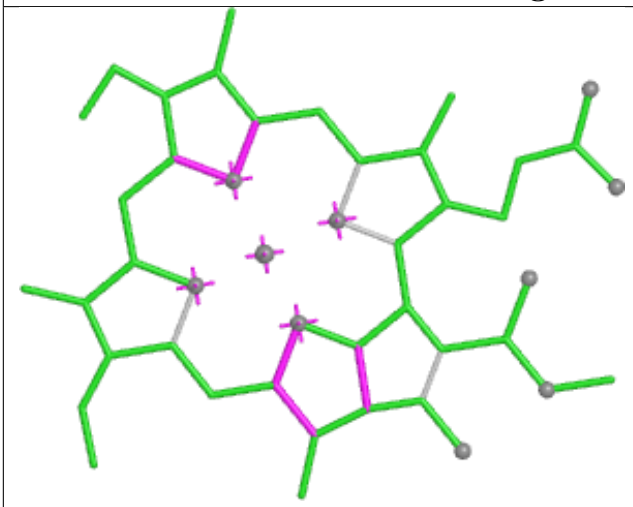

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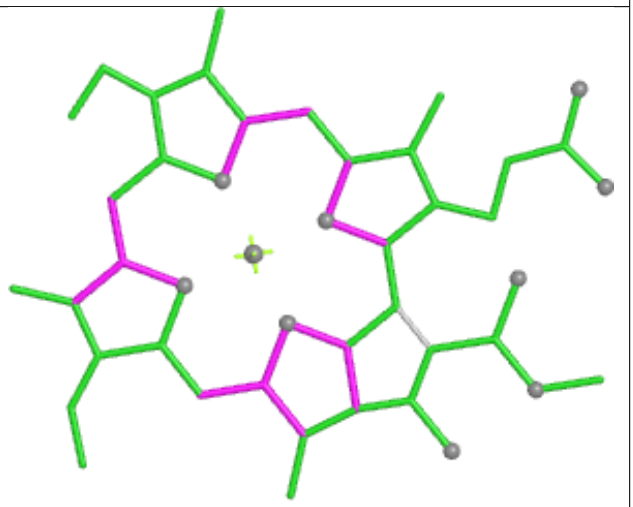
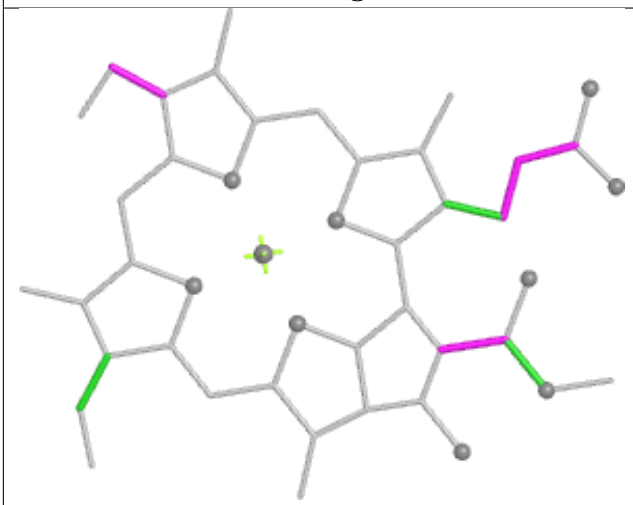


Bond angles



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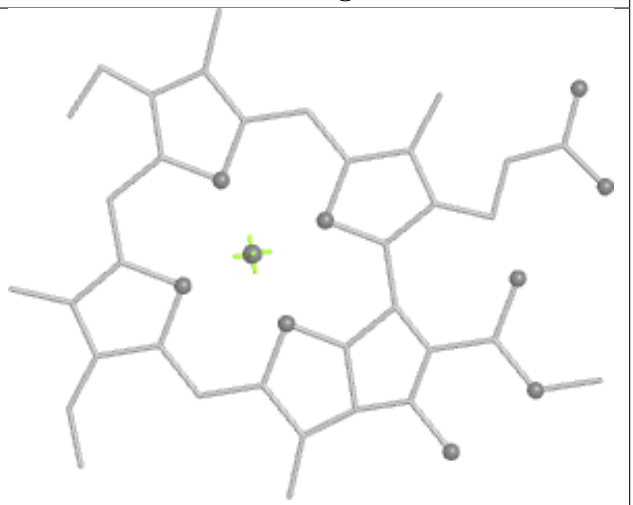
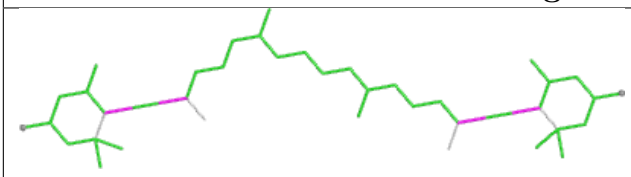
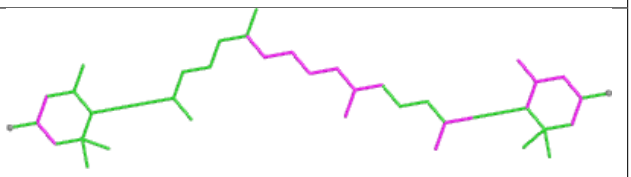
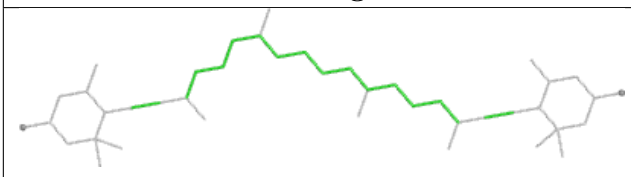
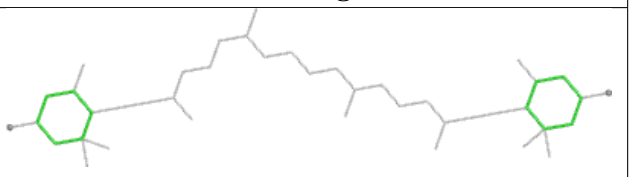
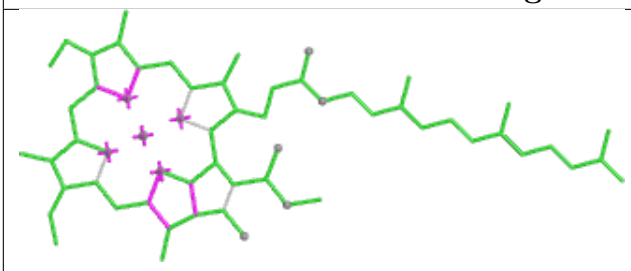
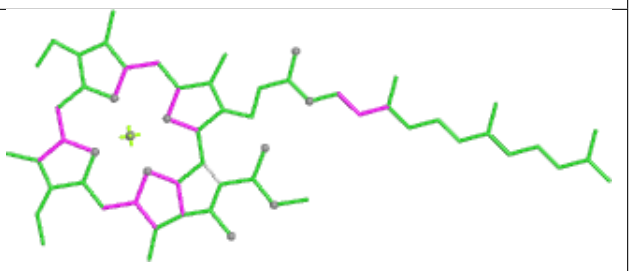
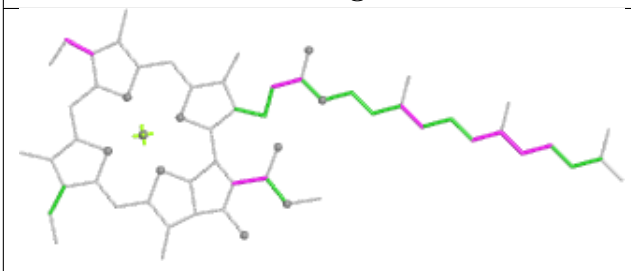
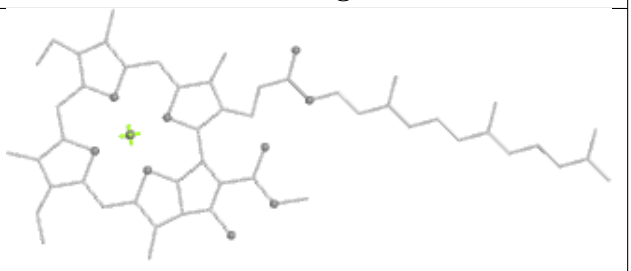


Rings

Ligand II0 e 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

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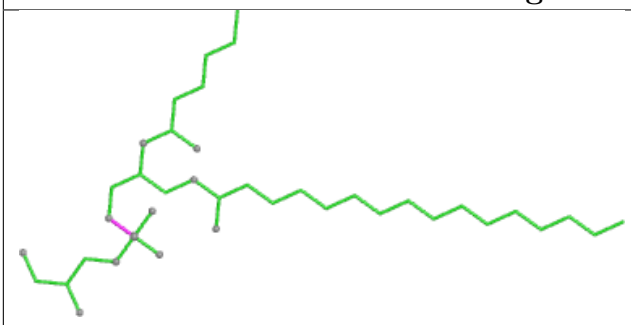

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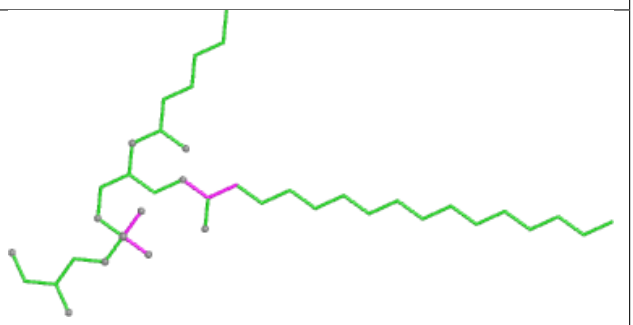

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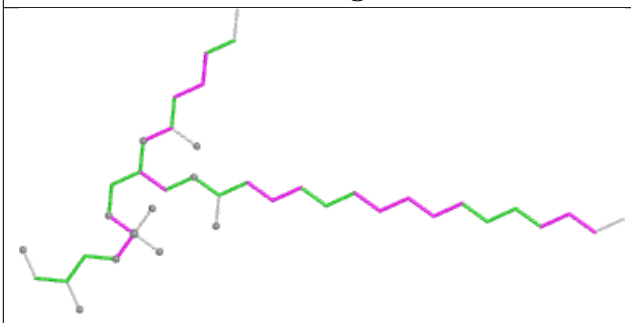

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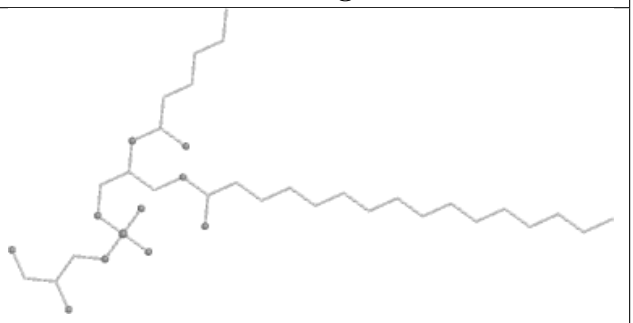

Rings

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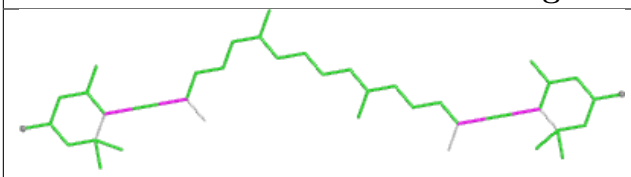

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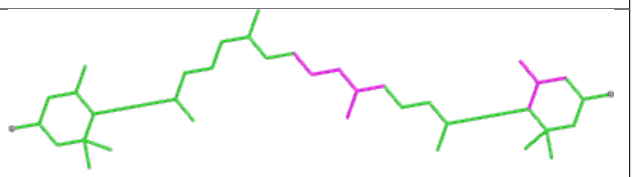

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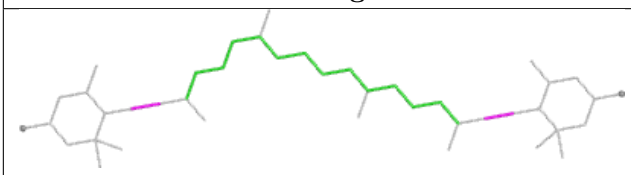

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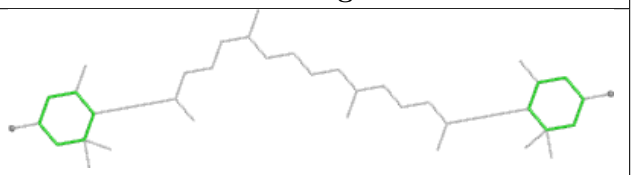

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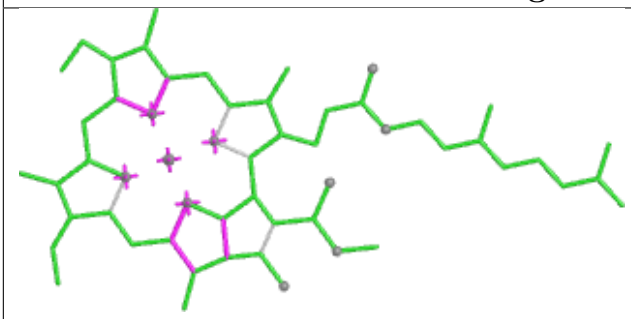

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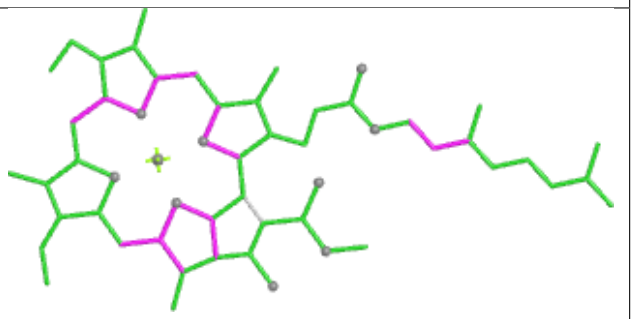

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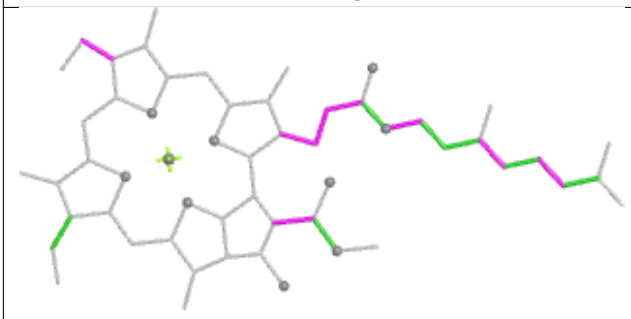

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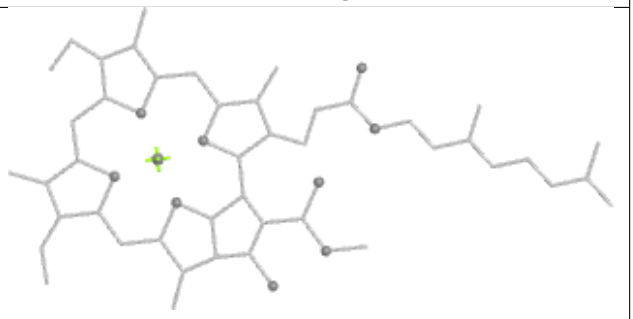

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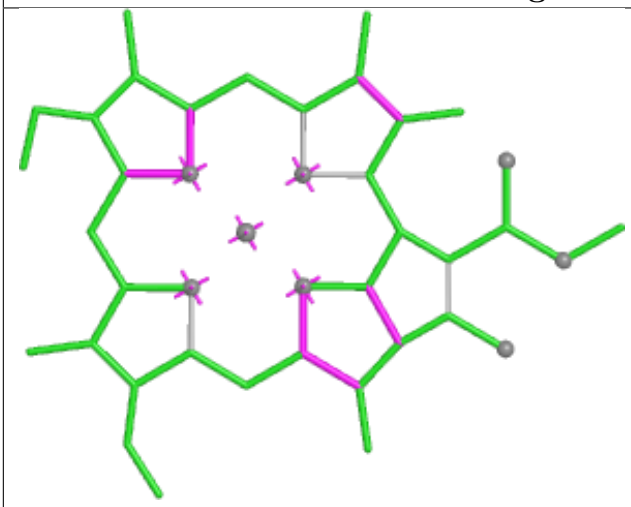

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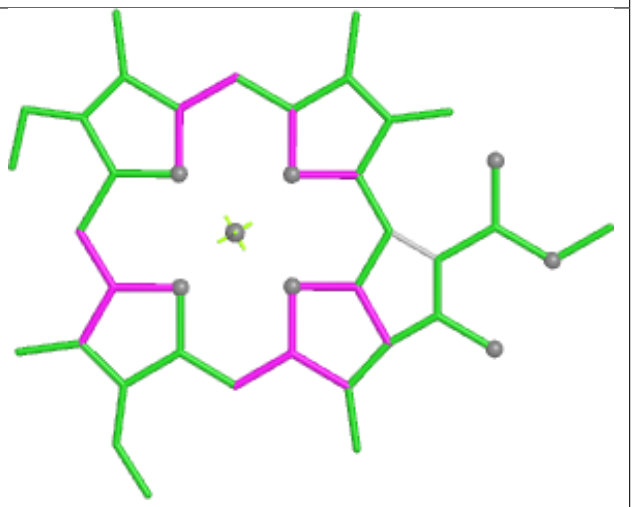

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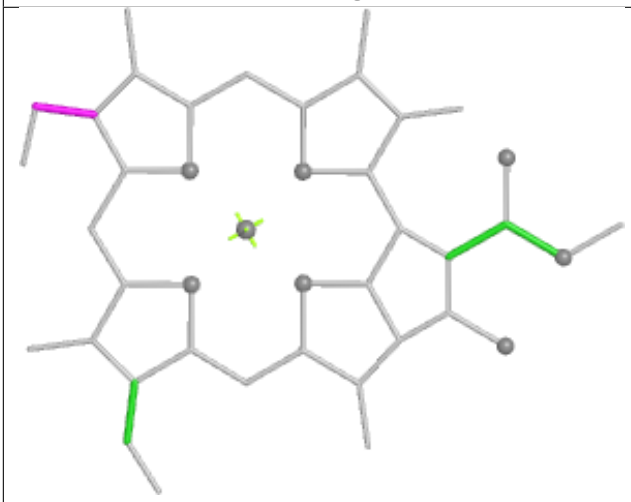

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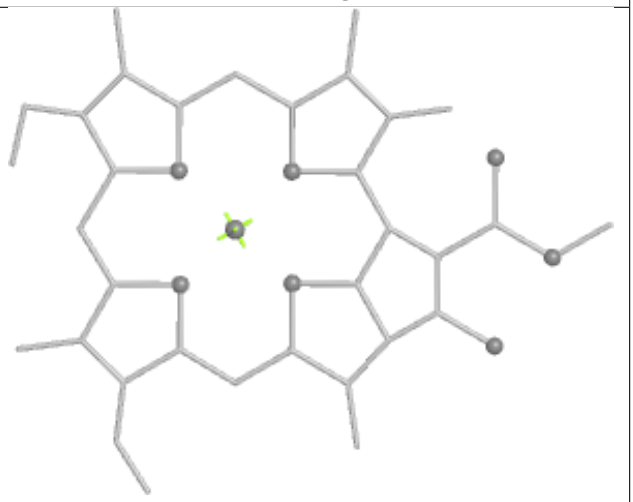

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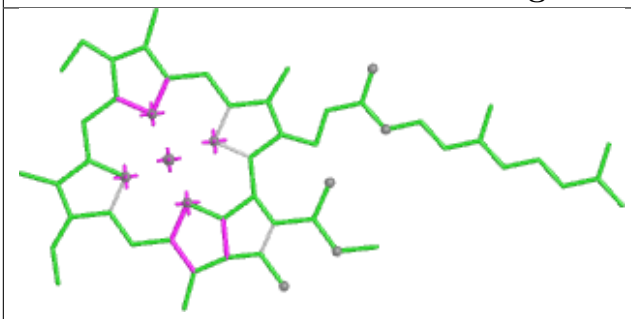

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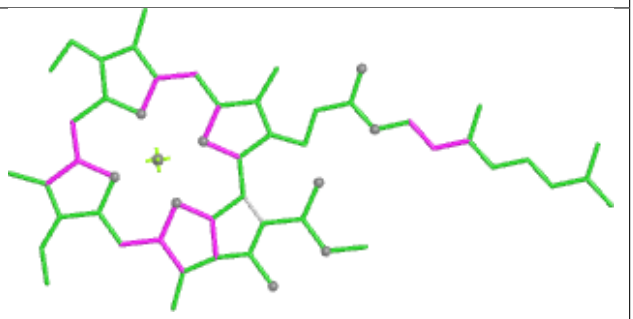

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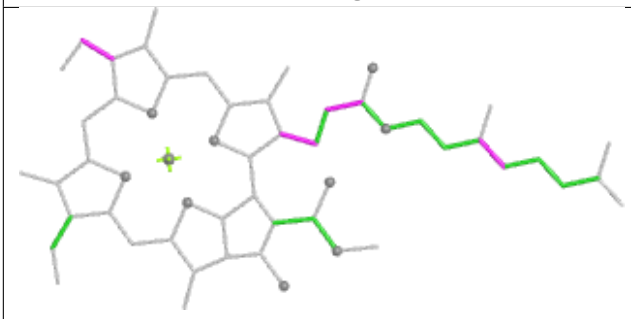

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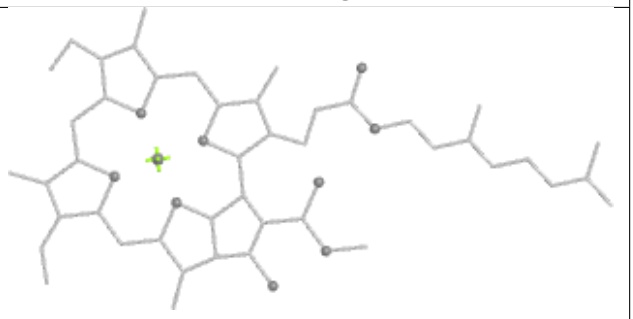
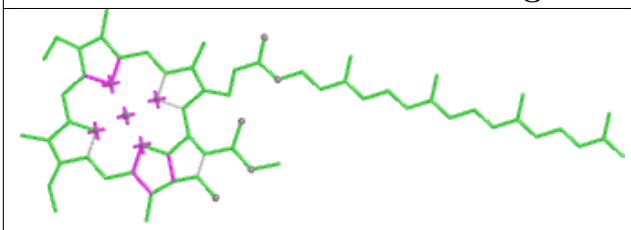


Rings

Ligand CLA A 837



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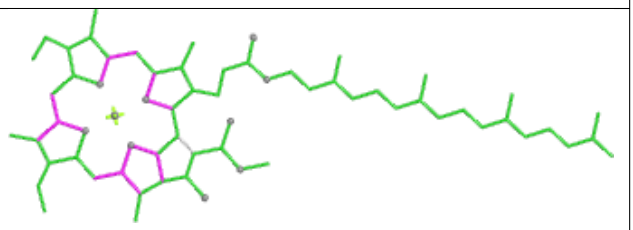

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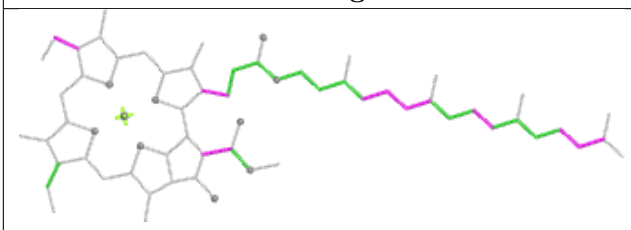

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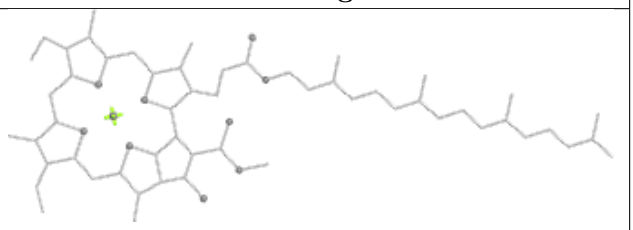

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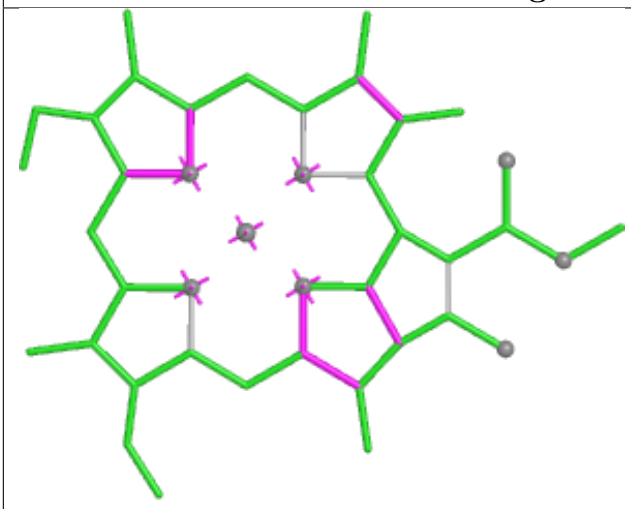

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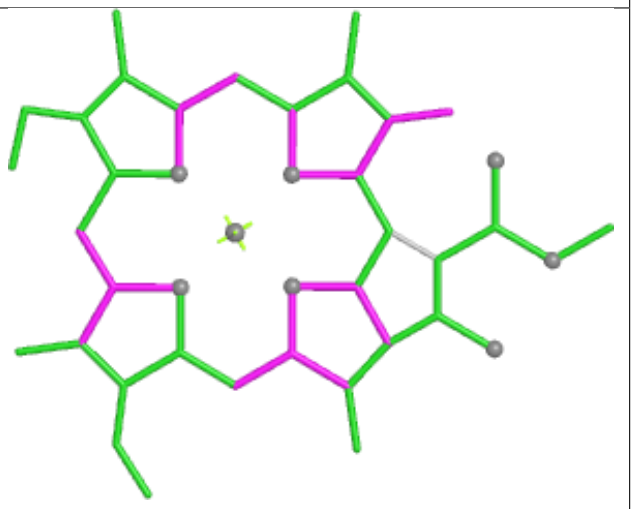

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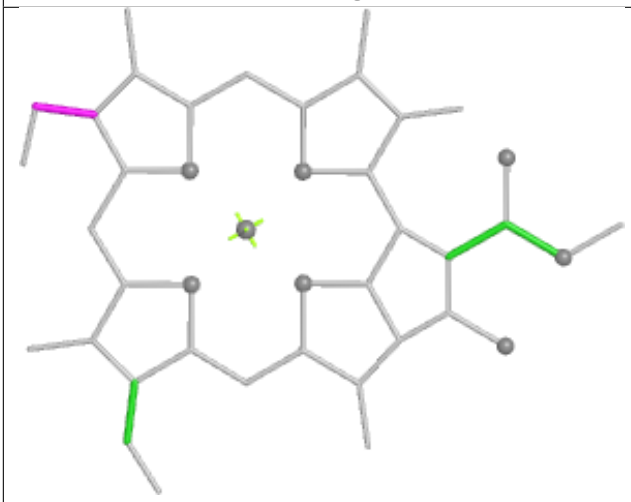

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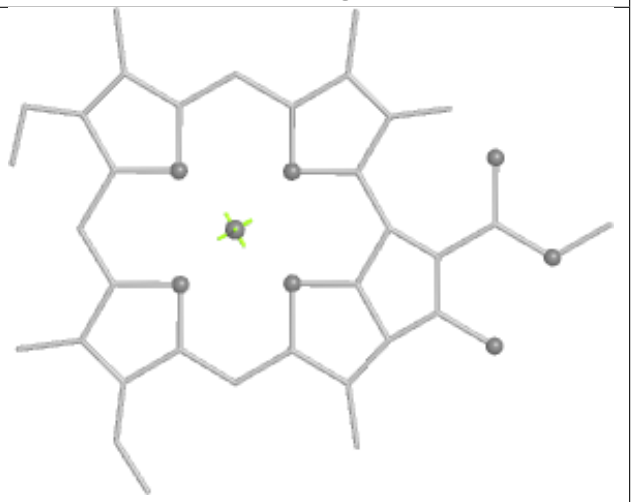

Rings

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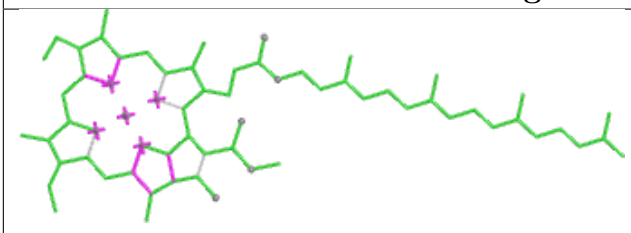

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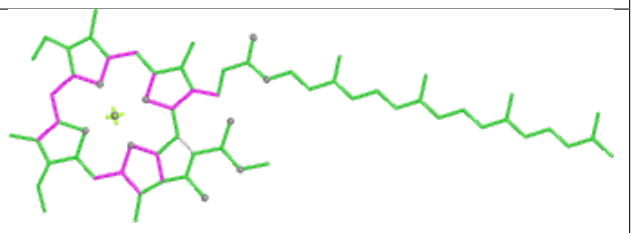

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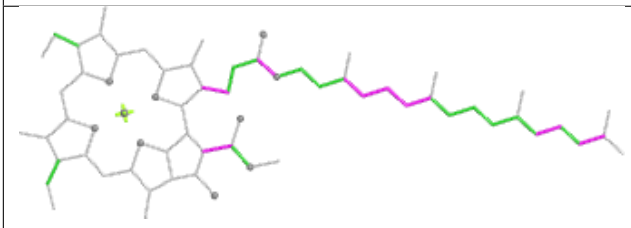

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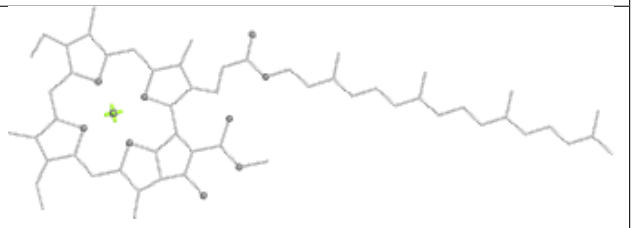

Rings

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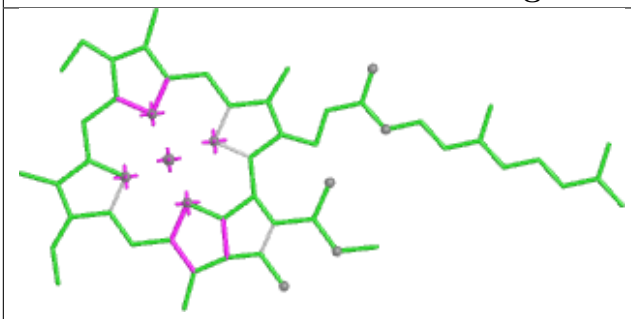

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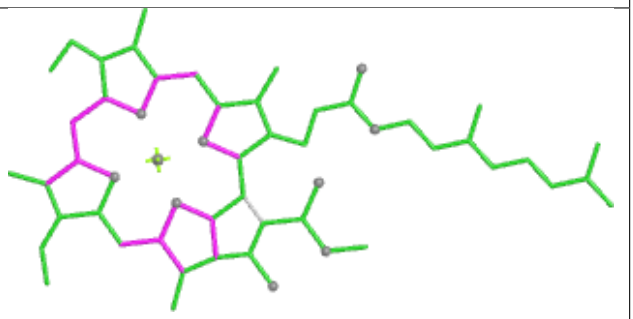

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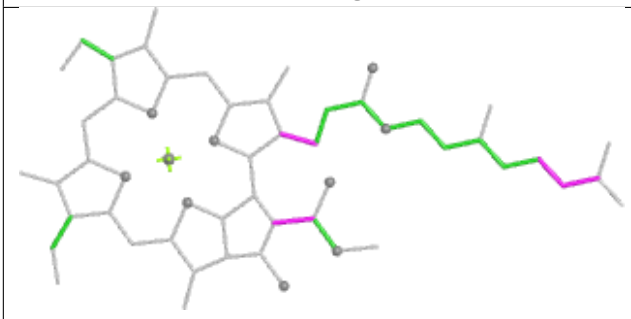

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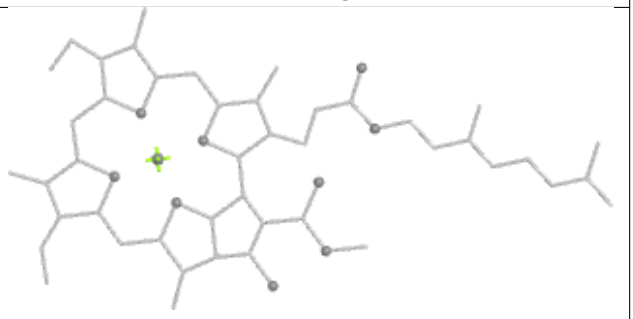
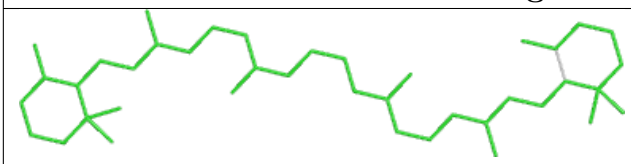


Rings

Ligand 8CT R 201



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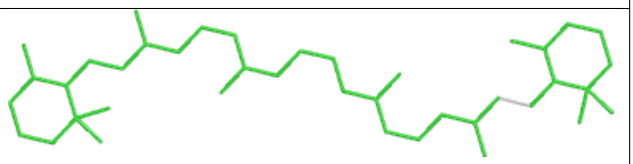

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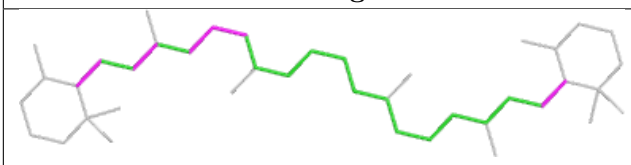

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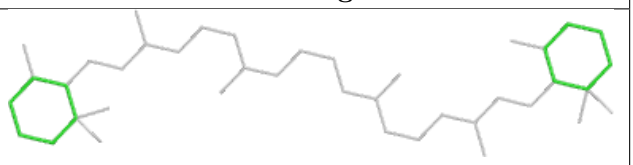
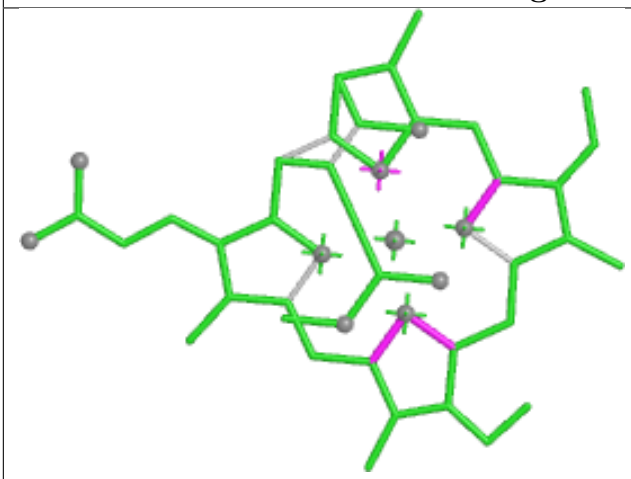


Rings

Ligand KC2 6 613



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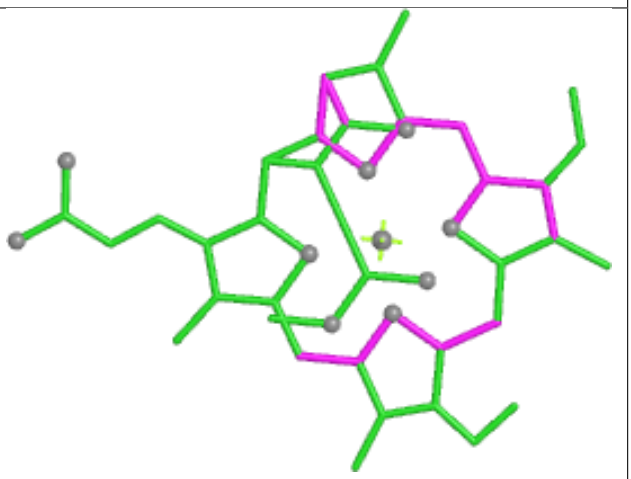

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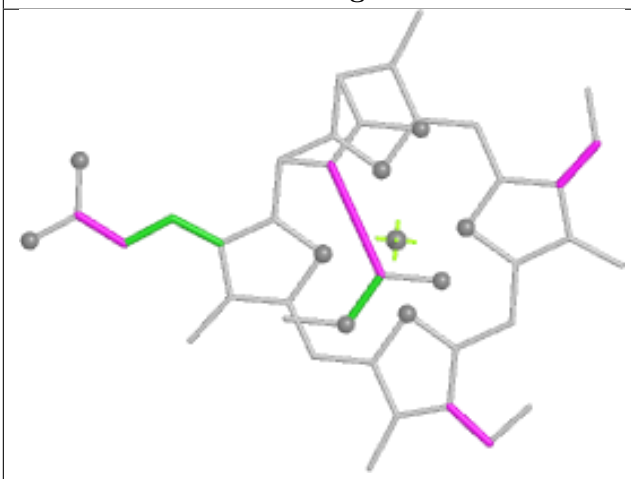

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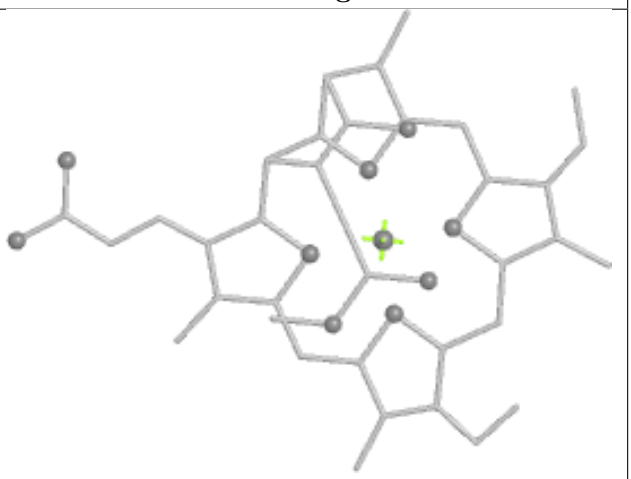

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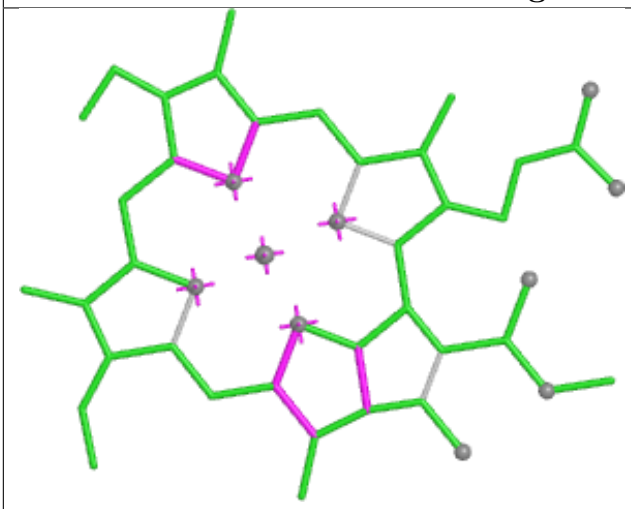
Ligand CLA 5 605



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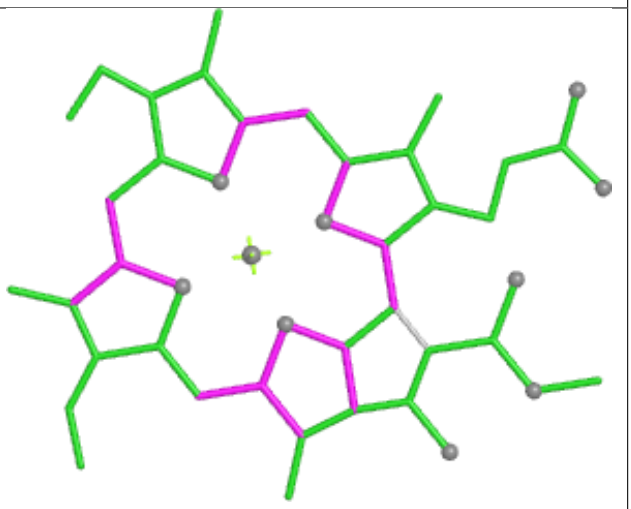

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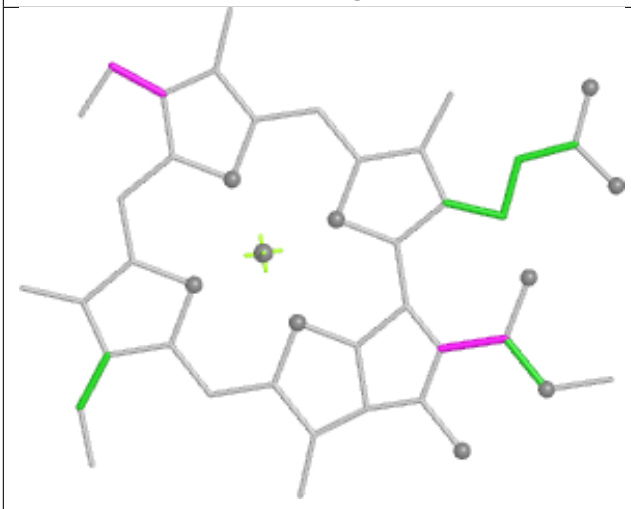
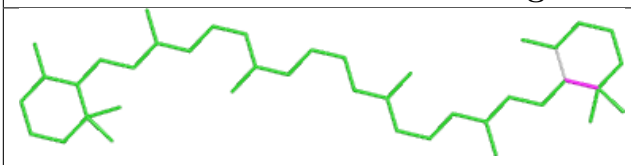


Torsions



Rings

Ligand 8CT B 850



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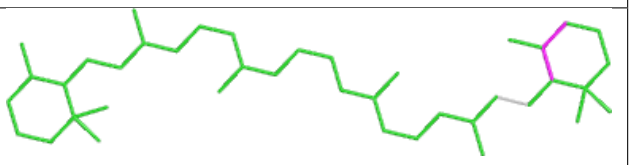
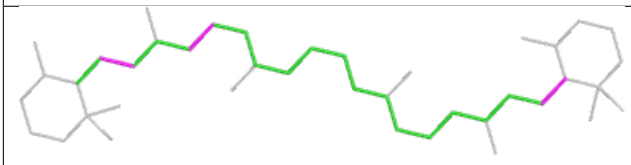


Bond angles



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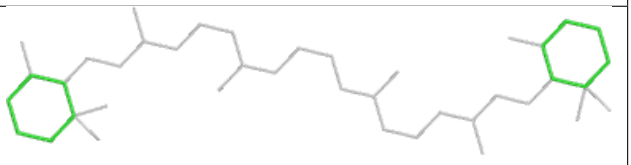

Rings

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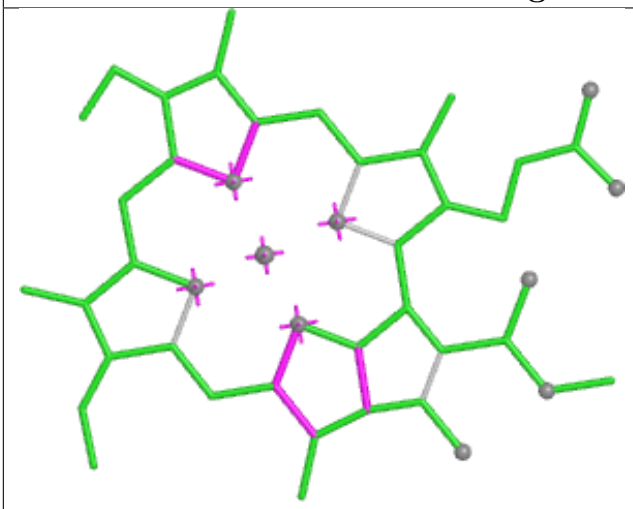

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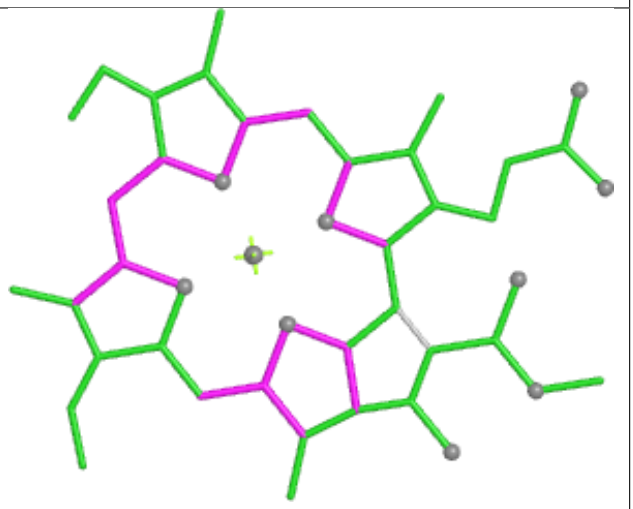
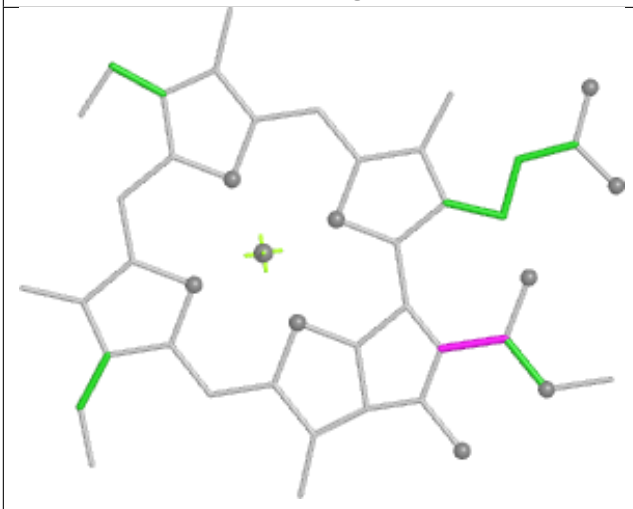


Bond angles



Torsions



Rings

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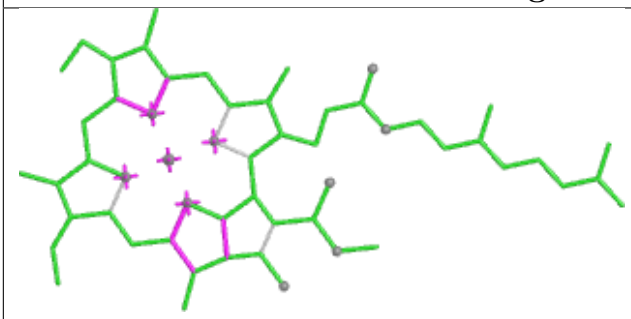

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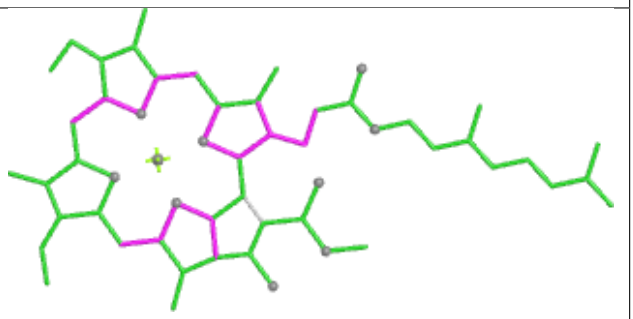

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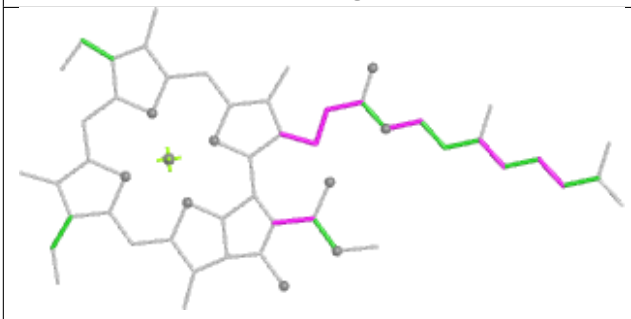

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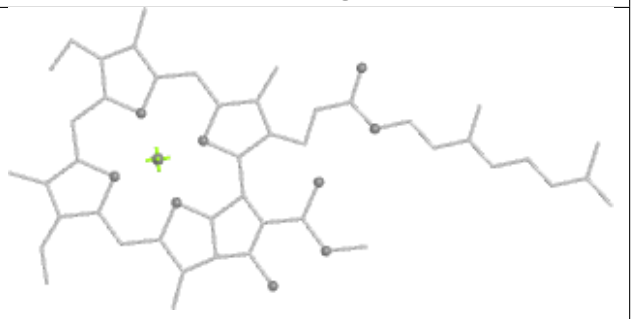

Rings

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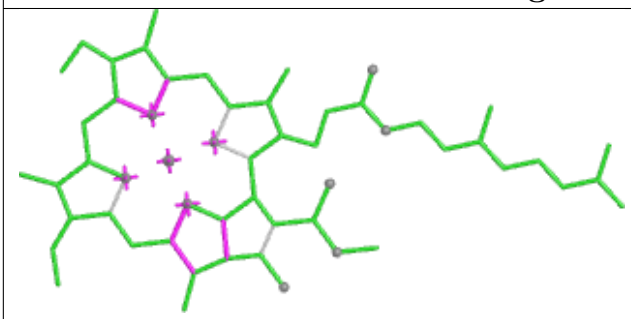

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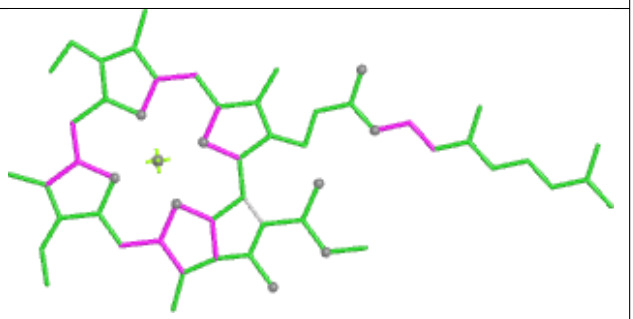

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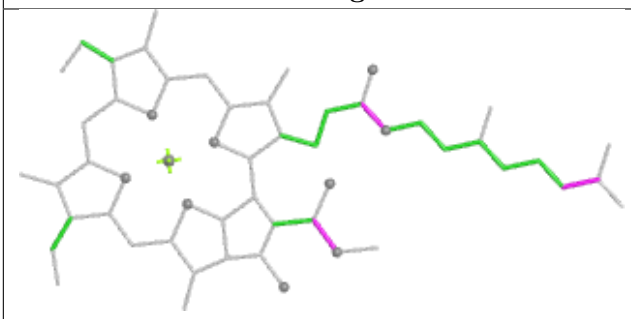

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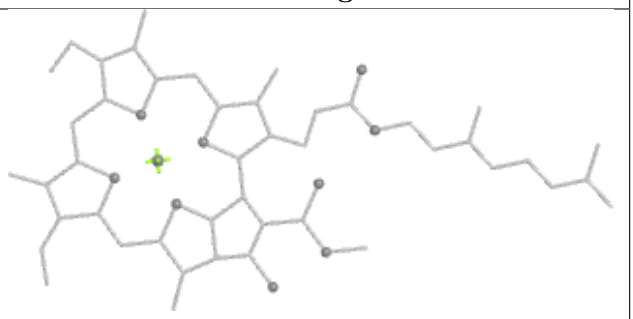

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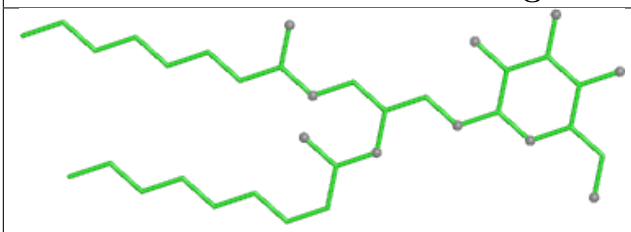
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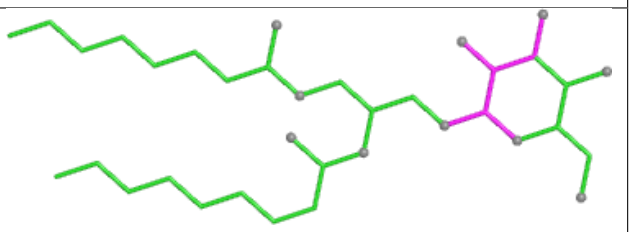
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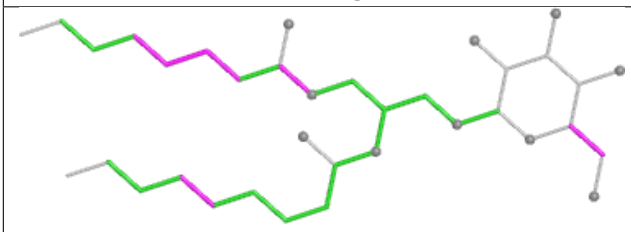
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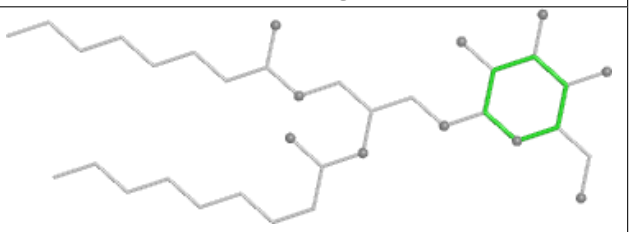
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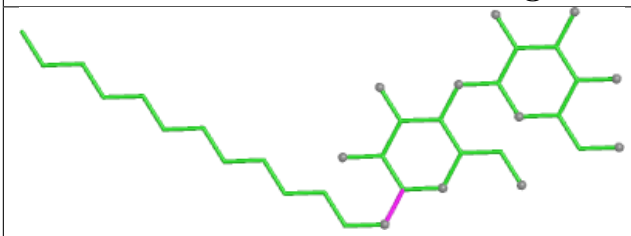
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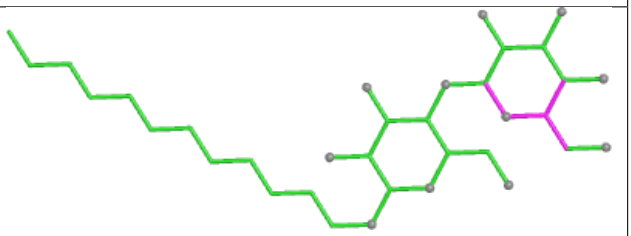
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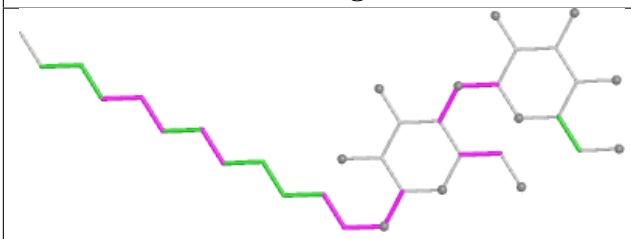
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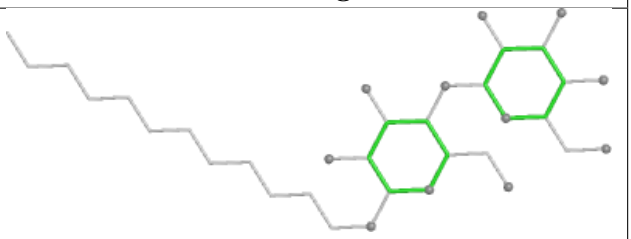
Rings

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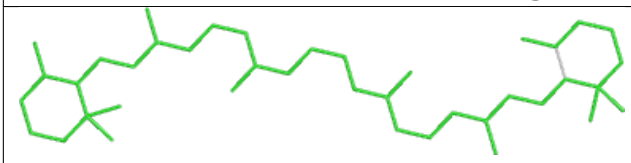
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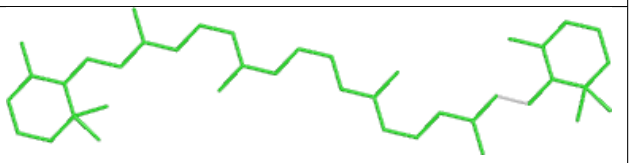
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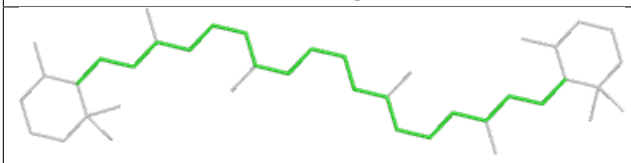
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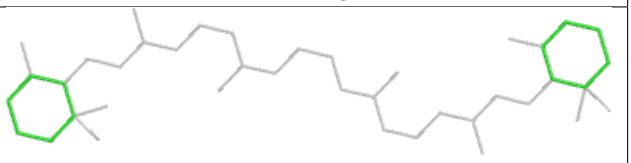
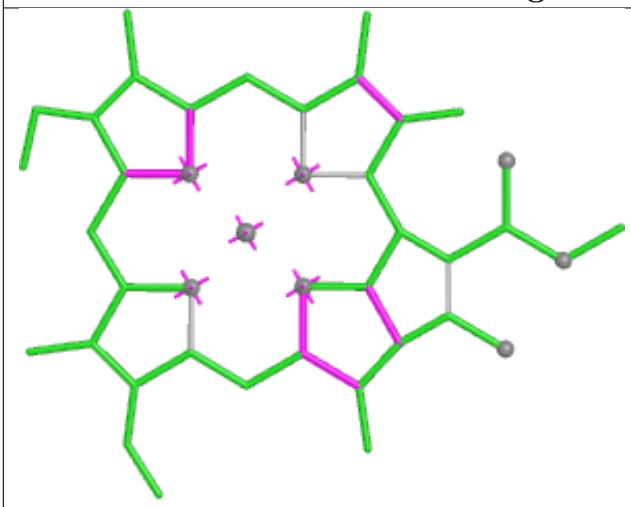

Rings

Ligand CLA d 609



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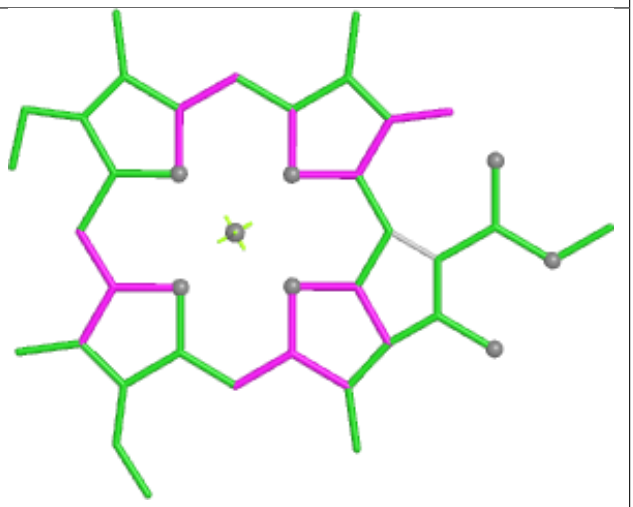

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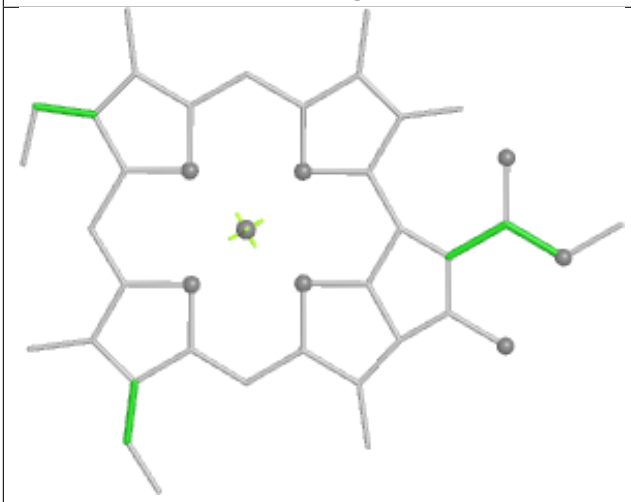

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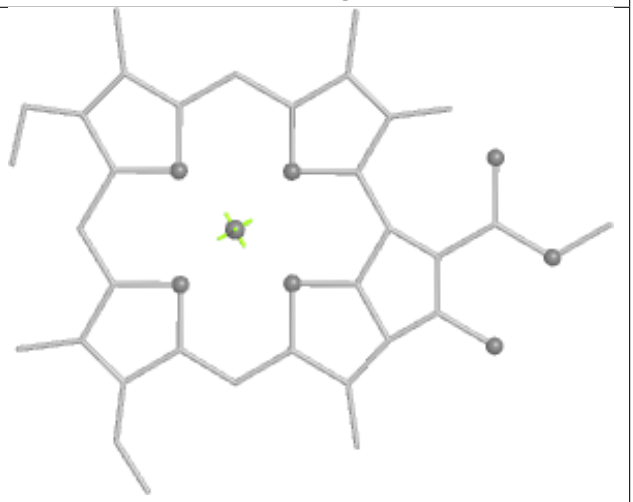

Rings

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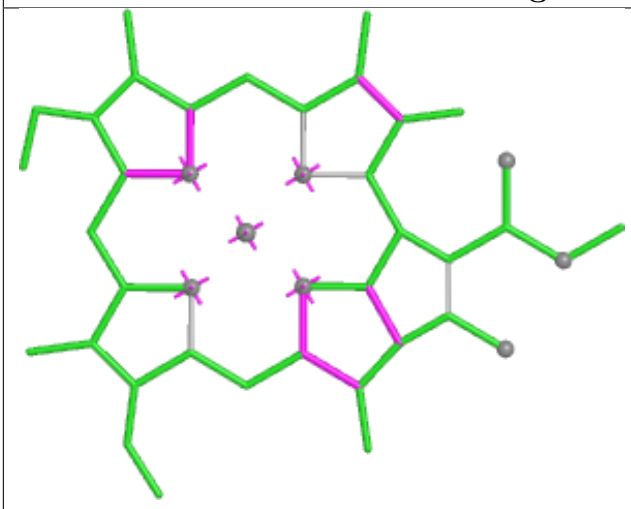

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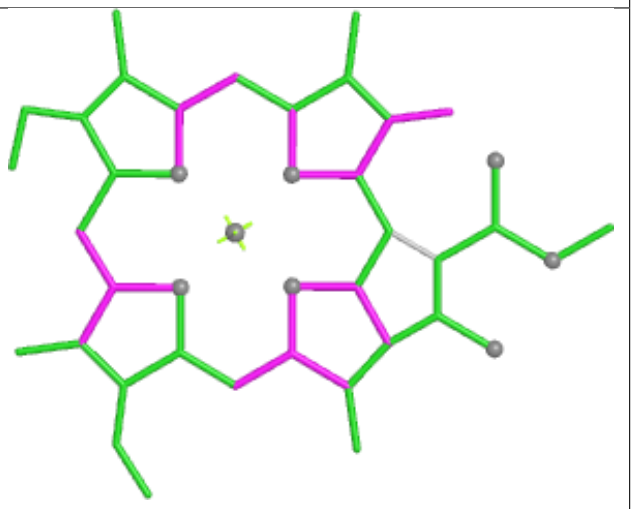

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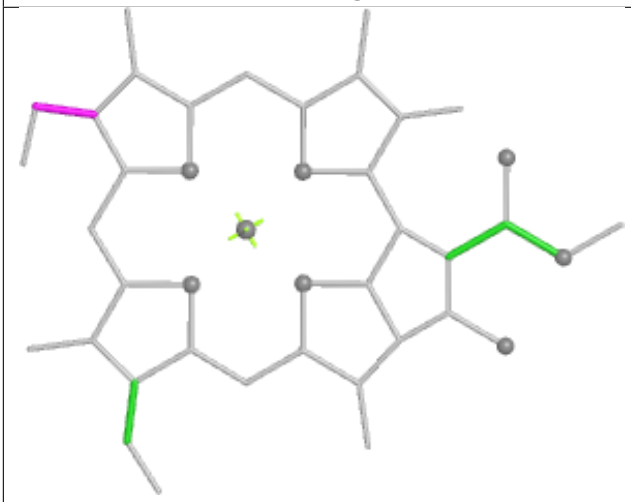

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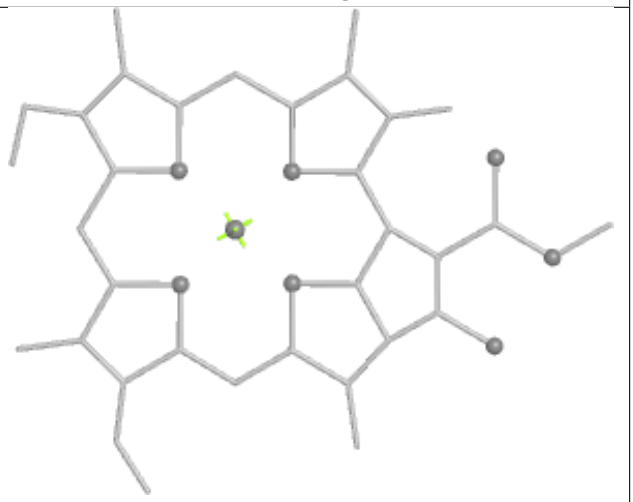

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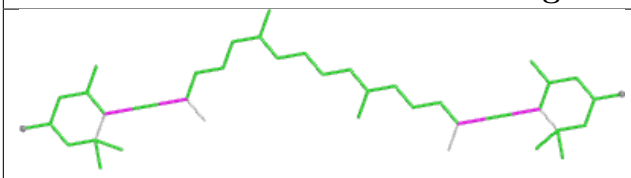

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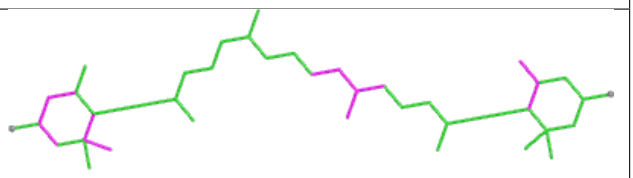

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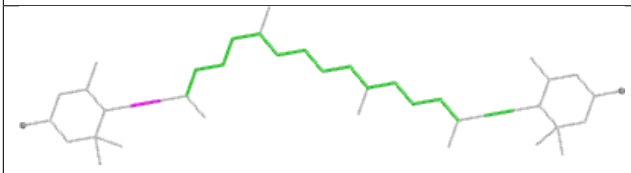

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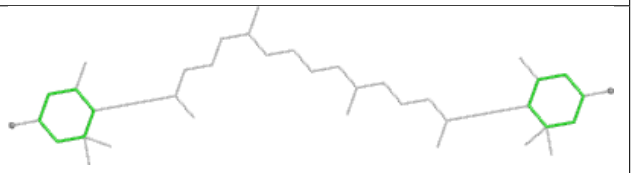

Rings

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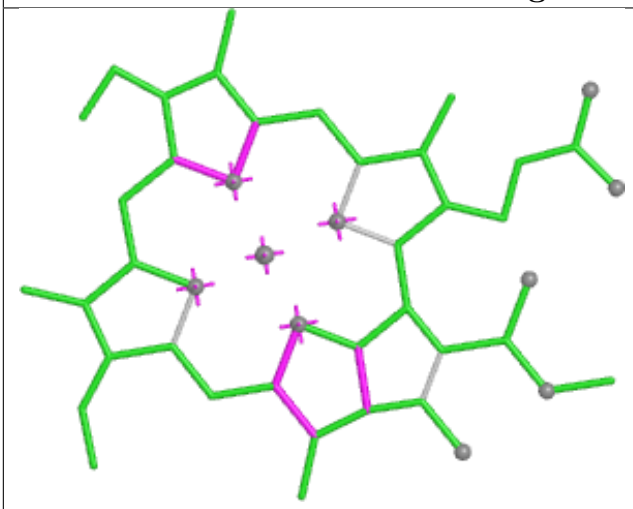

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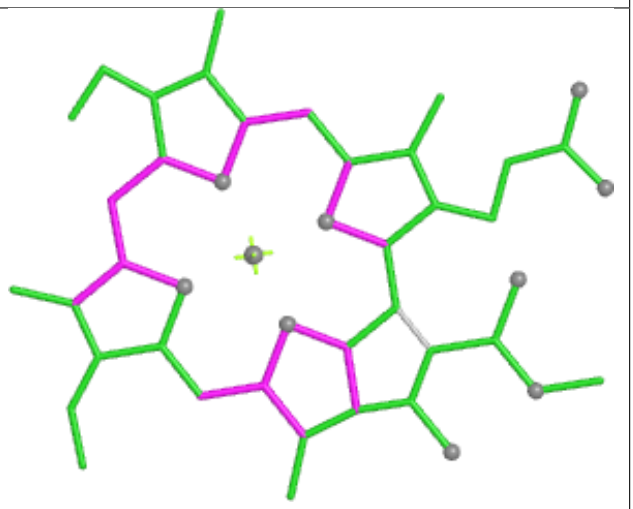

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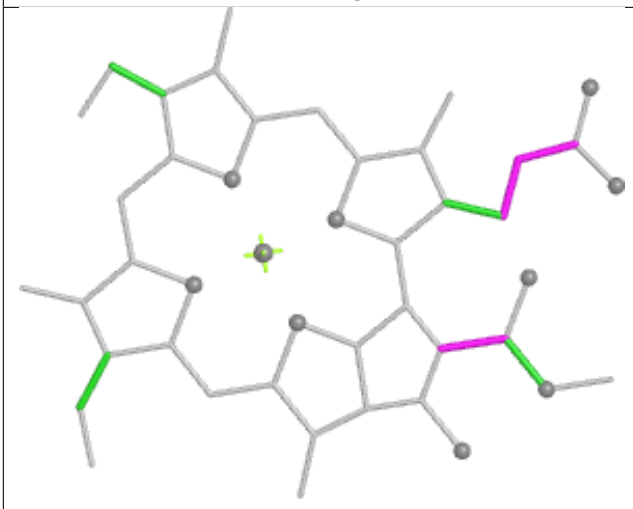

Torsions



Rings

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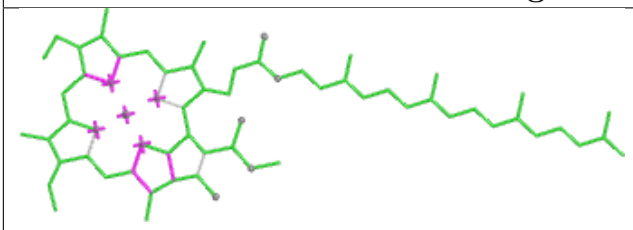

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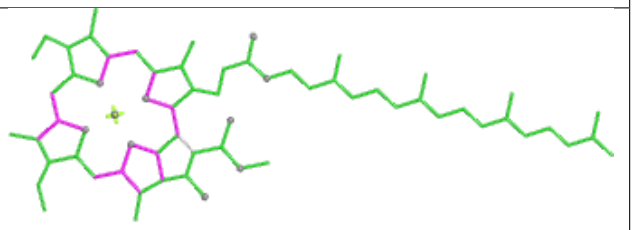

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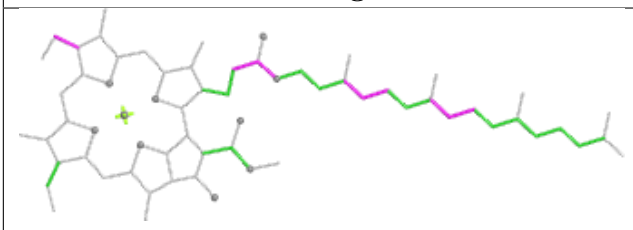

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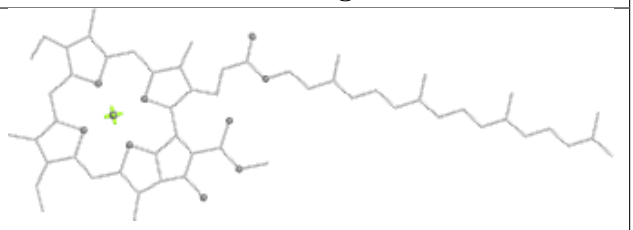

Rings

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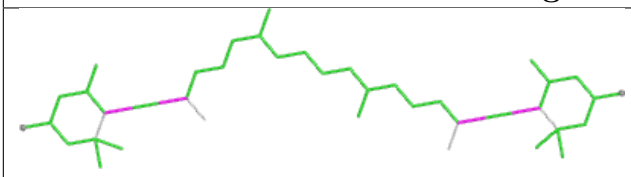

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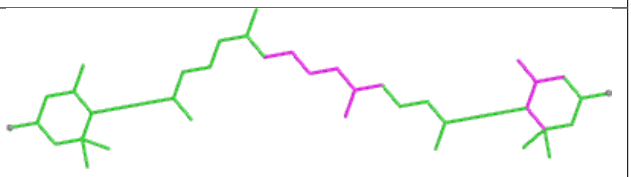

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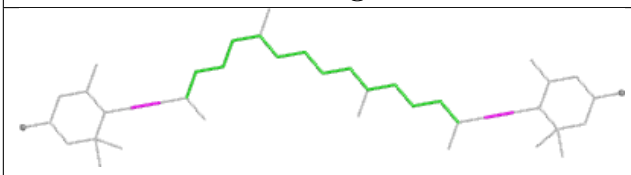

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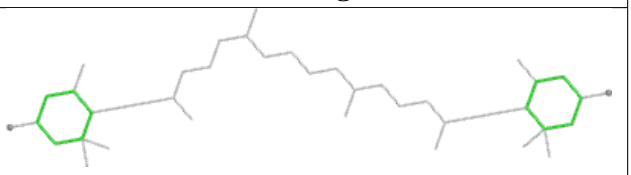

Rings

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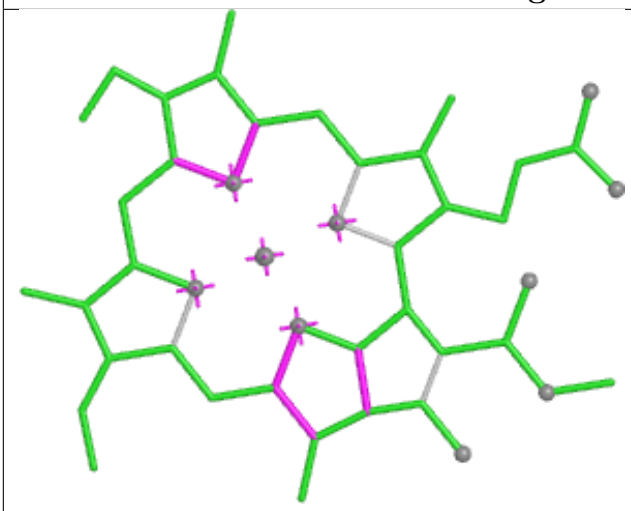

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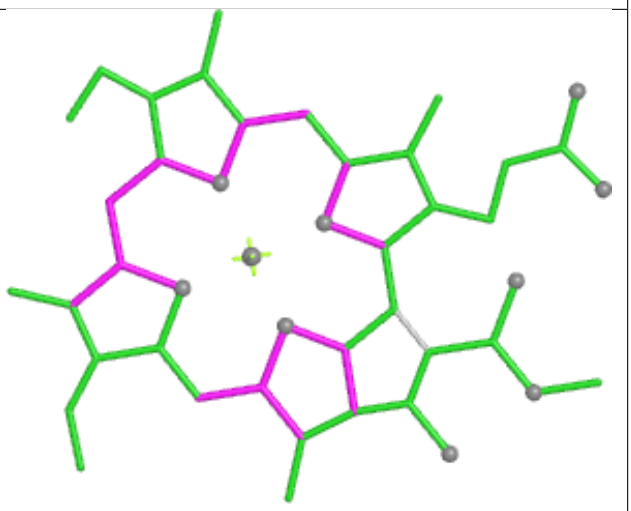

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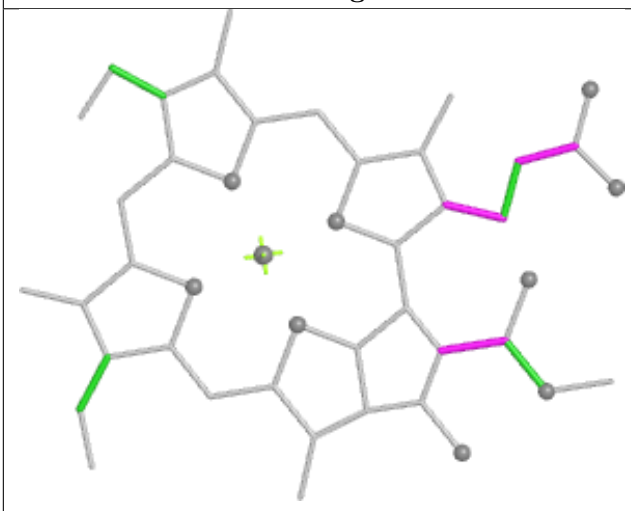

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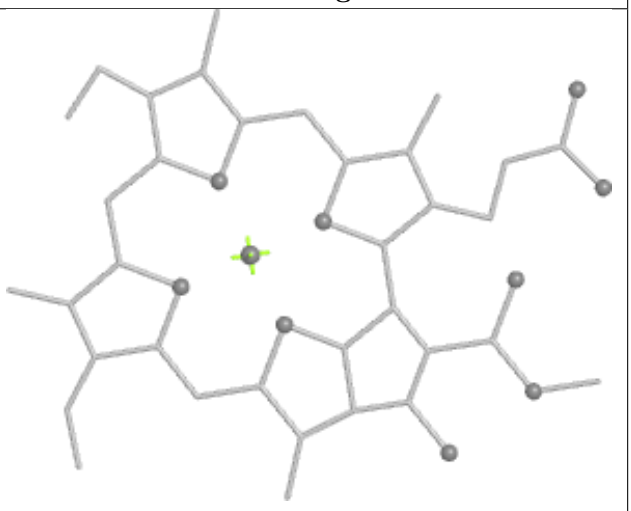

Rings

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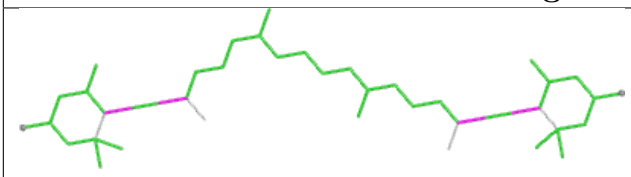
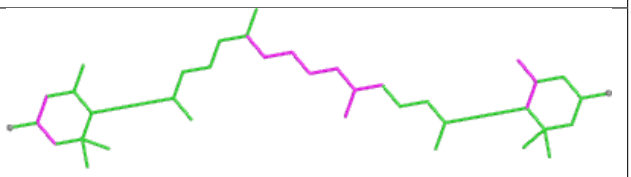
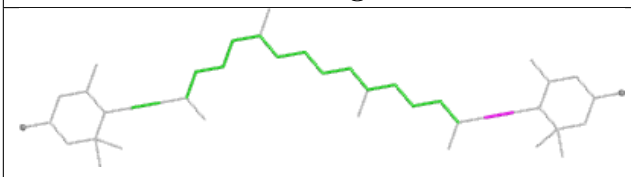
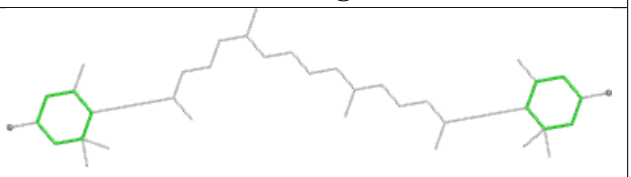
 Bond lengths	 Bond angles
 Torsions	 Rings

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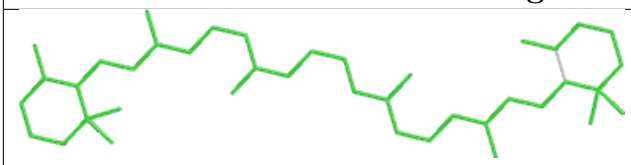
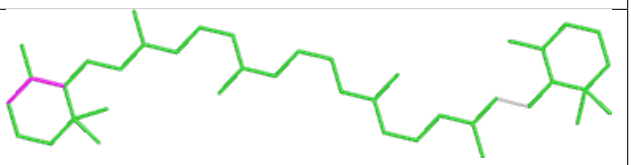
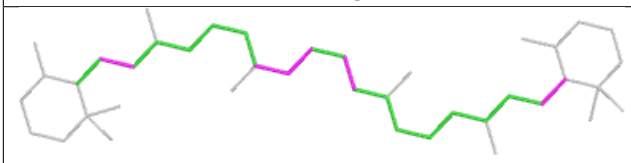
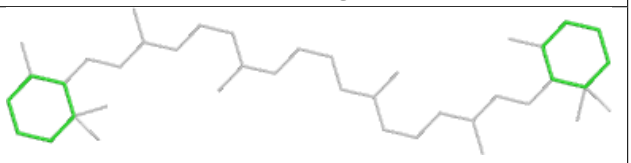
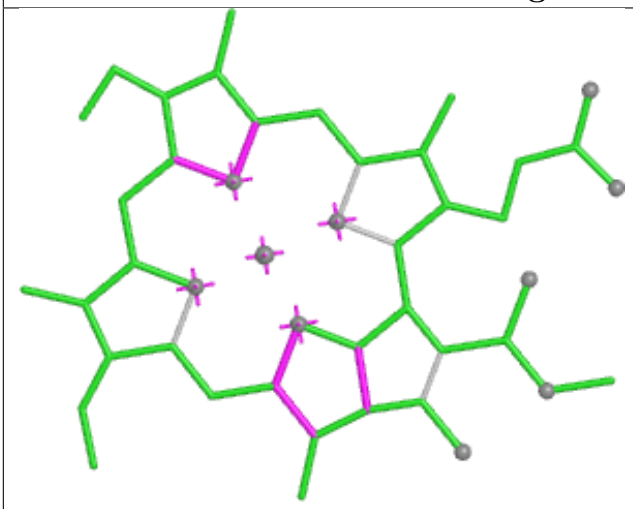
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 611



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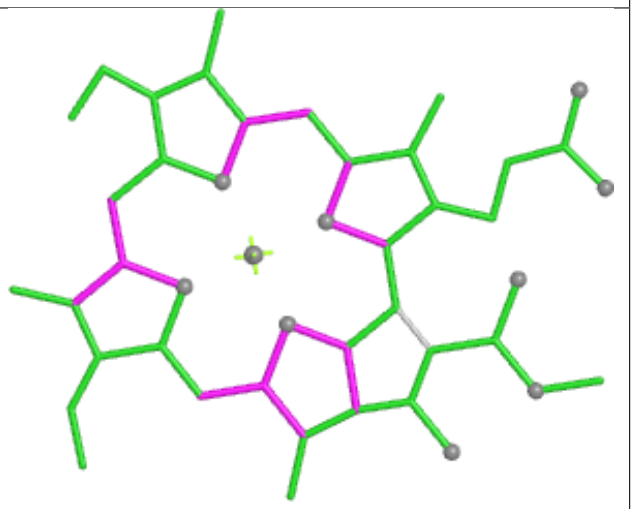
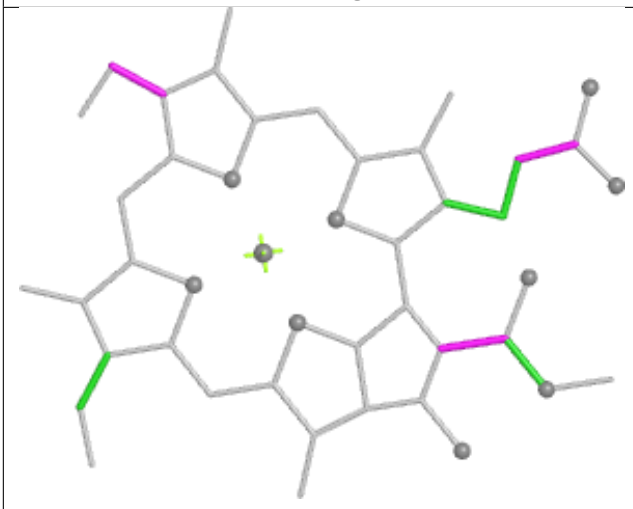


Bond angles

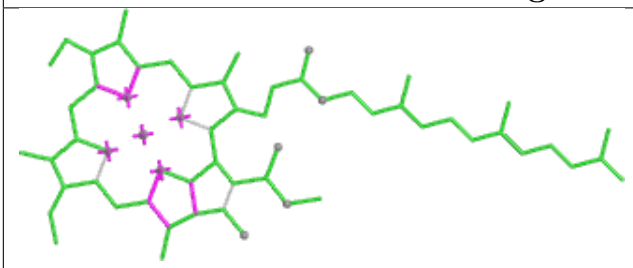


Torsions



Rings

Ligand CLA 3 603



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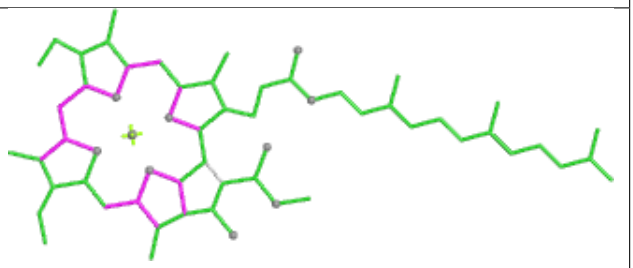

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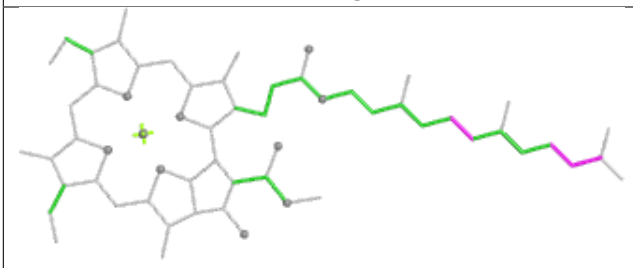

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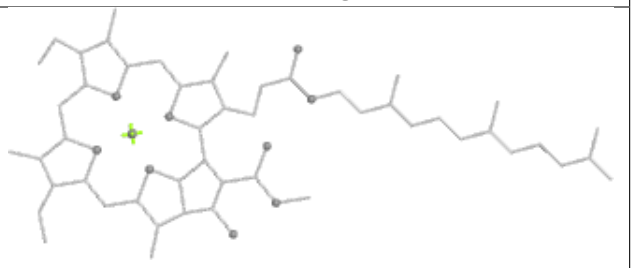
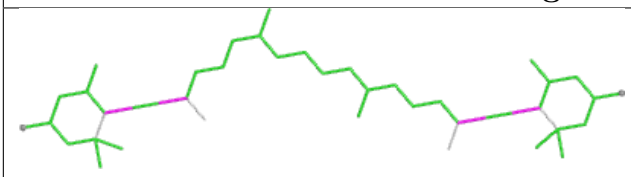


Rings

Ligand II0 8 612



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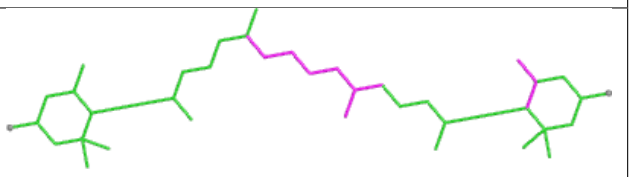

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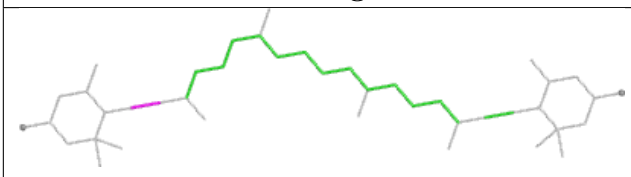

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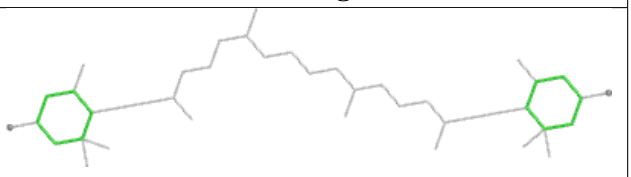
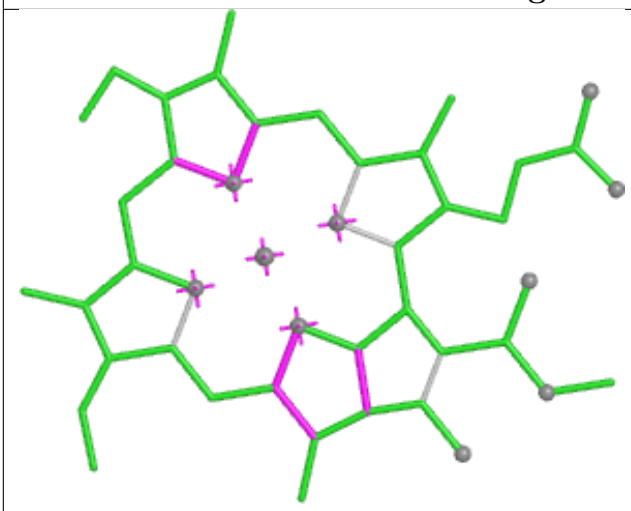


Rings

Ligand CLA 1 601



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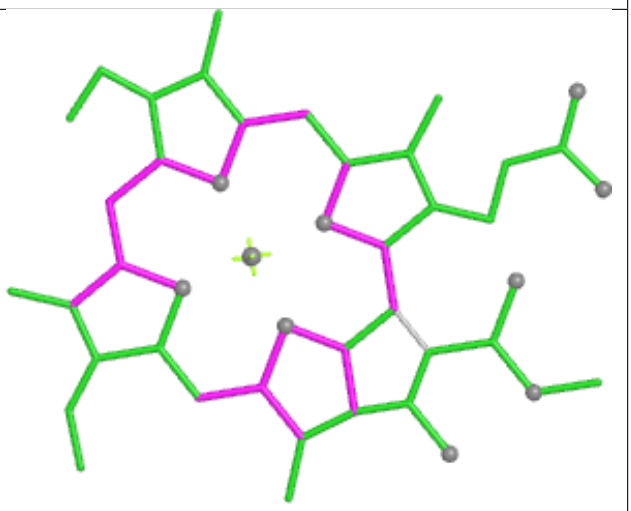

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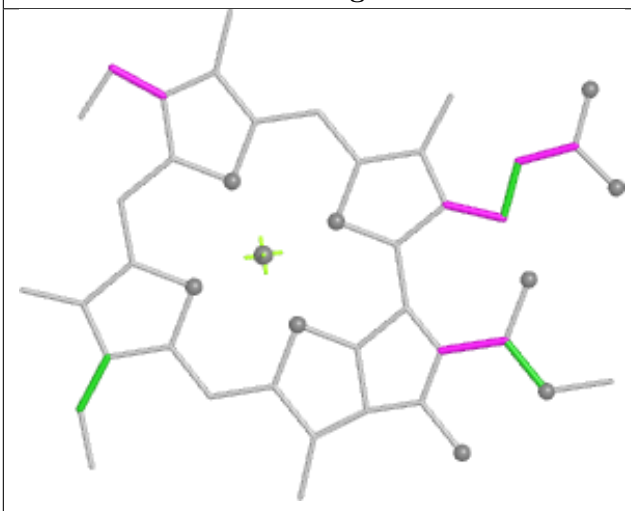

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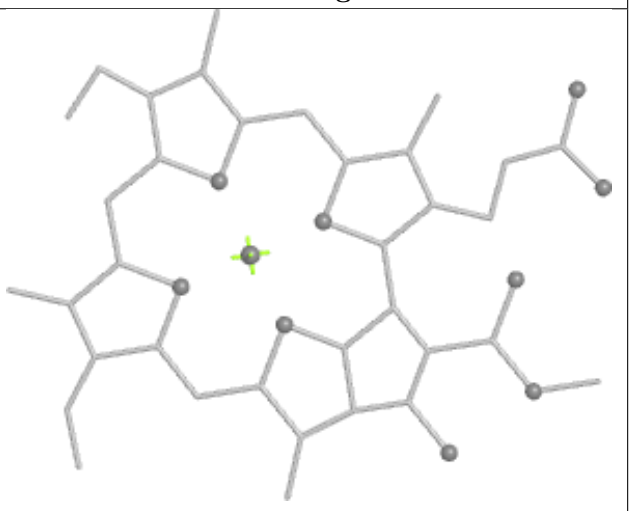
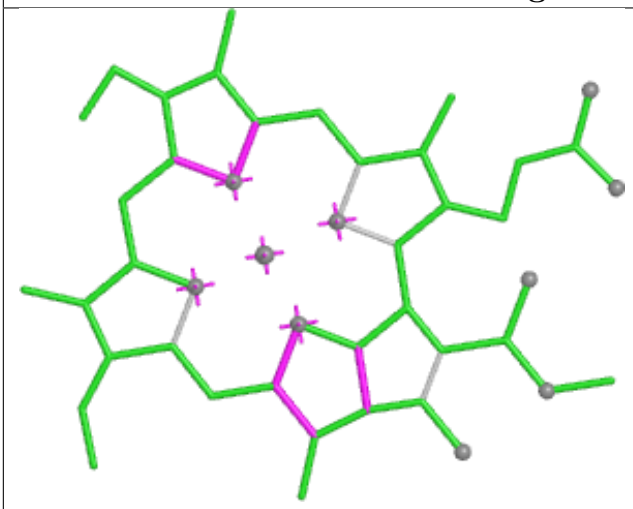


Rings

Ligand CLA 6 603



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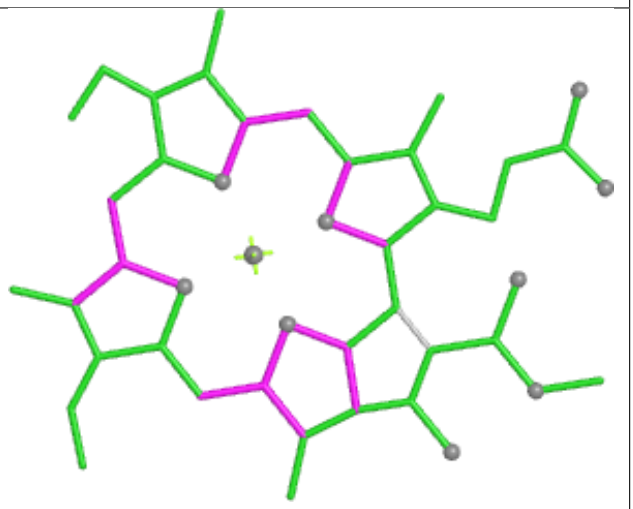

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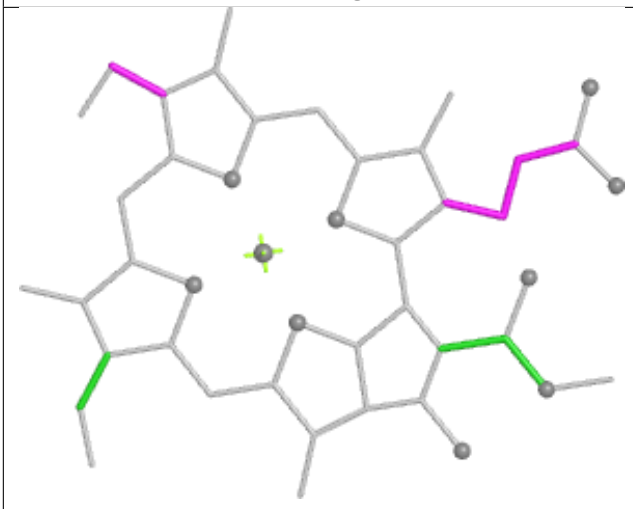
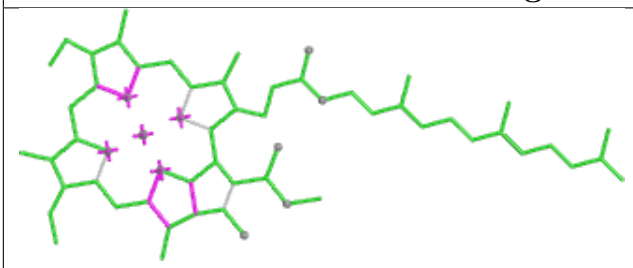


Torsions



Rings

Ligand CLA B 819



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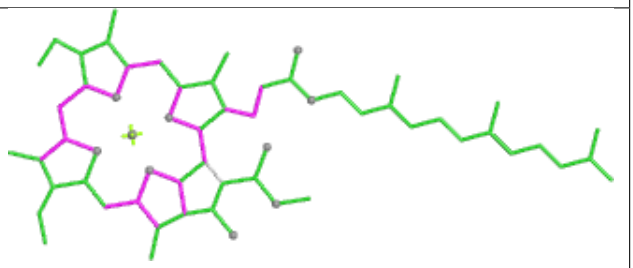

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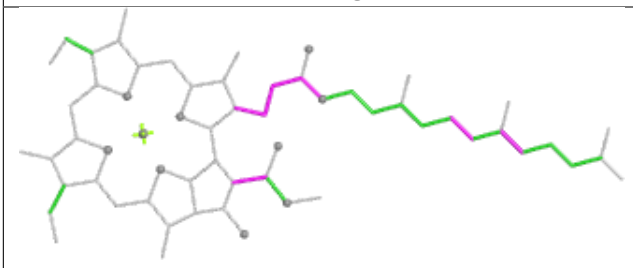

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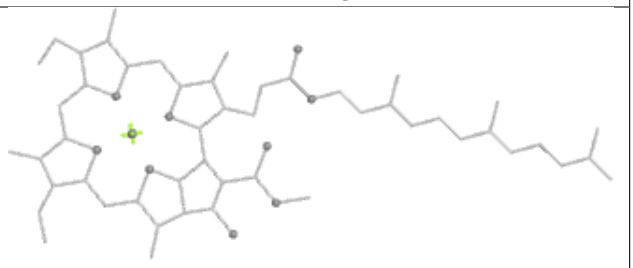
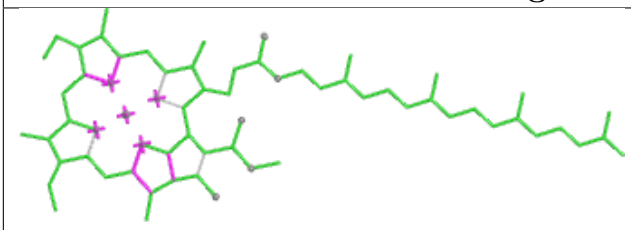


Rings

Ligand CLA 9 607



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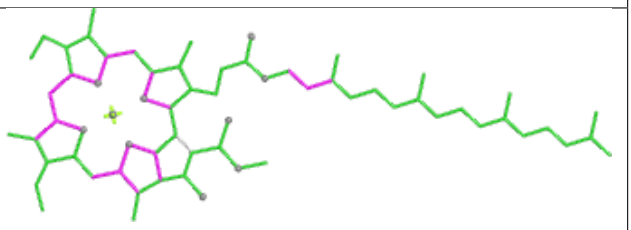

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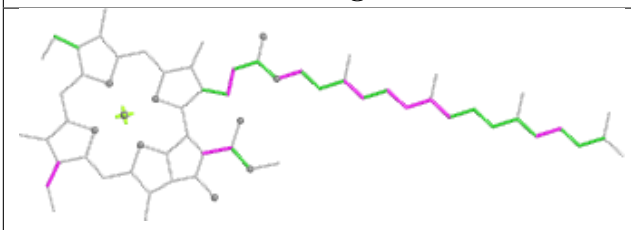

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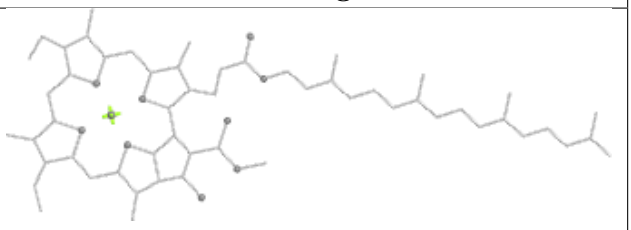

Rings

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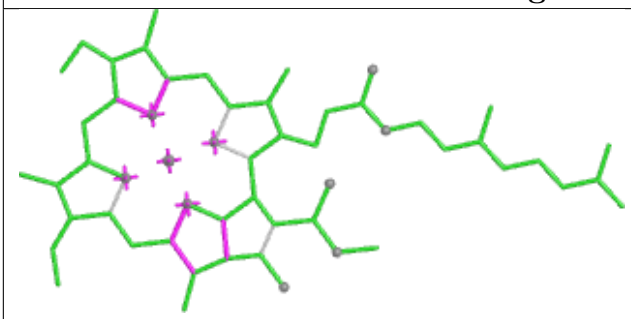

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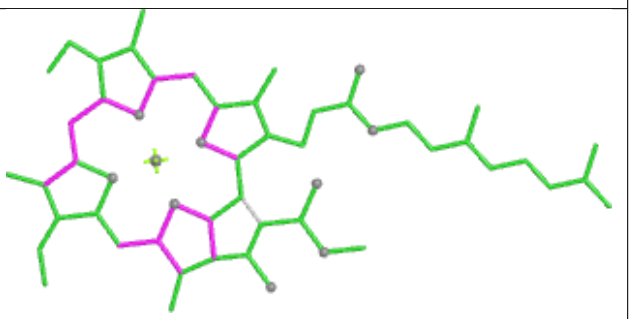

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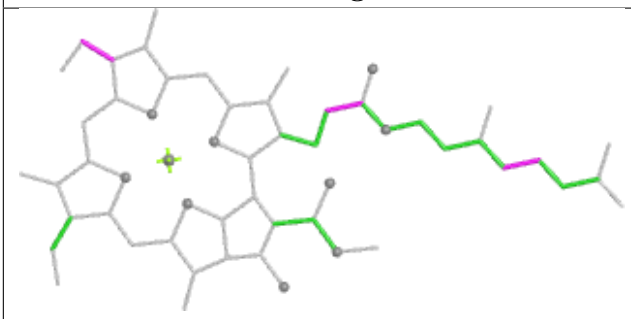

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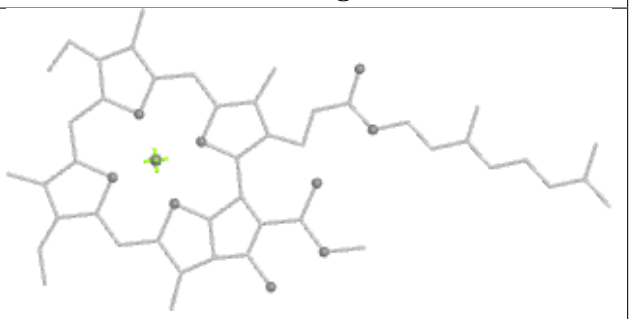
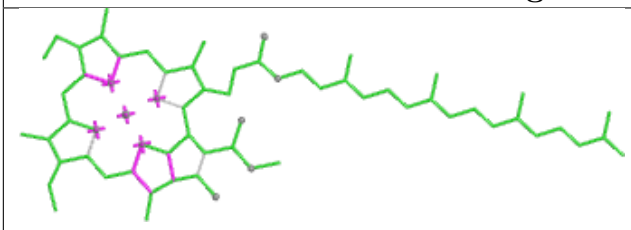


Rings

Ligand CLA L 201



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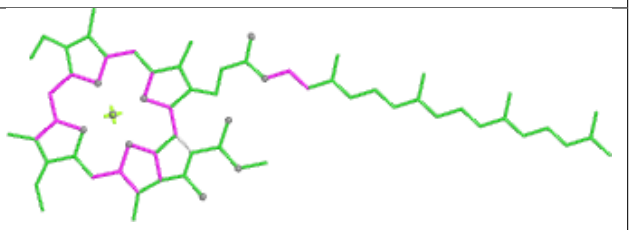

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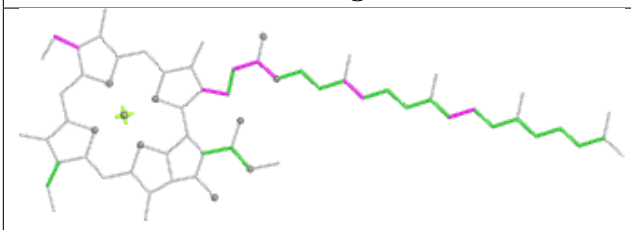

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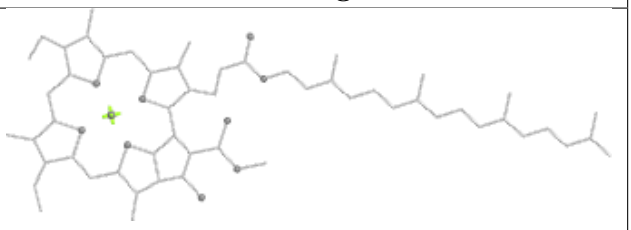

Rings

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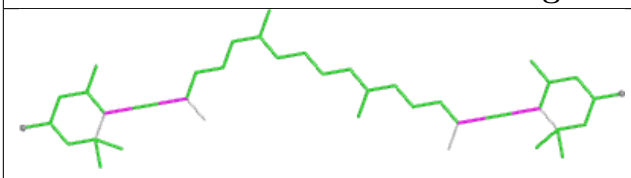

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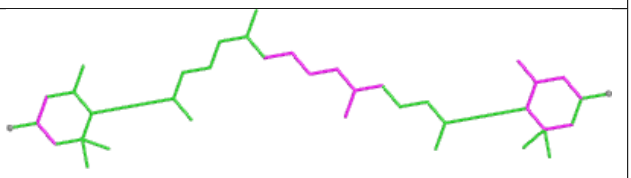

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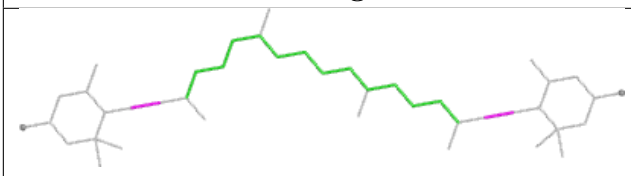

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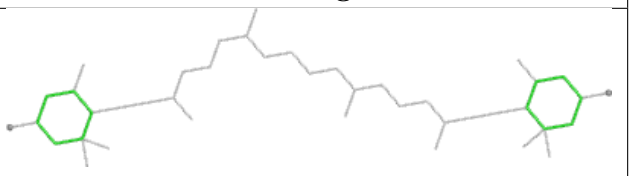

Rings

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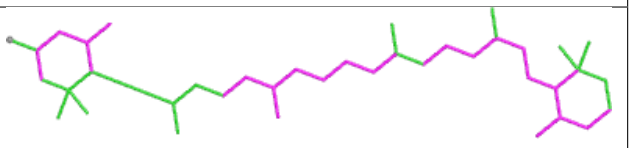
Bond lengths



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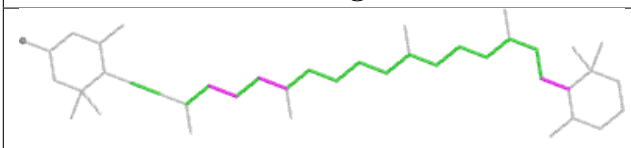

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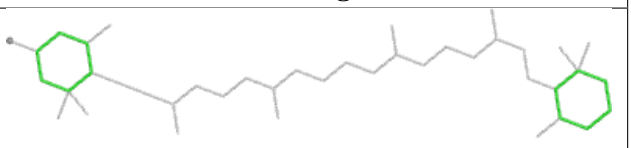

Rings

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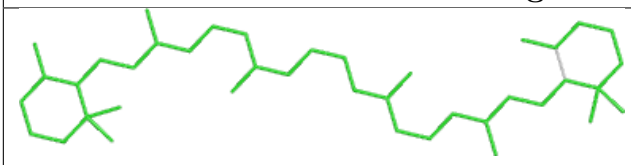

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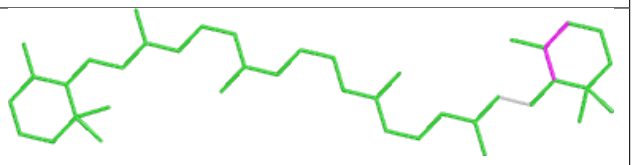

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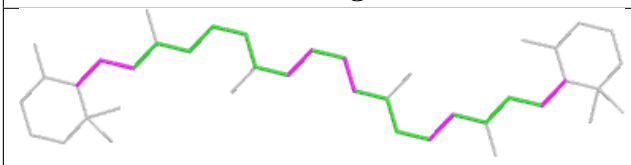

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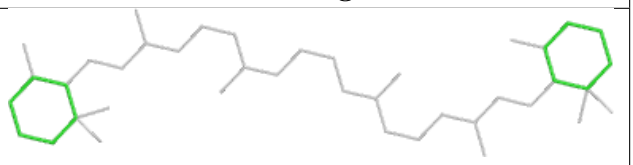
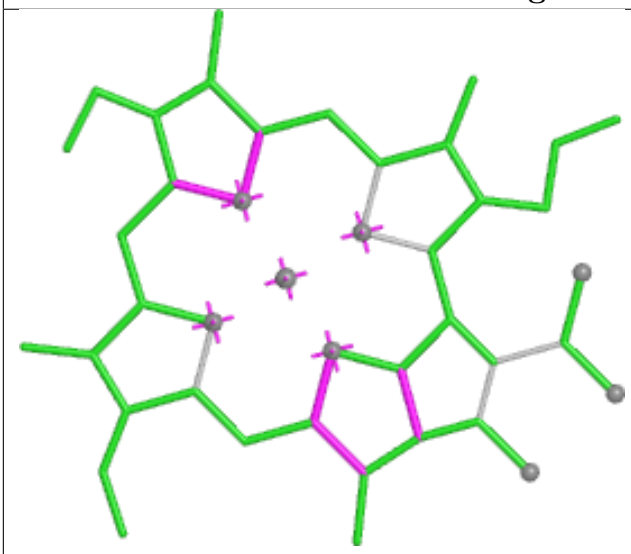


Rings

Ligand CLA 1 605



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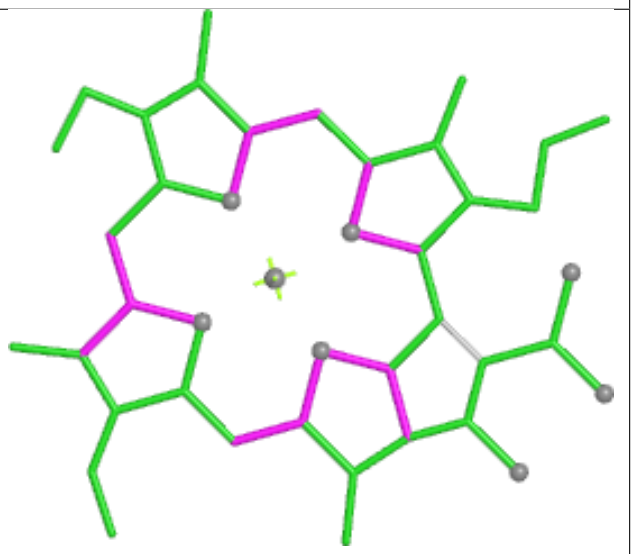

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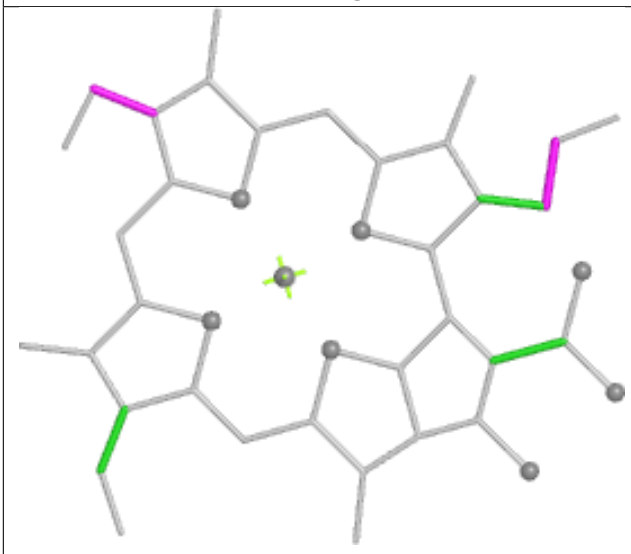

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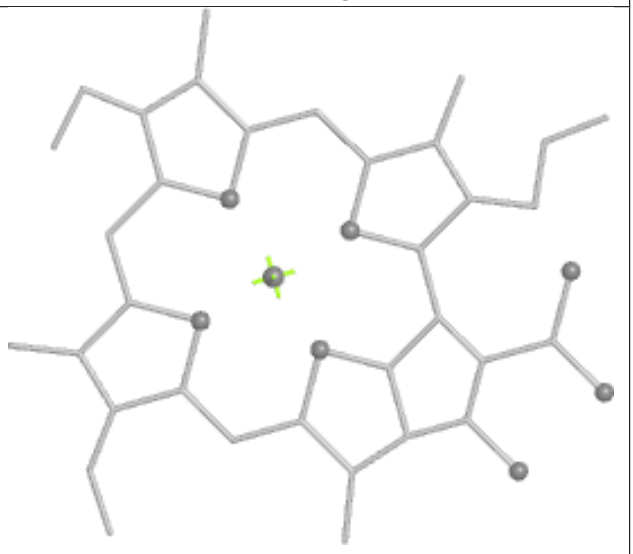

Rings

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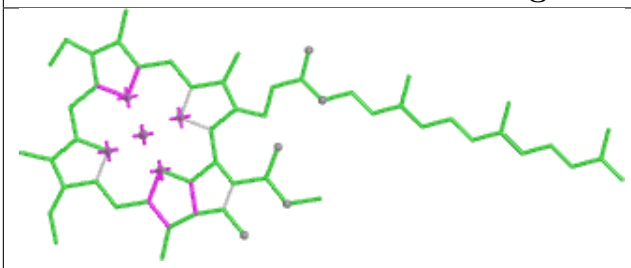

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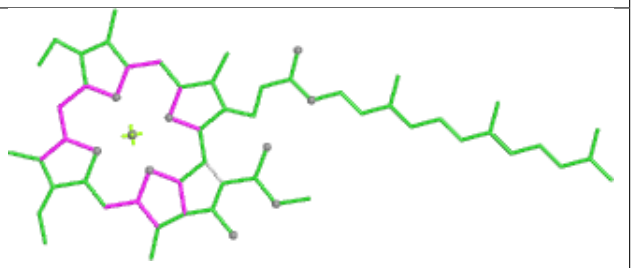

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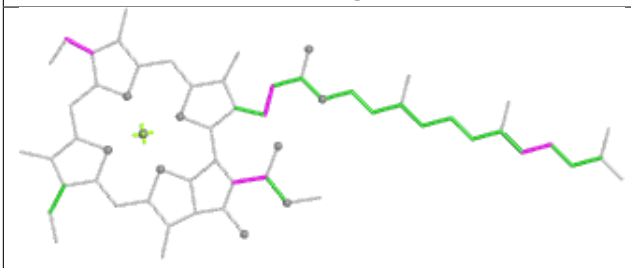

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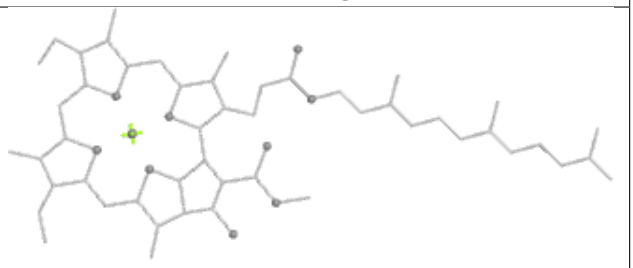

Rings

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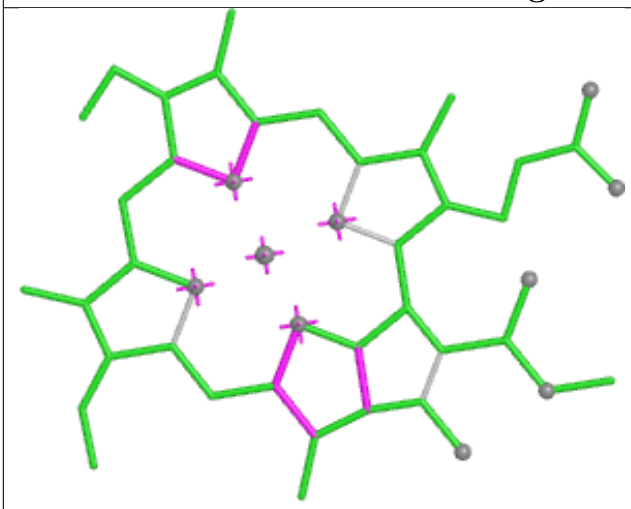

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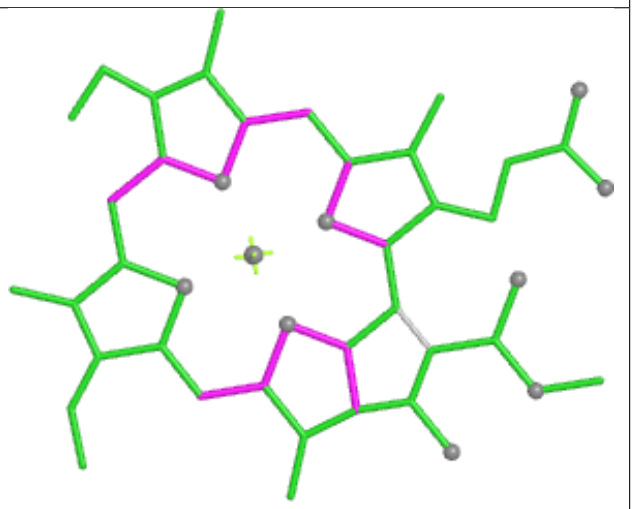
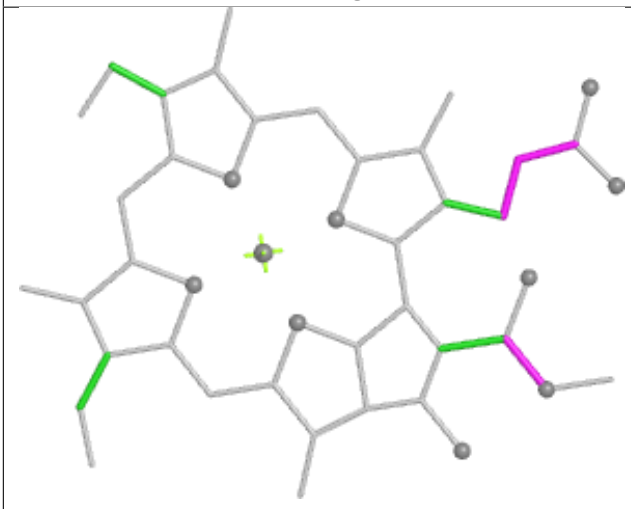


Bond angles

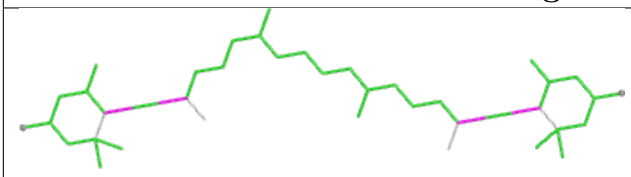


Torsions



Rings

Ligand II0 6 615



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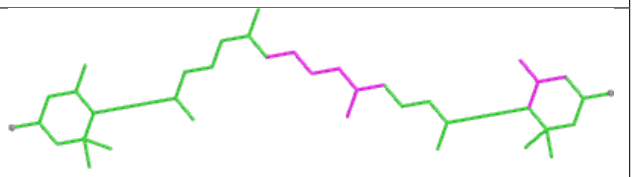

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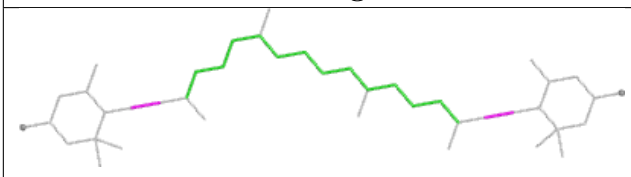

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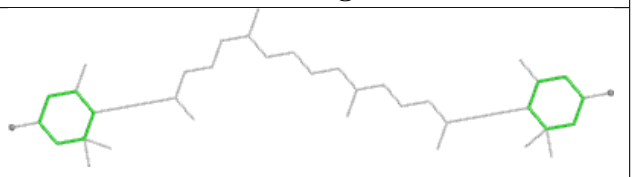

Rings

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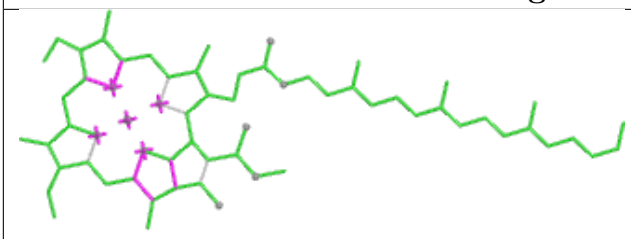

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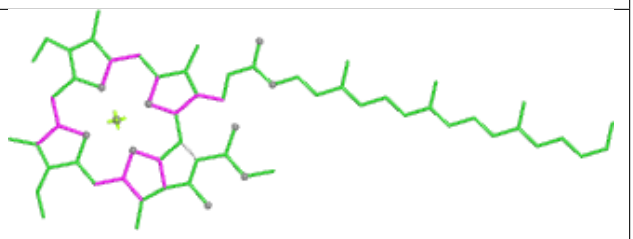
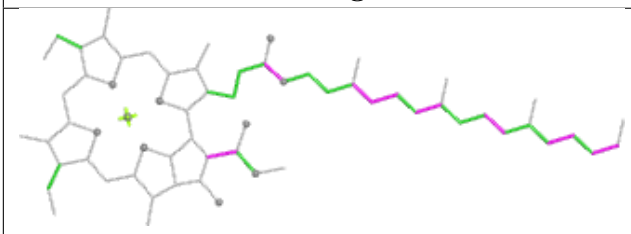
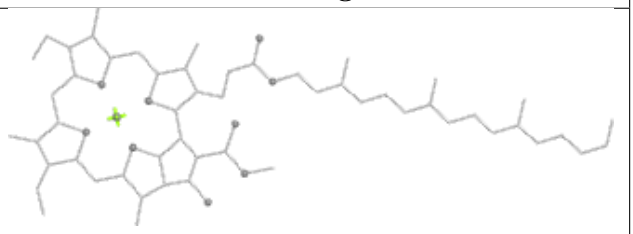


Bond angles

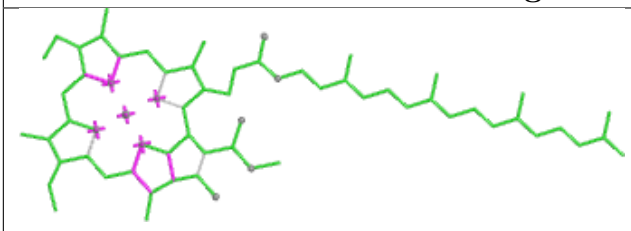


Torsions



Rings

Ligand CLA B 815



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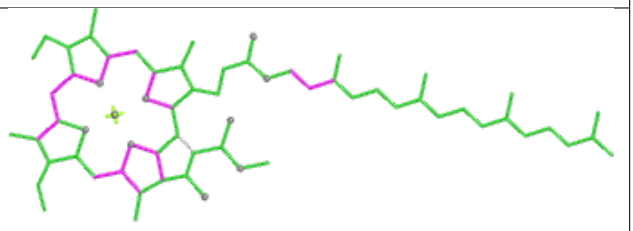

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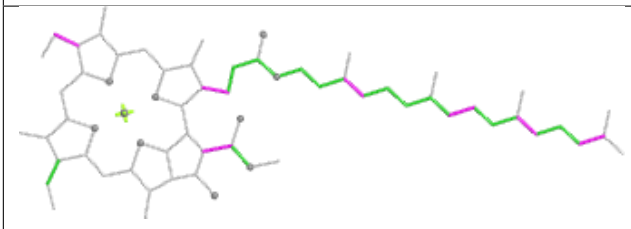

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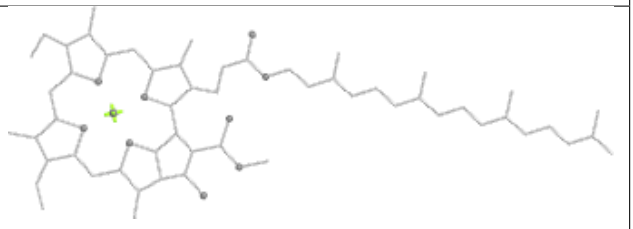
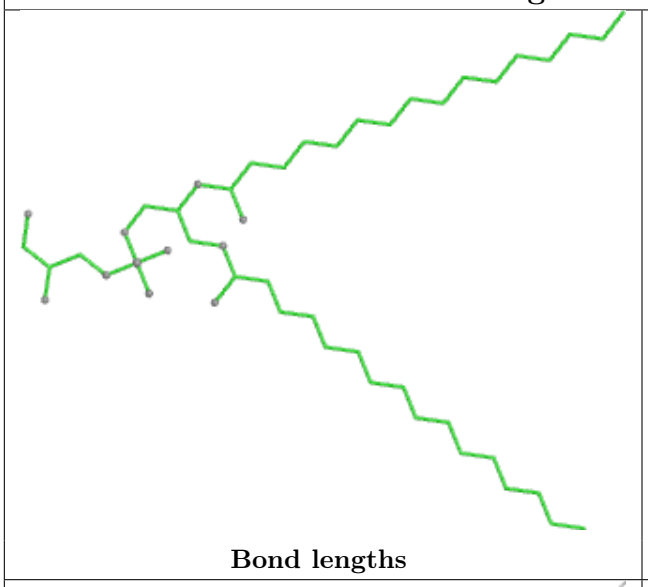


Rings

Ligand LHG 3 619



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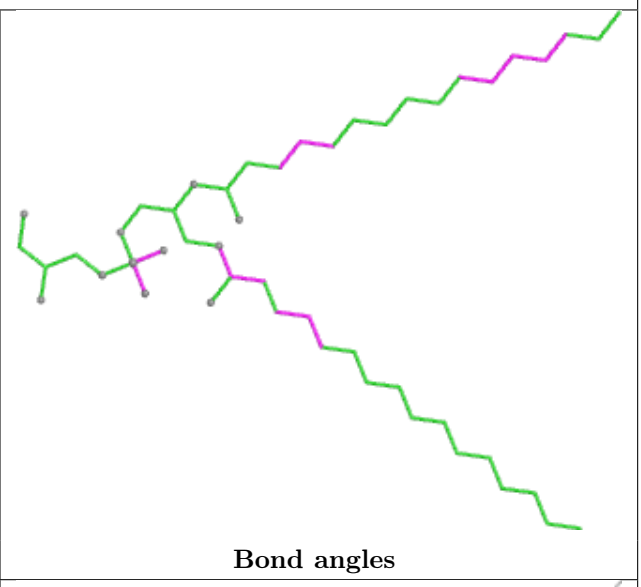

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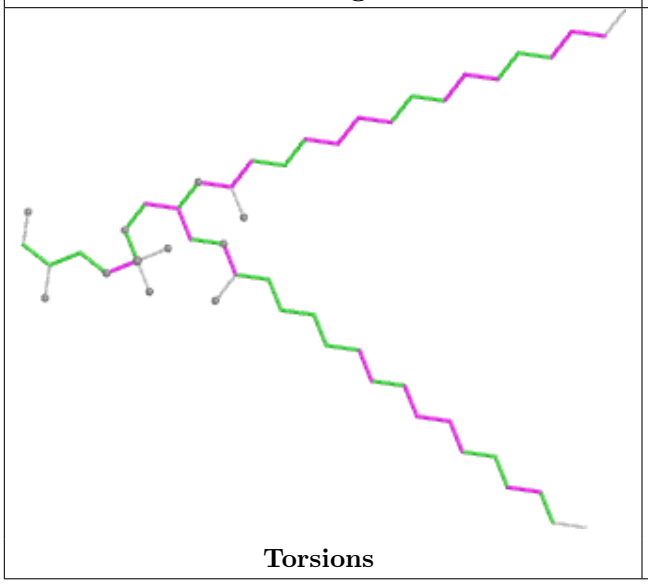

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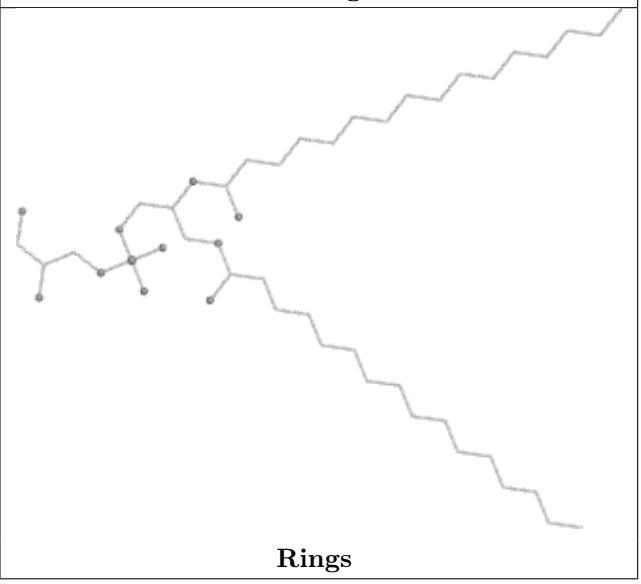
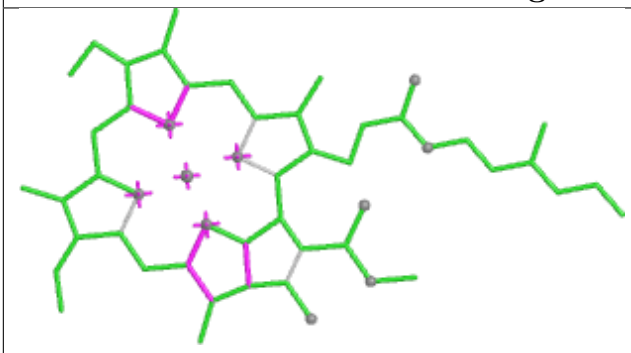


Rings

Ligand CLA 1 603



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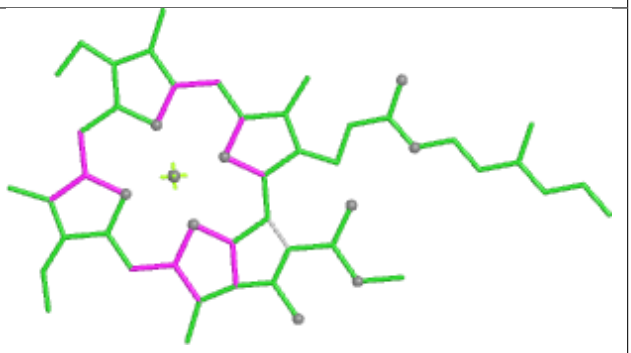

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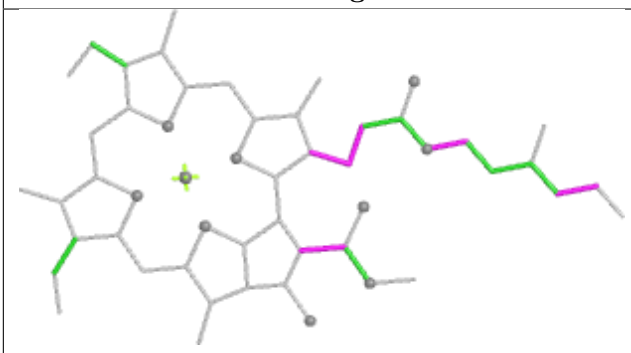

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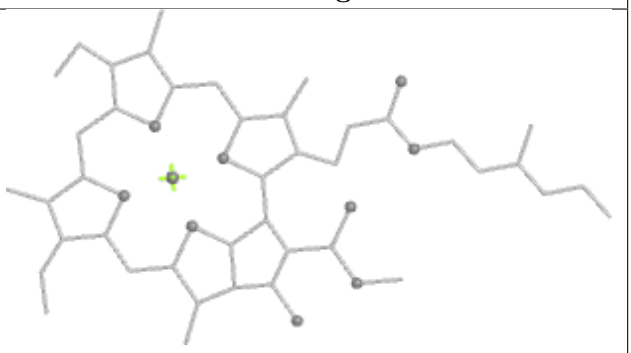
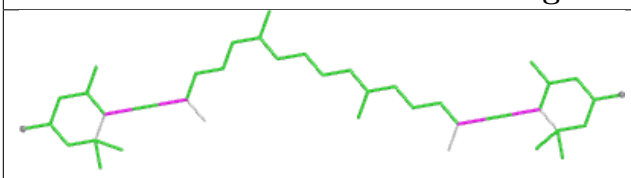


Rings

Ligand II0 5 617



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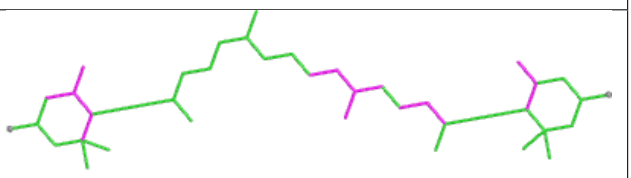
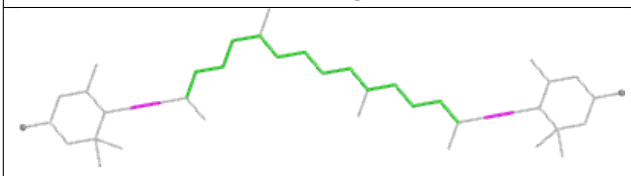


Bond angles



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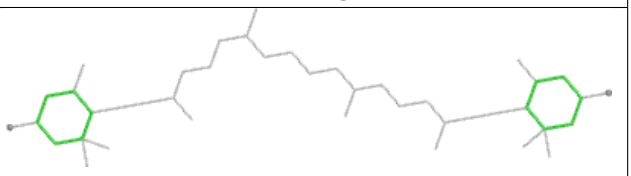

Rings

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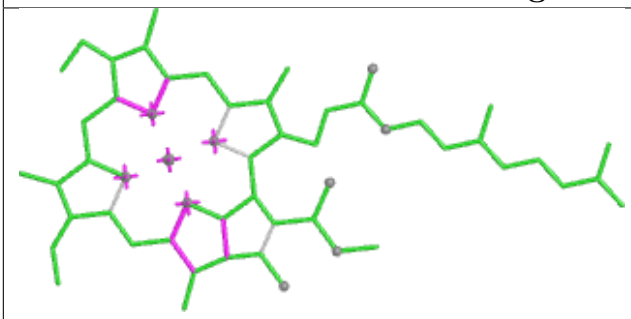

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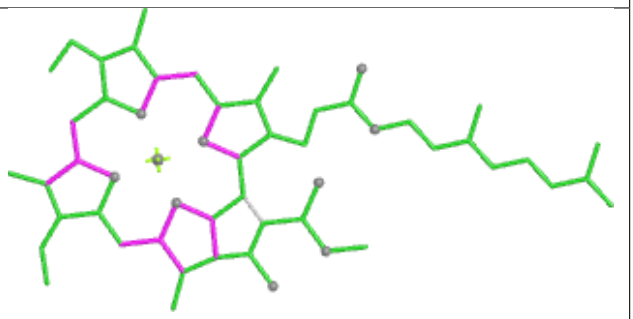

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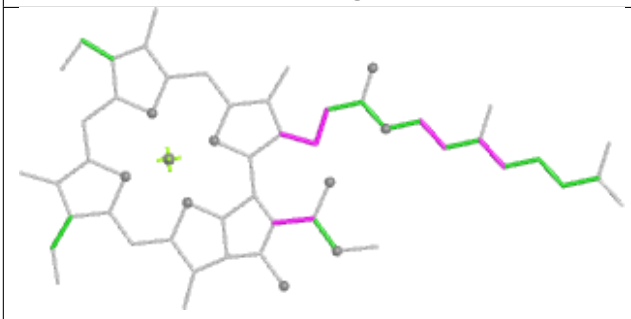

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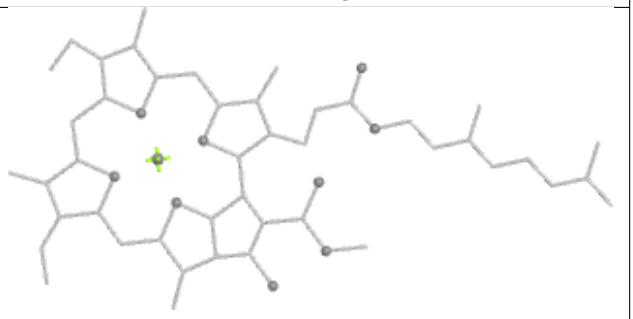
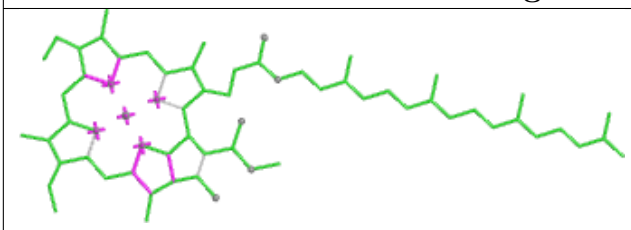


Rings

Ligand CLA A 833



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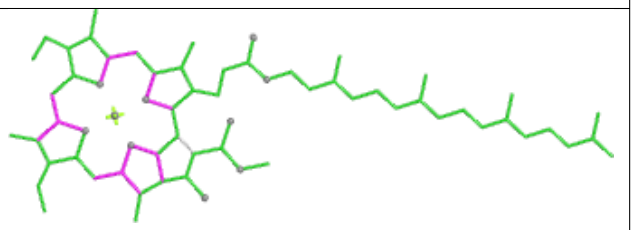

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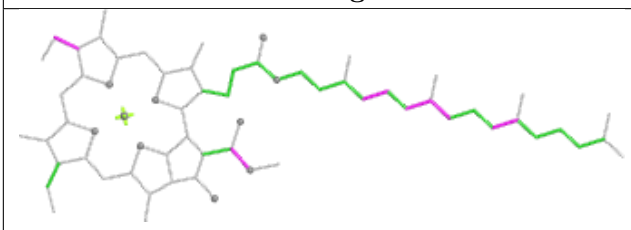

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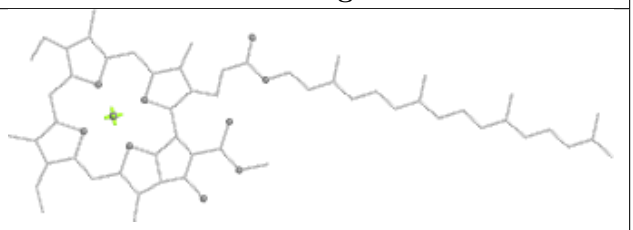
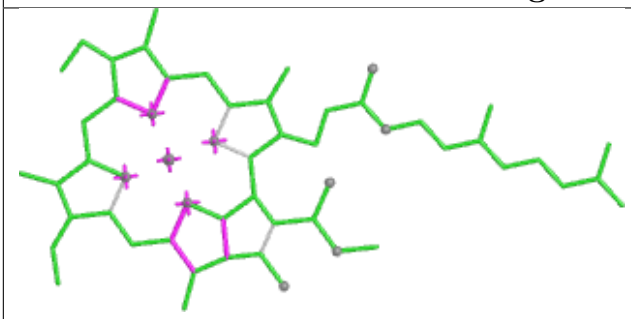


Rings

Ligand CLA 5 602



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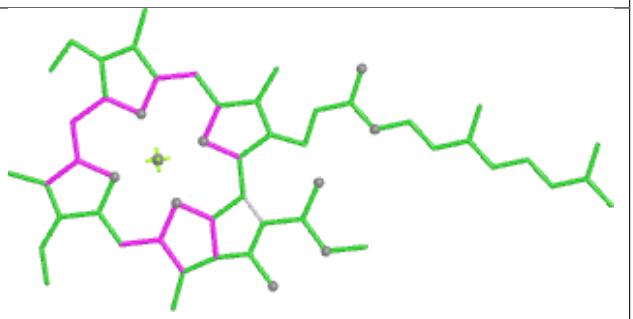

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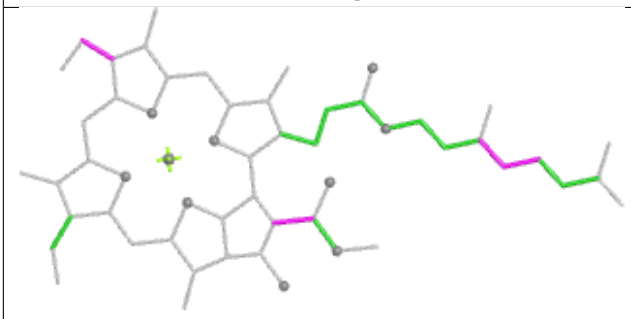

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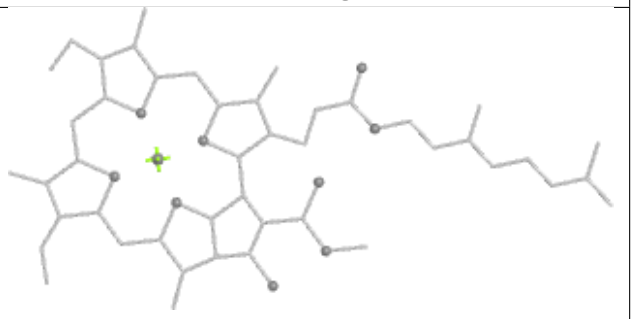
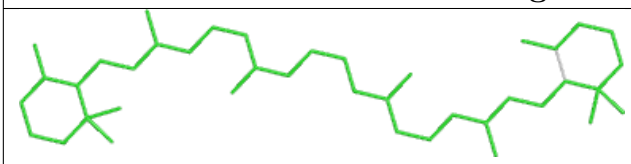


Rings

Ligand 8CT L 206



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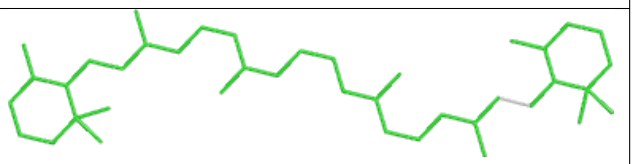
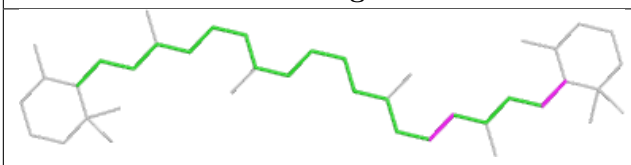


Bond angles



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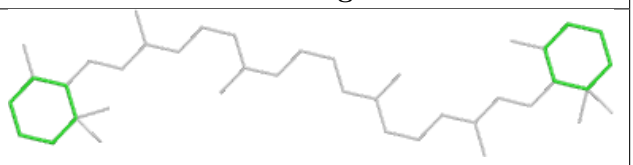
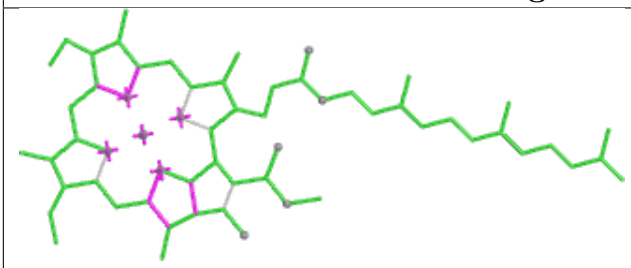


Rings

Ligand CLA 2 605



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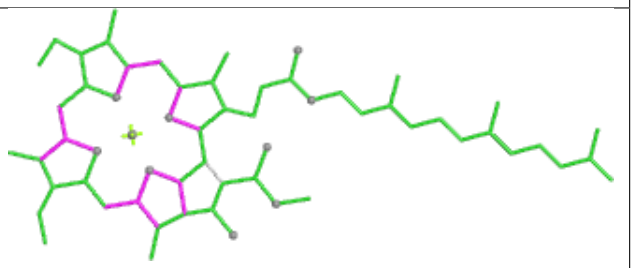

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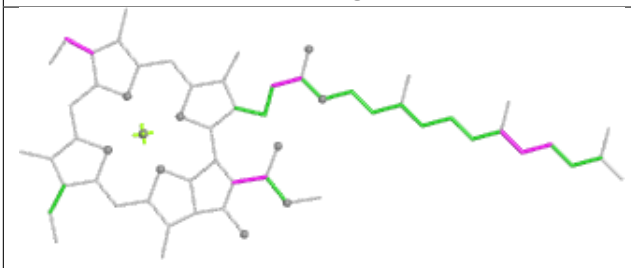

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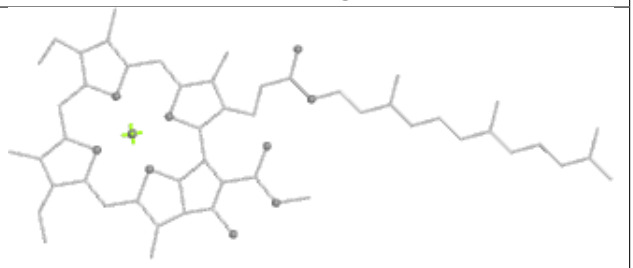
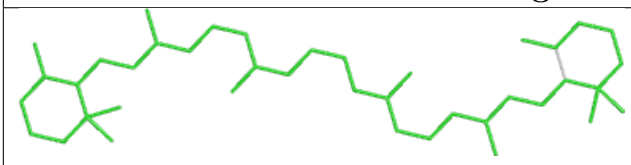


Rings

Ligand 8CT e 616



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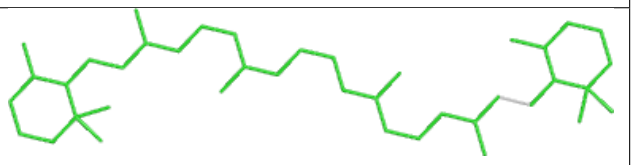

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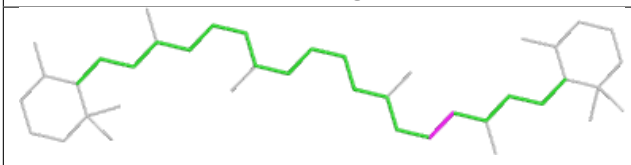

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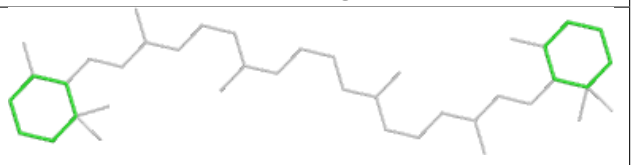
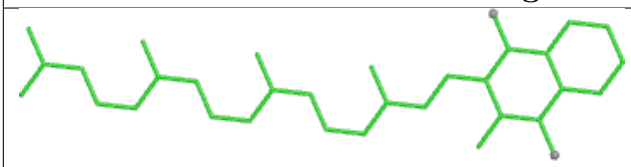


Rings

Ligand PQN B 842



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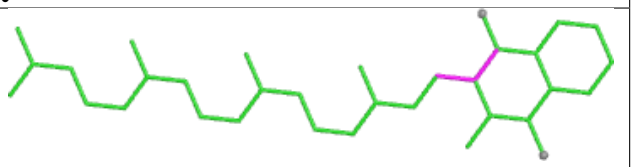
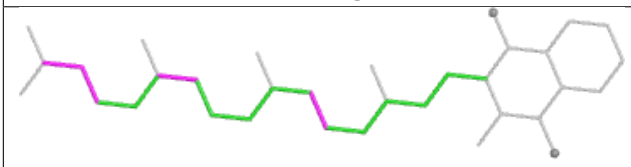


Bond angles



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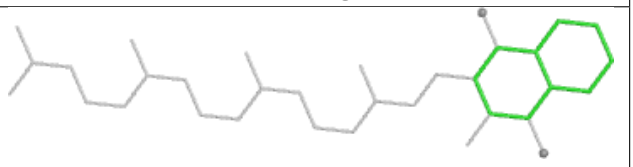
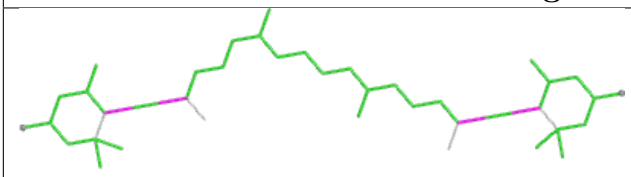


Rings

Ligand II0 a 616



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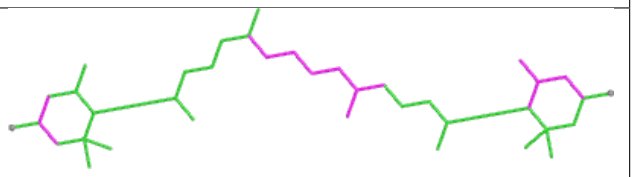
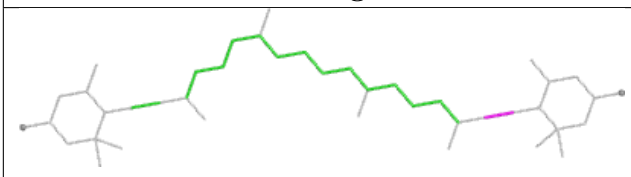


Bond angles



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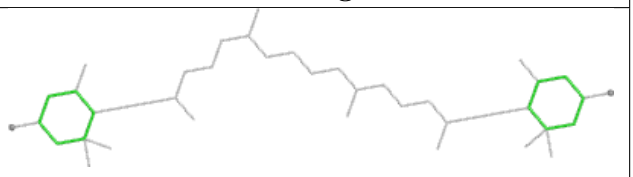
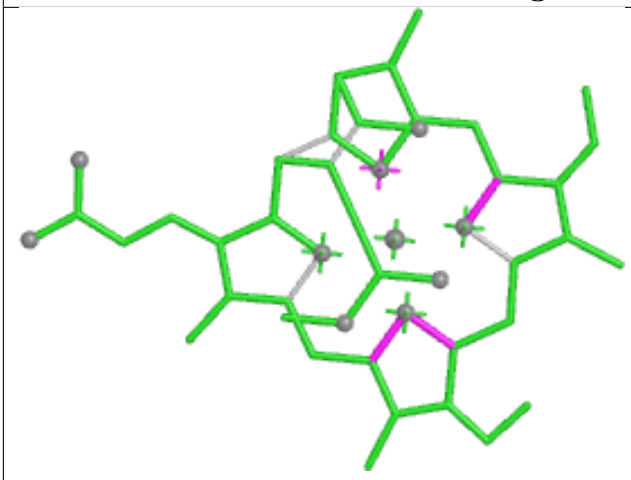


Rings

Ligand KC2 d 610



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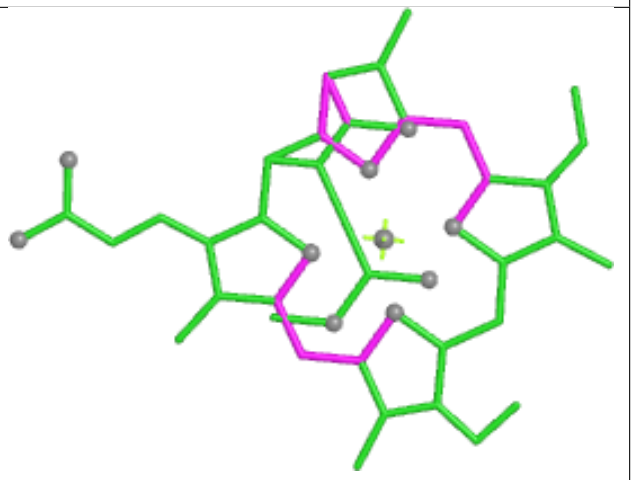
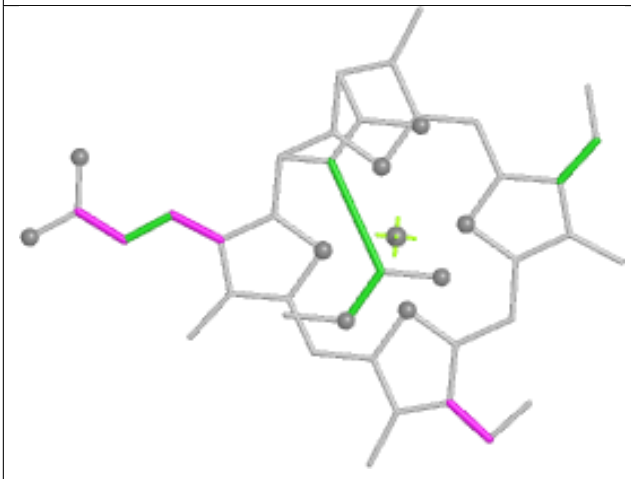


Bond angles



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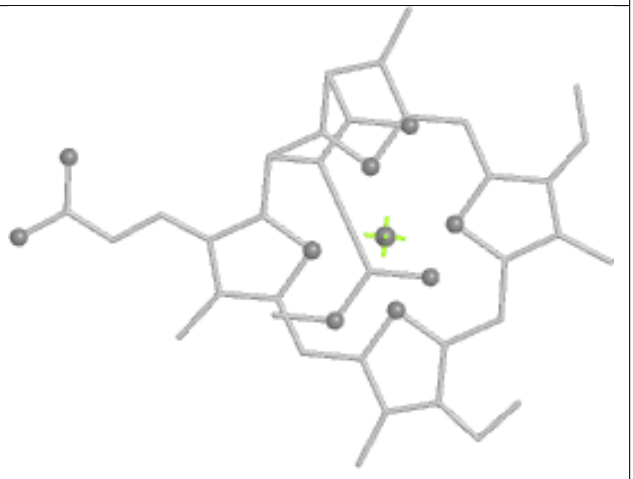
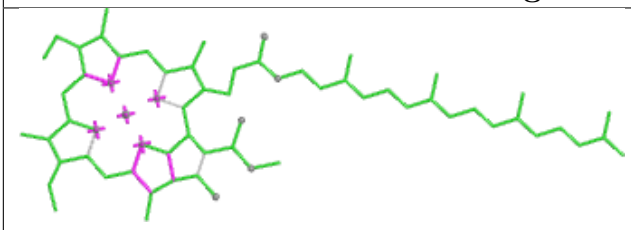


Rings

Ligand CLA A 818



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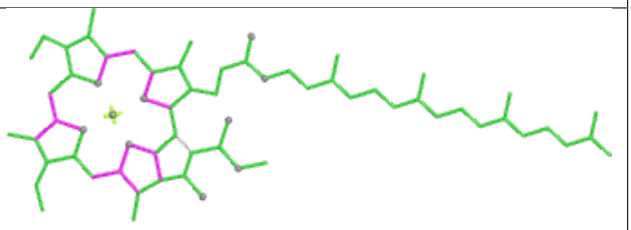
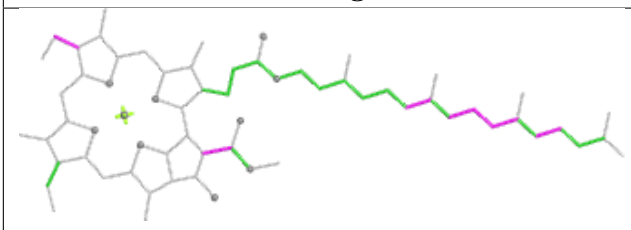


Bond angles



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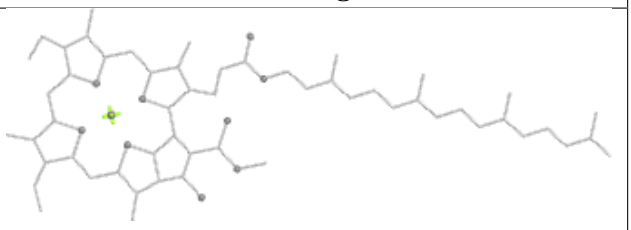
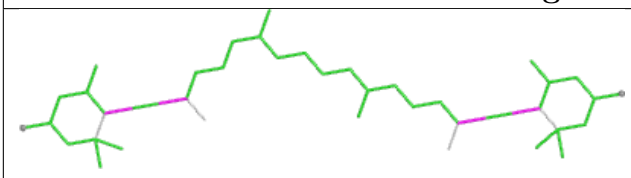


Rings

Ligand II0 6 616



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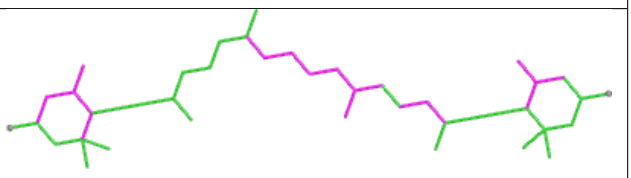

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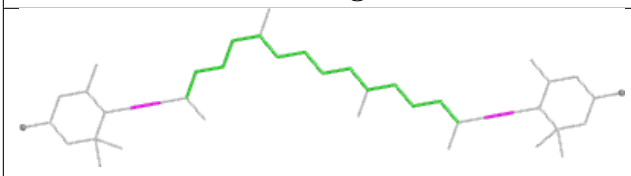
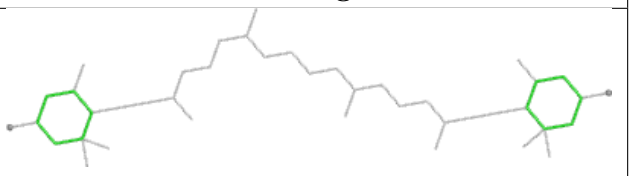
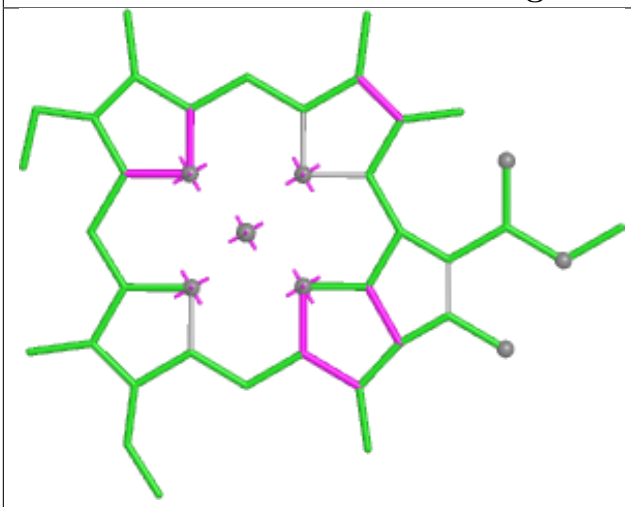


Torsions



Rings

Ligand CLA L 207



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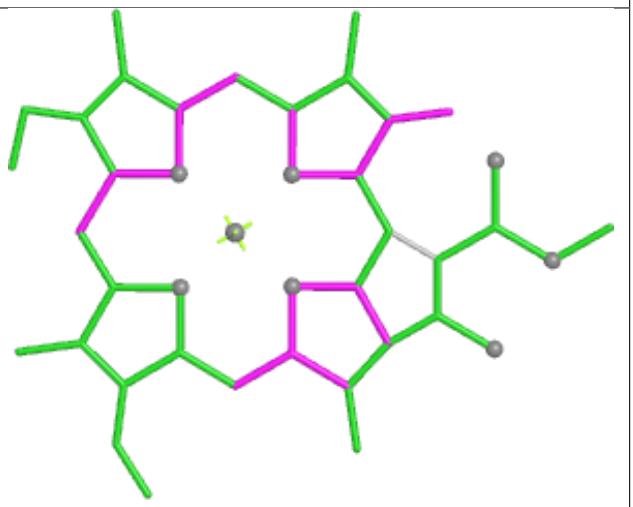

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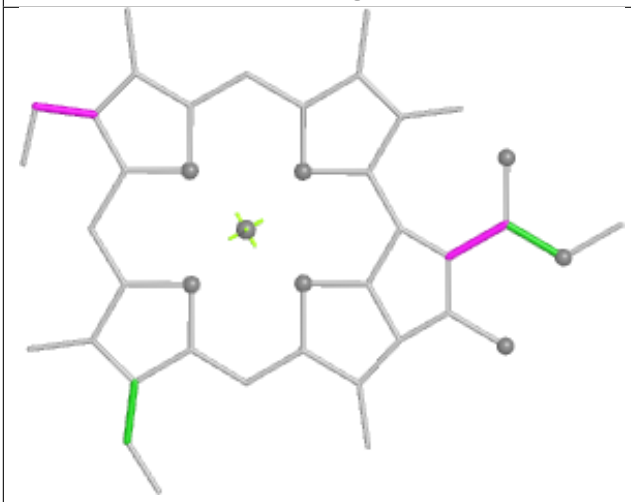

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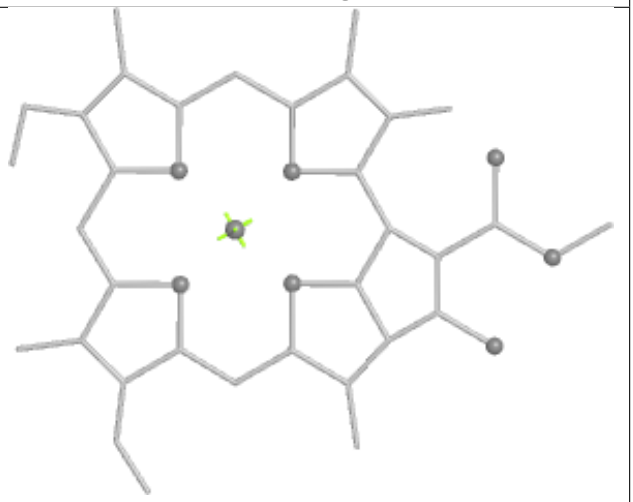

Rings

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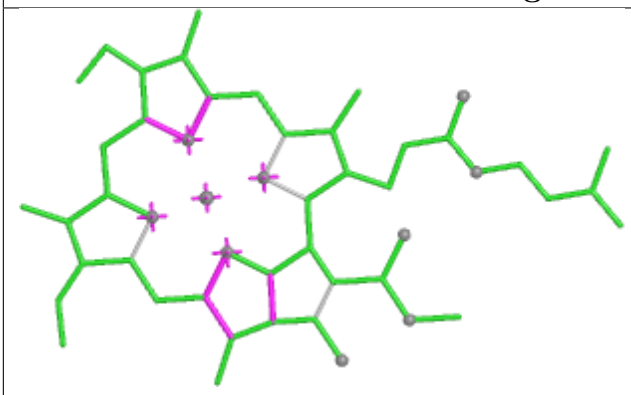

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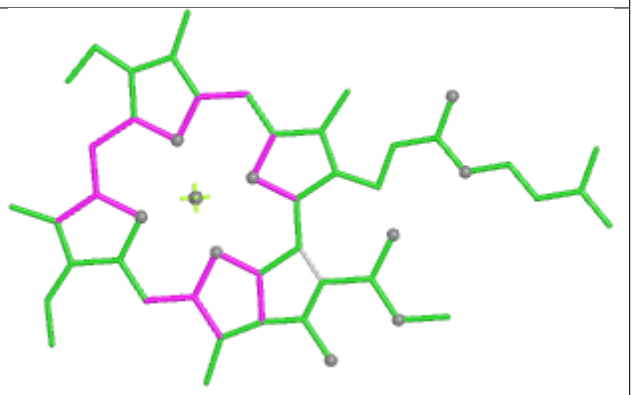

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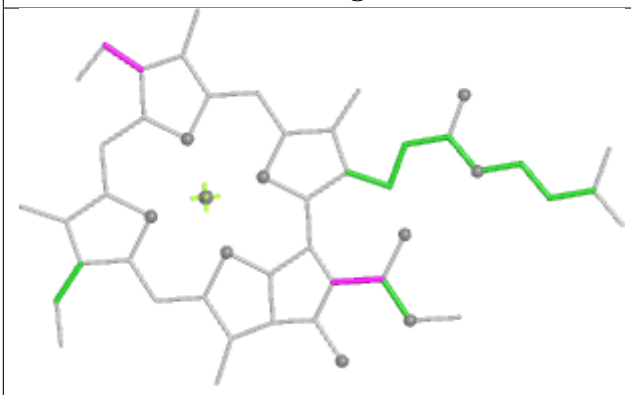

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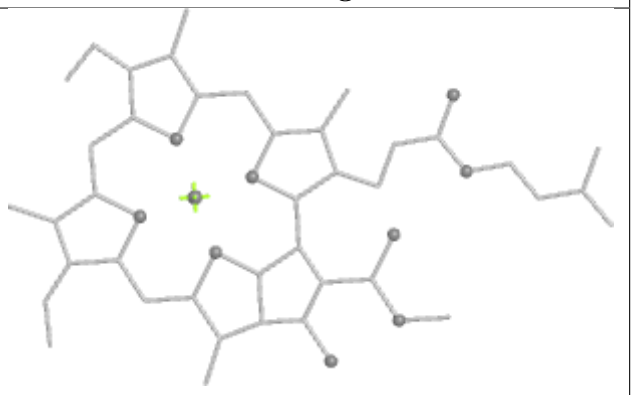
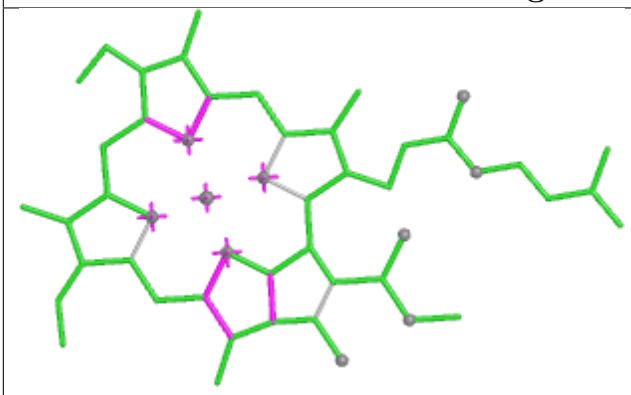


Rings

Ligand CLA d 611



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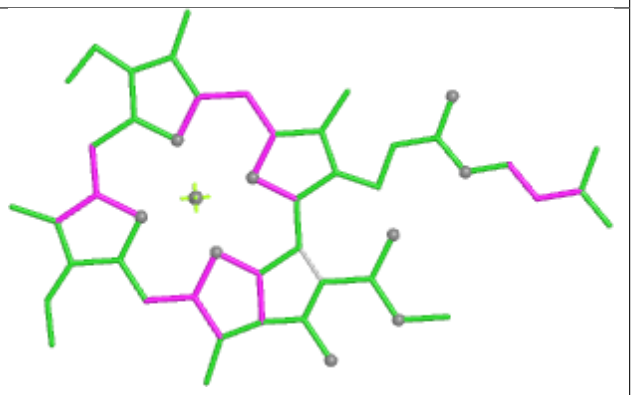

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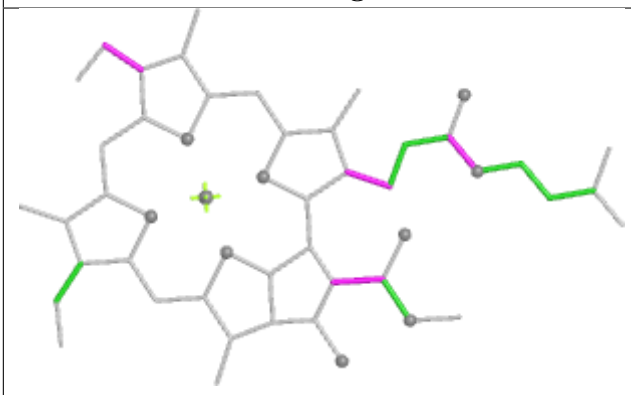

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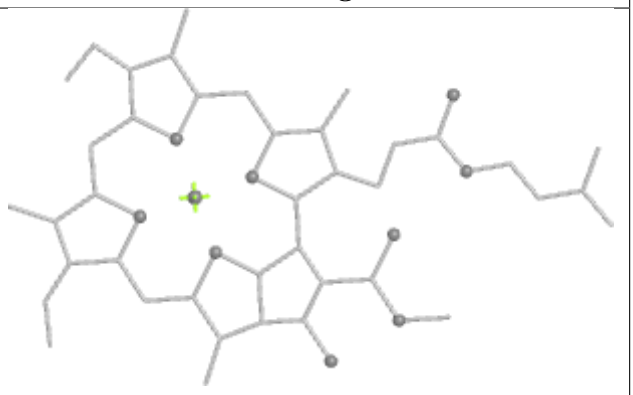
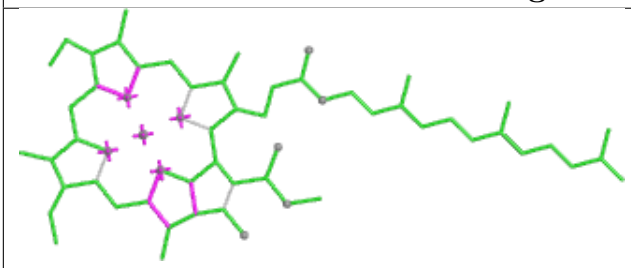


Rings

Ligand CLA a 609



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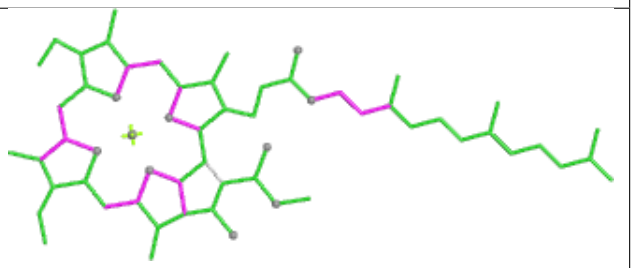

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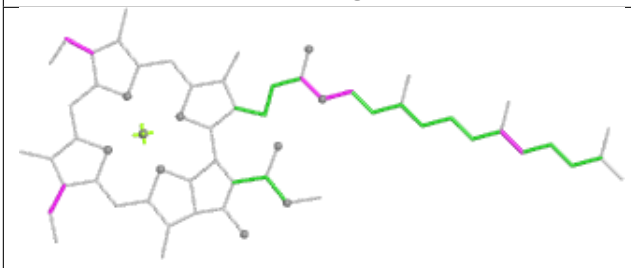

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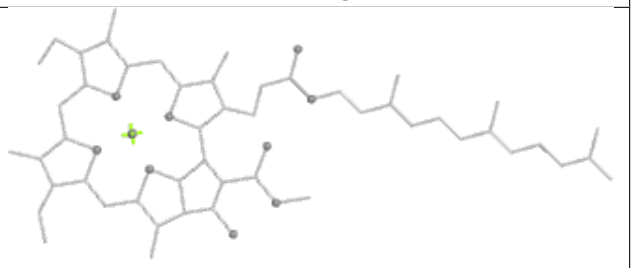
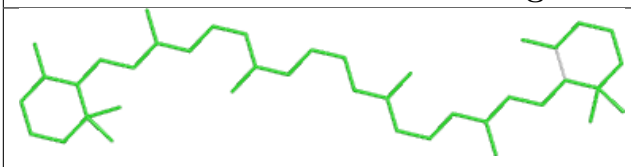


Rings

Ligand 8CT A 845



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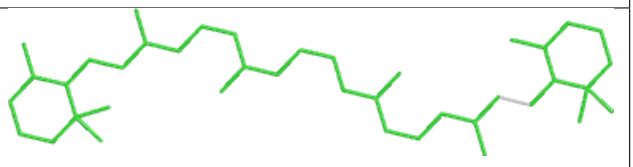

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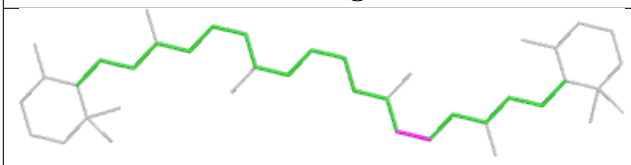

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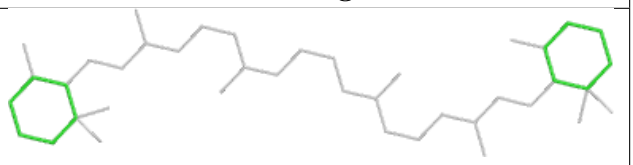
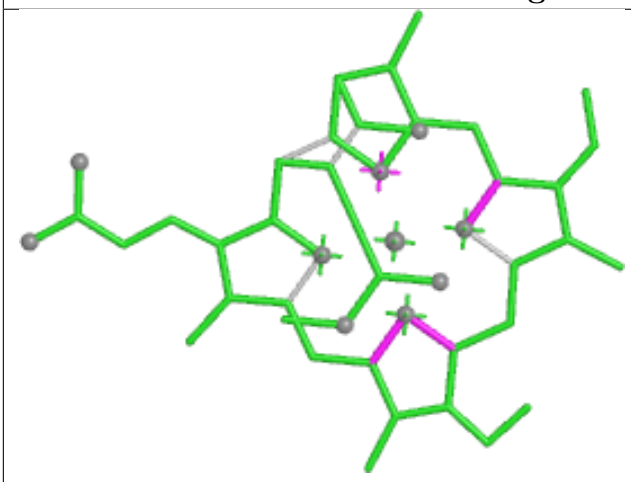


Rings

Ligand KC2 Z 307



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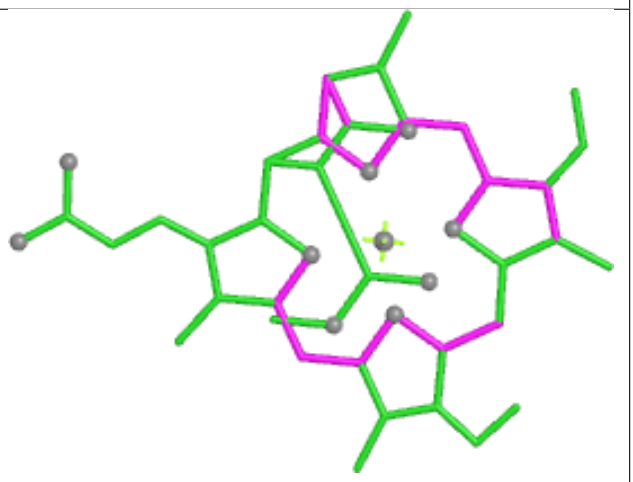

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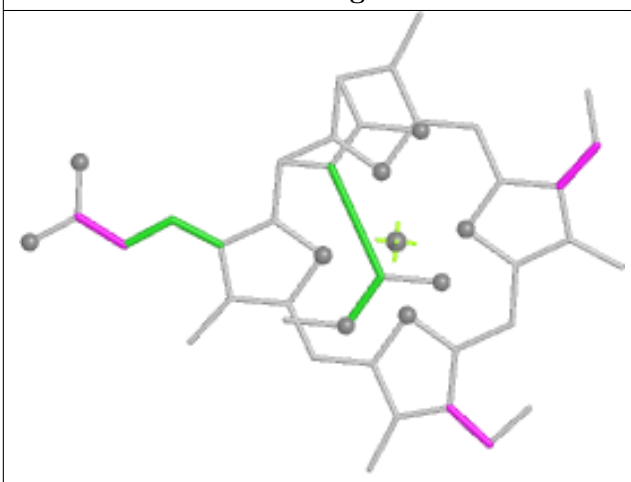

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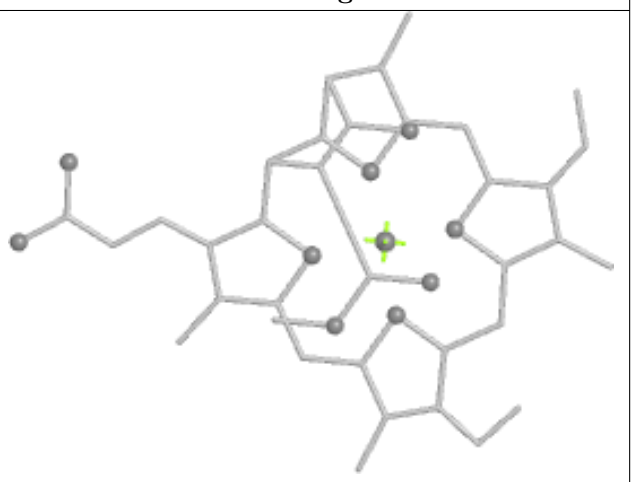

Rings

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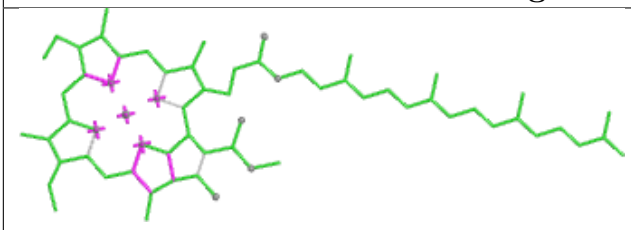
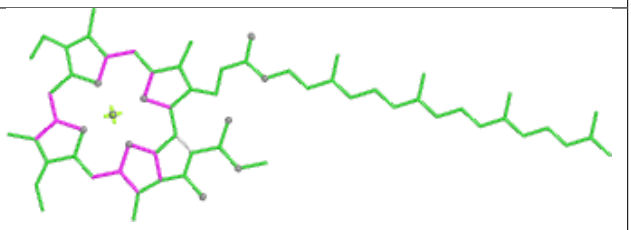
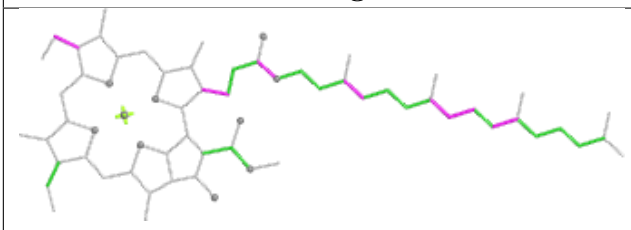
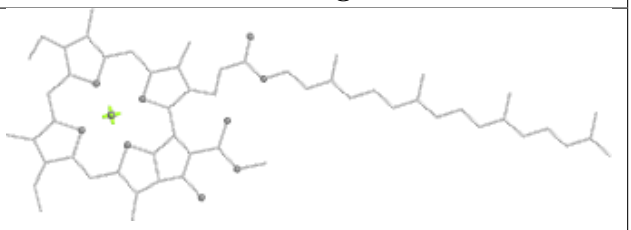
 Bond lengths	 Bond angles
 Torsions	 Rings

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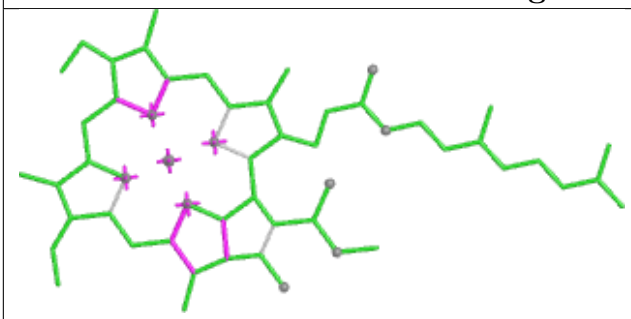
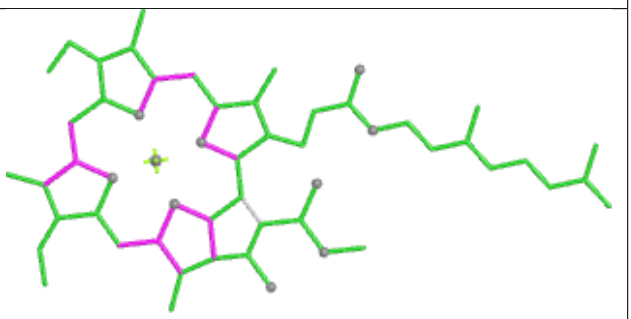
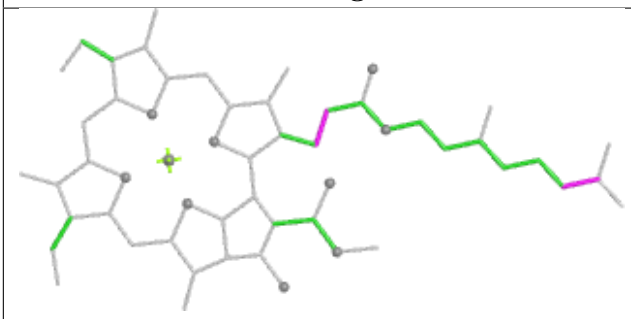
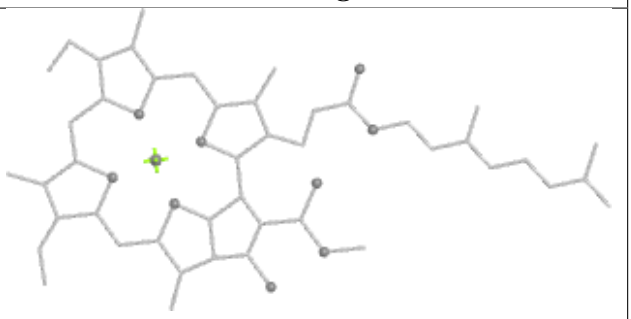
 Bond lengths	 Bond angles
 Torsions	 Rings

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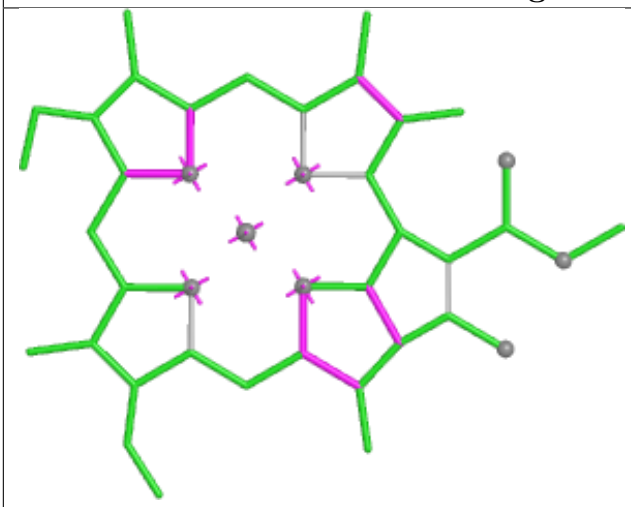

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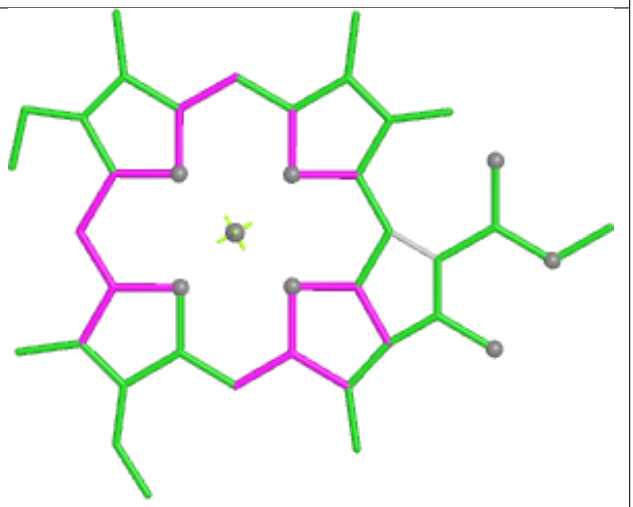

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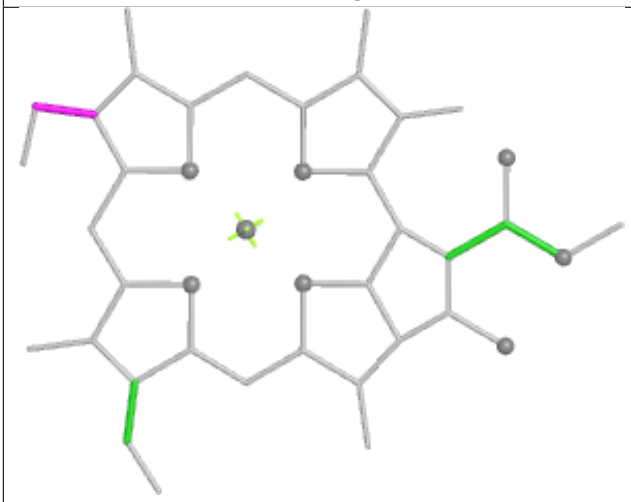

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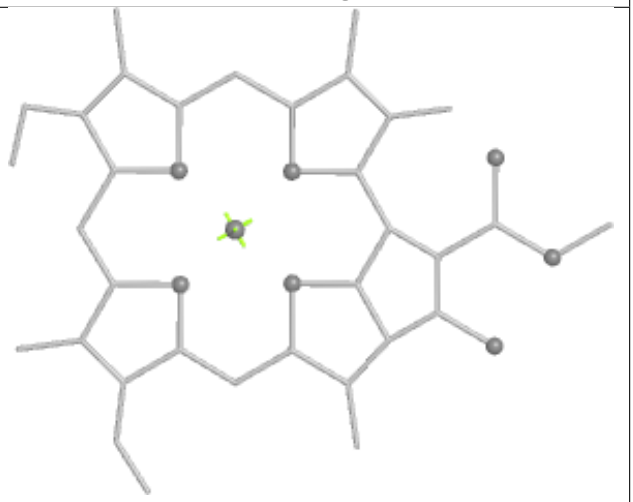
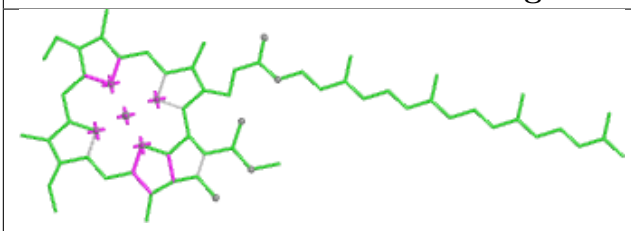


Rings

Ligand CLA B 828



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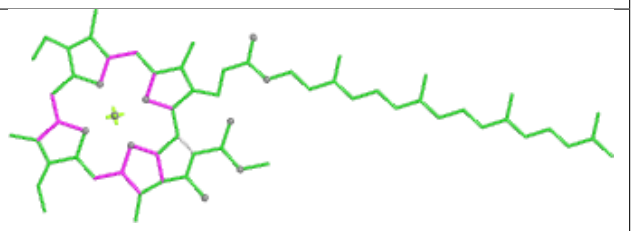

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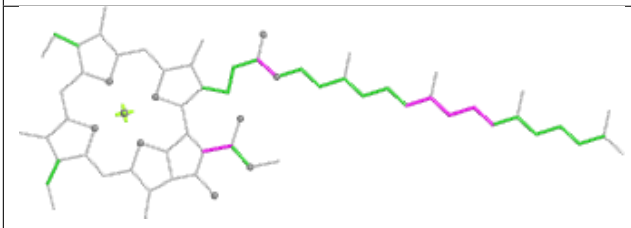

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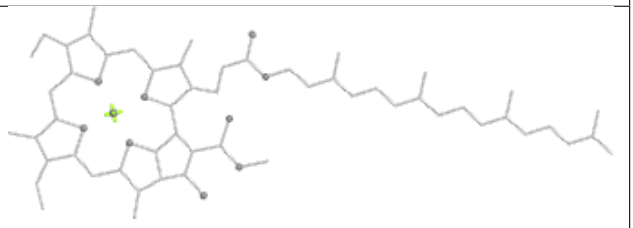
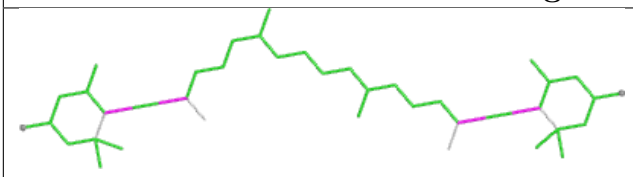


Rings

Ligand II0 c 619



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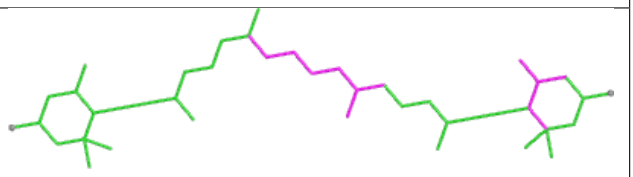

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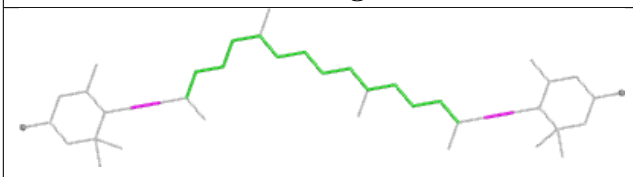

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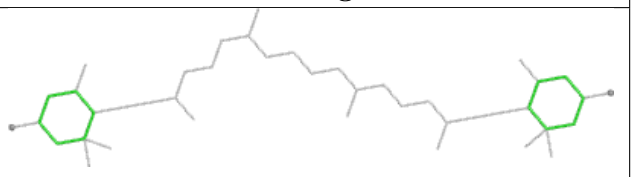
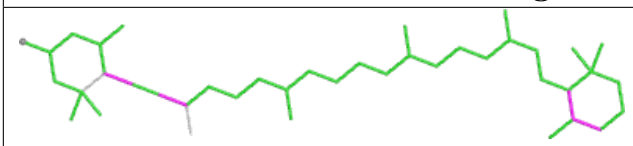


Rings

Ligand IHT 8 609



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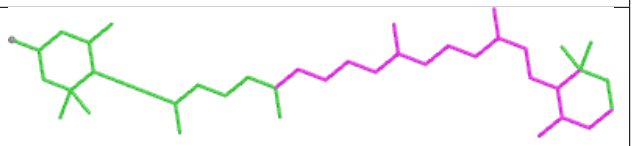


Bond angles

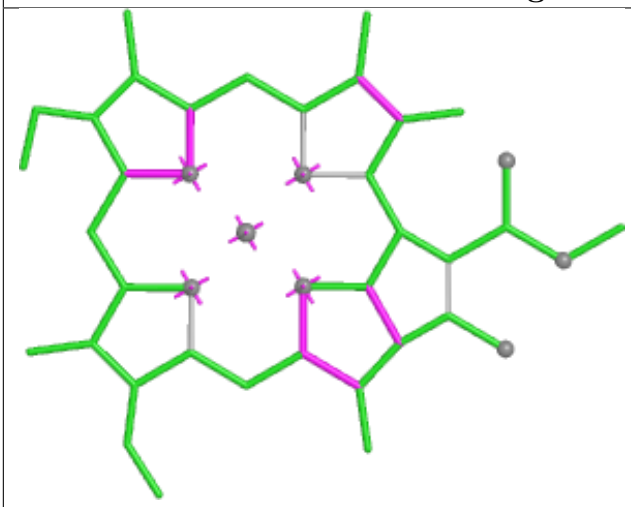


Torsions



Rings

Ligand CLA d 606



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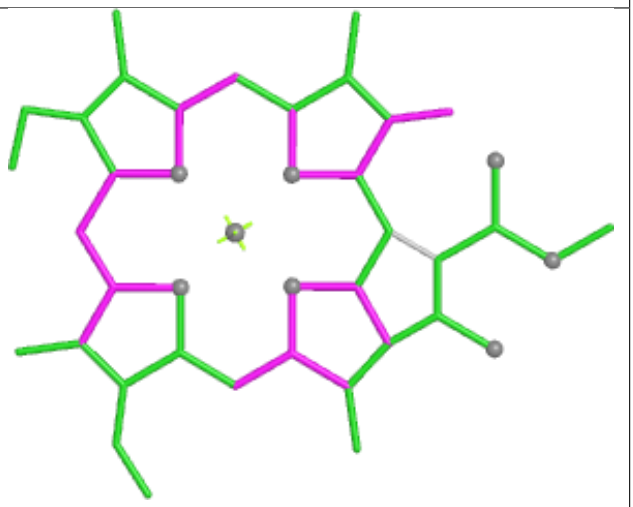
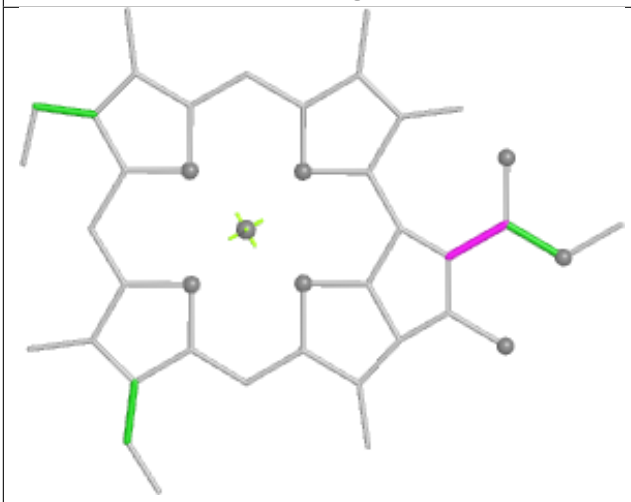


Bond angles



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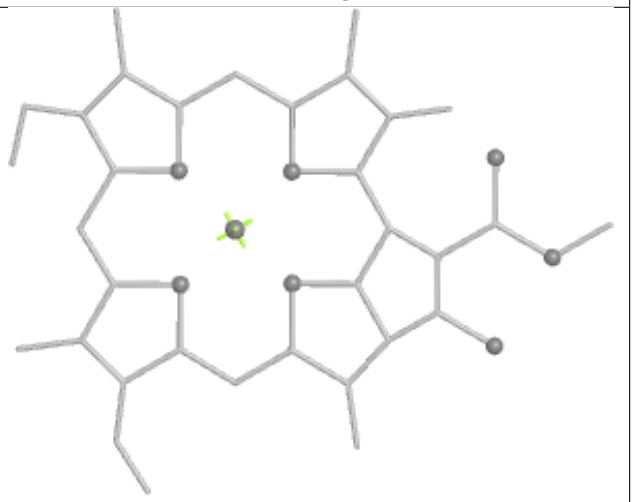
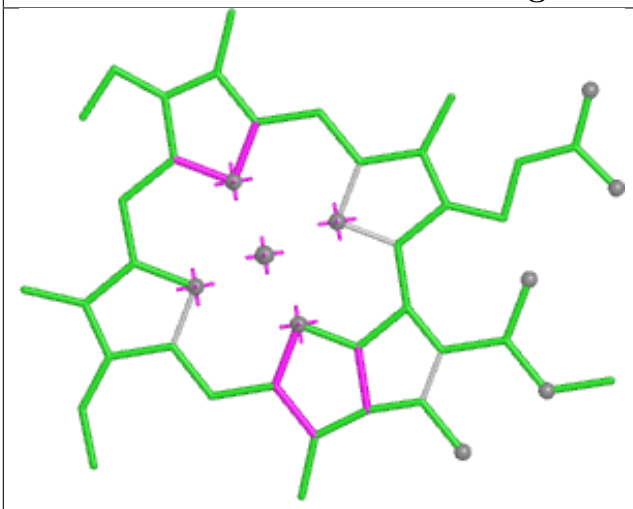


Rings

Ligand CLA 6 601



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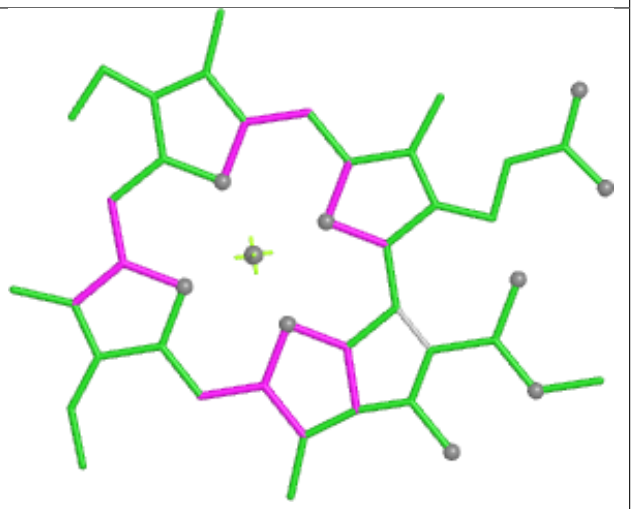

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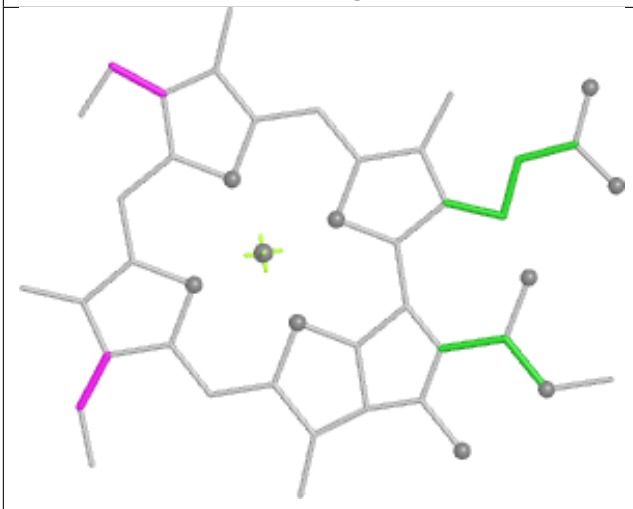
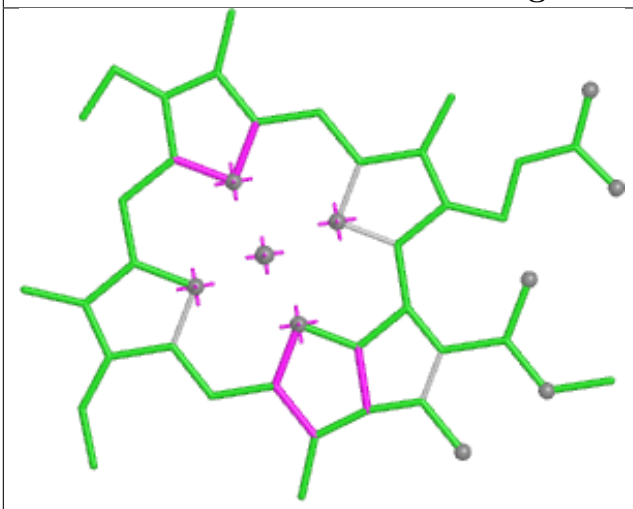


Torsions



Rings

Ligand CLA 3 612



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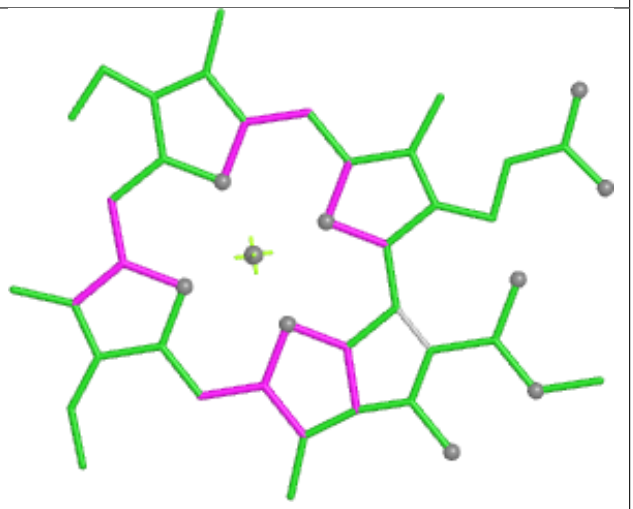
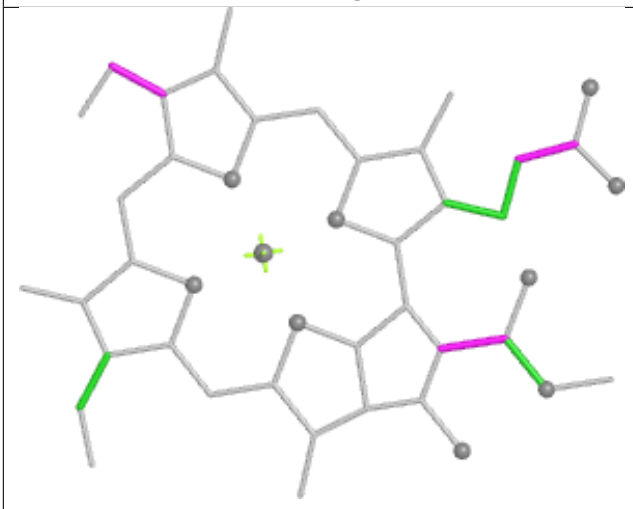


Bond angles



Torsions

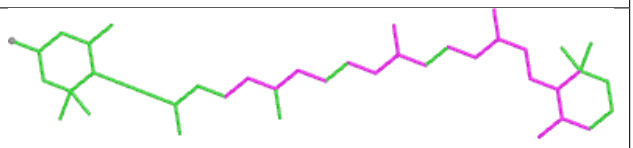


Rings

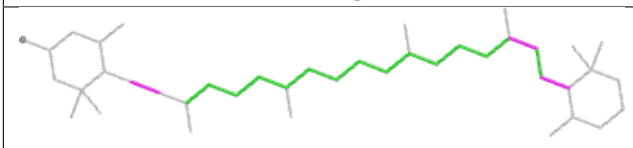
Ligand IHT 9 619



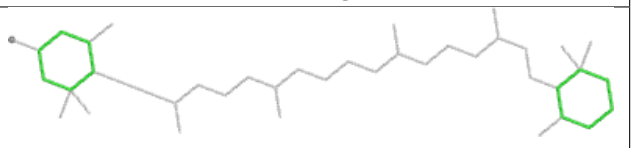
Bond lengths



Bond angles

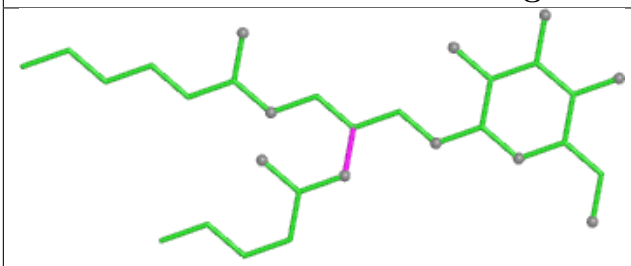


Torsions



Rings

Ligand LMG 3 618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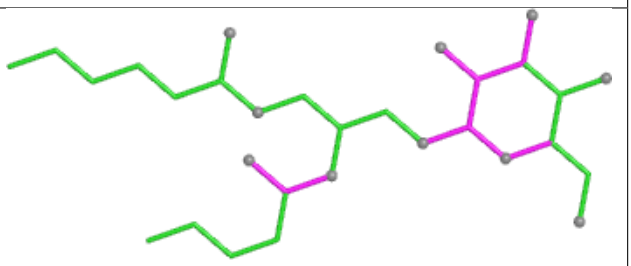
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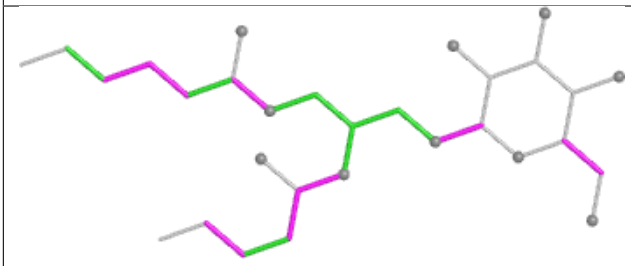
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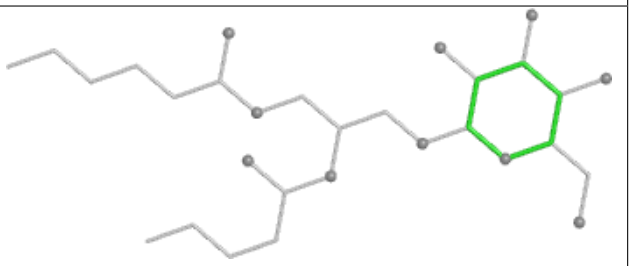
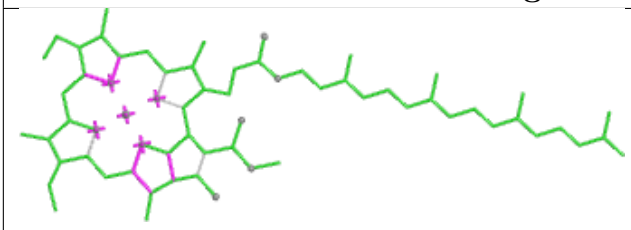

Rings

Ligand CLA A 831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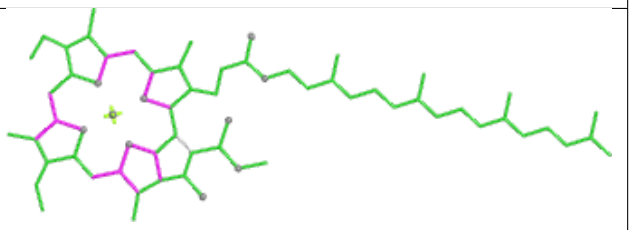
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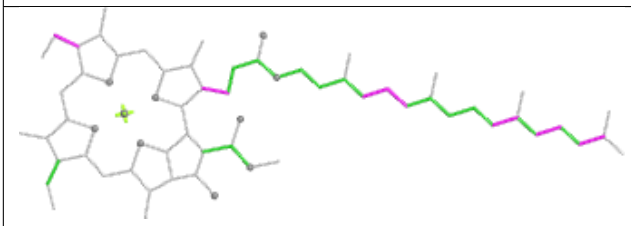
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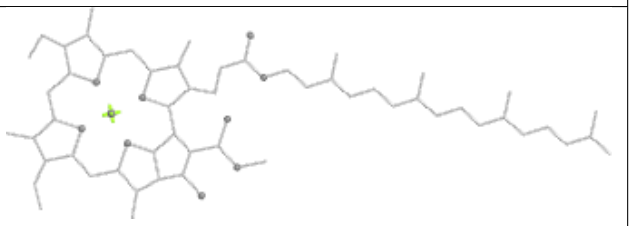
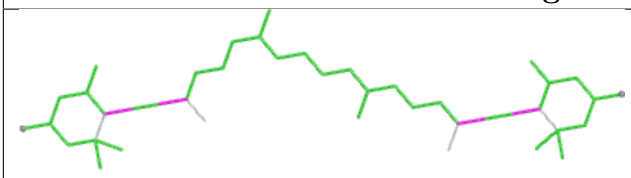

Rings

Ligand II0 3 616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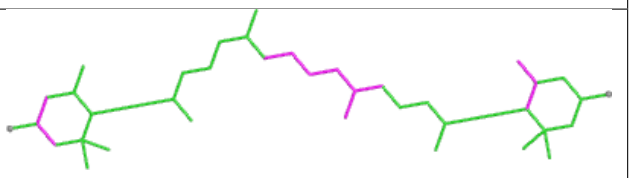
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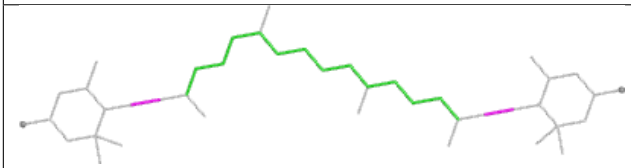
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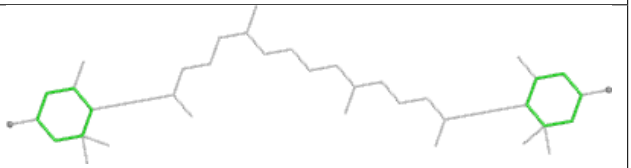
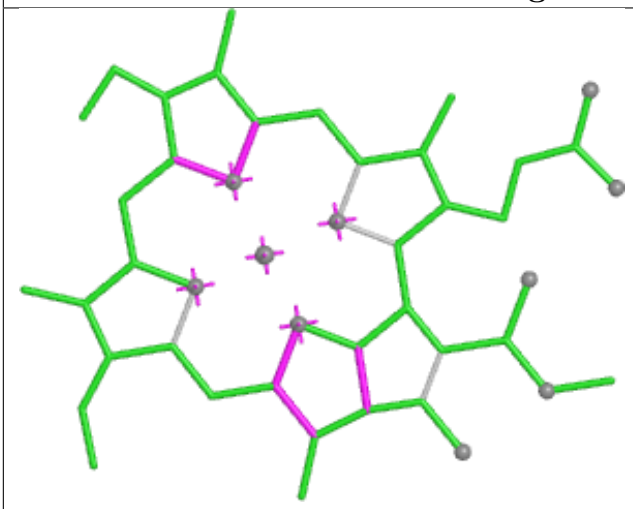

Rings

Ligand CLA 8 601



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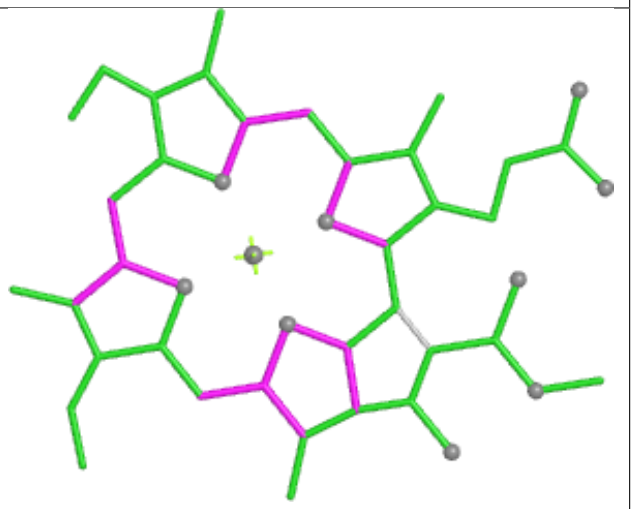

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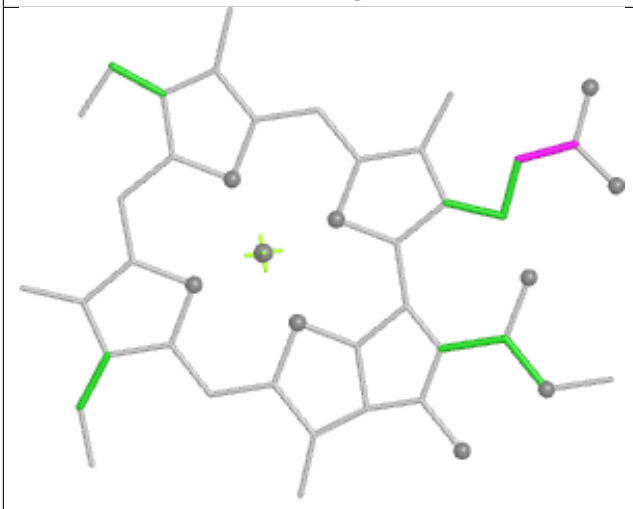
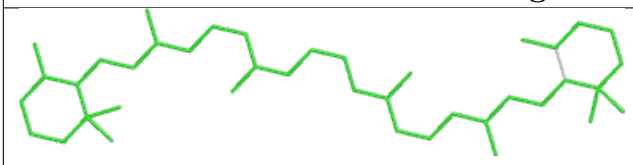


Torsions



Rings

Ligand 8CT Z 308



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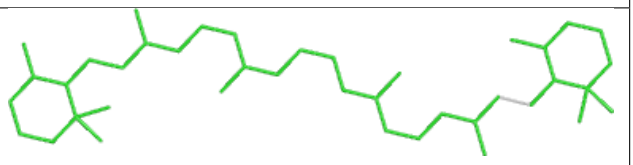

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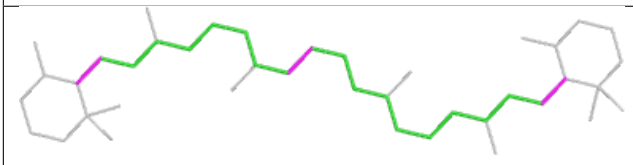

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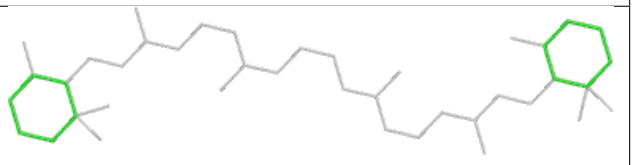
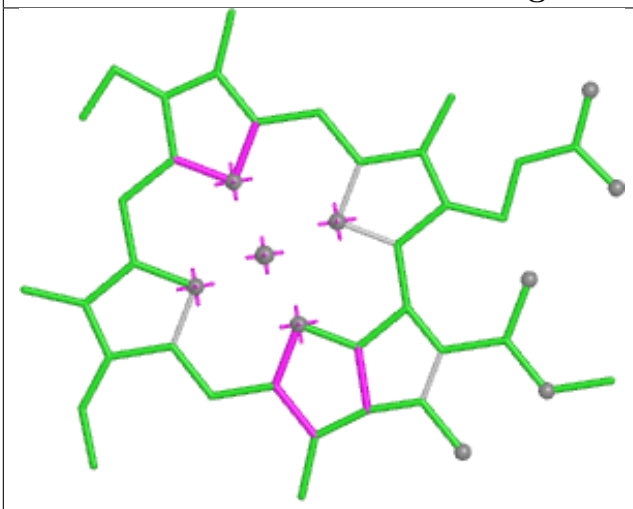


Rings

Ligand CLA 1 611



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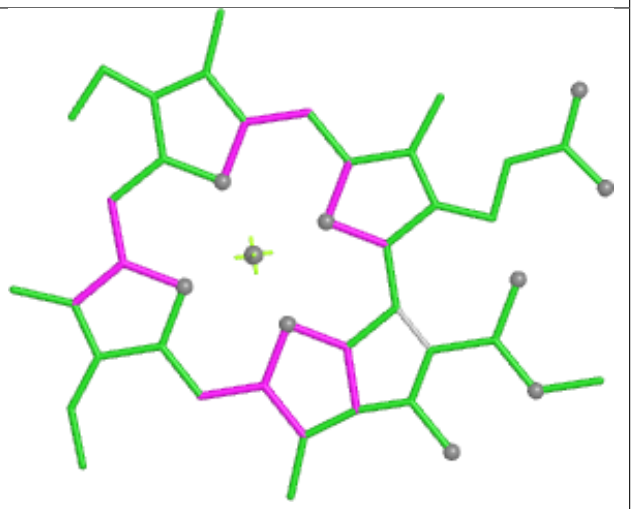

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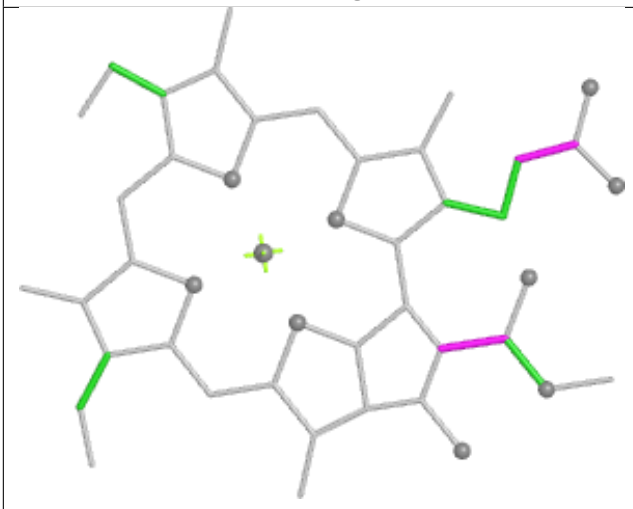
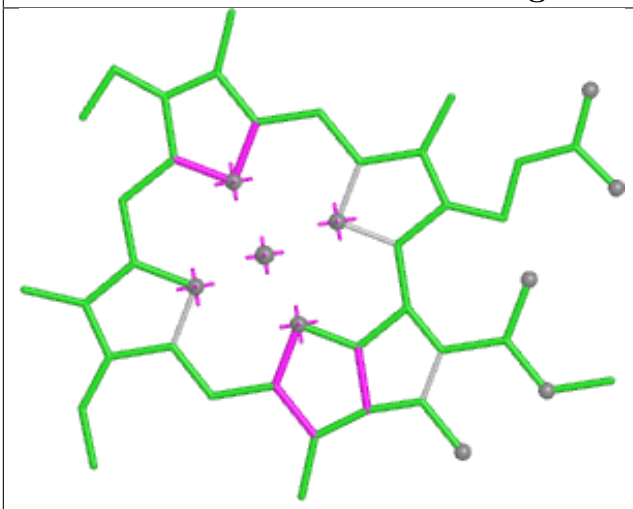


Torsions



Rings

Ligand CLA 5 603



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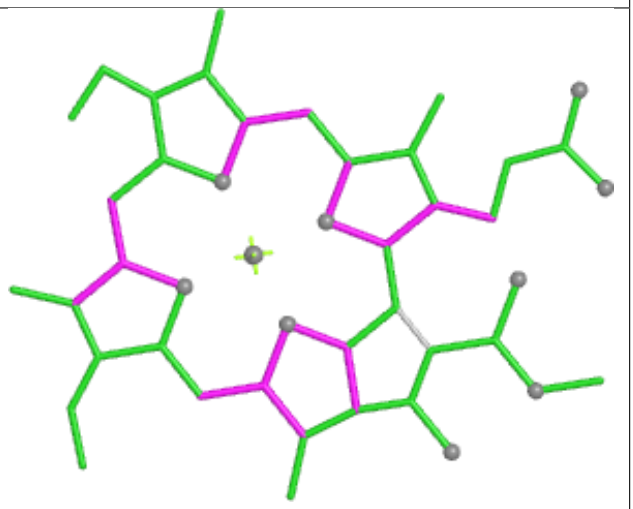

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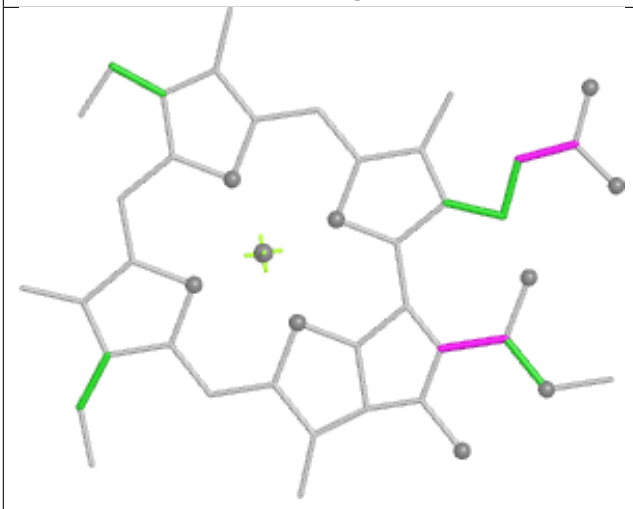
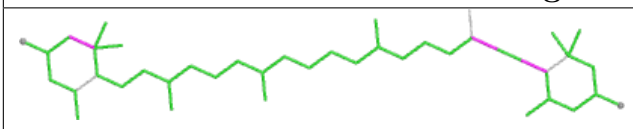


Torsions



Rings

Ligand II3 e 613



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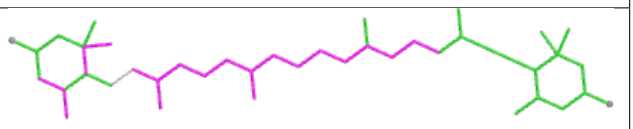
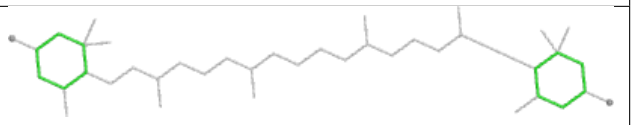


Bond angles

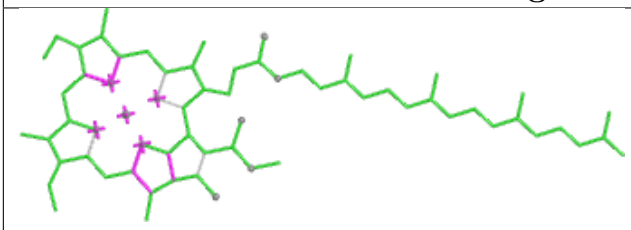


Torsions



Rings

Ligand CLA 4 610



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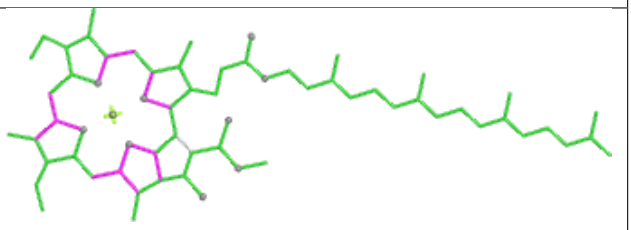
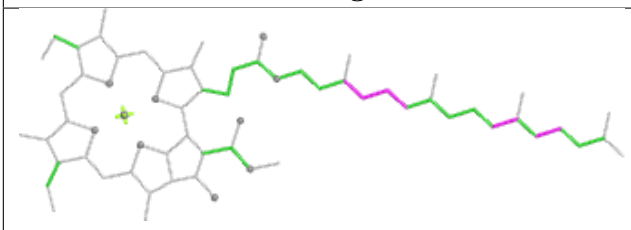


Bond angles



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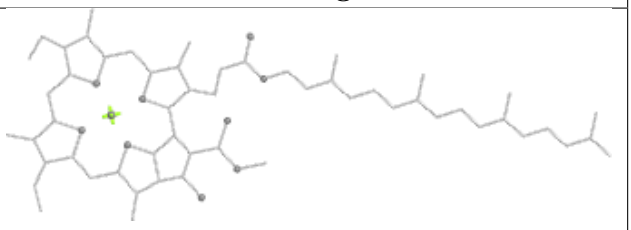
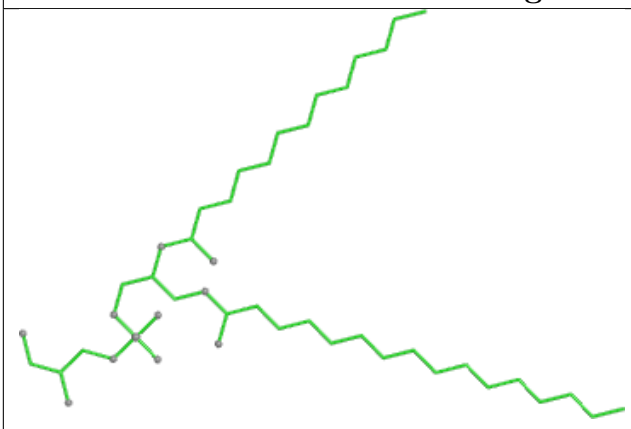


Rings

Ligand LHG Z 310



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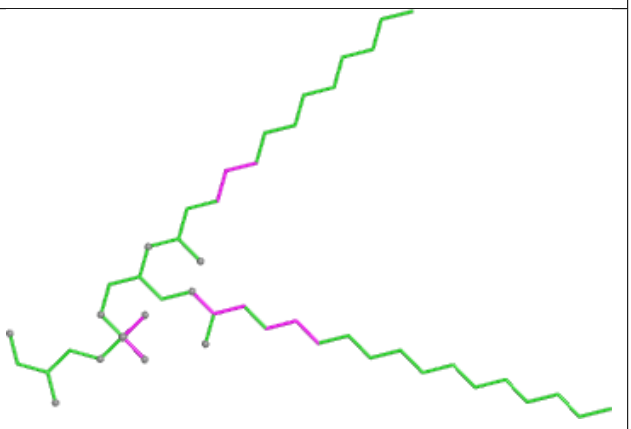

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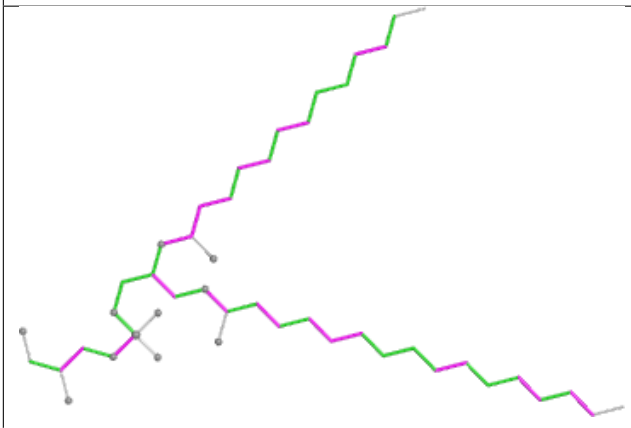

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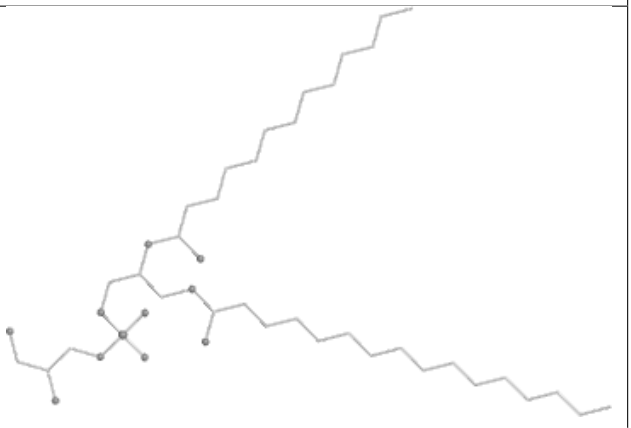
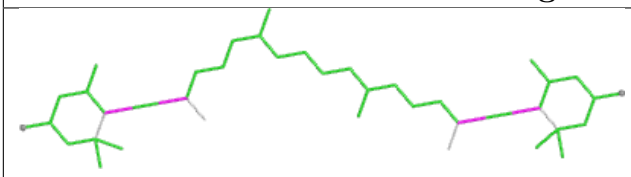


Rings

Ligand II0 R 204



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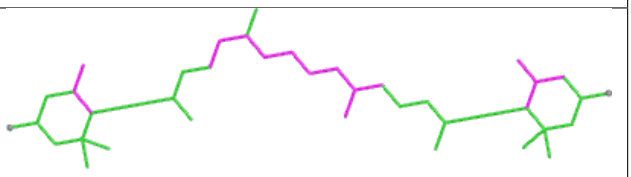

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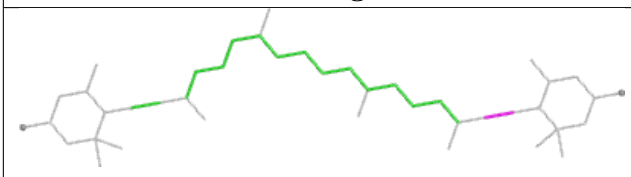

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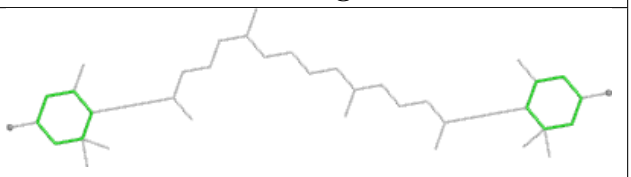
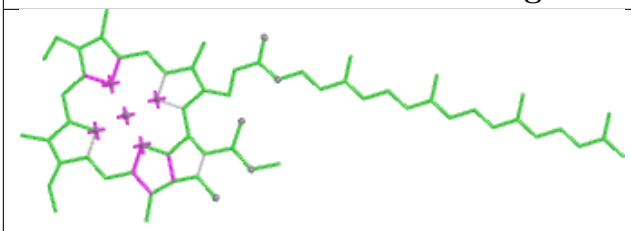


Rings

Ligand CLA B 835



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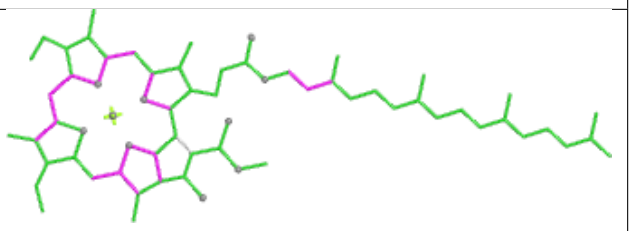
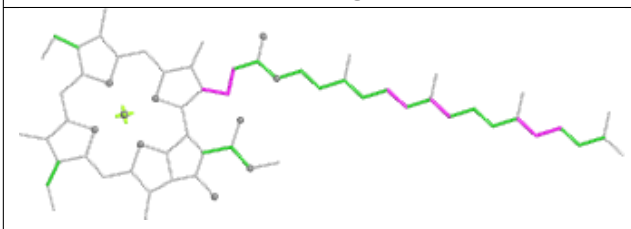


Bond angles



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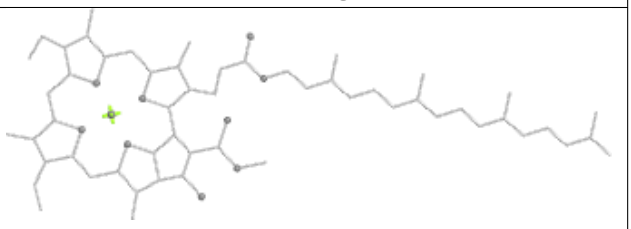
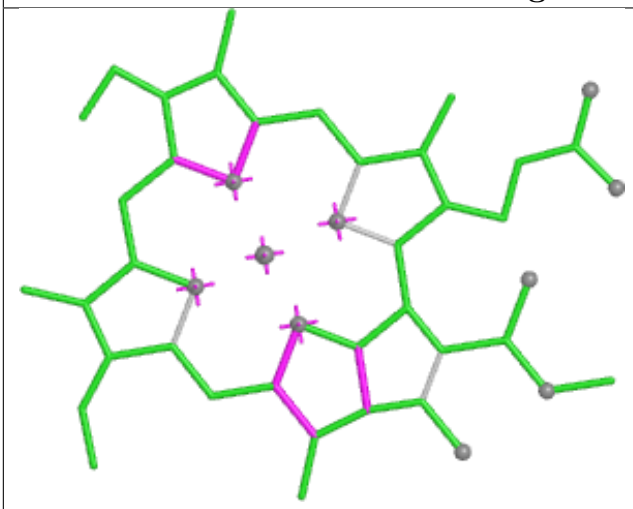


Rings

Ligand CLA 3 601



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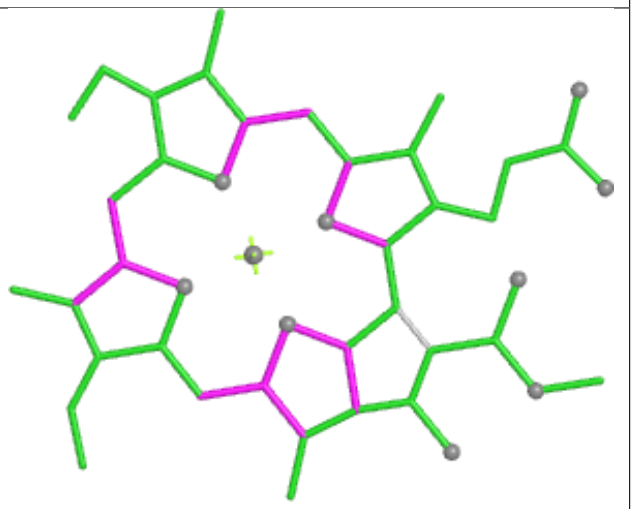

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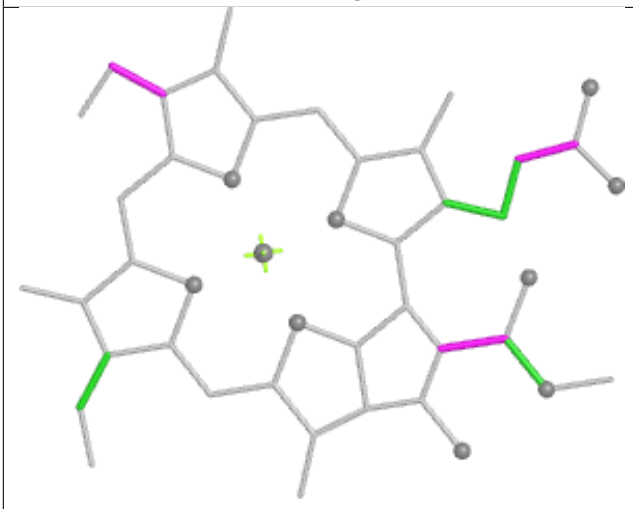
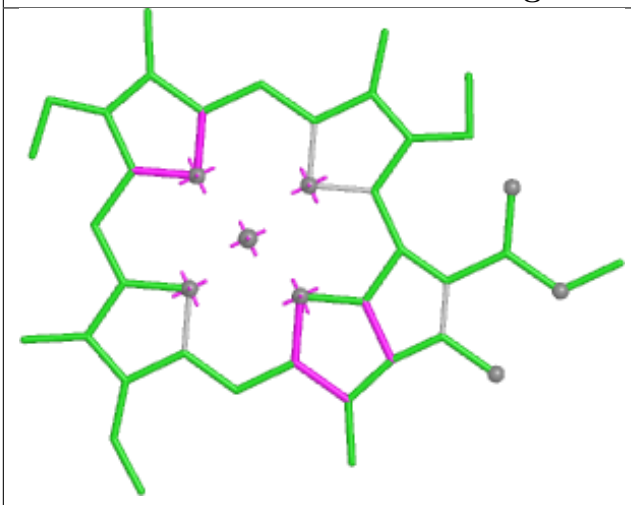


Torsions



Rings

Ligand CLA A 813



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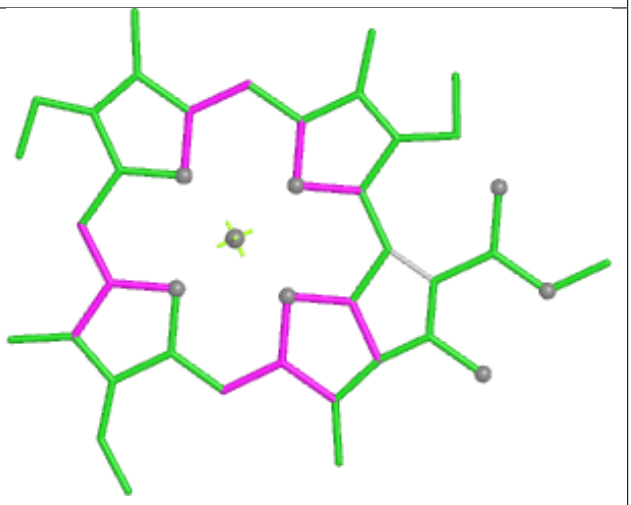
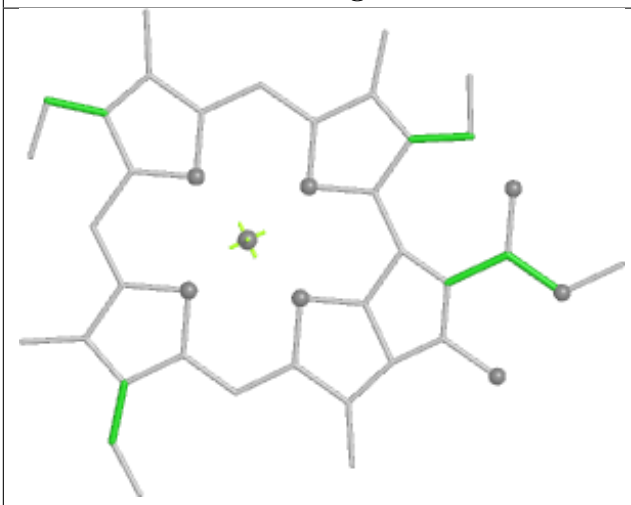


Bond angles

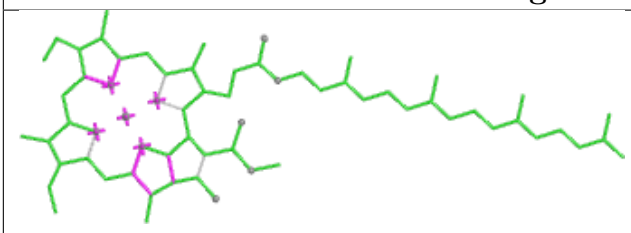


Torsions



Rings

Ligand CLA c 606



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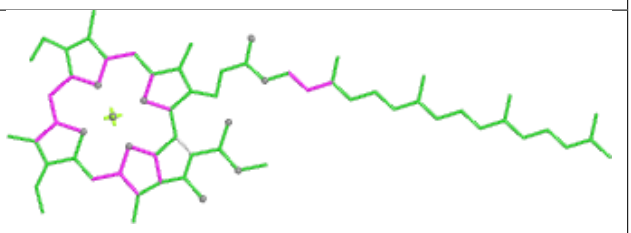
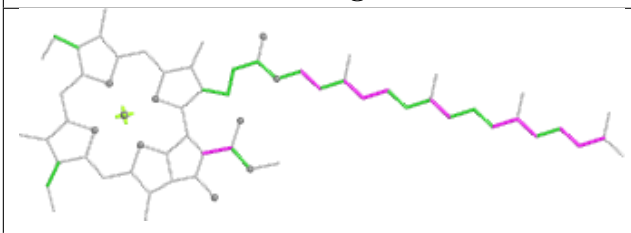


Bond angles



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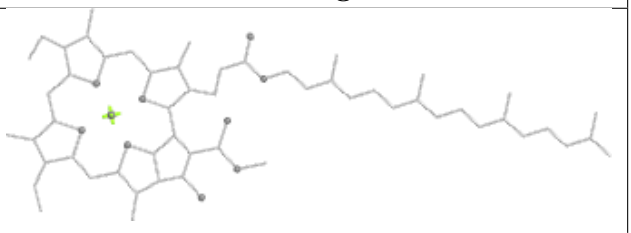
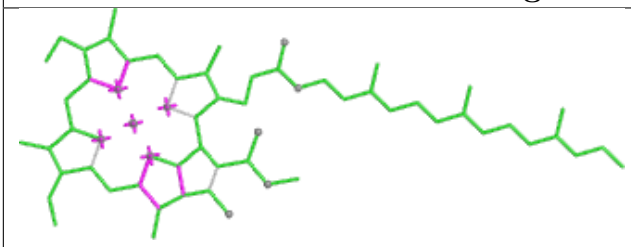


Rings

Ligand CLA A 815



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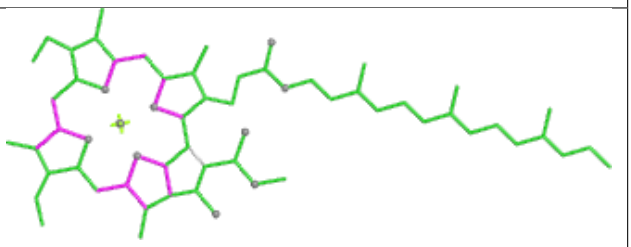
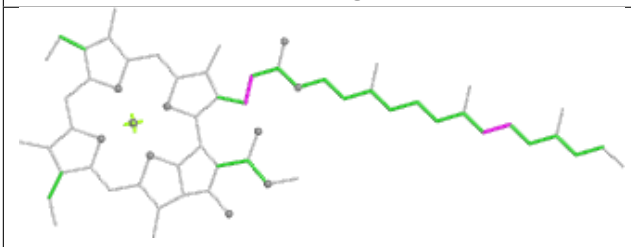
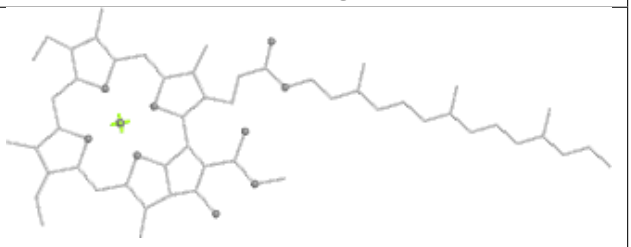


Bond angles

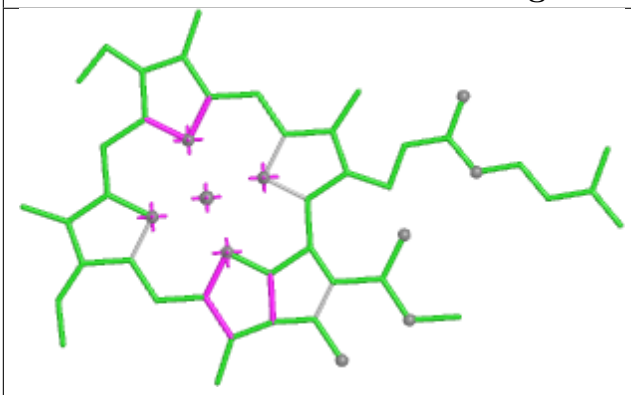


Torsions

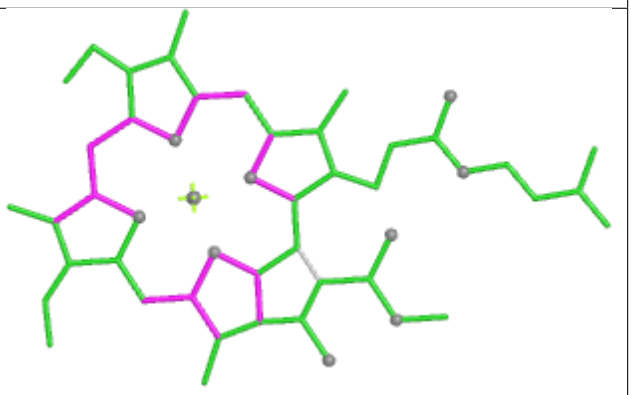


Rings

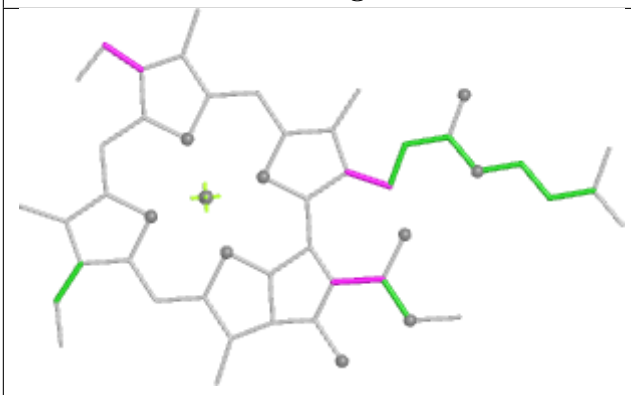
Ligand CLA 3 611



Bond lengths



Bond angles



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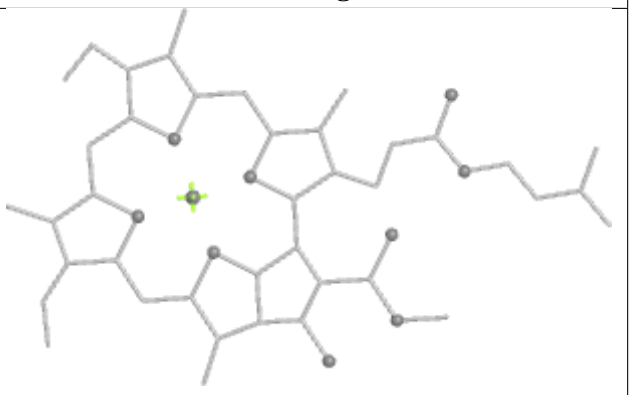
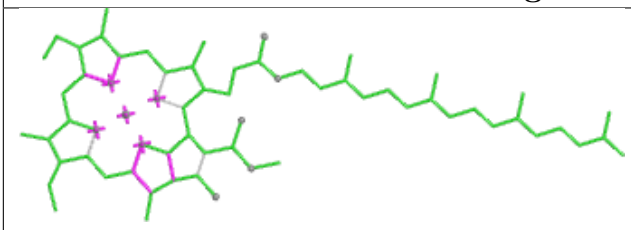


Rings

Ligand CLA B 826



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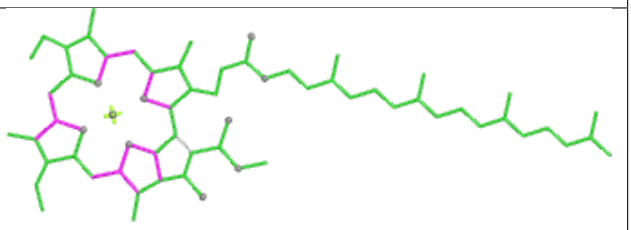
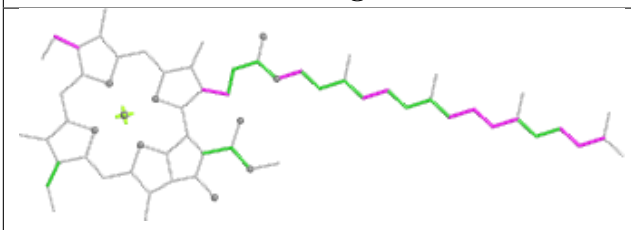


Bond angles



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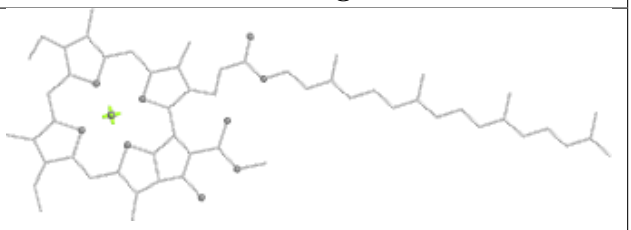
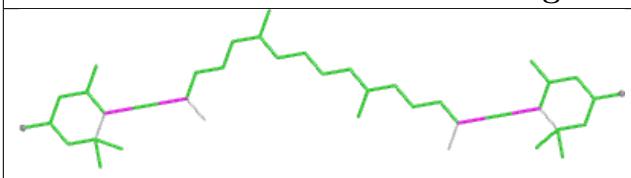


Rings

Ligand II0 4 613



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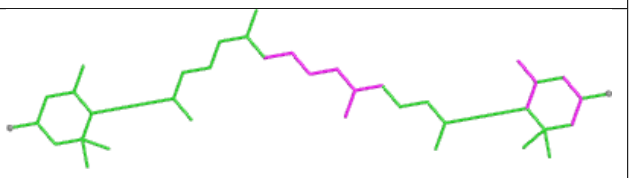
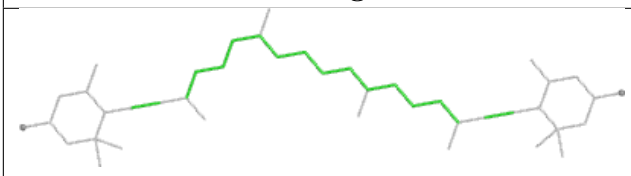


Bond angles



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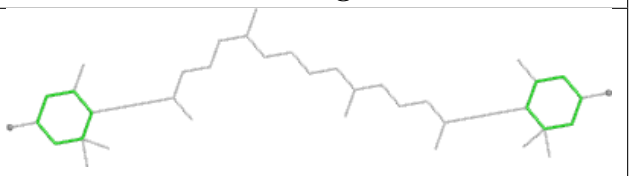
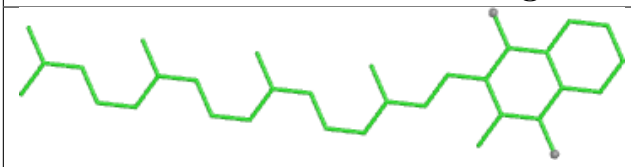


Rings

Ligand PQN A 849



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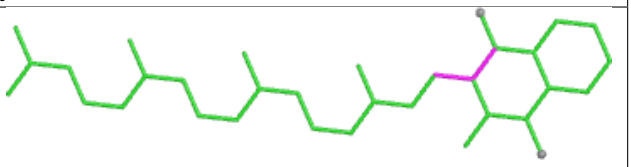
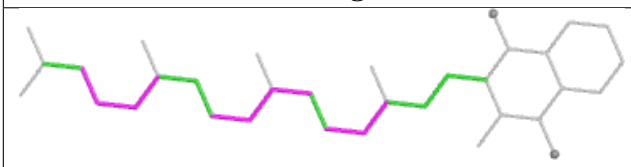
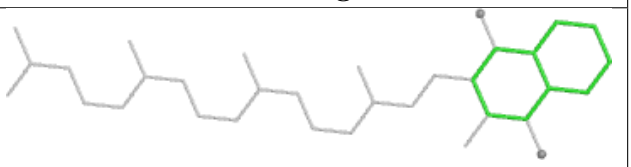


Bond angles



Torsions

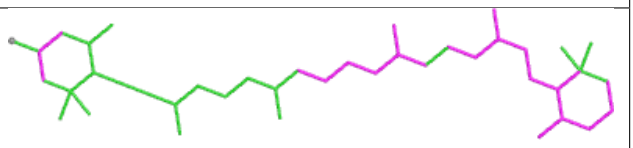


Rings

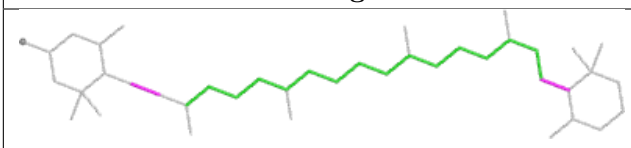
Ligand IHT Z 302



Bond lengths



Bond angles



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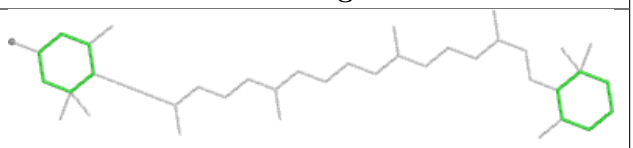
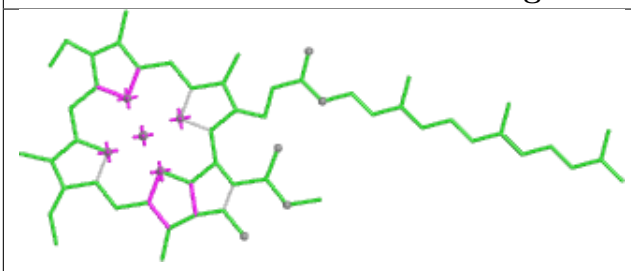


Rings

Ligand CLA A 816



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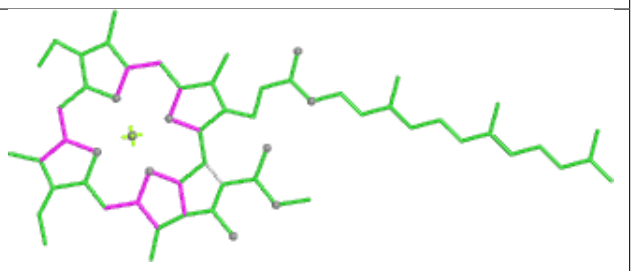
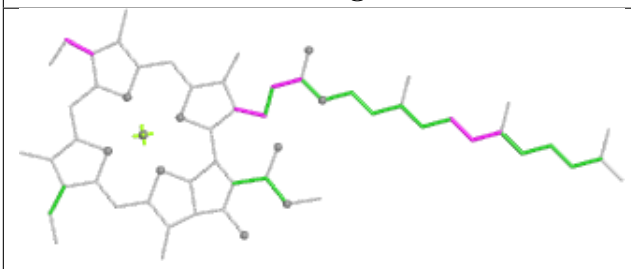


Bond angles



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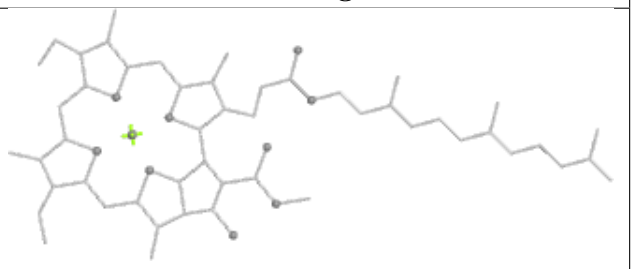
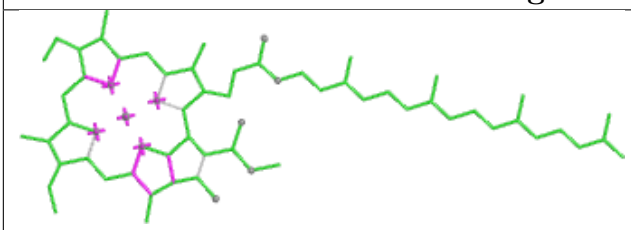


Rings

Ligand CLA b 604



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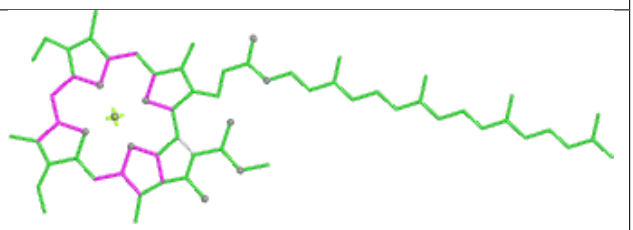
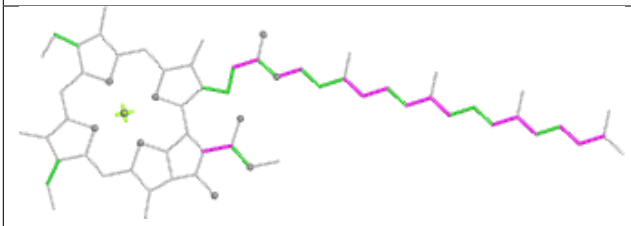


Bond angles



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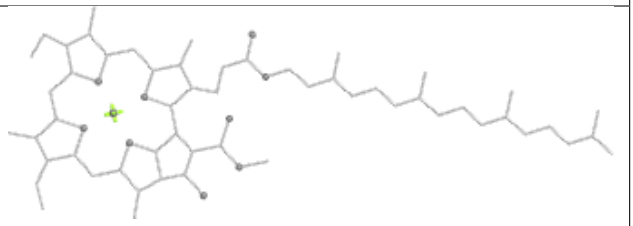
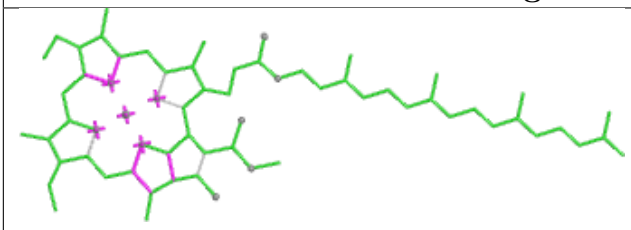


Rings

Ligand CLA A 838



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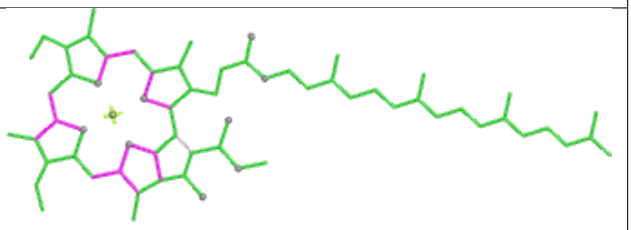
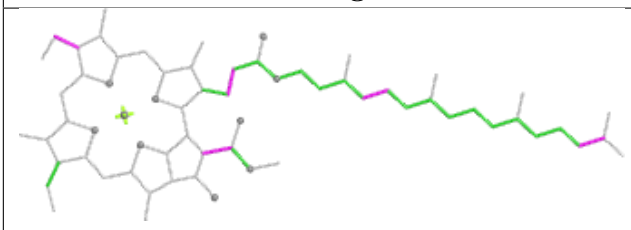


Bond angles



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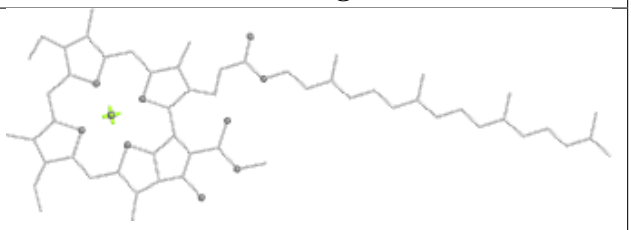
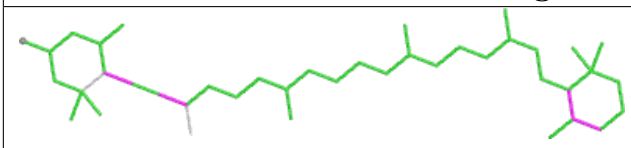
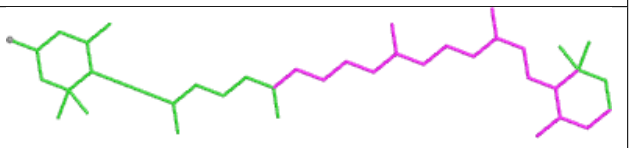


Rings

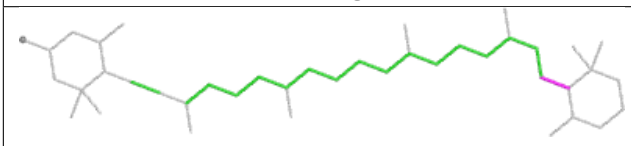
Ligand IHT c 620



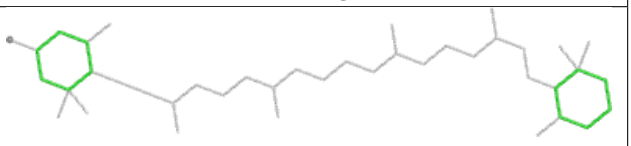
Bond lengths



Bond angles

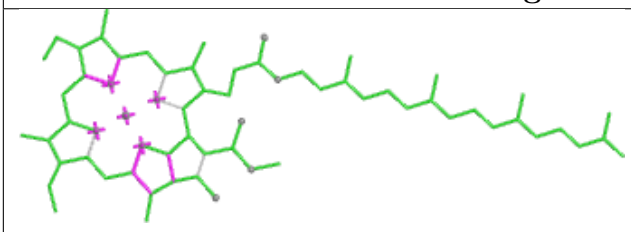


Torsions



Rings

Ligand CLA A 810



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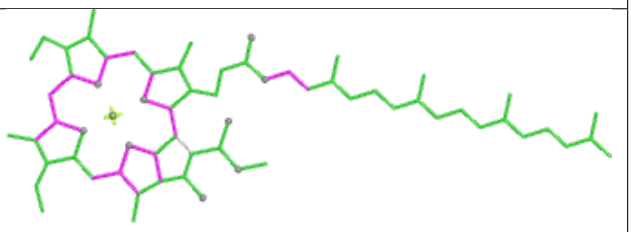
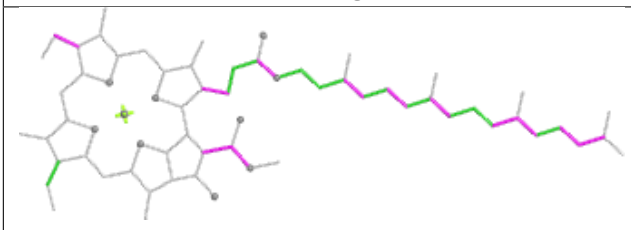


Bond angles



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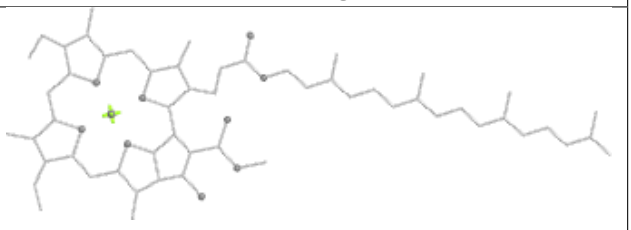
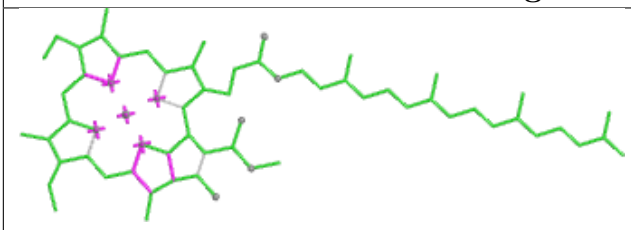


Rings

Ligand CLA B 837



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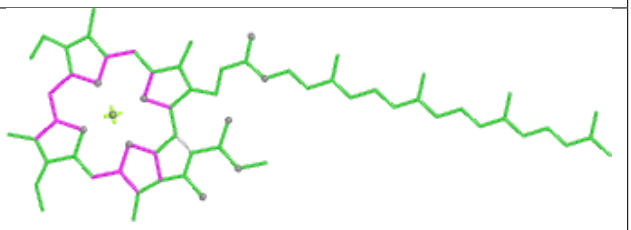
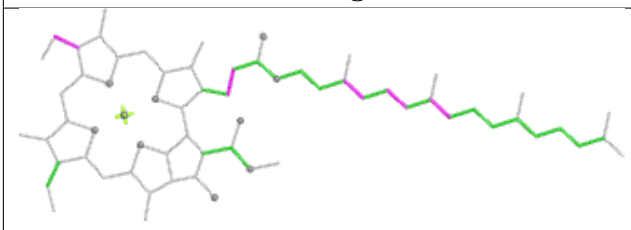


Bond angles



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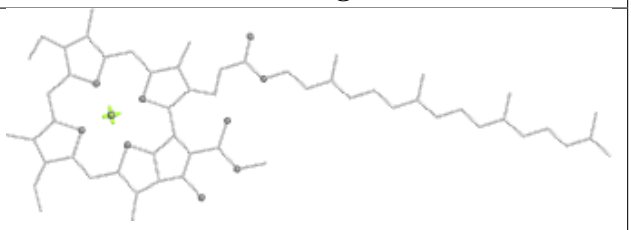
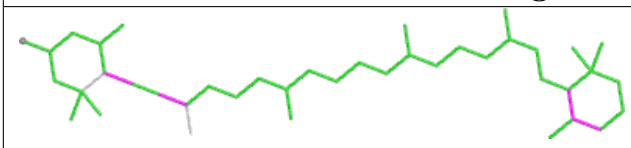


Rings

Ligand IHT L 205



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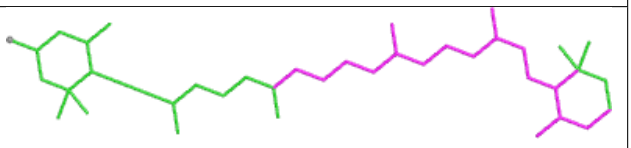
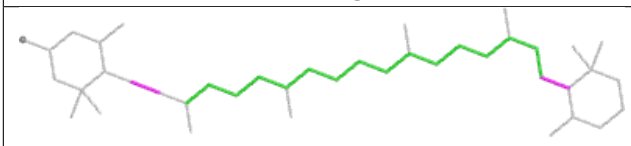


Bond angles



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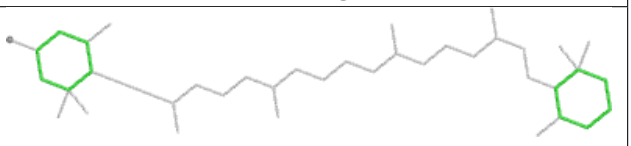
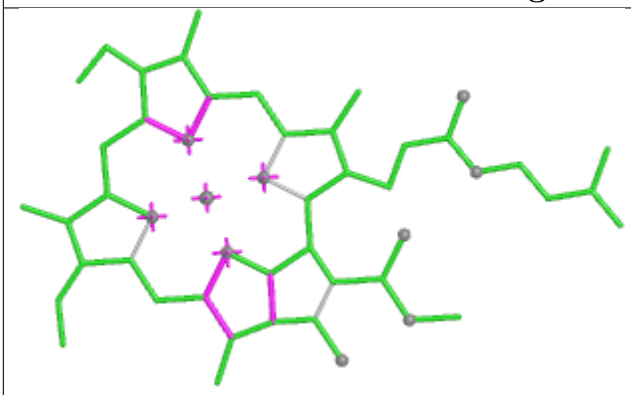
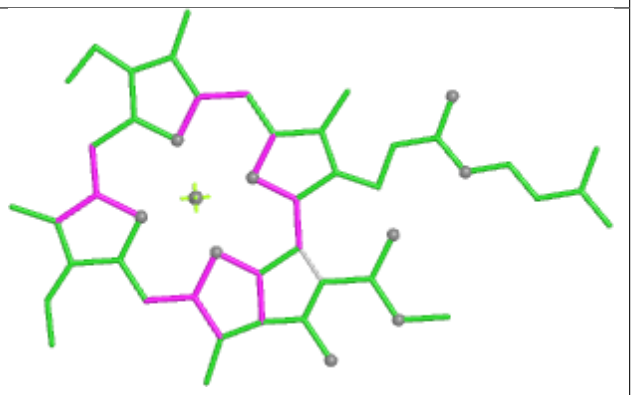


Rings

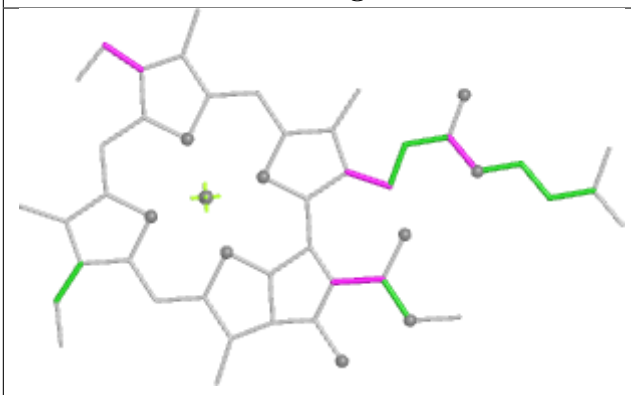
Ligand CLA 7 612



Bond lengths



Bond angles



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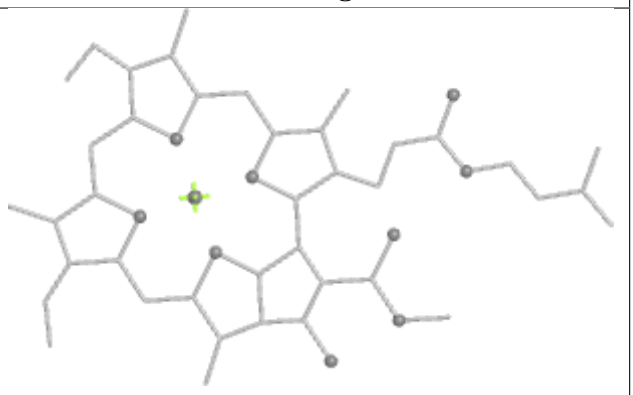
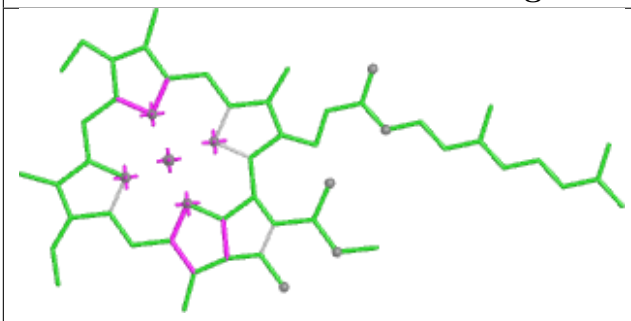
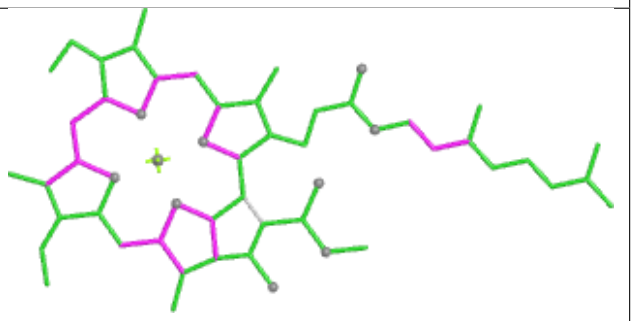


Rings

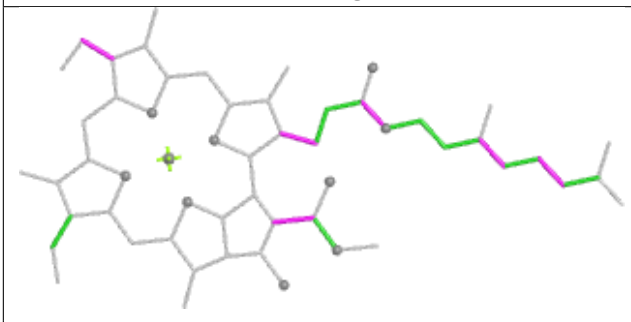
Ligand CLA B 831



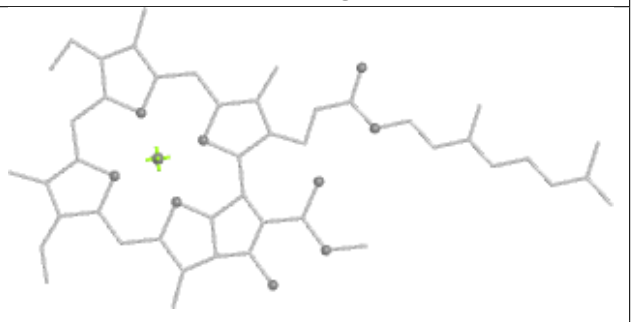
Bond lengths



Bond angles

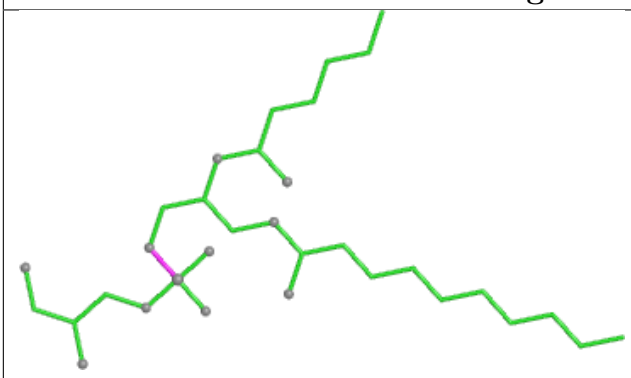


Torsions

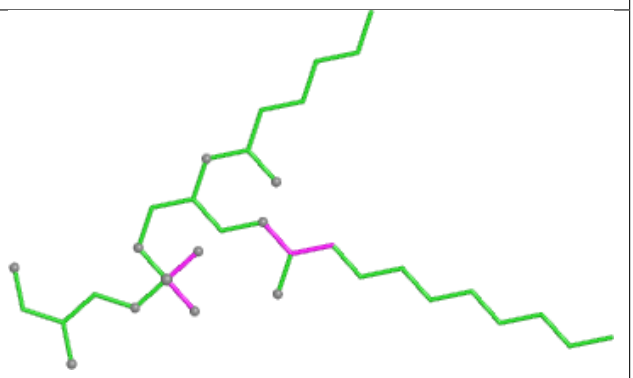


Rings

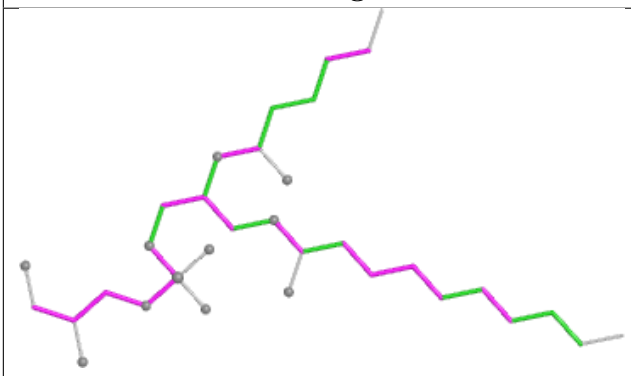
Ligand LHG 8 613



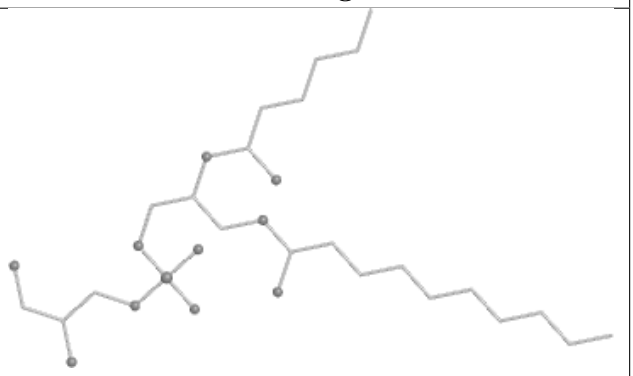
Bond lengths



Bond angles

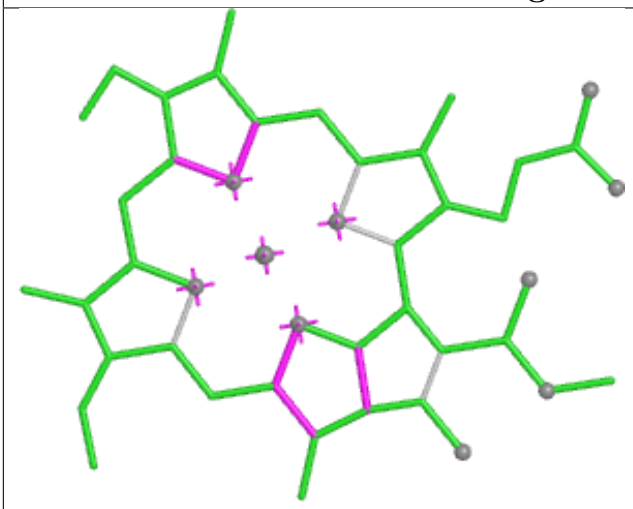


Torsions



Rings

Ligand CLA 1 613



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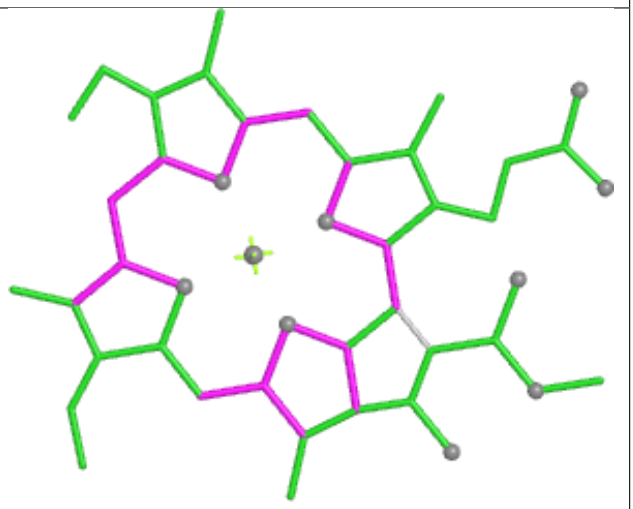
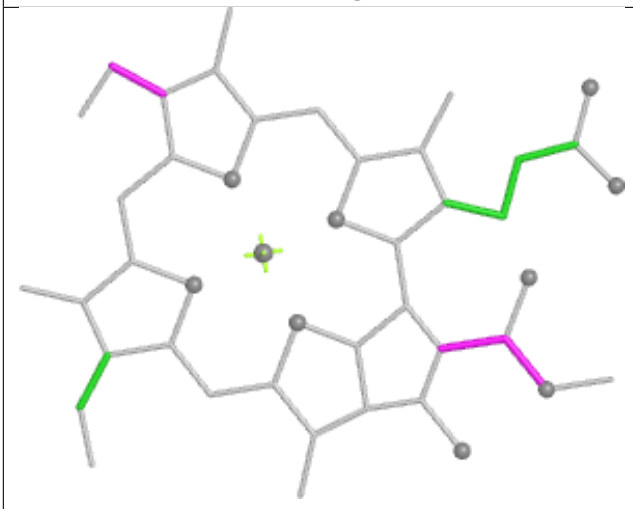


Bond angles

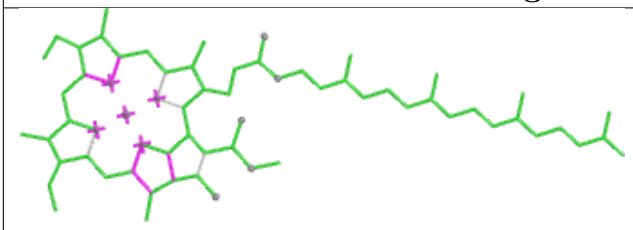


Torsions



Rings

Ligand CLA A 804



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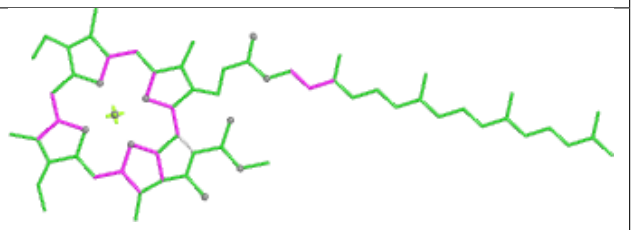
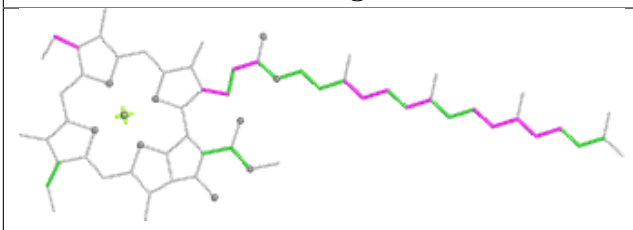


Bond angles



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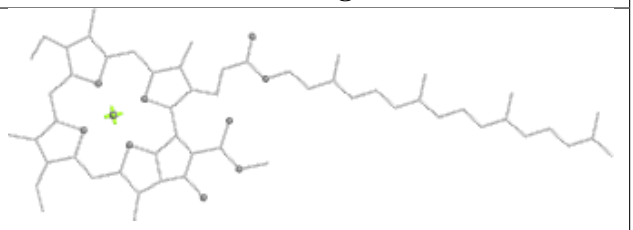
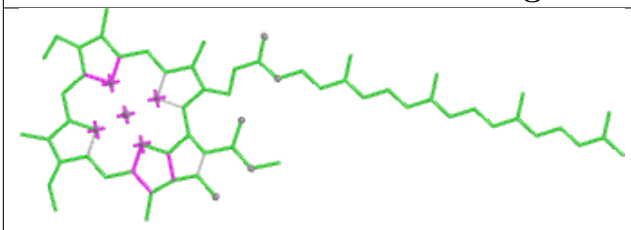


Rings

Ligand CLA A 832



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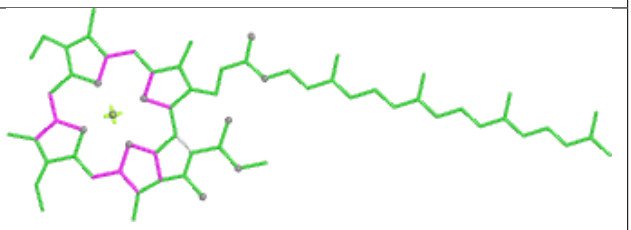
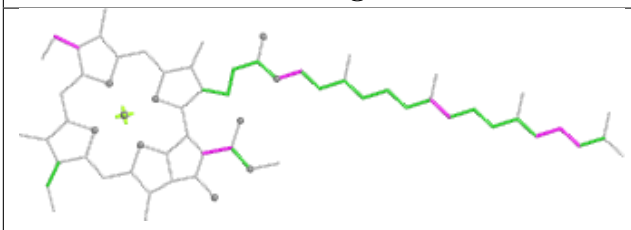


Bond angles



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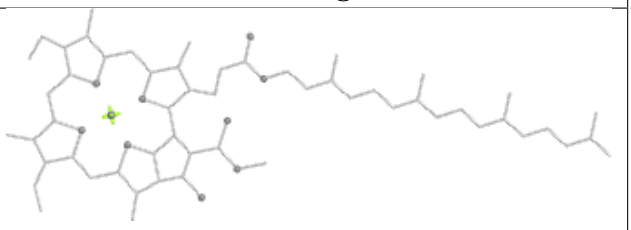
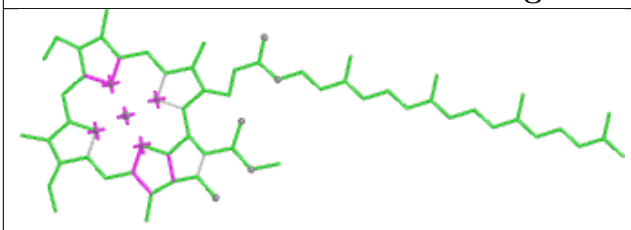


Rings

Ligand CLA B 806



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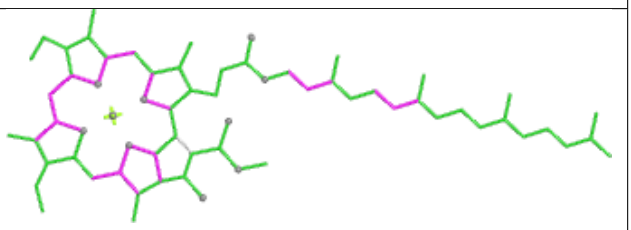
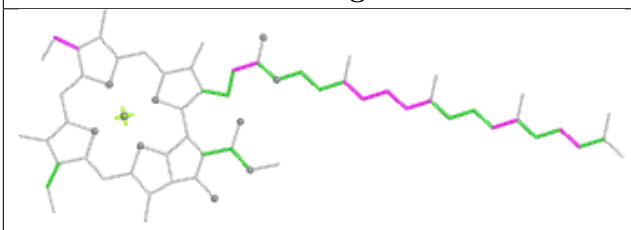


Bond angles



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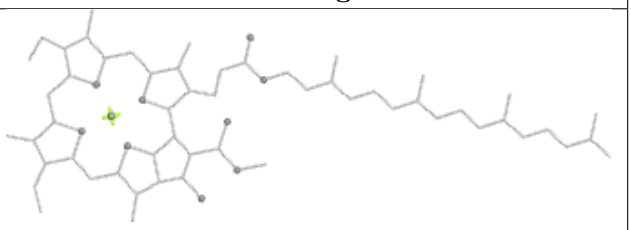
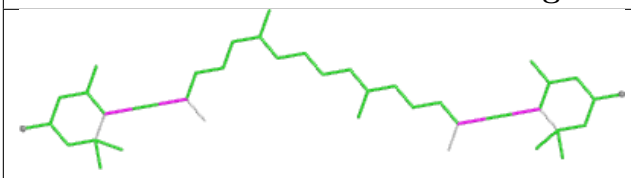


Rings

Ligand II0 5 620



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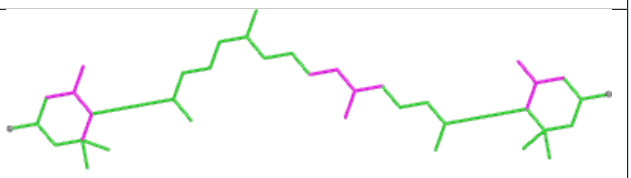
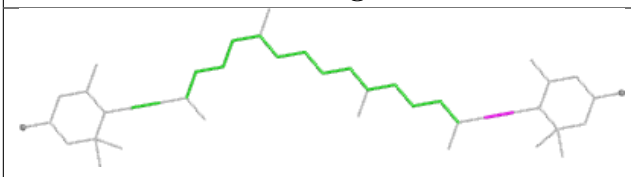


Bond angles



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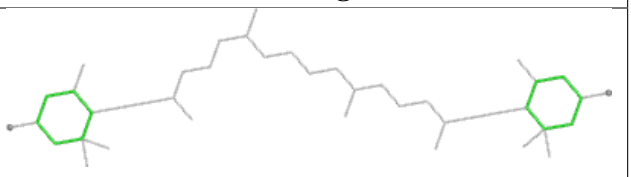
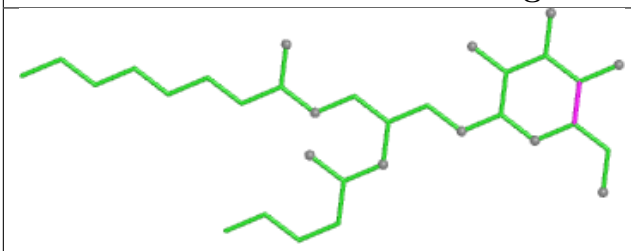


Rings

Ligand LMG 6 619



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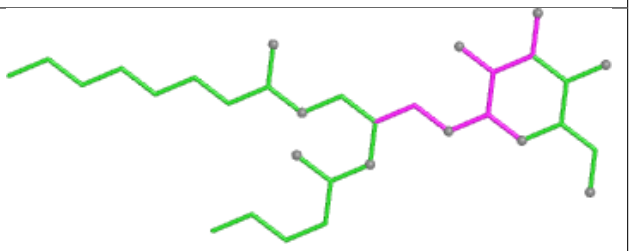
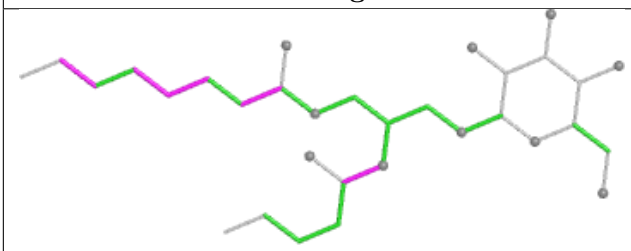


Bond angles



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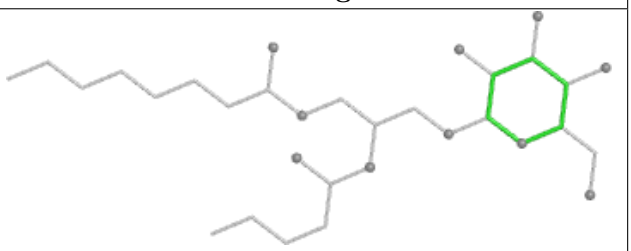
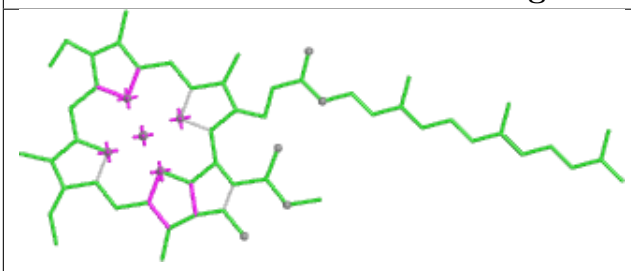


Rings

Ligand CLA 6 608



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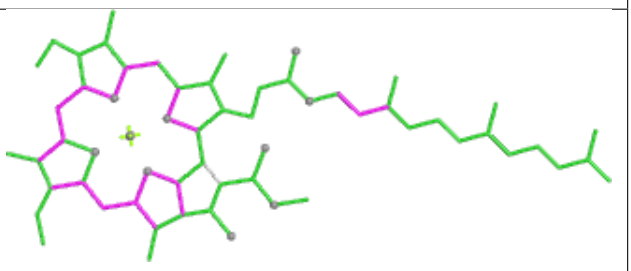
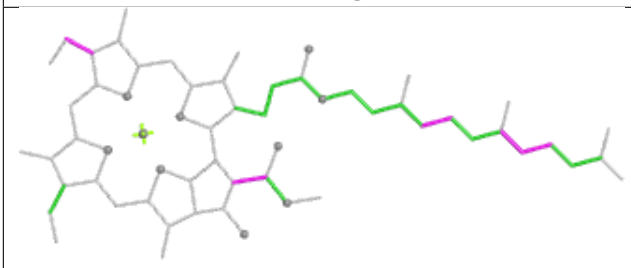


Bond angles



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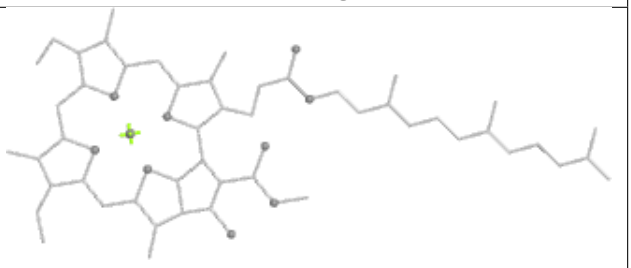
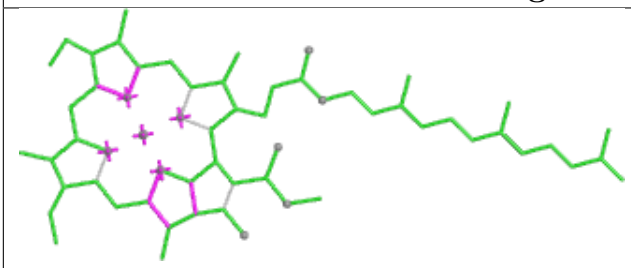


Rings

Ligand CLA 4 606



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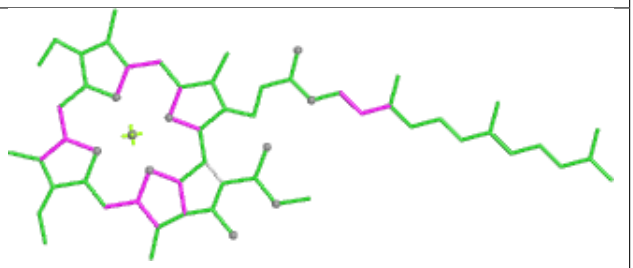
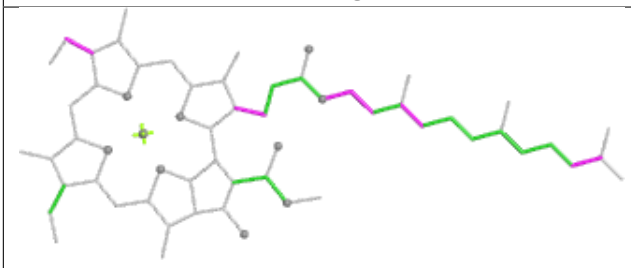


Bond angles



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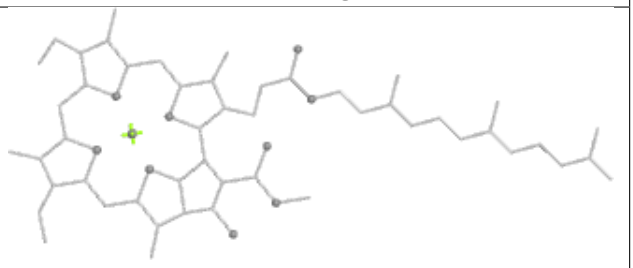
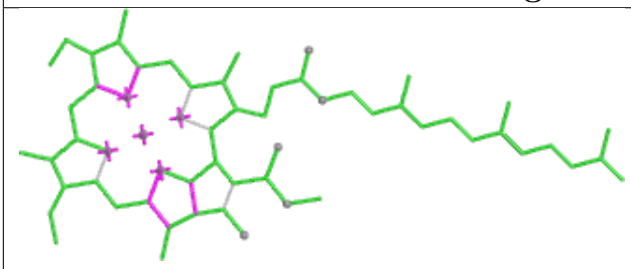


Rings

Ligand CLA B 830



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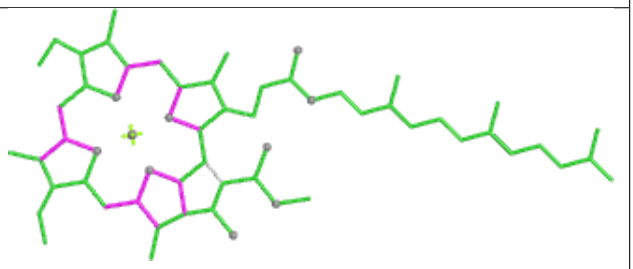
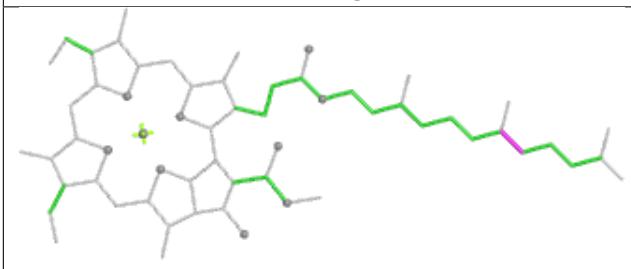


Bond angles



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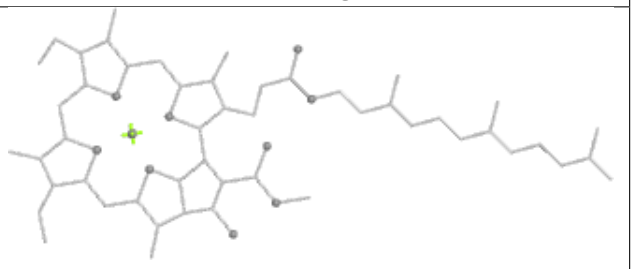
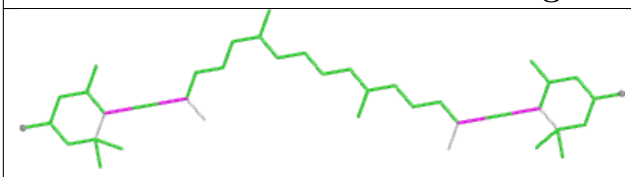


Rings

Ligand II0 9 616



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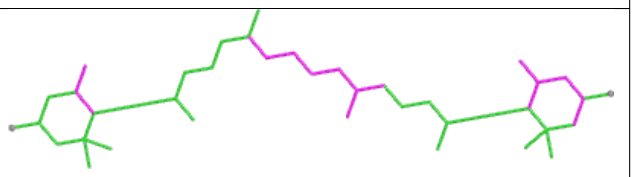

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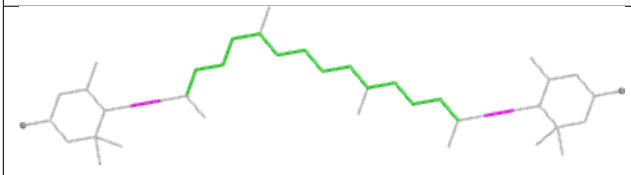

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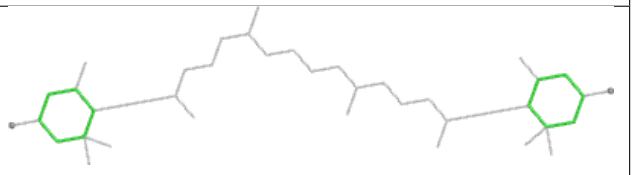
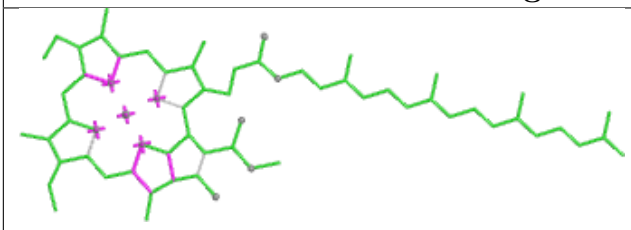


Rings

Ligand CLA A 825



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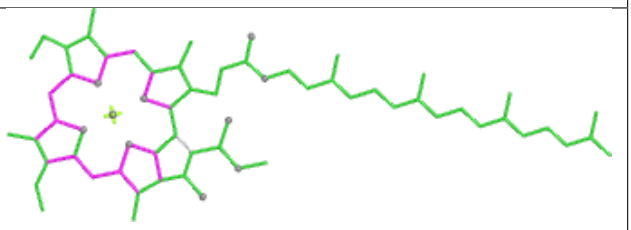
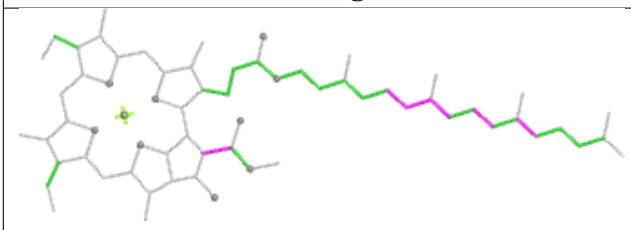


Bond angles



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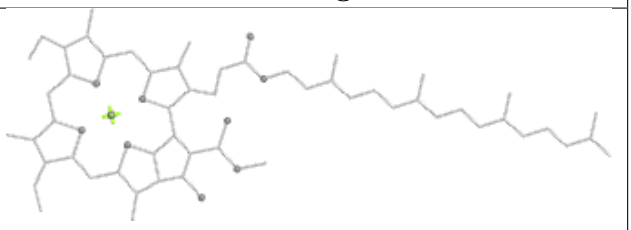
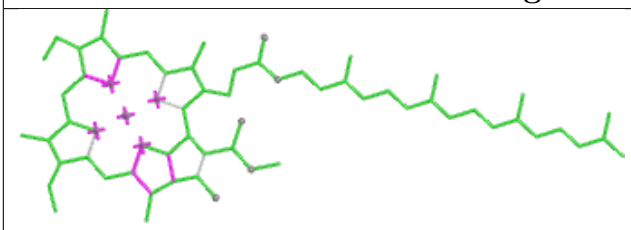


Rings

Ligand CLA A 811



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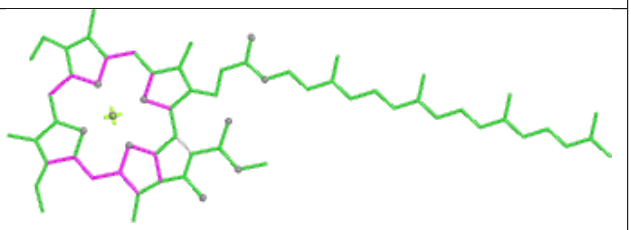
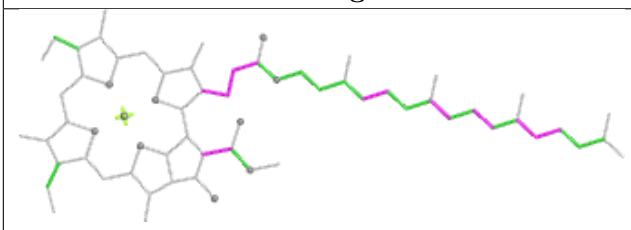


Bond angles



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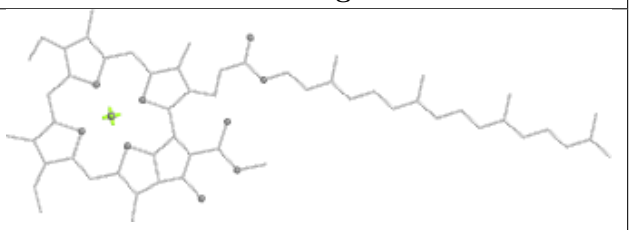
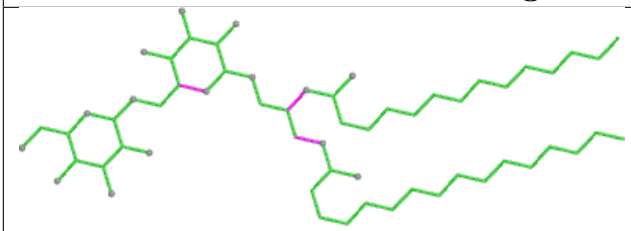
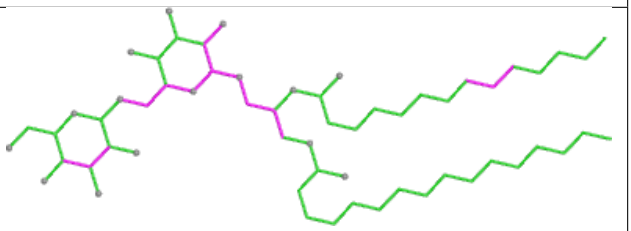


Rings

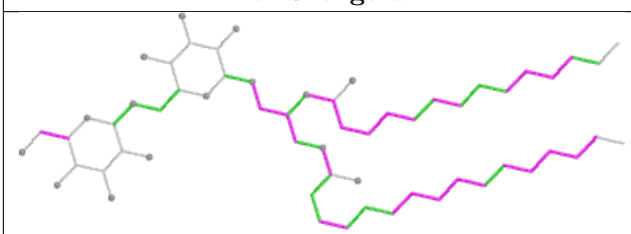
Ligand DGD Z 303



Bond lengths



Bond angles



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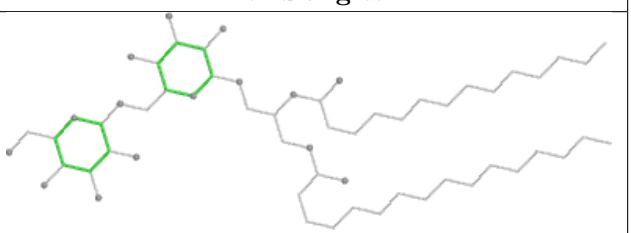
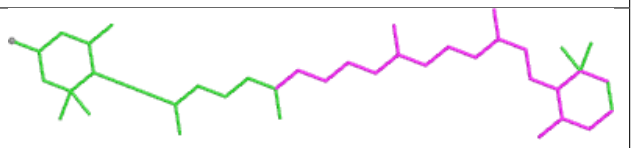


Rings

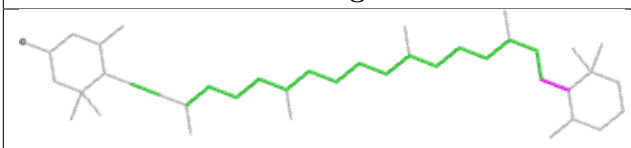
Ligand IHT d 617



Bond lengths



Bond angles



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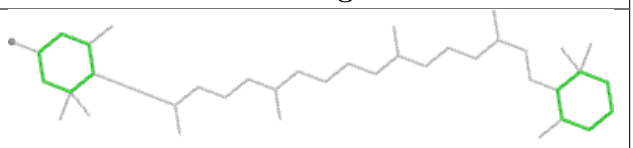
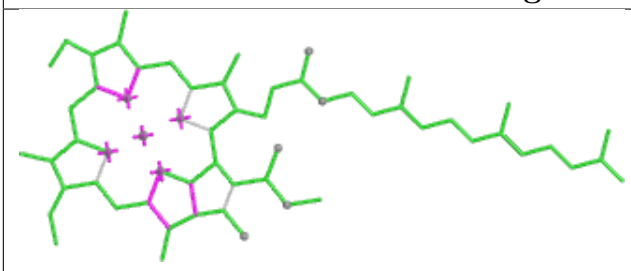
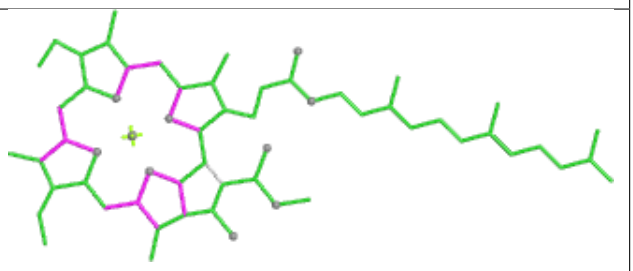


Rings

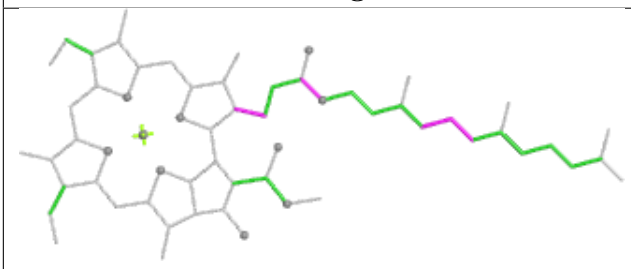
Ligand CLA A 830



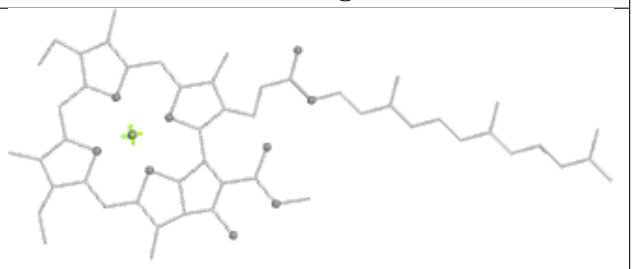
Bond lengths



Bond angles

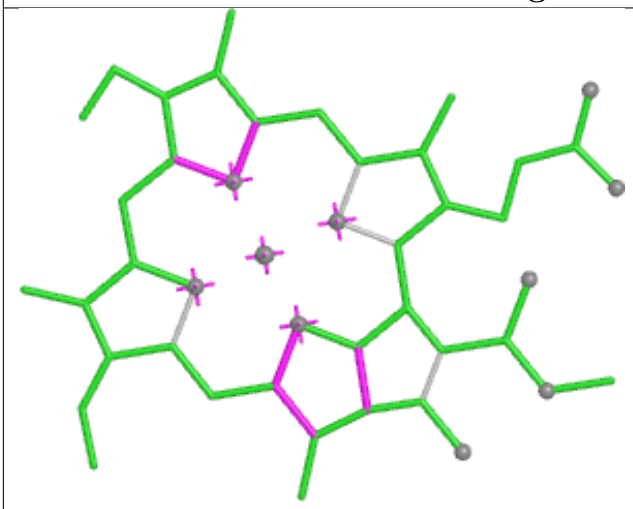


Torsions



Rings

Ligand CLA 9 613



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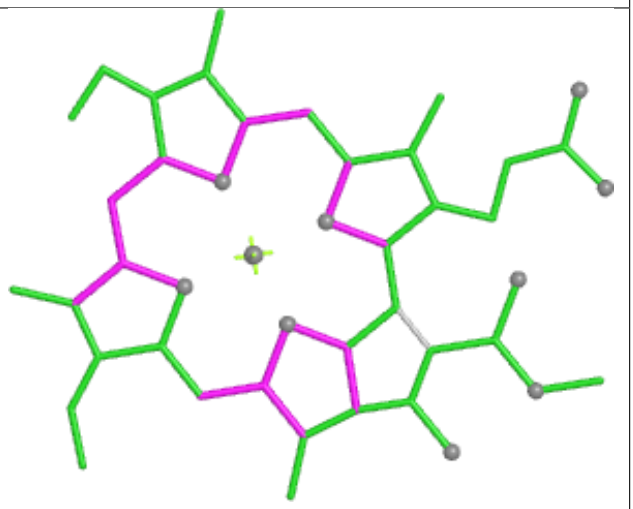

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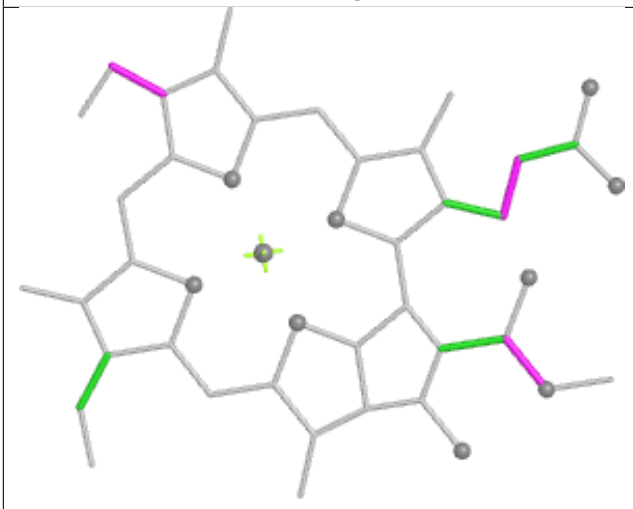
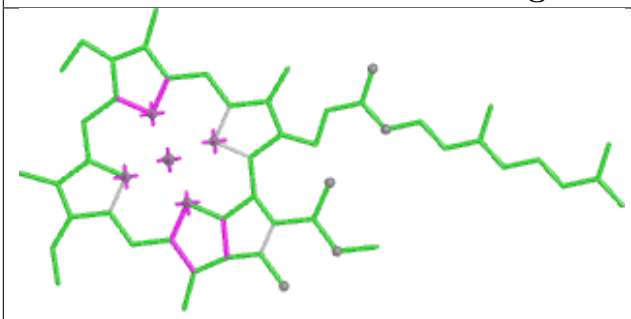


Torsions



Rings

Ligand CLA 7 611



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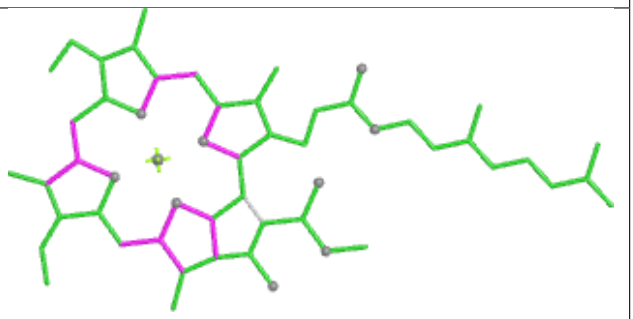

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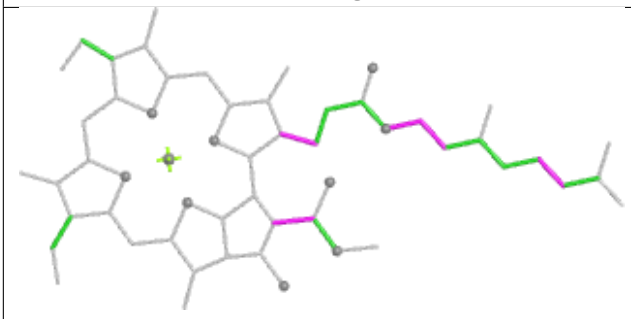

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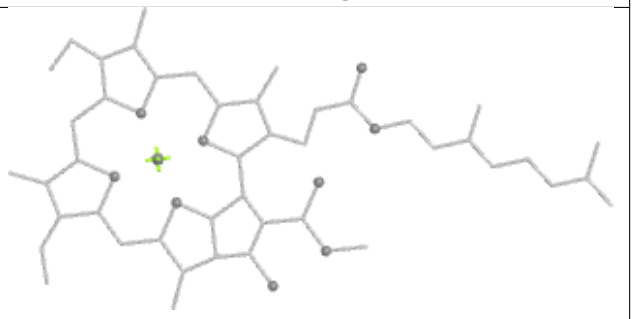
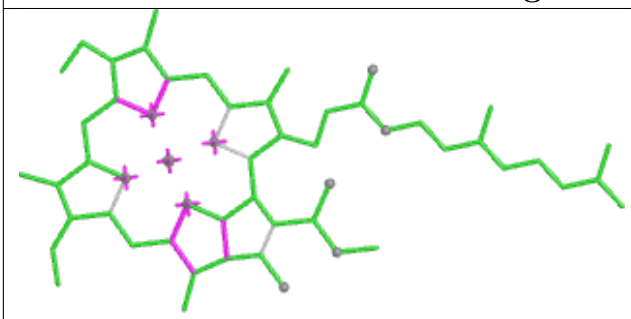


Rings

Ligand CLA R 202



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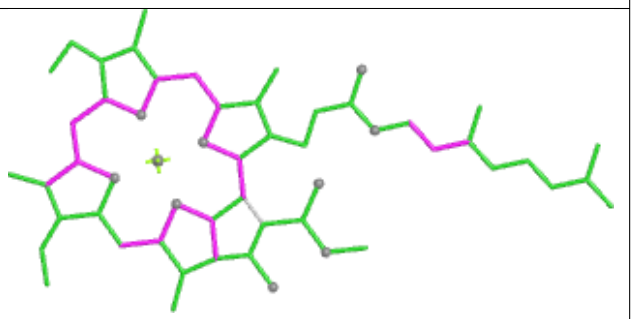

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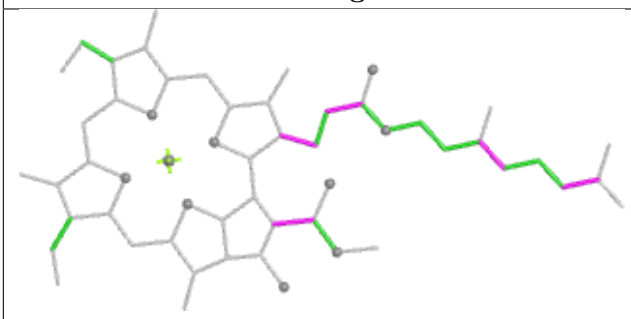

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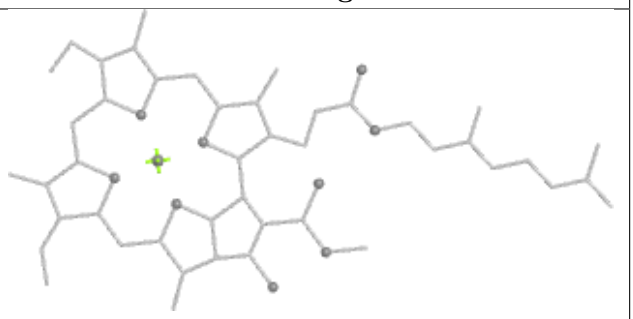
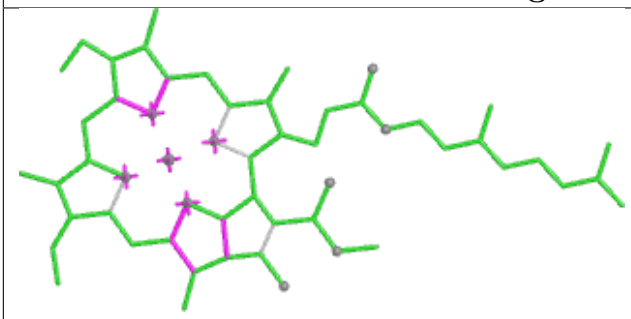


Rings

Ligand CLA 6 611



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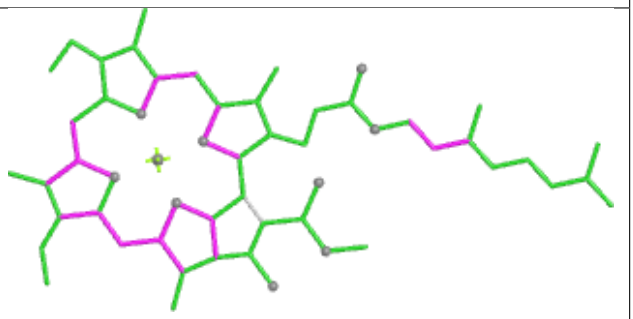

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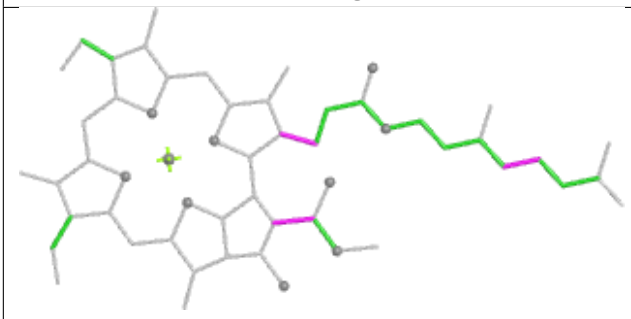

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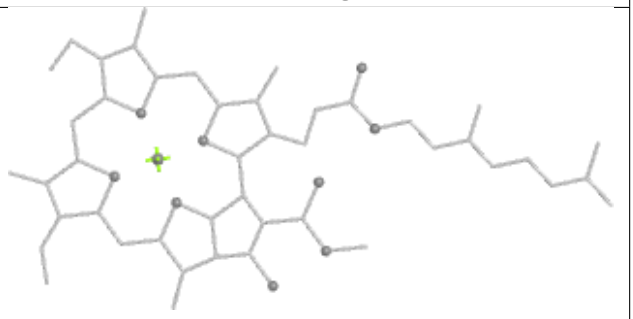

Rings

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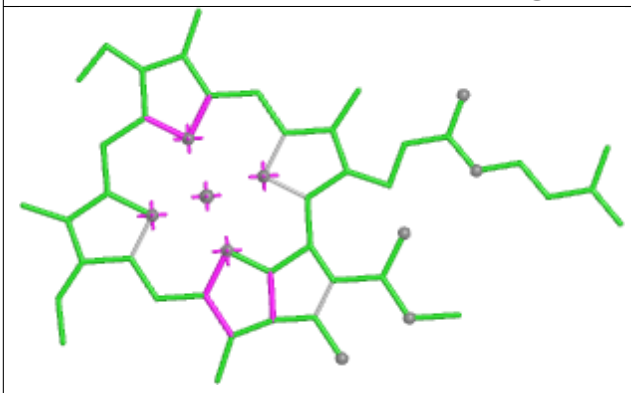

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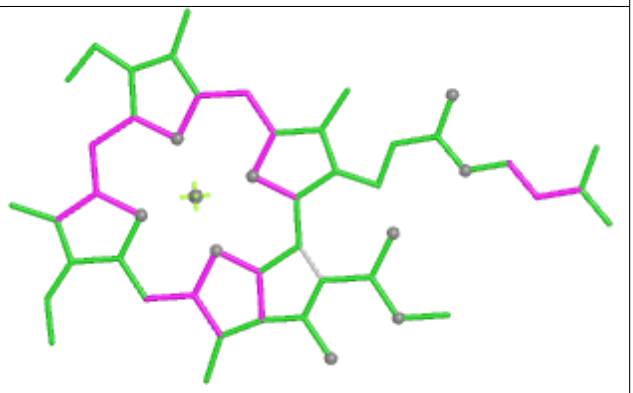

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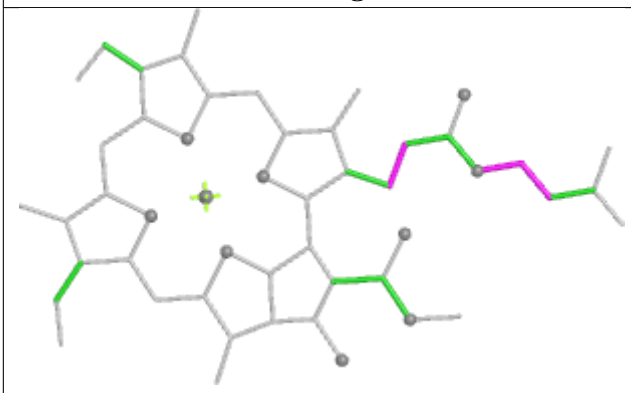

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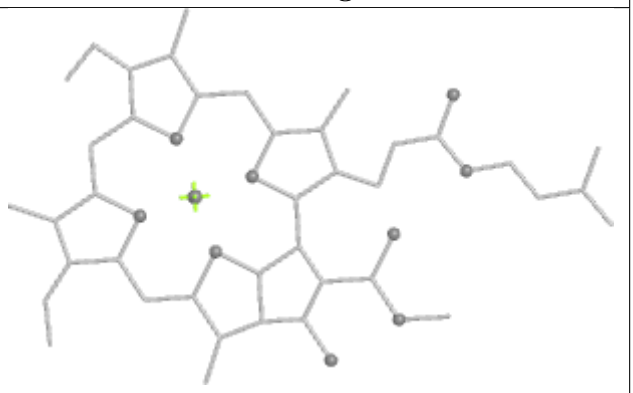
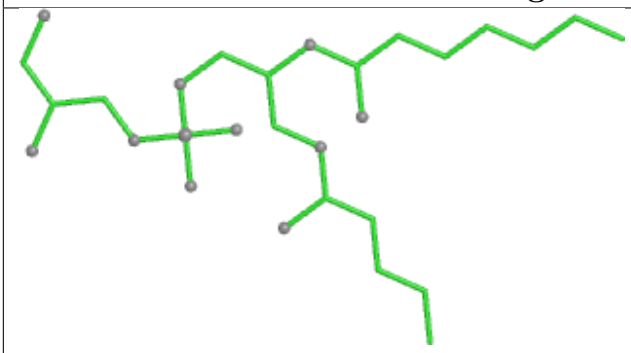


Rings

Ligand LHG c 621



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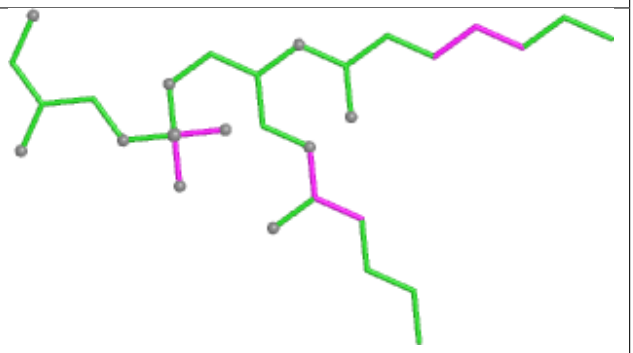

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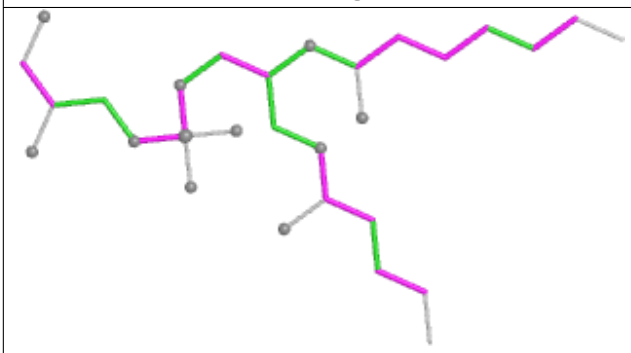

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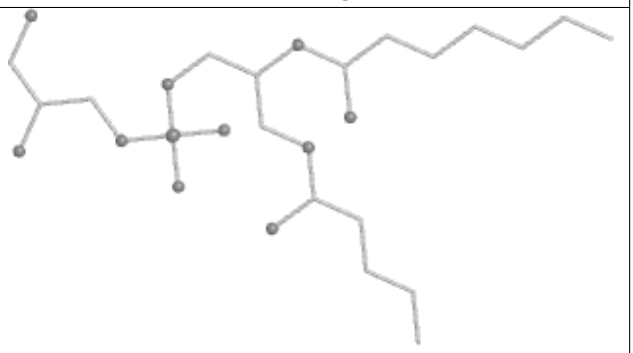
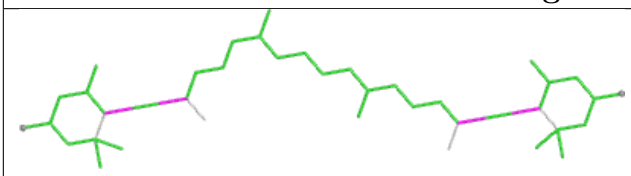


Rings

Ligand II0 4 612



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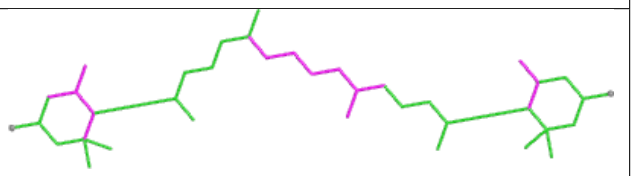

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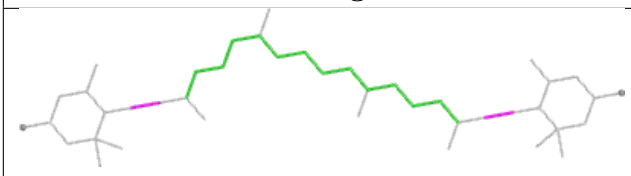

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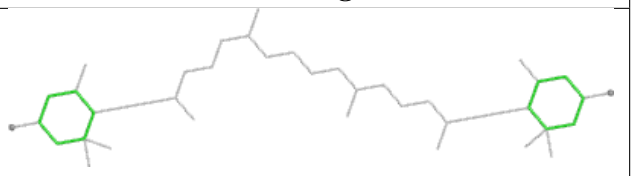
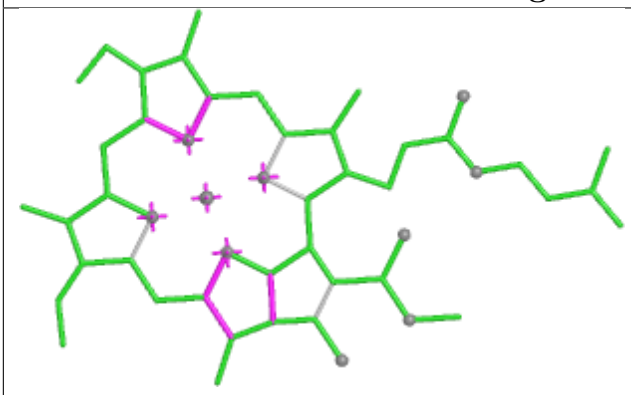


Rings

Ligand CLA e 603



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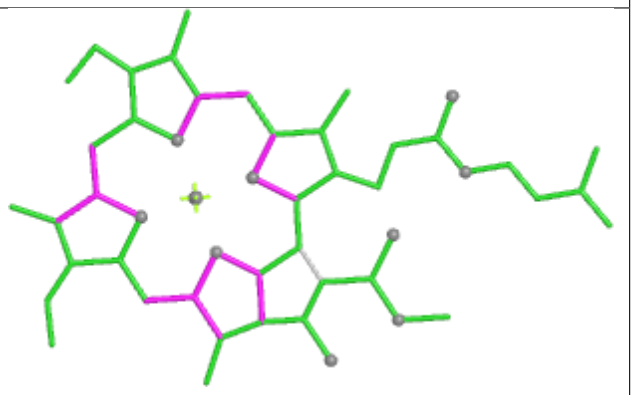

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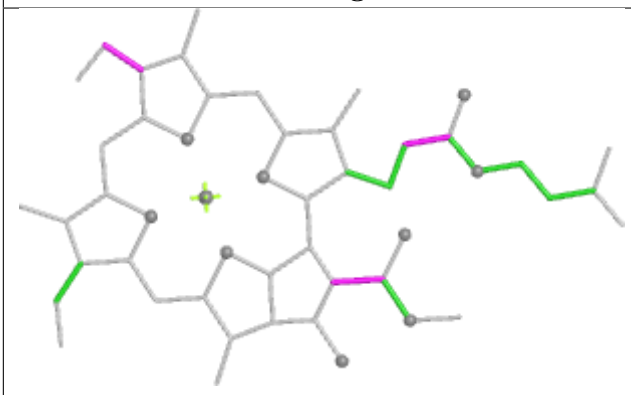

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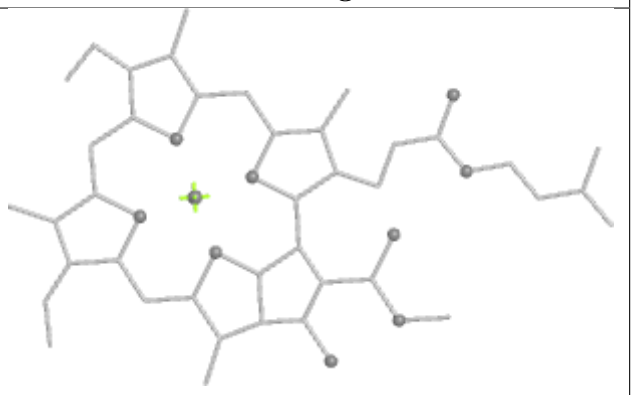
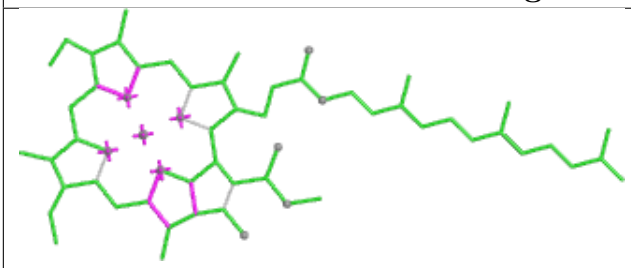


Rings

Ligand CLA B 824



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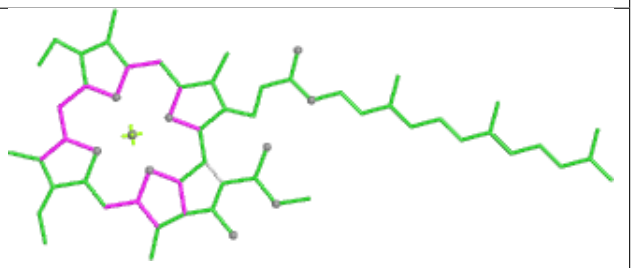

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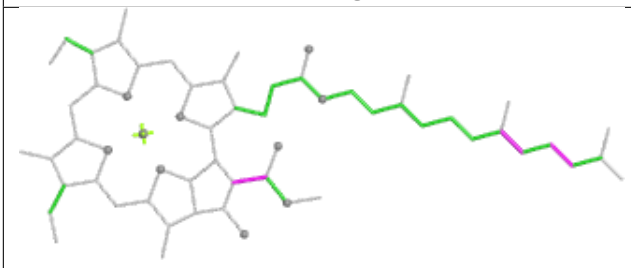

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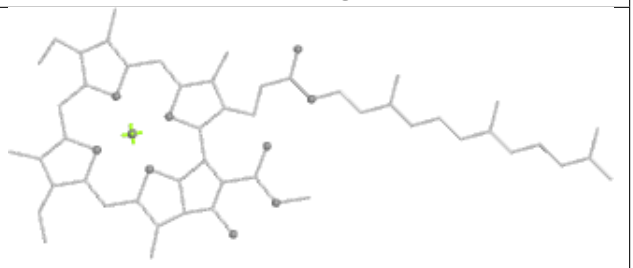
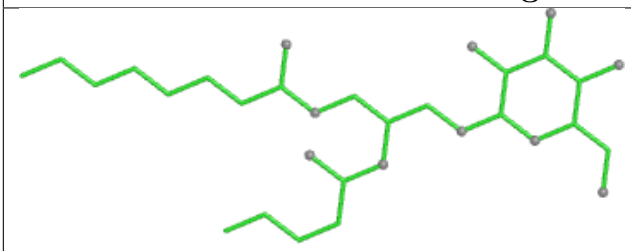


Rings

Ligand LMG F 205



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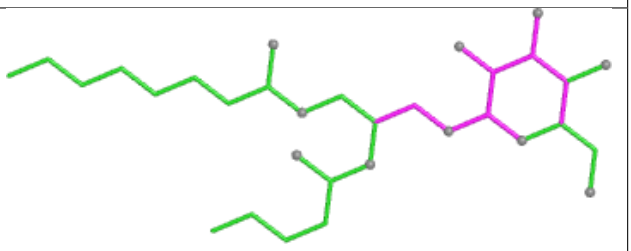

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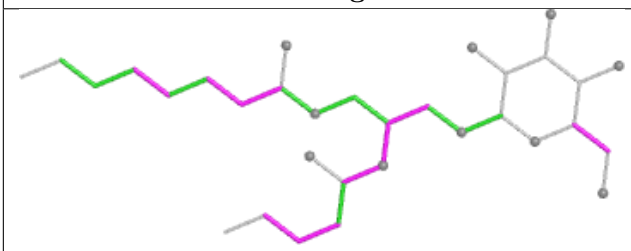

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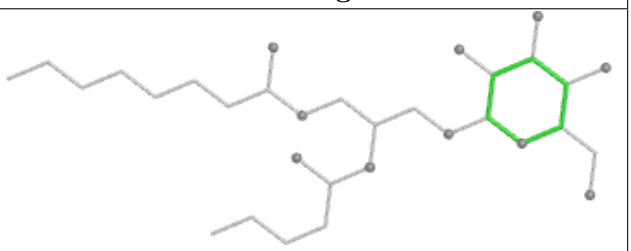
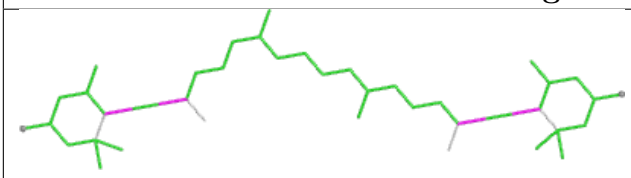


Rings

Ligand II0 2 615



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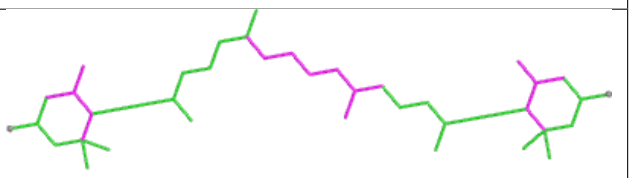

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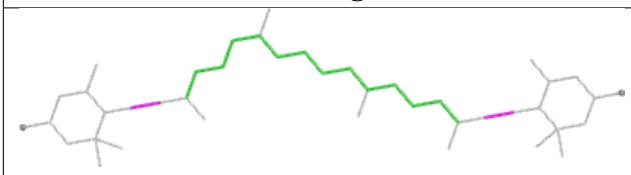

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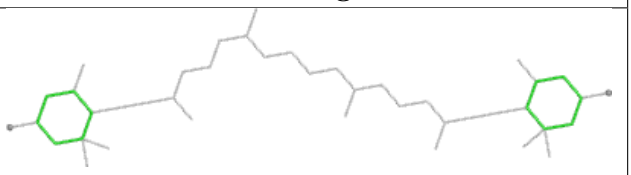
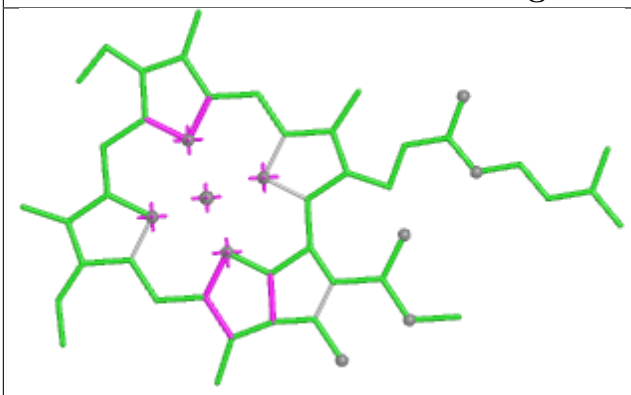


Rings

Ligand CLA 2 603



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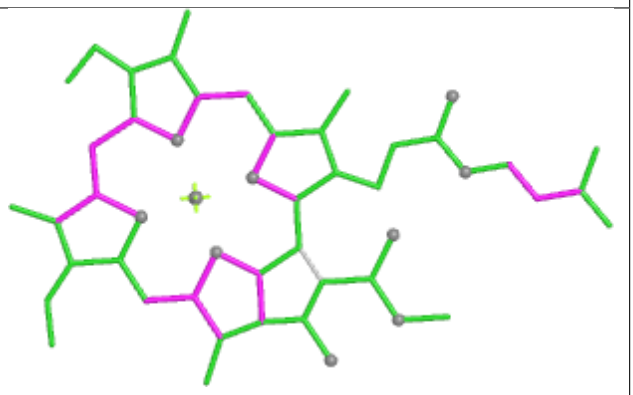
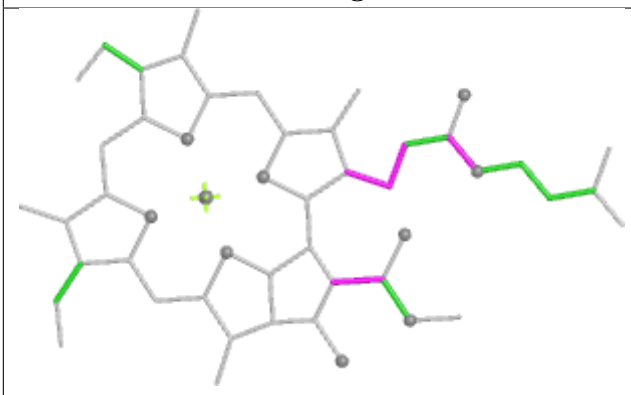


Bond angles



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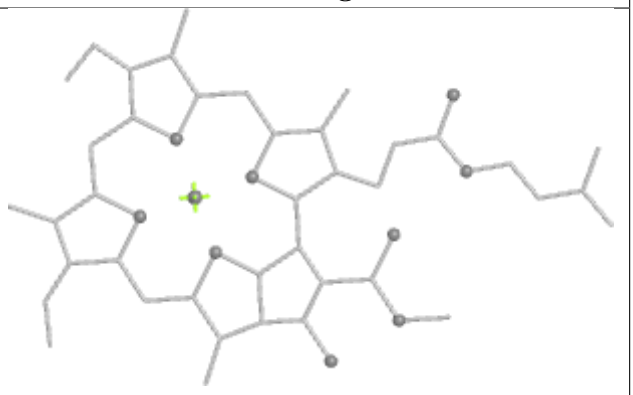
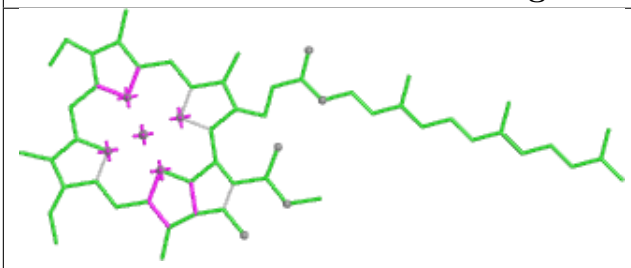


Rings

Ligand CLA 1 608



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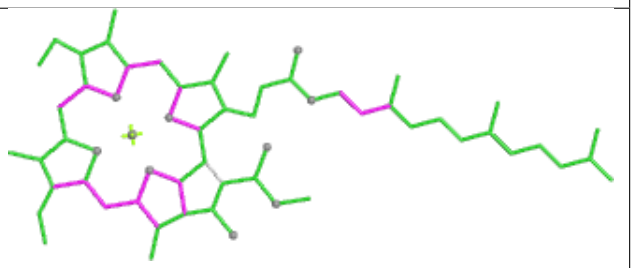
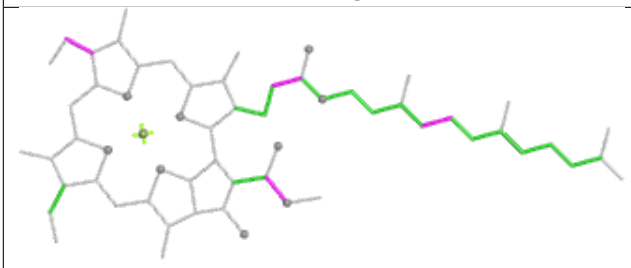


Bond angles



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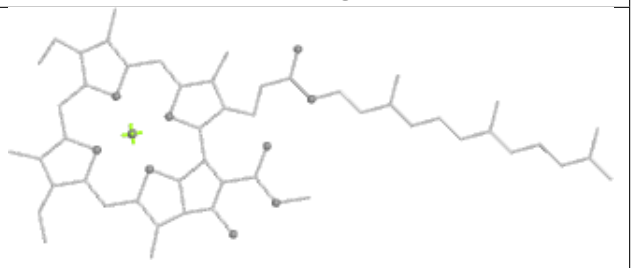
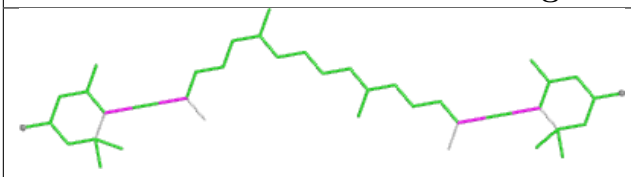


Rings

Ligand II0 d 613



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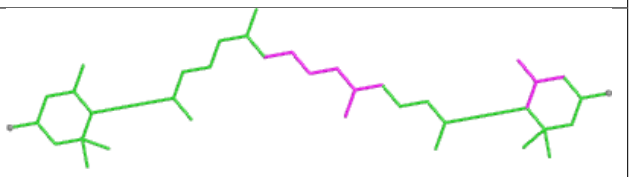
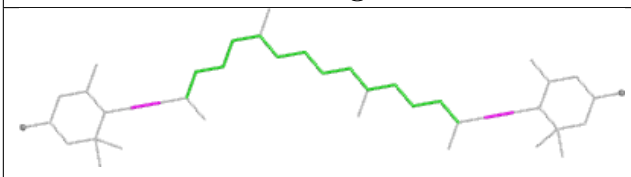


Bond angles



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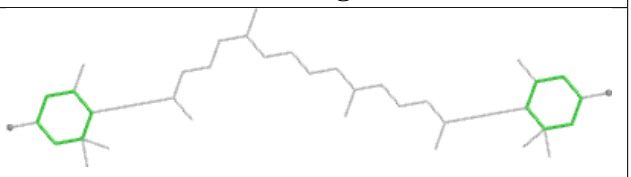
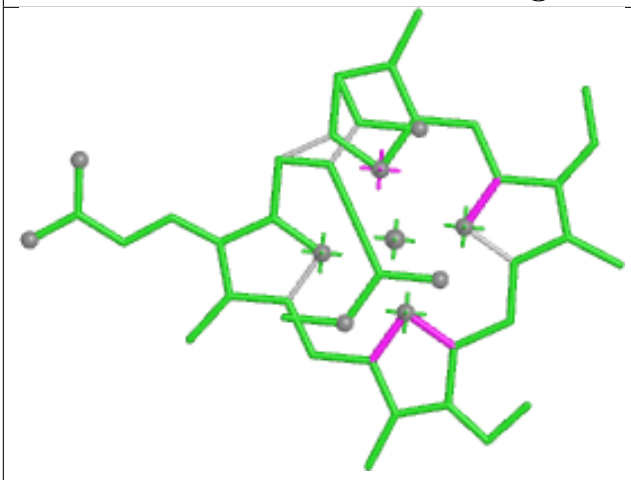


Rings

Ligand KC2 3 606



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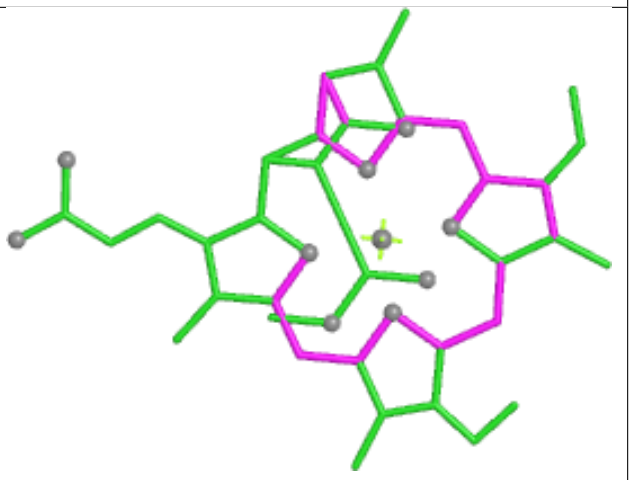
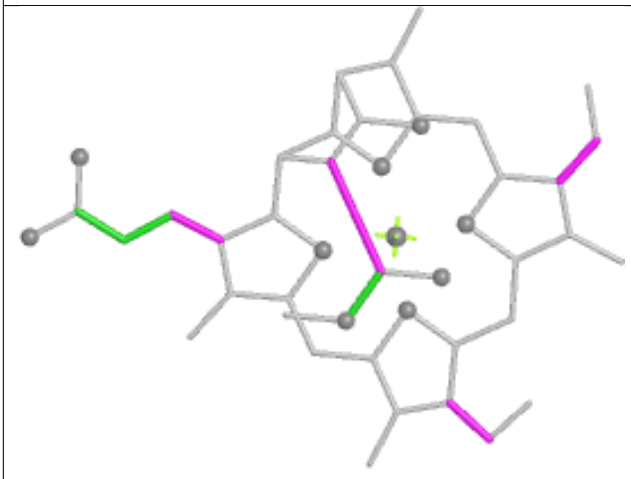
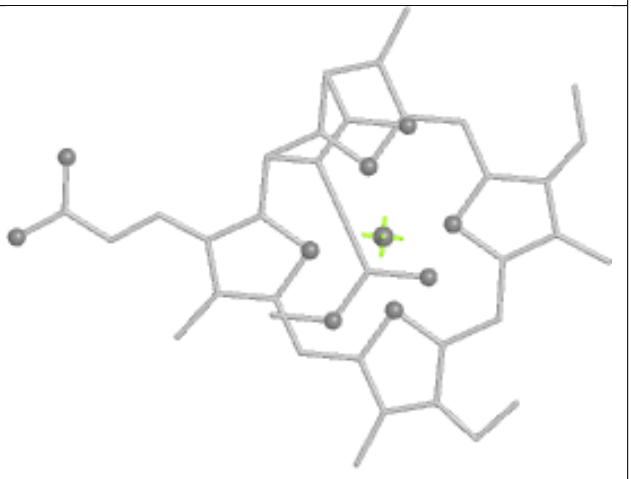


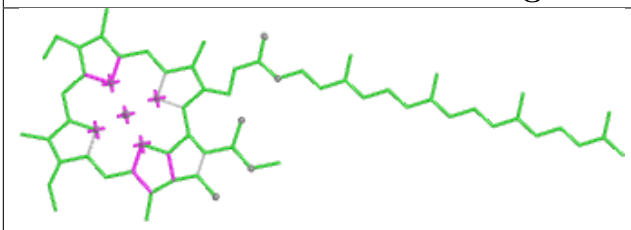
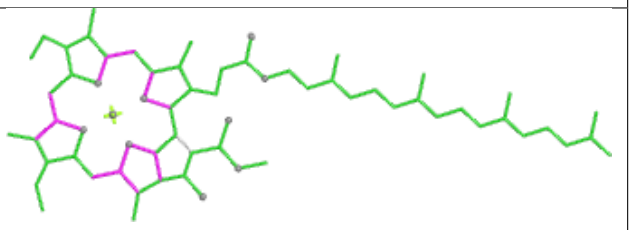
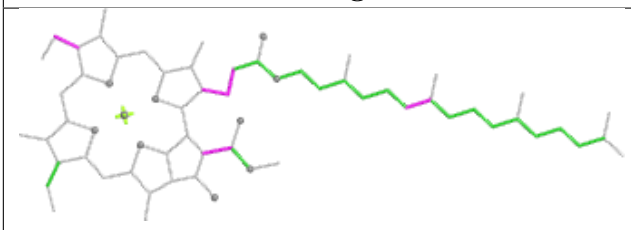
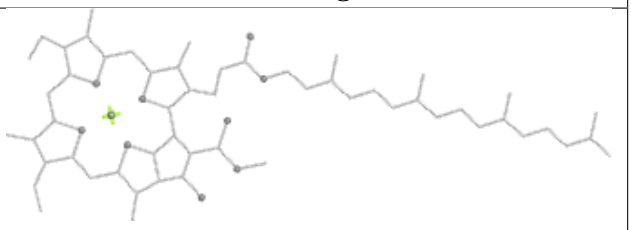
Bond angles

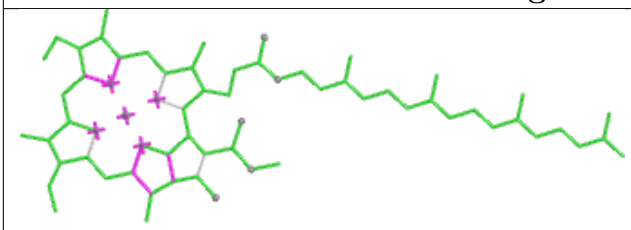
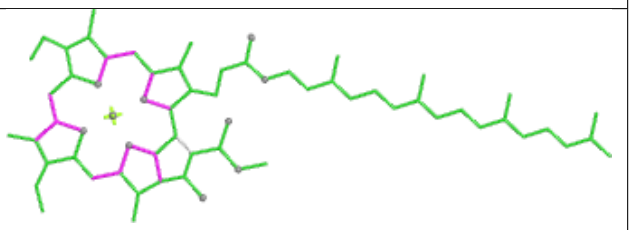
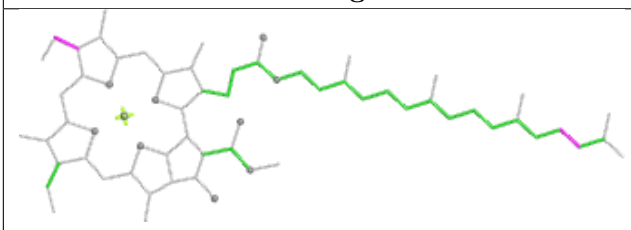
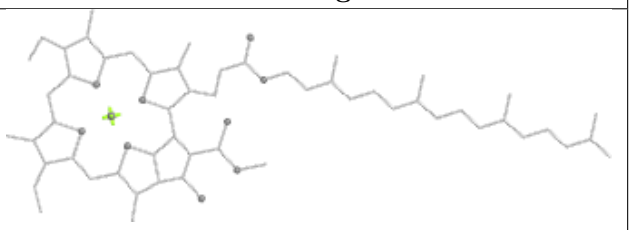


Torsions

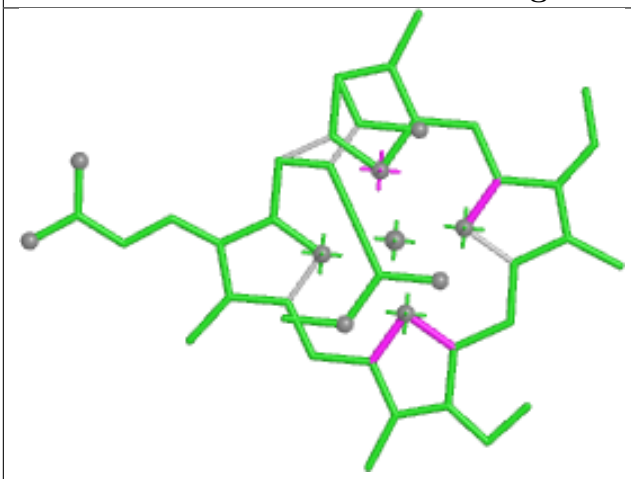


Rings

Ligand CLA A 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand KC2 7 606



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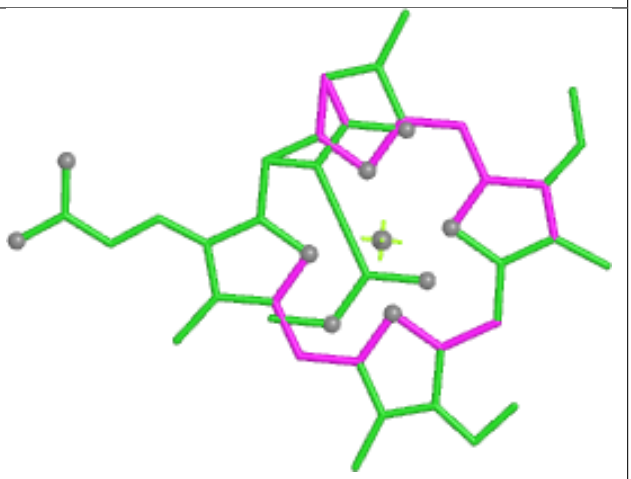

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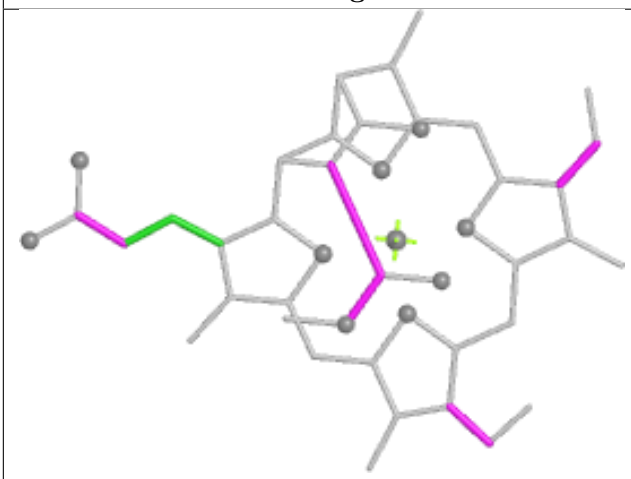

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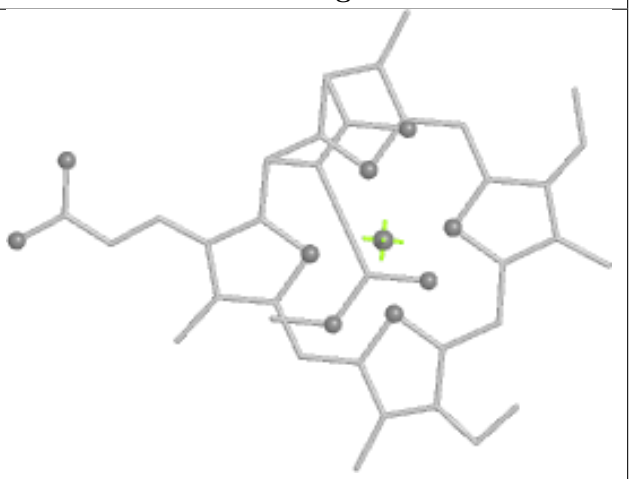
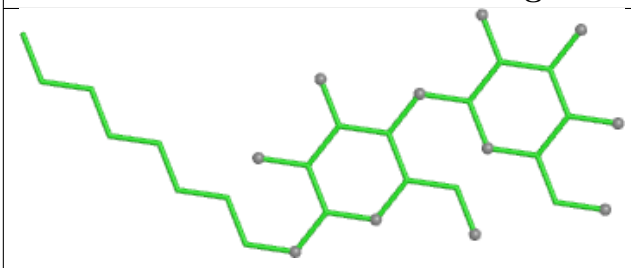


Rings

Ligand LMU e 617



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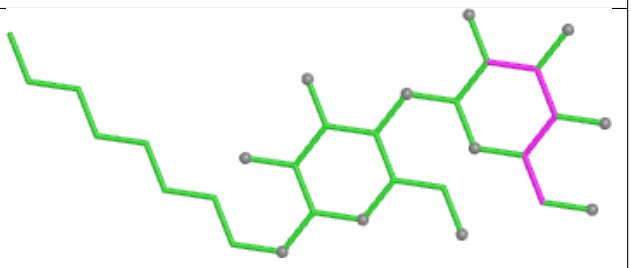

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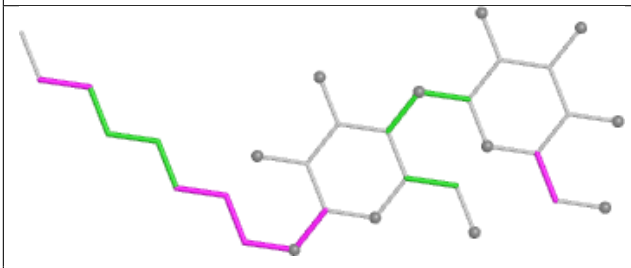

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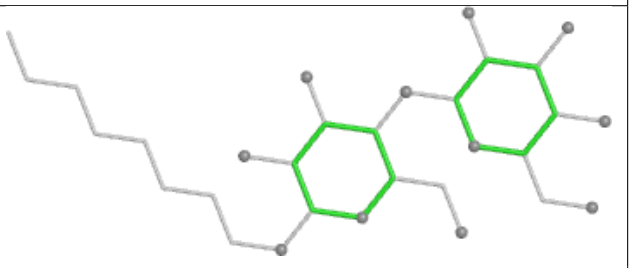
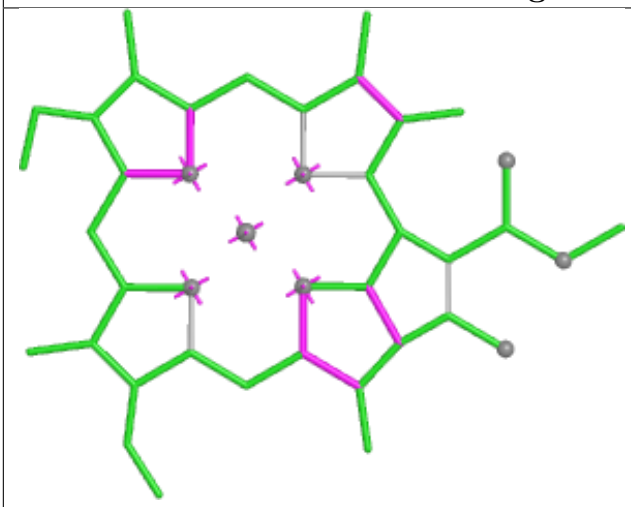


Rings

Ligand CLA 9 614



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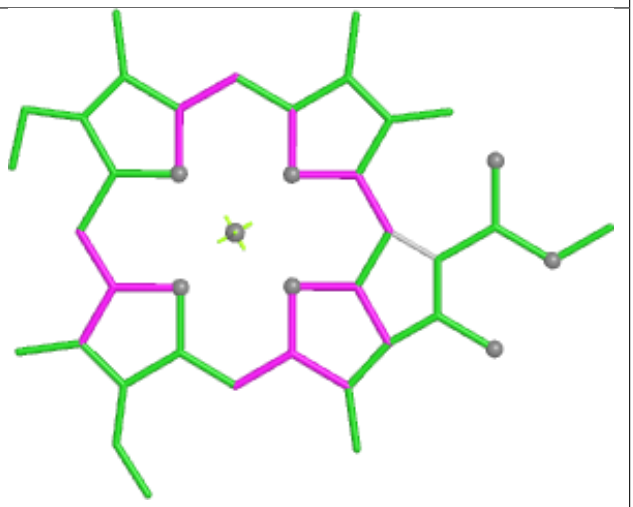
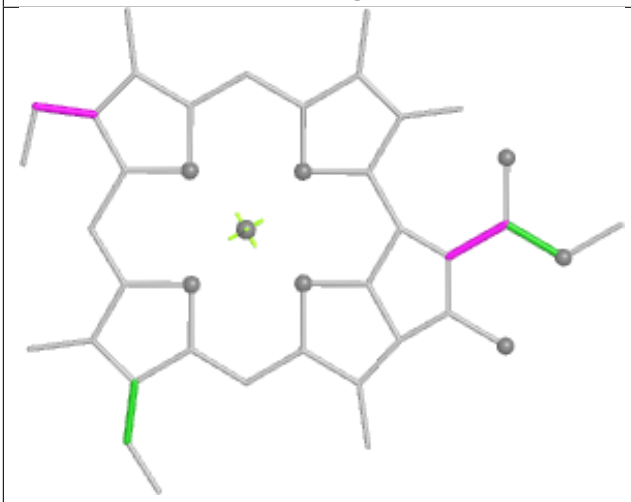


Bond angles



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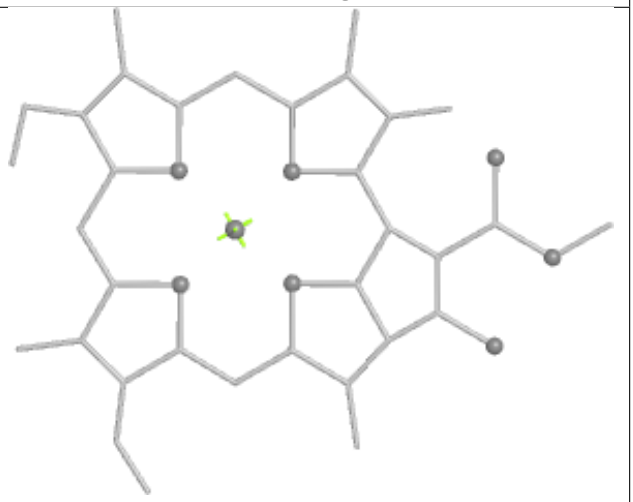
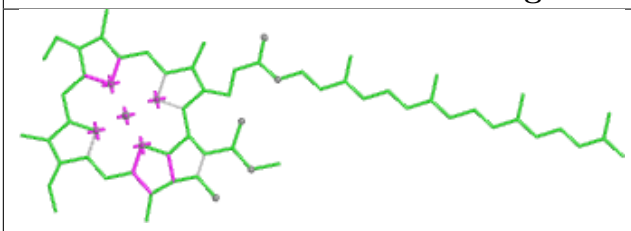


Rings

Ligand CLA B 808



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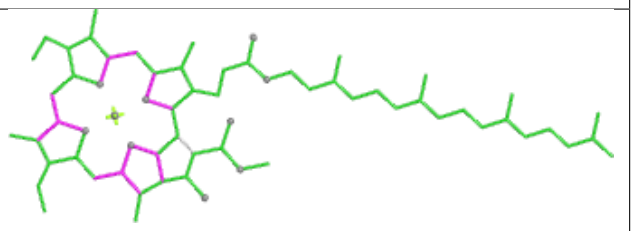
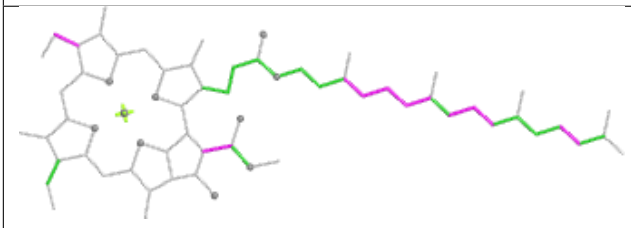


Bond angles



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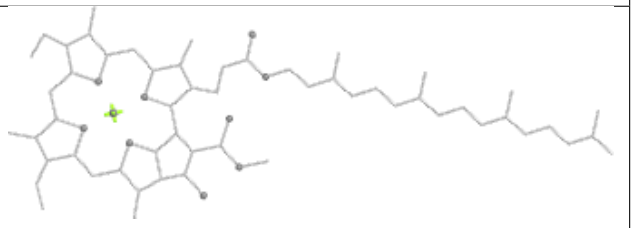

Rings

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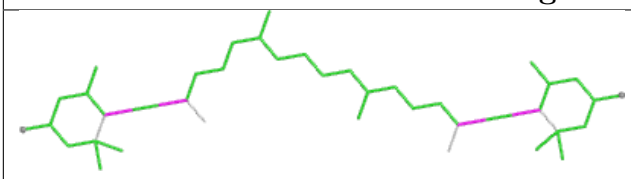

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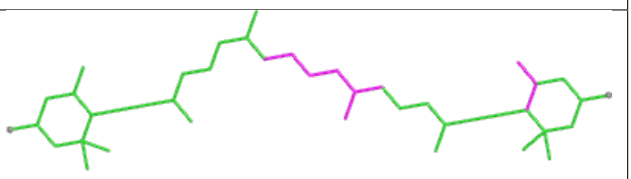

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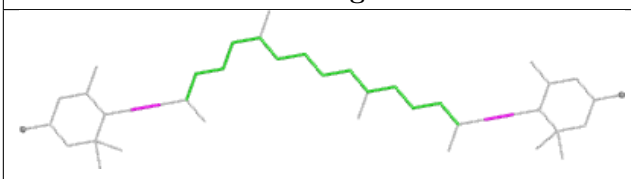

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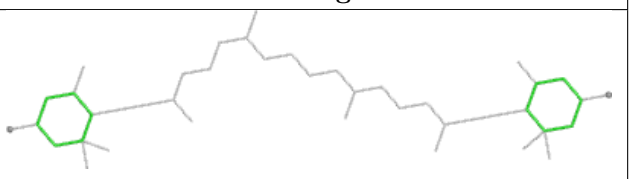
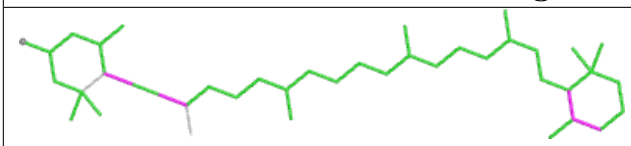


Rings

Ligand IHT 2 616



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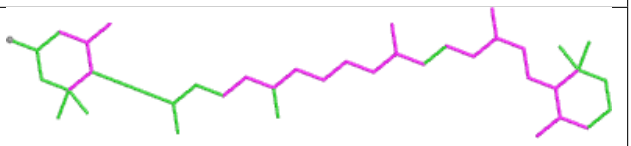
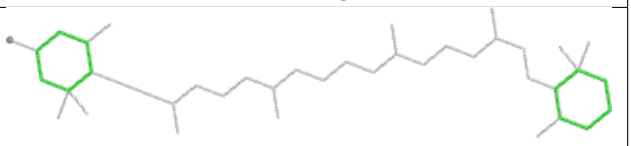


Bond angles

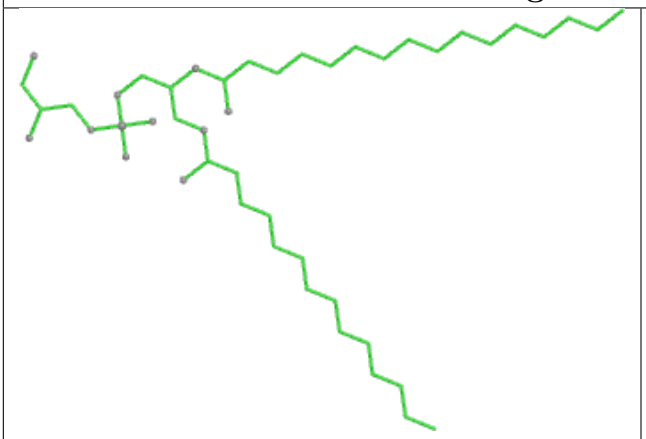


Torsions



Rings

Ligand LHG 4 617



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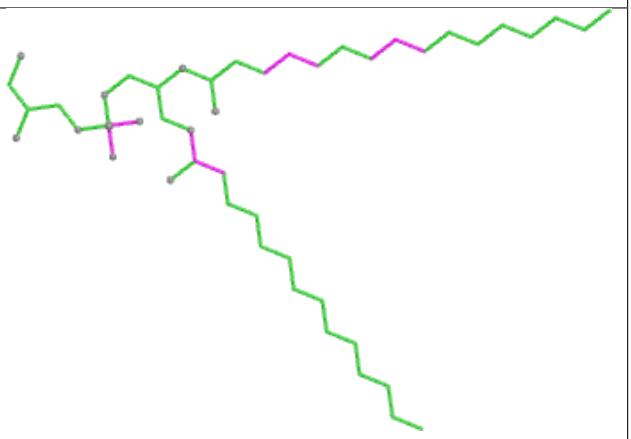
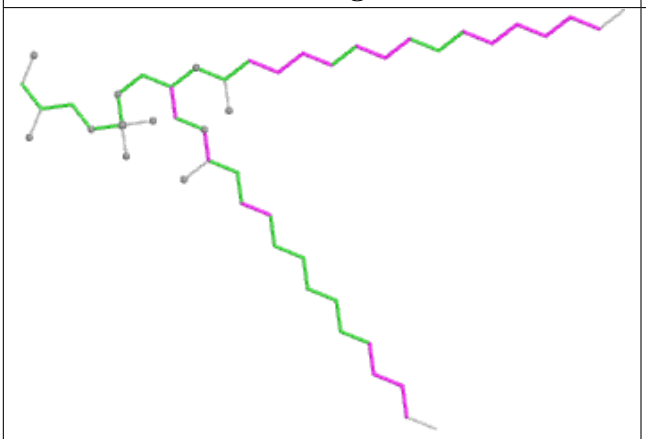


Bond angles



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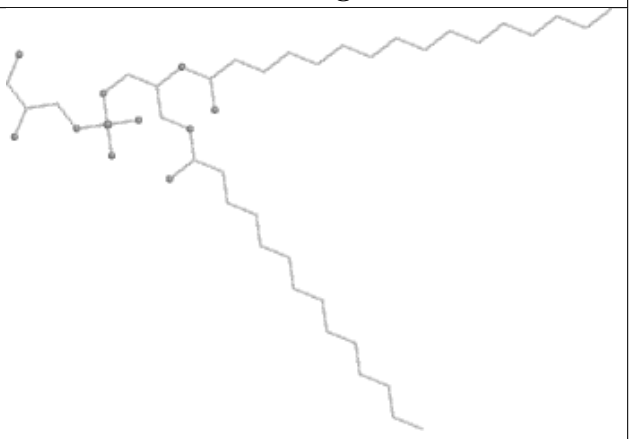
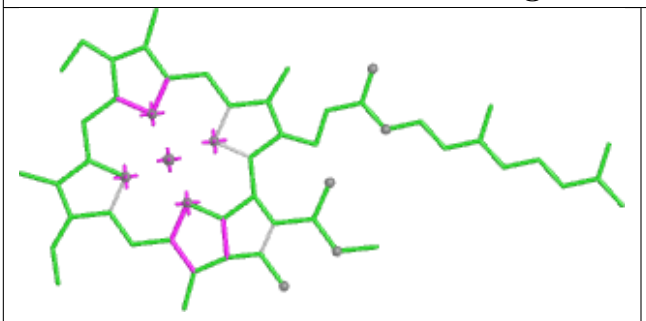


Rings

Ligand CLA A 836



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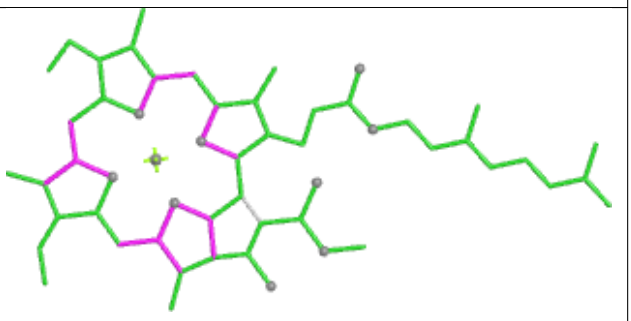
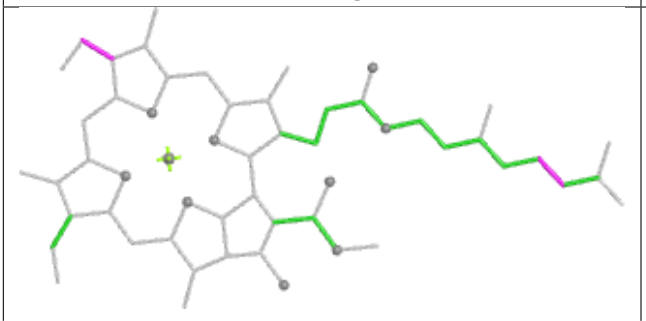


Bond angles



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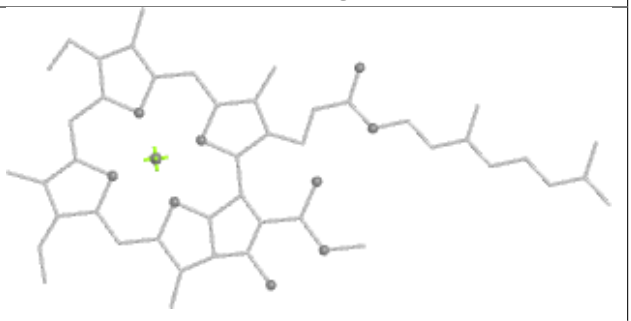
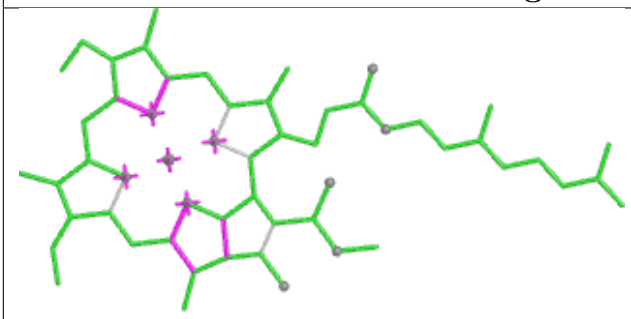


Rings

Ligand CLA B 811



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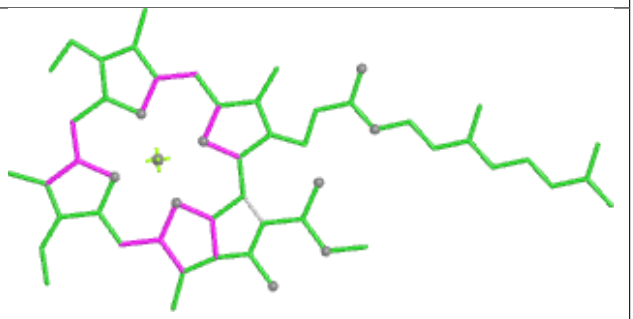
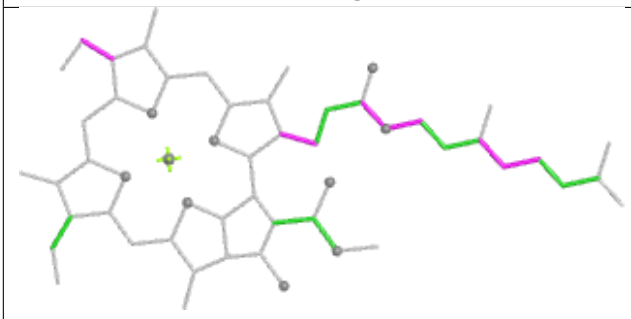


Bond angles



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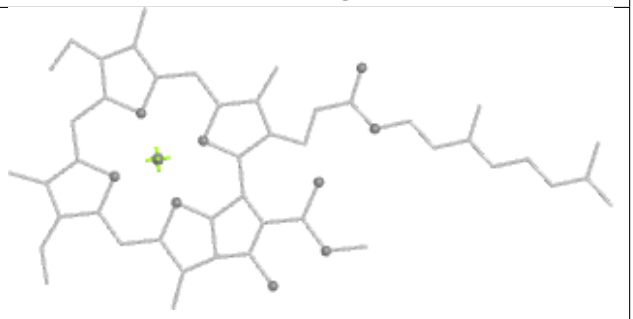
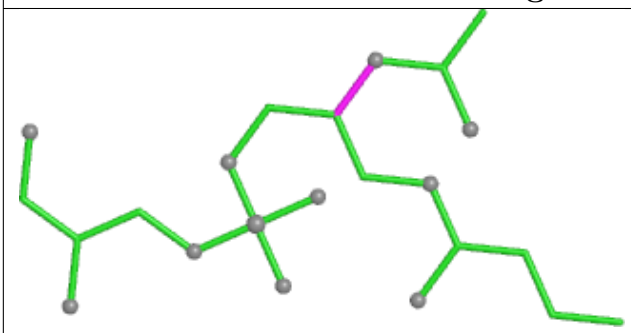


Rings

Ligand LHG 5 619



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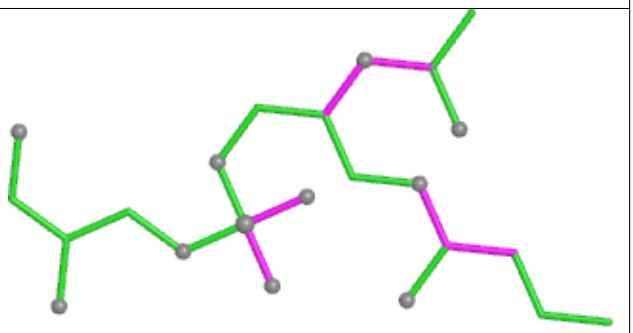
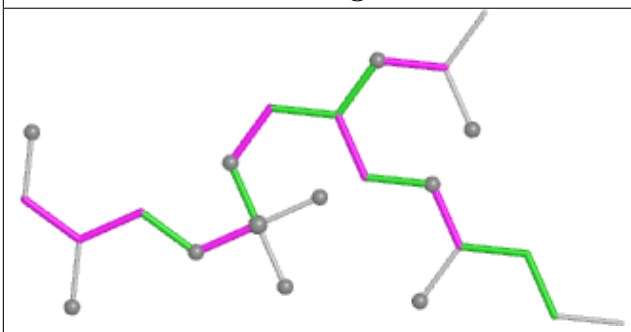


Bond angles



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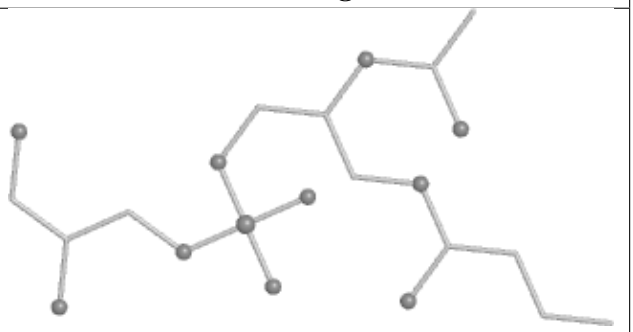
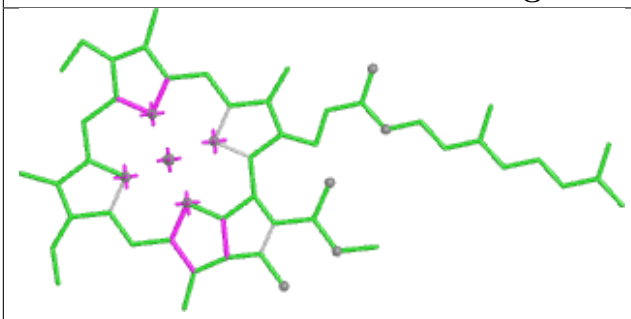


Rings

Ligand CLA A 821



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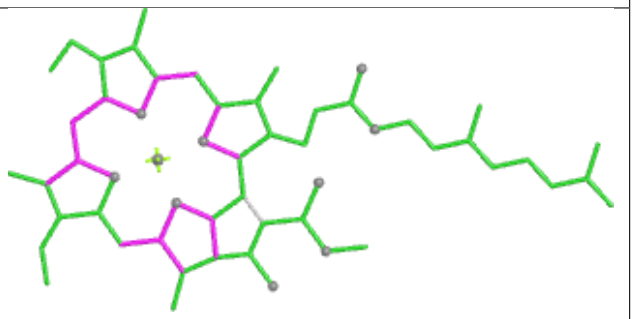
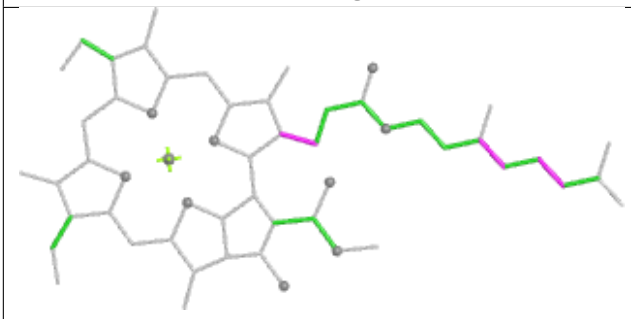


Bond angles



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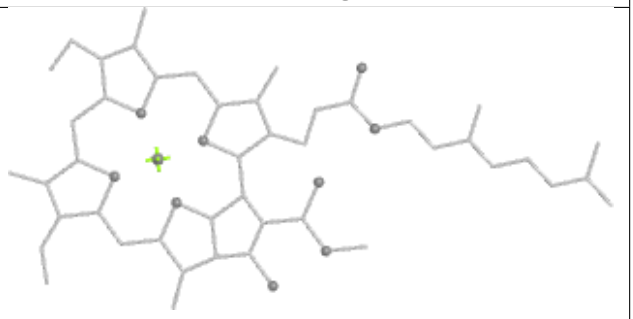
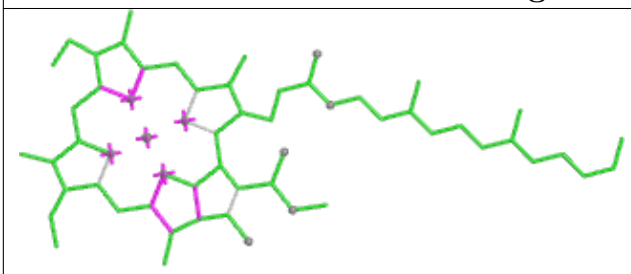


Rings

Ligand CLA 1 602



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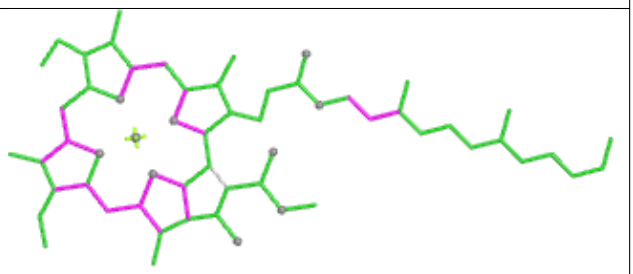
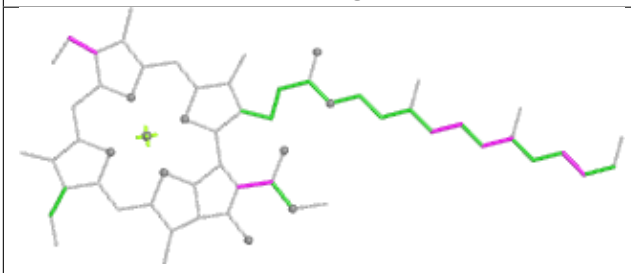


Bond angles



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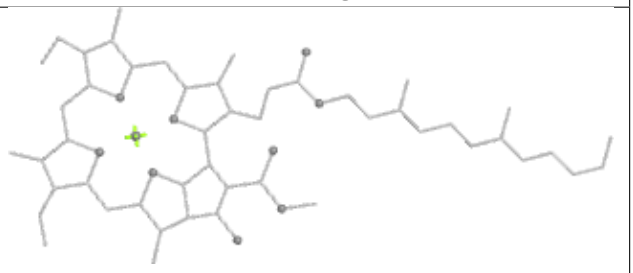
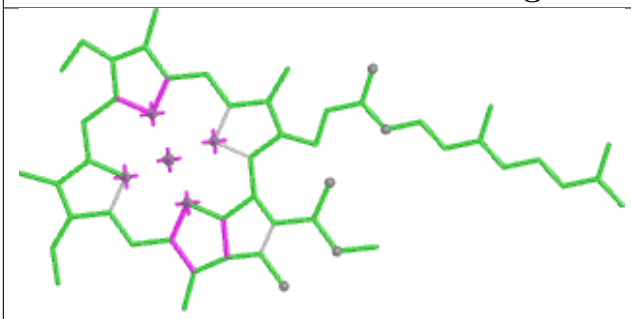
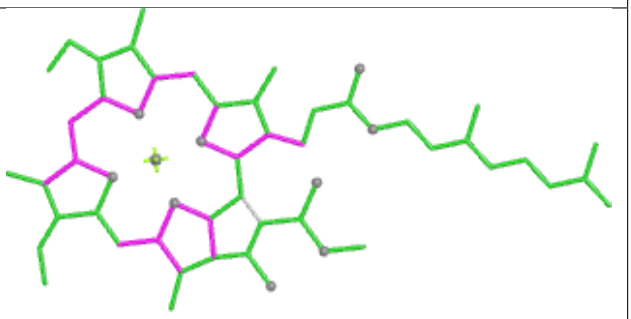
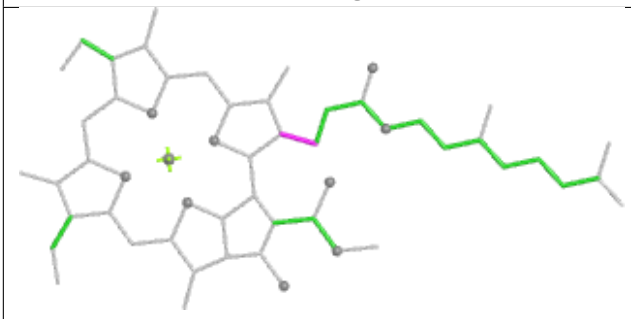
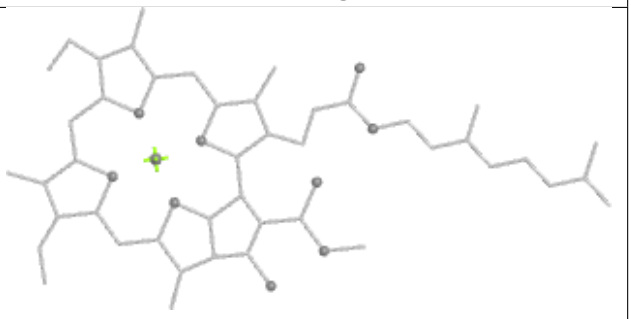


Rings

Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

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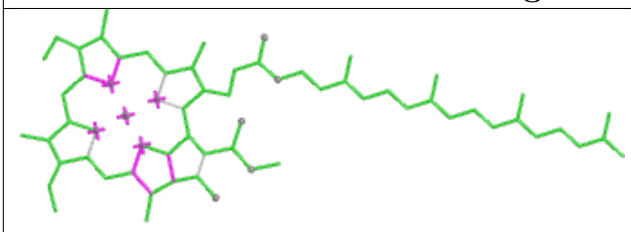
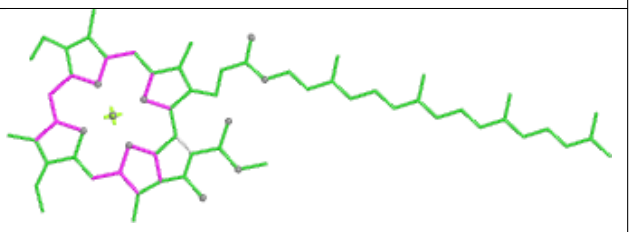
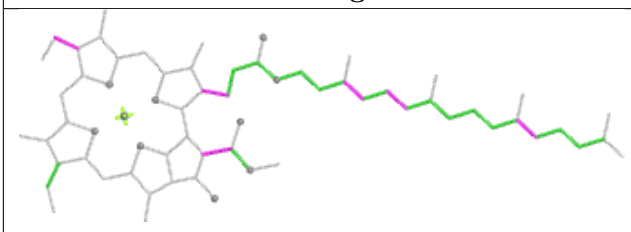
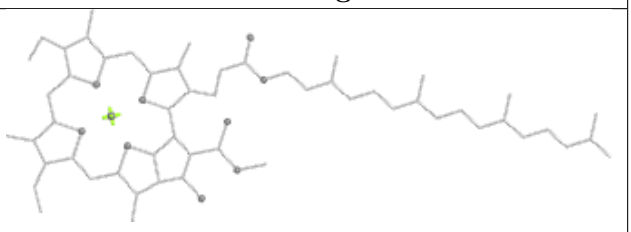
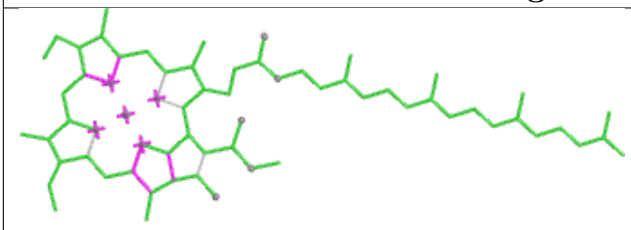
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 607



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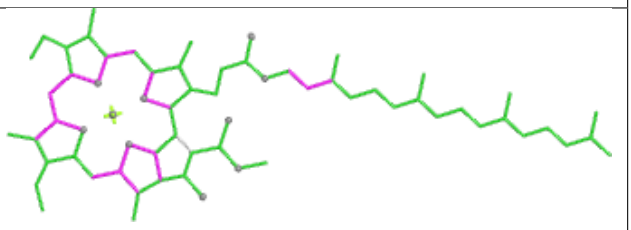

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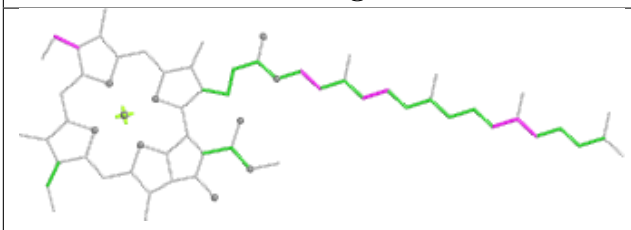

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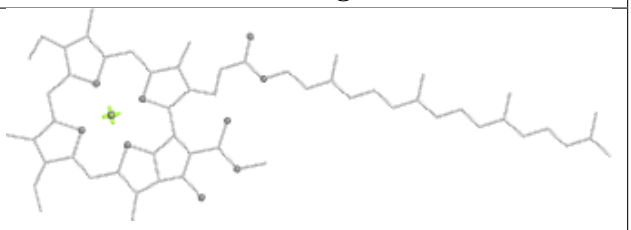
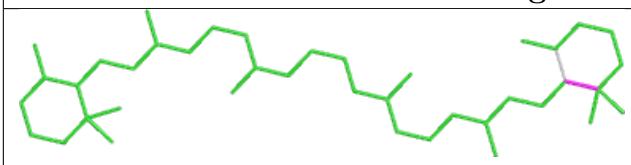


Rings

Ligand 8CT F 201



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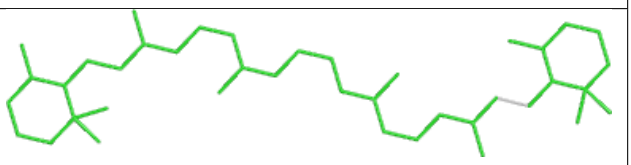

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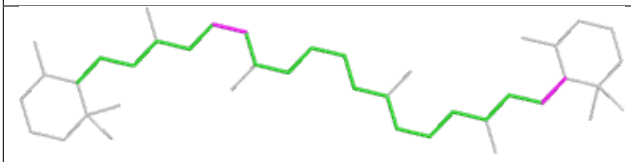

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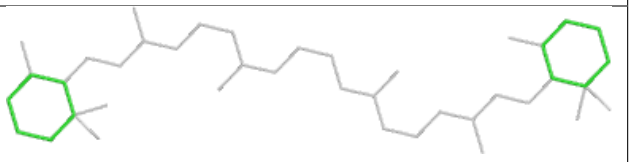
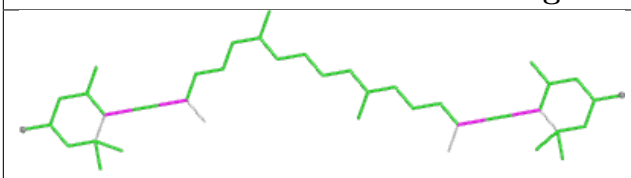


Rings

Ligand II0 a 619



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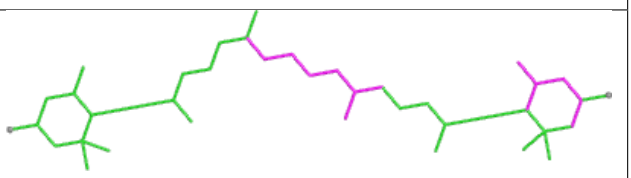

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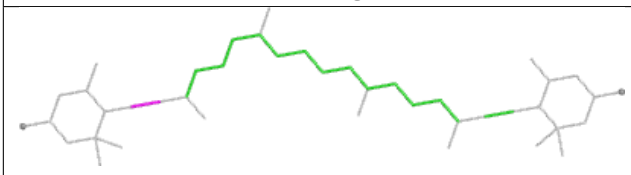

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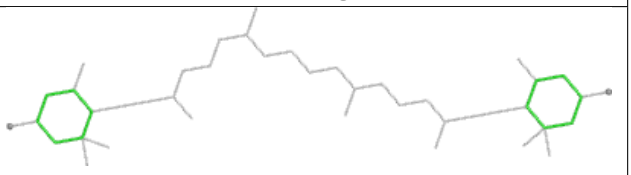
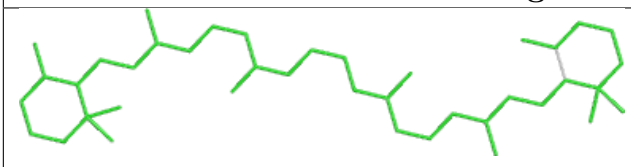


Rings

Ligand 8CT B 847



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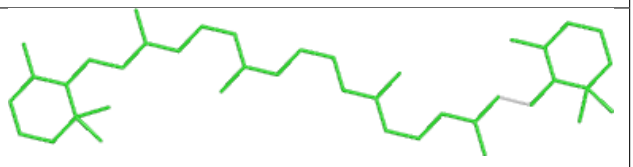

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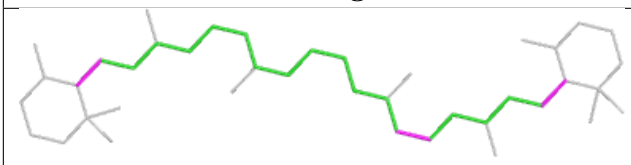

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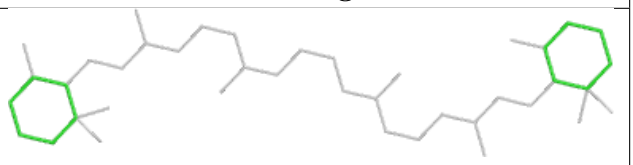
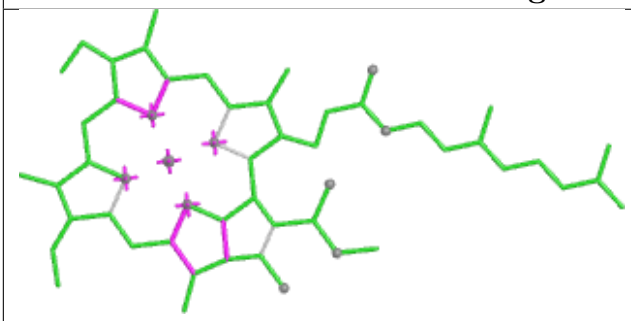


Rings

Ligand CLA 4 604



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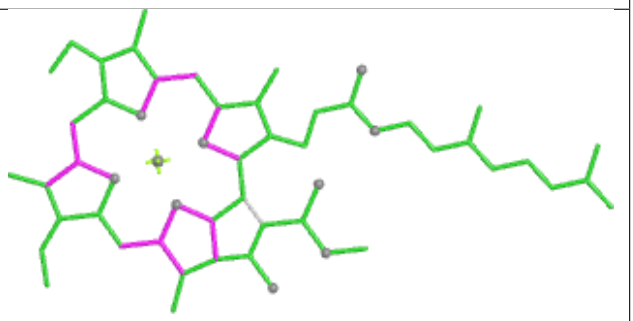

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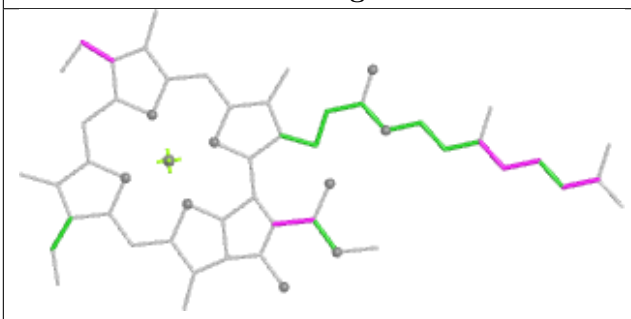

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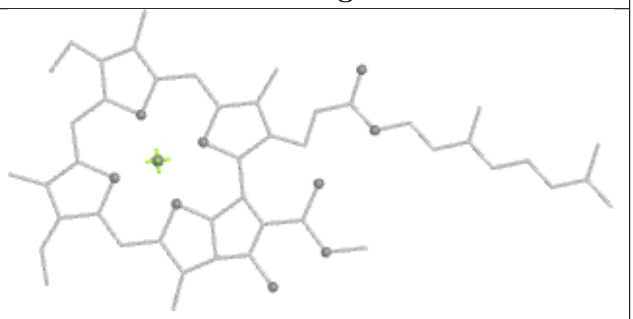
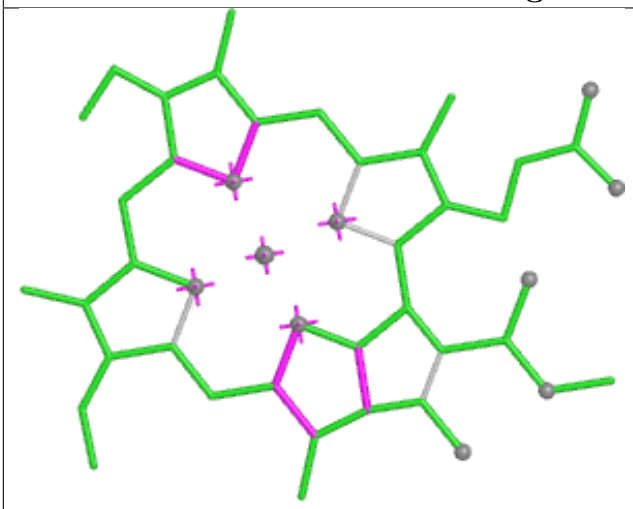


Rings

Ligand CLA F 203



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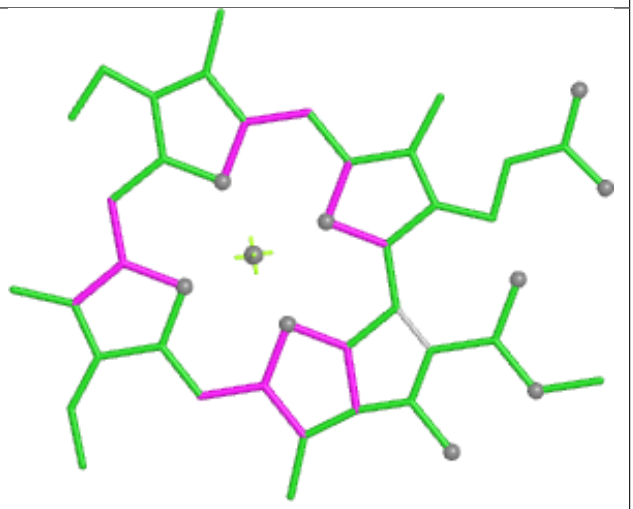
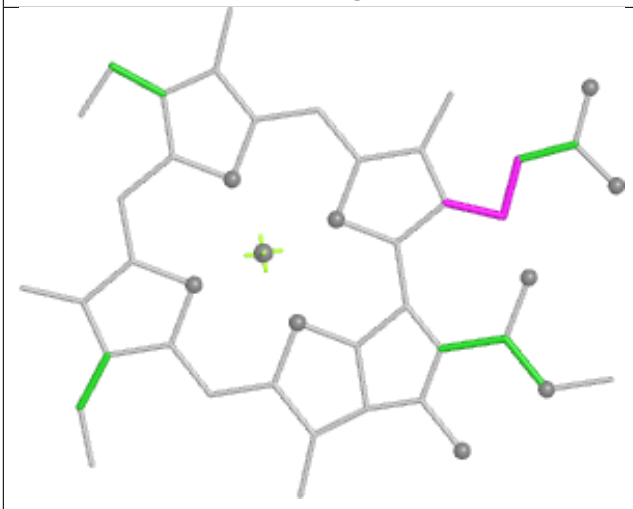


Bond angles

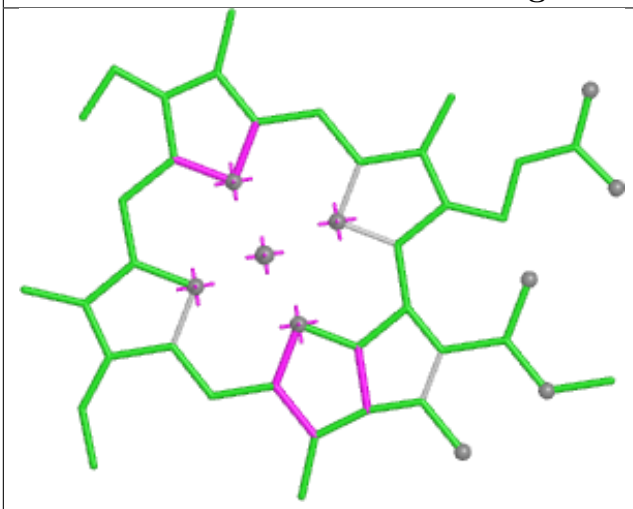


Torsions



Rings

Ligand CLA 2 607



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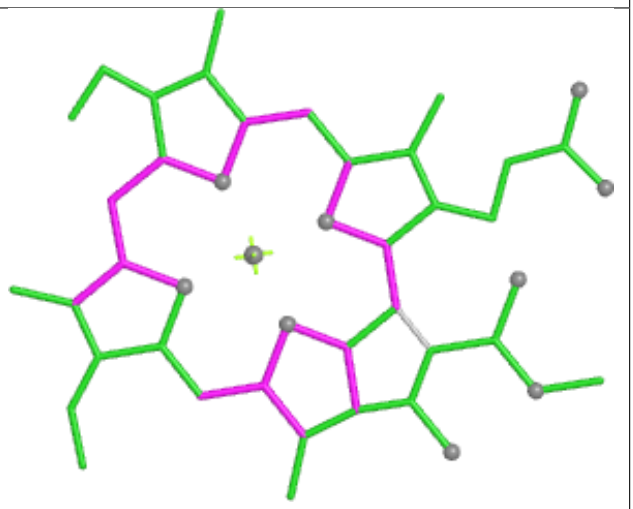
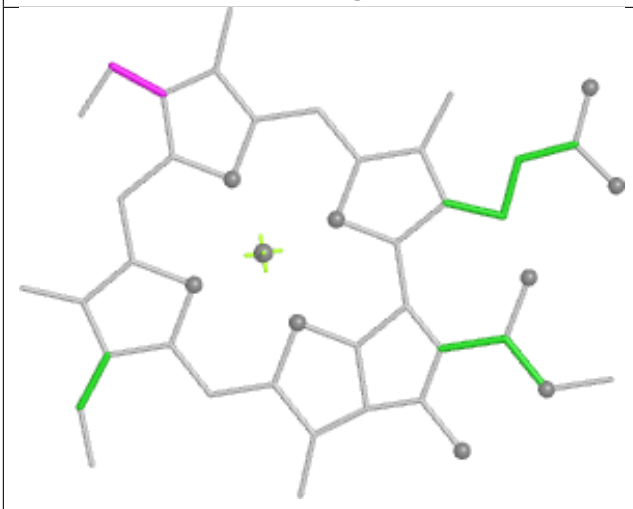


Bond angles

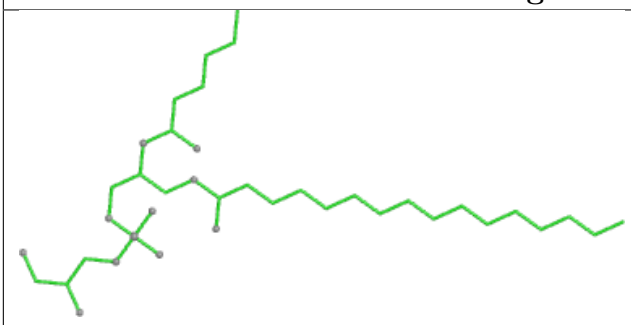


Torsions



Rings

Ligand LHG 7 619



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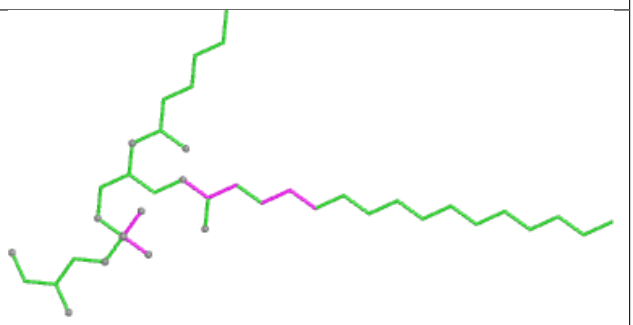
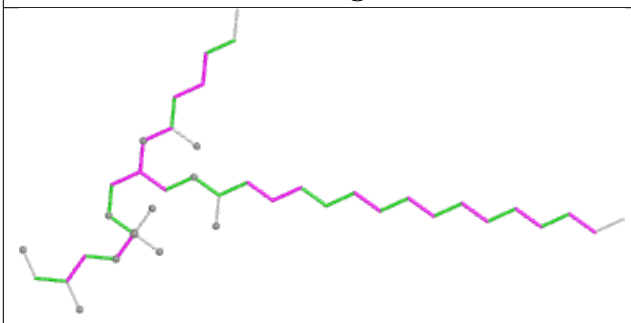


Bond angles



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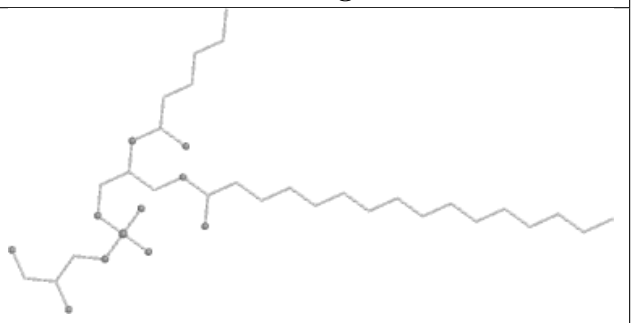
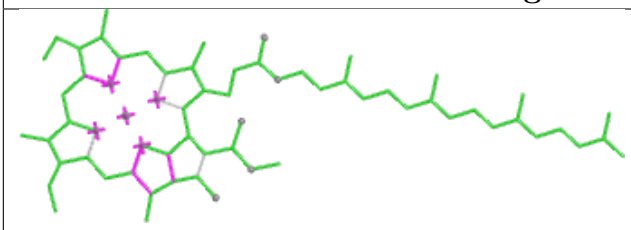


Rings

Ligand CLA A 803



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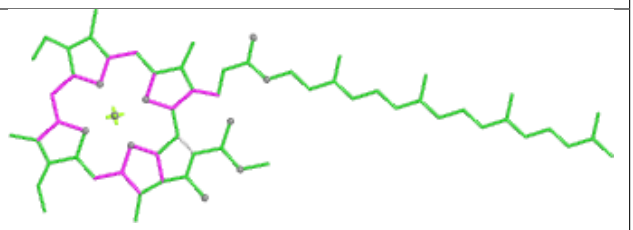

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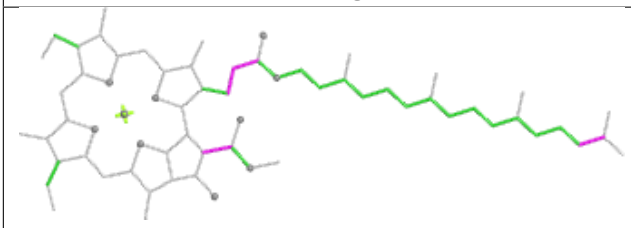

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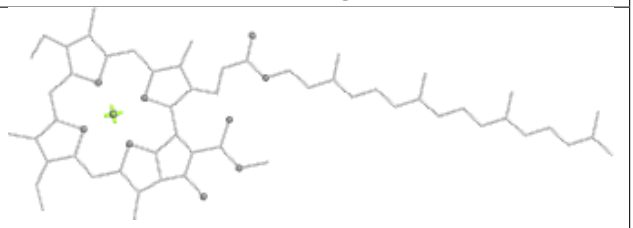
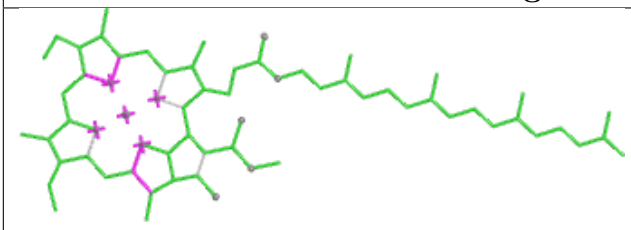


Rings

Ligand CLA A 801



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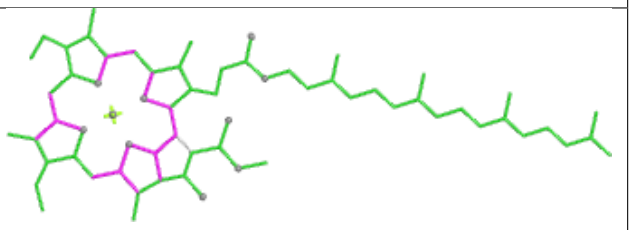
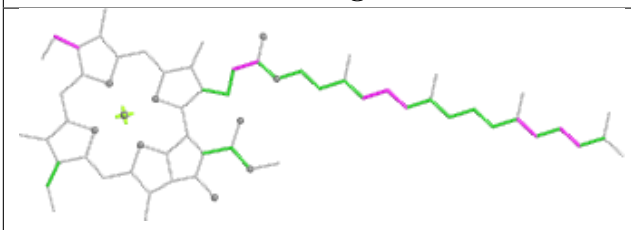


Bond angles



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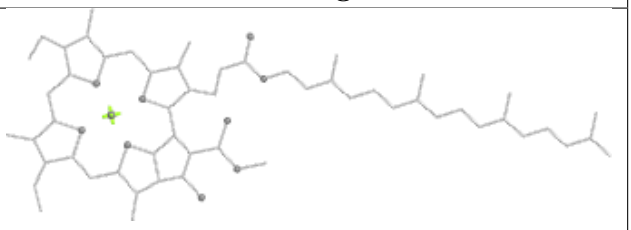
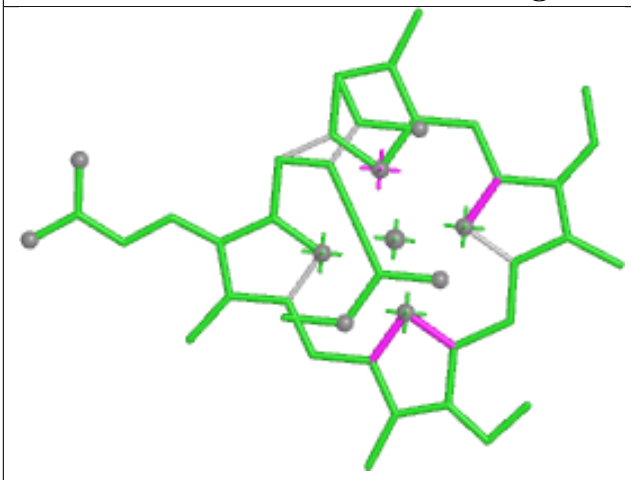


Rings

Ligand KC2 e 609



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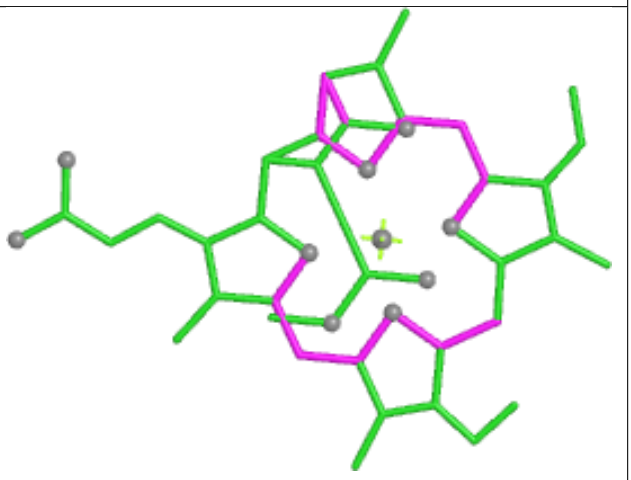
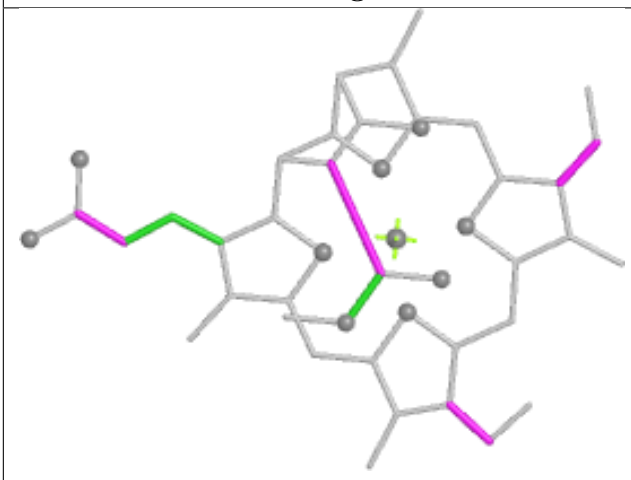


Bond angles



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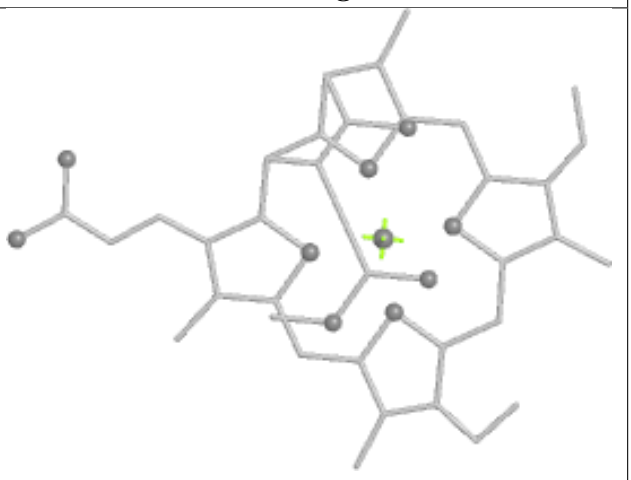
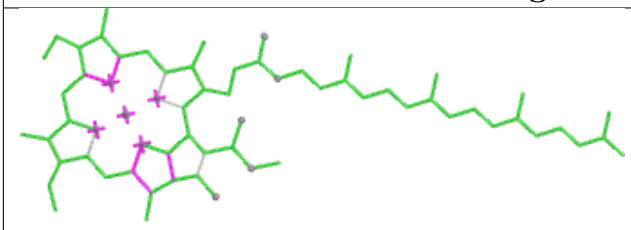
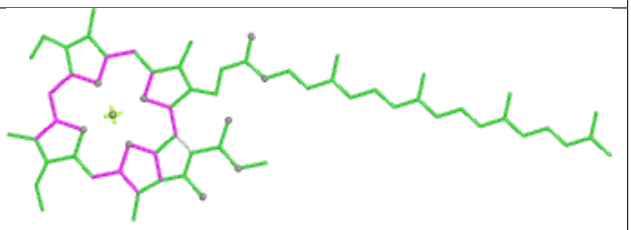
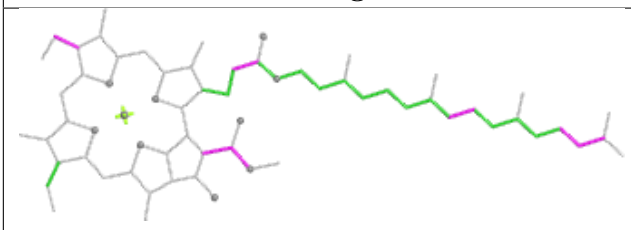
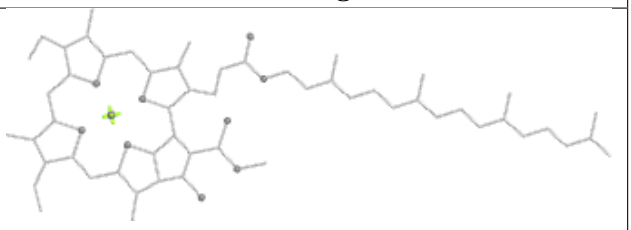
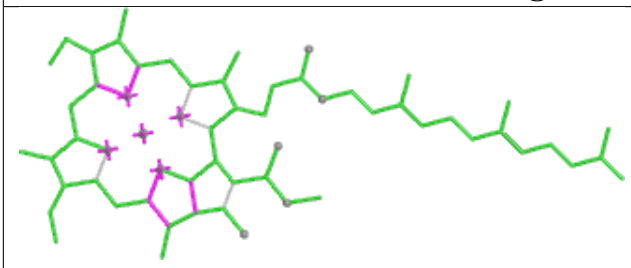
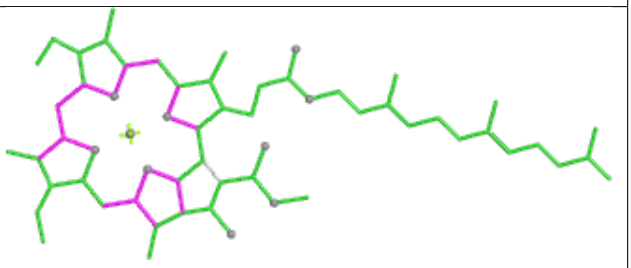
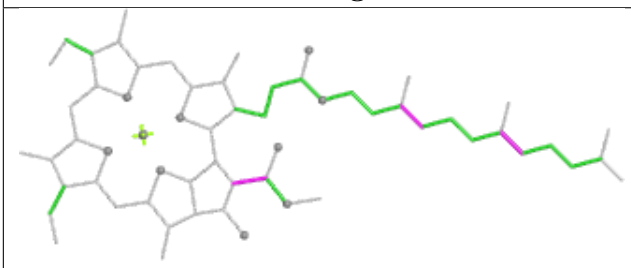
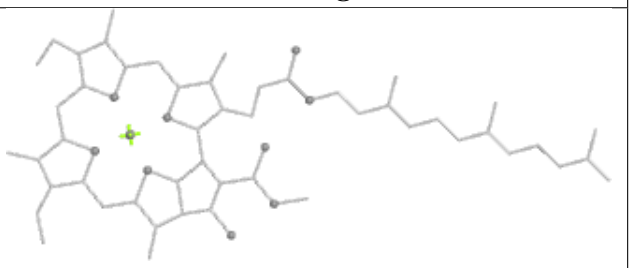
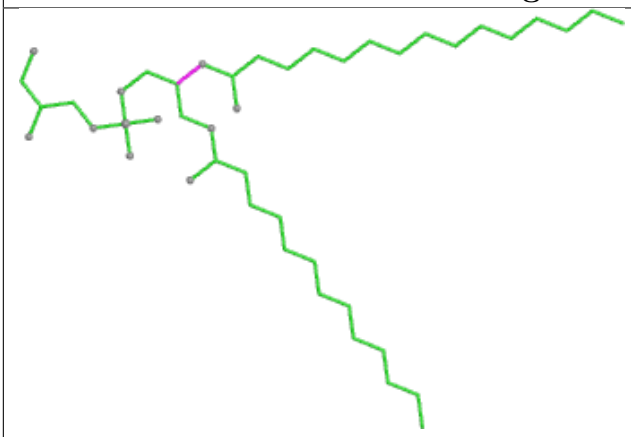


Rings

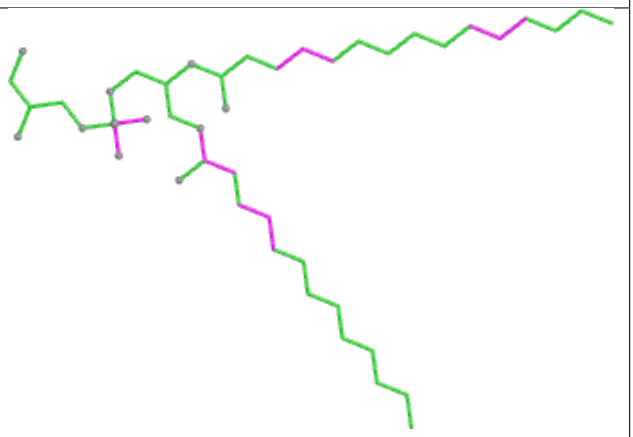
Ligand CLA e 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 6 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

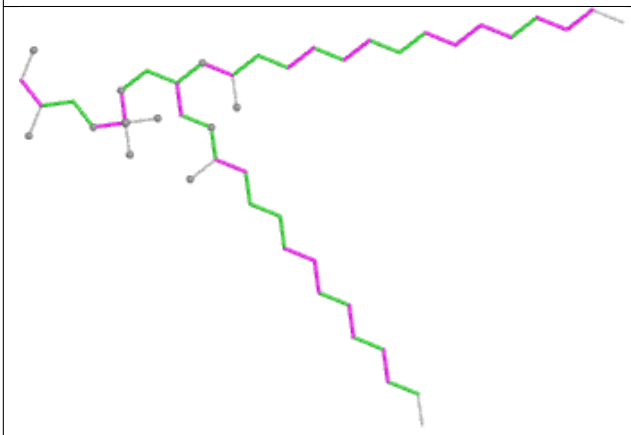
Ligand LHG B 849



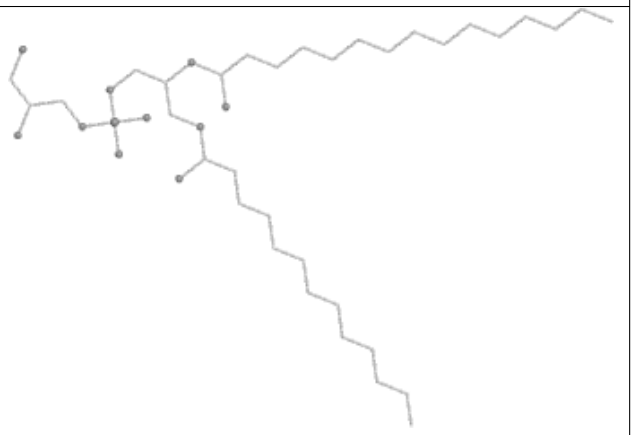
Bond lengths



Bond angles

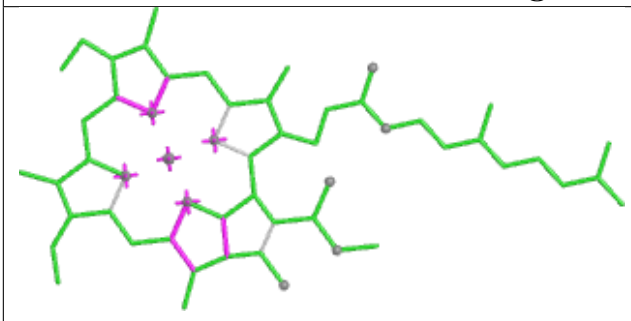


Torsions



Rings

Ligand CLA 7 603



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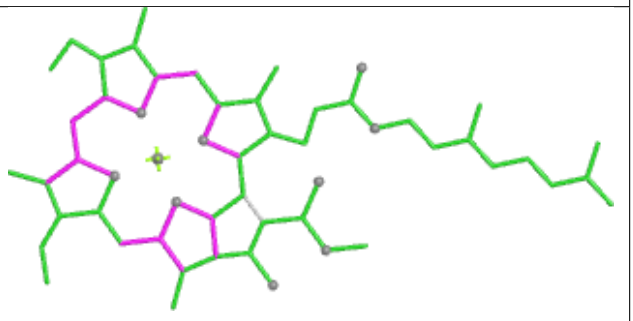
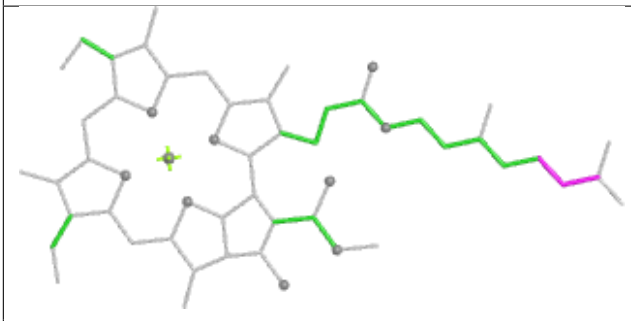


Bond angles



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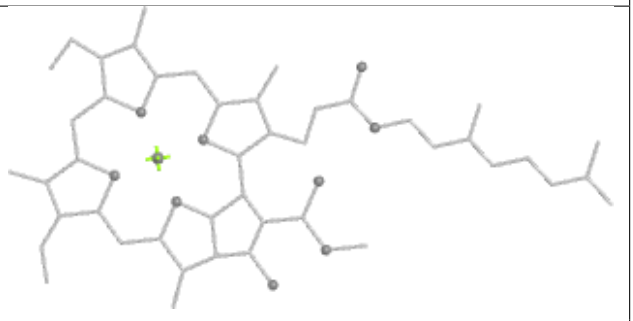
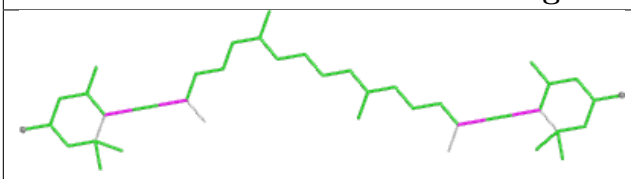


Rings

Ligand II0 7 613



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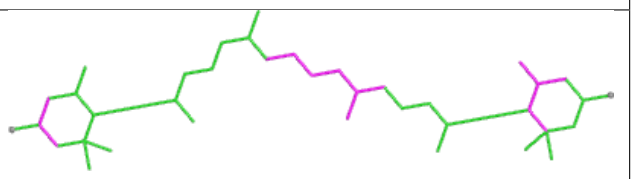
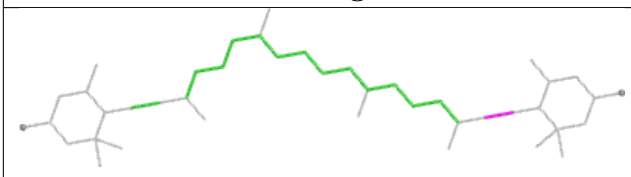


Bond angles



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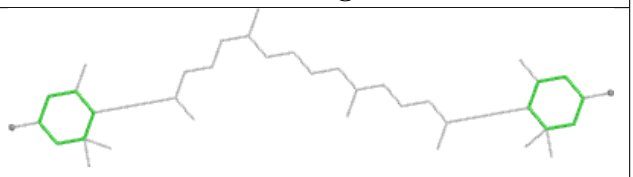
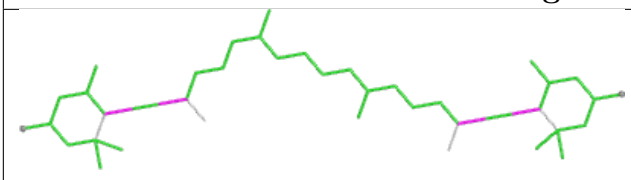


Rings

Ligand II0 1 616



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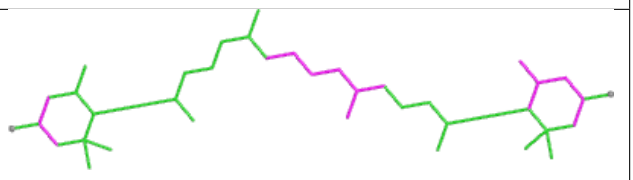
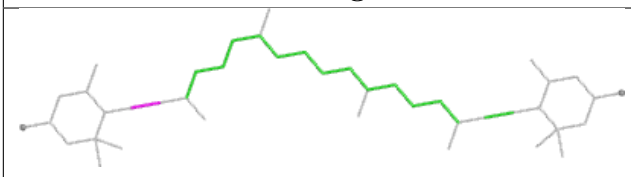


Bond angles



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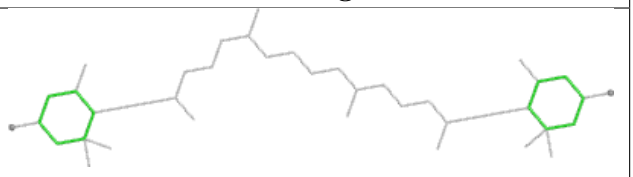
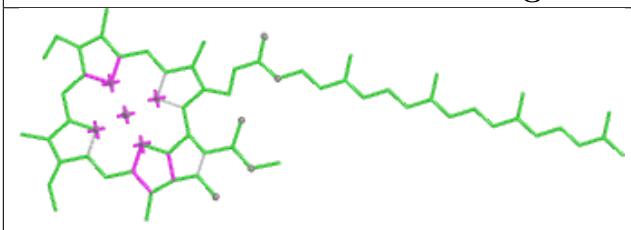


Rings

Ligand CLA A 827



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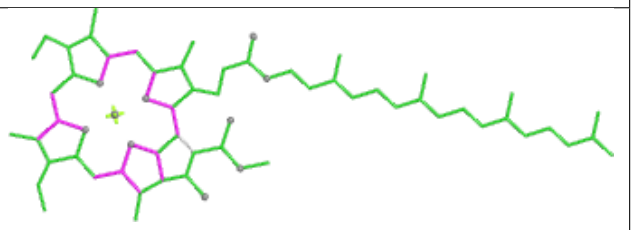
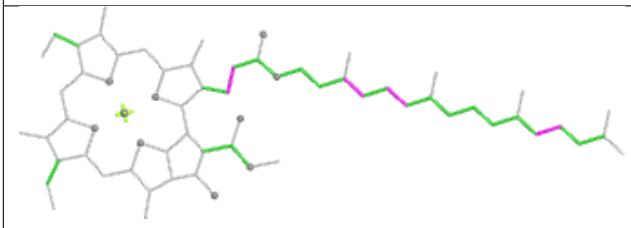


Bond angles



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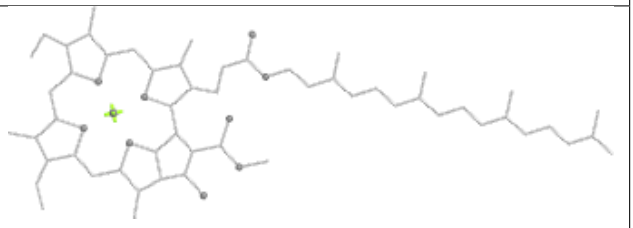
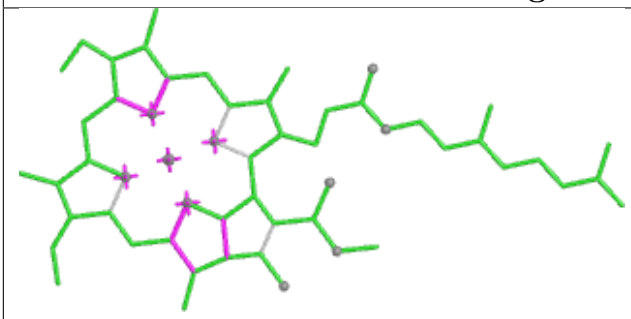
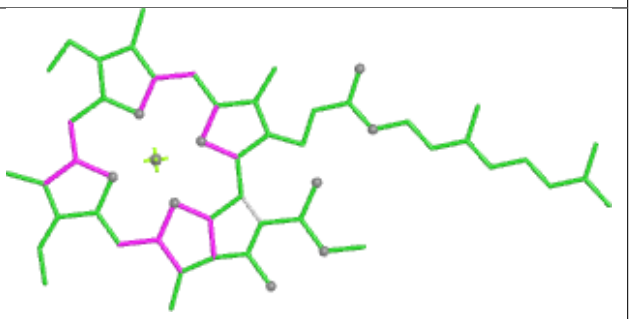
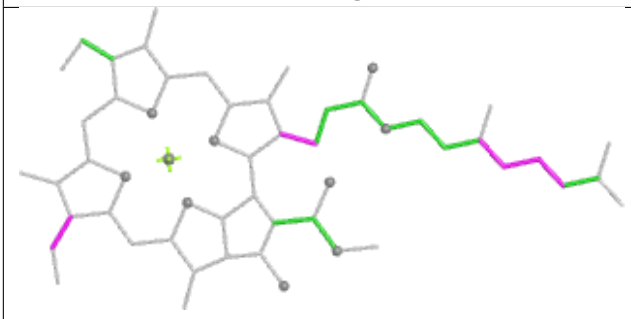
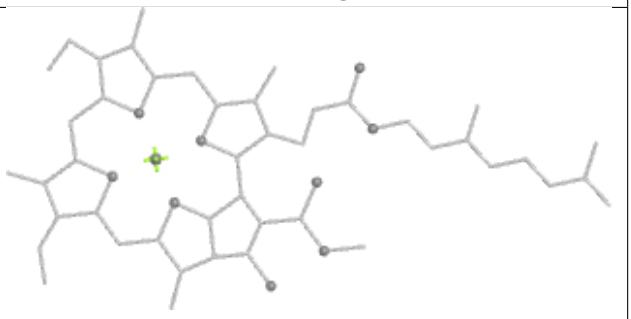


Rings

Ligand CLA 4 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

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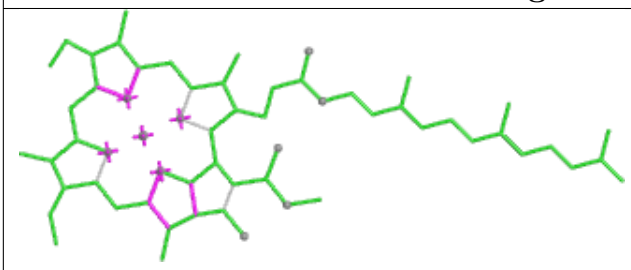
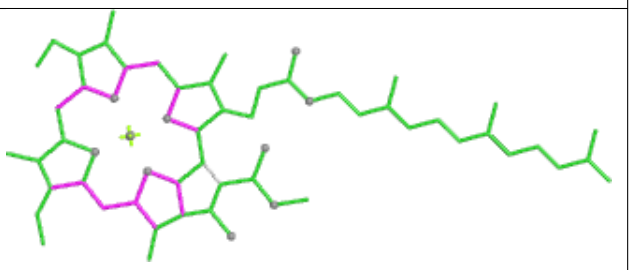
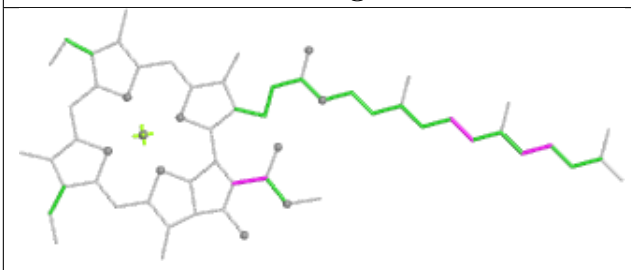
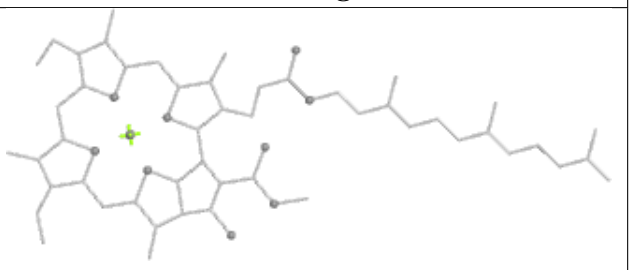
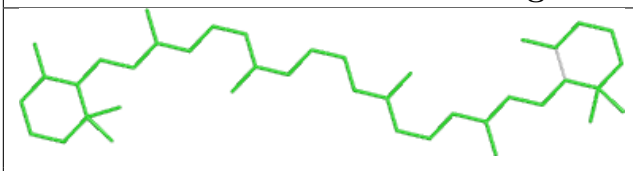
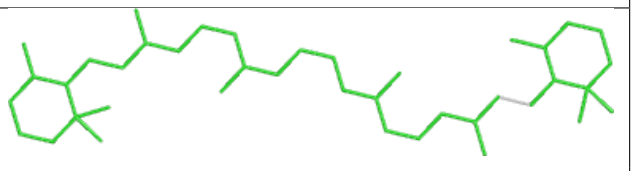
	
Bond lengths	Bond angles
	
Torsions	Rings

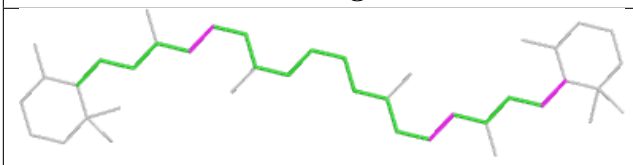
Ligand 8CT B 844



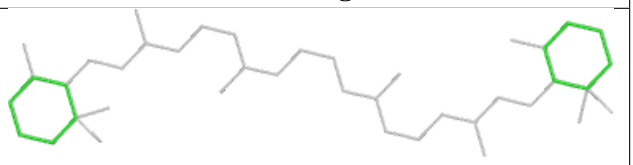
Bond lengths



Bond angles

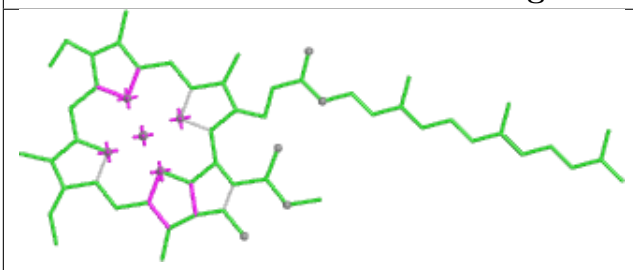


Torsions



Rings

Ligand CLA b 603



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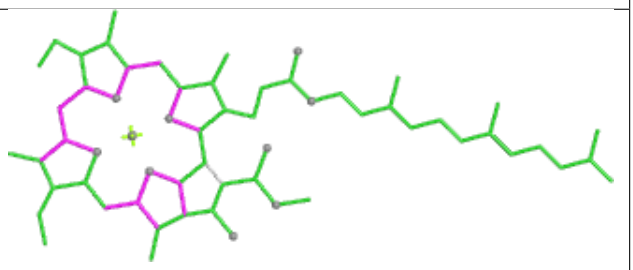
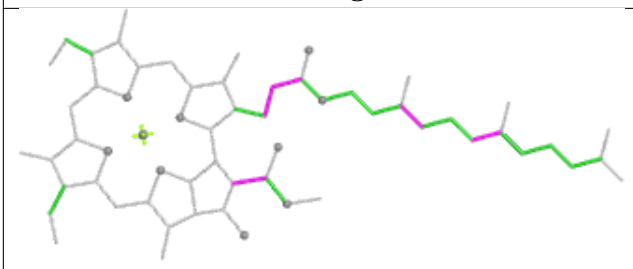


Bond angles



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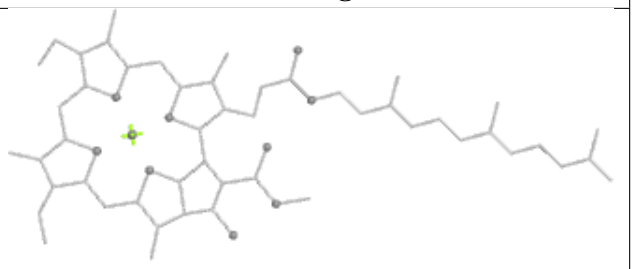
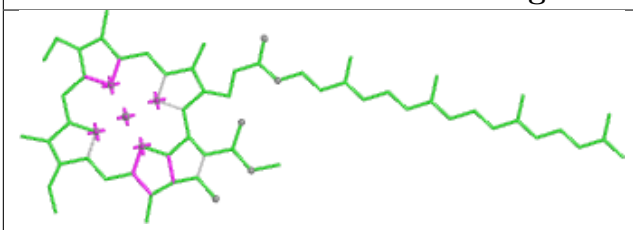


Rings

Ligand CLA 3 604



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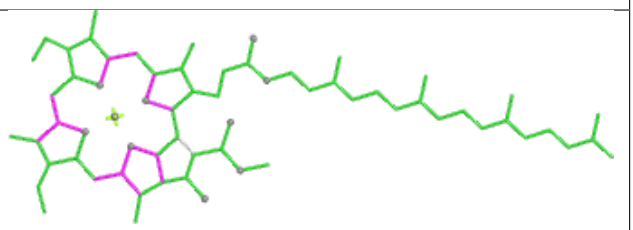
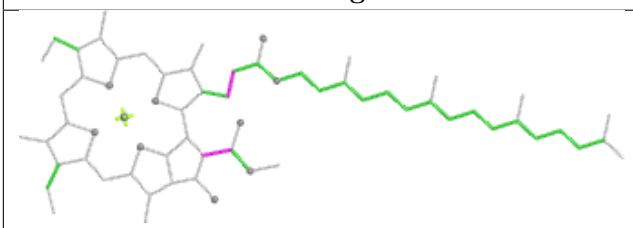


Bond angles



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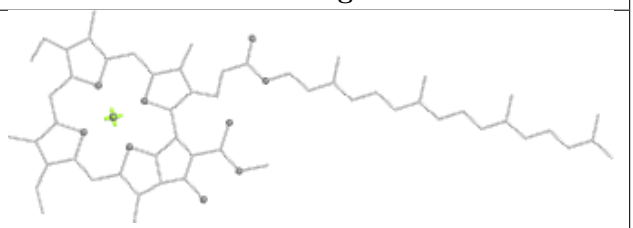
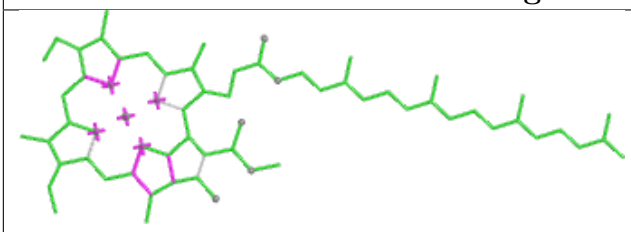


Rings

Ligand CLA A 842



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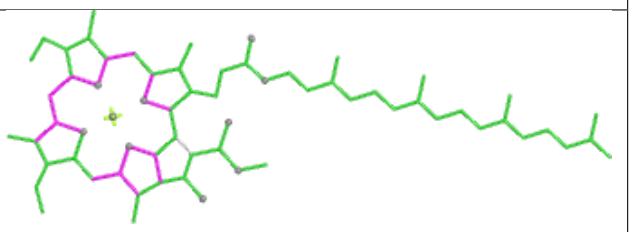
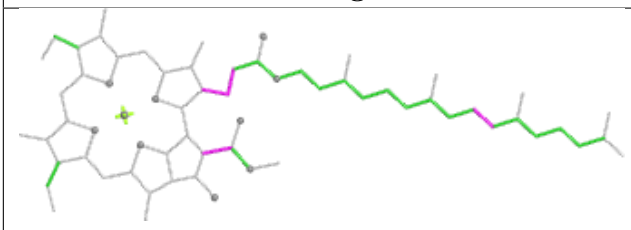


Bond angles



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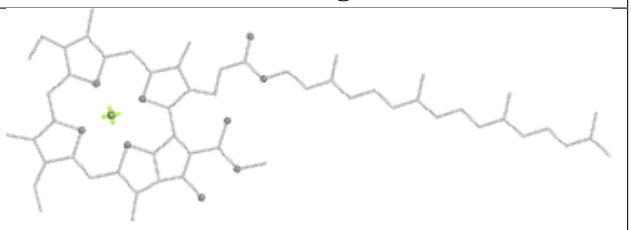
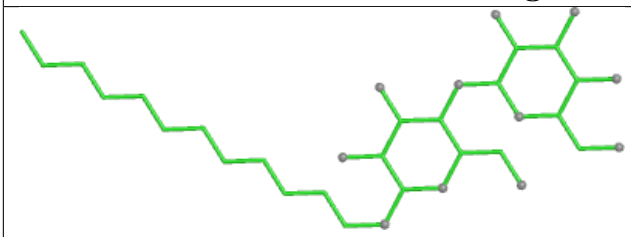


Rings

Ligand LMU 7 620



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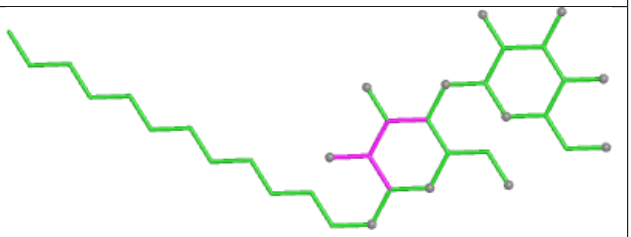

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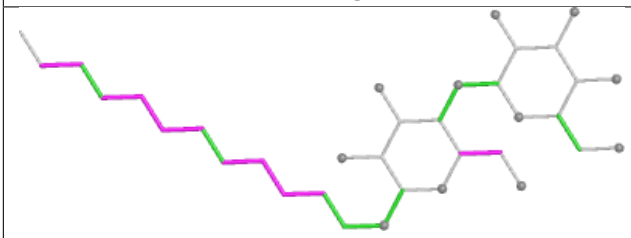

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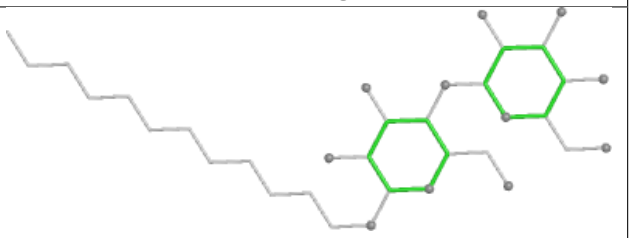
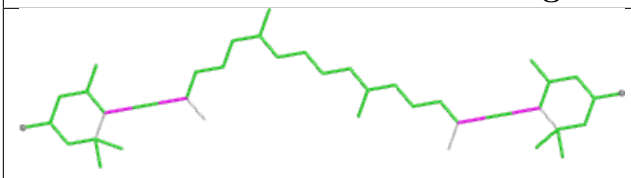


Rings

Ligand II0 8 610



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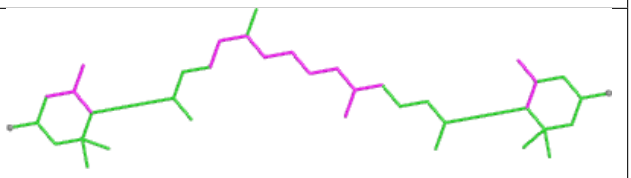
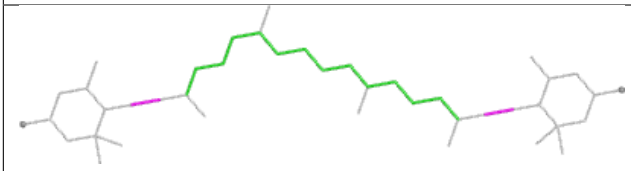


Bond angles



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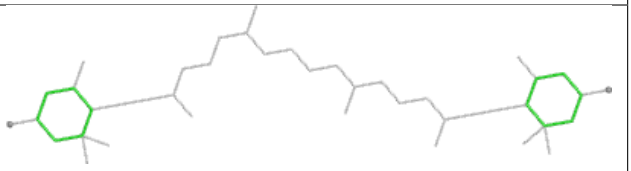
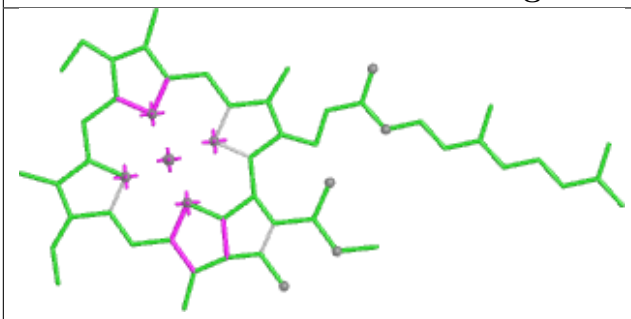
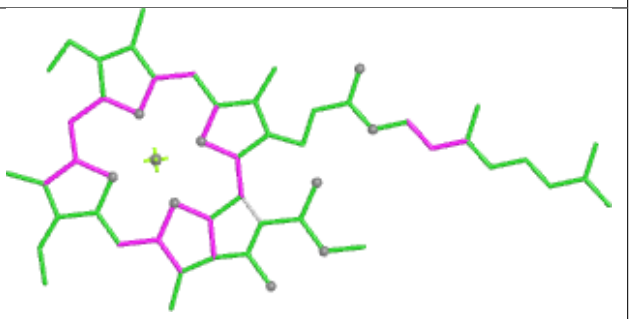
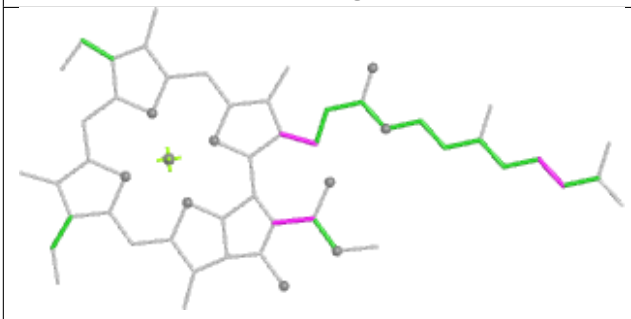
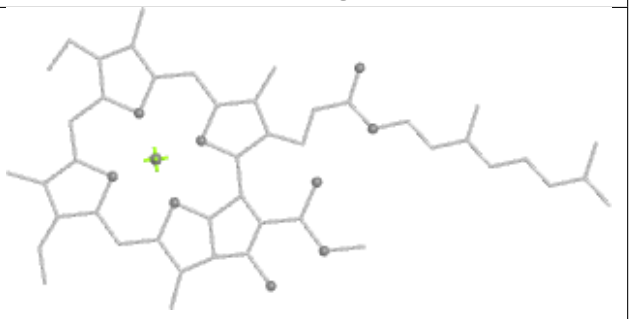
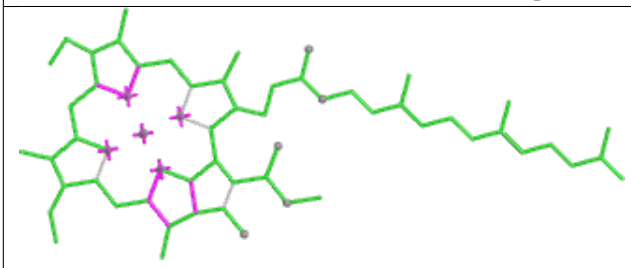
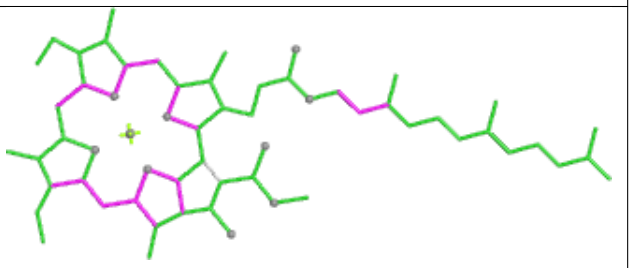
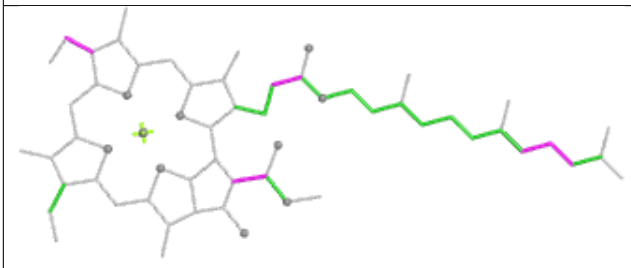
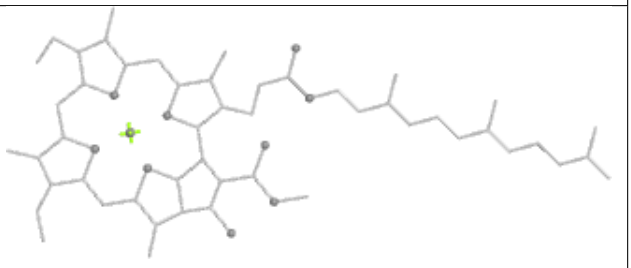
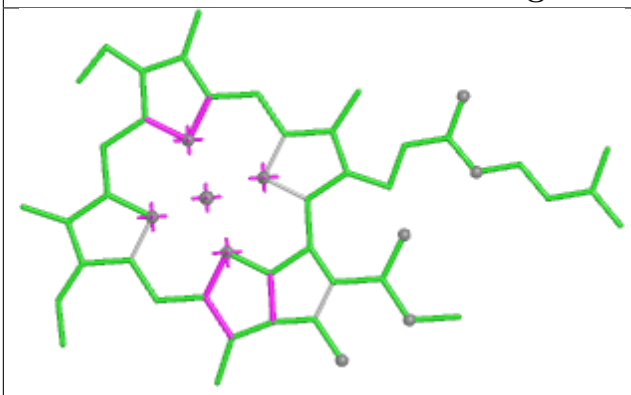


Rings

Ligand CLA A 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 603



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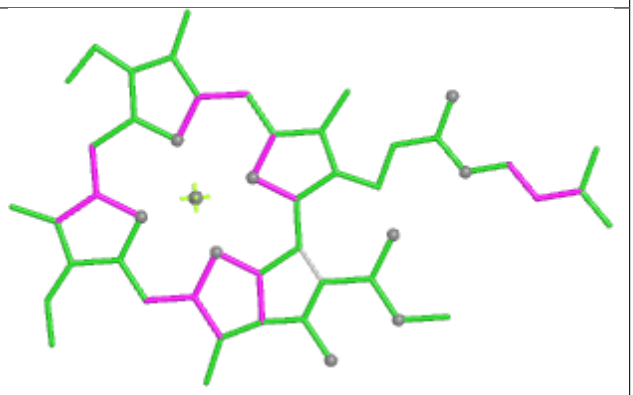

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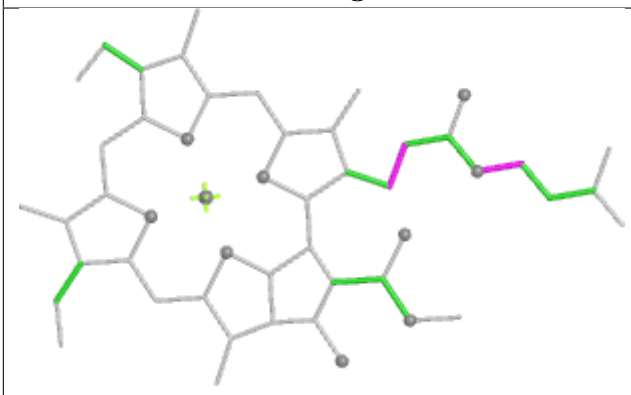

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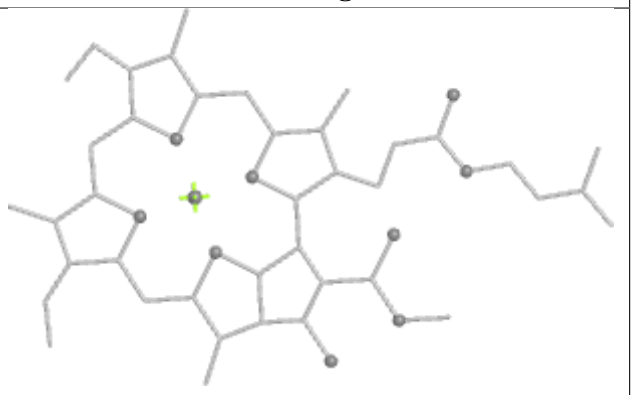
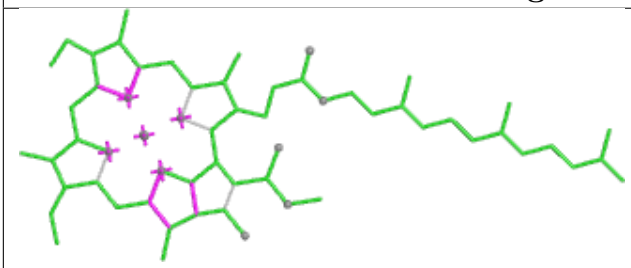


Rings

Ligand CLA d 604



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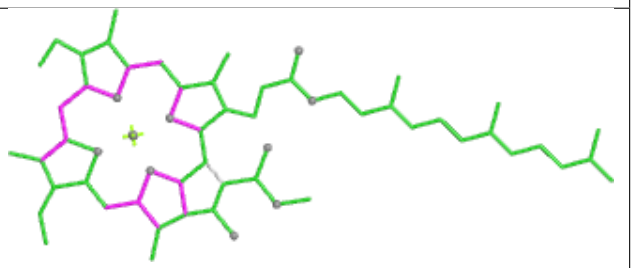

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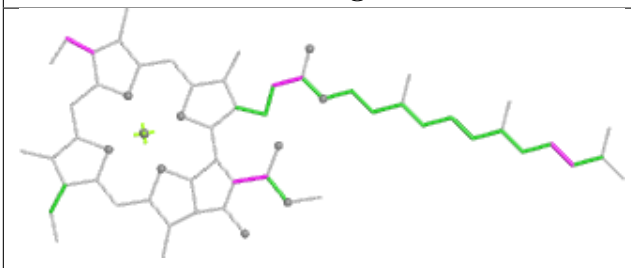

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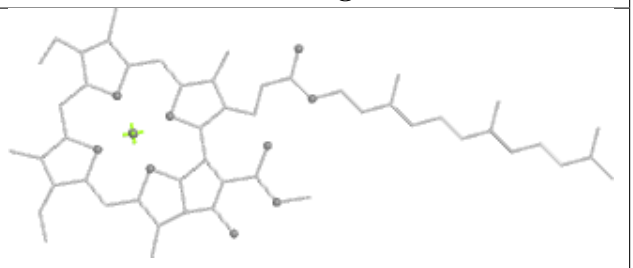

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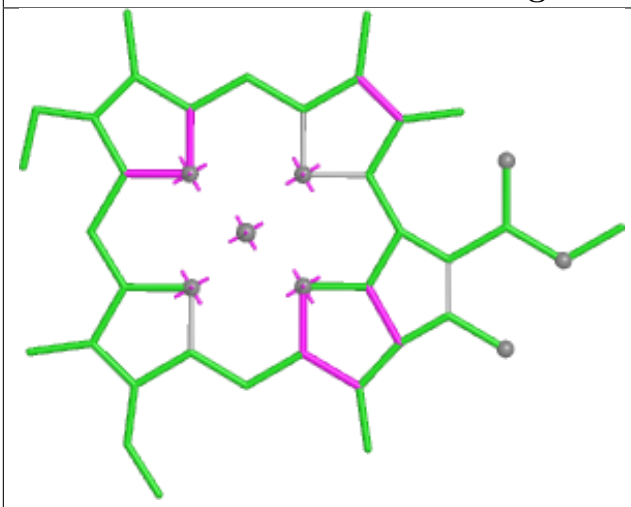

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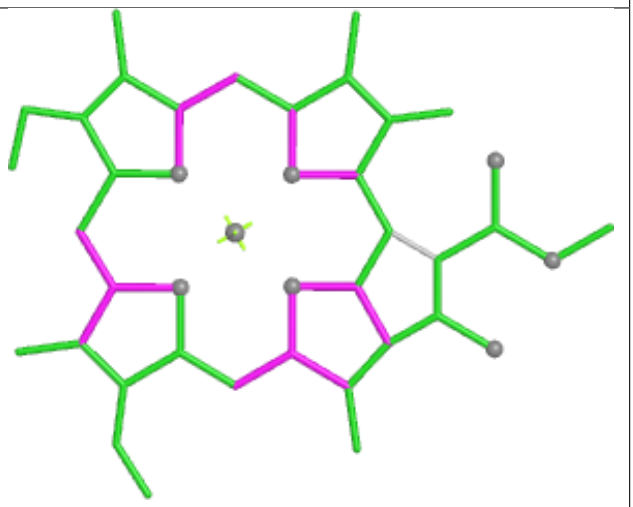

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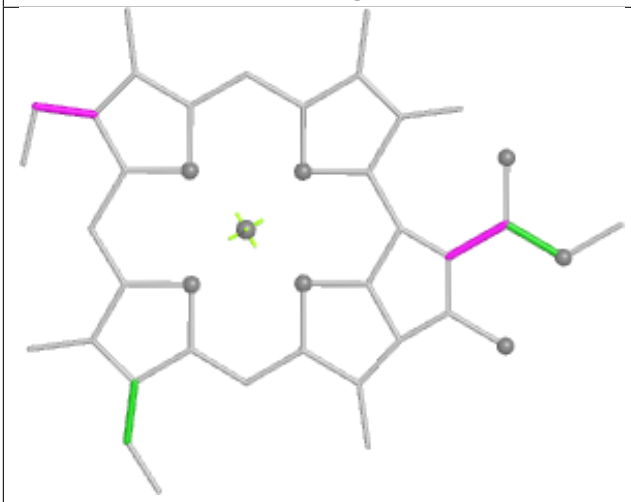

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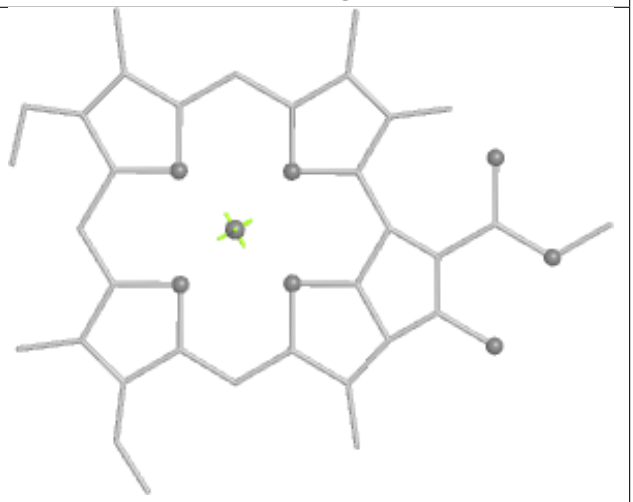

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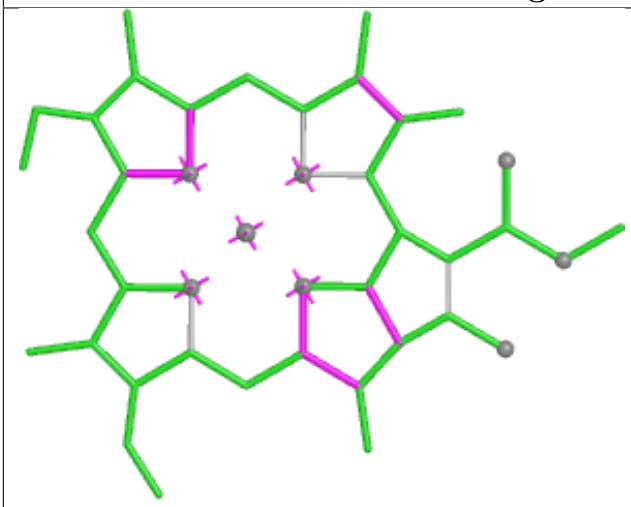

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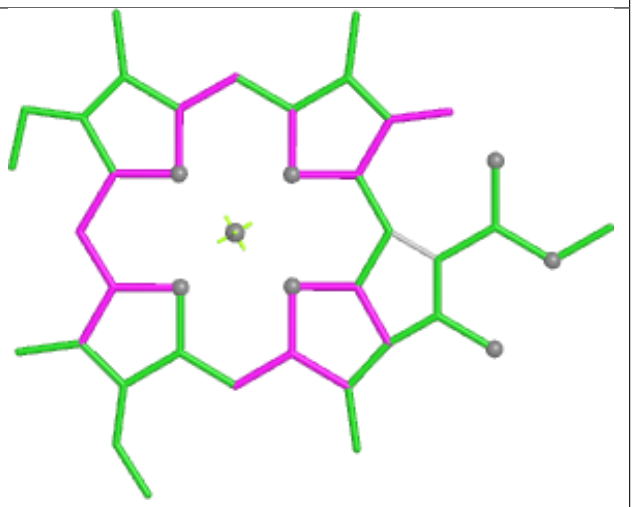

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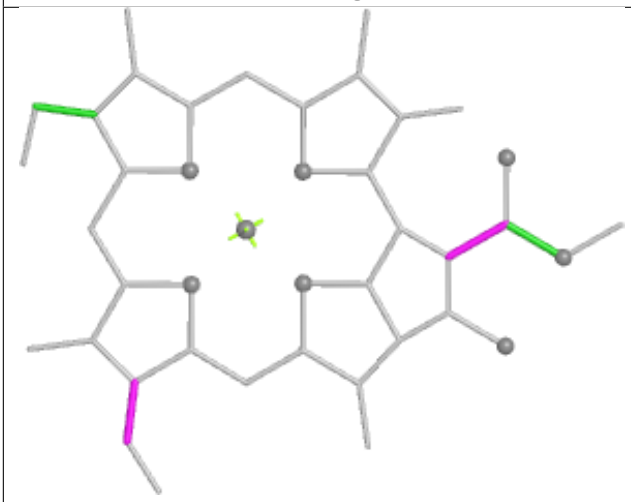

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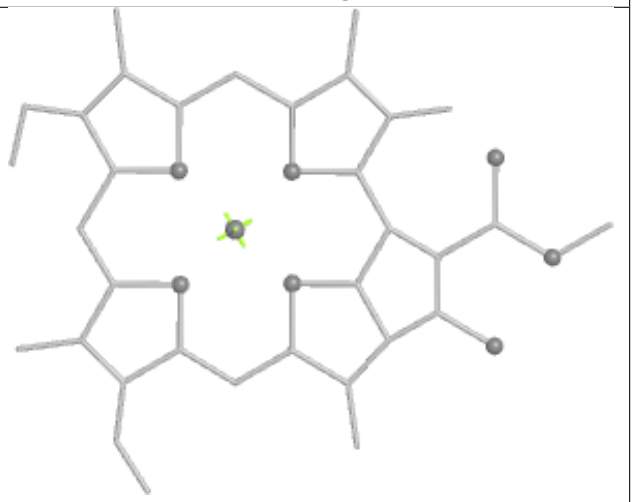

Rings

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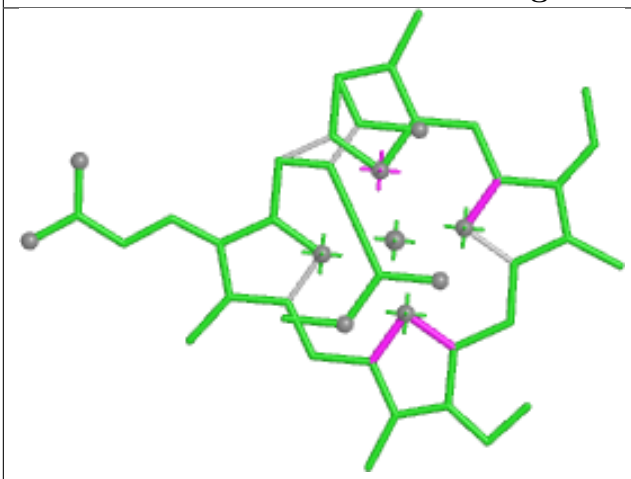

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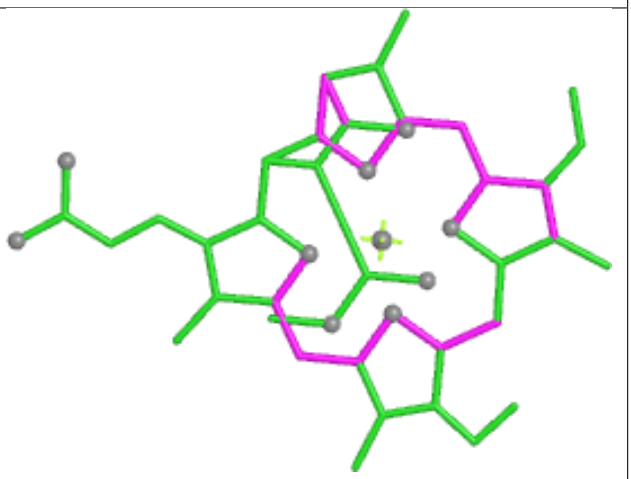

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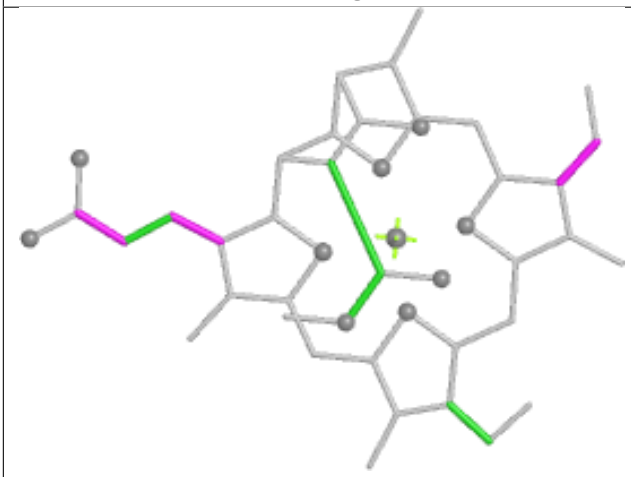

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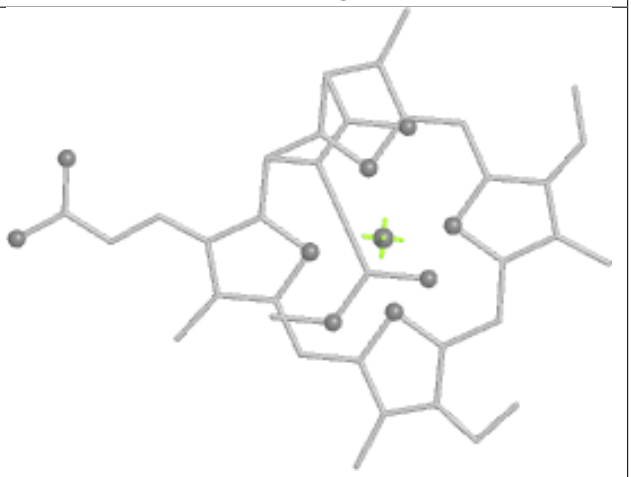

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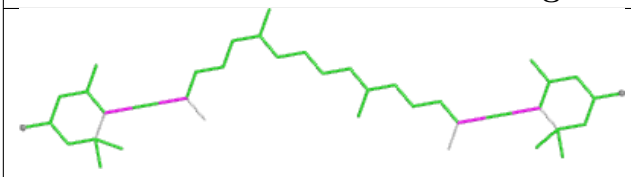

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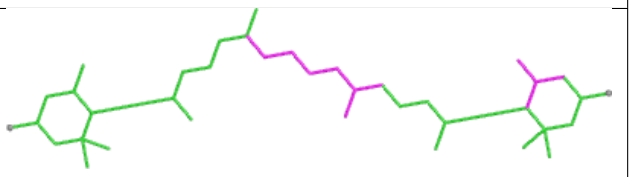

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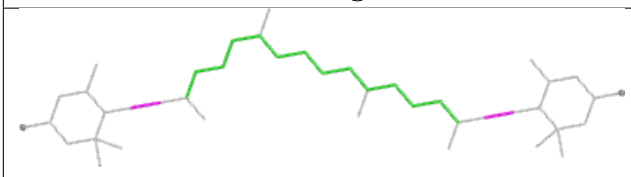

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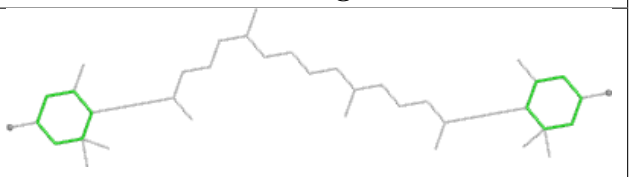
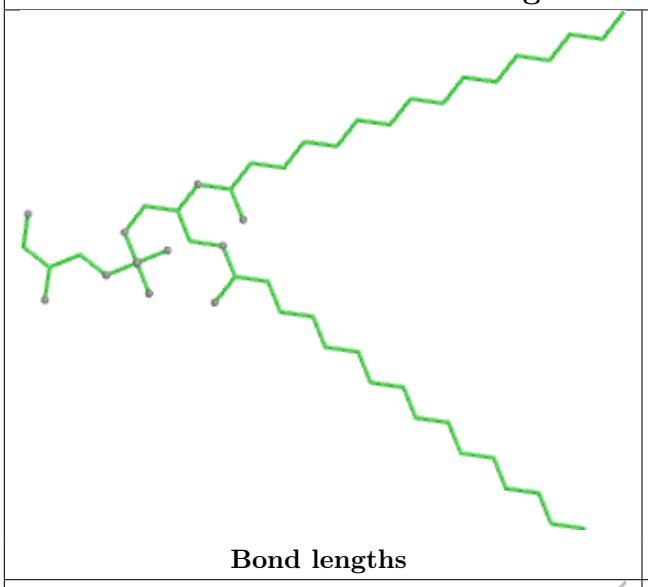


Rings

Ligand LHG A 850



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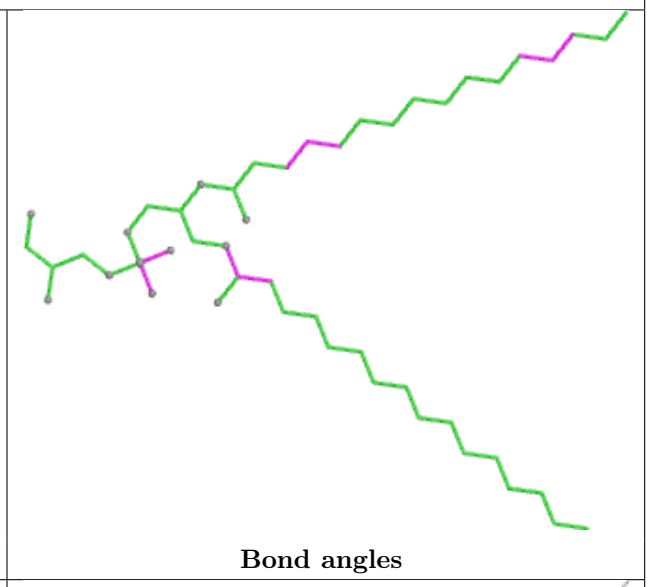

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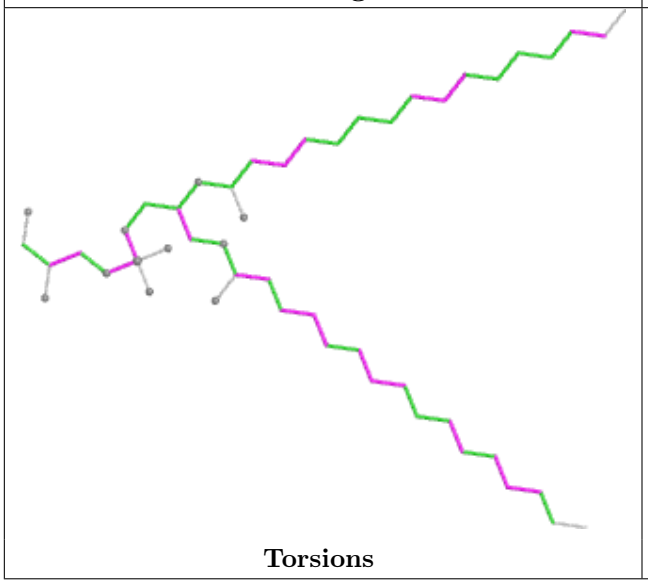

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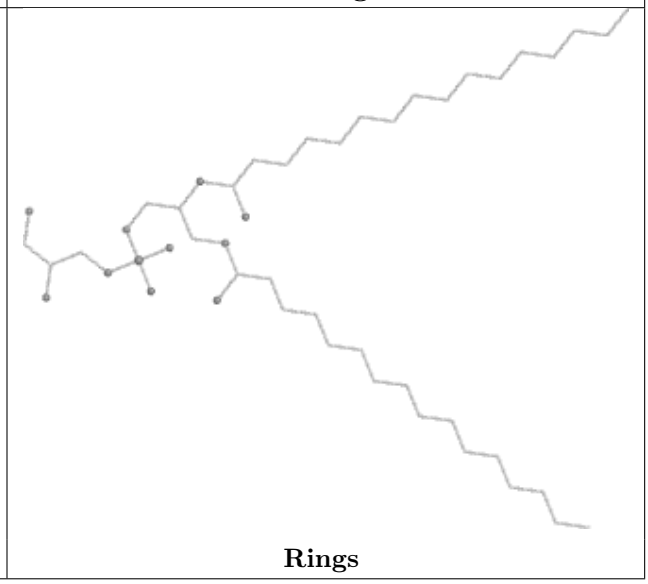
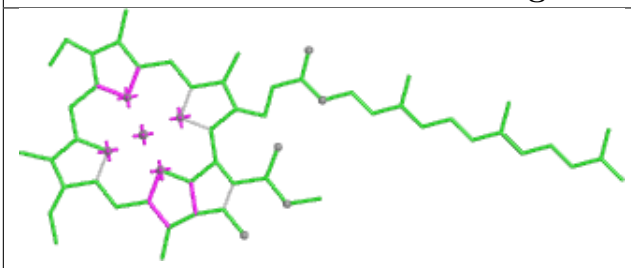
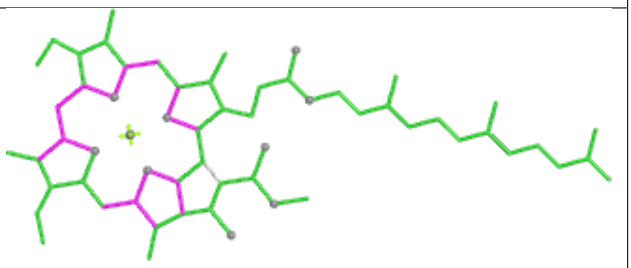
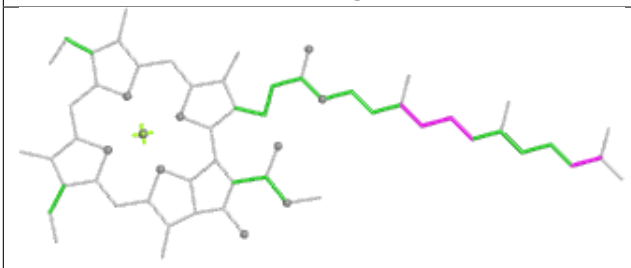
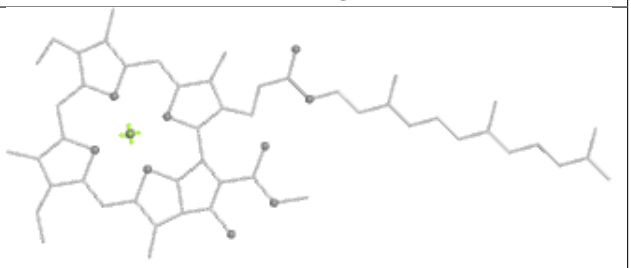


Rings

Ligand CLA 3 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

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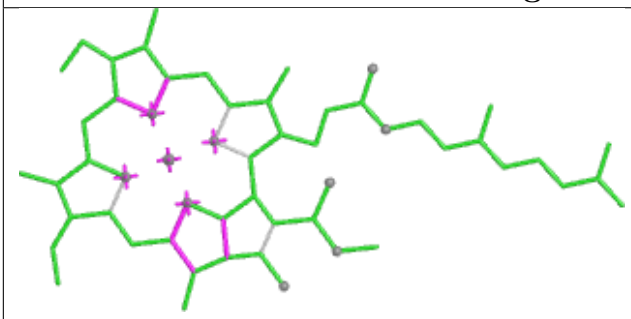
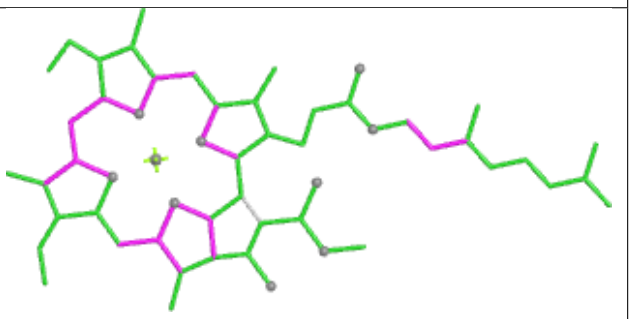
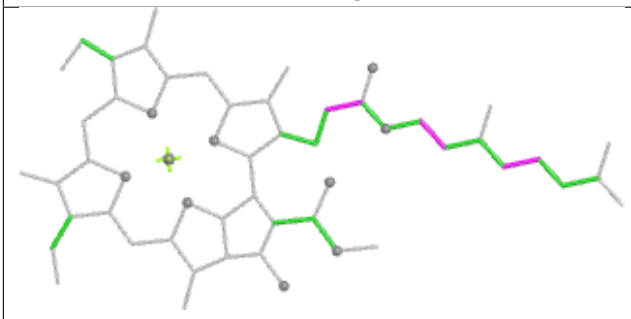
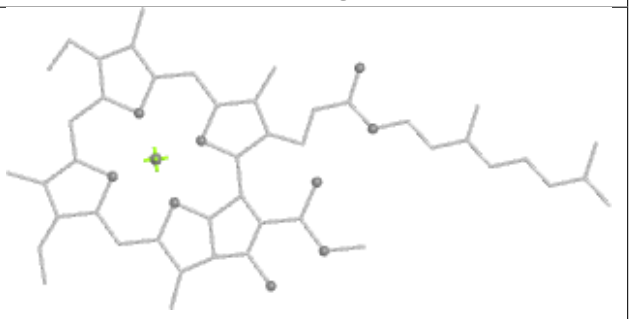
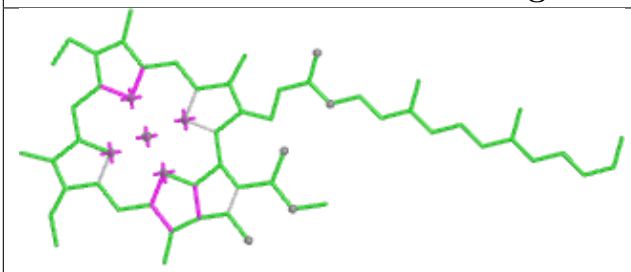
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 602



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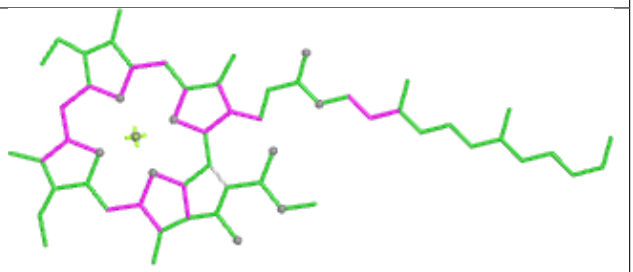
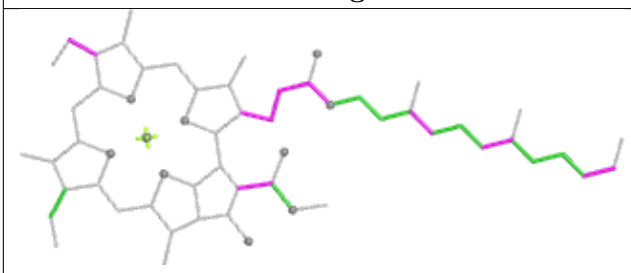


Bond angles



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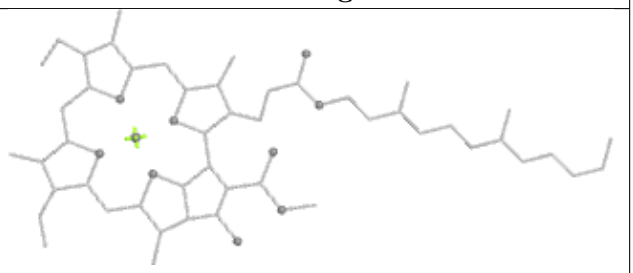
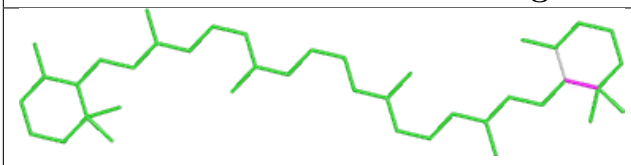


Rings

Ligand 8CT 7 617



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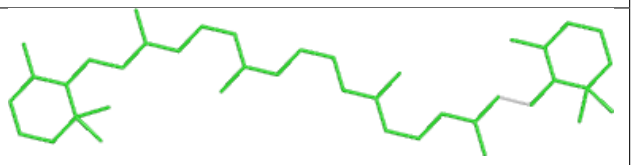

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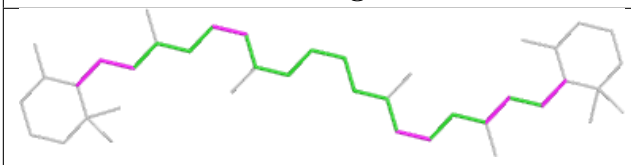

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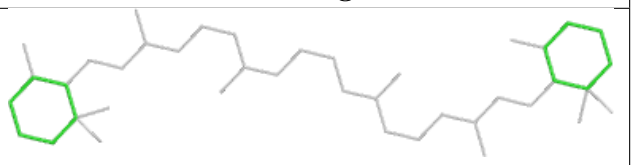
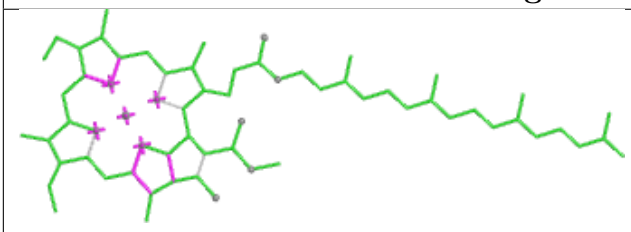


Rings

Ligand CLA B 827



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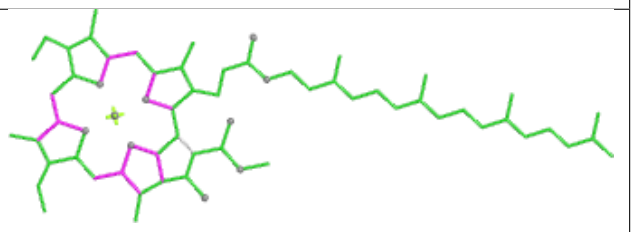
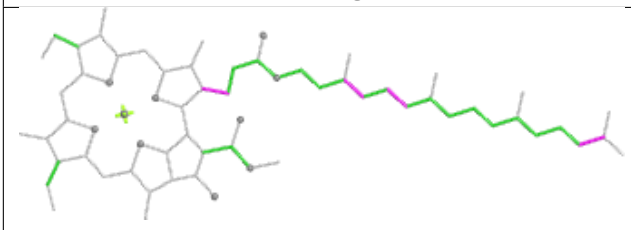


Bond angles



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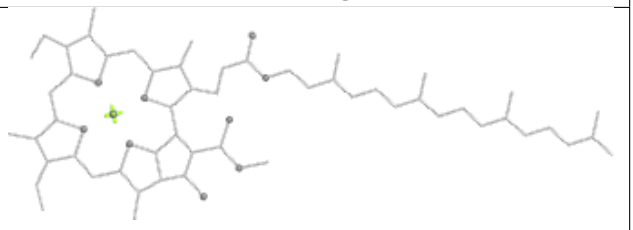
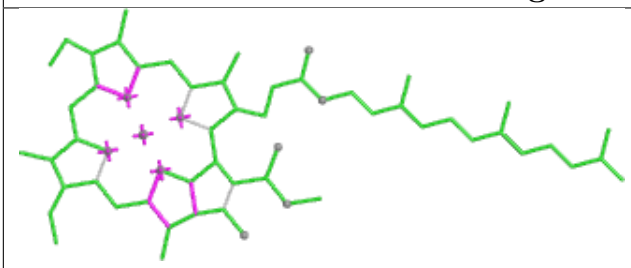
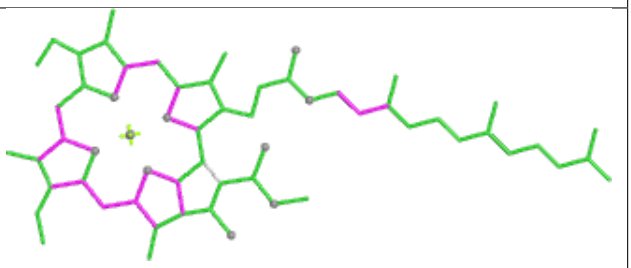
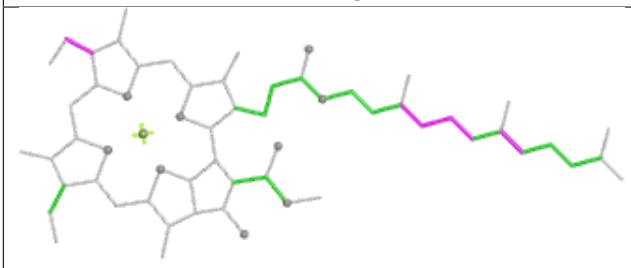
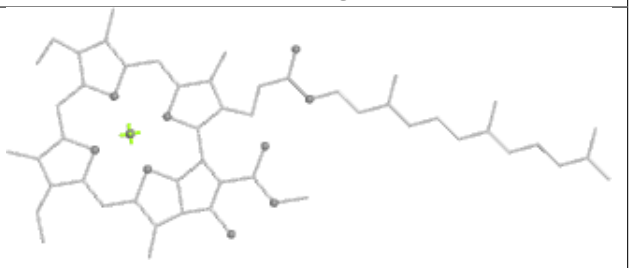


Rings

Ligand CLA 4 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

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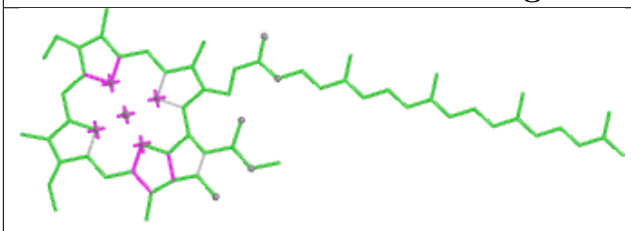
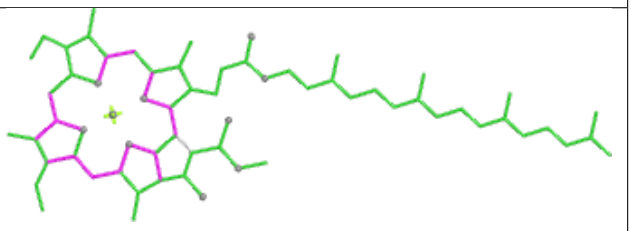
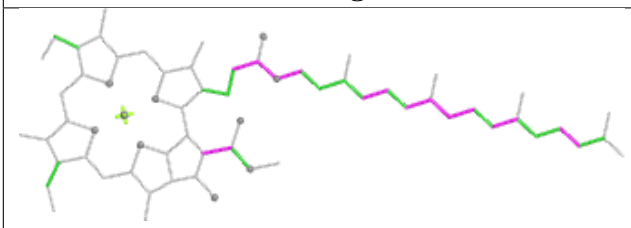
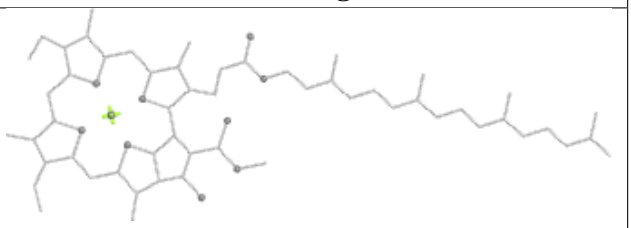
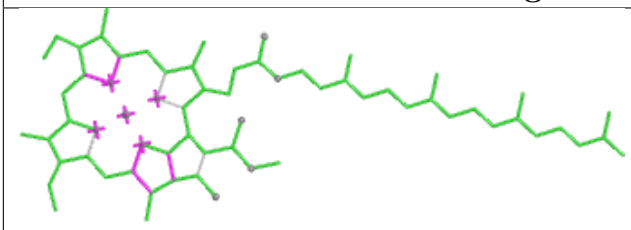
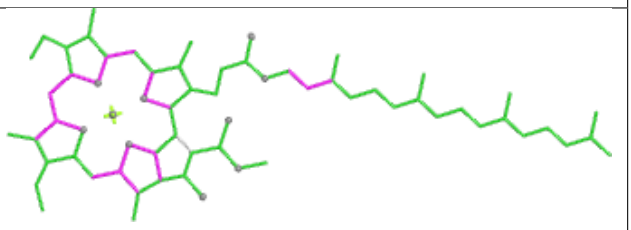
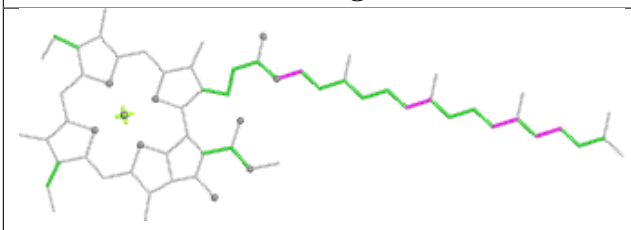
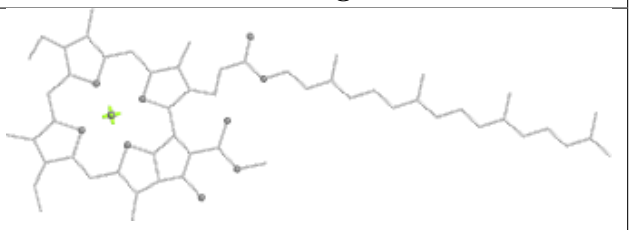
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

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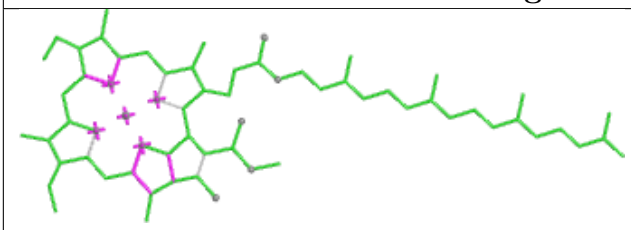
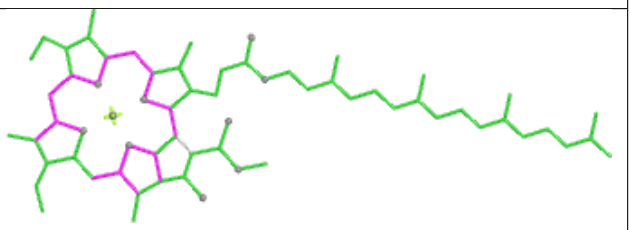
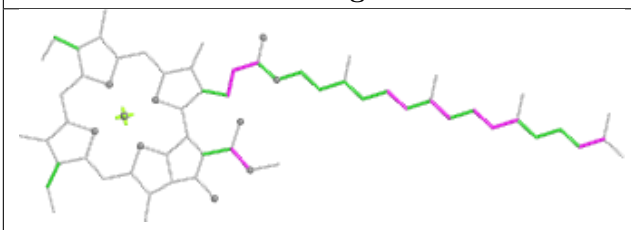
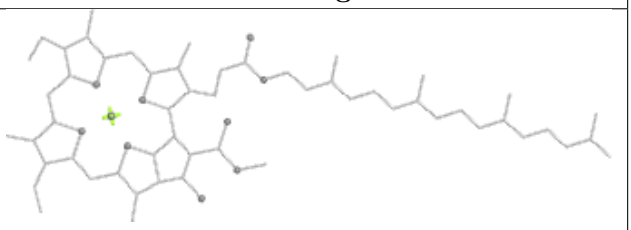
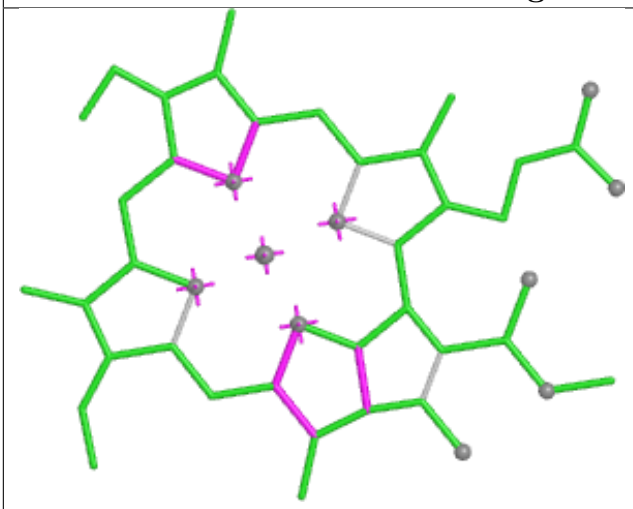
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 601



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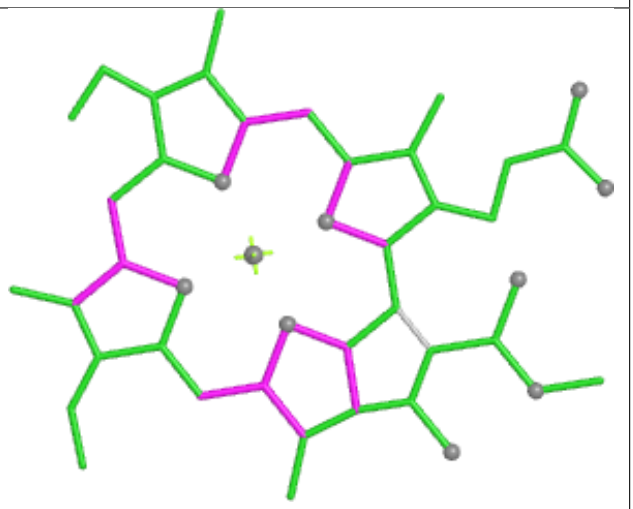

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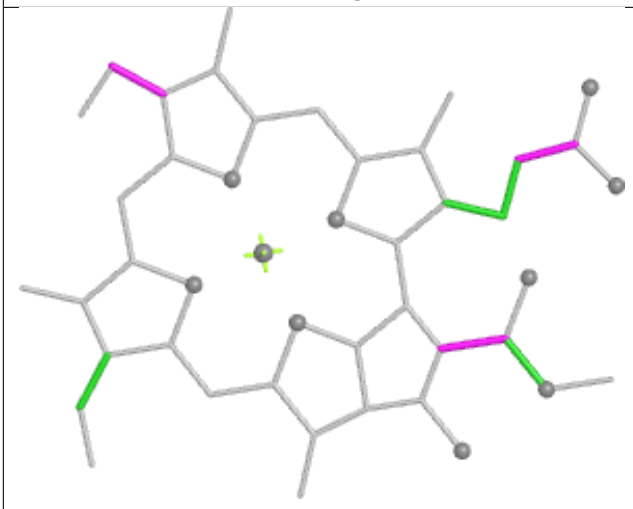

Torsions



Rings

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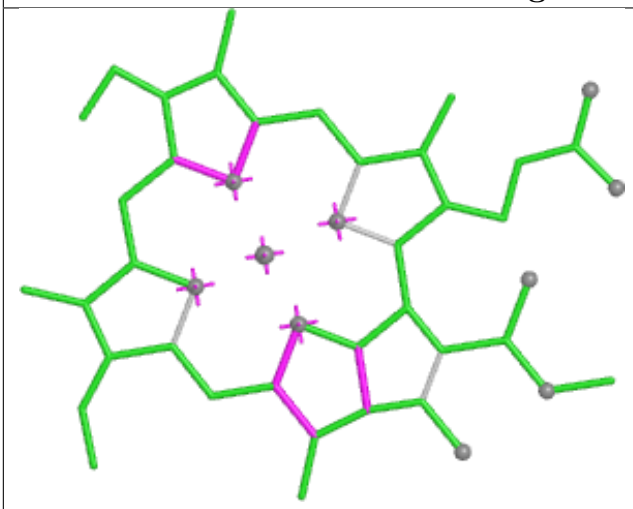

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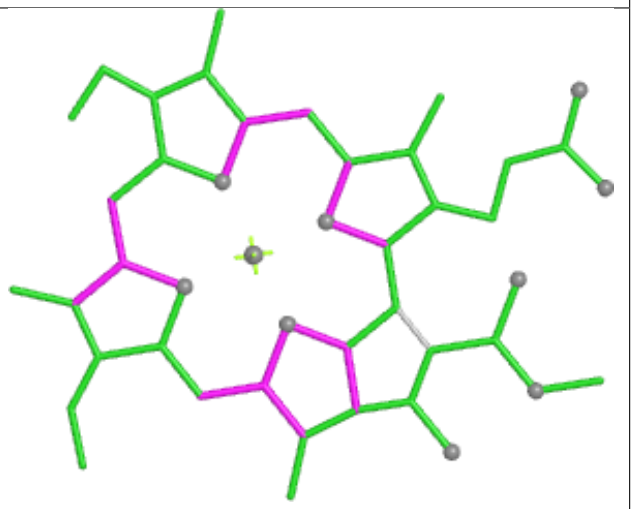
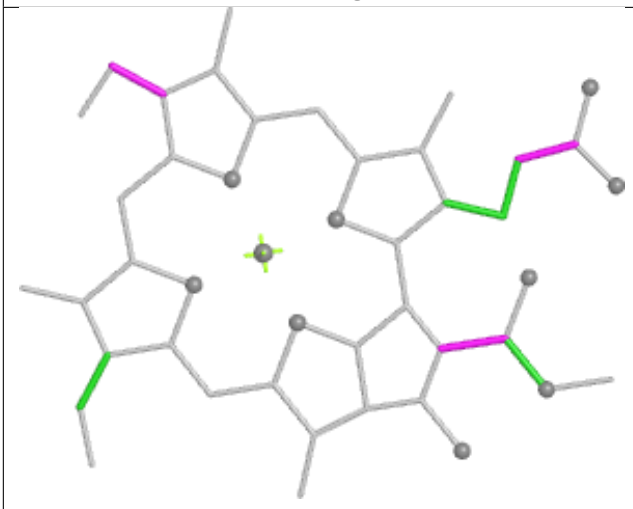


Bond angles



Torsions



Rings

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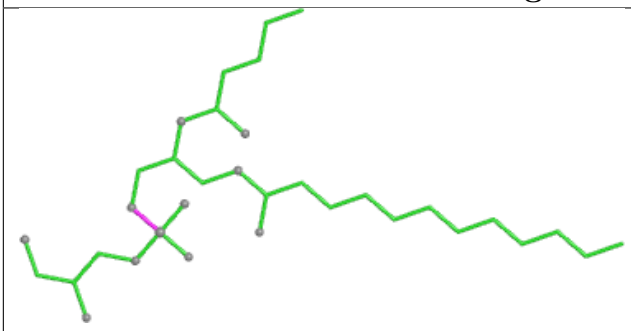

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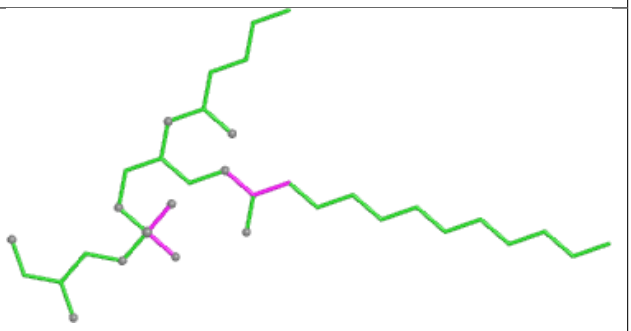

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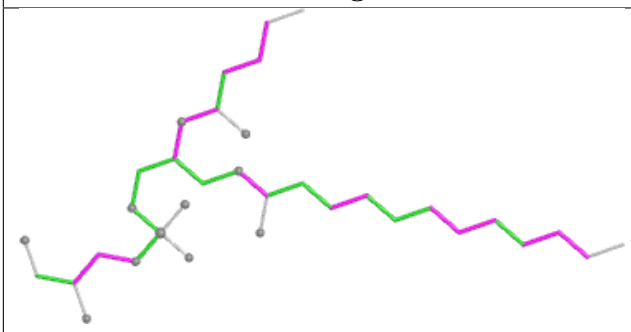
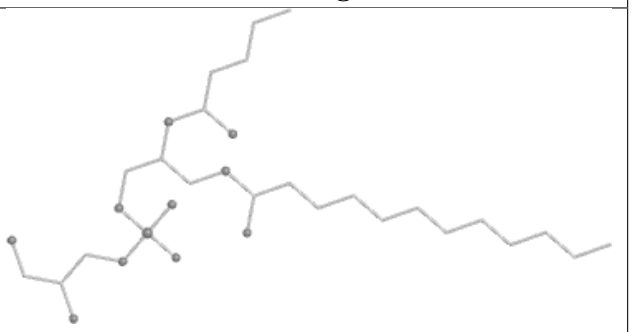
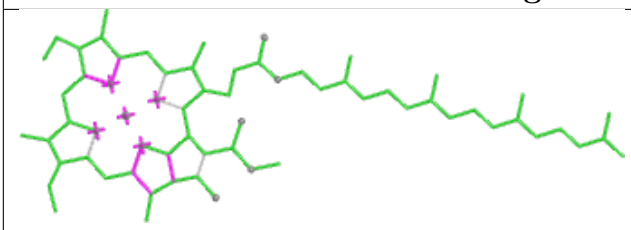


Torsions



Rings

Ligand CLA A 828



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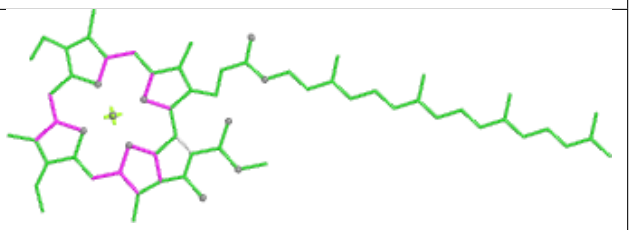

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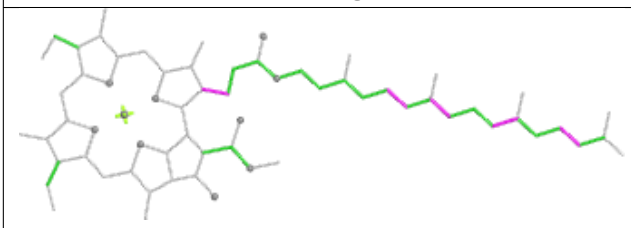

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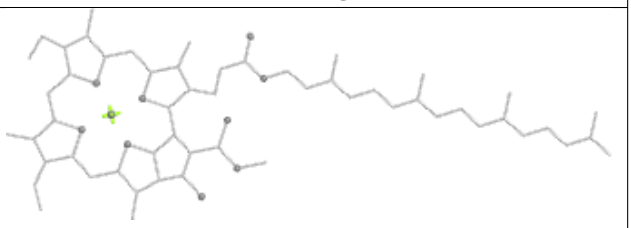
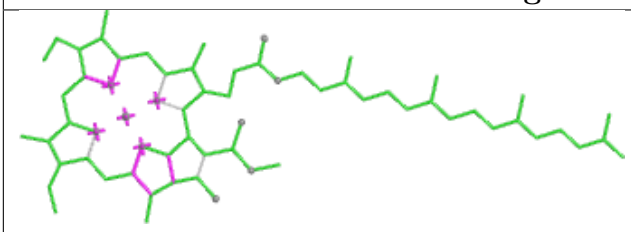


Rings

Ligand CLA A 844



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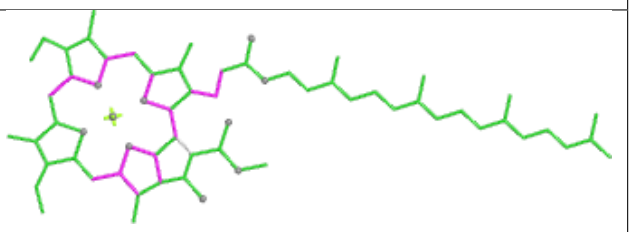
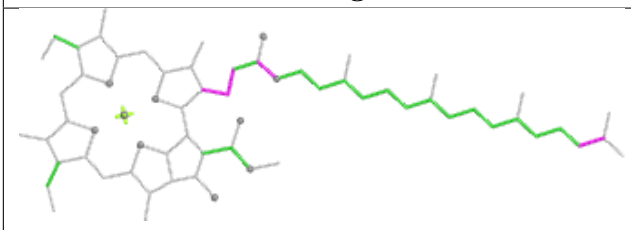


Bond angles



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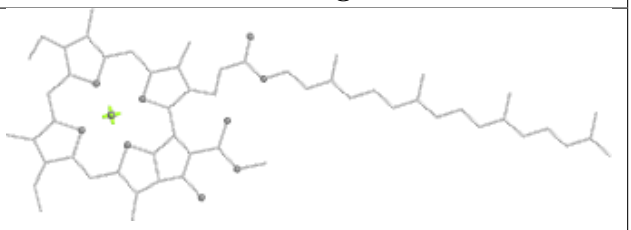
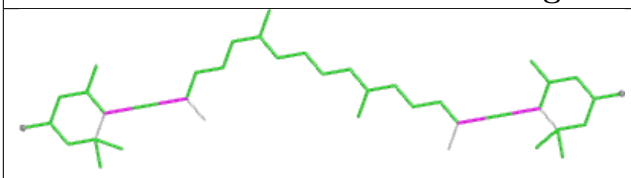


Rings

Ligand II0 e 615



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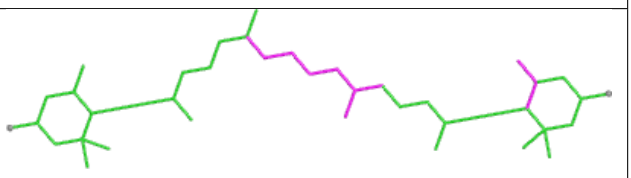

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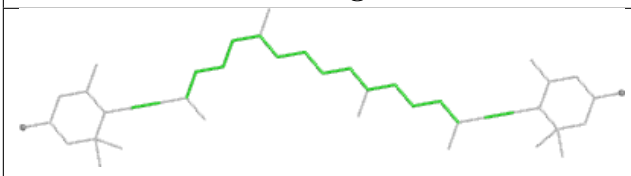

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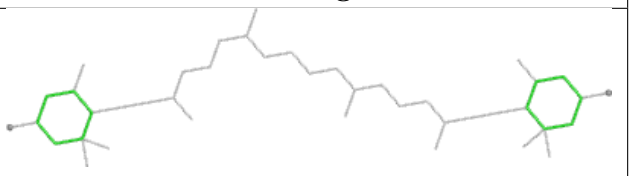
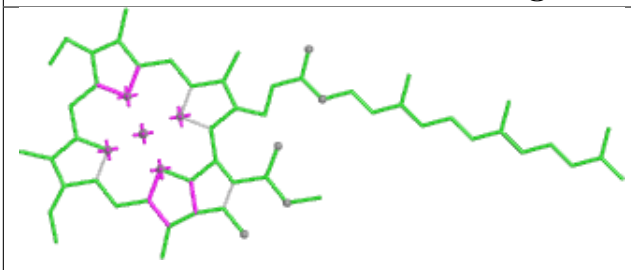


Rings

Ligand CLA 1 612



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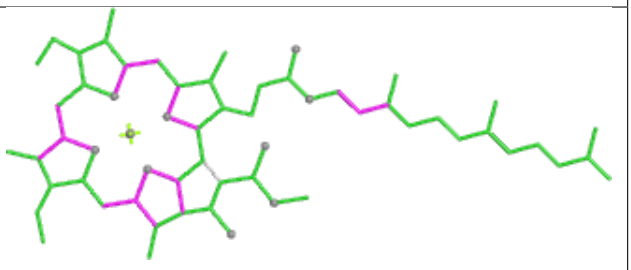
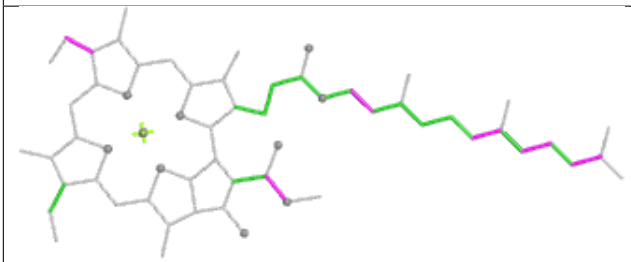


Bond angles



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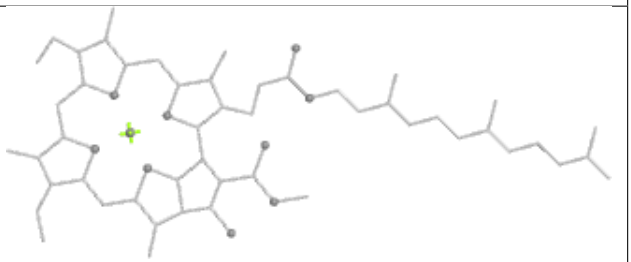
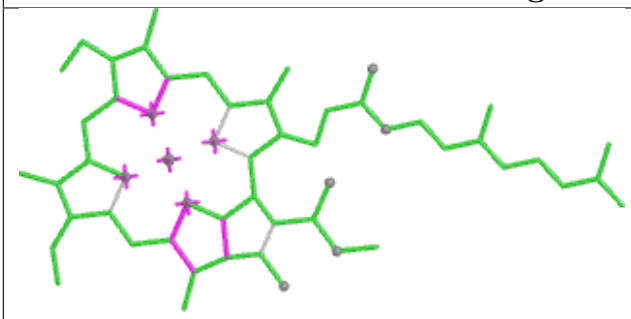


Rings

Ligand CLA b 611



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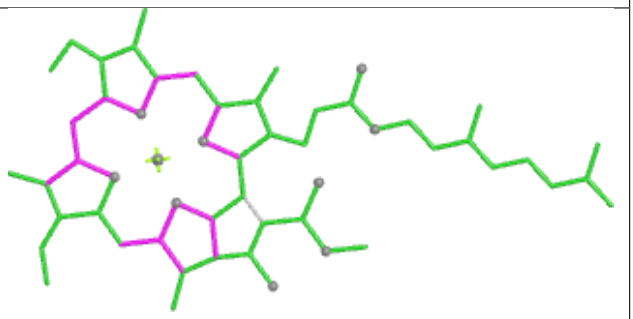

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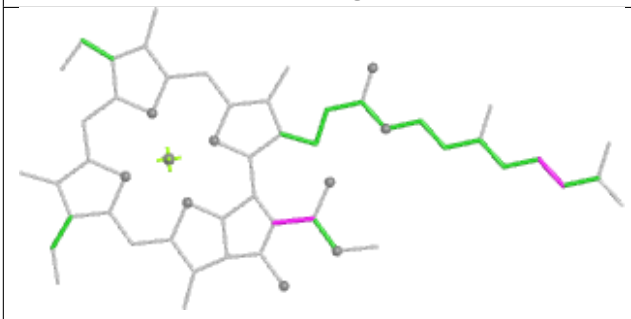

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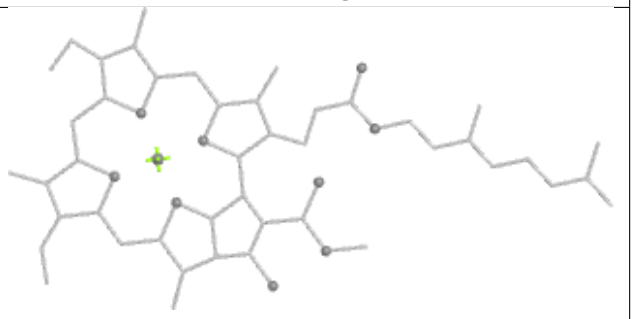

Rings

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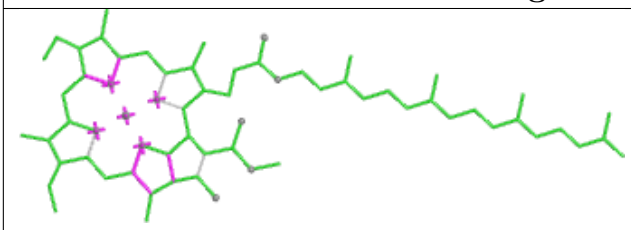

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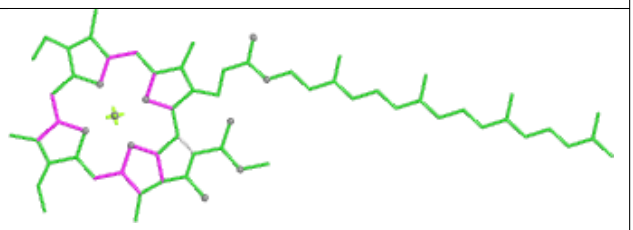

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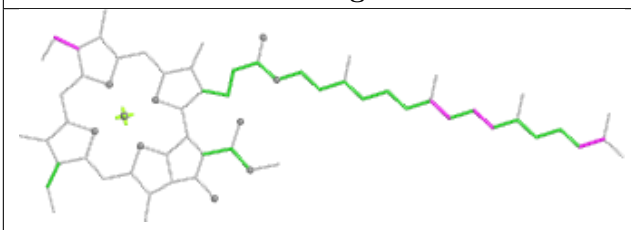

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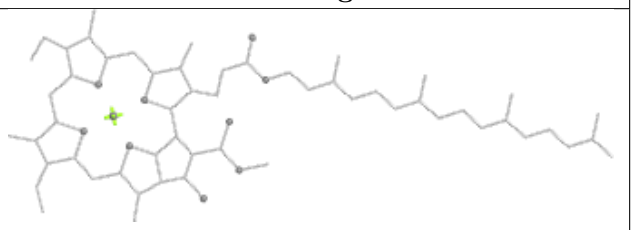

Rings

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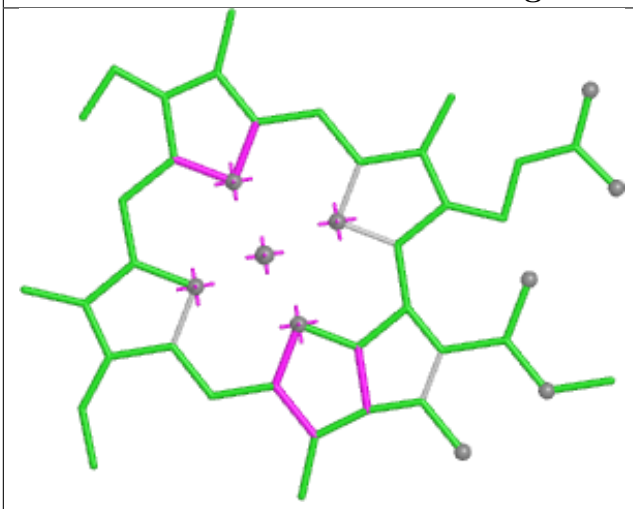

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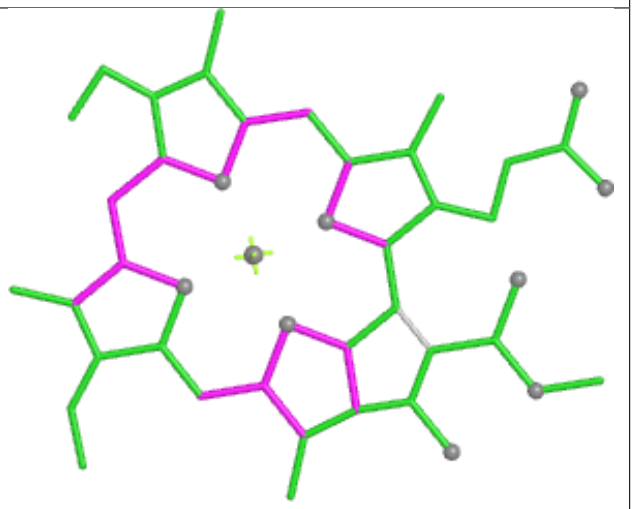

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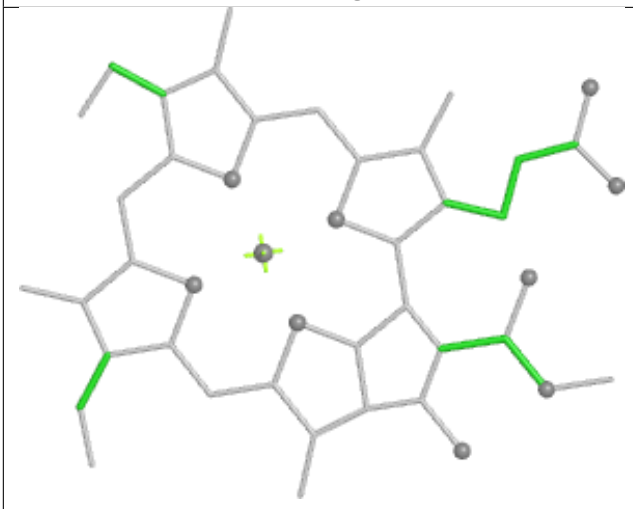
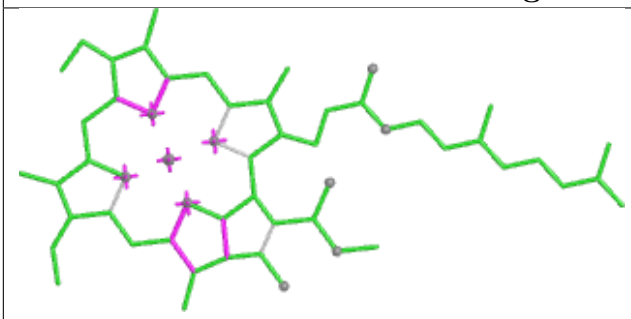


Torsions



Rings

Ligand CLA K 102



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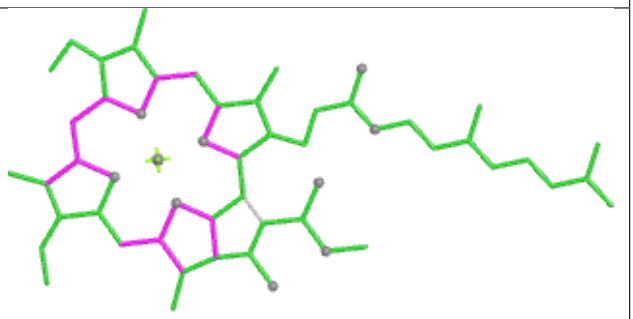

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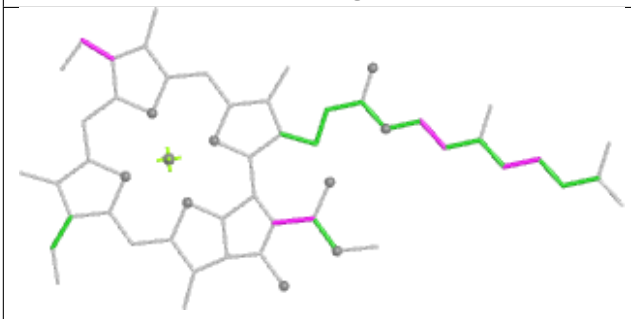

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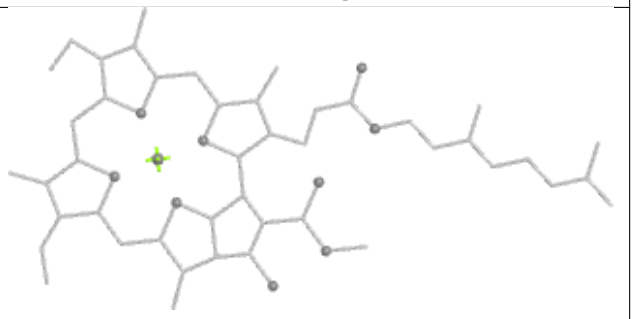
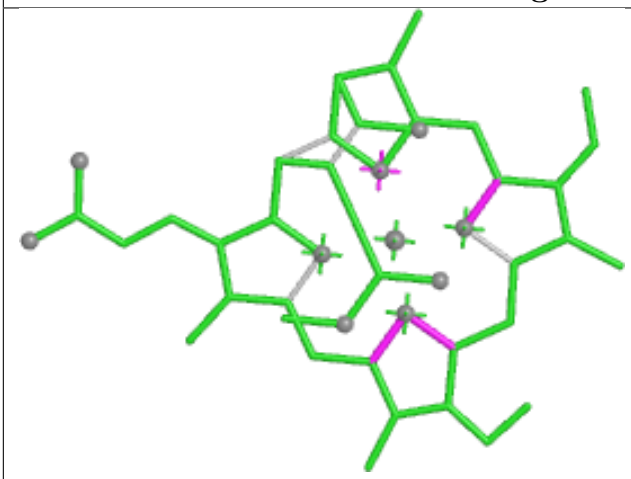


Rings

Ligand KC2 c 615



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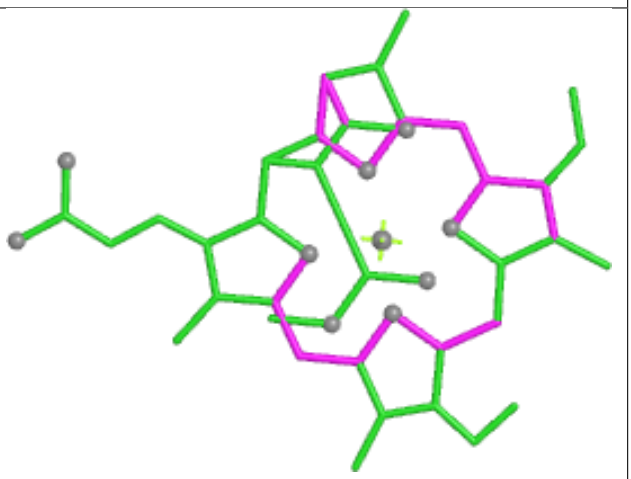
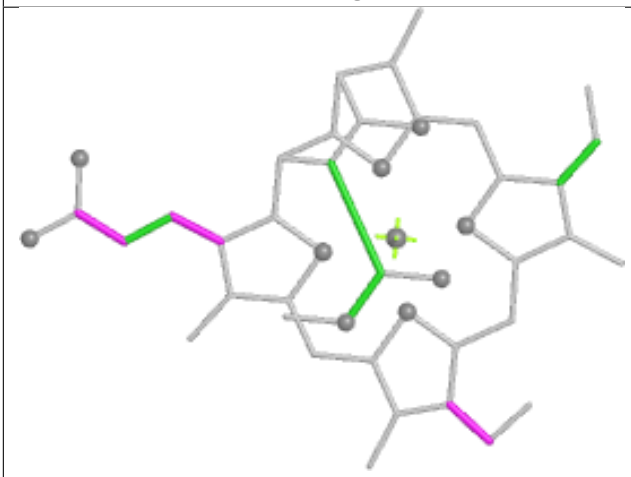


Bond angles



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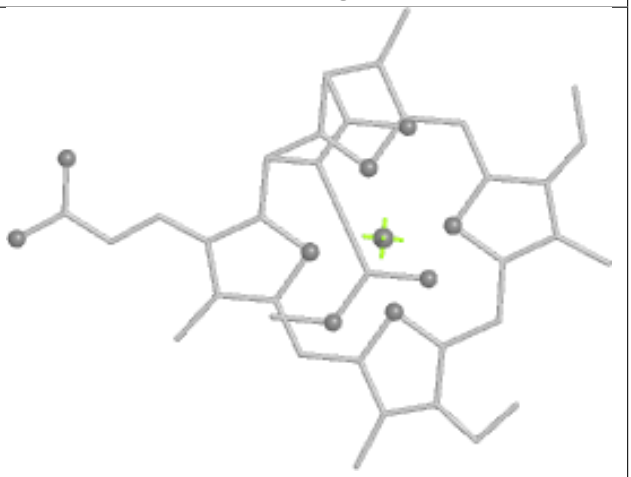
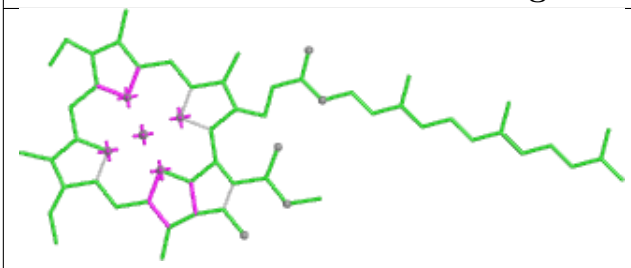


Rings

Ligand CLA e 606



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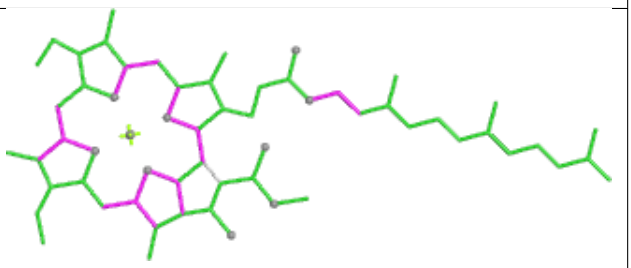
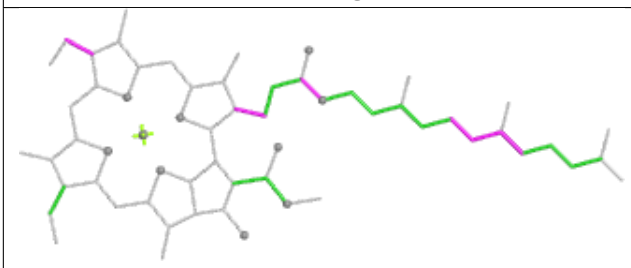


Bond angles



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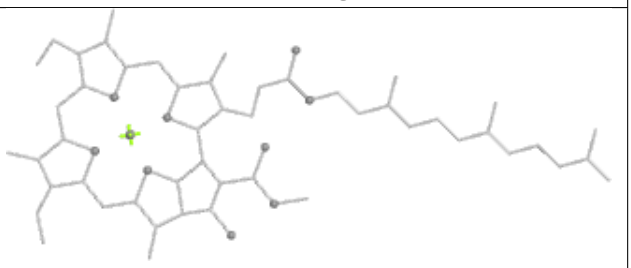
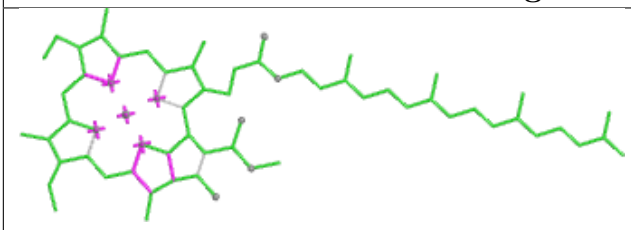
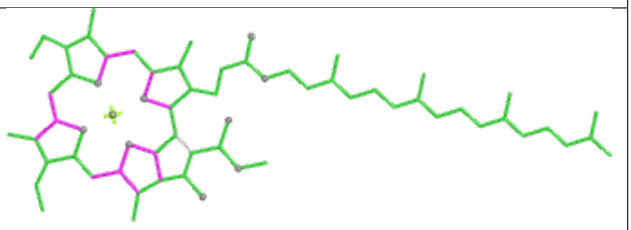


Rings

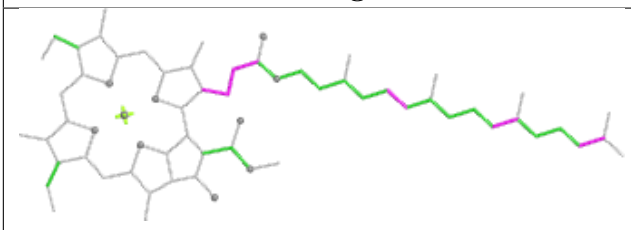
Ligand CLA B 809



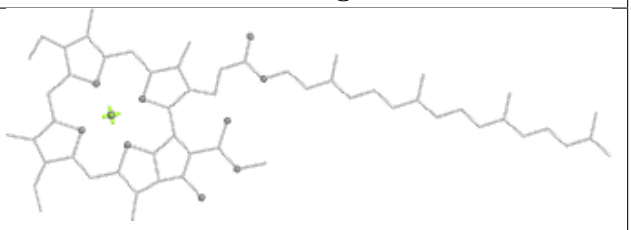
Bond lengths



Bond angles

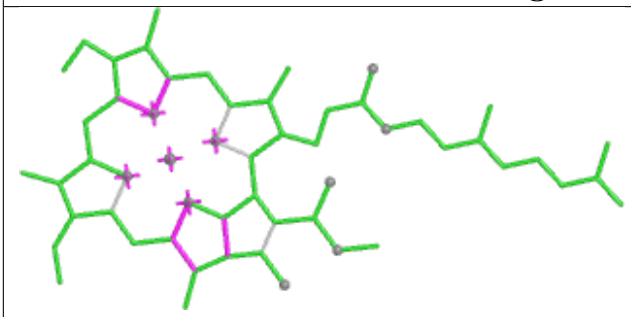


Torsions



Rings

Ligand CLA 5 604



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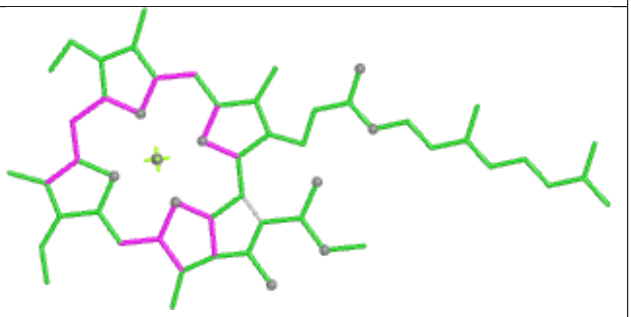

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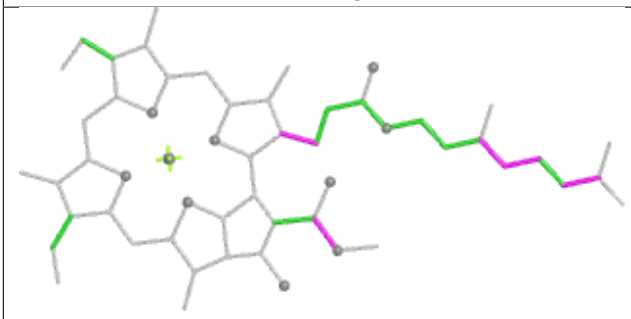

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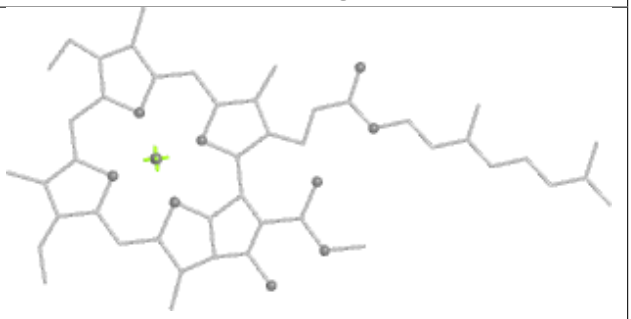

Rings

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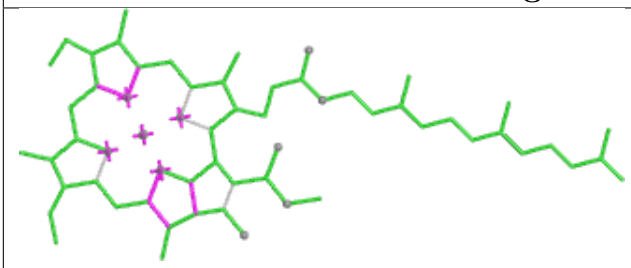

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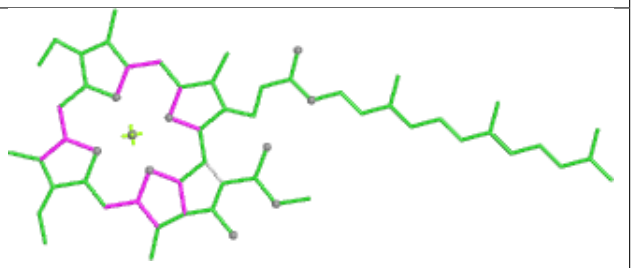

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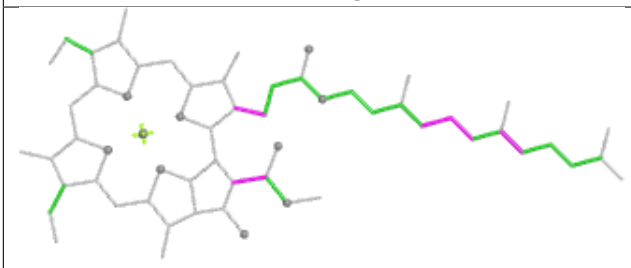

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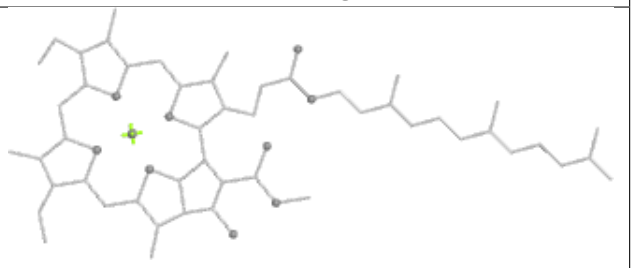

Rings

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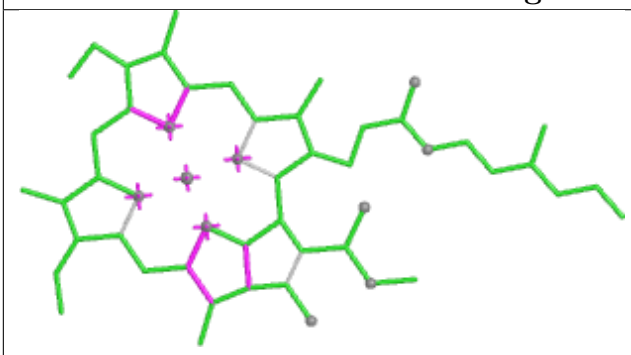

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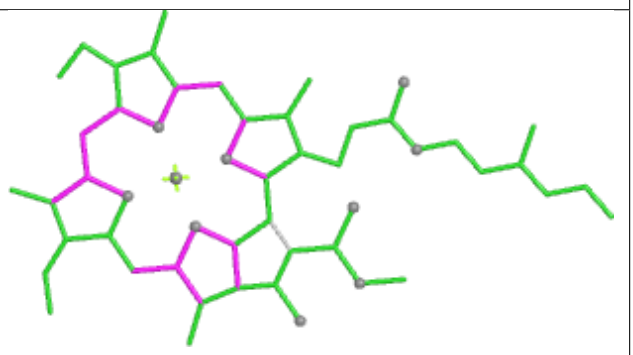

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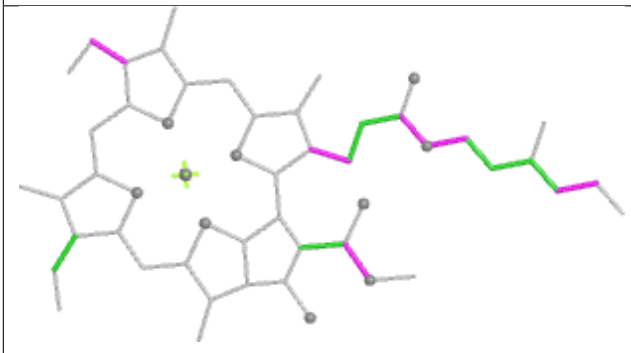

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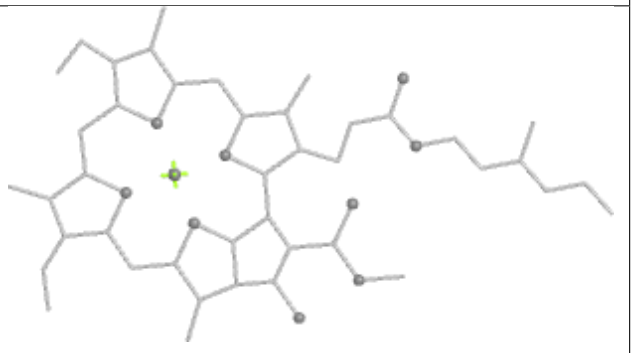
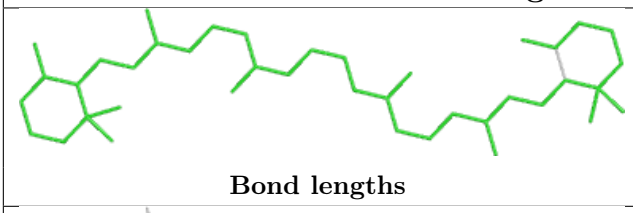


Rings

Ligand 8CT R 203



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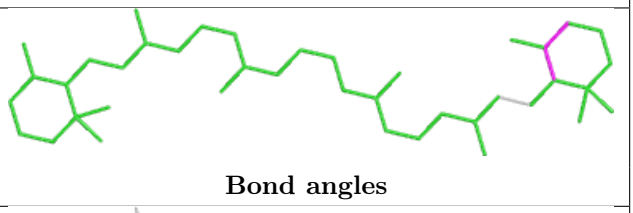

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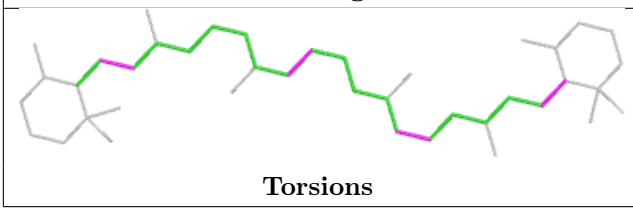

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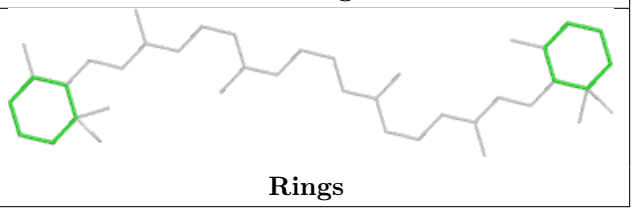
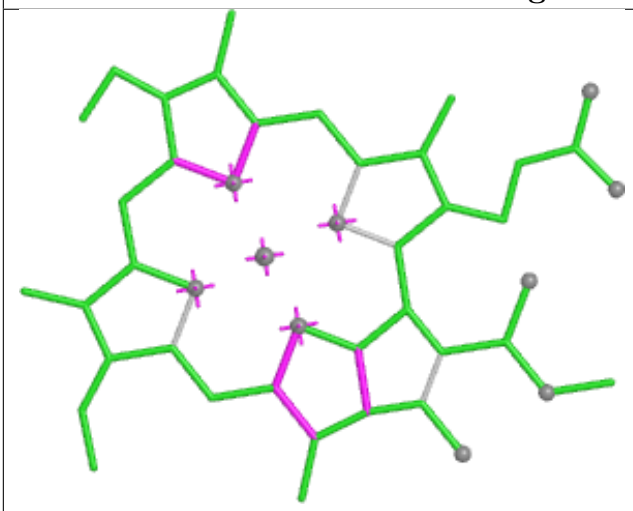


Rings

Ligand CLA 7 607



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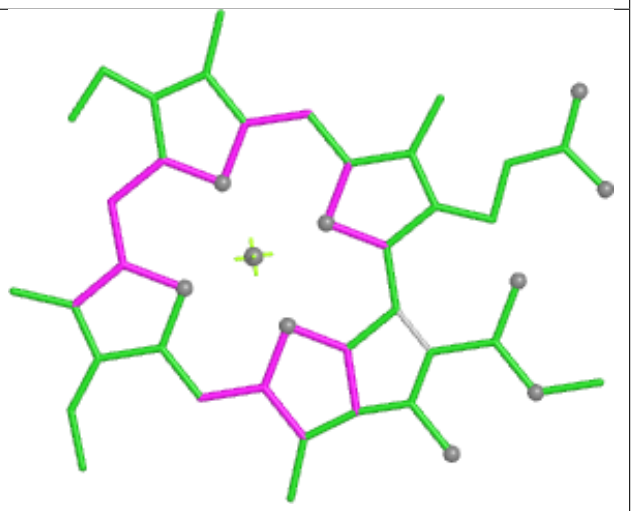

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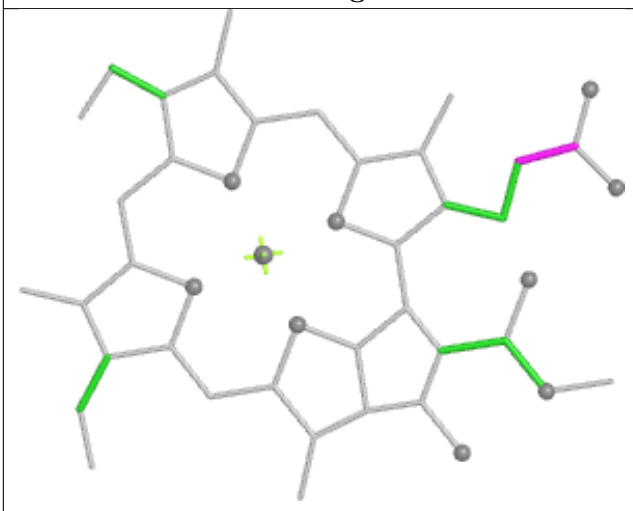

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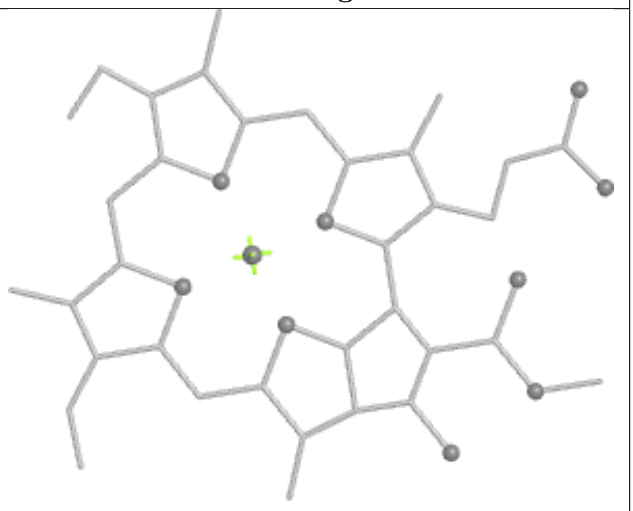
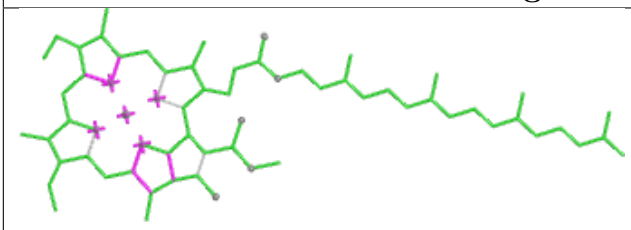


Rings

Ligand CLA A 806



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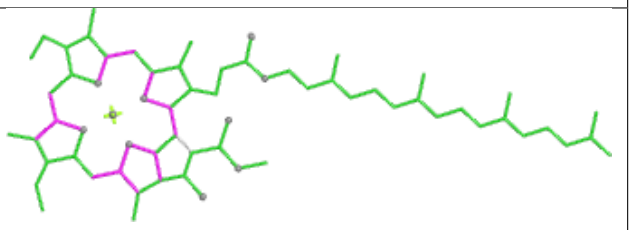

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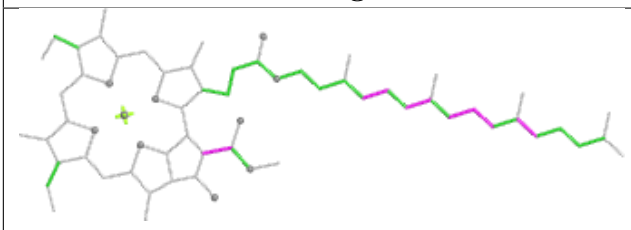

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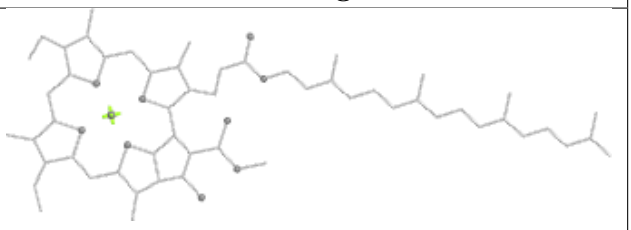
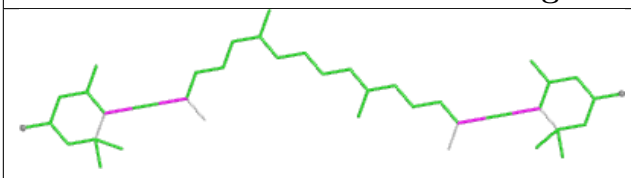


Rings

Ligand II0 d 616



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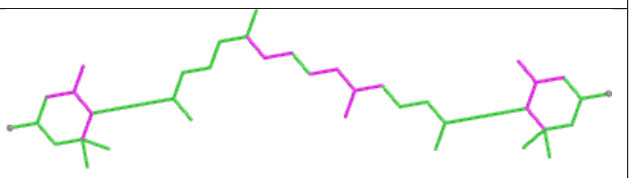

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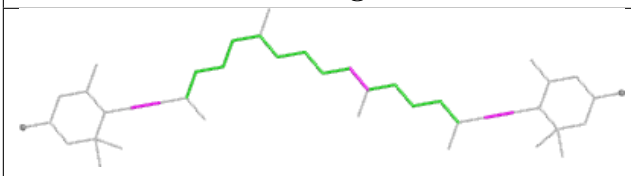

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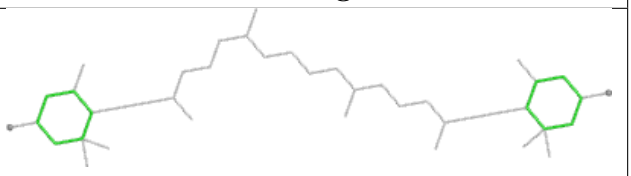
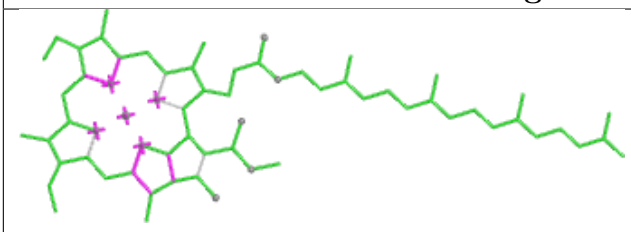


Rings

Ligand CLA B 822



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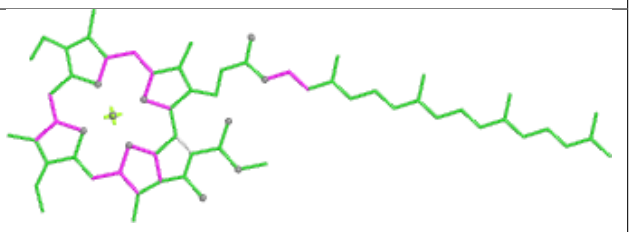

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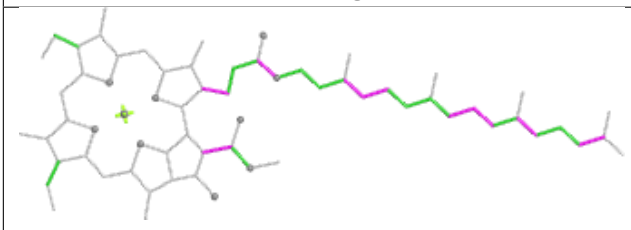

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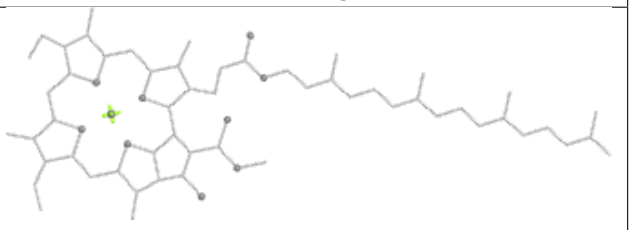
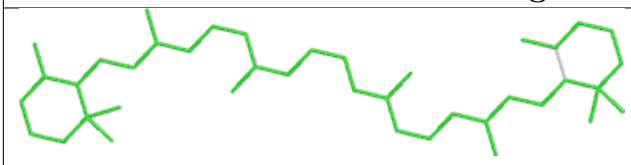


Rings

Ligand 8CT Z 309



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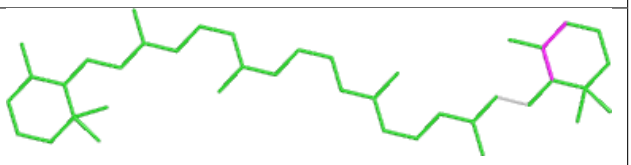

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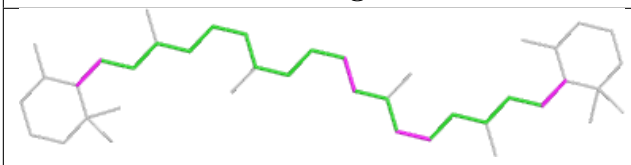

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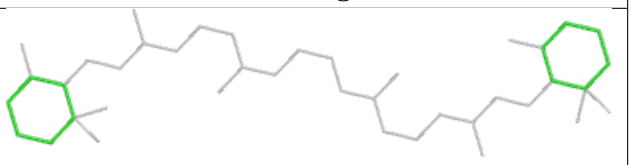
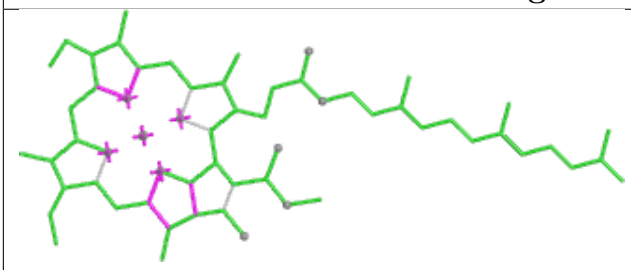


Rings

Ligand CLA 5 608



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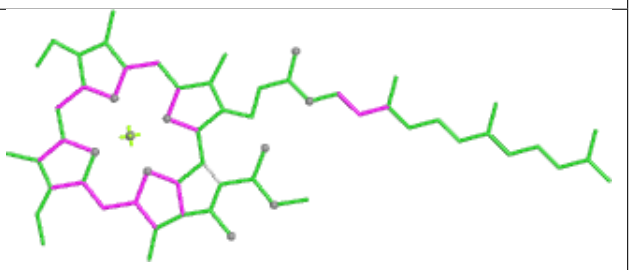

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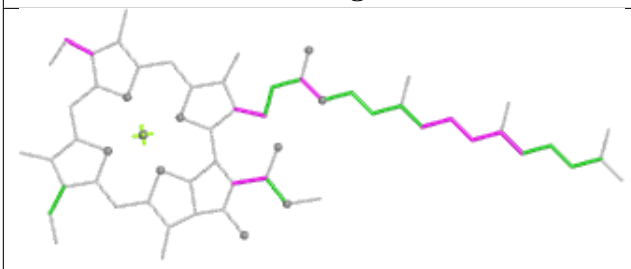

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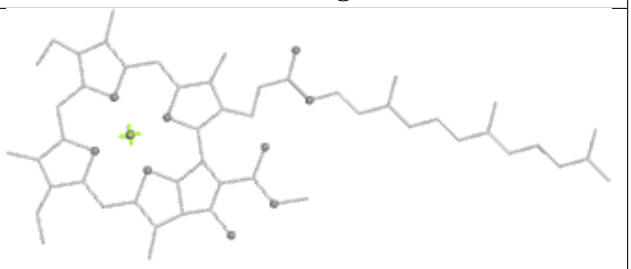
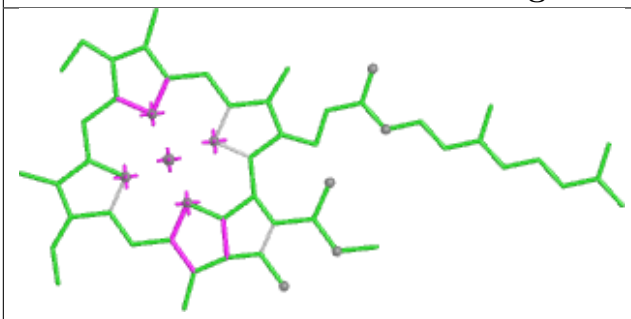


Rings

Ligand CLA 9 608



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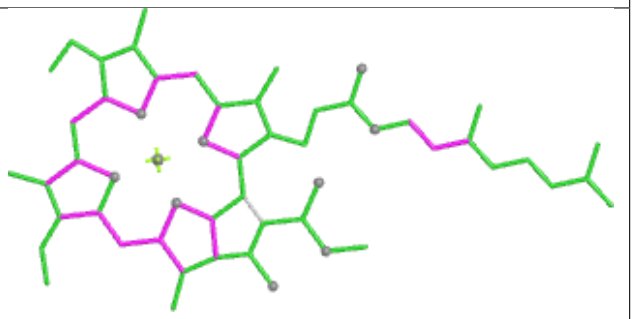

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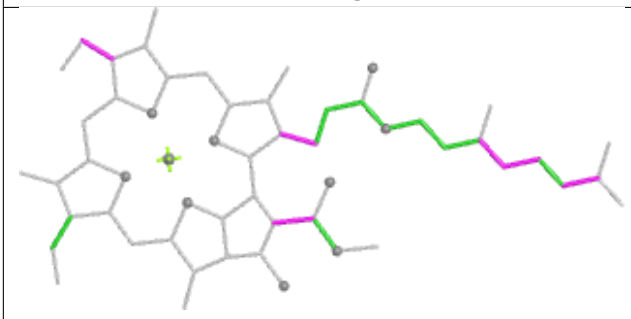

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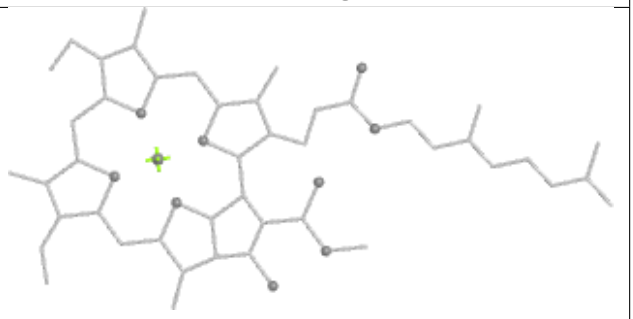
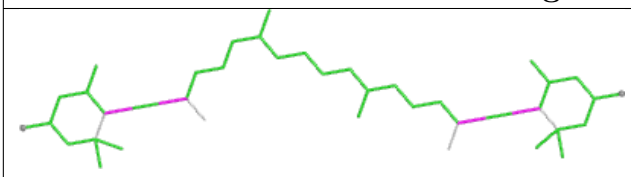


Rings

Ligand II0 7 615



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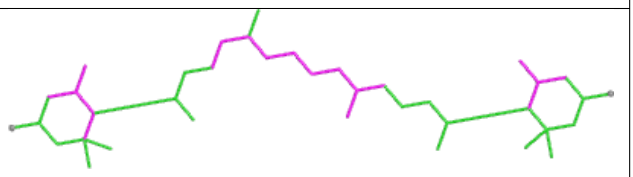
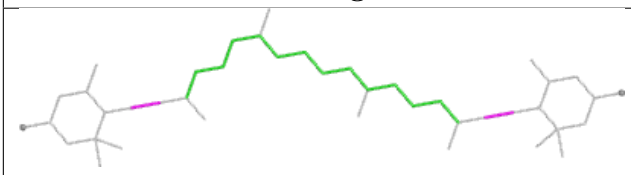


Bond angles



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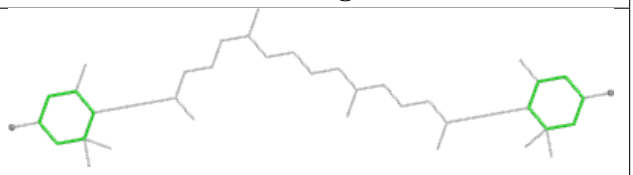
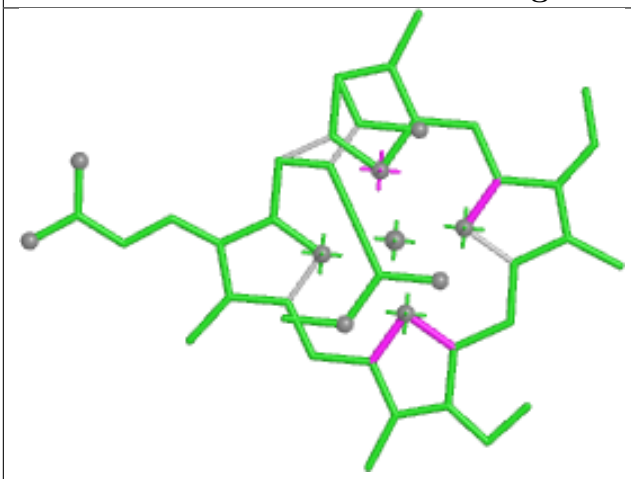


Rings

Ligand KC2 c 610



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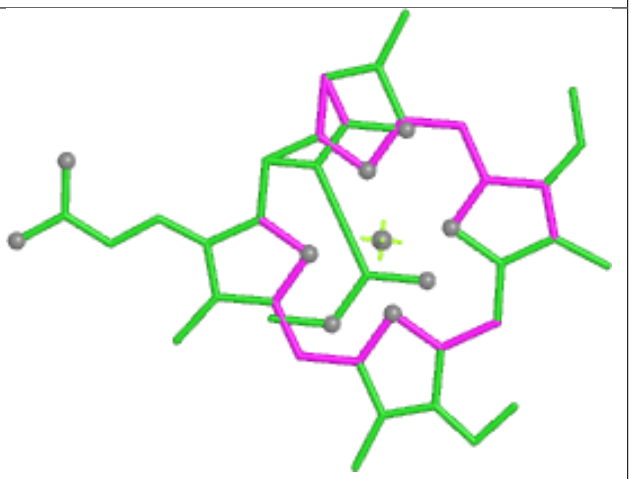

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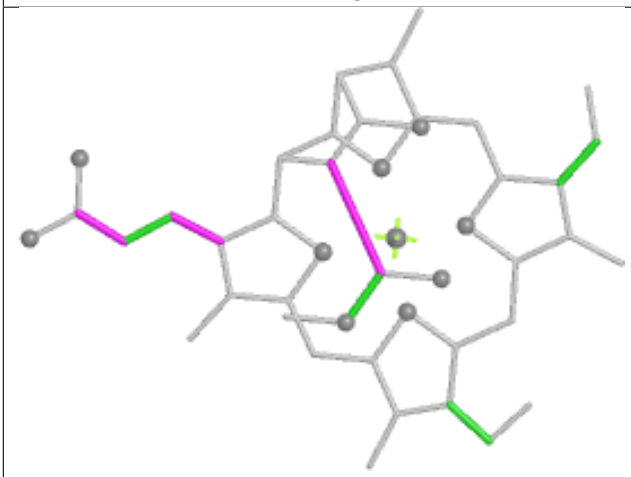

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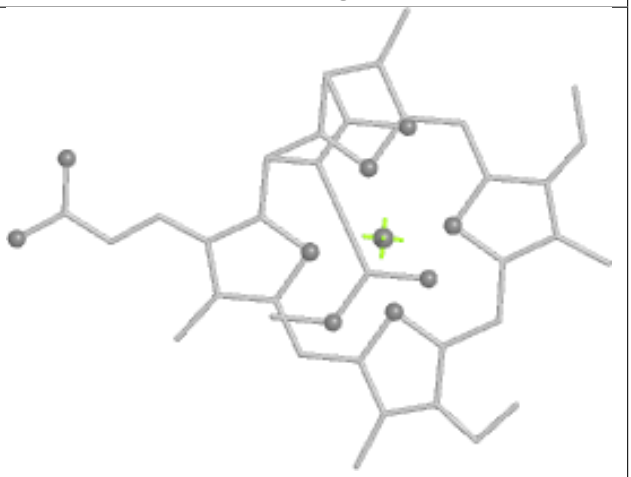
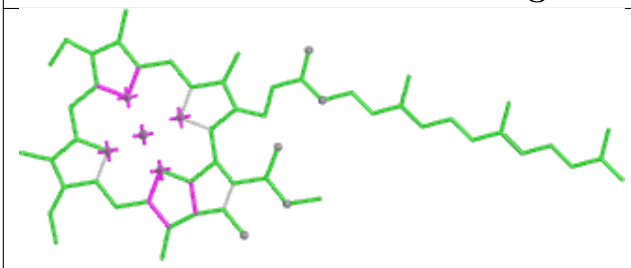


Rings

Ligand CLA 3 608



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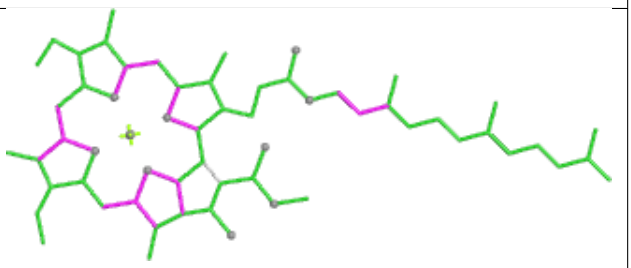
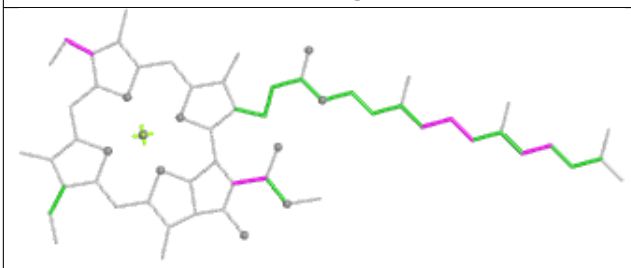


Bond angles



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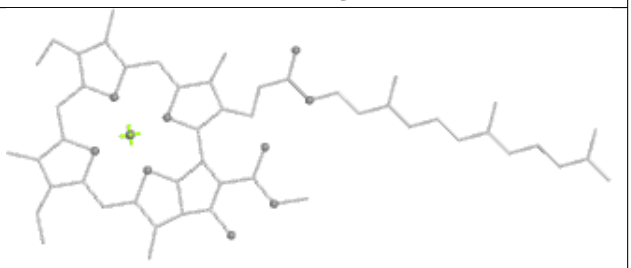
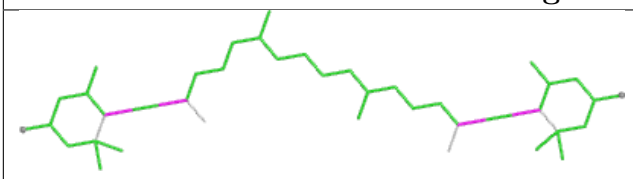


Rings

Ligand II0 3 615



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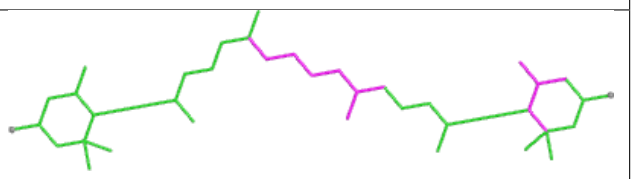

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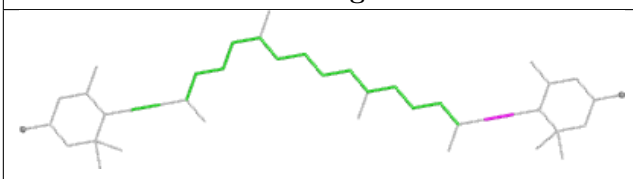
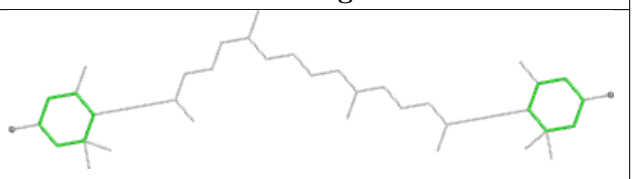
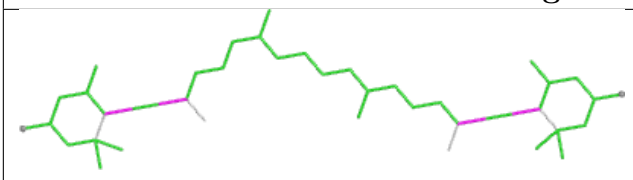


Torsions



Rings

Ligand II0 1 617



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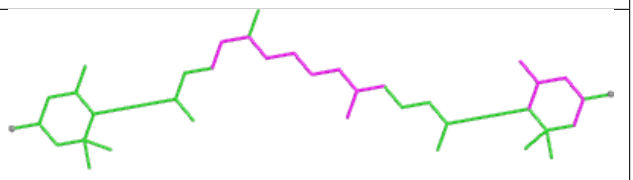

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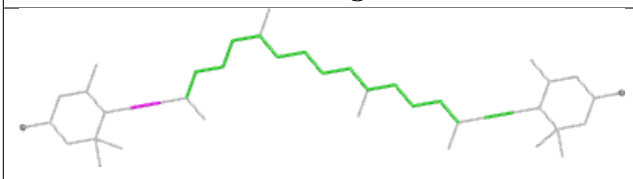

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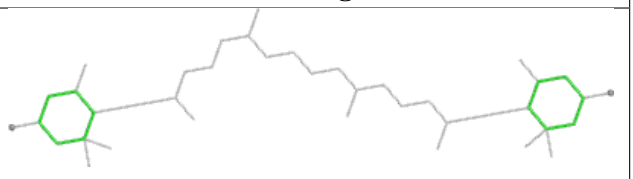
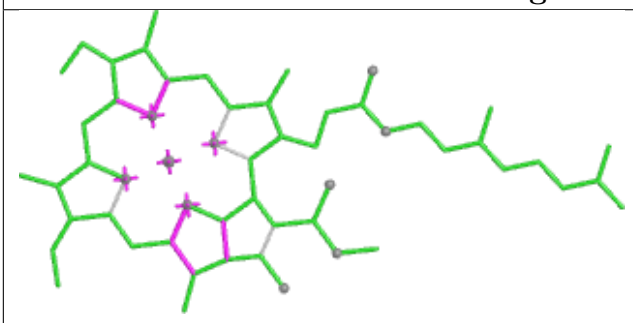


Rings

Ligand CLA c 612



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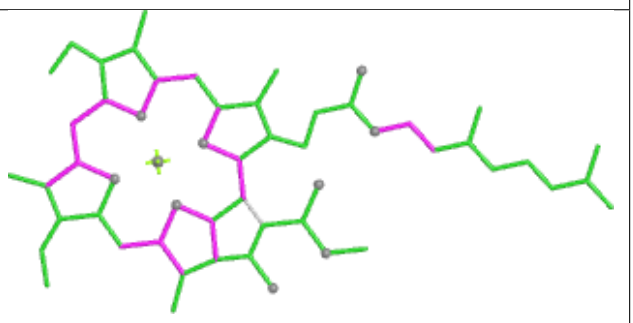

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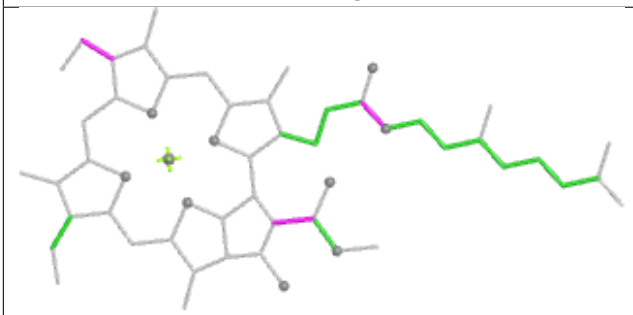

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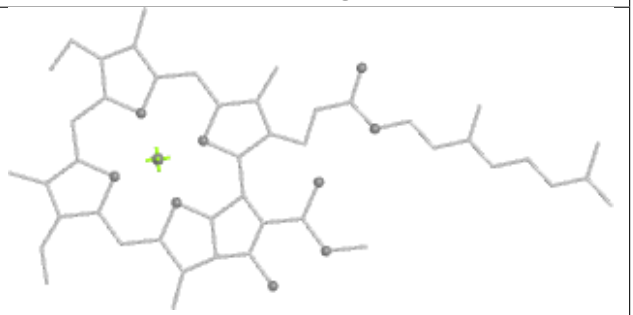

Rings

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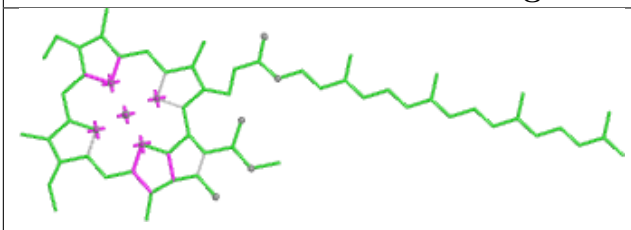
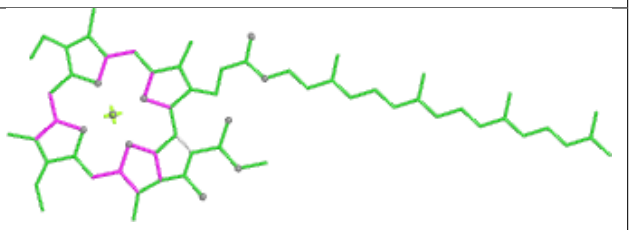
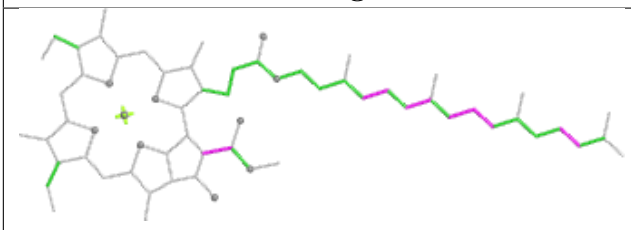
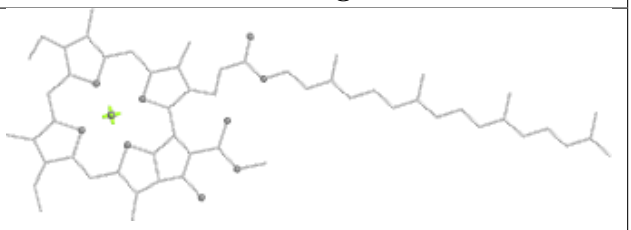
	
Bond lengths	Bond angles
	
Torsions	Rings

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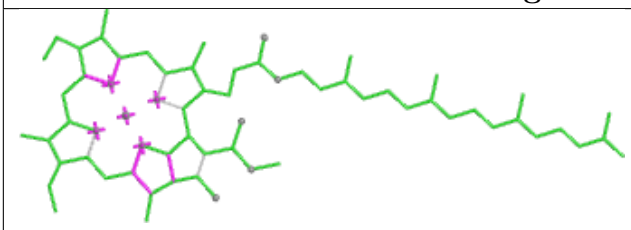	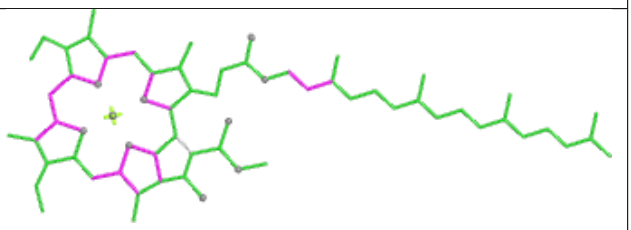
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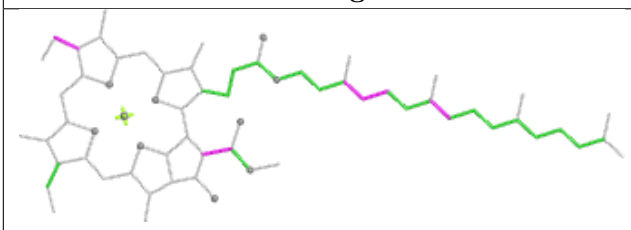
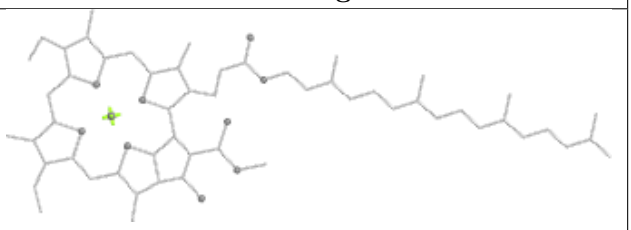
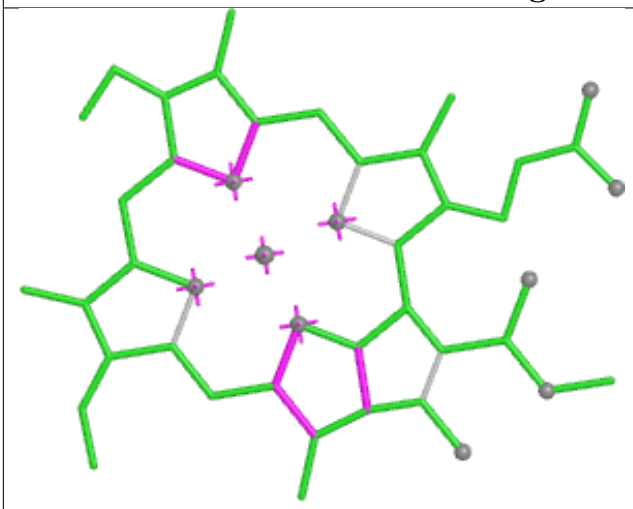
	
Torsions	Rings

Ligand CLA e 601



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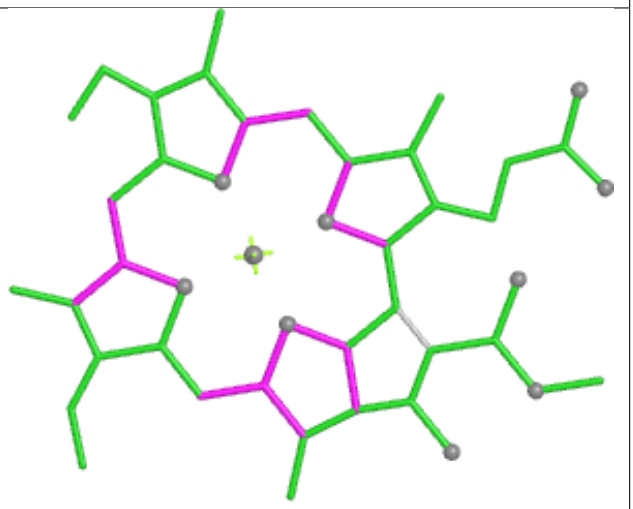
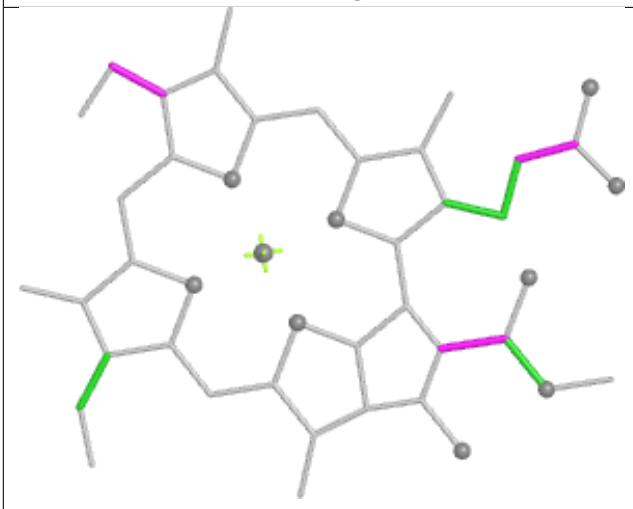


Bond angles

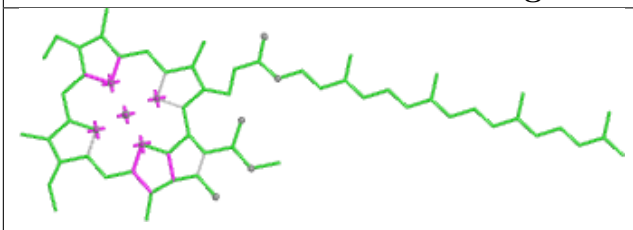


Torsions



Rings

Ligand CLA B 812



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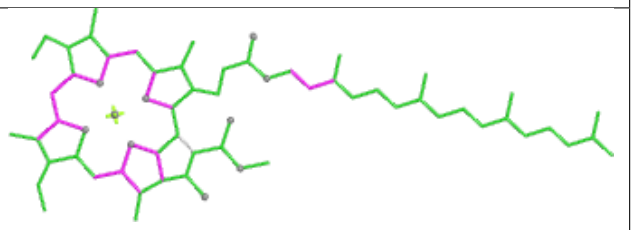

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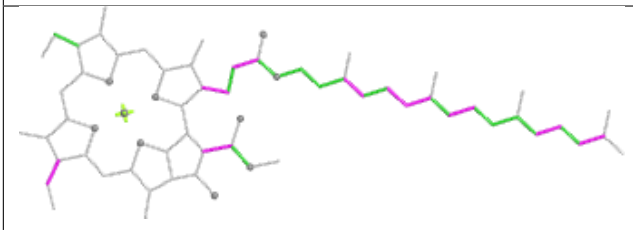

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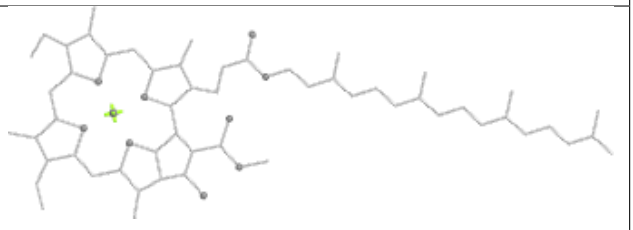
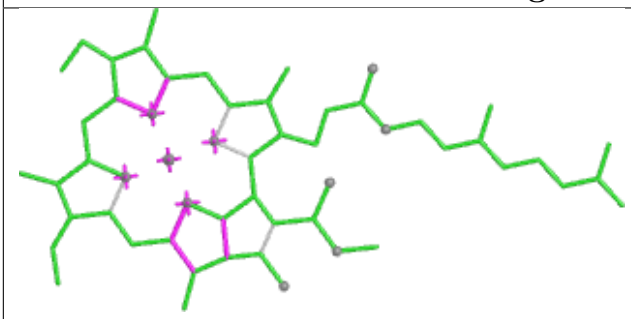


Rings

Ligand CLA 2 604



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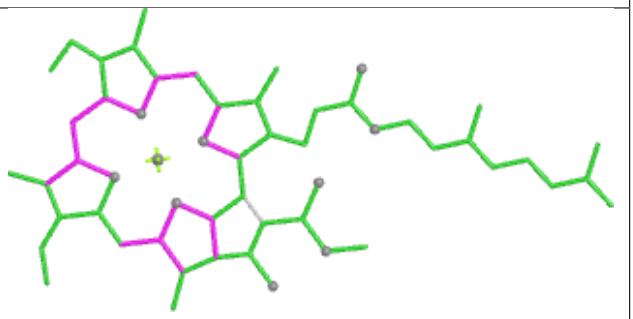

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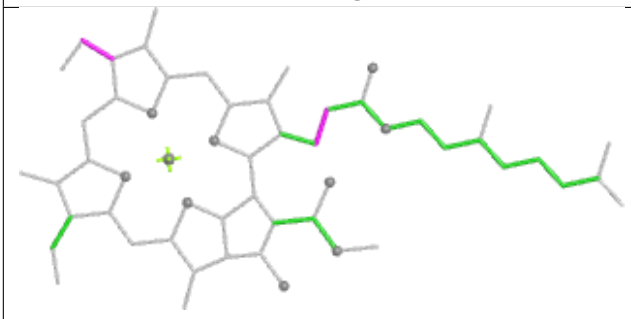

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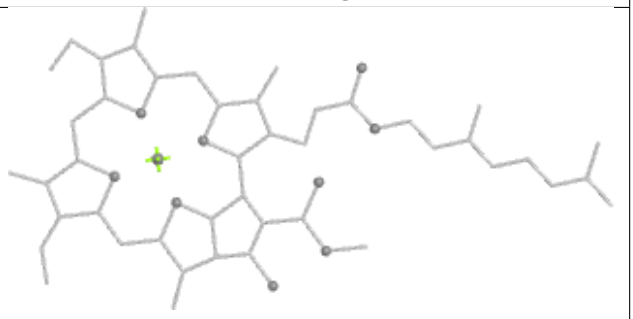
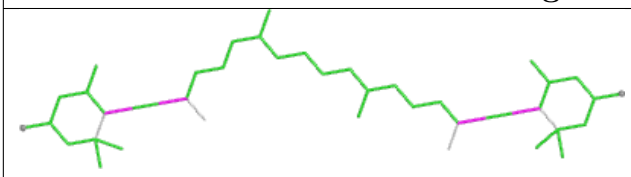


Rings

Ligand II0 J 101



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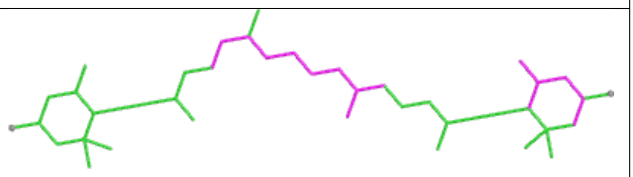

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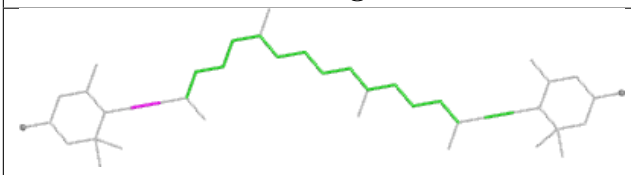

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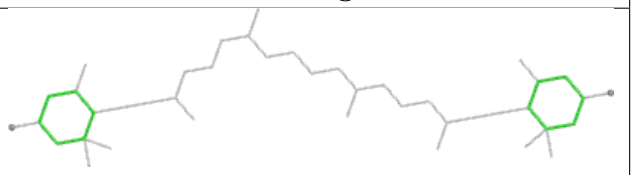
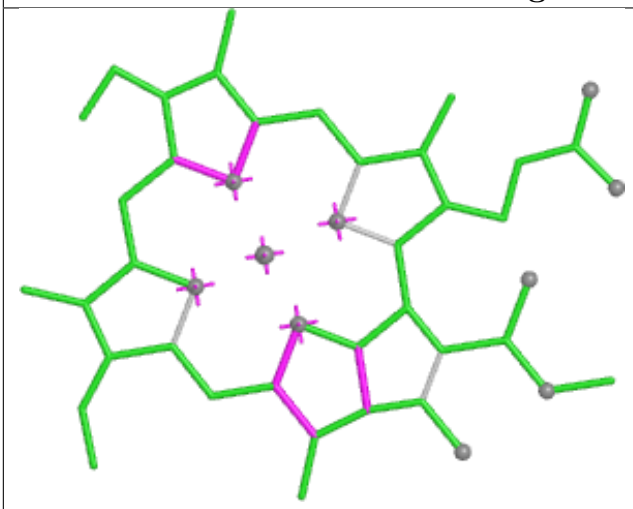


Rings

Ligand CLA 2 612



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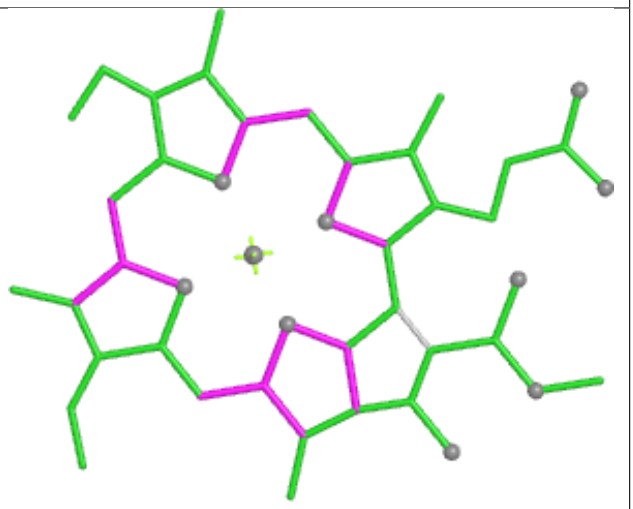
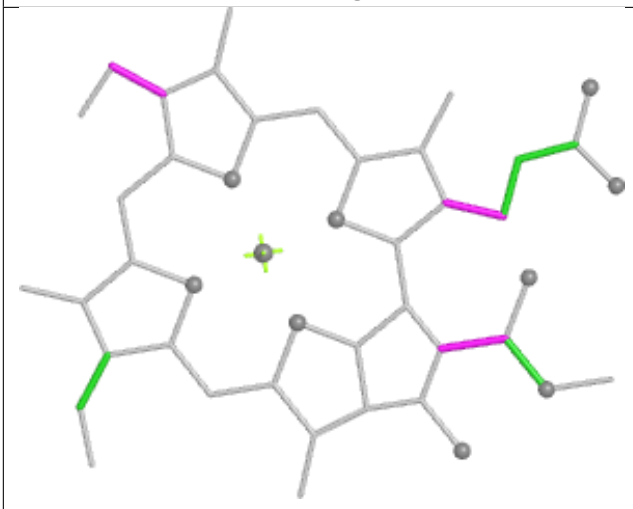


Bond angles



Torsions



Rings

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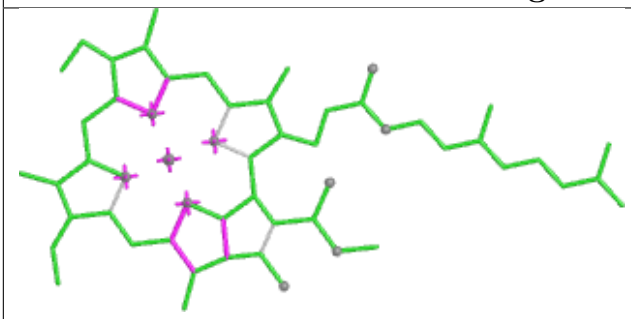

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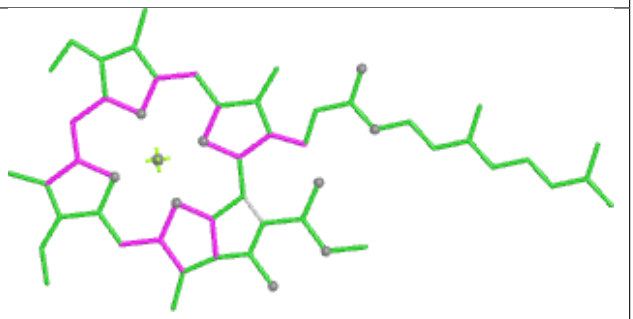

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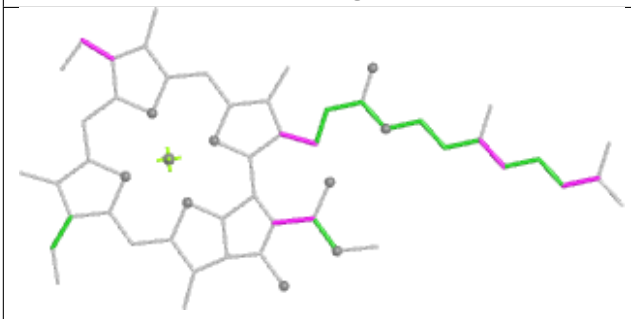

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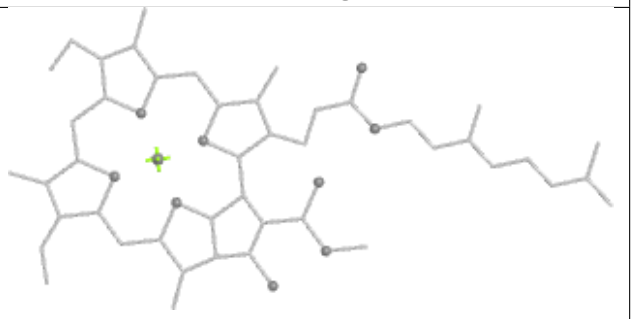
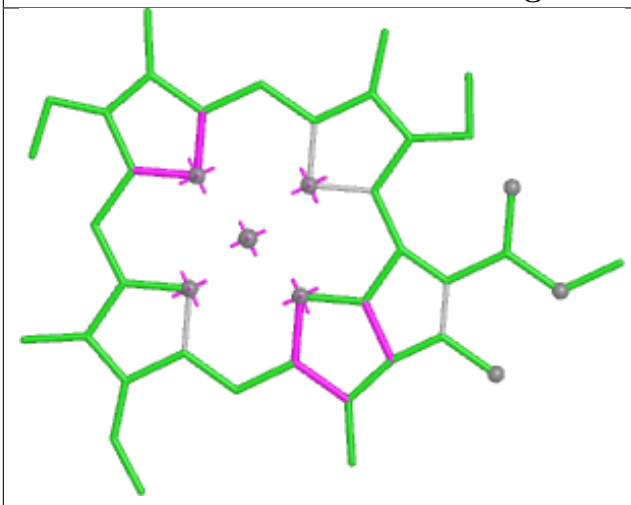


Rings

Ligand CLA B 814



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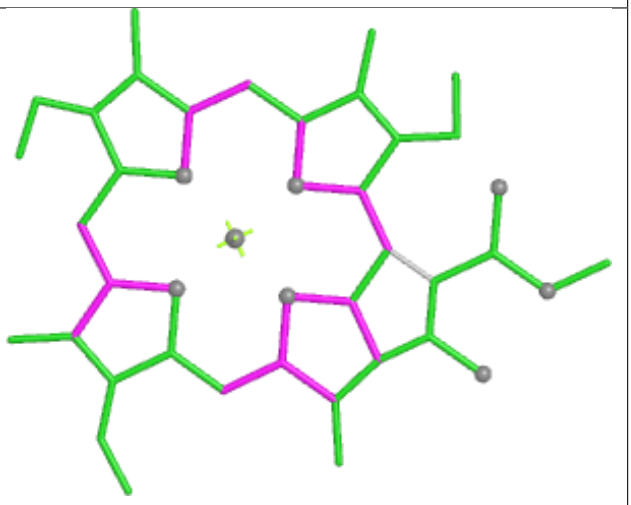

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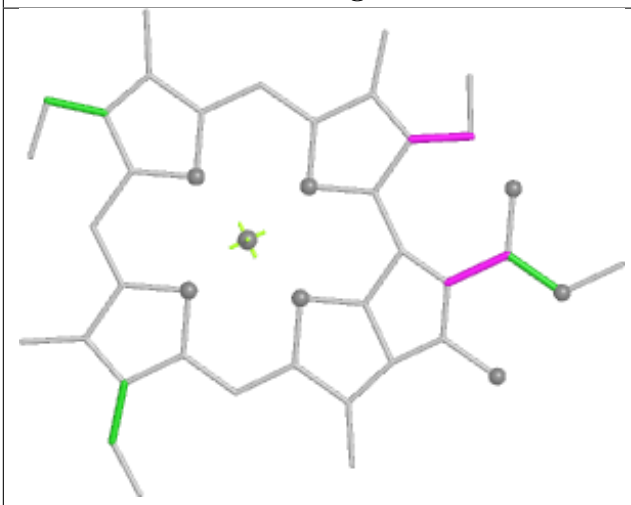
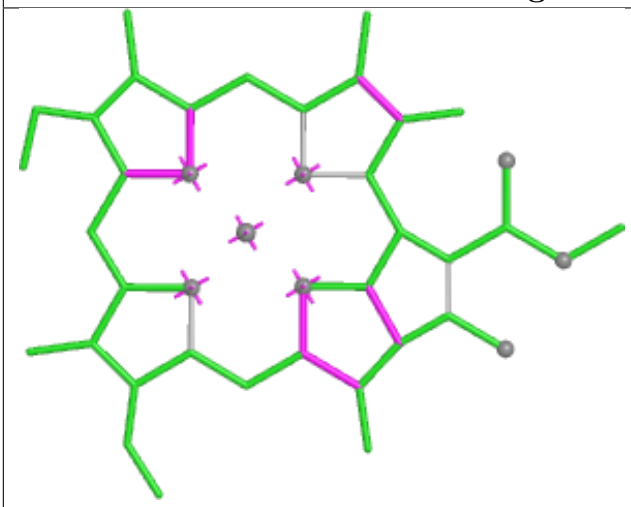


Torsions



Rings

Ligand CLA J 102



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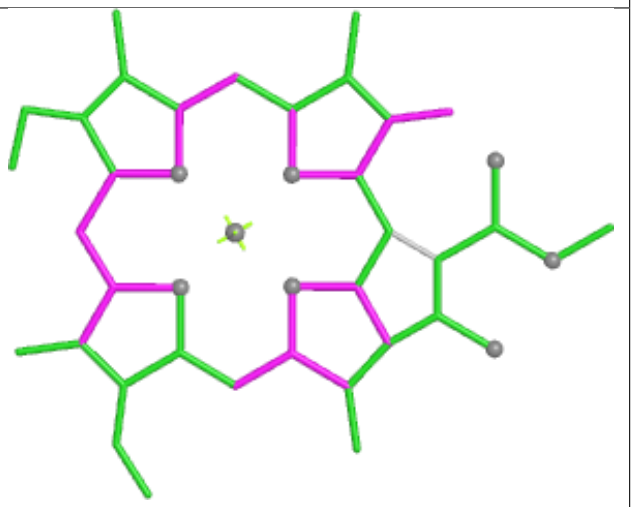
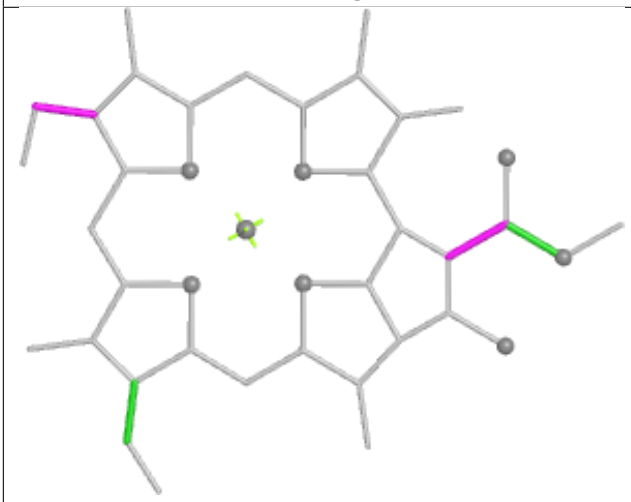


Bond angles



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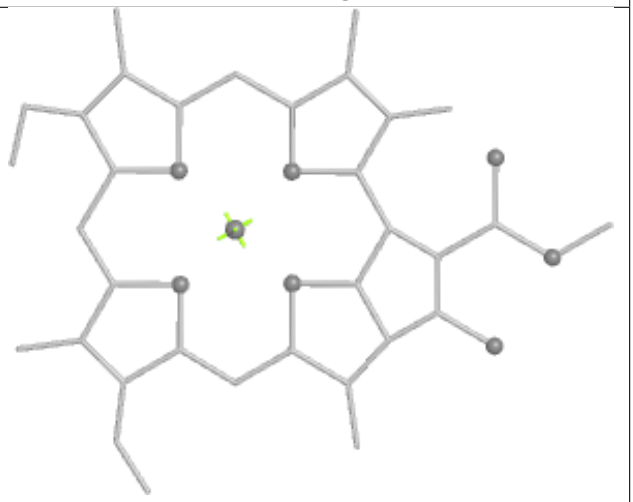
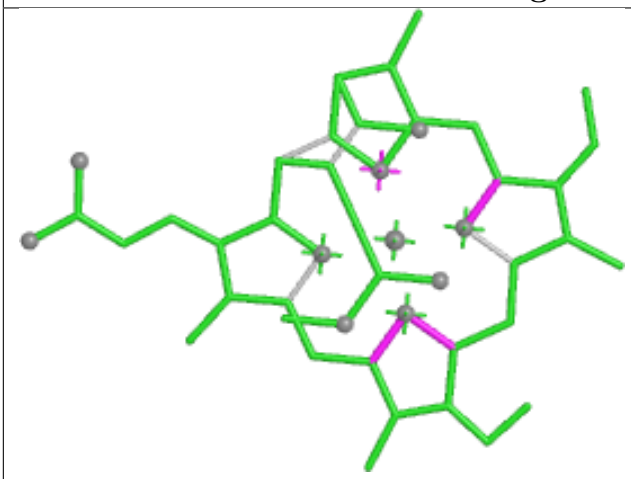


Rings

Ligand KC2 1 610



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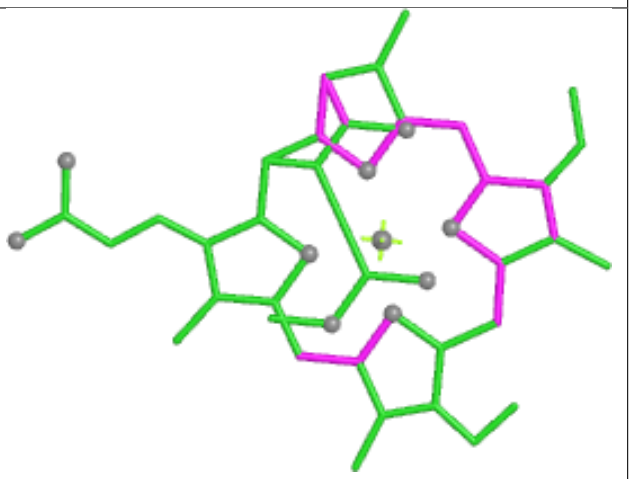
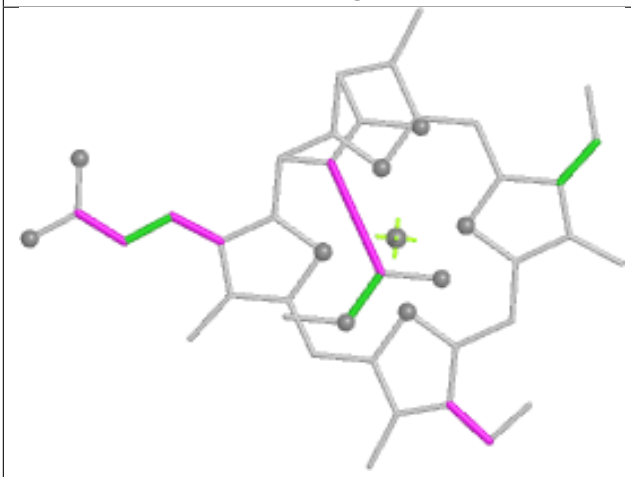


Bond angles



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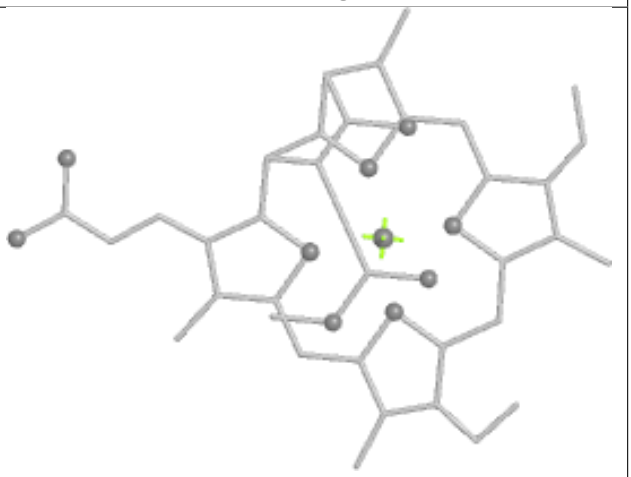
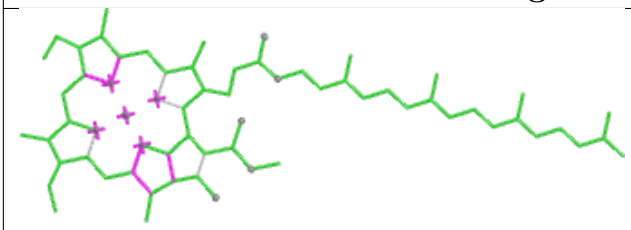


Rings

Ligand CLA 8 615



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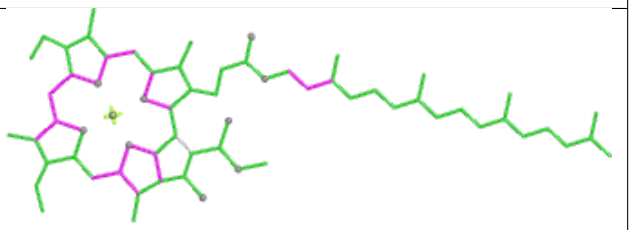

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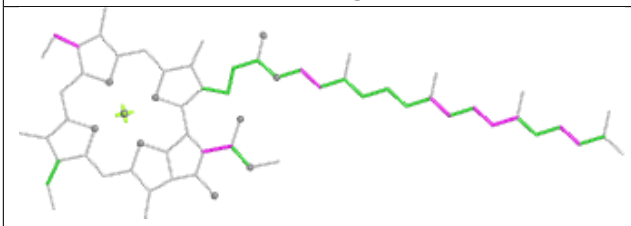

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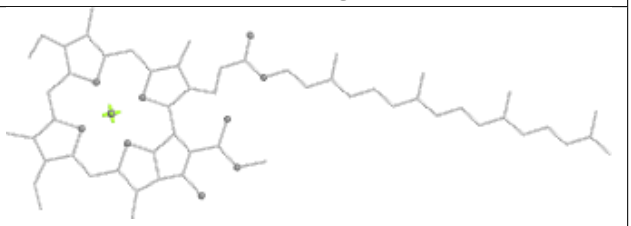
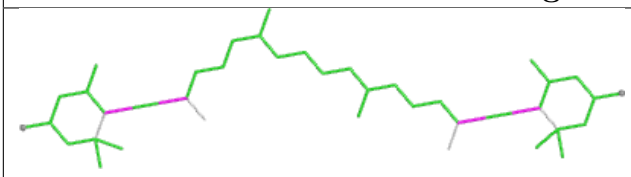


Rings

Ligand II0 1 614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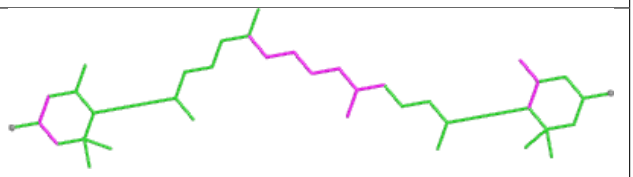
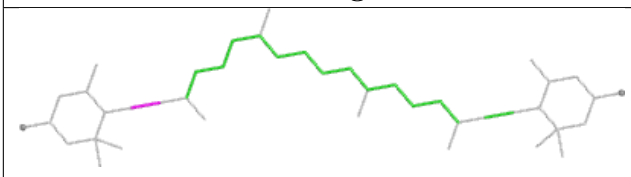

Bond angles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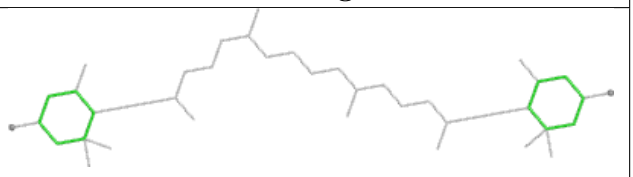
Rings

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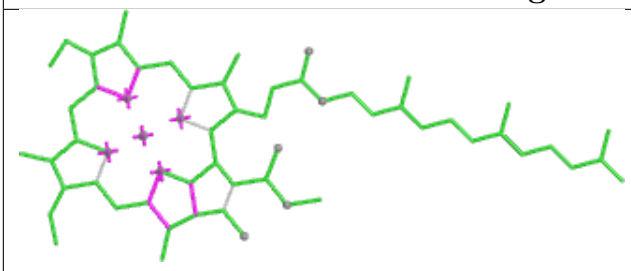
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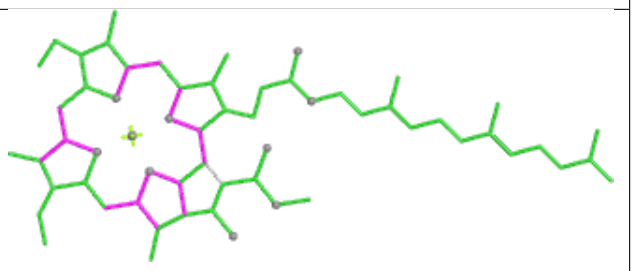
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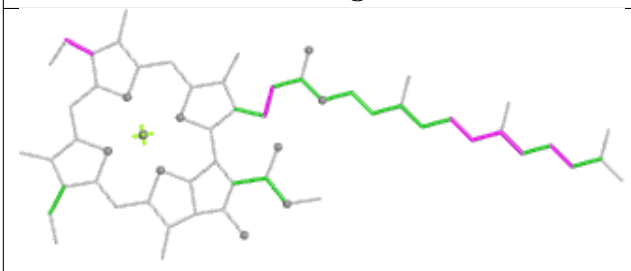
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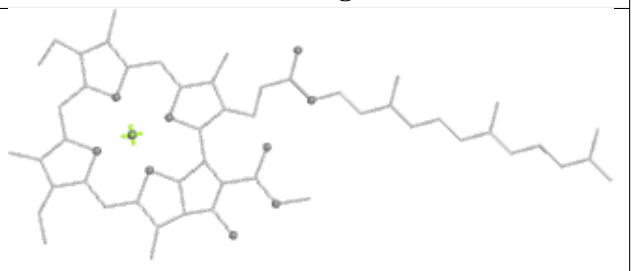
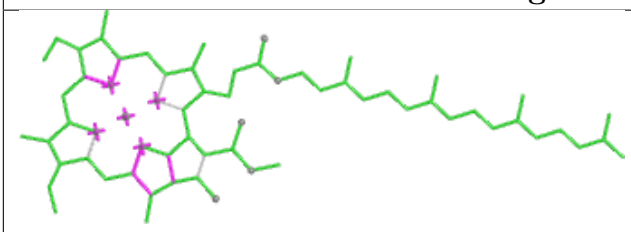

Rings

Ligand CLA 7 602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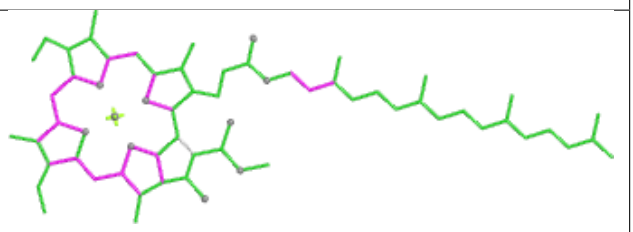
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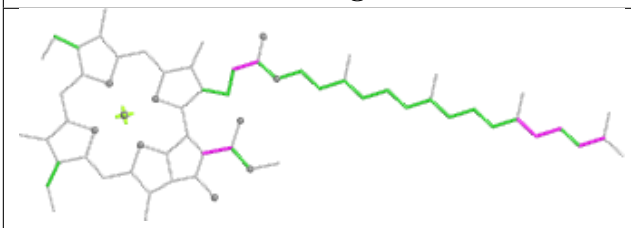
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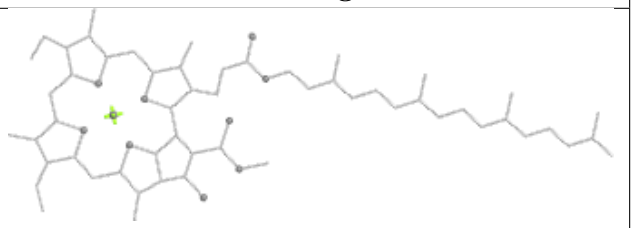
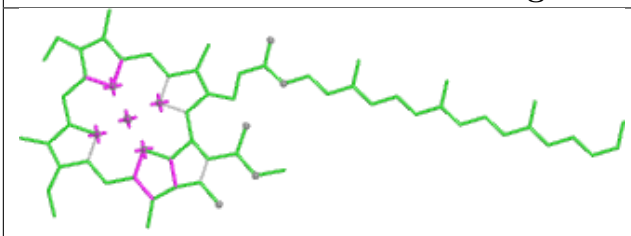

Rings

Ligand CLA b 602



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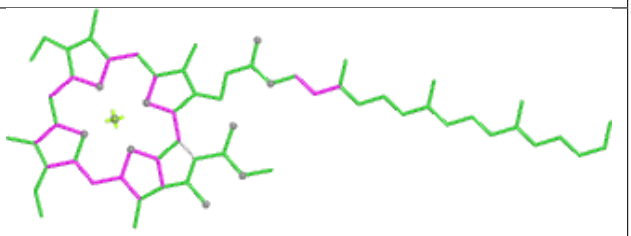

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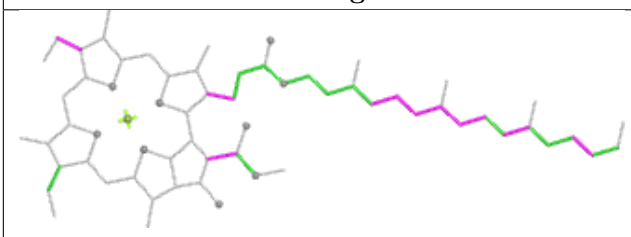

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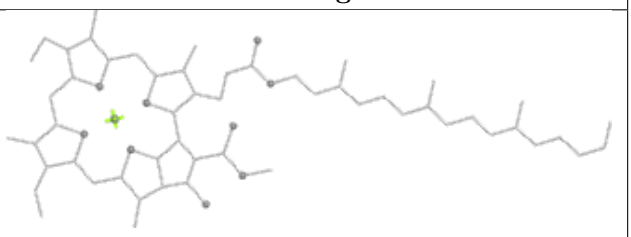

Rings

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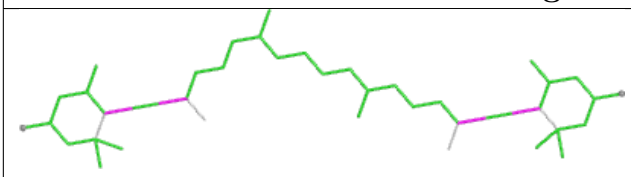

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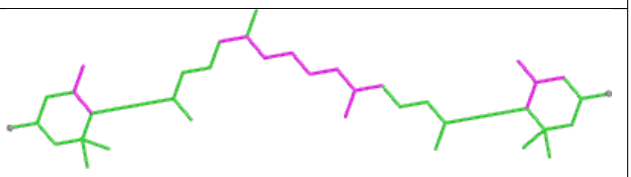

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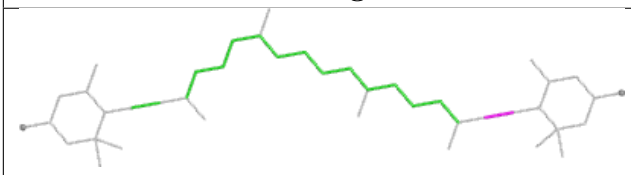

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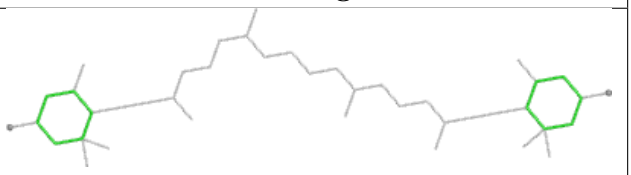

Rings

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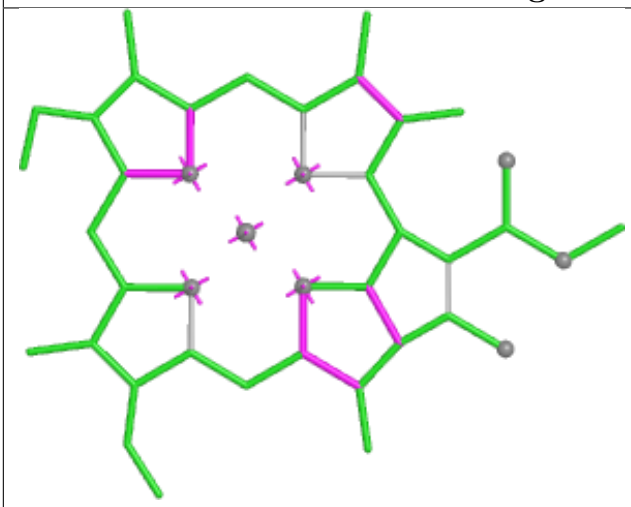

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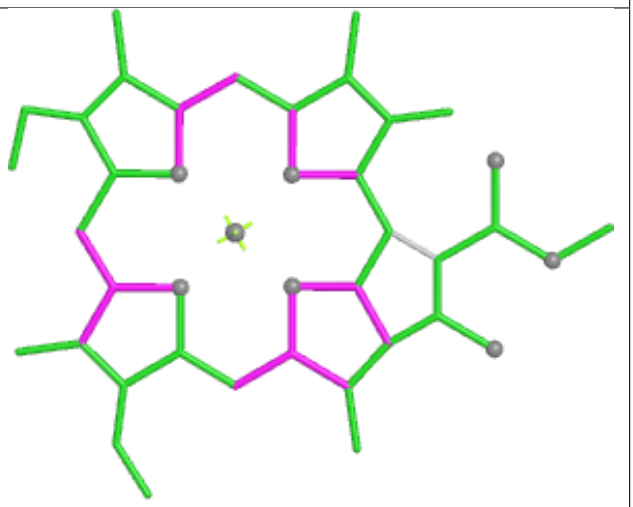

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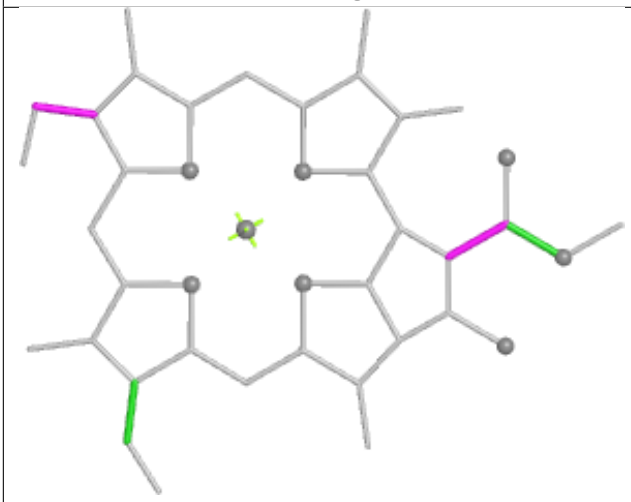

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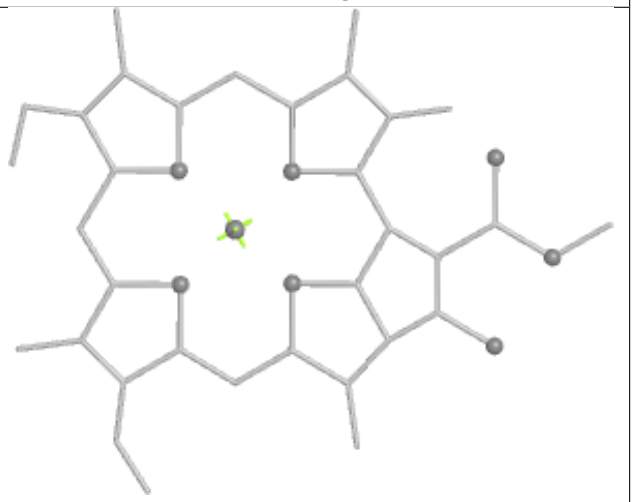

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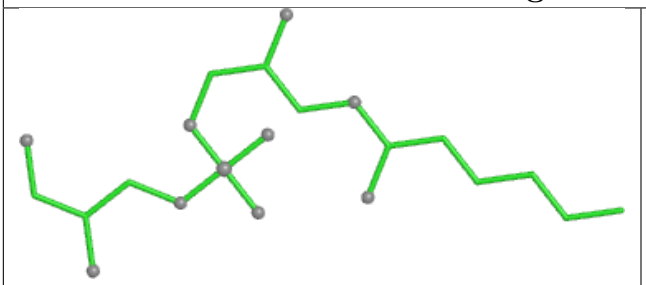

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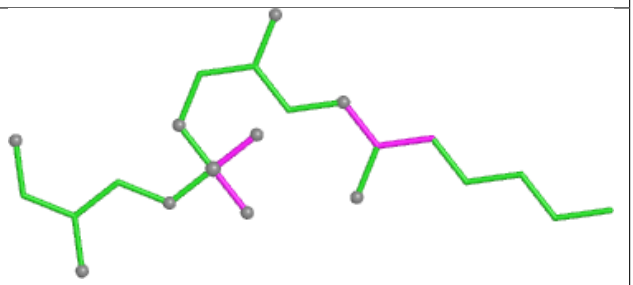

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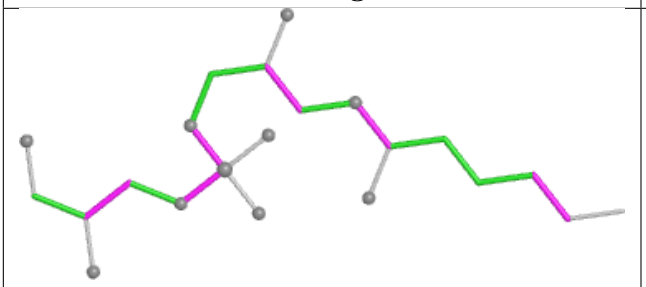

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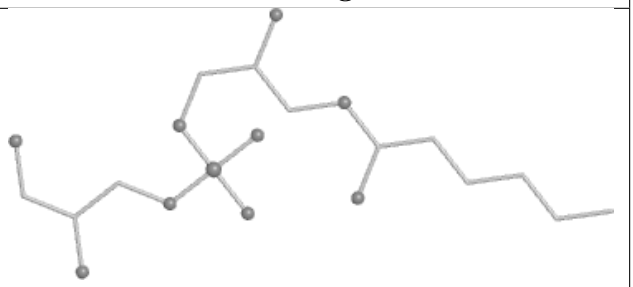

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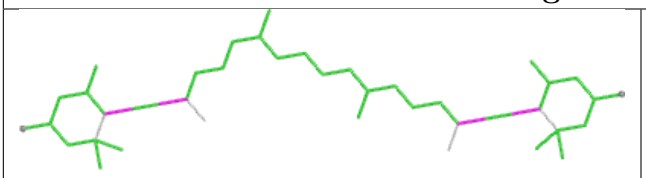

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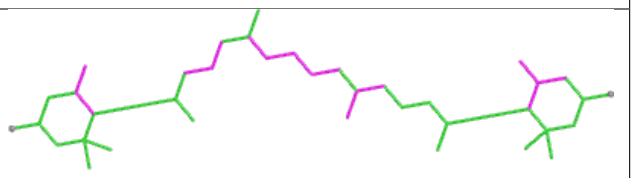

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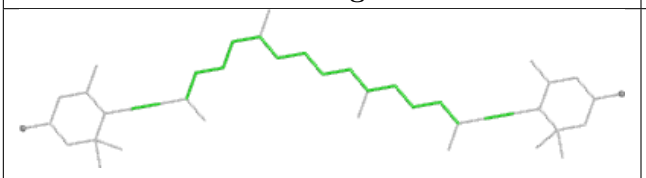

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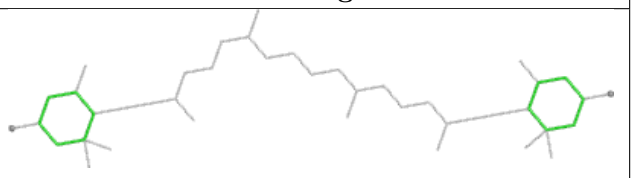
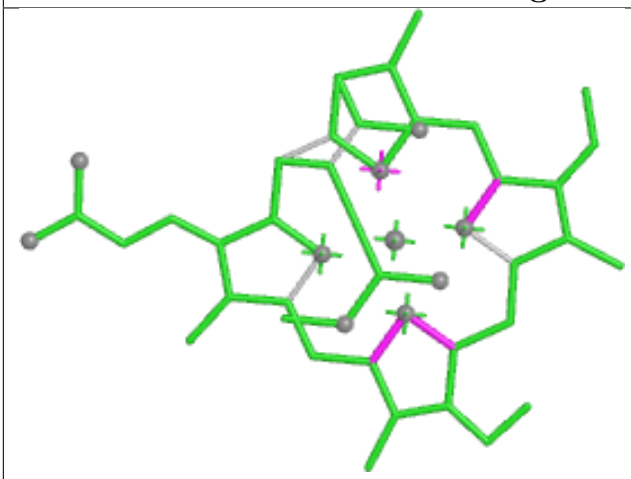


Rings

Ligand KC2 9 610



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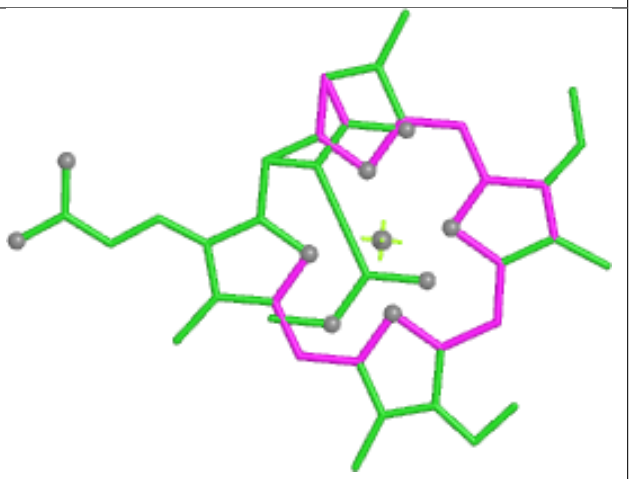

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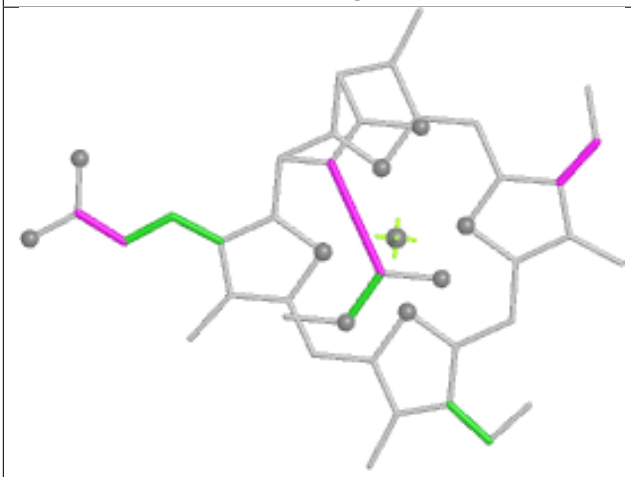

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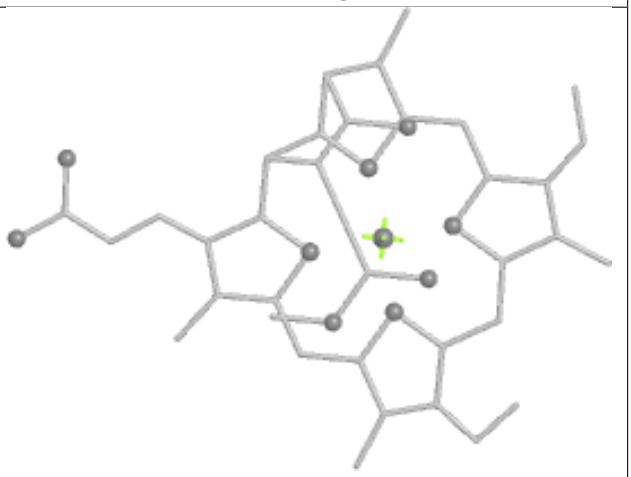
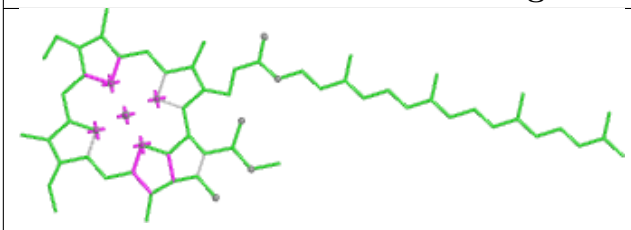


Rings

Ligand CLA d 608



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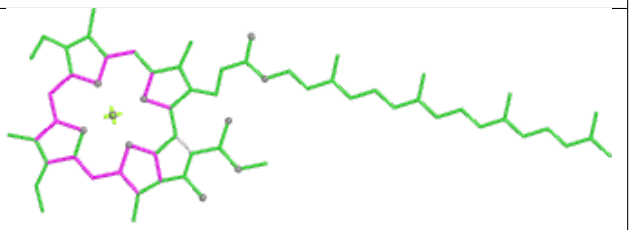

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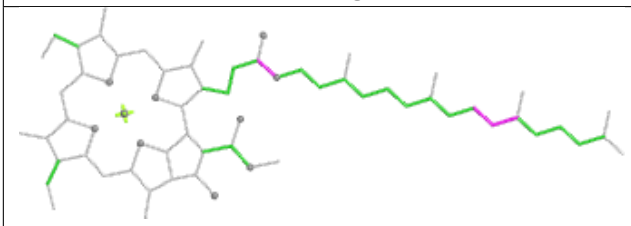

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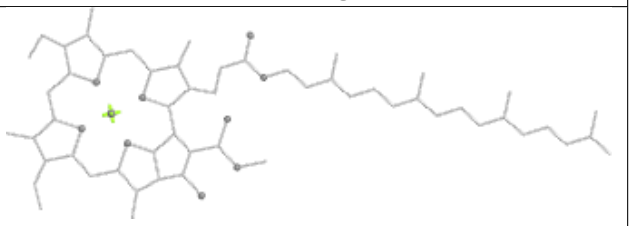

Rings

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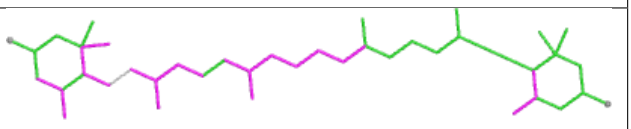
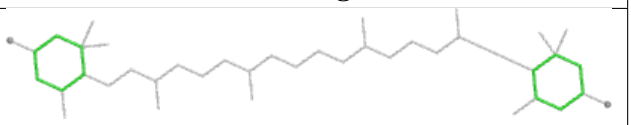
 Bond lengths	 Bond angles
 Torsions	 Rings

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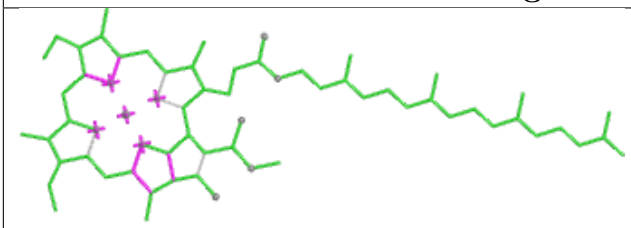
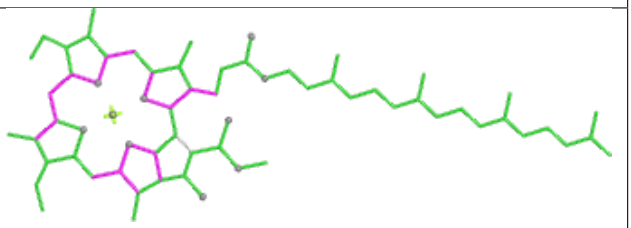
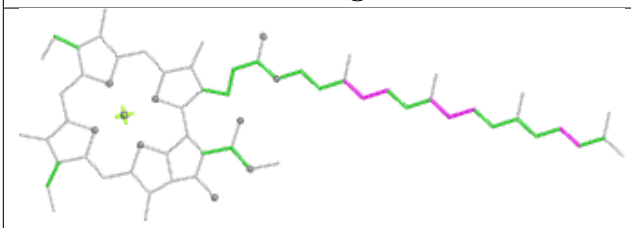
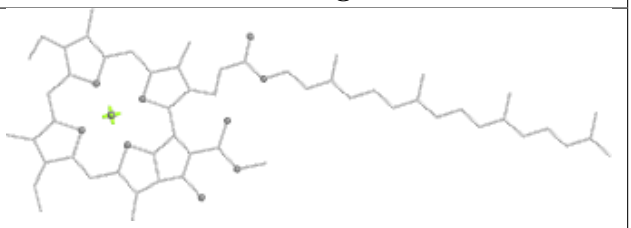
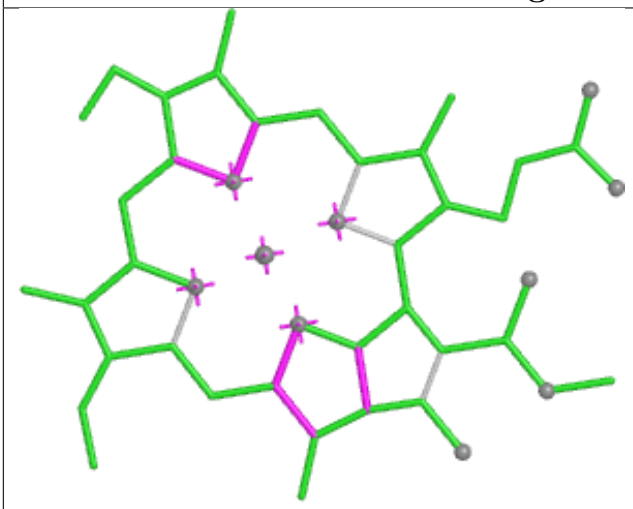
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 601



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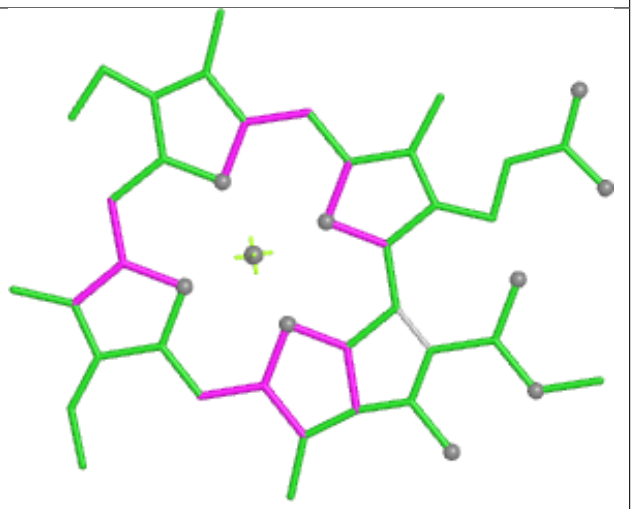
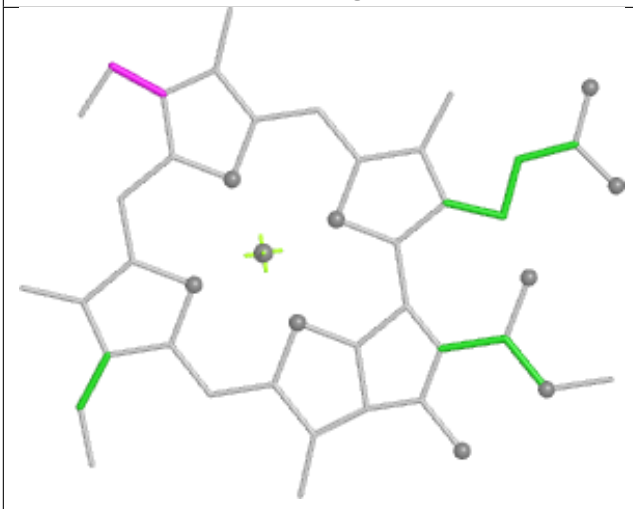


Bond angles

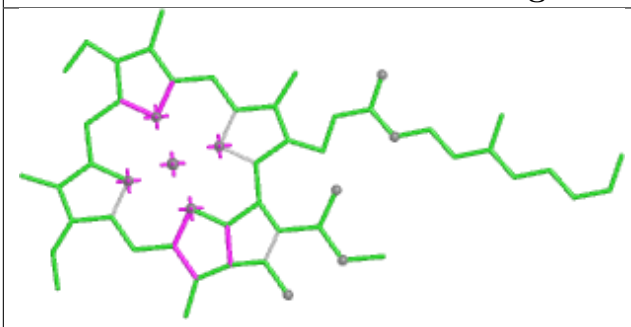


Torsions



Rings

Ligand CLA 4 603



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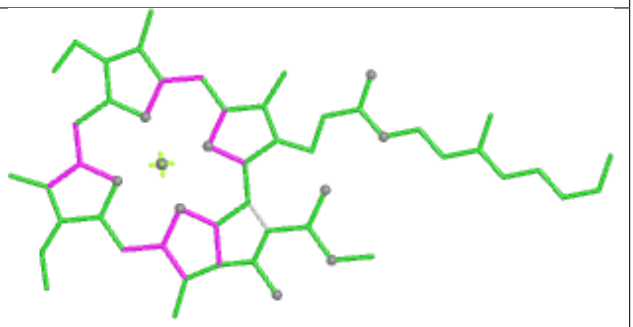

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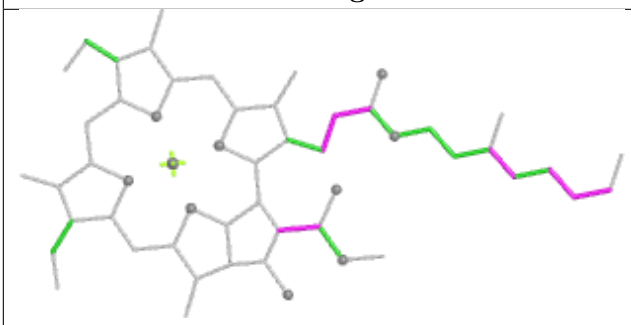

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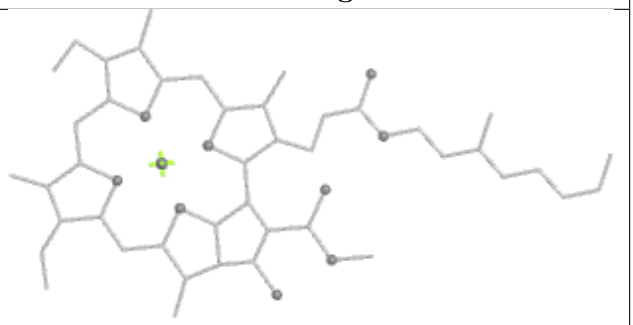
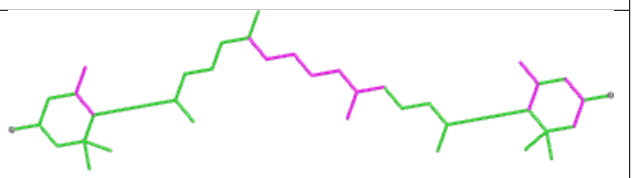


Rings

Ligand II0 9 618



Bond lengths



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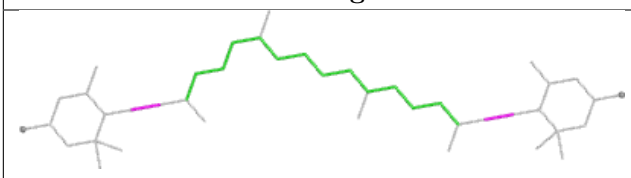

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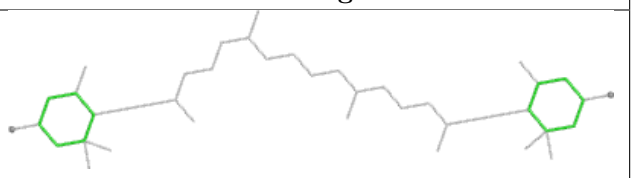
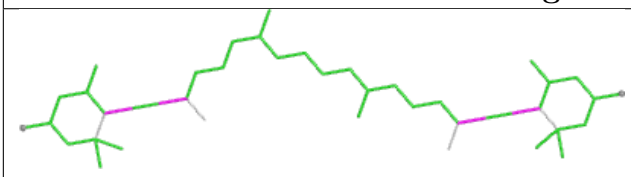


Rings

Ligand II0 1 619



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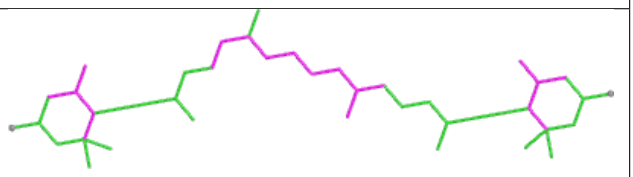
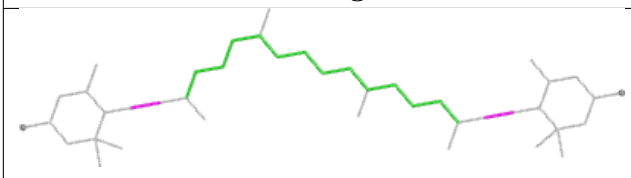


Bond angles



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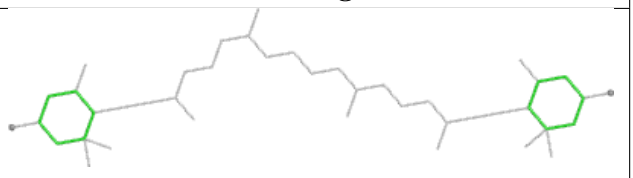
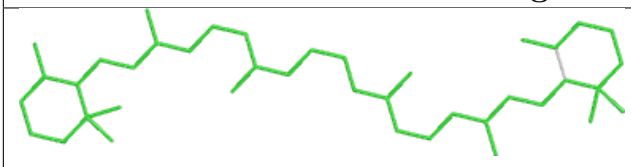
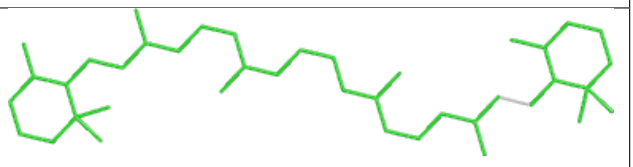


Rings

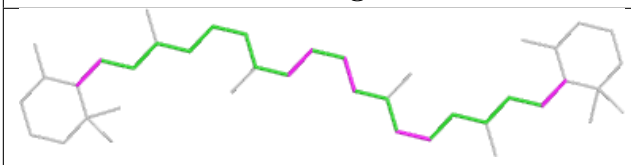
Ligand 8CT J 103



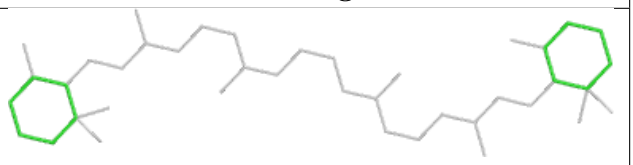
Bond lengths



Bond angles

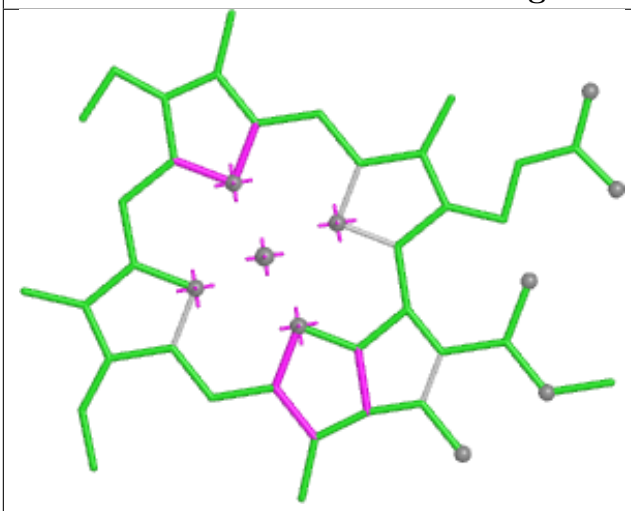


Torsions



Rings

Ligand CLA a 601



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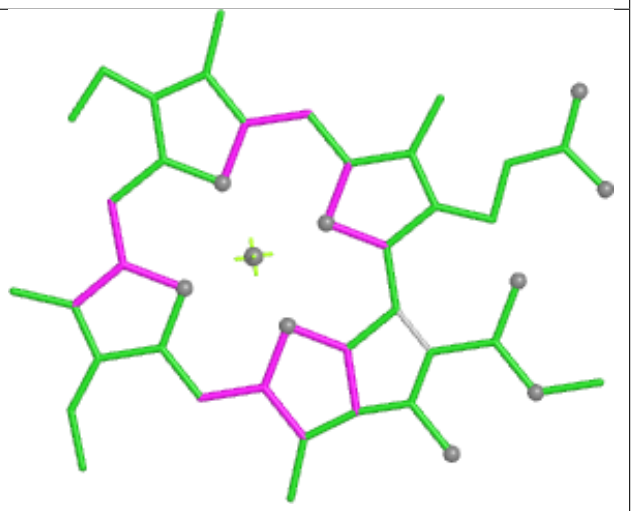

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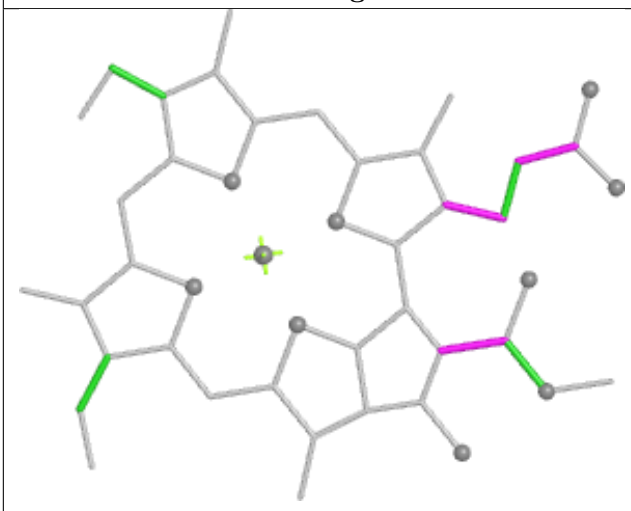

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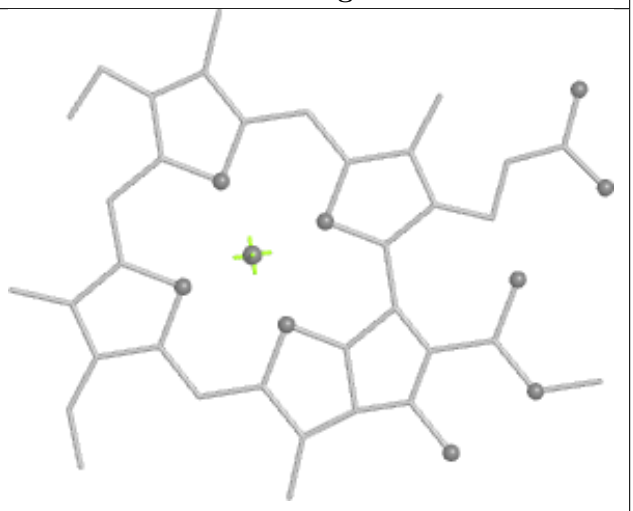
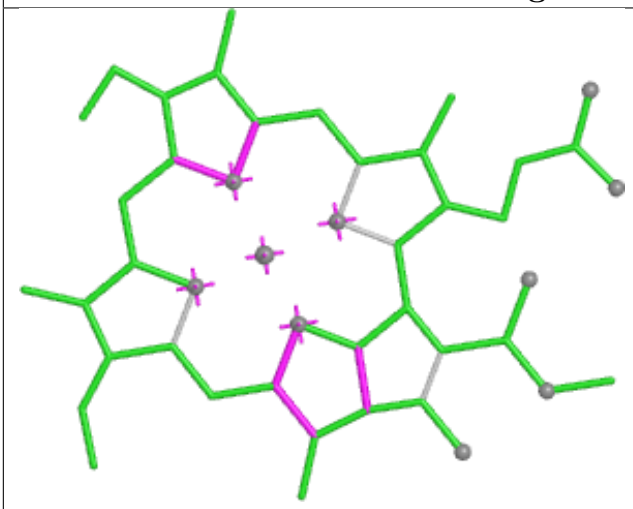


Rings

Ligand CLA 6 612



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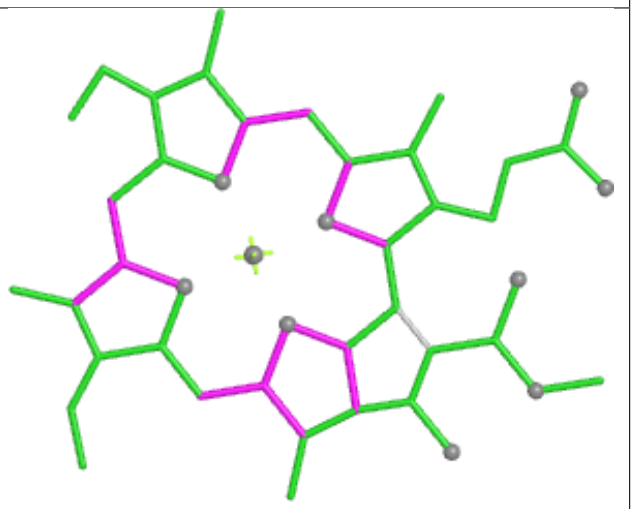

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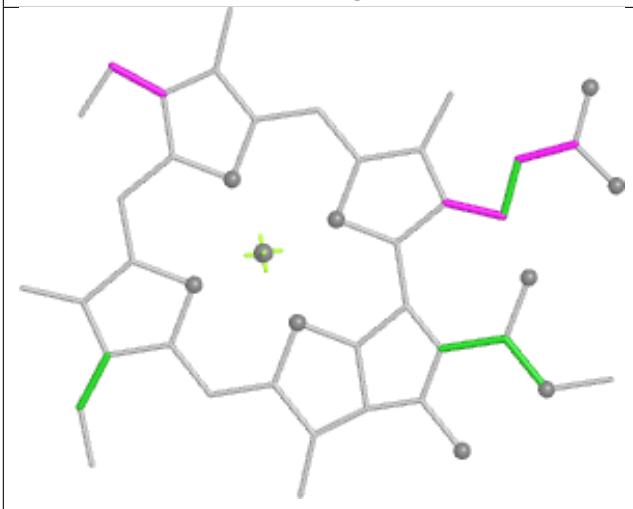
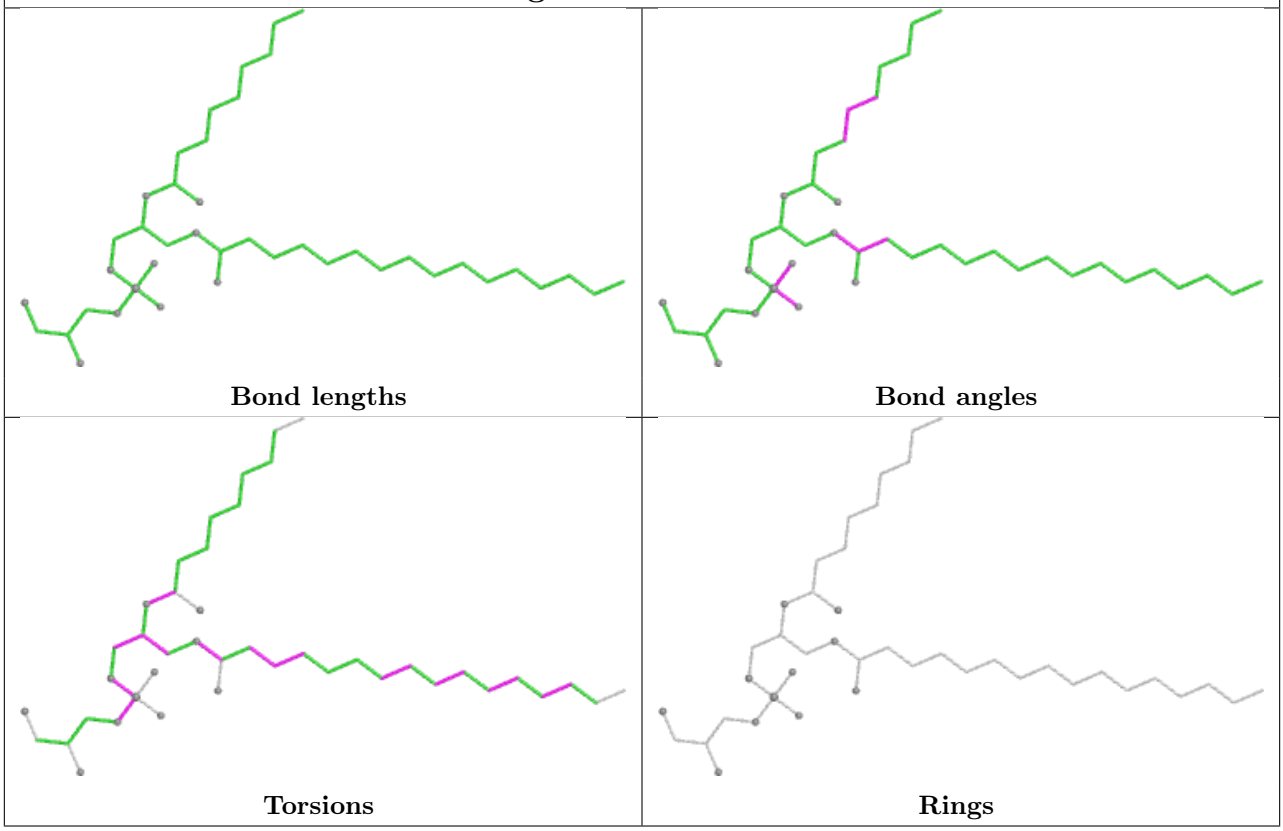


Torsions



Rings

Ligand LHG 2 620



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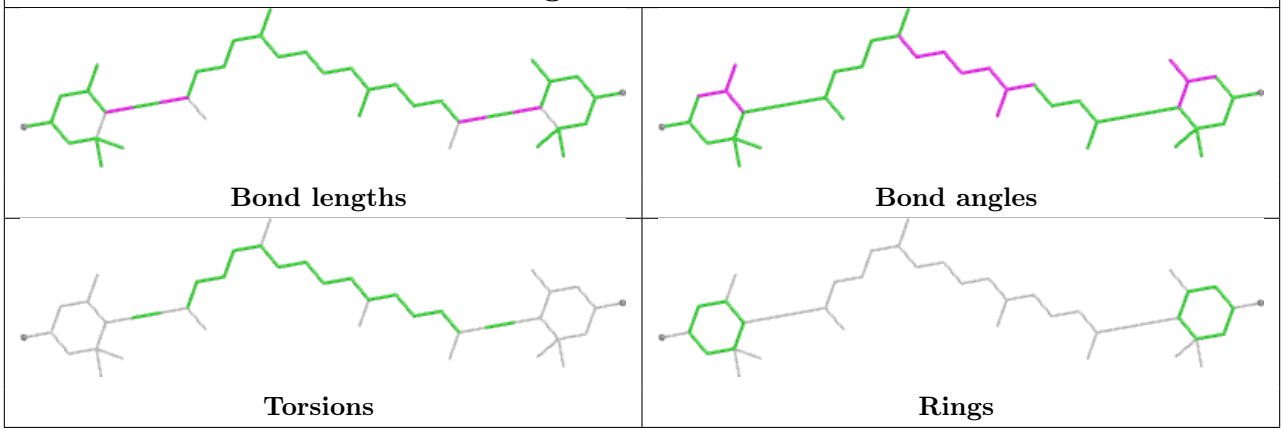

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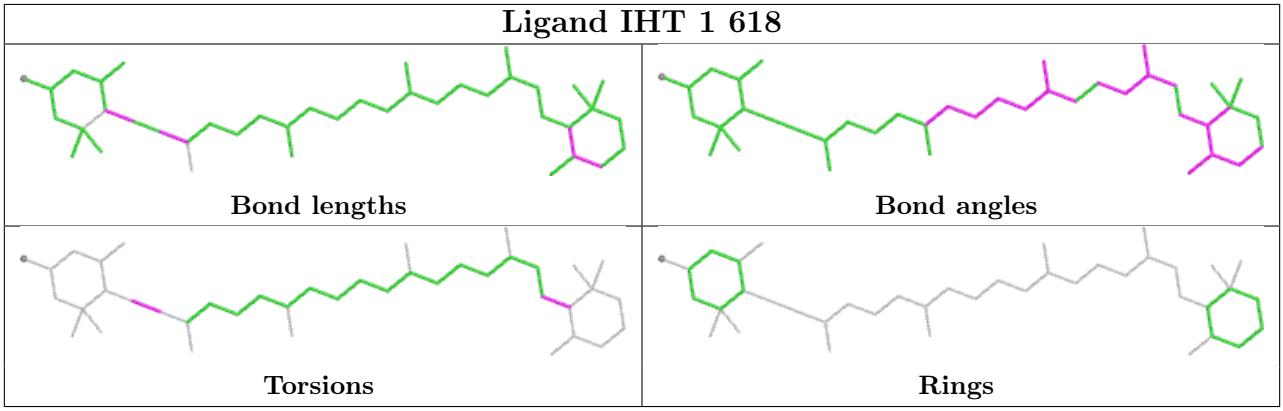
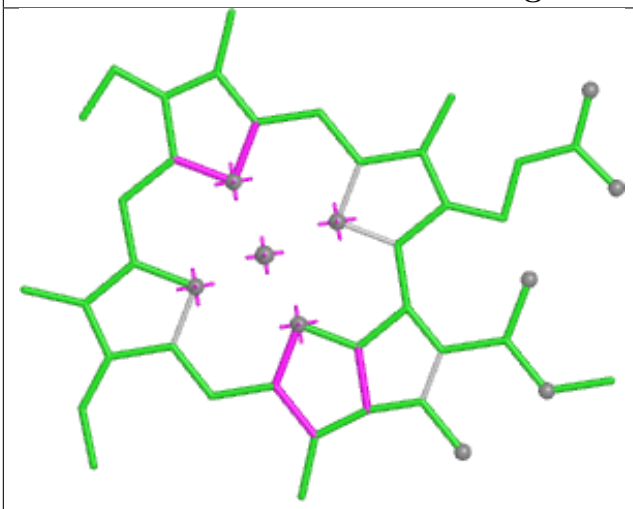


Ligand CLA B 804



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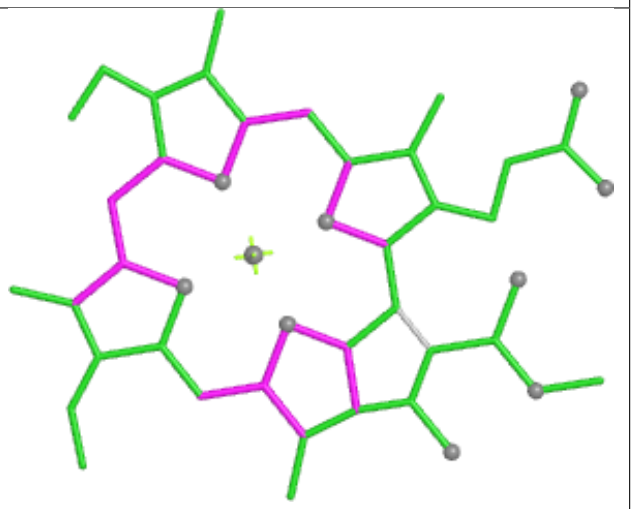

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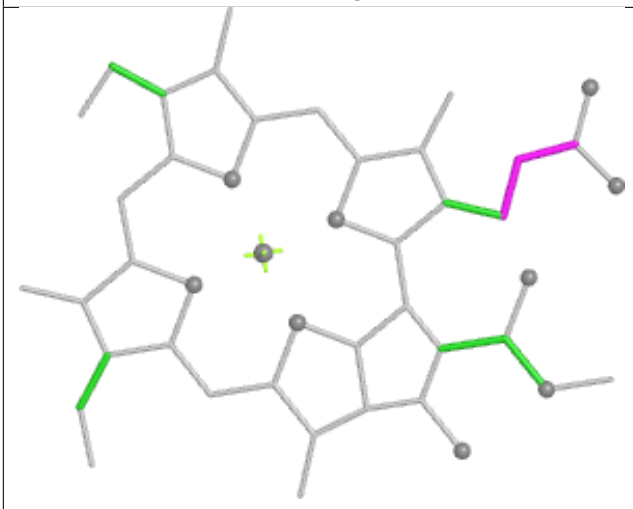
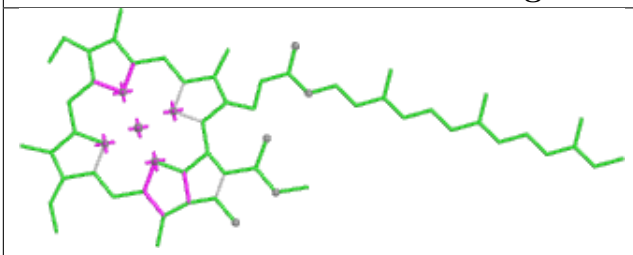


Torsions



Rings

Ligand CLA B 813



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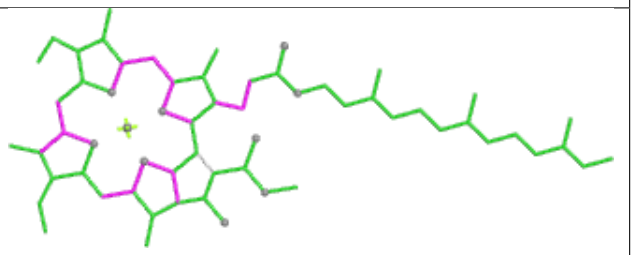

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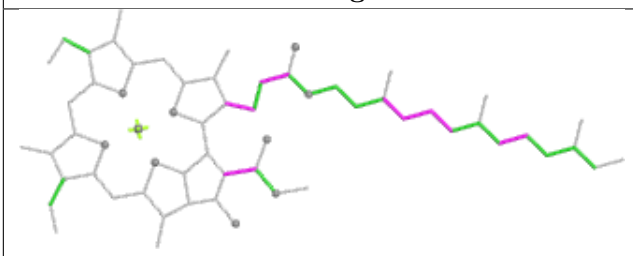

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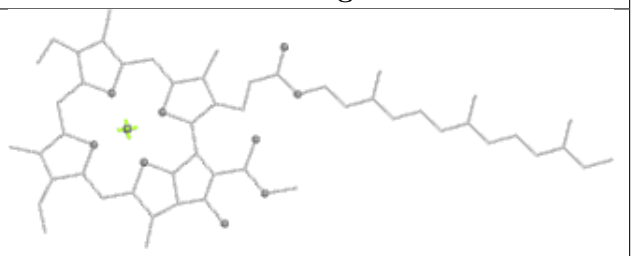
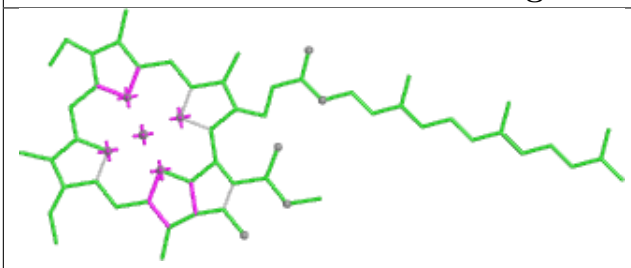
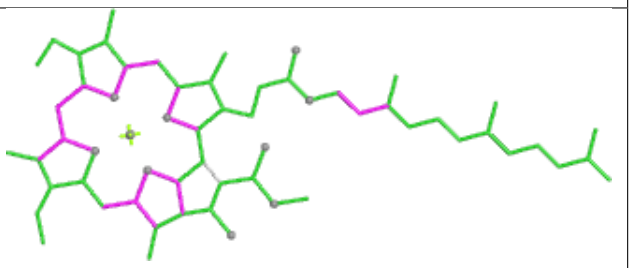
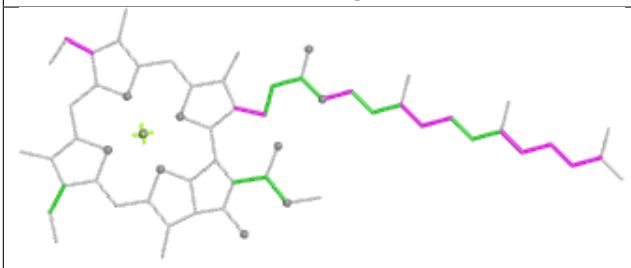
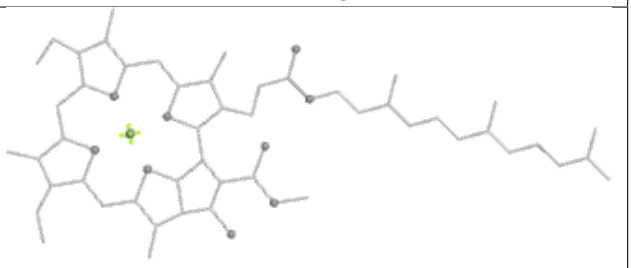
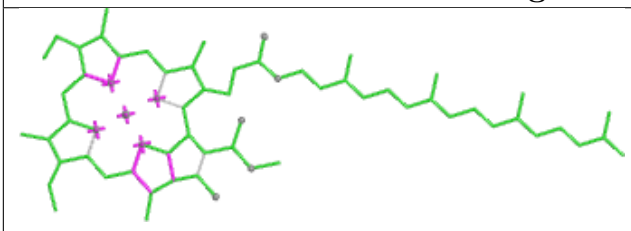
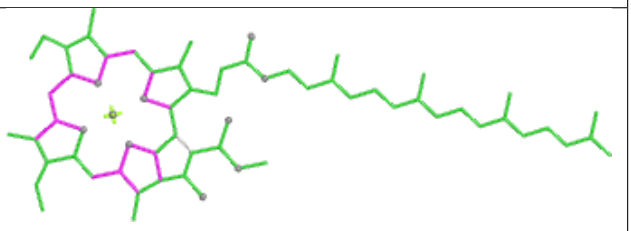
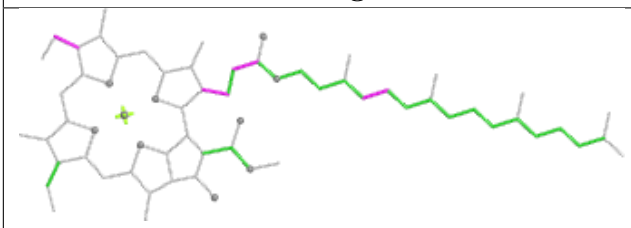
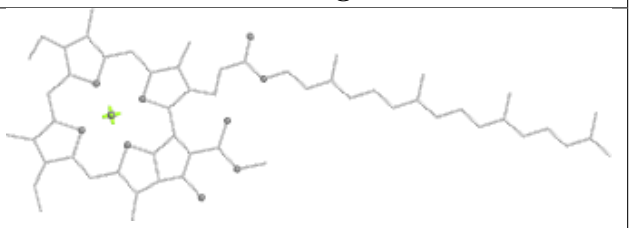
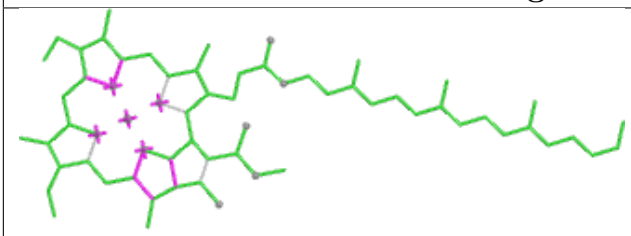


Rings

Ligand CLA F 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 602



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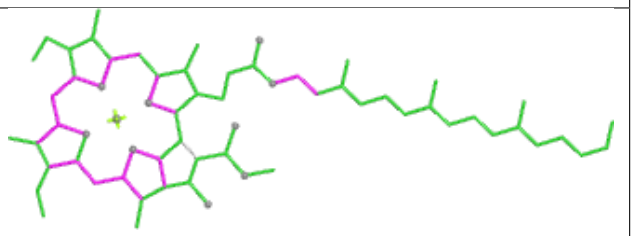
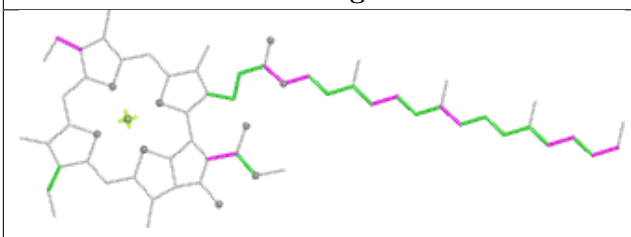


Bond angles



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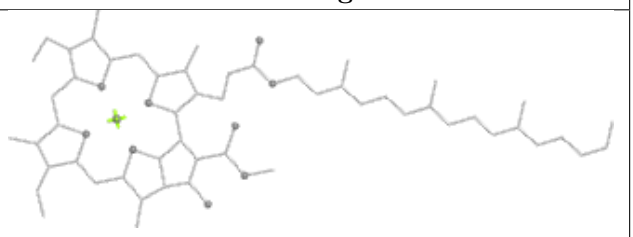
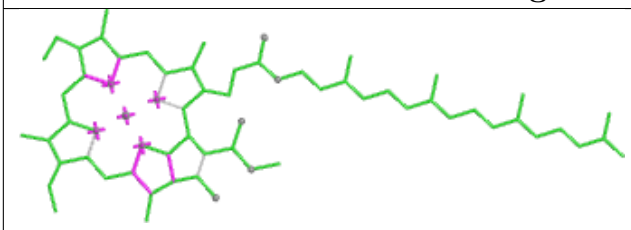


Rings

Ligand CLA c 602



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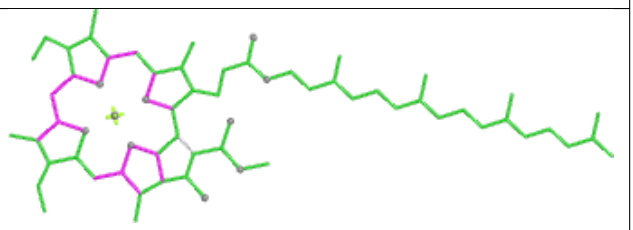

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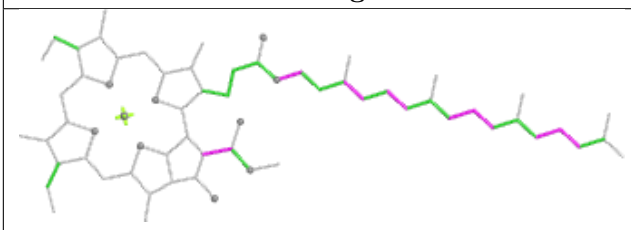

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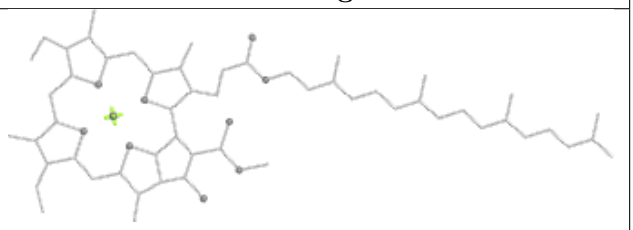
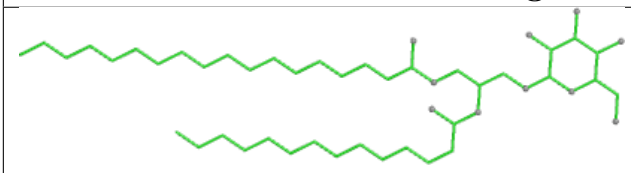


Rings

Ligand LMG I 102



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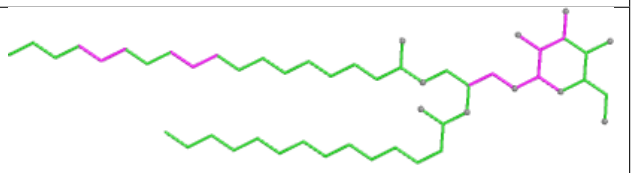

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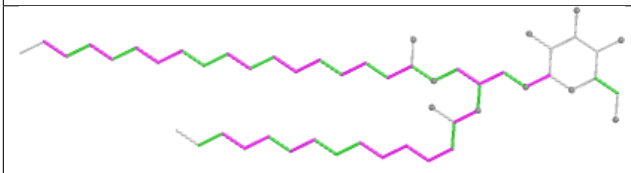

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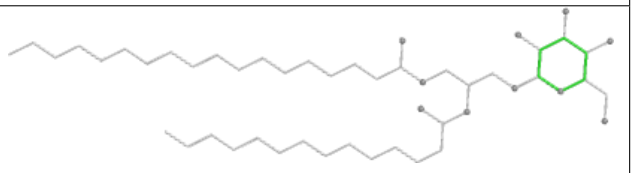
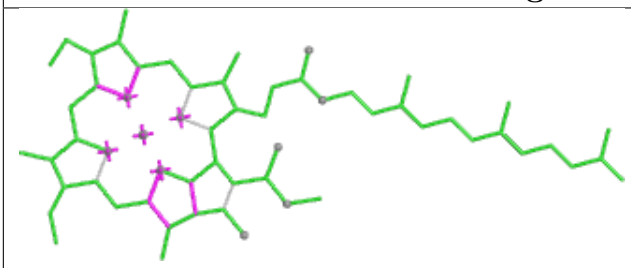


Rings

Ligand CLA L 203



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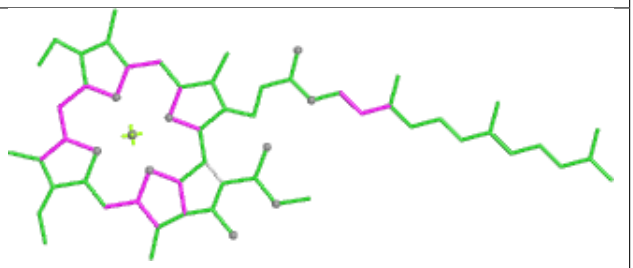

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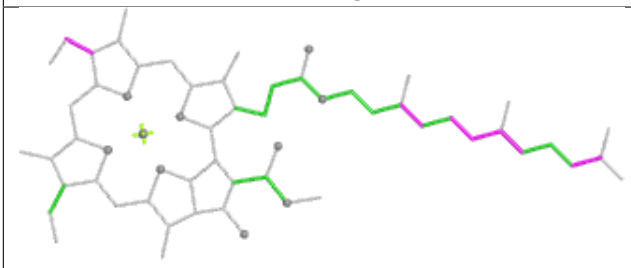

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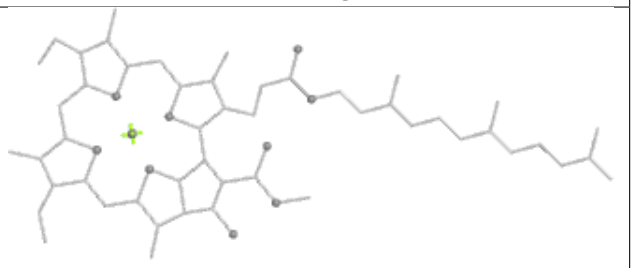
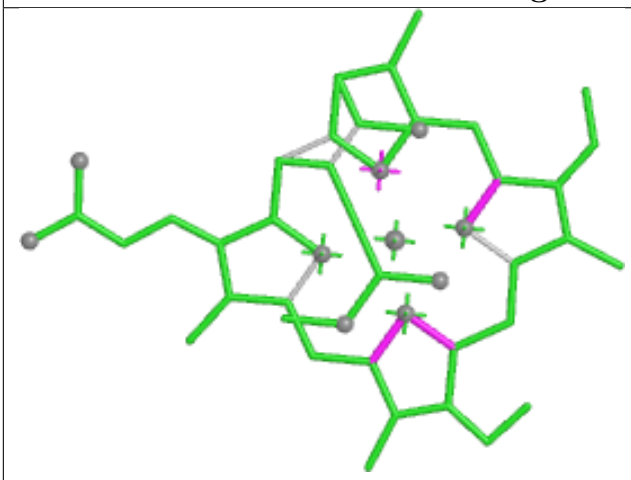


Rings

Ligand KC2 a 610



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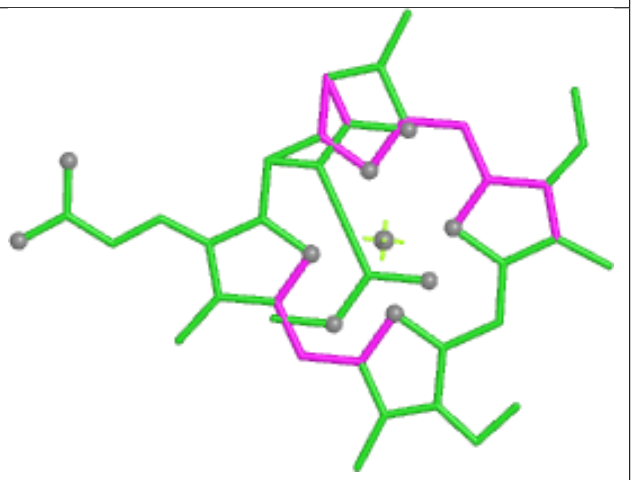
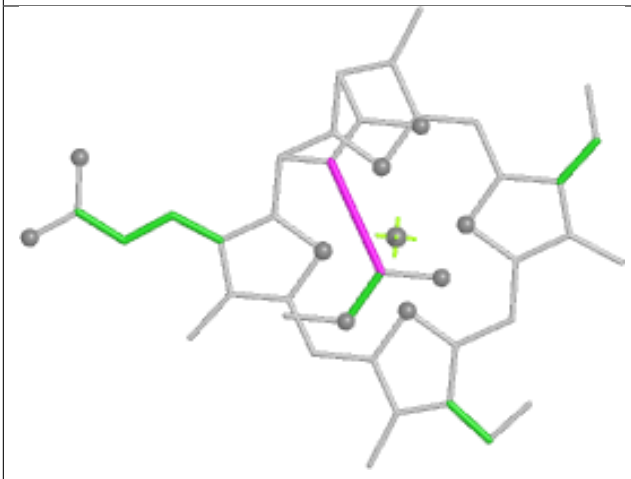


Bond angles



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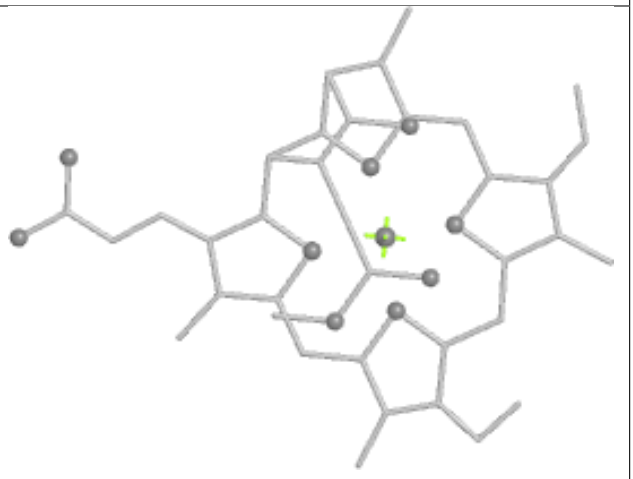
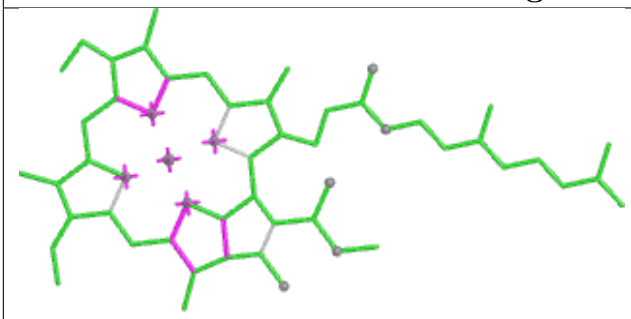
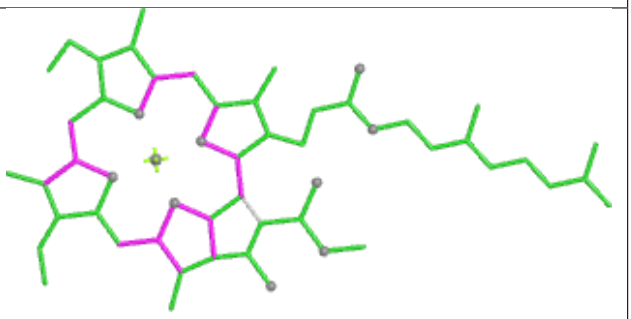
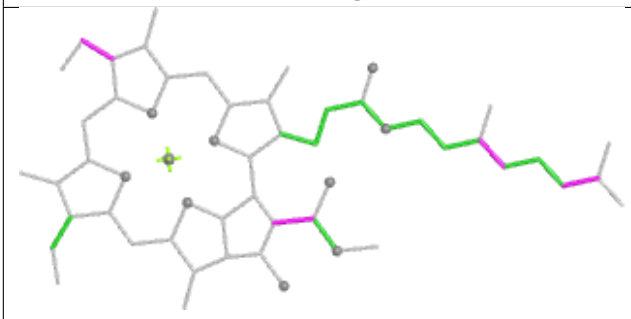
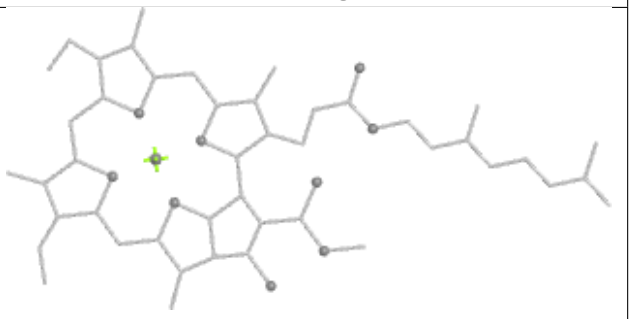
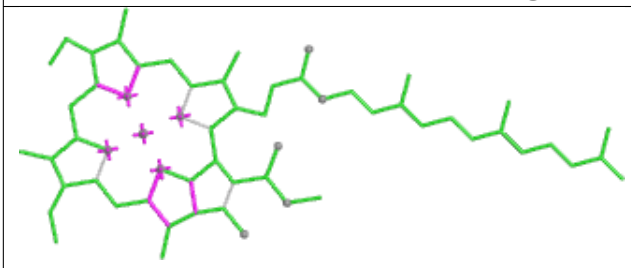
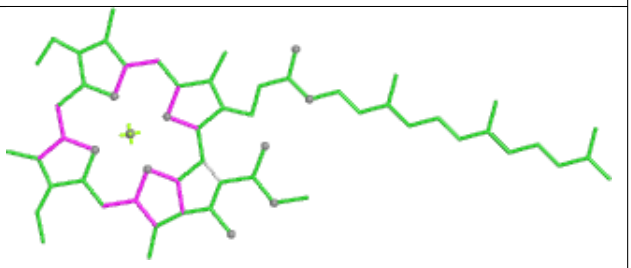
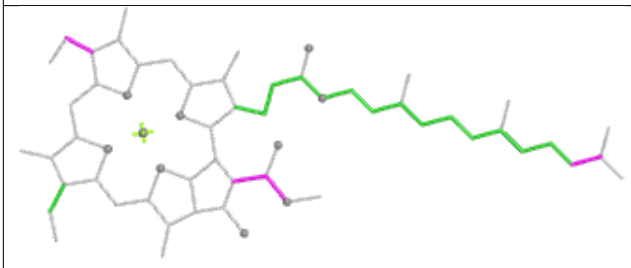
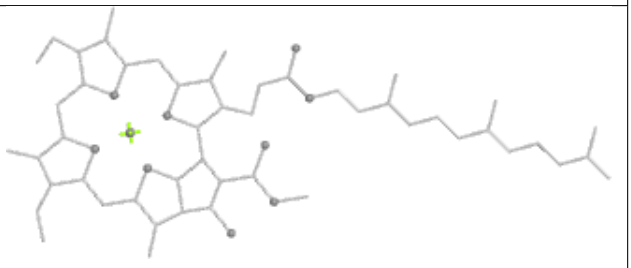
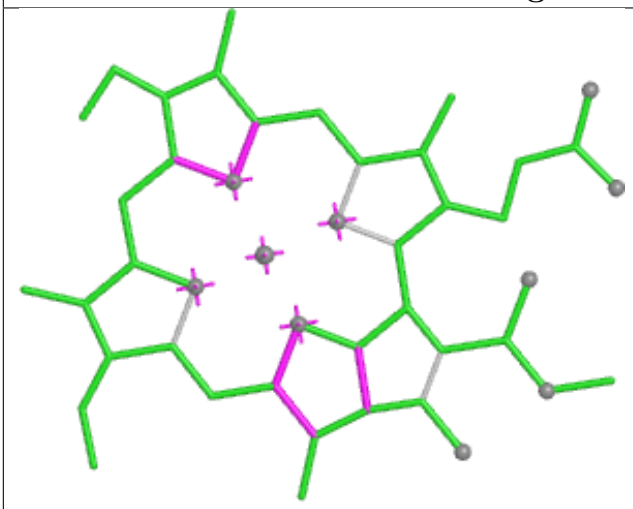


Rings

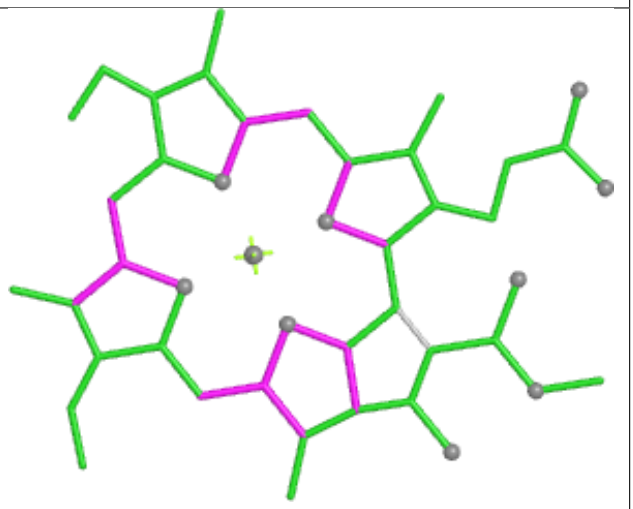
Ligand CLA F 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

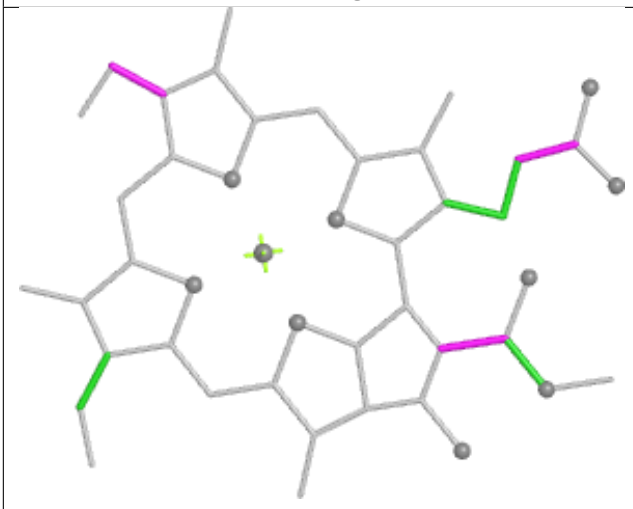
Ligand CLA b 601



Bond lengths



Bond angles

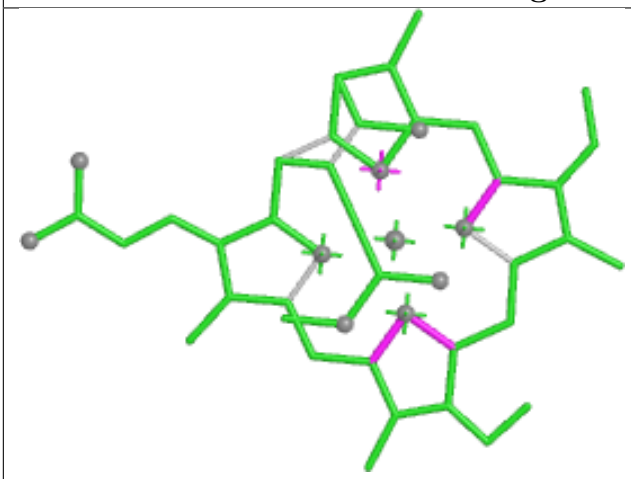


Torsions

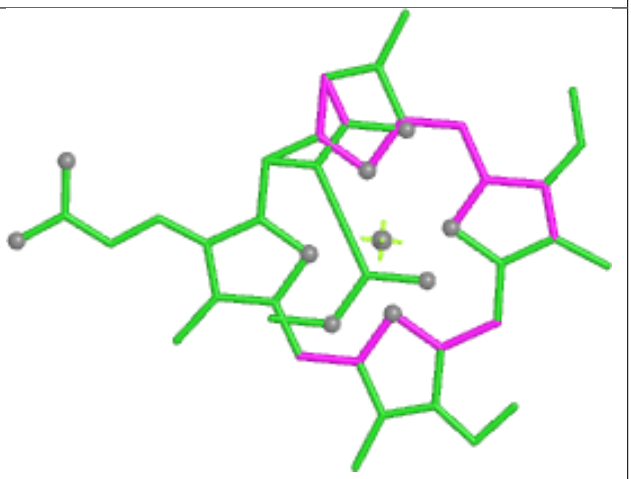


Rings

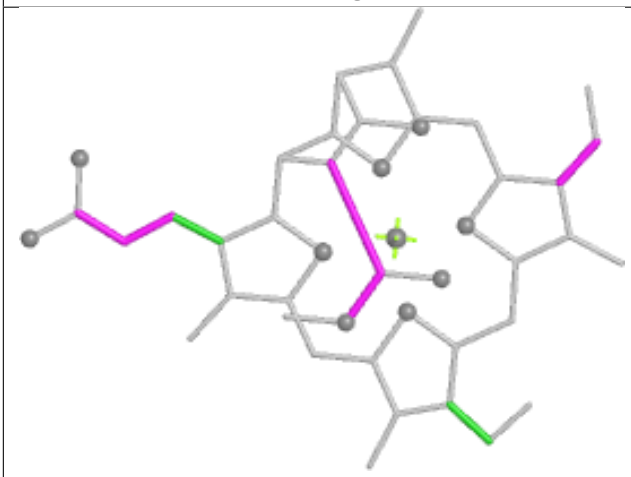
Ligand KC2 2 610



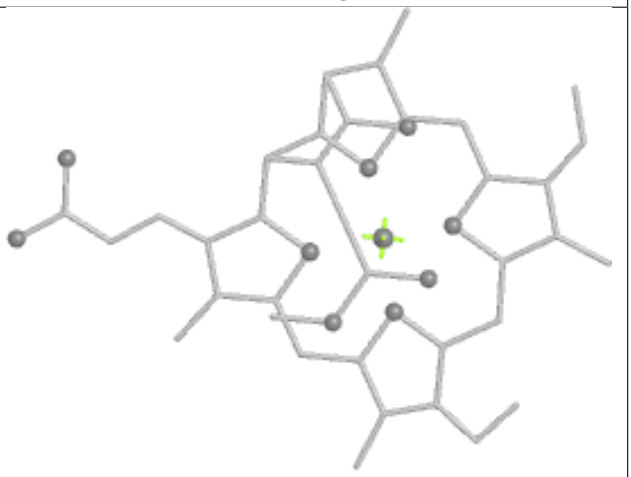
Bond lengths



Bond angles

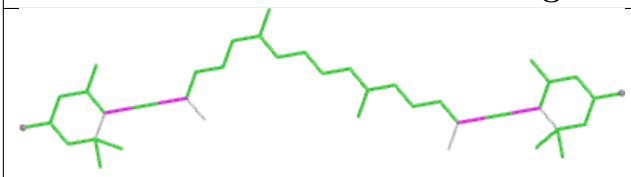


Torsions



Rings

Ligand II0 7 616



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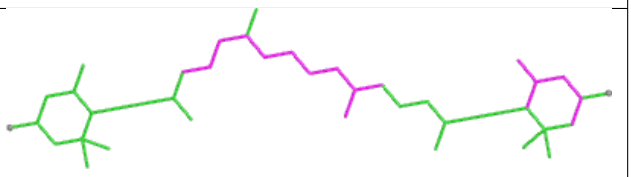

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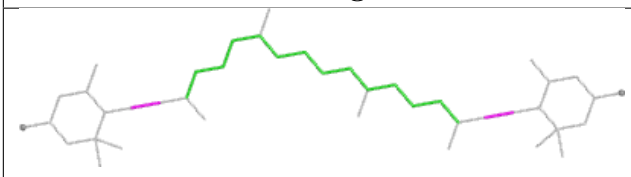

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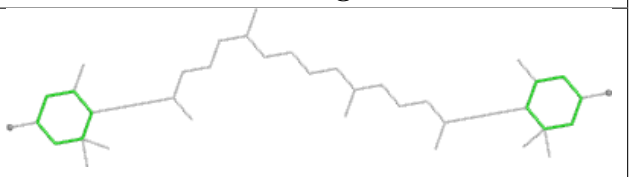
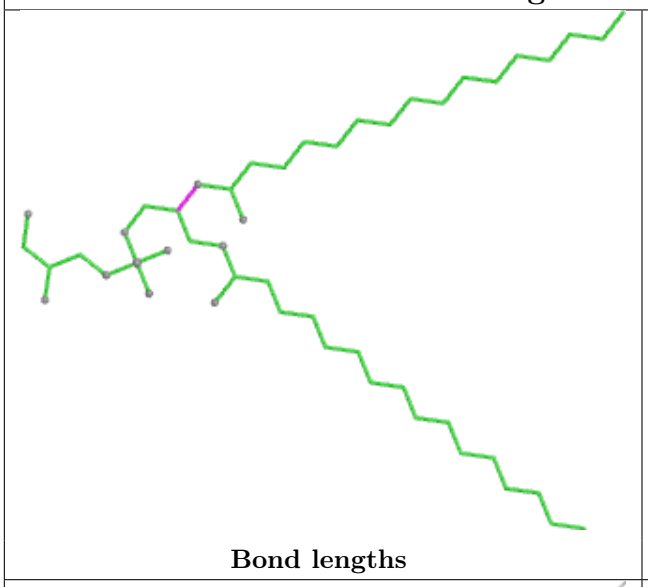


Rings

Ligand LHG 3 623



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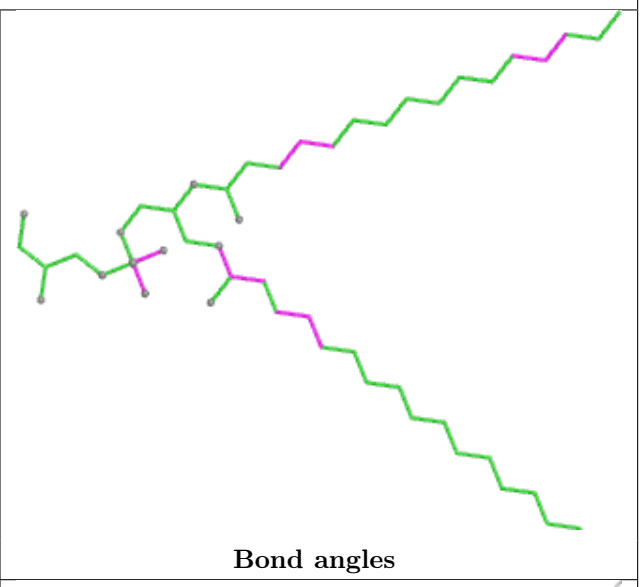

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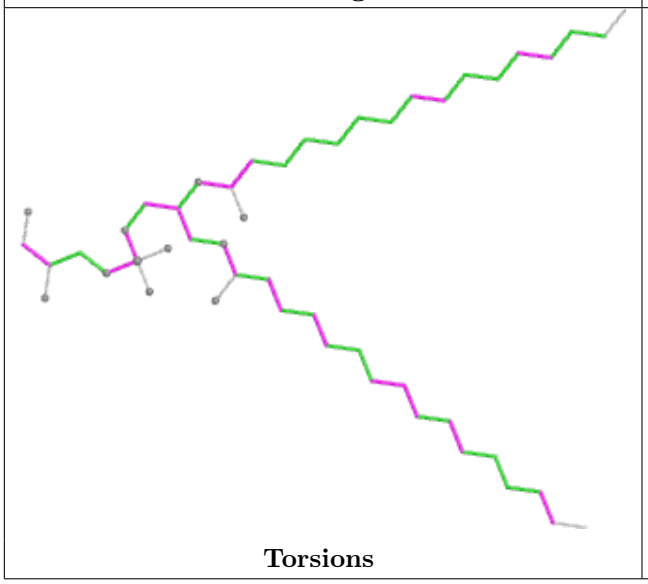

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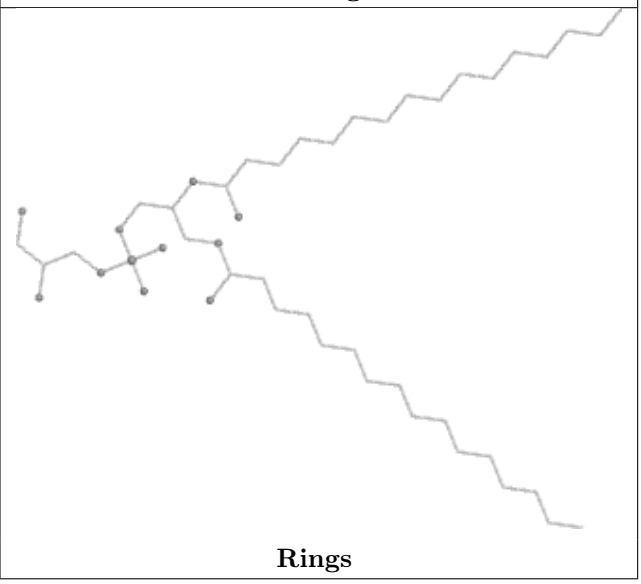
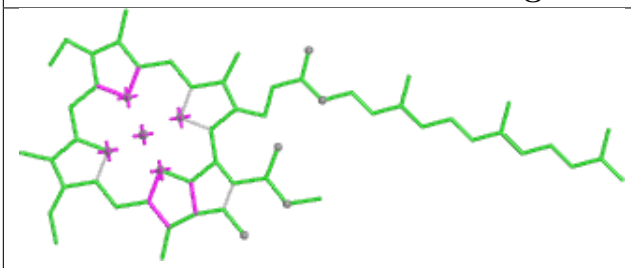


Rings

Ligand CLA B 810



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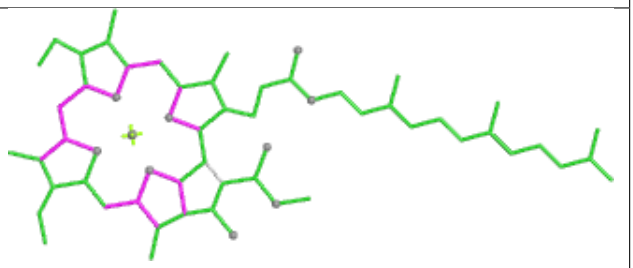
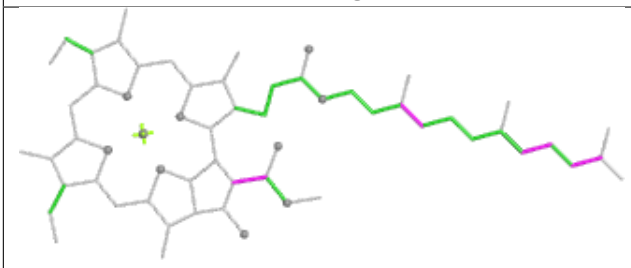


Bond angles



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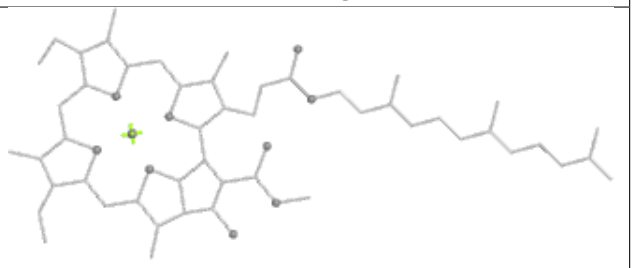
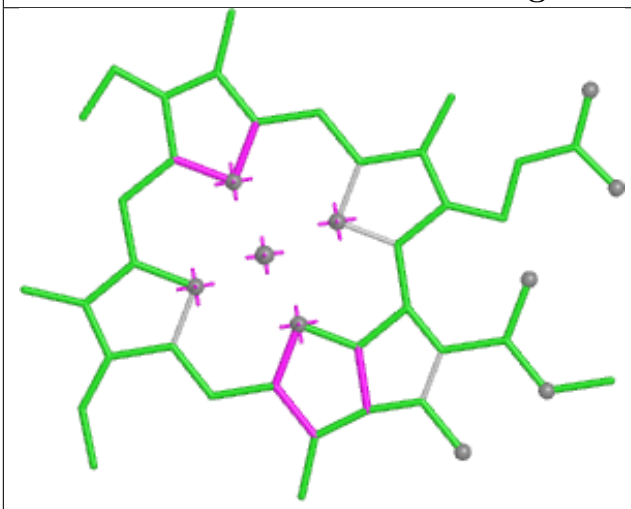


Rings

Ligand CLA 1 604



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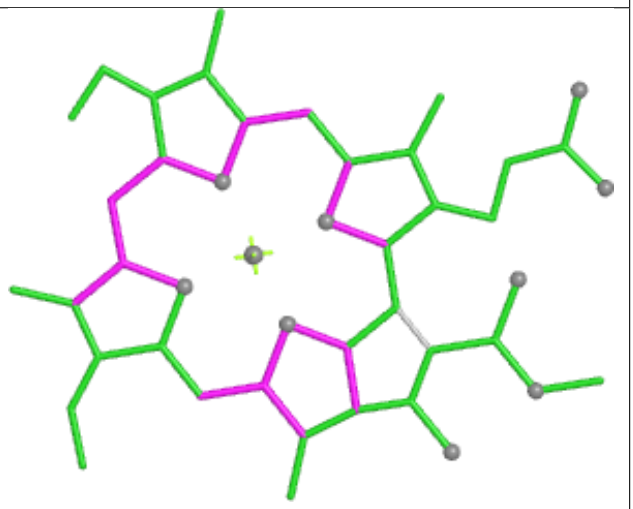

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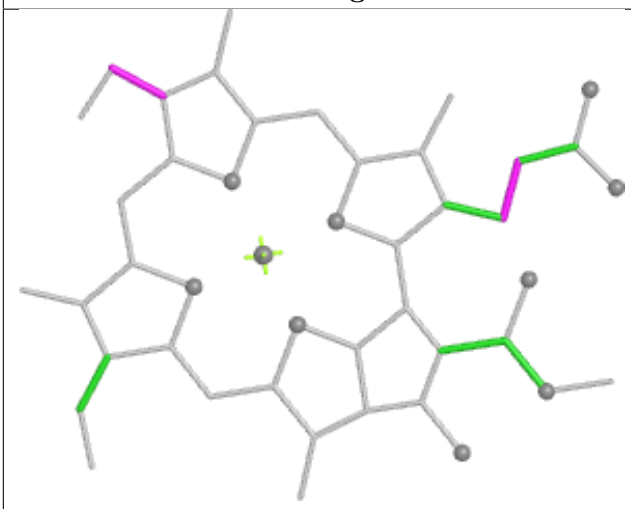

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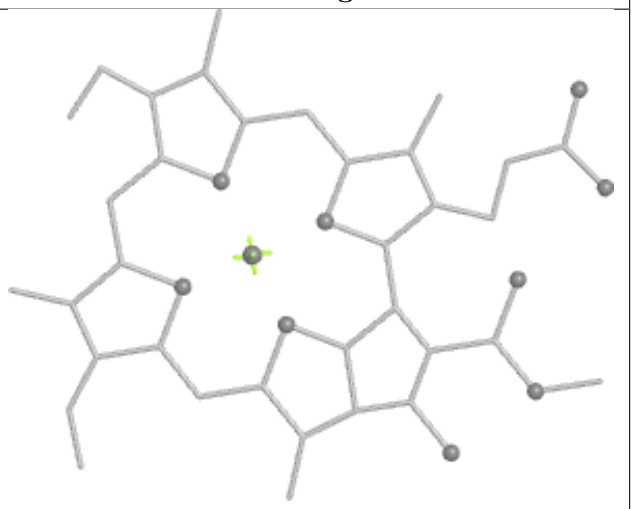

Rings

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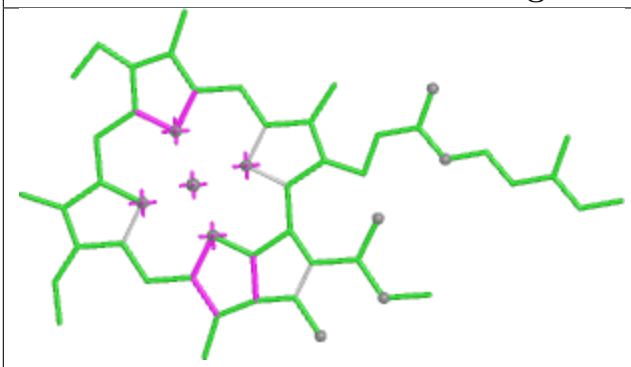

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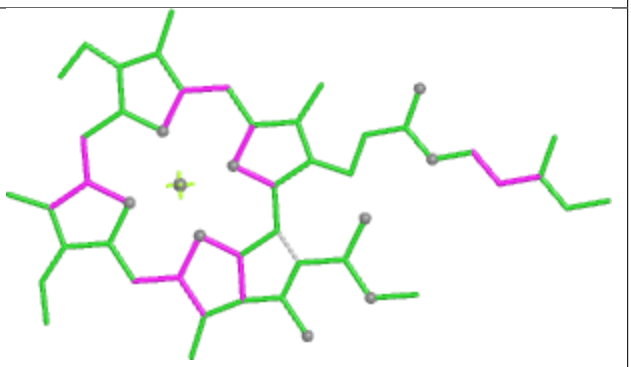
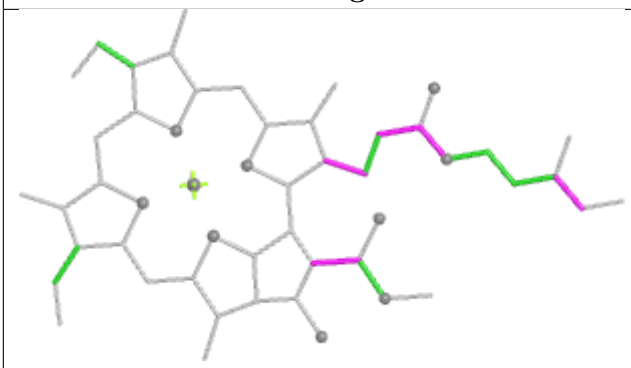


Bond angles



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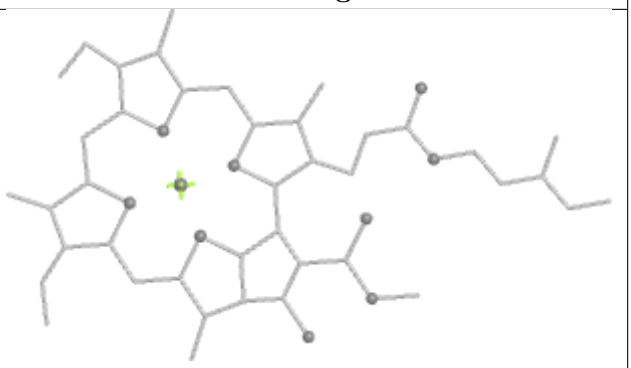

Rings

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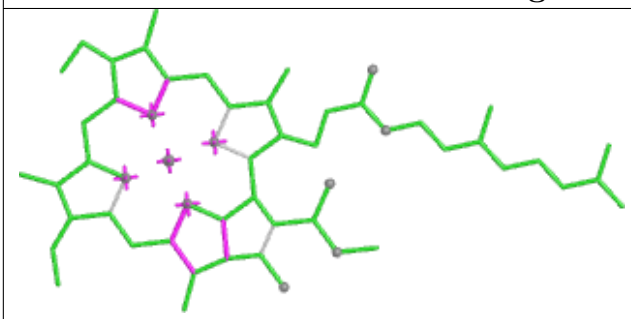

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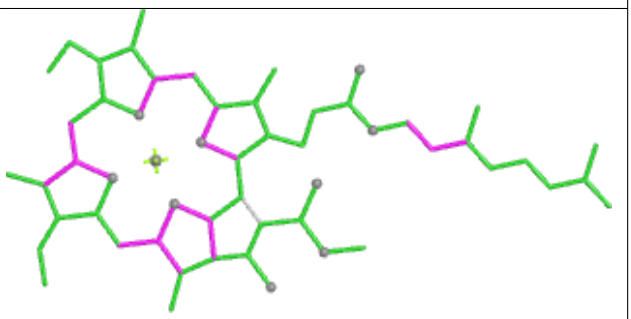

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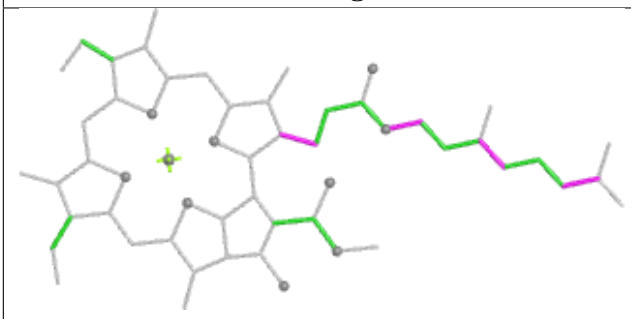

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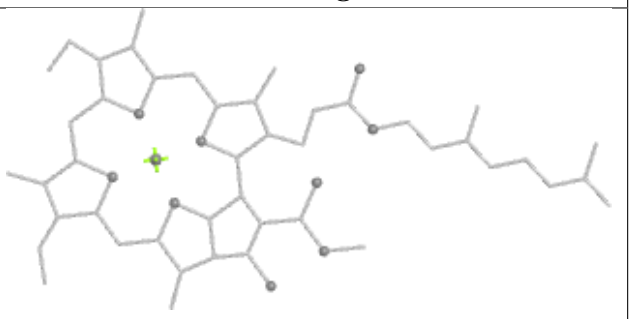

Rings

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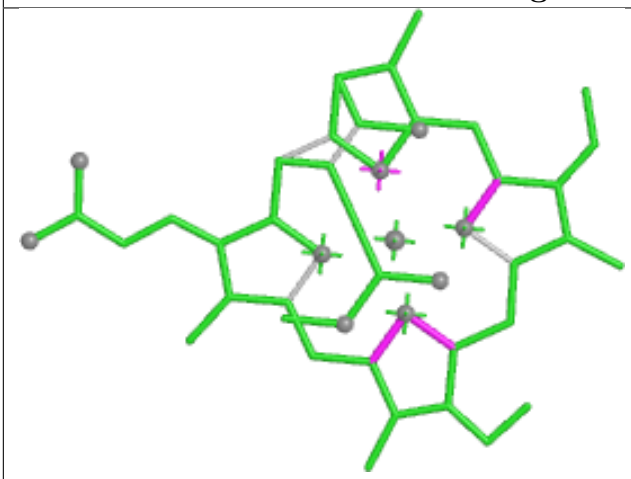

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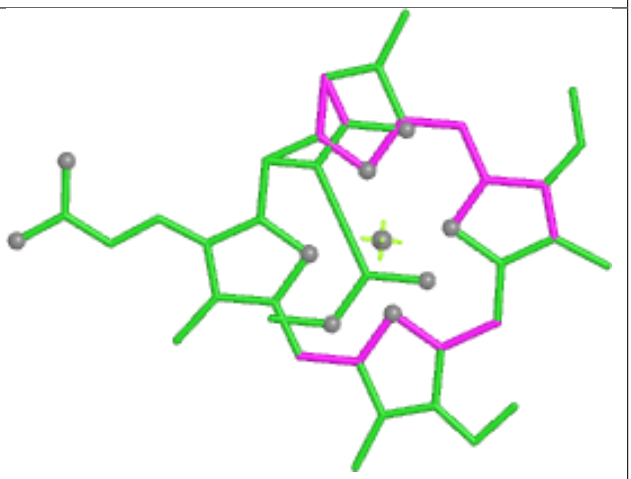

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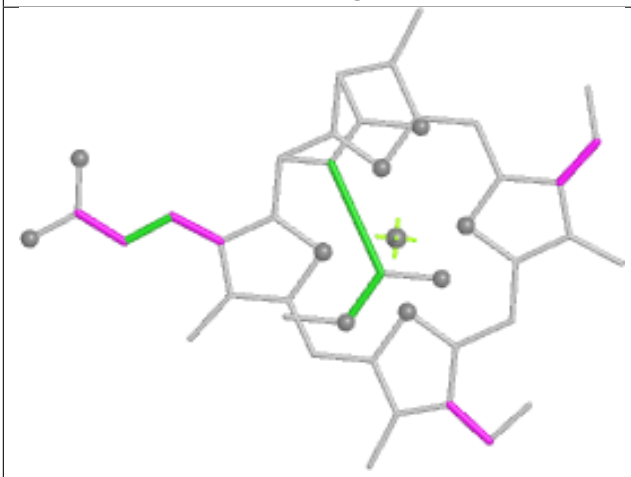

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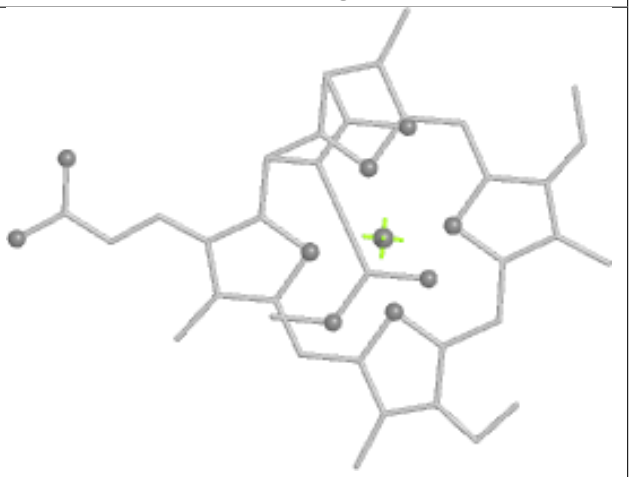
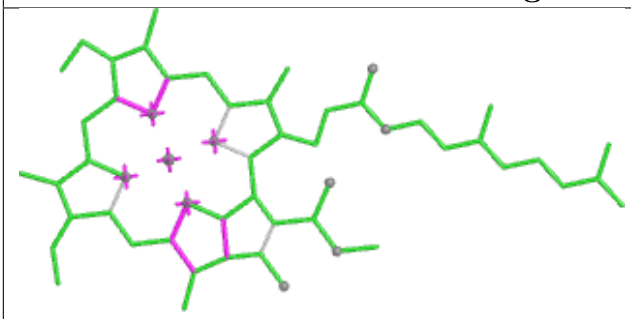


Rings

Ligand CLA A 840



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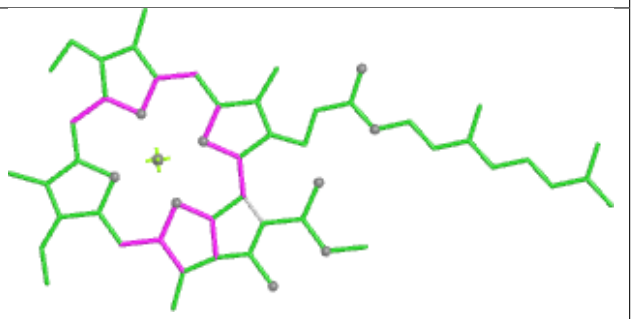

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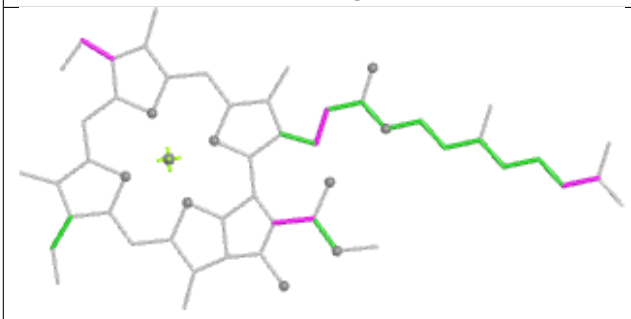

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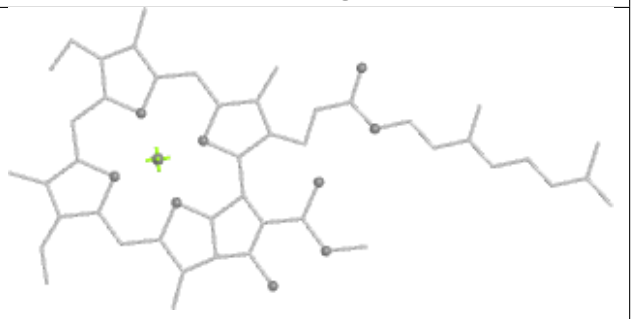
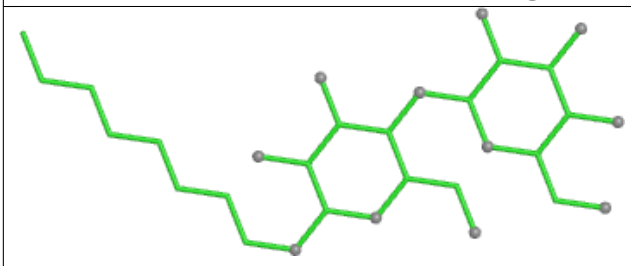


Rings

Ligand LMU J 104



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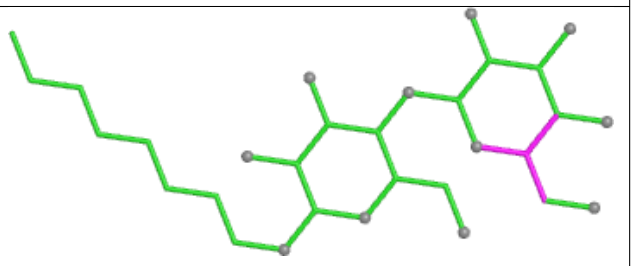

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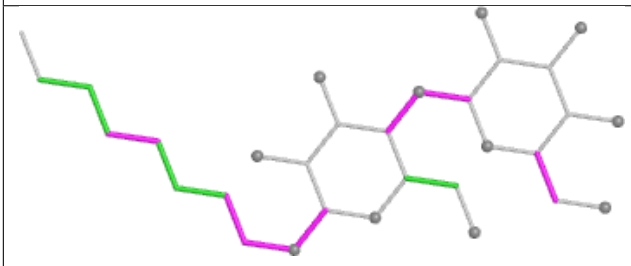

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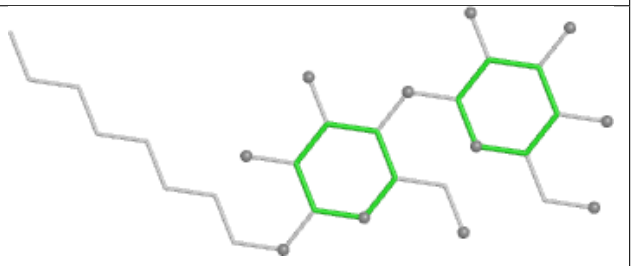
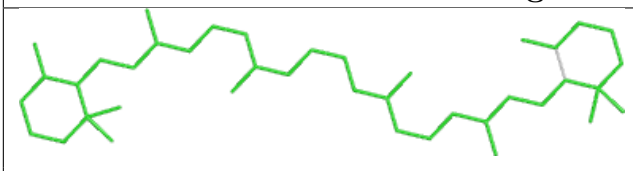


Rings

Ligand 8CT A 846



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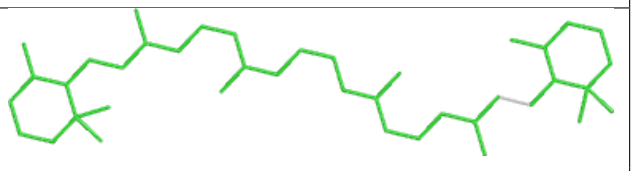
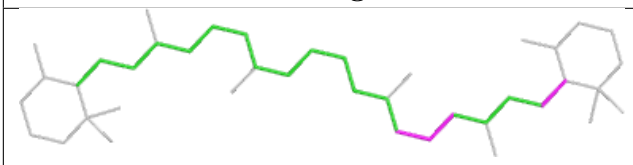


Bond angles



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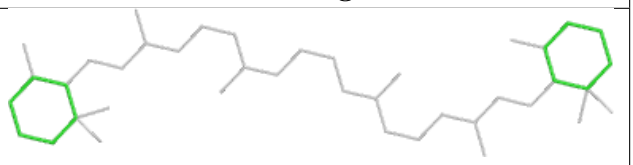
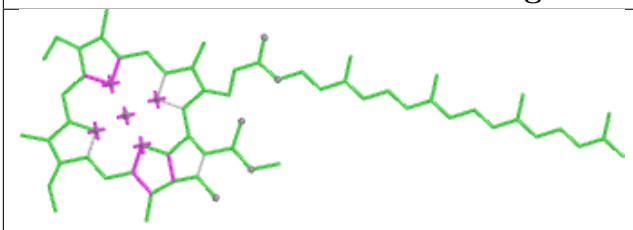


Rings

Ligand CLA B 832



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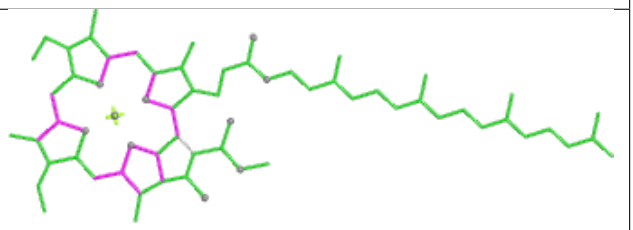
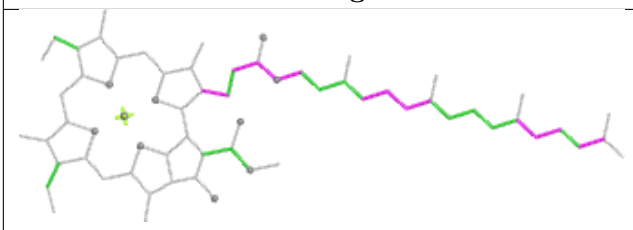


Bond angles



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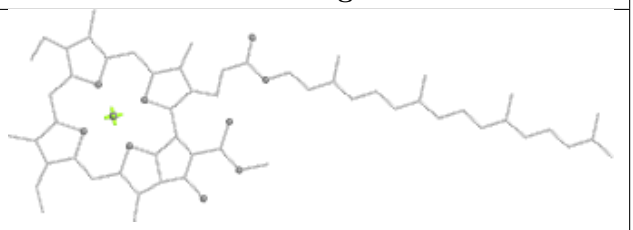
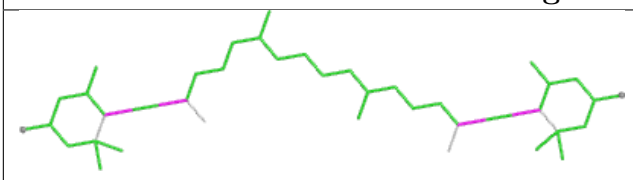


Rings

Ligand II0 3 613



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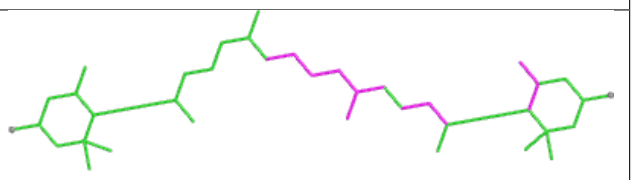
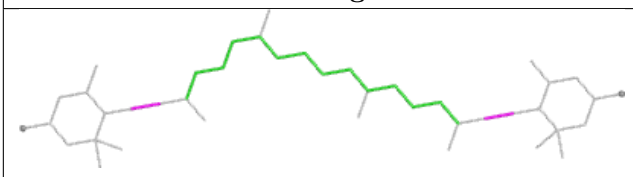


Bond angles



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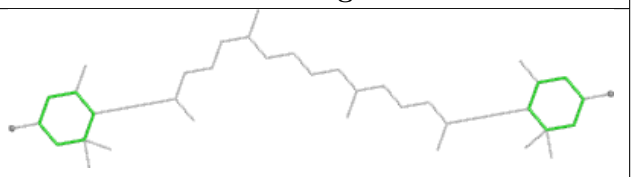
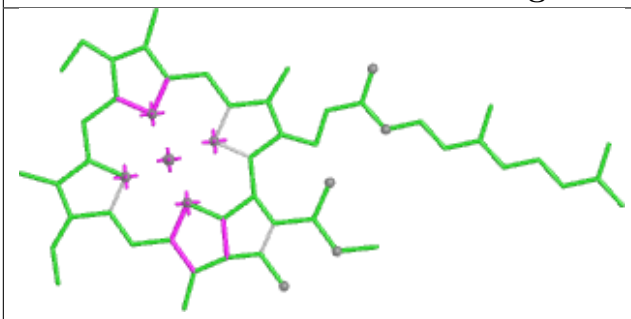
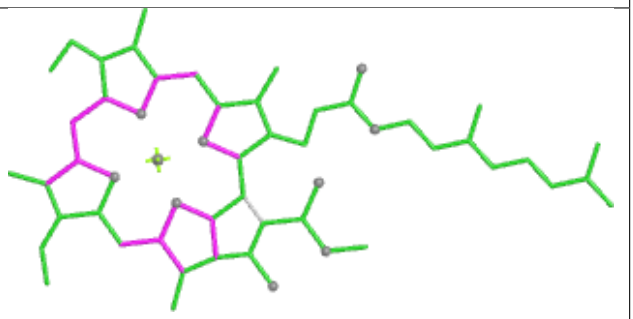


Rings

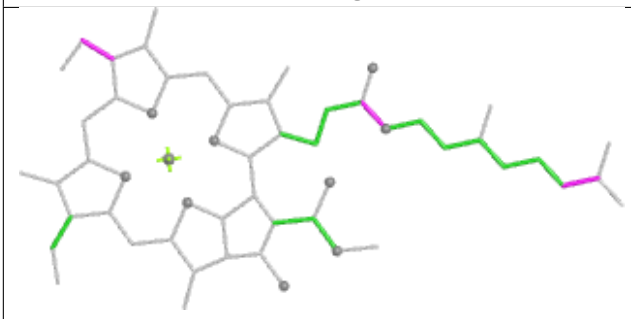
Ligand CLA 6 607



Bond lengths



Bond angles



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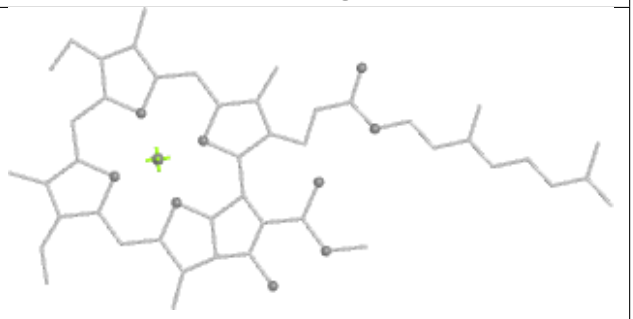
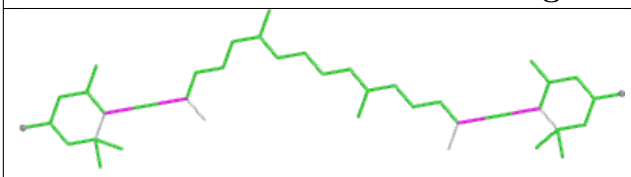
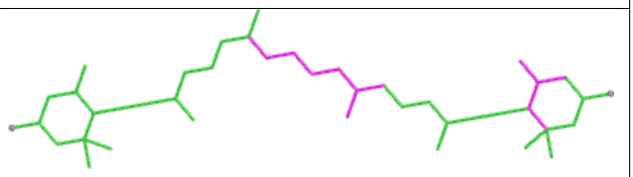


Rings

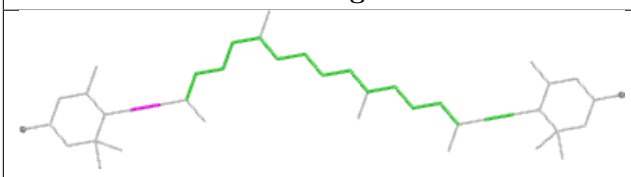
Ligand II0 6 614



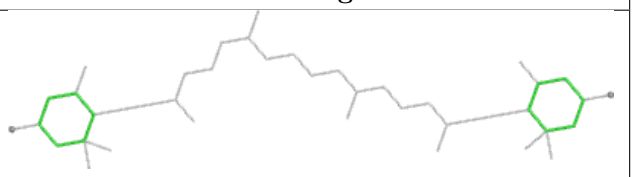
Bond lengths



Bond angles

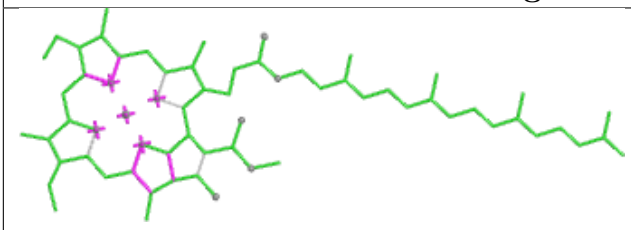


Torsions

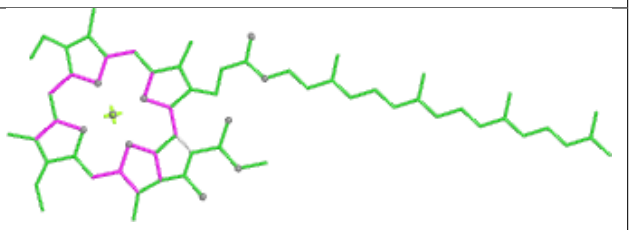


Rings

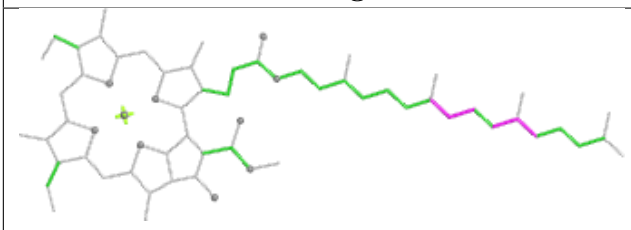
Ligand CLA A 826



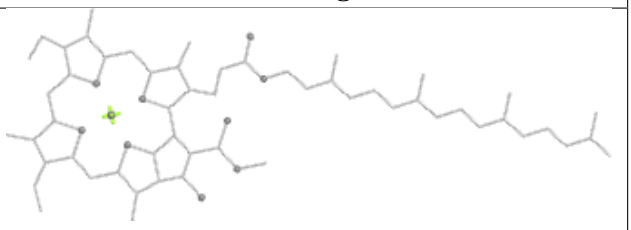
Bond lengths



Bond angles

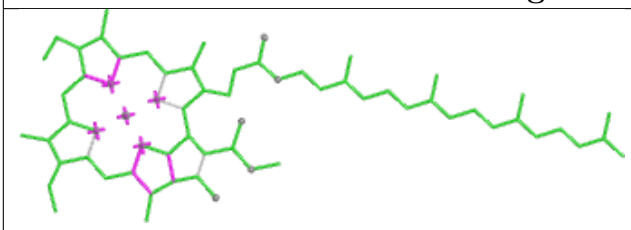


Torsions

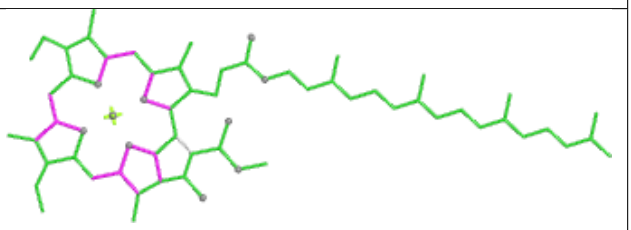


Rings

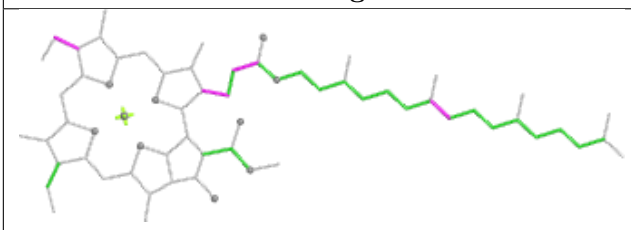
Ligand CLA b 606



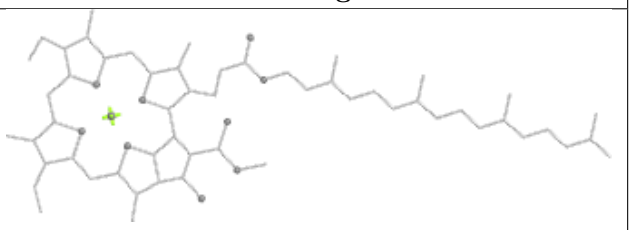
Bond lengths



Bond angles



Torsions



Rings

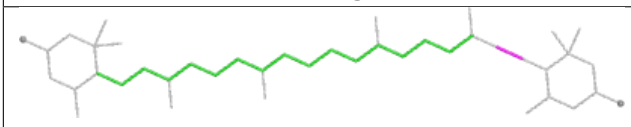
Ligand II3 b 613



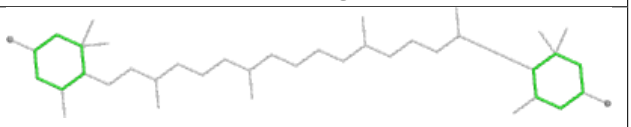
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

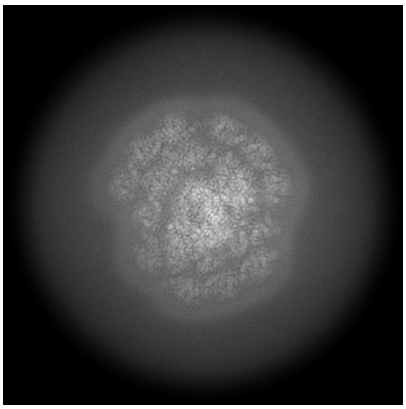
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33659. These allow visual inspection of the internal detail of the map and identification of artifacts.

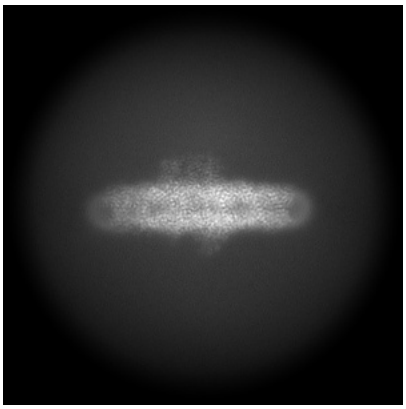
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

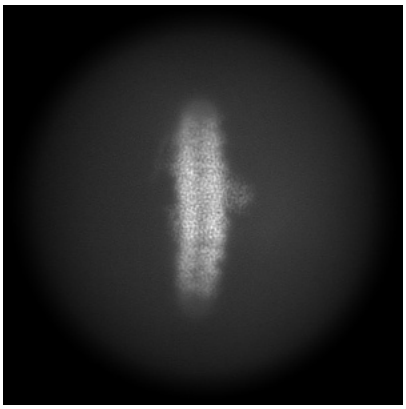
6.1.1 Primary map



X

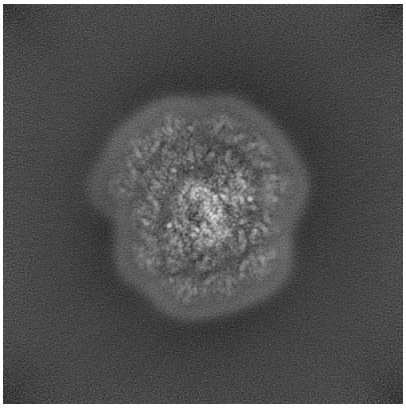


Y

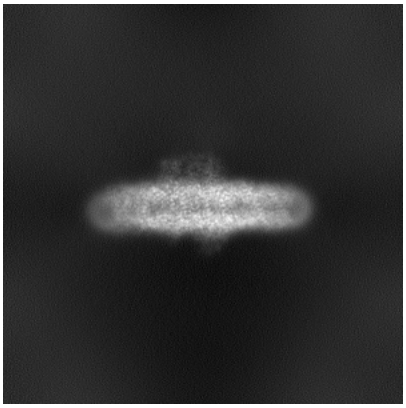


Z

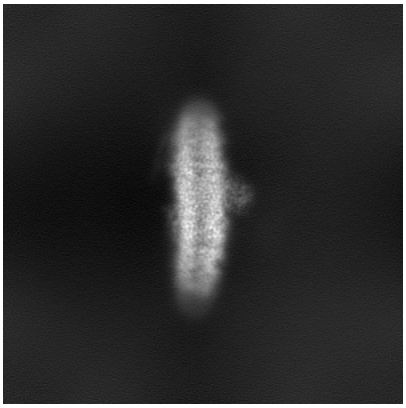
6.1.2 Raw map



X



Y

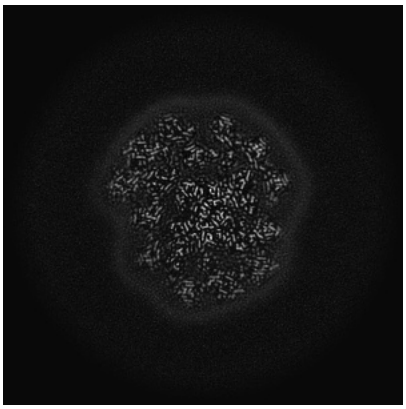


Z

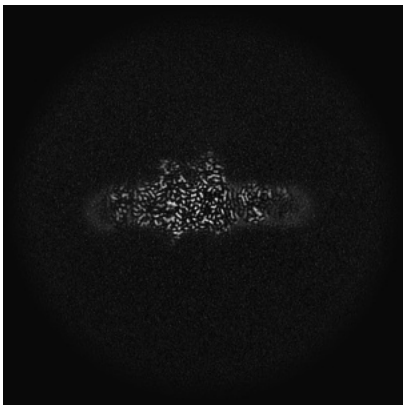
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 200

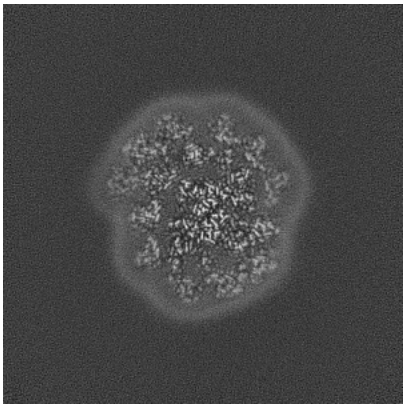


Y Index: 200

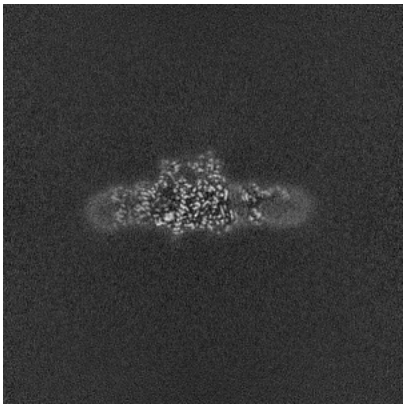


Z Index: 200

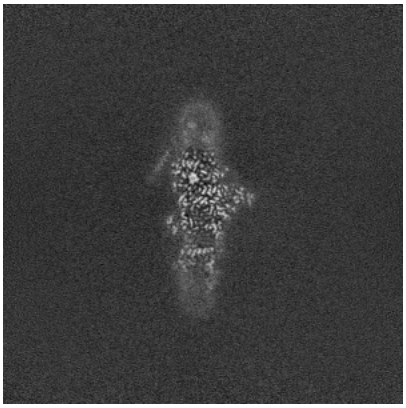
6.2.2 Raw map



X Index: 200



Y Index: 200

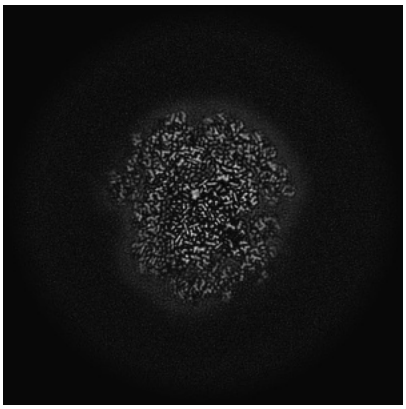


Z Index: 200

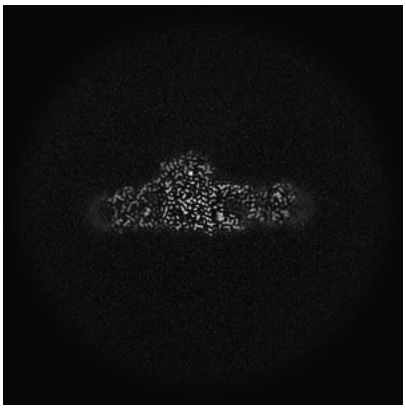
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

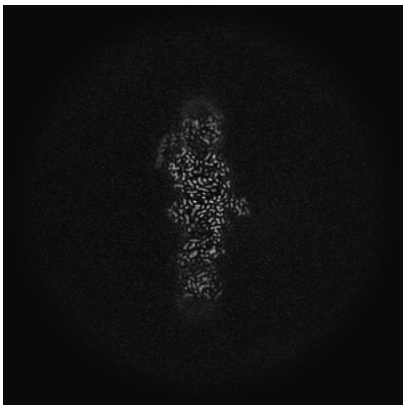
6.3.1 Primary map



X Index: 210

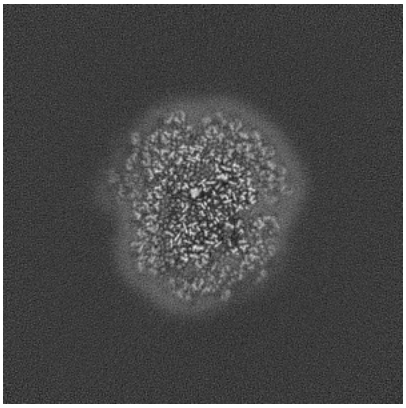


Y Index: 212

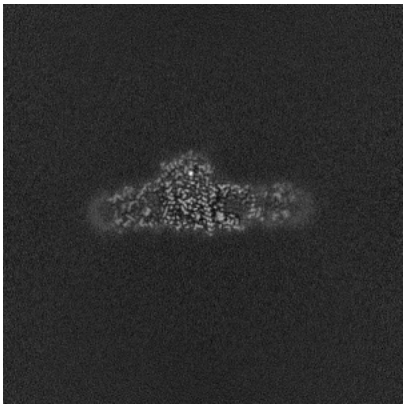


Z Index: 215

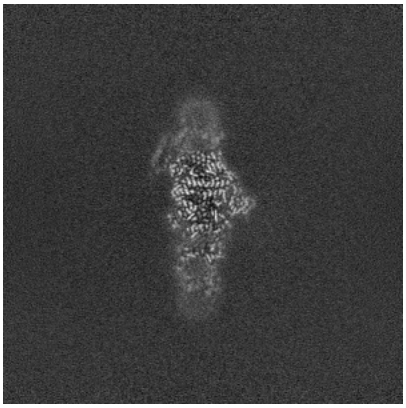
6.3.2 Raw map



X Index: 209



Y Index: 211

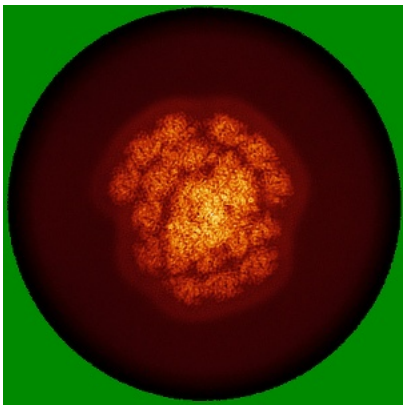


Z Index: 207

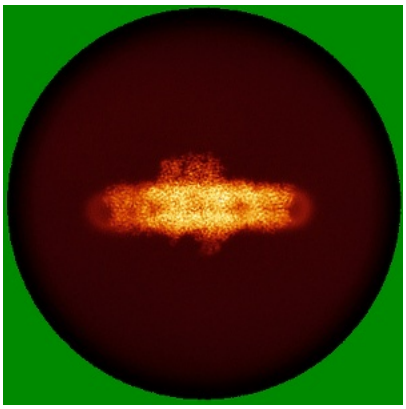
The images above show the largest variance slices of the map in three orthogonal directions.

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

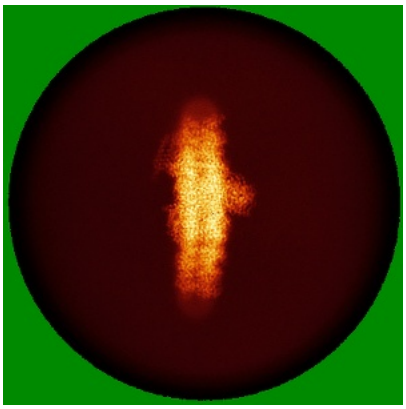
6.4.1 Primary map



X

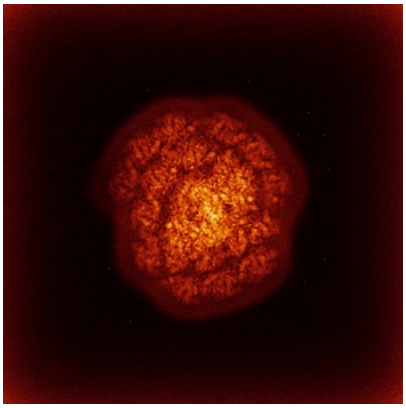


Y

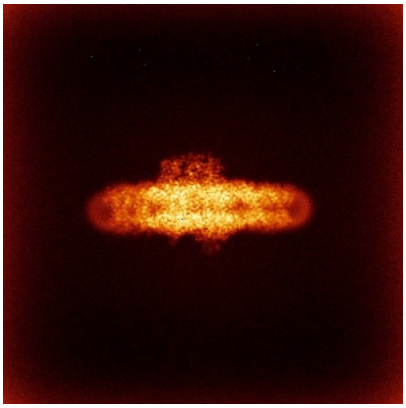


Z

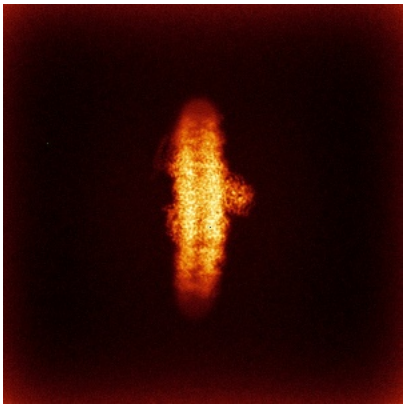
6.4.2 Raw map



X



Y

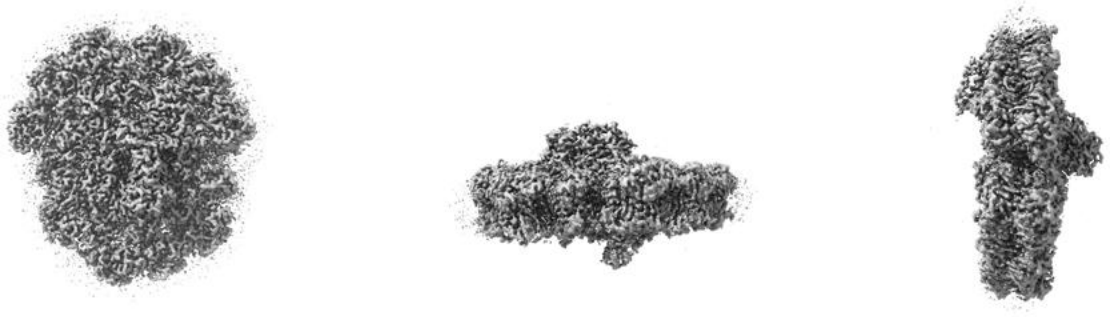


Z

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 0.35. 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.

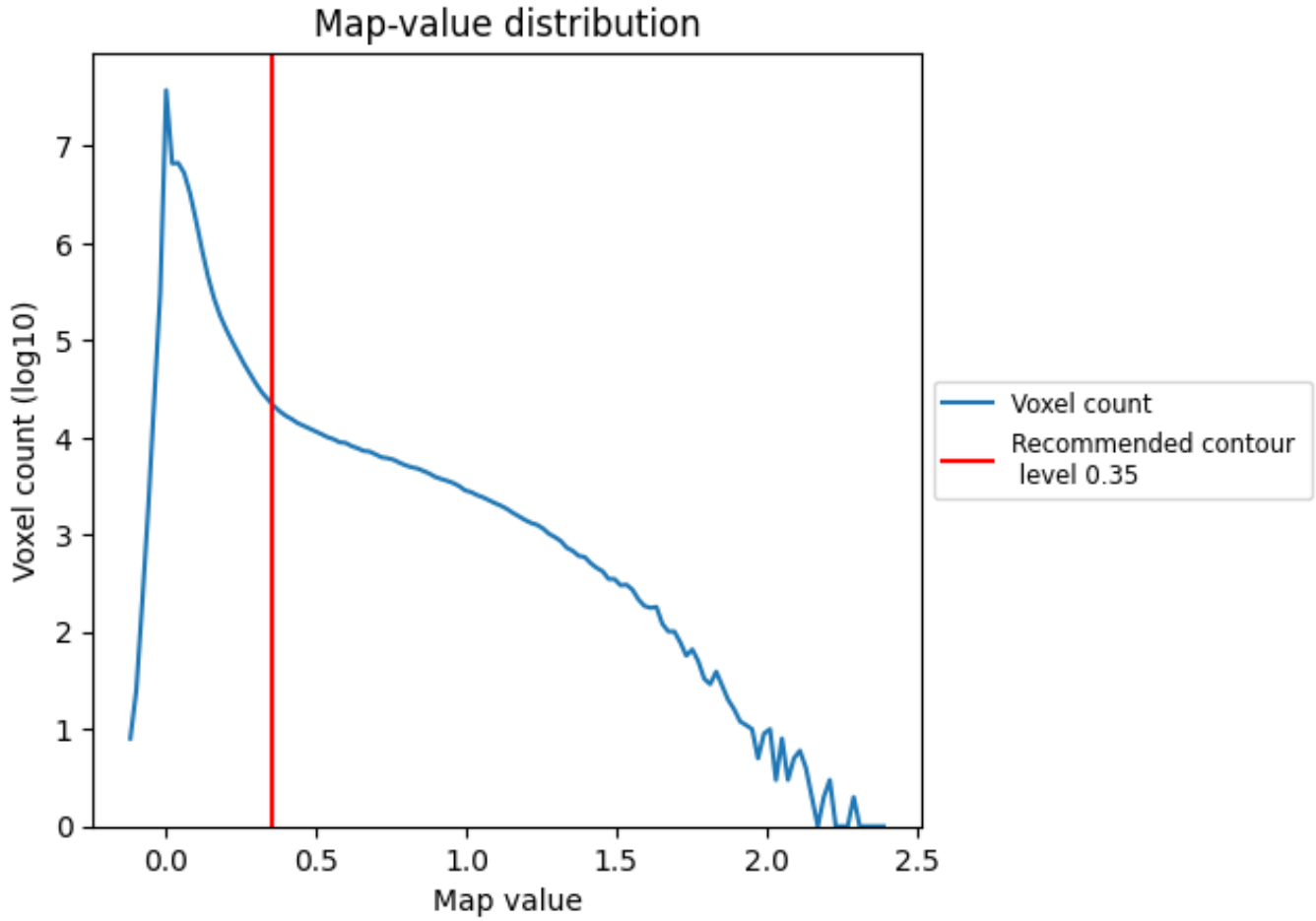
6.6 Mask visualisation (i)

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

7 Map analysis

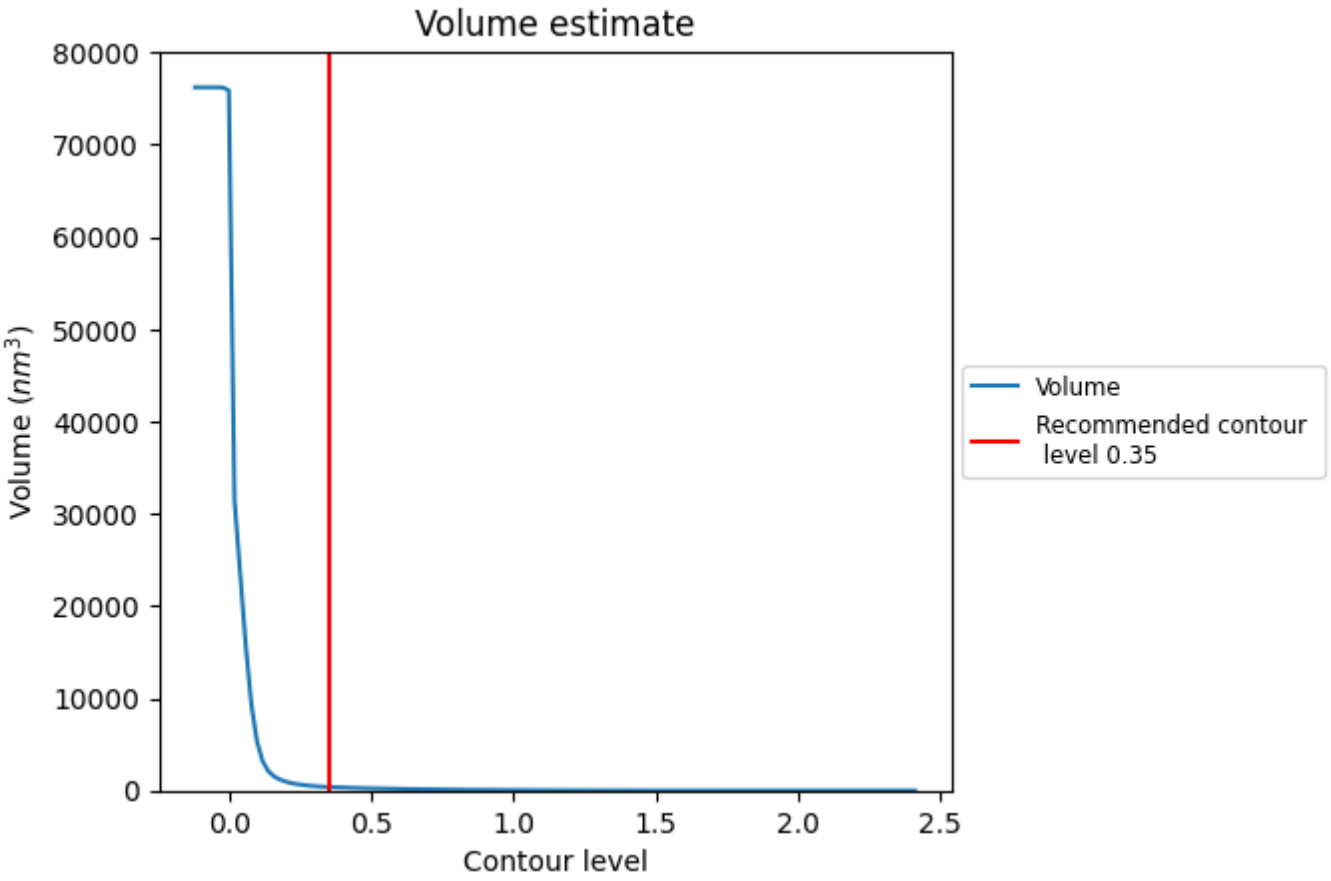
This section contains the results of statistical analysis of the map.

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.

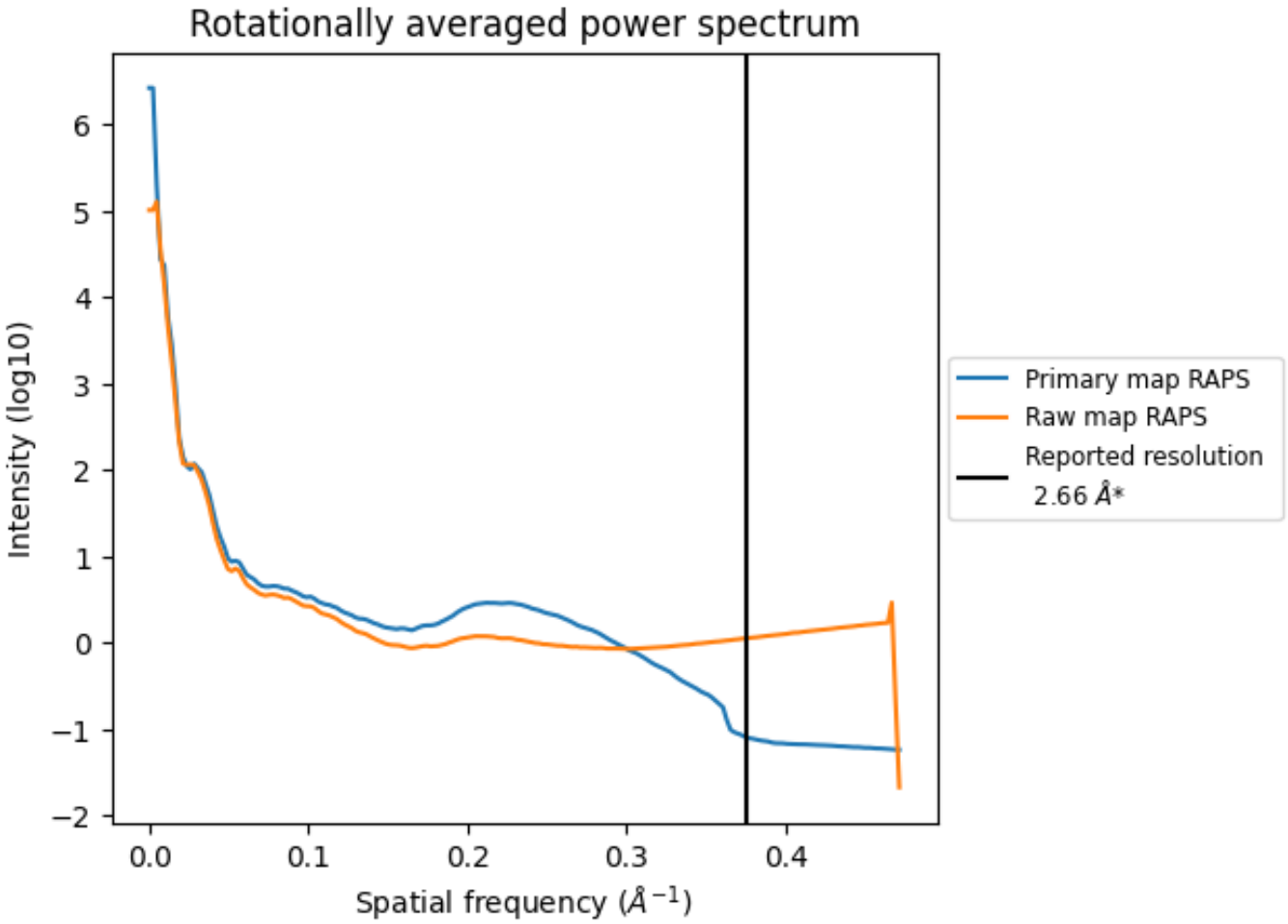
7.2 Volume estimate



The volume at the recommended contour level is 384 nm^3; this corresponds to an approximate mass of 347 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)

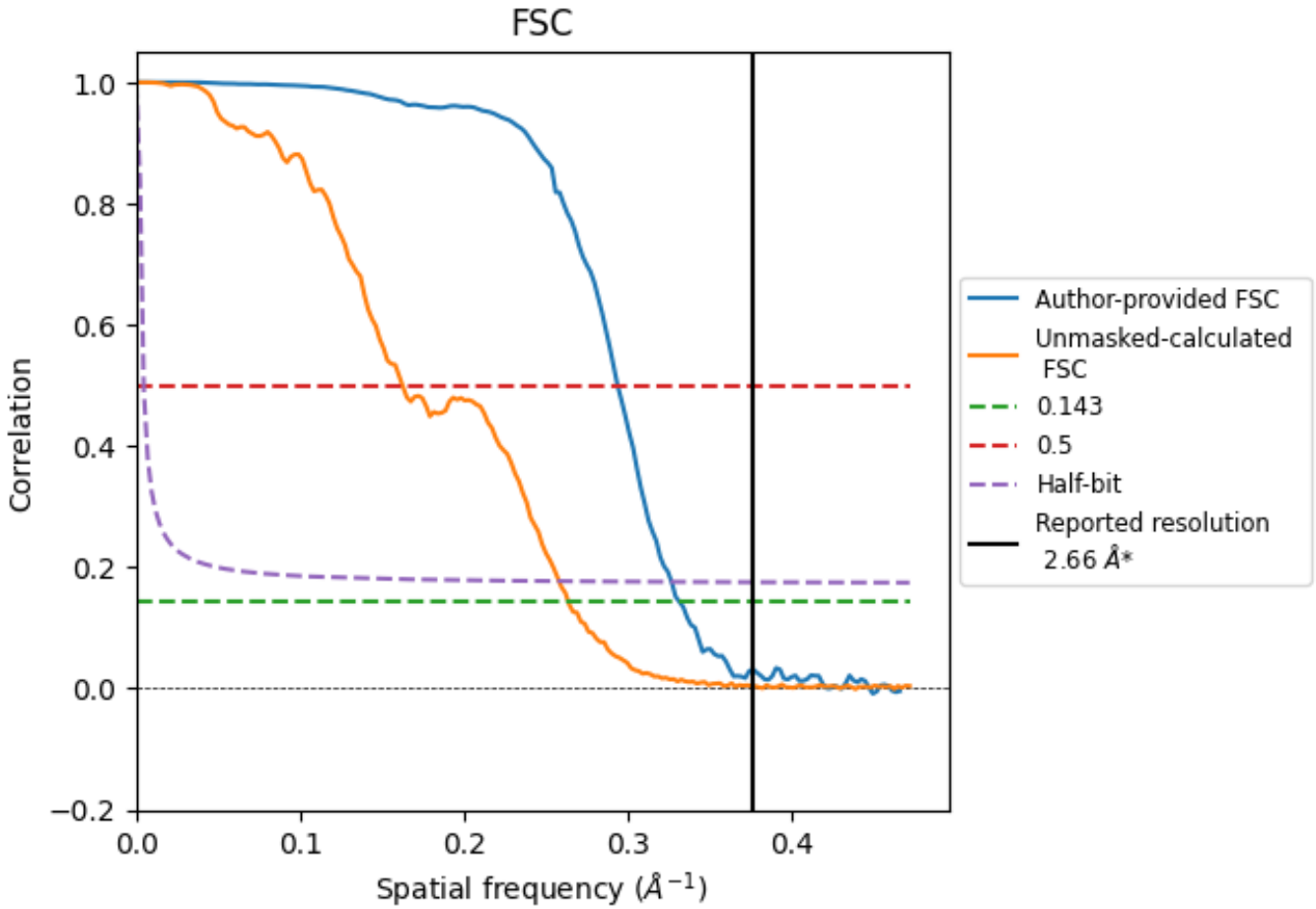


*Reported resolution corresponds to spatial frequency of 0.376 Å^{-1}

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 0.376 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	3.02	3.41	3.06
Unmasked-calculated*	3.80	6.16	3.88

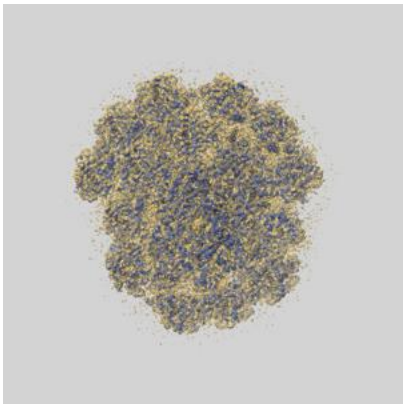
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 2.66 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.66 by more than 10 %

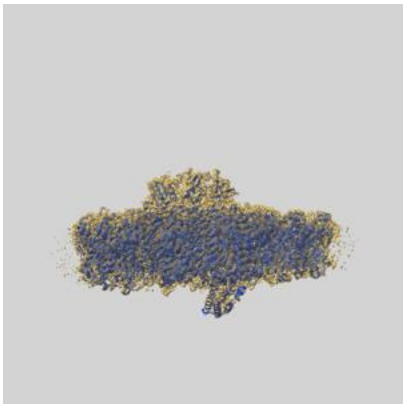
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33659 and PDB model 7Y7B. Per-residue inclusion information can be found in section 3 on page 35.

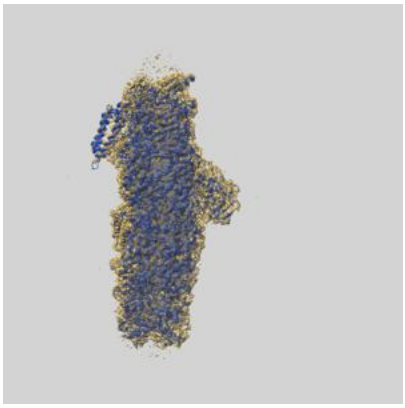
9.1 Map-model overlay



X



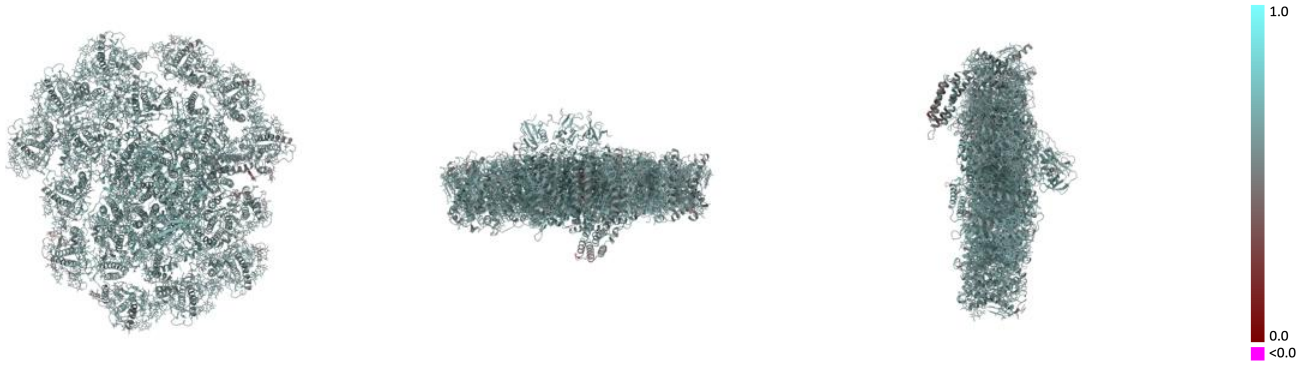
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

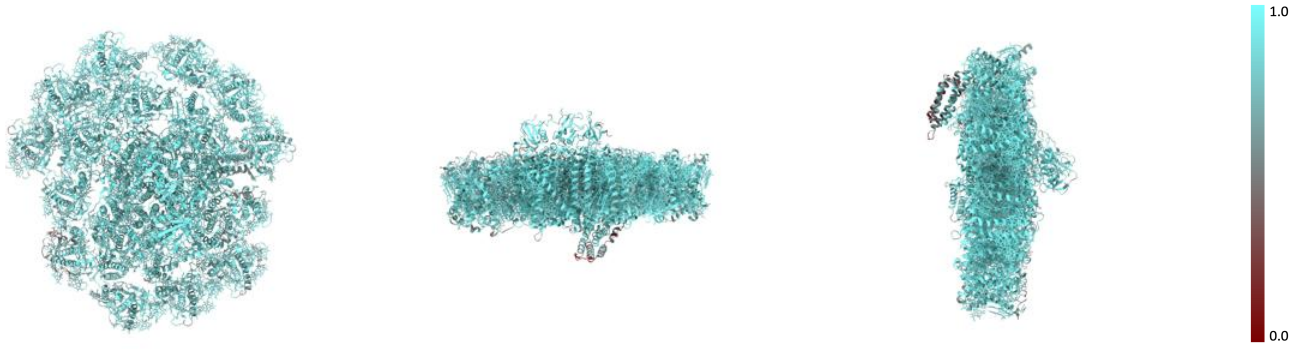
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

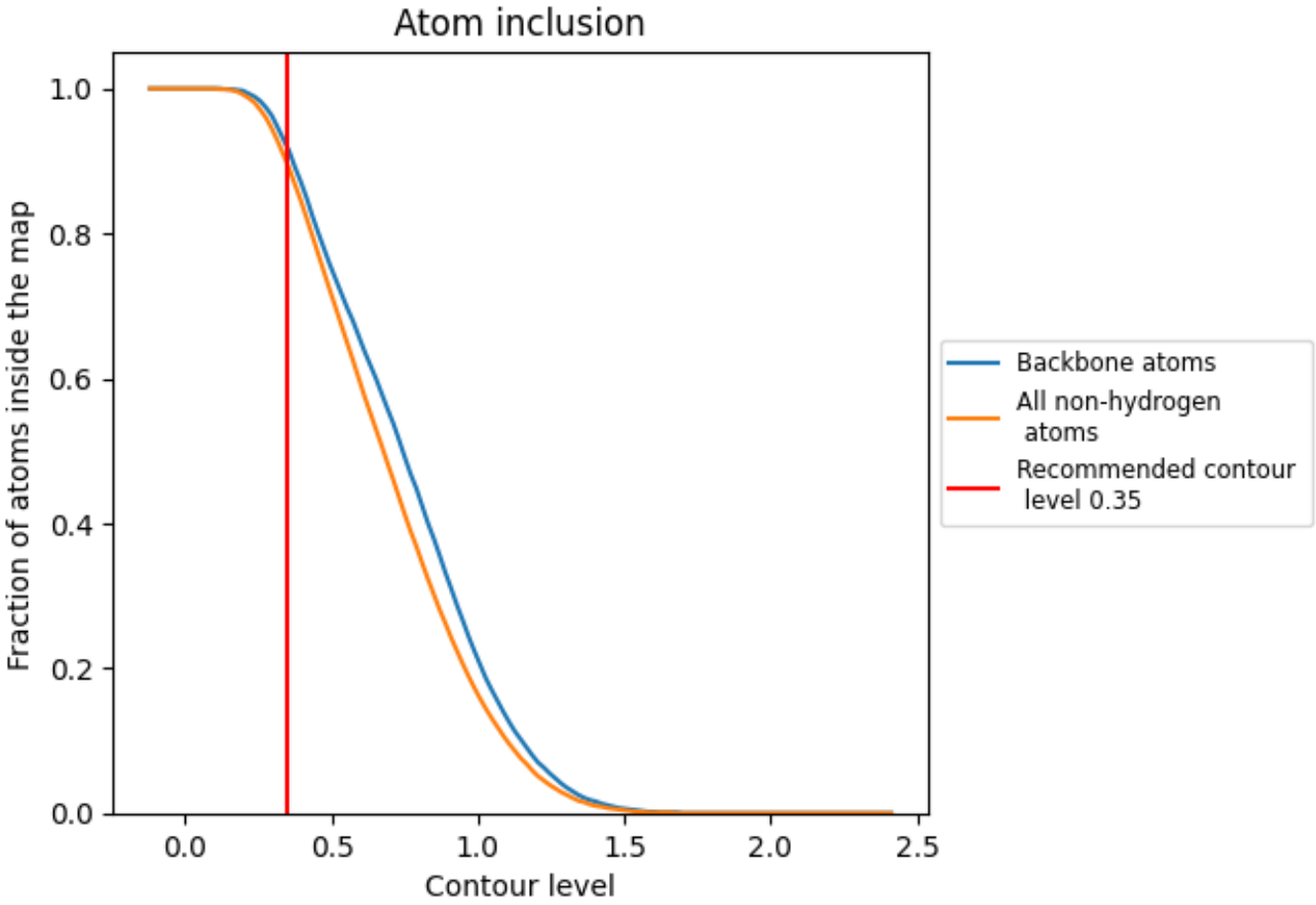
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.6070
1	0.7250	0.5490
2	0.9010	0.6030
3	0.9390	0.6270
4	0.9380	0.6130
5	0.8570	0.5600
6	0.8970	0.5810
7	0.8520	0.5580
8	0.8610	0.5920
9	0.7980	0.5750
A	0.9650	0.6450
B	0.9720	0.6440
C	0.9490	0.6110
D	0.8930	0.6030
E	0.8550	0.6070
F	0.9160	0.6230
I	0.9370	0.6280
J	0.9430	0.6340
K	0.8640	0.6050
L	0.9120	0.6160
M	0.9510	0.6260
O	0.8750	0.6090
R	0.9350	0.6080
X	0.6110	0.5150
Z	0.8810	0.6030
a	0.8970	0.5970
b	0.9060	0.5930
c	0.8000	0.5840
d	0.8270	0.5950
e	0.8160	0.5770

