Full wwPDB EM Validation Report (i)

Sep 15, 2026 – 07:16 PM JST

PDB ID	:	9UOF / pdb_00009uof
EMDB ID	:	EMD-64378
Title	:	PSI-6 FCPI supercomplex from haptophyte Chrysotila roscoffensis
Authors	:	La Rocca, R.; Tsai, P.-C.; Kato, K.; Nakajima, Y.; Akita, F.; Shen, J.-R.
Deposited on	:	2025-04-25
Resolution	:	1.89 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 (i) 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 (i)) were used in the production of this report:

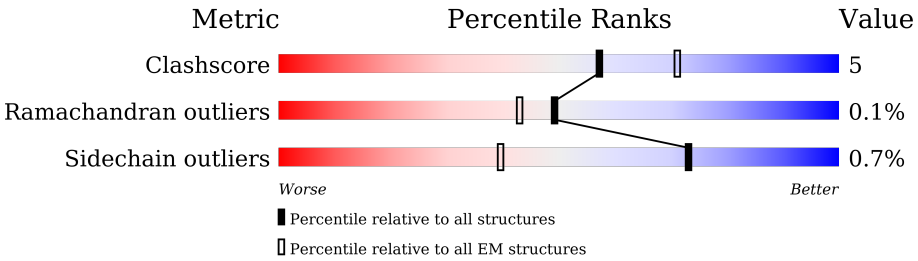
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

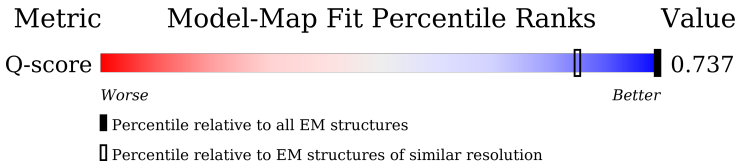
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.89 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	1004 (1.39 - 2.38)

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

Mol	Chain	Length	Quality of chain
1	A	752	92% 6% •
2	B	734	94% 6%
3	C	81	96% • •
4	D	142	88% 9% •

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Mol	Chain	Length	Quality of chain
5	E	67	93%
6	F	184	82% 6% 12%
7	I	35	86% 11%
8	J	39	92% 8%
9	L	141	89% 11%
10	M	29	93% 7%
11	O	201	81% 6% 12%
12	P	231	78% 5% 16%
13	Q	197	75% 9% 15%
14	R	90	96%
15	S	215	68% 8% 23%
16	U	191	70% 26%
17	T	202	41% 8% 51%

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 36741 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5813	3807	984	994	28	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	732	5805	3823	977	984	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	599	366	106	116	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	138	1092	697	188	204	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	64	494	314	86	93	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	161	1246	802	209	229	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	34	266	183	35	46	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	39	305	204	45	54	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	140	1056	693	168	194	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	29	216	144	34	37	1	0	0

- Molecule 11 is a protein called Fucoxanthin chlorophyll a/c binding protein III (FCPI-3).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	176	1341	872	217	244	8	0	0

- Molecule 12 is a protein called Fucoxanthin chlorophyll a/c binding protein VI (FCPI-6), GLY-CYS-PRO.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	193	1441	927	239	264	11	0	0

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c binding protein IV (FCPI-4).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Q	167	1257	809	202	234	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	R	88	664	434	106	123	1	0	0

- Molecule 15 is a protein called Fucoxanthin chlorophyll a/c binding protein II (FCPI-2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	S	165	1238	802	204	226	6	0	0

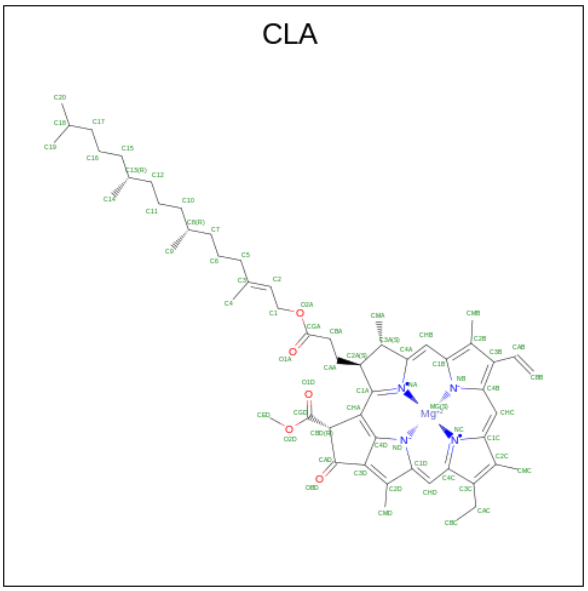
- Molecule 16 is a protein called Fucoxanthin chlorophyll a/c binding protein I (FCPI-1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	U	141	1082	692	183	198	9	0	0

- Molecule 17 is a protein called Fucoxanthin chlorophyll a/c binding protein V (FCPI-5).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	T	99	731	471	122	130	8	0	0

- Molecule 18 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
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
18	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
18	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	45	35	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	54	44	1	4	5	0
18	B	1	55	45	1	4	5	0
18	B	1	54	44	1	4	5	0
18	B	1	49	39	1	4	5	0
18	B	1	55	45	1	4	5	0
18	B	1	59	49	1	4	5	0
18	B	1	60	50	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	46	36	1	4	5	0
18	B	1	53	43	1	4	5	0
18	B	1	63	53	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	B	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	F	1	48	38	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	F	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	J	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
18	L	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
18	L	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	L	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
18	O	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	P	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
18	P	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
18	P	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
18	P	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	P	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	P	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	P	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	R	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	65	55	1	4	5	0

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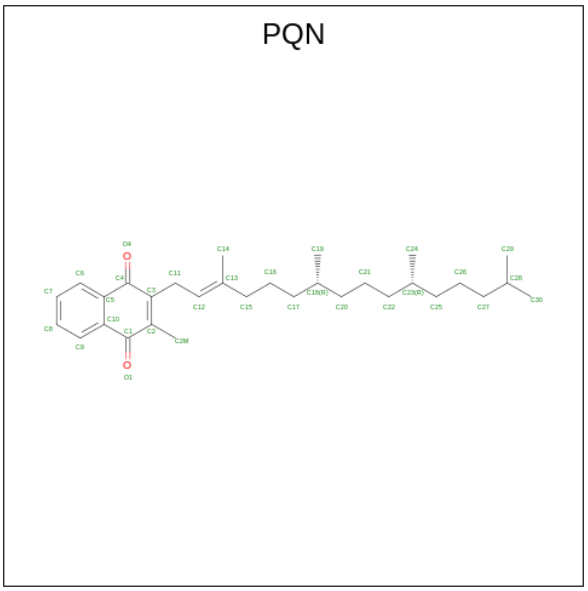
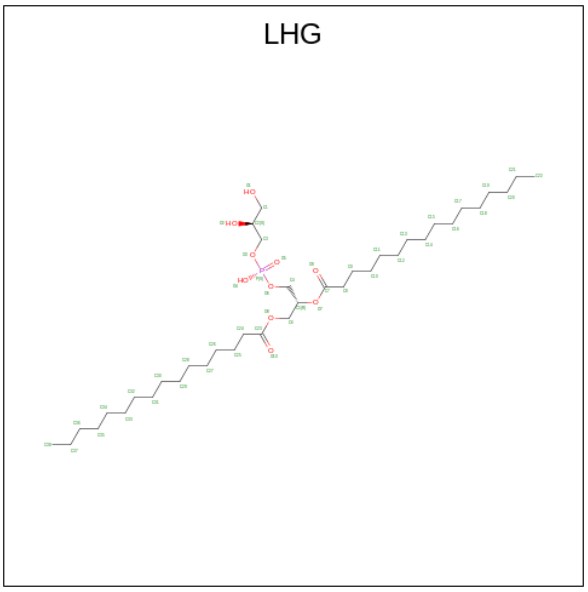
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	U	1	61	51	1	4	5	0
18	U	1	65	55	1	4	5	0
18	U	1	45	35	1	4	5	0
18	U	1	65	55	1	4	5	0
18	U	1	46	36	1	4	5	0
18	U	1	42	34	1	4	3	0
18	U	1	65	55	1	4	5	0
18	U	1	52	42	1	4	5	0
18	T	1	42	34	1	4	3	0
18	T	1	41	33	1	4	3	0
18	T	1	46	36	1	4	5	0
18	T	1	57	47	1	4	5	0
18	T	1	46	36	1	4	5	0
18	T	1	42	34	1	4	3	0
18	T	1	65	55	1	4	5	0
18	T	1	41	33	1	4	3	0
18	T	1	46	36	1	4	5	0
18	T	1	47	37	1	4	5	0

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	A	1	48	37	10	1	0

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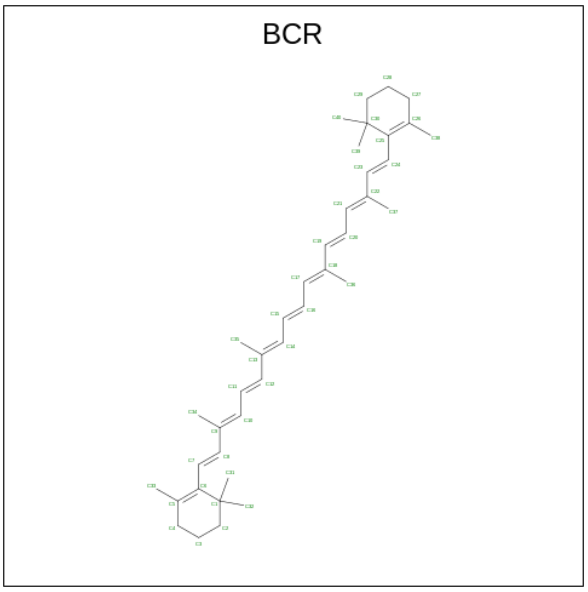
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	A	1	27	16	10	1	0
			Total	C	O	P	
20	R	1	49	38	10	1	0

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
21	A	1	40	40	0
			Total	C	
21	A	1	40	40	0
			Total	C	
21	A	1	40	40	0
			Total	C	
21	A	1	40	40	0
			Total	C	
21	B	1	40	40	0
			Total	C	
21	B	1	40	40	0
			Total	C	
21	B	1	40	40	0
			Total	C	
21	B	1	40	40	0
			Total	C	
21	B	1	40	40	0

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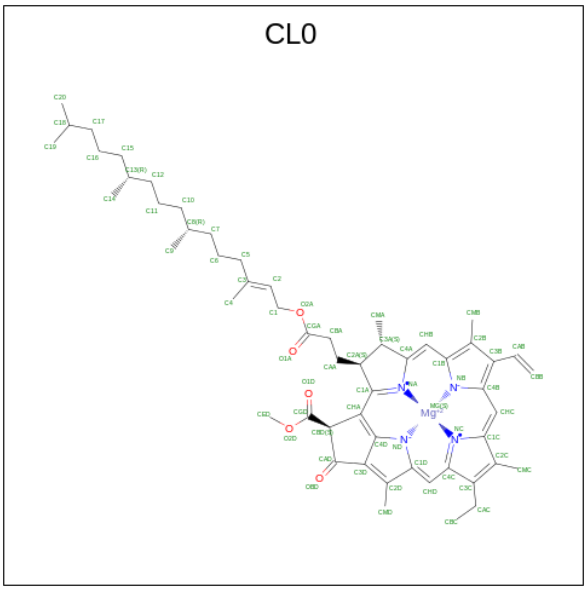
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
21	F	1	40	40	0
			Total	C	
21	F	1	40	40	0
			Total	C	
21	I	1	40	40	0
			Total	C	
21	I	1	40	40	0
			Total	C	
21	J	1	40	40	0
			Total	C	
21	L	1	40	40	0
			Total	C	
21	L	1	40	40	0
			Total	C	
21	M	1	40	40	0
			Total	C	
21	R	1	39	39	0

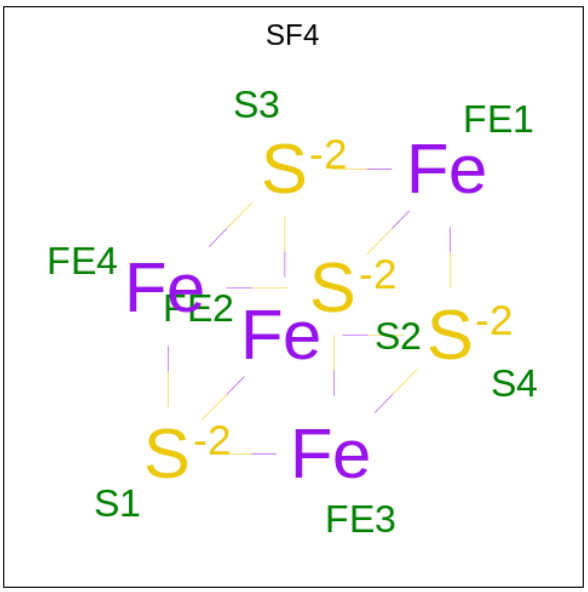
- Molecule 22 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

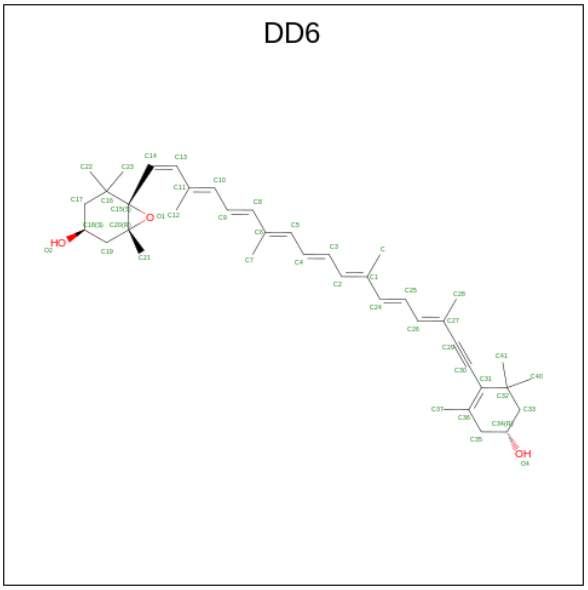
- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as

"Ligand of Interest" by depositor).



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

- Molecule 24 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	A	1	43	40	3	0
24	J	1	43	40	3	0
24	O	1	43	40	3	0
24	O	1	43	40	3	0
24	O	1	43	40	3	0
24	O	1	43	40	3	0
24	O	1	43	40	3	0
24	P	1	43	40	3	0
24	P	1	43	40	3	0
24	P	1	43	40	3	0
24	P	1	23	21	2	0
24	Q	1	43	40	3	0
24	Q	1	43	40	3	0
24	S	1	43	40	3	0
24	S	1	43	40	3	0
24	S	1	43	40	3	0
24	S	1	43	40	3	0
24	S	1	43	40	3	0
24	U	1	43	40	3	0
24	U	1	43	40	3	0
24	U	1	26	25	1	0
24	T	1	43	40	3	0

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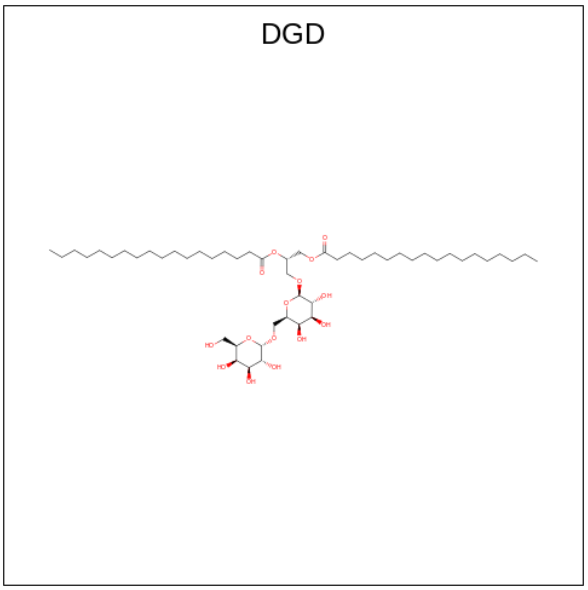
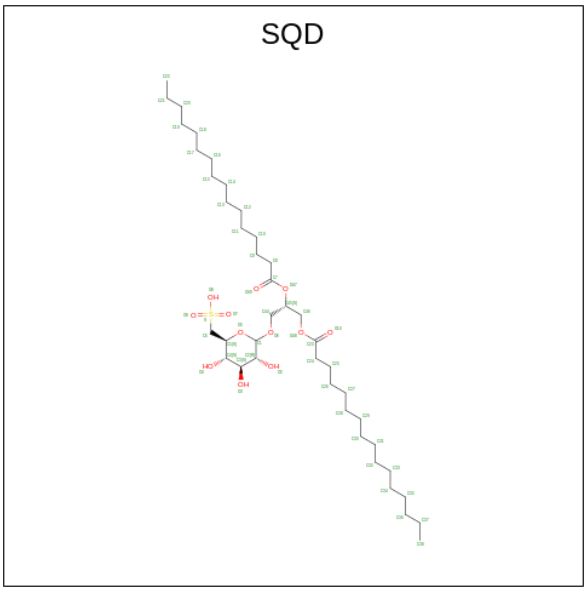
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	T	1	43	40	3	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



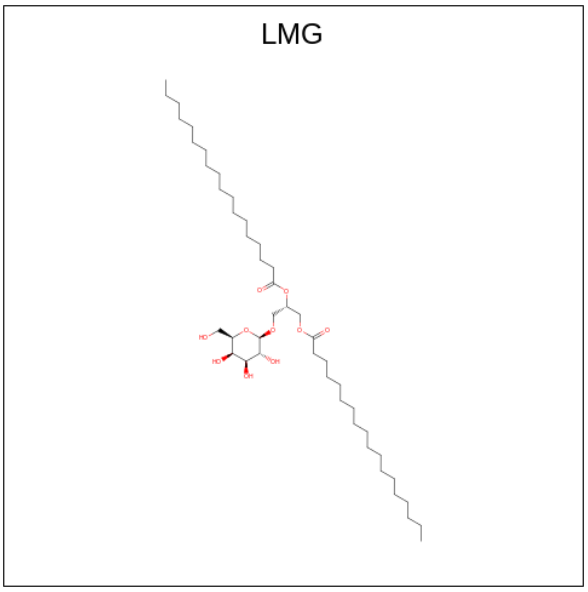
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	B	1	60	45	15	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	S	0
			50	37	12	1	
26	M	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			25	15	10	

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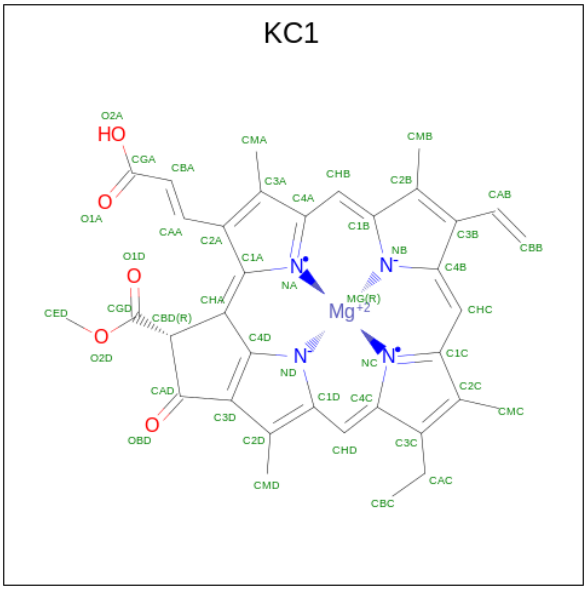
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	J	1	39	29	10	0
			Total	C	O	
27	P	1	34	24	10	0
			Total	C	O	
27	Q	1	55	45	10	0
			Total	C	O	
27	S	1	49	39	10	0
			Total	C	O	
27	U	1	32	22	10	0

- Molecule 28 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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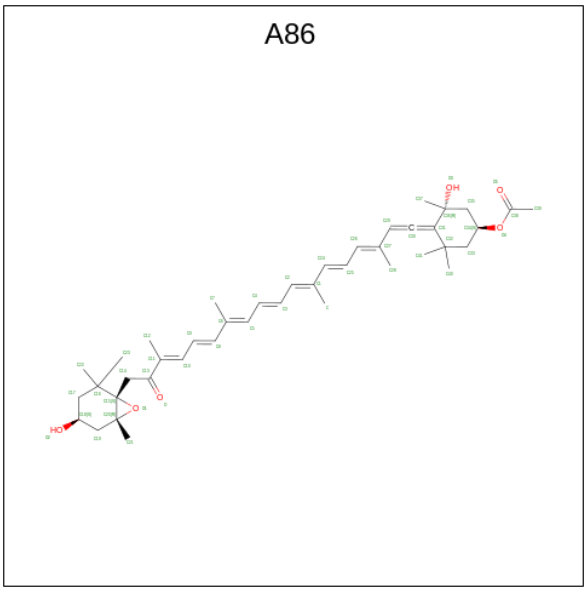
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
28	S	1	45	35	1	4	5	0
28	U	1	45	35	1	4	5	0
28	T	1	45	35	1	4	5	0

- Molecule 29 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	P	1	48	42	6	0
29	Q	1	48	42	6	0
29	Q	1	48	42	6	0
29	R	1	44	40	4	0
29	R	1	48	42	6	0
29	U	1	48	42	6	0
29	T	1	48	42	6	0

- Molecule 30 is water.

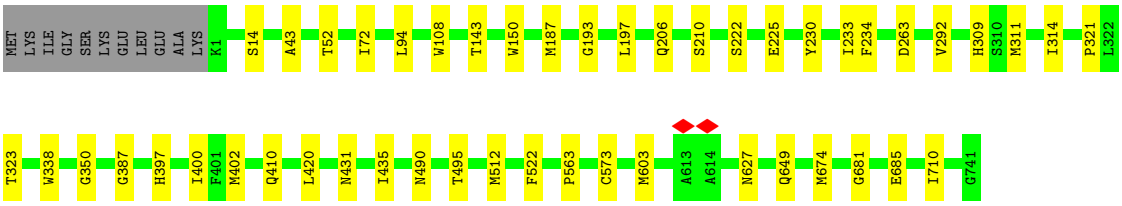
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
30	A	189	189	189	0
			Total	O	
30	B	286	286	286	0
			Total	O	
30	C	59	59	59	0
			Total	O	
30	D	39	39	39	0
			Total	O	
30	E	13	13	13	0
			Total	O	
30	F	33	33	33	0
			Total	O	
30	I	2	2	2	0
			Total	O	
30	J	2	2	2	0
			Total	O	
30	L	23	23	23	0
			Total	O	
30	M	5	5	5	0
			Total	O	
30	O	22	22	22	0
			Total	O	
30	P	30	30	30	0
			Total	O	
30	Q	19	19	19	0
			Total	O	
30	R	27	27	27	0
			Total	O	
30	S	25	25	25	0
			Total	O	
30	U	9	9	9	0
			Total	O	
30	T	7	7	7	0

3 Residue-property plots (i)

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

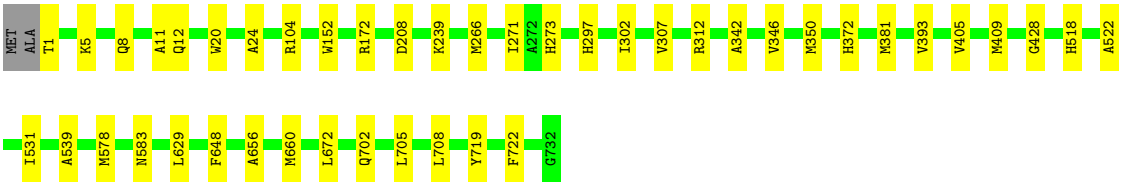
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 (psaA)

Chain A: 92% 6%



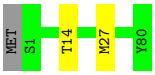
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 (psaB)

Chain B: 94% 6%



• Molecule 3: Photosystem I iron-sulfur center (psaC)

Chain C: 96%

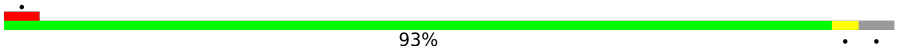


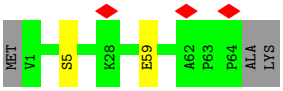
• Molecule 4: Photosystem I reaction center subunit II (psaD)

Chain D: 88% 9%

• Molecule 5: Photosystem I reaction center subunit IV (psaE)

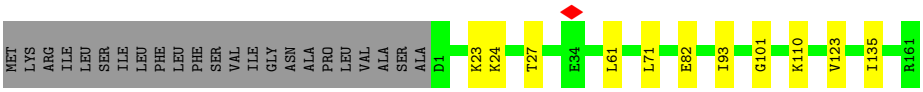
Chain E:





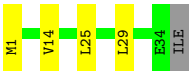
• Molecule 6: Photosystem I reaction center subunit III (psaF)

Chain F:



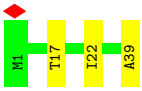
• Molecule 7: Photosystem I reaction center subunit VIII (psaI)

Chain I:



• Molecule 8: Photosystem I reaction center subunit IX (psaJ)

Chain J:

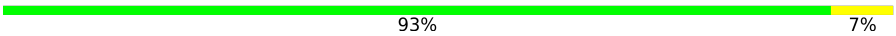


• Molecule 9: Photosystem I reaction center subunit XI (psaL)

Chain L:

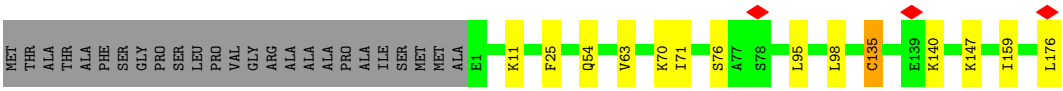
• Molecule 10: Photosystem I reaction center subunit XII (psaM)

Chain M:



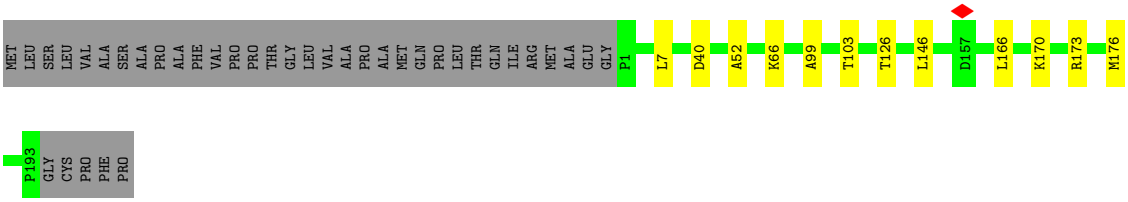
• Molecule 11: Fucoxanthin chlorophyll a/c binding protein III (FCPI-3)

Chain O:



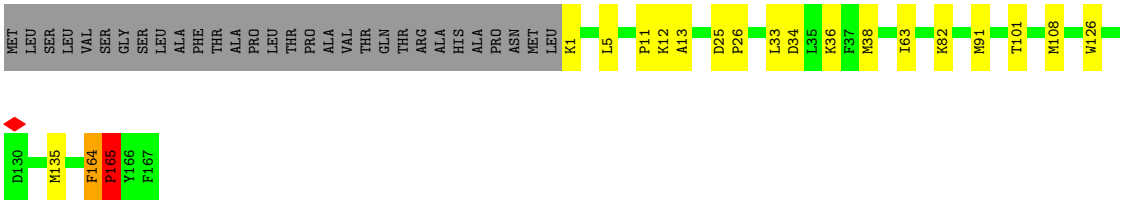
• Molecule 12: Fucoxanthin chlorophyll a/c binding protein VI (FCPI-6), GLY-CYS-PRO

Chain P:



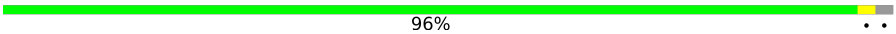
• Molecule 13: Fucoxanthin chlorophyll a/c binding protein IV (FCPI-4)

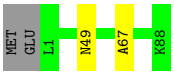
Chain Q:



• Molecule 14: Photosystem I reaction center subunit psaR

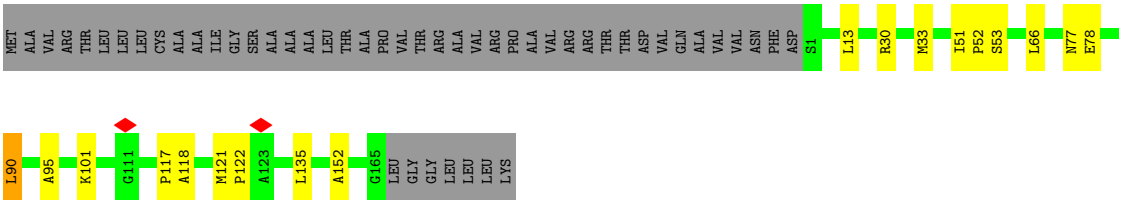
Chain R:





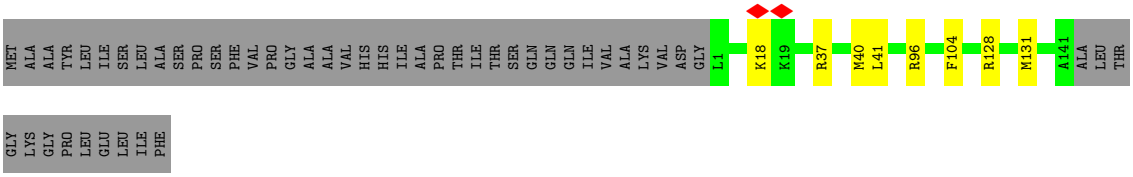
• Molecule 15: Fucoxanthin chlorophyll a/c binding protein II (FCPI-2)

Chain S:



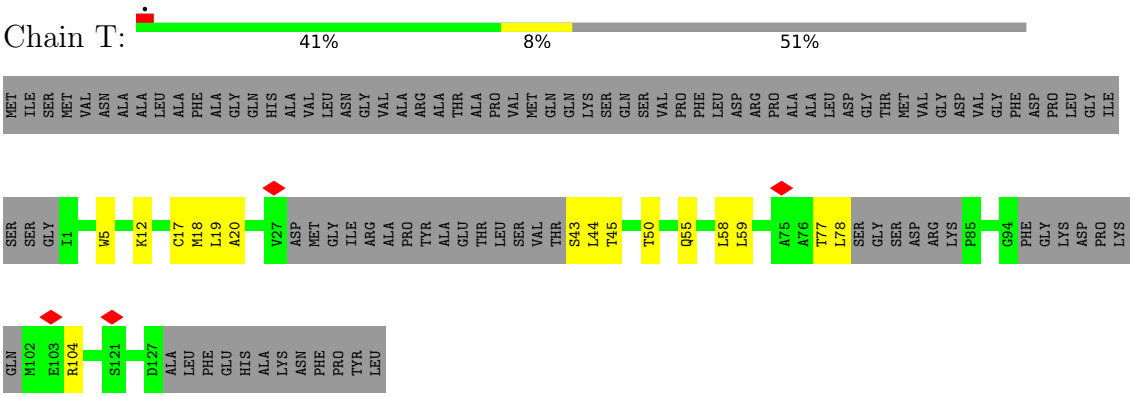
• Molecule 16: Fucoxanthin chlorophyll a/c binding protein I (FCPI-1)

Chain U:



• Molecule 17: Fucoxanthin chlorophyll a/c binding protein V (FCPI-5)

Chain T:


41%
8%
51%
MET ILE SER MET VAL ASN ALA ALA LEU ALA PHE ALA GLY GLN HIS ALA VAL LEU ASN GLY VAL ALA ARG ALA THR ALA PRO VAL MET GLN GLN LYS SER GLN SER VAL PRO PHE LEU ASP ARG PRO ALA ALA LEU ASP GLY THR MET VAL GLY ASP VAL GLY PHE ASP PRO LEU GLY ILE
SER SER GLY I1 W5 K12 C17 M18 L19 A20 V27 ASP MET GLY ILE ARG ALA PRO TYR ALA GLU THR LEU SER VAL THR S43 L44 T45 T50 Q55 L58 L59 A75 A76 T77 L78 SER GLY SER ASP ARG LYS P85 G94 PHE GLY LYS ASP PRO LYS
GLN M102 E103 R104 S121 D127 ALA LEU PHE GLU HIS ALA LYS ASN PHE PRO TYR LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	114380	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.114	Depositor
Minimum map value	-0.354	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, PQN, KC1, DD6, CLA, LHG, BCR, SF4, DGD, SQD, LMG, A86

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.26	0/6007	0.48	0/8185
2	B	0.25	0/6015	0.47	0/8205
3	C	0.21	0/609	0.45	0/826
4	D	0.21	0/1116	0.50	0/1503
5	E	0.22	0/505	0.41	0/689
6	F	0.24	0/1275	0.47	0/1728
7	I	0.26	0/273	0.53	0/373
8	J	0.26	0/313	0.55	0/427
9	L	0.24	0/1081	0.52	0/1470
10	M	0.21	0/218	0.34	0/295
11	O	0.24	0/1376	0.51	0/1865
12	P	0.22	0/1480	0.49	0/2010
13	Q	0.30	0/1285	0.58	2/1736 (0.1%)
14	R	0.26	0/681	0.47	0/930
15	S	0.20	0/1272	0.41	0/1732
16	U	0.24	0/1109	0.49	0/1499
17	T	0.28	0/741	0.60	1/999 (0.1%)
All	All	0.25	0/25356	0.49	3/34472 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	Q	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	19	LEU	N-CA-C	-5.92	106.70	114.04
13	Q	91	MET	CB-CG-SD	5.04	127.83	112.70
13	Q	165	PRO	CA-N-CD	-5.00	105.00	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	Q	164	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5813	0	5698	32	0
2	B	5805	0	5634	36	0
3	C	599	0	577	1	0
4	D	1092	0	1096	7	0
5	E	494	0	488	1	0
6	F	1246	0	1256	8	0
7	I	266	0	278	4	0
8	J	305	0	310	3	0
9	L	1056	0	1068	14	0
10	M	216	0	234	3	0
11	O	1341	0	1347	10	0
12	P	1441	0	1421	8	0
13	Q	1257	0	1260	11	0
14	R	664	0	668	2	0
15	S	1238	0	1217	12	0
16	U	1082	0	1058	6	0
17	T	731	0	749	11	0
18	A	2615	0	2651	59	0
18	B	2399	0	2438	70	0
18	F	94	0	69	1	0
18	J	42	0	31	2	0
18	L	164	0	150	4	0
18	O	495	0	475	13	0
18	P	403	0	337	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Q	609	0	566	13	0
18	R	110	0	105	4	0
18	S	384	0	358	13	0
18	T	473	0	379	13	0
18	U	441	0	417	13	0
19	A	33	0	46	2	0
19	B	33	0	46	1	0
20	A	75	0	93	2	0
20	R	49	0	74	2	0
21	A	160	0	224	5	0
21	B	200	0	280	7	0
21	F	80	0	112	4	0
21	I	80	0	112	4	0
21	J	40	0	56	1	0
21	L	80	0	112	6	0
21	M	40	0	56	4	0
21	R	39	0	53	3	0
22	A	65	0	72	3	0
23	A	8	0	0	0	0
23	C	16	0	0	0	0
24	A	43	0	0	0	0
24	J	43	0	0	0	0
24	O	215	0	0	0	0
24	P	152	0	0	1	0
24	Q	86	0	0	0	0
24	S	215	0	0	0	0
24	T	86	0	0	0	0
24	U	112	0	0	0	0
25	B	60	0	81	5	0
26	B	50	0	67	3	0
26	M	46	0	56	3	0
27	B	25	0	20	2	0
27	J	39	0	48	2	0
27	P	34	0	38	1	0
27	Q	55	0	86	6	0
27	S	49	0	68	6	0
27	U	32	0	34	2	0
28	O	45	0	0	1	0
28	P	134	0	0	0	0
28	Q	45	0	0	0	0
28	S	90	0	0	0	0
28	T	45	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	U	45	0	0	0	0
29	P	48	0	0	0	0
29	Q	96	0	0	0	0
29	R	92	0	0	2	0
29	T	48	0	0	0	0
29	U	48	0	0	1	0
30	A	189	0	0	1	0
30	B	286	0	0	1	0
30	C	59	0	0	0	0
30	D	39	0	0	1	0
30	E	13	0	0	0	0
30	F	33	0	0	1	0
30	I	2	0	0	0	0
30	J	2	0	0	0	0
30	L	23	0	0	0	0
30	M	5	0	0	0	0
30	O	22	0	0	0	0
30	P	30	0	0	0	0
30	Q	19	0	0	0	0
30	R	27	0	0	0	0
30	S	25	0	0	0	0
30	T	7	0	0	0	0
30	U	9	0	0	0	0
All	All	36741	0	34169	336	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 5.

All (336) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLY:O	1:A:197:LEU:HB2	1.87	0.75
27:U:201:LMG:H321	18:U:211:CLA:H42	1.74	0.69
1:A:522:PHE:HA	18:A:833:CLA:HED1	1.75	0.69
18:A:838:CLA:HED1	18:U:210:CLA:HAA2	1.76	0.68
18:Q:206:CLA:H42	27:Q:217:LMG:H182	1.76	0.67
5:E:5:SER:OG	5:E:59:GLU:OE2	2.13	0.66
18:A:835:CLA:H101	8:J:17:THR:HG23	1.78	0.65
18:B:818:CLA:HMD2	21:B:837:BCR:HC7	1.80	0.64
18:A:824:CLA:H13	18:A:845:CLA:H203	1.78	0.64
18:B:846:CLA:H42	15:S:66:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:846:CLA:HED3	18:B:846:CLA:H51	1.80	0.63
13:Q:11:PRO:HG2	13:Q:25:ASP:HB3	1.79	0.63
18:S:204:CLA:HBB2	18:S:214:CLA:HAB	1.80	0.62
21:M:101:BCR:H383	27:S:211:LMG:H301	1.82	0.61
9:L:25:ALA:HB2	16:U:104:PHE:HB3	1.84	0.60
18:B:824:CLA:H52	21:B:838:BCR:H23C	1.84	0.60
15:S:152:ALA:HA	27:S:211:LMG:HC2	1.84	0.60
18:A:803:CLA:H72	21:A:842:BCR:HC8	1.84	0.59
18:A:816:CLA:HBB2	18:A:816:CLA:H151	1.85	0.59
18:B:831:CLA:H152	21:F:804:BCR:H23C	1.83	0.59
18:A:808:CLA:HBB2	18:A:811:CLA:HMA3	1.84	0.59
9:L:51:MET:HB3	21:L:205:BCR:H12C	1.85	0.59
18:B:819:CLA:HBB2	18:B:835:CLA:H52	1.85	0.58
15:S:117:PRO:HB2	18:S:215:CLA:HED3	1.85	0.58
18:U:211:CLA:HED3	18:U:211:CLA:H12	1.85	0.58
18:Q:208:CLA:HBC3	27:Q:217:LMG:H452	1.86	0.58
4:D:135:ASN:ND2	4:D:138:ASP:OD2	2.36	0.58
17:T:59:LEU:HD11	18:T:205:CLA:H71	1.86	0.58
27:B:849:LMG:HC61	12:P:52:ALA:HB3	1.86	0.58
9:L:32:ASN:HB3	18:L:202:CLA:HAC1	1.85	0.57
19:A:837:PQN:H141	18:A:853:CLA:HBB2	1.86	0.57
17:T:104:ARG:NH2	28:T:209:KC1:OBD	2.38	0.57
6:F:71:LEU:HD22	6:F:82:GLU:HG2	1.86	0.57
18:B:819:CLA:H52	18:B:844:CLA:HBC1	1.86	0.57
4:D:20:ARG:NH2	30:D:201:HOH:O	2.37	0.56
1:A:321:PRO:HB3	9:L:1:SER:HB2	1.87	0.56
1:A:187:MET:HG3	1:A:311:MET:HE1	1.88	0.56
18:T:212:CLA:HHC	18:T:212:CLA:HBB1	1.89	0.55
1:A:230:TYR:HA	1:A:233:ILE:HG22	1.89	0.55
17:T:18:MET:HE1	18:T:208:CLA:HAB	1.89	0.55
26:M:102:SQD:H92	15:S:13:LEU:HG	1.88	0.55
12:P:173:ARG:HA	12:P:176:MET:HE3	1.89	0.55
18:B:810:CLA:H42	18:O:205:CLA:H52	1.88	0.55
9:L:51:MET:HE1	18:L:202:CLA:HED2	1.90	0.54
1:A:338:TRP:HB3	18:A:803:CLA:HAC1	1.90	0.54
18:Q:207:CLA:HHC	18:Q:207:CLA:HBB1	1.89	0.54
1:A:490:ASN:HB2	18:A:831:CLA:HED2	1.90	0.54
1:A:512:MET:HE1	1:A:603:MET:HE1	1.88	0.54
30:B:911:HOH:O	10:M:1:MET:SD	2.59	0.53
1:A:649:GLN:NE2	30:A:903:HOH:O	2.39	0.53
18:A:815:CLA:H141	18:A:823:CLA:H201	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:VAL:HG13	2:B:539:ALA:HB1	1.90	0.53
2:B:719:TYR:HB2	18:B:802:CLA:HED2	1.91	0.53
18:A:816:CLA:HBC3	18:A:825:CLA:H121	1.91	0.53
2:B:297:HIS:HB3	2:B:302:ILE:HD11	1.90	0.53
18:B:846:CLA:H43	9:L:76:ILE:HD12	1.89	0.53
13:Q:38:MET:HE3	18:Q:205:CLA:H11	1.91	0.52
27:S:211:LMG:H402	27:S:211:LMG:H211	1.90	0.52
18:T:202:CLA:HHC	18:T:202:CLA:HBB1	1.91	0.52
11:O:54:GLN:HE22	18:O:208:CLA:HHD	1.75	0.52
16:U:41:LEU:HD22	18:U:207:CLA:H93	1.91	0.52
1:A:72:ILE:HG12	18:A:807:CLA:H171	1.91	0.52
18:B:819:CLA:H3A	18:B:835:CLA:HED3	1.92	0.52
18:S:204:CLA:HHC	18:S:204:CLA:HBB1	1.90	0.52
18:R:205:CLA:HAA1	18:R:205:CLA:HED2	1.91	0.52
18:B:834:CLA:HHC	18:B:834:CLA:HBB1	1.90	0.52
11:O:147:LYS:NZ	28:O:210:KC1:O2A	2.42	0.52
18:B:827:CLA:HBC3	21:F:804:BCR:H362	1.92	0.52
27:J:102:LMG:H161	27:J:102:LMG:H211	1.91	0.52
18:O:203:CLA:HHC	18:O:203:CLA:HBB1	1.92	0.52
2:B:273:HIS:HB3	18:B:815:CLA:HMB2	1.92	0.52
18:B:821:CLA:H143	18:B:835:CLA:H192	1.92	0.52
18:A:853:CLA:HHC	18:A:853:CLA:HBB1	1.91	0.51
1:A:206:GLN:HA	1:A:210:SER:HB2	1.90	0.51
1:A:397:HIS:HA	1:A:400:ILE:HD12	1.92	0.51
18:A:817:CLA:HHC	18:A:817:CLA:HBB1	1.92	0.51
11:O:135:CYS:HA	11:O:140:LYS:HB3	1.93	0.51
13:Q:5:LEU:HD21	13:Q:26:PRO:HG3	1.93	0.51
18:U:209:CLA:HHC	18:U:209:CLA:HBB1	1.92	0.51
4:D:105:LYS:O	4:D:110:ARG:NH2	2.43	0.51
18:B:835:CLA:HHC	18:B:835:CLA:HBB1	1.91	0.51
18:B:848:CLA:HHC	18:B:848:CLA:HBB1	1.93	0.51
6:F:123:VAL:HB	27:J:102:LMG:HC72	1.93	0.51
11:O:63:VAL:HG11	11:O:176:LEU:HB3	1.92	0.51
18:A:845:CLA:HBC2	2:B:583:ASN:HB2	1.92	0.51
18:B:807:CLA:HBB1	18:B:808:CLA:H202	1.93	0.51
18:S:206:CLA:HED2	18:S:207:CLA:HMD1	1.93	0.51
18:J:103:CLA:HHC	18:J:103:CLA:HBB1	1.93	0.51
18:B:833:CLA:HHC	18:B:833:CLA:HBB1	1.93	0.50
15:S:118:ALA:HB1	15:S:122:PRO:HB3	1.93	0.50
1:A:495:THR:HG23	18:A:830:CLA:HED3	1.93	0.50
18:B:829:CLA:HHC	18:B:829:CLA:HBB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:818:CLA:H52	18:A:847:CLA:H2	1.93	0.50
18:B:846:CLA:HHC	18:B:846:CLA:HBB1	1.92	0.50
18:A:835:CLA:HHC	18:A:835:CLA:HBB1	1.93	0.50
18:Q:208:CLA:H3A	27:Q:217:LMG:H342	1.94	0.50
18:T:207:CLA:HHC	18:T:207:CLA:HBB1	1.93	0.50
1:A:309:HIS:HB3	1:A:314:ILE:HD11	1.93	0.50
15:S:90:LEU:HB3	18:S:201:CLA:H193	1.94	0.50
27:S:211:LMG:H352	18:S:214:CLA:H93	1.94	0.49
17:T:104:ARG:HG2	18:T:202:CLA:HED1	1.94	0.49
18:F:803:CLA:HHC	18:F:803:CLA:HBB1	1.93	0.49
9:L:28:LEU:HD21	16:U:96:ARG:HD2	1.95	0.49
1:A:292:VAL:HG11	18:A:846:CLA:H91	1.94	0.49
18:B:806:CLA:H8	25:B:842:DGD:HBN2	1.94	0.49
18:B:808:CLA:HHC	18:B:808:CLA:HBB1	1.95	0.49
18:B:822:CLA:HBB1	18:B:822:CLA:HHC	1.95	0.49
7:I:25:LEU:HD21	26:M:102:SQD:H122	1.94	0.49
18:B:846:CLA:H143	9:L:83:GLY:HA2	1.94	0.49
18:O:207:CLA:HHC	18:O:207:CLA:HBB1	1.94	0.49
1:A:402:MET:HE1	1:A:420:LEU:HD11	1.94	0.49
15:S:30:ARG:HA	15:S:33:MET:HE3	1.95	0.49
18:A:814:CLA:HHC	18:A:814:CLA:HBB1	1.94	0.49
18:U:205:CLA:H51	18:U:206:CLA:H3A	1.95	0.48
18:A:820:CLA:HHC	18:A:820:CLA:HBB1	1.94	0.48
18:A:831:CLA:HHC	18:A:831:CLA:HBB1	1.95	0.48
18:A:847:CLA:HHC	18:A:847:CLA:HBB1	1.94	0.48
18:B:848:CLA:HBA1	13:Q:101:THR:HG21	1.94	0.48
1:A:222:SER:OG	1:A:225:GLU:OE1	2.32	0.48
18:A:822:CLA:H91	21:A:844:BCR:H23C	1.96	0.48
2:B:405:VAL:O	2:B:409:MET:HG2	2.13	0.48
18:O:202:CLA:HHC	18:O:202:CLA:HBB1	1.95	0.48
18:R:202:CLA:HHC	18:R:202:CLA:HBB1	1.96	0.48
18:B:835:CLA:HED1	18:B:844:CLA:HHC	1.96	0.48
1:A:108:TRP:CD2	18:A:807:CLA:HED3	2.48	0.48
18:A:813:CLA:HHC	18:A:813:CLA:HBB1	1.96	0.48
18:B:821:CLA:H172	18:B:827:CLA:HBC1	1.96	0.48
11:O:11:LYS:HB3	11:O:11:LYS:HE3	1.61	0.48
2:B:522:ALA:HB2	18:B:831:CLA:HMA1	1.95	0.48
18:U:208:CLA:HHC	18:U:208:CLA:HBB1	1.95	0.48
18:B:821:CLA:H43	18:B:829:CLA:HBB2	1.96	0.47
26:B:847:SQD:H262	18:O:208:CLA:H12	1.95	0.47
18:U:206:CLA:HHC	18:U:206:CLA:HBB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:810:CLA:HHC	18:A:810:CLA:HBB1	1.95	0.47
18:A:851:CLA:H101	18:A:851:CLA:H171	1.96	0.47
2:B:409:MET:HG3	21:R:203:BCR:H402	1.96	0.47
18:A:824:CLA:H142	18:A:826:CLA:H18	1.95	0.47
2:B:342:ALA:HB2	18:B:820:CLA:H43	1.97	0.47
1:A:338:TRP:CE2	18:A:821:CLA:H18	2.50	0.47
18:A:826:CLA:H202	18:A:835:CLA:HHB	1.96	0.47
9:L:5:LYS:HG3	9:L:17:SER:HB3	1.97	0.47
11:O:70:LYS:NZ	11:O:76:SER:O	2.45	0.47
12:P:40:ASP:OD1	24:P:304:DD6:O2	2.33	0.47
13:Q:34:ASP:HB3	13:Q:108:MET:HE1	1.96	0.47
18:Q:208:CLA:HAA2	27:Q:217:LMG:H321	1.96	0.47
18:T:211:CLA:HHC	18:T:211:CLA:HBB1	1.96	0.47
18:B:827:CLA:HHC	18:B:827:CLA:HBB1	1.96	0.47
16:U:128:ARG:HA	16:U:131:MET:HE3	1.96	0.47
3:C:14:THR:HG22	3:C:27:MET:HG3	1.96	0.47
21:L:201:BCR:H15C	21:L:201:BCR:H351	1.81	0.47
18:U:207:CLA:H152	18:U:210:CLA:H142	1.96	0.47
4:D:86:ILE:HG12	4:D:92:ILE:HG12	1.97	0.46
18:A:815:CLA:HHC	18:A:815:CLA:HBB1	1.98	0.46
18:A:823:CLA:H152	18:A:834:CLA:H191	1.97	0.46
18:B:819:CLA:H42	18:B:820:CLA:H121	1.96	0.46
27:S:211:LMG:H322	18:S:214:CLA:H41	1.97	0.46
16:U:37:ARG:HA	16:U:40:MET:HE3	1.97	0.46
18:B:815:CLA:HHC	18:B:815:CLA:HBB1	1.96	0.46
18:U:210:CLA:H2	18:U:210:CLA:H62	1.80	0.46
18:A:801:CLA:HMD3	2:B:531:ILE:HG12	1.98	0.46
18:Q:208:CLA:HBA1	27:Q:217:LMG:H361	1.96	0.46
1:A:350:GLY:HA2	1:A:387:GLY:HA2	1.98	0.46
18:B:845:CLA:HBB1	18:B:845:CLA:HHC	1.98	0.46
11:O:98:LEU:HD23	18:O:207:CLA:HBC3	1.98	0.46
1:A:431:ASN:HD22	2:B:672:LEU:HD11	1.81	0.46
18:A:836:CLA:H152	21:I:102:BCR:H17C	1.98	0.46
4:D:9:PRO:HG2	4:D:57:LEU:HD23	1.97	0.46
10:M:8:PHE:HB3	21:M:101:BCR:H381	1.97	0.46
1:A:43:ALA:HB2	20:A:839:LHG:HC82	1.97	0.46
2:B:172:ARG:HB2	18:B:843:CLA:HBC2	1.98	0.46
18:A:834:CLA:H121	21:A:843:BCR:H12C	1.98	0.45
18:B:817:CLA:H162	18:B:817:CLA:H121	1.76	0.45
11:O:25:PHE:HE1	18:O:202:CLA:HBC3	1.81	0.45
15:S:121:MET:HE1	15:S:135:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:12:LYS:HE3	13:Q:13:ALA:HB2	1.99	0.45
17:T:55:GLN:HG3	17:T:58:LEU:HD12	1.98	0.45
7:I:1:MET:HB2	18:S:214:CLA:HBA1	1.98	0.45
9:L:53:HIS:HA	9:L:56:PHE:CE2	2.51	0.45
18:O:209:CLA:H41	18:O:209:CLA:H62	1.47	0.45
18:T:208:CLA:HED2	18:T:208:CLA:HBD	1.80	0.45
2:B:578:MET:HG3	2:B:708:LEU:HD21	1.99	0.45
6:F:110:LYS:HA	6:F:110:LYS:HD3	1.72	0.45
18:S:201:CLA:HAA1	18:S:201:CLA:H8	1.97	0.45
18:Q:206:CLA:H62	18:Q:206:CLA:H41	1.57	0.45
18:A:833:CLA:H151	18:A:852:CLA:H192	1.97	0.45
18:B:819:CLA:HHB	18:B:835:CLA:O1D	2.16	0.45
29:U:202:A86:C5	18:U:207:CLA:H2	2.47	0.45
18:B:846:CLA:H61	18:B:846:CLA:H41	1.71	0.45
21:I:102:BCR:H15C	21:I:102:BCR:H351	1.88	0.45
18:T:210:CLA:HHC	18:T:210:CLA:HBB1	1.99	0.45
18:B:808:CLA:H92	21:B:841:BCR:HC7	1.99	0.45
18:B:827:CLA:H42	21:F:804:BCR:H353	1.99	0.45
1:A:681:GLY:O	1:A:685:GLU:HG3	2.16	0.45
2:B:312:ARG:HA	27:B:849:LMG:HC4	1.99	0.45
18:B:807:CLA:H122	18:B:807:CLA:H161	1.75	0.45
14:R:49:ASN:OD1	29:R:204:A86:O3	2.35	0.45
18:A:833:CLA:H143	18:A:833:CLA:H112	1.87	0.45
18:T:208:CLA:H61	18:T:208:CLA:H41	1.51	0.45
18:A:833:CLA:H41	18:A:833:CLA:H61	1.78	0.44
18:B:817:CLA:H142	18:B:817:CLA:H111	1.78	0.44
18:B:846:CLA:H8	18:B:846:CLA:H52	1.80	0.44
20:R:201:LHG:H322	20:R:201:LHG:H352	1.66	0.44
18:A:836:CLA:H111	18:A:836:CLA:H72	1.79	0.44
22:A:848:CL0:O1D	18:B:802:CLA:HBB2	2.17	0.44
18:A:834:CLA:H13	18:A:847:CLA:H12	1.98	0.44
18:B:833:CLA:HBB2	19:B:836:PQN:H141	1.97	0.44
26:B:847:SQD:H141	26:B:847:SQD:H172	1.73	0.44
18:O:205:CLA:H112	18:O:205:CLA:H91	1.74	0.44
6:F:23:LYS:O	6:F:27:THR:OG1	2.26	0.44
18:B:821:CLA:H72	18:B:835:CLA:H191	1.99	0.44
13:Q:82:LYS:HB2	13:Q:82:LYS:HE3	1.69	0.44
21:A:843:BCR:H20C	21:A:843:BCR:H361	1.77	0.44
18:R:205:CLA:H62	18:R:205:CLA:H41	1.51	0.44
2:B:702:GLN:HG3	25:B:842:DGD:HA22	1.99	0.44
6:F:61:LEU:HD21	8:J:39:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:51:ILE:HG21	15:S:78:GLU:HA	2.00	0.44
17:T:50:THR:HG21	18:T:205:CLA:HAA2	2.00	0.44
17:T:104:ARG:NH2	28:T:209:KC1:O2D	2.51	0.44
18:O:209:CLA:H42	18:O:209:CLA:C3B	2.48	0.44
12:P:166:LEU:HG	12:P:170:LYS:HD2	1.99	0.44
18:A:845:CLA:H41	18:A:845:CLA:H61	1.70	0.43
2:B:8:GLN:O	2:B:12:GLN:HG3	2.18	0.43
21:L:205:BCR:H20C	21:L:205:BCR:H361	1.81	0.43
2:B:372:HIS:HE2	18:B:824:CLA:C1B	2.31	0.43
18:S:201:CLA:H2	18:S:201:CLA:H61	1.87	0.43
1:A:233:ILE:HG23	1:A:234:PHE:CD1	2.54	0.43
18:A:852:CLA:H41	18:L:203:CLA:H161	1.99	0.43
18:B:807:CLA:H12	7:I:14:VAL:HG21	1.99	0.43
18:S:206:CLA:HED3	18:S:207:CLA:HBC2	1.99	0.43
17:T:44:LEU:HD12	17:T:45:THR:HG23	2.01	0.43
9:L:123:PHE:HE2	15:S:95:ALA:HA	1.84	0.43
18:T:211:CLA:HED2	18:T:211:CLA:HBD	1.83	0.43
2:B:346:VAL:HG21	18:B:824:CLA:HHD	2.00	0.43
10:M:8:PHE:CE2	27:S:211:LMG:HC1	2.54	0.43
21:B:837:BCR:H20C	21:B:837:BCR:H361	1.84	0.43
21:B:839:BCR:H24C	21:B:839:BCR:H371	1.77	0.43
18:P:307:CLA:H41	18:P:307:CLA:H61	1.74	0.43
15:S:66:LEU:HD22	18:S:201:CLA:HMA1	1.99	0.43
17:T:5:TRP:HB2	17:T:78:LEU:HD11	2.01	0.43
1:A:150:TRP:CG	18:A:814:CLA:HAA2	2.54	0.43
1:A:563:PRO:HB3	1:A:710:ILE:HB	2.00	0.43
18:B:843:CLA:H141	18:B:843:CLA:H162	1.78	0.43
8:J:22:ILE:HA	18:J:103:CLA:HBB2	2.00	0.43
18:P:306:CLA:H61	18:P:306:CLA:H41	1.79	0.43
1:A:233:ILE:HG23	1:A:234:PHE:HD1	1.84	0.43
1:A:674:MET:HB2	18:A:801:CLA:C1C	2.48	0.43
2:B:271:ILE:HG23	18:B:816:CLA:HMA3	2.00	0.43
2:B:409:MET:HE2	21:R:203:BCR:H402	2.00	0.43
21:I:101:BCR:H15C	21:I:101:BCR:H351	1.88	0.43
2:B:20:TRP:CG	2:B:702:GLN:HE22	2.37	0.42
21:J:104:BCR:H15C	21:J:104:BCR:H351	1.93	0.42
2:B:266:MET:HE1	18:B:815:CLA:HED3	2.01	0.42
11:O:71:ILE:HD11	18:O:206:CLA:H43	2.01	0.42
1:A:323:THR:HG21	20:A:840:LHG:HC11	2.00	0.42
18:A:828:CLA:H142	21:B:841:BCR:H17C	2.00	0.42
22:A:848:CL0:H2	22:A:848:CL0:H14	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:830:CLA:H92	18:B:830:CLA:H61	1.78	0.42
4:D:73:ARG:HD3	4:D:79:GLN:HG3	2.00	0.42
12:P:7:LEU:HG	27:P:301:LMG:HC61	2.02	0.42
18:R:205:CLA:HED2	18:R:205:CLA:HBD	1.82	0.42
27:U:201:LMG:H302	18:U:211:CLA:H11	2.01	0.42
21:L:201:BCR:H20C	21:L:201:BCR:H361	1.83	0.42
19:A:837:PQN:H222	19:A:837:PQN:H18	1.58	0.42
7:I:29:LEU:HB3	26:M:102:SQD:H242	2.01	0.42
16:U:18:LYS:H	16:U:18:LYS:HG2	1.62	0.42
2:B:705:LEU:HD23	25:B:842:DGD:HA21	2.02	0.42
18:B:820:CLA:H11	18:B:843:CLA:H92	2.00	0.42
18:B:834:CLA:H41	18:B:834:CLA:H61	1.76	0.42
6:F:24:LYS:NZ	30:F:901:HOH:O	2.32	0.42
13:Q:164:PHE:CD2	13:Q:165:PRO:HD2	2.55	0.42
18:A:811:CLA:H143	18:A:811:CLA:H112	1.77	0.42
2:B:152:TRP:CD1	26:B:847:SQD:H3	2.55	0.42
2:B:660:MET:HB2	18:B:803:CLA:C1C	2.50	0.42
2:B:350:MET:HE3	2:B:350:MET:HB3	1.98	0.42
2:B:518:HIS:CG	18:B:831:CLA:HED3	2.55	0.42
18:B:803:CLA:H191	21:I:101:BCR:H19C	2.02	0.42
13:Q:36:LYS:HB2	13:Q:36:LYS:HE3	1.71	0.42
18:Q:216:CLA:H152	18:Q:216:CLA:H112	1.87	0.42
18:A:804:CLA:H62	18:A:804:CLA:H102	1.88	0.42
2:B:629:LEU:HD21	2:B:648:PHE:CG	2.55	0.42
18:B:830:CLA:H91	18:B:830:CLA:H111	1.83	0.42
12:P:99:ALA:O	12:P:103:THR:OG1	2.28	0.42
18:A:833:CLA:H202	18:A:833:CLA:H162	1.94	0.41
22:A:848:CL0:H32	18:B:801:CLA:C1D	2.50	0.41
21:M:101:BCR:H11C	21:M:101:BCR:H341	1.89	0.41
18:P:313:CLA:HBA1	18:P:313:CLA:H3A	1.85	0.41
18:B:848:CLA:HMA1	27:Q:217:LMG:H351	2.02	0.41
13:Q:126:TRP:CE3	18:Q:209:CLA:H42	2.55	0.41
14:R:67:ALA:O	29:R:206:A86:O2	2.38	0.41
17:T:12:LYS:NZ	18:T:207:CLA:O1D	2.35	0.41
1:A:263:ASP:OD1	1:A:263:ASP:N	2.42	0.41
18:A:801:CLA:H18	21:F:801:BCR:H14C	2.01	0.41
1:A:94:LEU:HD21	1:A:143:THR:HA	2.03	0.41
18:B:807:CLA:HHB	18:B:808:CLA:HMB3	2.01	0.41
18:B:834:CLA:H162	18:B:834:CLA:H122	1.48	0.41
18:B:835:CLA:H3A	20:R:201:LHG:H321	2.02	0.41
18:Q:208:CLA:HBB2	18:Q:212:CLA:H203	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:52:PRO:O	15:S:77:ASN:ND2	2.53	0.41
18:U:210:CLA:H161	18:U:210:CLA:H141	1.86	0.41
2:B:1:THR:HG22	2:B:11:ALA:O	2.20	0.41
2:B:381:MET:HE1	21:B:840:BCR:H361	2.01	0.41
12:P:126:THR:HB	12:P:146:LEU:HD22	2.03	0.41
21:A:841:BCR:H24C	21:A:841:BCR:H371	1.93	0.41
9:L:41:SER:O	9:L:45:ARG:HG3	2.20	0.41
18:S:215:CLA:H141	18:S:215:CLA:H162	1.86	0.41
2:B:629:LEU:HD22	2:B:722:PHE:HA	2.03	0.41
18:A:823:CLA:H91	18:A:823:CLA:H112	1.88	0.41
18:A:828:CLA:H191	25:B:842:DGD:HA81	2.02	0.41
2:B:656:ALA:HB3	18:B:803:CLA:HBB2	2.02	0.41
18:B:828:CLA:H111	6:F:93:ILE:HD11	2.02	0.41
9:L:5:LYS:NZ	9:L:17:SER:OG	2.53	0.41
12:P:66:LYS:HD2	18:P:315:CLA:C3D	2.51	0.41
18:A:849:CLA:H172	6:F:101:GLY:HA2	2.03	0.41
2:B:239:LYS:HA	2:B:239:LYS:HD2	1.86	0.41
18:B:825:CLA:H142	18:B:825:CLA:H112	1.88	0.41
18:Q:203:CLA:HBA1	18:Q:203:CLA:H11	1.54	0.41
17:T:17:CYS:HA	17:T:20:ALA:HB3	2.01	0.41
18:A:801:CLA:O1A	2:B:428:GLY:HA3	2.21	0.41
2:B:208:ASP:OD1	2:B:208:ASP:N	2.54	0.41
9:L:52:ALA:HA	21:L:205:BCR:H16C	2.03	0.41
11:O:159:ILE:HD12	11:O:159:ILE:HA	1.91	0.41
18:Q:216:CLA:H192	18:Q:216:CLA:H161	1.83	0.41
18:B:816:CLA:H91	18:B:816:CLA:H111	1.90	0.40
4:D:39:VAL:HG22	4:D:49:ILE:HG12	2.03	0.40
13:Q:126:TRP:HB3	13:Q:135:MET:HE2	2.03	0.40
18:A:824:CLA:H122	18:A:824:CLA:H8	1.94	0.40
21:M:101:BCR:H15C	21:M:101:BCR:H351	1.83	0.40
18:O:204:CLA:H172	18:O:204:CLA:H13	1.67	0.40
18:B:812:CLA:H12	18:B:812:CLA:H52	1.92	0.40
21:L:205:BCR:H15C	21:L:205:BCR:H351	1.90	0.40
1:A:431:ASN:O	1:A:435:ILE:HG13	2.22	0.40
18:A:818:CLA:H112	18:A:818:CLA:H91	1.90	0.40
18:A:852:CLA:H91	18:A:852:CLA:H112	1.90	0.40
18:A:852:CLA:H72	18:L:203:CLA:H12	2.03	0.40
2:B:24:ALA:HB2	25:B:842:DGD:HA32	2.02	0.40
21:R:203:BCR:H11C	21:R:203:BCR:H341	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/752 (98%)	722 (98%)	17 (2%)	0	100	100
2	B	730/734 (100%)	714 (98%)	16 (2%)	0	100	100
3	C	78/81 (96%)	78 (100%)	0	0	100	100
4	D	136/142 (96%)	132 (97%)	4 (3%)	0	100	100
5	E	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
6	F	159/184 (86%)	157 (99%)	2 (1%)	0	100	100
7	I	32/35 (91%)	32 (100%)	0	0	100	100
8	J	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
9	L	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
10	M	27/29 (93%)	27 (100%)	0	0	100	100
11	O	174/201 (87%)	171 (98%)	3 (2%)	0	100	100
12	P	191/231 (83%)	190 (100%)	1 (0%)	0	100	100
13	Q	165/197 (84%)	157 (95%)	6 (4%)	2 (1%)	10	4
14	R	86/90 (96%)	86 (100%)	0	0	100	100
15	S	163/215 (76%)	161 (99%)	2 (1%)	0	100	100
16	U	139/191 (73%)	138 (99%)	1 (1%)	0	100	100
17	T	91/202 (45%)	90 (99%)	1 (1%)	0	100	100
All	All	3147/3531 (89%)	3089 (98%)	56 (2%)	2 (0%)	49	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	Q	165	PRO
13	Q	33	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/612 (98%)	598 (99%)	5 (1%)	73	75
2	B	590/591 (100%)	587 (100%)	3 (0%)	81	84
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	118/122 (97%)	118 (100%)	0	100	100
5	E	53/55 (96%)	53 (100%)	0	100	100
6	F	133/152 (88%)	132 (99%)	1 (1%)	73	75
7	I	31/32 (97%)	31 (100%)	0	100	100
8	J	32/32 (100%)	32 (100%)	0	100	100
9	L	111/112 (99%)	111 (100%)	0	100	100
10	M	21/21 (100%)	21 (100%)	0	100	100
11	O	145/161 (90%)	143 (99%)	2 (1%)	59	59
12	P	144/173 (83%)	144 (100%)	0	100	100
13	Q	133/157 (85%)	131 (98%)	2 (2%)	57	56
14	R	71/73 (97%)	71 (100%)	0	100	100
15	S	125/162 (77%)	122 (98%)	3 (2%)	43	38
16	U	110/148 (74%)	110 (100%)	0	100	100
17	T	73/153 (48%)	71 (97%)	2 (3%)	39	34
All	All	2561/2825 (91%)	2543 (99%)	18 (1%)	73	78

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	52	THR
1	A	410	GLN
1	A	573	CYS
1	A	627	ASN
2	B	5	LYS
2	B	104	ARG

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Mol	Chain	Res	Type
2	B	307	VAL
6	F	135	ILE
11	O	95	LEU
11	O	135	CYS
13	Q	1	LYS
13	Q	63	ILE
15	S	53	SER
15	S	90	LEU
15	S	101	LYS
17	T	43	SER
17	T	77	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	431	ASN
2	B	39	ASN
2	B	169	ASN
2	B	641	GLN
3	C	3	ASN
3	C	37	GLN
4	D	115	ASN
6	F	15	ASN
6	F	31	ASN
6	F	45	GLN
9	L	32	ASN
11	O	54	GLN
12	P	186	HIS
14	R	49	ASN
14	R	85	GLN
15	S	46	GLN
15	S	72	ASN
16	U	120	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

220 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	$\#\|Z\| > 2$
21	BCR	B	840	-	41,41,41	1.03	2 (4%)	56,56,56	1.25	7 (12%)
18	CLA	B	834	2	69,73,73	1.27	9 (13%)	83,113,113	1.02	4 (4%)
21	BCR	J	104	-	41,41,41	1.05	2 (4%)	56,56,56	1.12	4 (7%)
18	CLA	A	820	1	55,59,73	1.40	7 (12%)	66,96,113	1.20	6 (9%)
18	CLA	Q	212	13	69,73,73	1.25	8 (11%)	83,113,113	1.04	7 (8%)
18	CLA	T	202	-	46,50,73	1.46	7 (15%)	55,85,113	1.26	5 (9%)
18	CLA	Q	207	13	50,54,73	1.41	7 (14%)	60,90,113	1.23	5 (8%)
18	CLA	A	826	1	69,73,73	1.32	8 (11%)	83,113,113	0.88	3 (3%)
23	SF4	A	850	2,1	0,12,12	-	-	-		
28	KC1	U	213	16	49,53,53	1.76	10 (20%)	63,89,89	1.02	4 (6%)
18	CLA	Q	204	-	65,69,73	1.21	6 (9%)	78,108,113	1.02	6 (7%)
18	CLA	A	846	1	64,68,73	1.40	9 (14%)	77,107,113	0.91	4 (5%)
18	CLA	B	843	2	69,73,73	1.30	8 (11%)	83,113,113	0.97	3 (3%)
24	DD6	S	203	-	39,45,45	1.65	8 (20%)	52,67,67	1.91	13 (25%)
18	CLA	Q	213	30	61,65,73	1.26	7 (11%)	73,103,113	1.04	5 (6%)
18	CLA	B	814	2	59,63,73	1.43	8 (13%)	71,101,113	1.03	4 (5%)
24	DD6	O	214	-	39,45,45	1.54	8 (20%)	52,67,67	1.57	12 (23%)
29	A86	R	204	-	40,46,50	1.75	4 (10%)	45,70,76	2.08	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	B	848	2	54,58,73	1.37	8 (14%)	65,95,113	1.20	6 (9%)
18	CLA	A	845	30	69,73,73	1.18	8 (11%)	83,113,113	0.98	3 (3%)
24	DD6	P	317	-	20,24,45	1.80	6 (30%)	27,37,67	1.92	6 (22%)
18	CLA	B	819	2	57,61,73	1.31	7 (12%)	68,98,113	1.05	5 (7%)
18	CLA	A	829	1	69,73,73	1.23	8 (11%)	83,113,113	0.97	4 (4%)
18	CLA	L	202	9	53,57,73	1.39	8 (15%)	62,93,113	1.39	6 (9%)
18	CLA	U	209	16	46,50,73	1.48	7 (15%)	55,85,113	1.17	5 (9%)
26	SQD	M	102	-	45,46,54	0.99	4 (8%)	54,57,65	1.62	10 (18%)
18	CLA	B	810	2	58,62,73	1.44	9 (15%)	73,100,113	0.94	3 (4%)
18	CLA	A	806	1	69,73,73	1.16	7 (10%)	83,113,113	0.95	4 (4%)
18	CLA	Q	211	13	45,49,73	1.49	8 (17%)	54,84,113	1.24	6 (11%)
24	DD6	P	314	-	39,45,45	1.68	7 (17%)	52,67,67	1.99	10 (19%)
18	CLA	A	847	1	69,73,73	1.22	9 (13%)	83,113,113	1.10	6 (7%)
18	CLA	A	808	1	60,64,73	1.33	9 (15%)	72,102,113	1.29	7 (9%)
24	DD6	P	316	-	39,45,45	1.64	6 (15%)	52,67,67	1.81	12 (23%)
18	CLA	P	308	-	56,60,73	1.30	7 (12%)	67,97,113	1.08	5 (7%)
18	CLA	T	208	17	69,73,73	1.18	7 (10%)	83,113,113	1.16	7 (8%)
28	KC1	O	210	11	49,53,53	1.75	10 (20%)	63,89,89	1.17	5 (7%)
20	LHG	A	839	-	47,47,48	0.65	0	50,53,54	1.19	5 (10%)
18	CLA	A	821	-	69,73,73	1.24	8 (11%)	83,113,113	1.02	6 (7%)
18	CLA	L	204	-	54,58,73	1.36	8 (14%)	65,95,113	1.14	5 (7%)
18	CLA	P	310	12	54,58,73	1.33	7 (12%)	65,95,113	1.14	3 (4%)
18	CLA	B	835	30	69,73,73	1.23	7 (10%)	83,113,113	1.10	8 (9%)
18	CLA	B	831	2	69,73,73	1.23	8 (11%)	83,113,113	0.94	3 (3%)
18	CLA	L	203	9	69,73,73	1.22	8 (11%)	83,113,113	0.97	4 (4%)
18	CLA	B	826	2	54,58,73	1.45	8 (14%)	65,95,113	1.08	4 (6%)
18	CLA	A	828	1	69,73,73	1.25	7 (10%)	83,113,113	0.95	4 (4%)
18	CLA	B	830	2	62,66,73	1.31	8 (12%)	74,104,113	1.04	5 (6%)
18	CLA	Q	206	13	54,59,73	1.40	7 (12%)	64,96,113	0.99	3 (4%)
18	CLA	Q	216	30	69,73,73	1.17	8 (11%)	83,113,113	0.99	4 (4%)
21	BCR	A	841	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
18	CLA	A	835	1	69,73,73	1.25	7 (10%)	83,113,113	0.99	4 (4%)
18	CLA	A	825	1	69,73,73	1.26	8 (11%)	83,113,113	0.90	3 (3%)
18	CLA	A	823	1	69,73,73	1.25	8 (11%)	83,113,113	0.89	4 (4%)
18	CLA	O	208	11	64,68,73	1.19	8 (12%)	77,107,113	1.07	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	BCR	A	842	-	41,41,41	1.06	2 (4%)	56,56,56	1.12	4 (7%)
18	CLA	U	207	-	69,73,73	1.16	6 (8%)	83,113,113	1.18	8 (9%)
21	BCR	L	201	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	4 (7%)
18	CLA	S	201	30	69,73,73	1.15	7 (10%)	83,113,113	1.13	7 (8%)
18	CLA	A	810	1	58,62,73	1.29	7 (12%)	69,99,113	1.09	6 (8%)
18	CLA	A	833	1	69,73,73	1.27	9 (13%)	83,113,113	1.12	6 (7%)
18	CLA	Q	208	13	54,58,73	1.33	9 (16%)	65,95,113	1.08	5 (7%)
28	KC1	P	305	12	49,53,53	2.06	11 (22%)	63,89,89	1.20	7 (11%)
18	CLA	B	820	-	67,71,73	1.23	8 (11%)	80,110,113	1.06	6 (7%)
21	BCR	I	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	8 (14%)
24	DD6	U	214	-	24,26,45	1.63	6 (25%)	30,35,67	1.62	6 (20%)
18	CLA	P	313	12	49,53,73	1.44	6 (12%)	59,89,113	1.17	5 (8%)
25	DGD	B	842	-	61,61,67	0.98	1 (1%)	75,75,81	1.35	7 (9%)
18	CLA	Q	205	13	64,68,73	1.20	8 (12%)	77,107,113	1.04	4 (5%)
21	BCR	F	801	-	41,41,41	1.05	2 (4%)	56,56,56	1.29	6 (10%)
27	LMG	J	102	-	39,39,55	0.86	1 (2%)	47,47,63	1.21	2 (4%)
18	CLA	B	846	2	69,73,73	1.21	8 (11%)	83,113,113	1.25	7 (8%)
24	DD6	U	203	-	39,45,45	1.63	8 (20%)	52,67,67	1.91	13 (25%)
20	LHG	A	840	18	26,26,48	0.84	1 (3%)	29,32,54	1.33	3 (10%)
18	CLA	R	202	30	49,53,73	1.43	8 (16%)	59,89,113	1.20	6 (10%)
18	CLA	T	211	17	50,54,73	1.42	7 (14%)	60,90,113	1.27	7 (11%)
18	CLA	O	207	11	50,54,73	1.39	8 (16%)	60,90,113	1.15	4 (6%)
18	CLA	Q	209	13	69,73,73	1.15	6 (8%)	83,113,113	1.00	3 (3%)
18	CLA	S	205	15	50,54,73	1.47	8 (16%)	60,90,113	1.08	3 (5%)
18	CLA	U	204	-	65,69,73	1.23	7 (10%)	78,108,113	0.95	5 (6%)
18	CLA	A	851	1	69,73,73	1.22	8 (11%)	83,113,113	0.95	3 (3%)
23	SF4	C	101	3	0,12,12	-	-	-		
18	CLA	A	815	1	69,73,73	1.24	7 (10%)	83,113,113	1.00	5 (6%)
24	DD6	S	213	-	39,45,45	1.65	8 (20%)	52,67,67	1.71	13 (25%)
27	LMG	S	211	-	49,49,55	0.73	1 (2%)	57,57,63	1.25	4 (7%)
18	CLA	S	204	15	50,54,73	1.38	7 (14%)	60,90,113	1.13	4 (6%)
18	CLA	T	210	17	45,49,73	1.42	5 (11%)	54,84,113	1.35	7 (12%)
18	CLA	A	807	1	69,73,73	1.22	8 (11%)	83,113,113	1.02	5 (6%)
18	CLA	B	818	2	50,54,73	1.42	8 (16%)	60,90,113	1.23	6 (10%)
18	CLA	B	811	2	59,63,73	1.28	7 (11%)	71,101,113	0.99	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
18	CLA	B	816	2	64,68,73	1.28	8 (12%)	77,107,113	1.00	4 (5%)
18	CLA	B	813	2	53,57,73	1.43	9 (16%)	62,93,113	1.14	4 (6%)
18	CLA	B	845	2	69,73,73	1.29	9 (13%)	83,113,113	1.02	5 (6%)
18	CLA	P	307	12	60,64,73	1.29	8 (13%)	72,102,113	1.07	6 (8%)
18	CLA	B	802	2	69,73,73	1.29	7 (10%)	83,113,113	0.84	4 (4%)
18	CLA	P	312	12	45,49,73	1.45	7 (15%)	54,84,113	1.27	5 (9%)
21	BCR	B	841	-	41,41,41	1.07	2 (4%)	56,56,56	1.08	4 (7%)
18	CLA	A	803	1	69,73,73	1.21	8 (11%)	83,113,113	1.04	4 (4%)
18	CLA	B	815	2	63,67,73	1.24	7 (11%)	75,105,113	1.12	6 (8%)
18	CLA	B	823	2	69,73,73	1.26	7 (10%)	83,113,113	0.96	4 (4%)
18	CLA	B	825	2	69,73,73	1.29	8 (11%)	83,113,113	0.96	5 (6%)
24	DD6	U	212	-	39,45,45	1.53	7 (17%)	52,67,67	1.85	10 (19%)
24	DD6	O	201	-	39,45,45	1.62	8 (20%)	52,67,67	1.61	9 (17%)
18	CLA	B	808	2	69,73,73	1.26	8 (11%)	83,113,113	0.93	3 (3%)
27	LMG	Q	217	-	55,55,55	0.75	1 (1%)	63,63,63	1.33	8 (12%)
18	CLA	S	214	30	69,73,73	1.17	6 (8%)	83,113,113	1.03	5 (6%)
29	A86	Q	201	-	44,50,50	1.68	5 (11%)	51,76,76	1.76	10 (19%)
18	CLA	T	212	-	51,55,73	1.37	6 (11%)	61,91,113	1.20	6 (9%)
18	CLA	A	814	30	49,53,73	1.42	8 (16%)	59,89,113	1.15	5 (8%)
18	CLA	O	211	11	45,49,73	1.49	7 (15%)	54,84,113	1.23	6 (11%)
18	CLA	B	805	2	69,73,73	1.22	9 (13%)	83,113,113	0.98	4 (4%)
21	BCR	I	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.17	4 (7%)
18	CLA	P	306	12	69,73,73	1.19	7 (10%)	83,113,113	1.05	5 (6%)
18	CLA	U	206	16	49,53,73	1.42	6 (12%)	59,89,113	1.14	5 (8%)
24	DD6	O	215	-	39,45,45	1.54	8 (20%)	52,67,67	1.68	12 (23%)
18	CLA	B	821	-	68,72,73	1.17	8 (11%)	81,111,113	0.96	5 (6%)
21	BCR	R	203	-	40,40,41	1.16	2 (5%)	54,54,56	1.44	11 (20%)
18	CLA	A	853	30	69,73,73	1.20	7 (10%)	83,113,113	1.07	7 (8%)
18	CLA	P	309	30	51,55,73	1.35	8 (15%)	61,91,113	1.05	4 (6%)
18	CLA	A	838	20	56,60,73	1.30	8 (14%)	67,97,113	1.06	3 (4%)
24	DD6	S	202	-	39,45,45	1.53	8 (20%)	52,67,67	1.55	8 (15%)
18	CLA	A	827	1	54,58,73	1.45	8 (14%)	65,95,113	1.06	4 (6%)
23	SF4	C	102	3	0,12,12	-	-	-		
24	DD6	J	101	-	39,45,45	1.53	8 (20%)	52,67,67	1.66	9 (17%)
24	DD6	Q	215	-	39,45,45	1.55	7 (17%)	52,67,67	1.58	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	BCR	F	804	-	41,41,41	1.02	2 (4%)	56,56,56	1.26	4 (7%)
18	CLA	A	849	1	69,73,73	1.25	6 (8%)	83,113,113	0.93	3 (3%)
28	KC1	T	209	17	49,53,53	1.80	11 (22%)	63,89,89	1.05	3 (4%)
18	CLA	B	817	-	69,73,73	1.24	7 (10%)	83,113,113	1.05	8 (9%)
18	CLA	S	207	15	56,60,73	1.28	7 (12%)	67,97,113	1.17	5 (7%)
18	CLA	B	803	-	69,73,73	1.18	7 (10%)	83,113,113	1.00	5 (6%)
21	BCR	M	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.29	8 (14%)
18	CLA	A	817	1	49,53,73	1.44	8 (16%)	59,89,113	1.15	5 (8%)
18	CLA	O	209	11	69,73,73	1.20	7 (10%)	83,113,113	1.26	7 (8%)
18	CLA	O	202	11	47,51,73	1.44	7 (14%)	56,86,113	1.17	5 (8%)
24	DD6	P	304	-	39,45,45	1.49	8 (20%)	52,67,67	1.53	10 (19%)
28	KC1	S	208	15	49,53,53	1.74	10 (20%)	63,89,89	1.16	4 (6%)
18	CLA	S	206	15	49,53,73	1.35	6 (12%)	59,89,113	1.09	5 (8%)
24	DD6	T	214	-	39,45,45	1.55	7 (17%)	52,67,67	1.92	11 (21%)
18	CLA	U	205	16	69,73,73	1.19	7 (10%)	83,113,113	0.95	3 (3%)
18	CLA	A	804	1	69,73,73	1.18	8 (11%)	83,113,113	1.04	6 (7%)
24	DD6	Q	202	-	39,45,45	1.56	8 (20%)	52,67,67	1.69	10 (19%)
18	CLA	T	204	17	50,54,73	1.46	7 (14%)	60,90,113	0.99	3 (5%)
19	PQN	A	837	-	34,34,34	0.39	0	42,45,45	0.45	0
18	CLA	T	203	17	45,49,73	1.44	7 (15%)	54,84,113	1.19	4 (7%)
21	BCR	A	843	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	3 (5%)
24	DD6	O	212	-	39,45,45	1.58	8 (20%)	52,67,67	1.73	9 (17%)
29	A86	T	201	-	44,50,50	1.64	6 (13%)	51,76,76	1.66	11 (21%)
21	BCR	B	839	-	41,41,41	1.04	2 (4%)	56,56,56	1.17	4 (7%)
18	CLA	A	836	30	69,73,73	1.20	9 (13%)	83,113,113	1.06	6 (7%)
18	CLA	A	834	1	69,73,73	1.34	9 (13%)	83,113,113	0.96	4 (4%)
18	CLA	A	824	1	66,70,73	1.23	8 (12%)	79,109,113	1.13	6 (7%)
18	CLA	B	804	2	49,53,73	1.48	8 (16%)	59,89,113	1.06	3 (5%)
24	DD6	A	854	-	39,45,45	1.51	8 (20%)	52,67,67	1.59	10 (19%)
21	BCR	B	837	-	41,41,41	1.07	2 (4%)	56,56,56	1.13	4 (7%)
24	DD6	S	209	-	39,45,45	1.51	8 (20%)	52,67,67	1.50	9 (17%)
24	DD6	S	212	-	39,45,45	1.53	8 (20%)	52,67,67	1.53	10 (19%)
18	CLA	A	811	1	69,73,73	1.24	8 (11%)	83,113,113	0.98	4 (4%)
18	CLA	T	206	-	50,54,73	1.37	8 (16%)	60,90,113	1.19	6 (10%)
18	CLA	U	211	16	56,60,73	1.32	7 (12%)	67,97,113	1.06	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	U	208	16	50,54,73	1.36	7 (14%)	60,90,113	1.18	5 (8%)
18	CLA	A	805	1	53,57,73	1.43	9 (16%)	62,93,113	1.12	4 (6%)
21	BCR	B	838	-	41,41,41	1.05	2 (4%)	56,56,56	1.19	7 (12%)
29	A86	Q	214	-	44,50,50	1.64	6 (13%)	51,76,76	1.49	10 (19%)
18	CLA	O	204	11	69,73,73	1.22	9 (13%)	83,113,113	0.95	5 (6%)
18	CLA	B	801	-	69,73,73	1.21	8 (11%)	83,113,113	0.98	5 (6%)
18	CLA	A	822	30	69,73,73	1.16	5 (7%)	83,113,113	1.01	4 (4%)
18	CLA	O	203	-	49,53,73	1.44	7 (14%)	59,89,113	1.14	5 (8%)
18	CLA	A	801	-	69,73,73	1.20	7 (10%)	83,113,113	0.96	4 (4%)
27	LMG	P	301	-	34,34,55	1.14	3 (8%)	42,42,63	1.30	2 (4%)
28	KC1	P	311	12	47,52,53	1.79	9 (19%)	57,87,89	1.41	8 (14%)
27	LMG	B	849	-	25,25,55	1.38	5 (20%)	33,33,63	1.24	5 (15%)
18	CLA	B	827	2	53,57,73	1.40	8 (15%)	62,93,113	1.12	5 (8%)
18	CLA	J	103	8	46,50,73	1.49	7 (15%)	55,85,113	1.15	4 (7%)
18	CLA	B	824	2	69,73,73	1.27	9 (13%)	83,113,113	1.71	11 (13%)
18	CLA	B	822	2	69,73,73	1.27	8 (11%)	83,113,113	1.00	5 (6%)
18	CLA	P	315	12	51,55,73	1.41	8 (15%)	61,91,113	1.18	5 (8%)
18	CLA	Q	203	13	52,56,73	1.35	6 (11%)	62,92,113	1.12	5 (8%)
18	CLA	B	806	2	69,73,73	1.27	8 (11%)	83,113,113	0.92	4 (4%)
26	SQD	B	847	-	49,50,54	1.01	6 (12%)	58,61,65	1.55	10 (17%)
28	KC1	S	210	15	49,53,53	1.71	10 (20%)	63,89,89	1.15	5 (7%)
18	CLA	O	206	-	69,73,73	1.17	8 (11%)	83,113,113	0.93	4 (4%)
21	BCR	A	844	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	5 (8%)
29	A86	R	206	-	44,50,50	1.59	6 (13%)	51,76,76	1.57	10 (19%)
18	CLA	T	205	-	61,65,73	1.23	7 (11%)	73,103,113	0.99	4 (5%)
18	CLA	A	831	1	49,53,73	1.38	7 (14%)	59,89,113	1.19	5 (8%)
18	CLA	B	828	2	62,66,73	1.32	8 (12%)	74,104,113	1.02	4 (5%)
18	CLA	B	807	2	69,73,73	1.22	8 (11%)	83,113,113	0.98	4 (4%)
18	CLA	A	819	1	47,51,73	1.45	8 (17%)	56,86,113	1.12	4 (7%)
18	CLA	A	852	1	69,73,73	1.19	8 (11%)	83,113,113	0.97	5 (6%)
18	CLA	F	802	30	52,56,73	1.42	7 (13%)	62,92,113	1.18	5 (8%)
18	CLA	B	844	2	69,73,73	1.28	8 (11%)	83,113,113	0.94	6 (7%)
18	CLA	B	832	2	51,55,73	1.44	8 (15%)	61,91,113	1.17	5 (8%)
18	CLA	B	809	2	69,73,73	1.21	8 (11%)	83,113,113	0.97	5 (6%)
21	BCR	L	205	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	A	832	1	55,59,73	1.41	8 (14%)	66,96,113	1.10	4 (6%)
18	CLA	A	809	1	66,70,73	1.25	8 (12%)	79,109,113	0.92	3 (3%)
28	KC1	Q	210	13	49,53,53	1.74	9 (18%)	63,89,89	1.30	8 (12%)
18	CLA	B	812	2	58,62,73	1.36	8 (13%)	69,99,113	1.06	4 (5%)
18	CLA	A	813	1	54,58,73	1.40	7 (12%)	65,95,113	1.17	7 (10%)
20	LHG	R	201	-	48,48,48	0.65	2 (4%)	51,54,54	1.25	5 (9%)
18	CLA	B	829	30	69,73,73	1.18	8 (11%)	83,113,113	1.05	6 (7%)
18	CLA	R	205	14	69,73,73	1.28	9 (13%)	83,113,113	0.98	4 (4%)
29	A86	P	303	-	44,50,50	1.65	6 (13%)	51,76,76	1.66	10 (19%)
18	CLA	A	802	1	59,63,73	1.34	8 (13%)	71,101,113	1.01	3 (4%)
27	LMG	U	201	-	32,32,55	1.01	0	40,40,63	1.15	4 (10%)
29	A86	U	202	-	44,50,50	1.60	6 (13%)	51,76,76	1.56	10 (19%)
18	CLA	U	210	16	69,73,73	1.17	8 (11%)	83,113,113	1.01	5 (6%)
18	CLA	T	207	17	46,50,73	1.44	6 (13%)	55,85,113	1.17	5 (9%)
24	DD6	T	213	-	39,45,45	1.62	7 (17%)	52,67,67	1.84	13 (25%)
22	CL0	A	848	1	69,73,73	1.44	6 (8%)	83,113,113	0.91	4 (4%)
24	DD6	O	213	-	39,45,45	1.49	7 (17%)	52,67,67	1.51	11 (21%)
18	CLA	S	215	15	69,73,73	1.18	7 (10%)	83,113,113	0.94	3 (3%)
18	CLA	A	830	1	54,58,73	1.34	8 (14%)	65,95,113	1.07	4 (6%)
18	CLA	F	803	6	50,54,73	1.40	7 (14%)	60,90,113	1.19	5 (8%)
18	CLA	O	205	11	69,73,73	1.21	7 (10%)	83,113,113	0.94	4 (4%)
18	CLA	A	818	30	69,73,73	1.20	7 (10%)	83,113,113	0.95	3 (3%)
18	CLA	B	833	-	69,73,73	1.21	8 (11%)	83,113,113	1.06	7 (8%)
19	PQN	B	836	-	34,34,34	0.41	0	42,45,45	0.35	0
18	CLA	A	812	1	49,53,73	1.48	8 (16%)	59,89,113	1.11	4 (6%)
28	KC1	P	302	12	49,53,53	1.80	11 (22%)	63,89,89	1.19	6 (9%)
18	CLA	A	816	1	69,73,73	1.24	8 (11%)	83,113,113	1.04	4 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	B	840	-	-	5/29/63/63	0/2/2/2
18	CLA	B	834	2	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	J	104	-	-	13/29/63/63	0/2/2/2
18	CLA	A	820	1	-	3/23/99/115	-
18	CLA	Q	212	13	-	15/39/115/115	-
18	CLA	T	202	-	-	1/12/88/115	-
18	CLA	Q	207	13	-	4/17/93/115	-
18	CLA	A	826	1	-	3/39/115/115	-
28	KC1	U	213	16	-	3/15/71/71	-
23	SF4	A	850	2,1	-	-	0/6/5/5
18	CLA	Q	204	-	-	10/35/111/115	-
18	CLA	A	846	1	-	9/33/109/115	-
18	CLA	B	843	2	-	5/39/115/115	-
24	DD6	S	203	-	-	8/26/80/80	0/3/3/3
18	CLA	Q	213	30	-	6/30/106/115	-
18	CLA	B	814	2	-	4/27/103/115	-
24	DD6	O	214	-	-	8/26/80/80	0/3/3/3
29	A86	R	204	-	-	1/30/84/90	0/3/3/3
18	CLA	B	848	2	-	7/21/97/115	-
18	CLA	A	845	30	-	6/39/115/115	-
24	DD6	P	317	-	-	10/15/46/80	0/2/2/3
18	CLA	B	819	2	-	8/25/101/115	-
18	CLA	A	829	1	-	4/39/115/115	-
18	CLA	L	202	9	-	8/20/96/115	-
18	CLA	U	209	16	-	2/12/88/115	-
26	SQD	M	102	-	-	16/41/61/69	0/1/1/1
18	CLA	B	810	2	-	2/25/101/115	-
18	CLA	A	806	1	-	5/39/115/115	-
18	CLA	Q	211	13	-	4/10/86/115	-
24	DD6	P	314	-	-	13/26/80/80	0/3/3/3
18	CLA	A	847	1	-	9/39/115/115	-
18	CLA	A	808	1	-	5/29/105/115	-
24	DD6	P	316	-	-	14/26/80/80	0/3/3/3
18	CLA	P	308	-	-	7/24/100/115	-
18	CLA	T	208	17	-	12/39/115/115	-
28	KC1	O	210	11	-	0/15/71/71	-
20	LHG	A	839	-	-	20/52/52/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	821	-	-	10/39/115/115	-
18	CLA	L	204	-	-	8/21/97/115	-
18	CLA	P	310	12	-	4/21/97/115	-
18	CLA	B	835	30	-	1/39/115/115	-
18	CLA	B	831	2	-	4/39/115/115	-
18	CLA	L	203	9	-	1/39/115/115	-
18	CLA	B	826	2	-	0/21/97/115	-
18	CLA	A	828	1	-	6/39/115/115	-
18	CLA	B	830	2	-	3/31/107/115	-
18	CLA	Q	206	13	-	7/22/98/115	-
18	CLA	Q	216	30	-	14/39/115/115	-
21	BCR	A	841	-	-	7/29/63/63	0/2/2/2
18	CLA	A	835	1	-	5/39/115/115	-
18	CLA	A	825	1	-	5/39/115/115	-
18	CLA	A	823	1	-	9/39/115/115	-
18	CLA	O	208	11	-	3/33/109/115	-
21	BCR	A	842	-	-	10/29/63/63	0/2/2/2
18	CLA	U	207	-	-	8/39/115/115	-
21	BCR	L	201	-	-	11/29/63/63	0/2/2/2
18	CLA	S	201	30	-	9/39/115/115	-
18	CLA	A	810	1	-	1/26/102/115	-
18	CLA	A	833	1	-	6/39/115/115	-
18	CLA	Q	208	13	-	2/21/97/115	-
28	KC1	P	305	12	-	3/15/71/71	-
18	CLA	B	820	-	-	5/37/113/115	-
21	BCR	I	101	-	-	6/29/63/63	0/2/2/2
24	DD6	U	214	-	-	8/14/37/80	0/1/1/3
18	CLA	P	313	12	-	0/15/91/115	-
25	DGD	B	842	-	-	20/49/89/95	0/2/2/2
18	CLA	Q	205	13	-	7/33/109/115	-
21	BCR	F	801	-	-	8/29/63/63	0/2/2/2
27	LMG	J	102	-	-	24/34/54/70	0/1/1/1
18	CLA	B	846	2	-	7/39/115/115	-
24	DD6	U	203	-	-	15/26/80/80	0/3/3/3
20	LHG	A	840	18	-	8/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	R	202	30	-	0/15/91/115	-
18	CLA	T	211	17	-	5/17/93/115	-
18	CLA	O	207	11	-	2/17/93/115	-
18	CLA	Q	209	13	-	8/39/115/115	-
18	CLA	S	205	15	-	5/17/93/115	-
18	CLA	U	204	-	-	12/35/111/115	-
18	CLA	A	851	1	-	11/39/115/115	-
24	DD6	S	213	-	-	10/26/80/80	0/3/3/3
18	CLA	A	815	1	-	12/39/115/115	-
27	LMG	S	211	-	-	26/44/64/70	0/1/1/1
23	SF4	C	101	3	-	-	0/6/5/5
18	CLA	S	204	15	-	0/17/93/115	-
18	CLA	T	210	17	-	0/10/86/115	-
18	CLA	A	807	1	-	7/39/115/115	-
18	CLA	B	818	2	-	2/17/93/115	-
18	CLA	B	811	2	-	0/27/103/115	-
18	CLA	B	816	2	-	2/33/109/115	-
18	CLA	B	813	2	-	4/20/96/115	-
18	CLA	B	845	2	-	2/39/115/115	-
18	CLA	P	307	12	-	11/29/105/115	-
18	CLA	B	802	2	-	3/39/115/115	-
18	CLA	P	312	12	-	2/10/86/115	-
21	BCR	B	841	-	-	5/29/63/63	0/2/2/2
18	CLA	A	803	1	-	5/39/115/115	-
18	CLA	B	815	2	-	8/32/108/115	-
18	CLA	B	823	2	-	7/39/115/115	-
18	CLA	B	825	2	-	7/39/115/115	-
24	DD6	U	212	-	-	11/26/80/80	0/3/3/3
24	DD6	O	201	-	-	3/26/80/80	0/3/3/3
18	CLA	B	808	2	-	5/39/115/115	-
27	LMG	Q	217	-	-	23/50/70/70	0/1/1/1
18	CLA	S	214	30	-	1/39/115/115	-
29	A86	Q	201	-	-	24/34/90/90	0/3/3/3
18	CLA	T	212	-	-	4/18/94/115	-
18	CLA	A	814	30	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	O	211	11	-	0/10/86/115	-
18	CLA	B	805	2	-	9/39/115/115	-
21	BCR	I	102	-	-	9/29/63/63	0/2/2/2
18	CLA	P	306	12	-	9/39/115/115	-
18	CLA	U	206	16	-	4/15/91/115	-
24	DD6	O	215	-	-	12/26/80/80	0/3/3/3
18	CLA	B	821	-	-	4/38/114/115	-
21	BCR	R	203	-	-	10/27/61/63	0/2/2/2
18	CLA	A	853	30	-	2/39/115/115	-
18	CLA	P	309	30	-	2/18/94/115	-
18	CLA	A	838	20	-	5/24/100/115	-
24	DD6	S	202	-	-	8/26/80/80	0/3/3/3
18	CLA	A	827	1	-	2/21/97/115	-
24	DD6	J	101	-	-	6/26/80/80	0/3/3/3
23	SF4	C	102	3	-	-	0/6/5/5
24	DD6	Q	215	-	-	8/26/80/80	0/3/3/3
21	BCR	F	804	-	-	9/29/63/63	0/2/2/2
18	CLA	A	849	1	-	7/39/115/115	-
28	KC1	T	209	17	-	2/15/71/71	-
18	CLA	B	817	-	-	7/39/115/115	-
18	CLA	S	207	15	-	5/24/100/115	-
18	CLA	B	803	-	-	6/39/115/115	-
21	BCR	M	101	-	-	4/29/63/63	0/2/2/2
18	CLA	A	817	1	-	0/15/91/115	-
18	CLA	O	209	11	-	12/39/115/115	-
18	CLA	O	202	11	-	2/13/89/115	-
24	DD6	P	304	-	-	8/26/80/80	0/3/3/3
28	KC1	S	208	15	-	1/15/71/71	-
18	CLA	S	206	15	-	2/15/91/115	-
24	DD6	T	214	-	-	12/26/80/80	0/3/3/3
18	CLA	U	205	16	-	8/39/115/115	-
18	CLA	A	804	1	-	12/39/115/115	-
24	DD6	Q	202	-	-	6/26/80/80	0/3/3/3
18	CLA	T	204	17	-	4/17/93/115	-
19	PQN	A	837	-	-	7/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	T	203	17	-	2/10/86/115	-
21	BCR	A	843	-	-	4/29/63/63	0/2/2/2
24	DD6	O	212	-	-	11/26/80/80	0/3/3/3
29	A86	T	201	-	-	18/34/90/90	0/3/3/3
21	BCR	B	839	-	-	4/29/63/63	0/2/2/2
18	CLA	A	836	30	-	3/39/115/115	-
18	CLA	A	834	1	-	9/39/115/115	-
18	CLA	A	824	1	-	6/36/112/115	-
18	CLA	B	804	2	-	4/15/91/115	-
24	DD6	A	854	-	-	13/26/80/80	0/3/3/3
21	BCR	B	837	-	-	9/29/63/63	0/2/2/2
24	DD6	S	209	-	-	6/26/80/80	0/3/3/3
24	DD6	S	212	-	-	16/26/80/80	0/3/3/3
18	CLA	A	811	1	-	6/39/115/115	-
18	CLA	T	206	-	-	5/17/93/115	-
18	CLA	U	211	16	-	3/24/100/115	-
18	CLA	U	208	16	-	2/17/93/115	-
18	CLA	A	805	1	-	2/20/96/115	-
21	BCR	B	838	-	-	7/29/63/63	0/2/2/2
29	A86	Q	214	-	-	8/34/90/90	0/3/3/3
18	CLA	O	204	11	-	5/39/115/115	-
18	CLA	B	801	-	-	1/39/115/115	-
18	CLA	A	822	30	-	2/39/115/115	-
18	CLA	O	203	-	-	1/15/91/115	-
18	CLA	A	801	-	-	6/39/115/115	-
27	LMG	P	301	-	-	12/29/49/70	0/1/1/1
28	KC1	P	311	12	-	4/12/68/71	-
27	LMG	B	849	-	-	8/19/39/70	0/1/1/1
18	CLA	B	827	2	-	3/20/96/115	-
18	CLA	J	103	8	-	3/12/88/115	-
18	CLA	B	824	2	-	9/39/115/115	-
18	CLA	B	822	2	-	0/39/115/115	-
18	CLA	P	315	12	-	1/18/94/115	-
18	CLA	Q	203	13	-	5/19/95/115	-
18	CLA	B	806	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	B	847	-	-	23/45/65/69	0/1/1/1
28	KC1	S	210	15	-	4/15/71/71	-
18	CLA	O	206	-	-	1/39/115/115	-
21	BCR	A	844	-	-	9/29/63/63	0/2/2/2
29	A86	R	206	-	-	4/34/90/90	0/3/3/3
18	CLA	T	205	-	-	11/30/106/115	-
18	CLA	A	831	1	-	2/15/91/115	-
18	CLA	B	828	2	-	3/31/107/115	-
18	CLA	B	807	2	-	2/39/115/115	-
18	CLA	A	819	1	-	1/13/89/115	-
18	CLA	A	852	1	-	4/39/115/115	-
18	CLA	F	802	30	-	5/19/95/115	-
18	CLA	B	844	2	-	2/39/115/115	-
18	CLA	B	832	2	-	2/18/94/115	-
18	CLA	B	809	2	-	9/39/115/115	-
21	BCR	L	205	-	-	8/29/63/63	0/2/2/2
18	CLA	A	832	1	-	0/23/99/115	-
18	CLA	A	809	1	-	2/36/112/115	-
28	KC1	Q	210	13	-	2/15/71/71	-
18	CLA	B	812	2	-	2/26/102/115	-
18	CLA	A	813	1	-	2/21/97/115	-
20	LHG	R	201	-	-	31/53/53/53	-
18	CLA	B	829	30	-	1/39/115/115	-
18	CLA	R	205	14	-	11/39/115/115	-
29	A86	P	303	-	-	14/34/90/90	0/3/3/3
18	CLA	A	802	1	-	3/27/103/115	-
27	LMG	U	201	-	-	17/27/47/70	0/1/1/1
29	A86	U	202	-	-	14/34/90/90	0/3/3/3
18	CLA	U	210	16	-	8/39/115/115	-
18	CLA	T	207	17	-	1/12/88/115	-
24	DD6	T	213	-	-	12/26/80/80	0/3/3/3
22	CL0	A	848	1	-	1/39/115/115	-
24	DD6	O	213	-	-	5/26/80/80	0/3/3/3
18	CLA	S	215	15	-	4/39/115/115	-
18	CLA	A	830	1	-	0/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	803	6	-	4/17/93/115	-
18	CLA	O	205	11	-	6/39/115/115	-
18	CLA	A	818	30	-	3/39/115/115	-
18	CLA	B	833	-	-	5/39/115/115	-
19	PQN	B	836	-	-	1/23/43/43	0/2/2/2
18	CLA	A	812	1	-	1/15/91/115	-
28	KC1	P	302	12	-	1/15/71/71	-
18	CLA	A	816	1	-	2/39/115/115	-

All (1468) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Q	214	A86	C13-C11	-6.67	1.36	1.49
29	T	201	A86	C13-C11	-6.53	1.37	1.49
29	U	202	A86	C13-C11	-6.42	1.37	1.49
29	R	206	A86	C13-C11	-6.40	1.37	1.49
29	P	303	A86	C13-C11	-6.37	1.37	1.49
29	Q	201	A86	C13-C11	-6.18	1.37	1.49
29	R	204	A86	C13-C11	-5.90	1.38	1.49
22	A	848	CL0	MG-NC	5.50	2.19	2.06
22	A	848	CL0	MG-NA	5.35	2.19	2.06
18	A	826	CLA	MG-NA	5.20	2.18	2.06
18	B	843	CLA	MG-NA	5.19	2.18	2.06
18	B	845	CLA	MG-NA	5.17	2.18	2.06
28	P	305	KC1	MG-NC	5.17	2.18	2.06
18	U	207	CLA	C4C-C3C	-5.09	1.36	1.45
28	U	213	KC1	C4D-ND	-4.95	1.30	1.37
18	B	825	CLA	MG-NA	4.93	2.18	2.06
18	B	844	CLA	MG-NA	4.92	2.18	2.06
18	A	846	CLA	MG-NA	4.88	2.17	2.06
18	A	834	CLA	MG-NA	4.87	2.17	2.06
28	P	305	KC1	MG-NA	4.83	2.17	2.06
29	R	204	A86	C5-C6	4.76	1.42	1.35
18	S	205	CLA	MG-NA	4.71	2.17	2.06
18	B	806	CLA	MG-NA	4.70	2.17	2.06
28	S	210	KC1	C1C-C2C	-4.69	1.35	1.44
18	B	814	CLA	MG-NA	4.67	2.17	2.06
18	A	833	CLA	MG-NA	4.66	2.17	2.06
18	B	846	CLA	C4C-C3C	-4.66	1.37	1.45
18	A	812	CLA	MG-NA	4.66	2.17	2.06
18	A	825	CLA	MG-NA	4.65	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	204	CLA	MG-NA	4.64	2.17	2.06
18	B	831	CLA	C4C-C3C	-4.64	1.37	1.45
18	B	808	CLA	C4C-C3C	-4.64	1.37	1.45
18	T	211	CLA	C1C-C2C	-4.64	1.35	1.44
18	A	832	CLA	MG-NA	4.64	2.17	2.06
18	Q	212	CLA	C1C-C2C	-4.64	1.35	1.44
18	T	208	CLA	C4C-C3C	-4.63	1.37	1.45
28	P	305	KC1	MG-NB	4.63	2.15	2.05
18	B	810	CLA	MG-NA	4.62	2.17	2.06
28	P	311	KC1	C4A-C3A	-4.62	1.35	1.44
29	R	204	A86	C2-C1	4.62	1.41	1.35
28	Q	210	KC1	C4D-ND	-4.61	1.31	1.37
18	B	812	CLA	MG-NA	4.61	2.17	2.06
18	A	832	CLA	C4C-C3C	-4.60	1.37	1.45
18	P	310	CLA	C4C-C3C	-4.60	1.37	1.45
18	F	802	CLA	MG-NA	4.60	2.17	2.06
18	A	820	CLA	MG-NA	4.60	2.17	2.06
18	U	210	CLA	C4C-C3C	-4.59	1.37	1.45
28	Q	210	KC1	C4C-C3C	-4.58	1.37	1.45
18	R	205	CLA	C4C-C3C	-4.58	1.37	1.45
18	O	205	CLA	C4C-C3C	-4.58	1.37	1.45
18	B	804	CLA	C4C-C3C	-4.57	1.37	1.45
18	L	202	CLA	C4C-C3C	-4.57	1.37	1.45
18	B	824	CLA	MG-NA	4.57	2.17	2.06
18	B	848	CLA	C4C-C3C	-4.57	1.37	1.45
22	A	848	CL0	C4C-C3C	-4.56	1.37	1.45
18	B	835	CLA	C4C-C3C	-4.56	1.37	1.45
29	Q	201	A86	C2-C1	4.56	1.41	1.35
18	A	849	CLA	C4C-C3C	-4.55	1.37	1.45
18	A	819	CLA	C4C-C3C	-4.55	1.37	1.45
18	Q	212	CLA	MG-NA	4.54	2.17	2.06
18	U	205	CLA	C1C-C2C	-4.54	1.35	1.44
18	S	205	CLA	C4C-C3C	-4.54	1.37	1.45
18	B	818	CLA	C4C-C3C	-4.54	1.37	1.45
28	S	208	KC1	C4C-C3C	-4.53	1.37	1.45
18	A	823	CLA	MG-NA	4.53	2.17	2.06
18	B	813	CLA	C4C-C3C	-4.53	1.37	1.45
18	S	215	CLA	C4C-C3C	-4.53	1.37	1.45
18	B	827	CLA	C4C-C3C	-4.52	1.37	1.45
18	U	209	CLA	C4C-C3C	-4.52	1.37	1.45
18	A	823	CLA	C1C-C2C	-4.51	1.35	1.44
18	A	806	CLA	C4C-C3C	-4.51	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	O	209	CLA	C4C-C3C	-4.51	1.37	1.45
18	A	805	CLA	C4C-C3C	-4.51	1.37	1.45
28	T	209	KC1	MG-NA	4.51	2.17	2.06
18	B	802	CLA	C4C-C3C	-4.51	1.37	1.45
18	A	846	CLA	C4C-C3C	-4.51	1.37	1.45
18	B	817	CLA	C4C-C3C	-4.51	1.37	1.45
18	B	826	CLA	C4C-C3C	-4.51	1.37	1.45
18	A	805	CLA	MG-NA	4.51	2.17	2.06
18	A	808	CLA	C4C-C3C	-4.51	1.37	1.45
18	A	849	CLA	C1C-C2C	-4.50	1.35	1.44
18	B	810	CLA	C4C-C3C	-4.50	1.37	1.45
18	B	807	CLA	C4C-C3C	-4.50	1.37	1.45
18	P	307	CLA	C4C-C3C	-4.50	1.37	1.45
18	A	823	CLA	C4C-C3C	-4.50	1.37	1.45
18	U	206	CLA	C1C-C2C	-4.50	1.35	1.44
18	B	824	CLA	C4C-C3C	-4.49	1.37	1.45
18	B	822	CLA	MG-NA	4.49	2.16	2.06
18	O	206	CLA	C4C-C3C	-4.49	1.37	1.45
18	S	214	CLA	C4C-C3C	-4.49	1.37	1.45
18	B	801	CLA	C4C-C3C	-4.49	1.37	1.45
18	B	803	CLA	C4C-C3C	-4.49	1.37	1.45
18	B	803	CLA	C1C-C2C	-4.49	1.35	1.44
18	A	838	CLA	C4C-C3C	-4.49	1.37	1.45
18	Q	203	CLA	C1C-C2C	-4.48	1.35	1.44
18	L	203	CLA	C1C-C2C	-4.48	1.35	1.44
18	B	806	CLA	C4C-C3C	-4.48	1.37	1.45
18	A	813	CLA	C4C-C3C	-4.48	1.37	1.45
18	A	851	CLA	C1C-C2C	-4.48	1.35	1.44
18	U	205	CLA	C4C-C3C	-4.48	1.37	1.45
18	A	811	CLA	MG-NA	4.48	2.16	2.06
18	B	811	CLA	C1C-C2C	-4.48	1.35	1.44
18	S	204	CLA	C4C-C3C	-4.48	1.37	1.45
18	R	202	CLA	C4C-C3C	-4.48	1.37	1.45
28	U	213	KC1	C4C-C3C	-4.48	1.37	1.45
18	A	802	CLA	MG-NA	4.48	2.16	2.06
18	O	204	CLA	C4C-C3C	-4.47	1.37	1.45
18	B	822	CLA	C1C-C2C	-4.47	1.35	1.44
18	B	834	CLA	C4C-C3C	-4.47	1.37	1.45
18	A	825	CLA	C4C-C3C	-4.46	1.37	1.45
18	A	815	CLA	C4C-C3C	-4.46	1.37	1.45
18	Q	207	CLA	C4C-C3C	-4.46	1.37	1.45
18	A	817	CLA	C4C-C3C	-4.46	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	810	CLA	C4C-C3C	-4.46	1.37	1.45
18	B	826	CLA	MG-NA	4.46	2.16	2.06
18	B	805	CLA	C4C-C3C	-4.46	1.37	1.45
18	A	827	CLA	C1C-C2C	-4.46	1.35	1.44
18	B	804	CLA	MG-NA	4.46	2.16	2.06
18	A	807	CLA	C4C-C3C	-4.46	1.37	1.45
18	A	809	CLA	C4C-C3C	-4.46	1.37	1.45
18	A	814	CLA	C4C-C3C	-4.45	1.37	1.45
18	L	203	CLA	C4C-C3C	-4.45	1.37	1.45
18	B	834	CLA	C1C-C2C	-4.45	1.35	1.44
18	T	207	CLA	C4C-C3C	-4.45	1.37	1.45
18	A	829	CLA	C1C-C2C	-4.45	1.36	1.44
18	B	828	CLA	C4C-C3C	-4.45	1.37	1.45
18	A	828	CLA	C4C-C3C	-4.45	1.37	1.45
18	U	206	CLA	C4C-C3C	-4.45	1.37	1.45
18	P	308	CLA	C4C-C3C	-4.45	1.37	1.45
18	Q	206	CLA	C1C-C2C	-4.44	1.36	1.44
18	B	832	CLA	C4C-C3C	-4.44	1.37	1.45
18	F	803	CLA	C4C-C3C	-4.44	1.37	1.45
18	P	313	CLA	MG-NA	4.44	2.16	2.06
24	P	314	DD6	C10-C11	4.44	1.41	1.35
18	A	821	CLA	C4C-C3C	-4.44	1.37	1.45
18	B	822	CLA	C4C-C3C	-4.44	1.37	1.45
18	A	812	CLA	C4C-C3C	-4.44	1.37	1.45
18	B	821	CLA	C4C-C3C	-4.43	1.37	1.45
28	P	311	KC1	C1C-C2C	-4.43	1.36	1.44
24	P	316	DD6	C2-C1	4.43	1.41	1.35
28	O	210	KC1	C1C-C2C	-4.43	1.36	1.44
18	P	309	CLA	C4C-C3C	-4.43	1.37	1.45
28	Q	210	KC1	C1C-C2C	-4.43	1.36	1.44
18	A	822	CLA	C4C-C3C	-4.43	1.37	1.45
28	O	210	KC1	C4C-C3C	-4.43	1.37	1.45
18	O	203	CLA	C4C-C3C	-4.42	1.37	1.45
18	T	212	CLA	C4C-C3C	-4.42	1.37	1.45
18	B	820	CLA	C1C-C2C	-4.42	1.36	1.44
28	T	209	KC1	C4D-ND	-4.42	1.31	1.37
18	Q	206	CLA	C4C-C3C	-4.42	1.37	1.45
18	A	835	CLA	C4C-C3C	-4.42	1.37	1.45
18	A	834	CLA	MG-NC	4.42	2.16	2.06
24	P	316	DD6	C5-C6	4.42	1.41	1.35
18	A	825	CLA	C1C-C2C	-4.42	1.36	1.44
18	B	828	CLA	MG-NA	4.42	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	U	211	CLA	C4C-C3C	-4.42	1.37	1.45
18	B	832	CLA	MG-NA	4.42	2.16	2.06
18	A	818	CLA	C1C-C2C	-4.42	1.36	1.44
18	B	802	CLA	MG-NA	4.41	2.16	2.06
18	S	201	CLA	C4C-C3C	-4.41	1.37	1.45
18	B	816	CLA	C1C-C2C	-4.41	1.36	1.44
18	O	205	CLA	C1C-C2C	-4.41	1.36	1.44
18	A	851	CLA	C4C-C3C	-4.41	1.37	1.45
18	A	845	CLA	C4C-C3C	-4.40	1.37	1.45
18	A	830	CLA	C4C-C3C	-4.40	1.37	1.45
28	P	302	KC1	C1C-C2C	-4.40	1.36	1.44
18	A	824	CLA	C4C-C3C	-4.40	1.37	1.45
18	Q	209	CLA	C4C-C3C	-4.40	1.37	1.45
18	T	205	CLA	C4C-C3C	-4.40	1.37	1.45
18	B	819	CLA	C4C-C3C	-4.40	1.37	1.45
18	A	847	CLA	C1C-C2C	-4.40	1.36	1.44
18	B	812	CLA	C4C-C3C	-4.40	1.37	1.45
18	Q	216	CLA	C4C-C3C	-4.40	1.37	1.45
18	B	819	CLA	C1C-C2C	-4.40	1.36	1.44
18	A	829	CLA	C4C-C3C	-4.40	1.37	1.45
18	A	852	CLA	C4C-C3C	-4.40	1.37	1.45
18	A	803	CLA	C1C-C2C	-4.39	1.36	1.44
18	A	834	CLA	C1C-C2C	-4.39	1.36	1.44
18	A	826	CLA	C1C-C2C	-4.39	1.36	1.44
18	B	816	CLA	C4C-C3C	-4.39	1.37	1.45
18	R	205	CLA	MG-NA	4.39	2.16	2.06
18	A	807	CLA	C1C-C2C	-4.39	1.36	1.44
18	B	828	CLA	C1C-C2C	-4.39	1.36	1.44
28	P	305	KC1	C1C-C2C	-4.39	1.36	1.44
24	S	203	DD6	C10-C11	4.39	1.41	1.35
18	A	801	CLA	C1C-C2C	-4.39	1.36	1.44
18	A	827	CLA	C4C-C3C	-4.39	1.37	1.45
18	A	818	CLA	C4C-C3C	-4.39	1.37	1.45
18	B	811	CLA	C4C-C3C	-4.39	1.37	1.45
18	O	211	CLA	C1C-C2C	-4.39	1.36	1.44
18	T	203	CLA	C4C-C3C	-4.38	1.37	1.45
18	F	802	CLA	C4C-C3C	-4.38	1.37	1.45
18	A	836	CLA	C4C-C3C	-4.38	1.37	1.45
18	T	204	CLA	C4C-C3C	-4.38	1.37	1.45
28	T	209	KC1	C1C-C2C	-4.38	1.36	1.44
18	B	815	CLA	C4C-C3C	-4.38	1.37	1.45
18	L	204	CLA	C4C-C3C	-4.38	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	314	DD6	C2-C1	4.38	1.41	1.35
28	O	210	KC1	C4D-ND	-4.38	1.31	1.37
18	B	808	CLA	C1C-C2C	-4.38	1.36	1.44
18	Q	204	CLA	C1C-C2C	-4.38	1.36	1.44
18	J	103	CLA	C4C-C3C	-4.37	1.37	1.45
18	A	833	CLA	C4C-C3C	-4.37	1.37	1.45
18	P	315	CLA	C4C-C3C	-4.37	1.37	1.45
18	A	820	CLA	C1C-C2C	-4.37	1.36	1.44
18	P	306	CLA	C4C-C3C	-4.37	1.37	1.45
18	Q	205	CLA	C4C-C3C	-4.37	1.37	1.45
18	A	811	CLA	C1C-C2C	-4.37	1.36	1.44
18	A	819	CLA	C1C-C2C	-4.37	1.36	1.44
18	U	204	CLA	C1C-C2C	-4.37	1.36	1.44
18	B	835	CLA	MG-NA	4.36	2.16	2.06
18	A	802	CLA	C4C-C3C	-4.36	1.37	1.45
18	A	846	CLA	C1C-C2C	-4.36	1.36	1.44
18	B	823	CLA	C4C-C3C	-4.36	1.37	1.45
18	P	309	CLA	C1C-C2C	-4.36	1.36	1.44
24	P	314	DD6	C5-C6	4.36	1.41	1.35
18	B	827	CLA	C1C-C2C	-4.36	1.36	1.44
18	A	804	CLA	C1C-C2C	-4.36	1.36	1.44
18	A	831	CLA	C4C-C3C	-4.36	1.37	1.45
18	P	306	CLA	C1C-C2C	-4.36	1.36	1.44
18	A	847	CLA	C4C-C3C	-4.36	1.37	1.45
18	Q	213	CLA	C1C-C2C	-4.36	1.36	1.44
18	P	312	CLA	C1C-C2C	-4.36	1.36	1.44
18	S	204	CLA	C1C-C2C	-4.35	1.36	1.44
18	B	809	CLA	C4C-C3C	-4.35	1.37	1.45
18	A	833	CLA	C1C-C2C	-4.35	1.36	1.44
18	Q	209	CLA	C1C-C2C	-4.35	1.36	1.44
18	A	830	CLA	C1C-C2C	-4.35	1.36	1.44
18	B	814	CLA	C1C-C2C	-4.35	1.36	1.44
18	O	208	CLA	C1C-C2C	-4.35	1.36	1.44
28	P	305	KC1	C4A-C3A	-4.35	1.36	1.44
18	A	827	CLA	MG-NA	4.35	2.16	2.06
18	B	813	CLA	C1C-C2C	-4.35	1.36	1.44
18	P	307	CLA	C1C-C2C	-4.35	1.36	1.44
18	B	809	CLA	C1C-C2C	-4.34	1.36	1.44
18	A	813	CLA	C1C-C2C	-4.34	1.36	1.44
18	B	844	CLA	C1C-C2C	-4.34	1.36	1.44
18	A	835	CLA	MG-NA	4.34	2.16	2.06
18	A	821	CLA	MG-NA	4.34	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	833	CLA	C1C-C2C	-4.34	1.36	1.44
18	U	210	CLA	C1C-C2C	-4.34	1.36	1.44
18	U	204	CLA	C4C-C3C	-4.34	1.37	1.45
18	B	815	CLA	C1C-C2C	-4.34	1.36	1.44
18	A	809	CLA	C1C-C2C	-4.34	1.36	1.44
18	A	815	CLA	MG-NA	4.33	2.16	2.06
18	T	205	CLA	C1C-C2C	-4.33	1.36	1.44
18	A	810	CLA	C1C-C2C	-4.33	1.36	1.44
18	P	308	CLA	C1C-C2C	-4.33	1.36	1.44
18	B	820	CLA	C4C-C3C	-4.33	1.37	1.45
18	A	831	CLA	C1C-C2C	-4.33	1.36	1.44
18	Q	208	CLA	C4C-C3C	-4.33	1.37	1.45
18	O	202	CLA	C1C-C2C	-4.33	1.36	1.44
18	P	313	CLA	C4C-C3C	-4.33	1.37	1.45
18	Q	205	CLA	C1C-C2C	-4.33	1.36	1.44
18	A	801	CLA	C4C-C3C	-4.33	1.37	1.45
18	U	207	CLA	C1C-C2C	-4.33	1.36	1.44
18	Q	212	CLA	C4C-C3C	-4.33	1.37	1.45
18	A	834	CLA	C4C-C3C	-4.33	1.37	1.45
18	A	853	CLA	C4C-C3C	-4.33	1.37	1.45
22	A	848	CL0	C1C-C2C	-4.32	1.36	1.44
18	T	202	CLA	C4C-C3C	-4.32	1.37	1.45
18	B	833	CLA	C4C-C3C	-4.32	1.37	1.45
18	Q	213	CLA	C4C-C3C	-4.32	1.37	1.45
24	T	214	DD6	C5-C6	4.32	1.41	1.35
18	S	206	CLA	C1C-C2C	-4.32	1.36	1.44
24	T	213	DD6	C5-C6	4.32	1.41	1.35
28	O	210	KC1	C4A-C3A	-4.32	1.36	1.44
28	P	311	KC1	C4D-ND	-4.32	1.31	1.37
18	A	816	CLA	C4C-C3C	-4.31	1.37	1.45
18	T	203	CLA	C1C-C2C	-4.31	1.36	1.44
18	O	203	CLA	C1C-C2C	-4.31	1.36	1.44
18	T	212	CLA	C1C-C2C	-4.31	1.36	1.44
18	T	206	CLA	C4C-C3C	-4.31	1.37	1.45
28	S	208	KC1	C4D-ND	-4.31	1.31	1.37
18	S	205	CLA	C1C-C2C	-4.31	1.36	1.44
18	A	813	CLA	MG-NA	4.31	2.16	2.06
18	T	210	CLA	C4C-C3C	-4.31	1.37	1.45
18	B	825	CLA	C4C-C3C	-4.30	1.37	1.45
18	L	202	CLA	C1C-C2C	-4.30	1.36	1.44
18	T	204	CLA	C1C-C2C	-4.30	1.36	1.44
18	B	824	CLA	C1C-C2C	-4.30	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	845	CLA	C4C-C3C	-4.30	1.37	1.45
18	O	207	CLA	C1C-C2C	-4.30	1.36	1.44
18	B	848	CLA	C1C-C2C	-4.30	1.36	1.44
28	S	208	KC1	C1C-C2C	-4.30	1.36	1.44
18	O	202	CLA	C4C-C3C	-4.30	1.37	1.45
18	O	211	CLA	C4C-C3C	-4.30	1.37	1.45
18	A	803	CLA	C4C-C3C	-4.29	1.37	1.45
18	A	838	CLA	C1C-C2C	-4.29	1.36	1.44
18	A	852	CLA	C1C-C2C	-4.29	1.36	1.44
18	U	211	CLA	C1C-C2C	-4.29	1.36	1.44
18	S	207	CLA	C4C-C3C	-4.29	1.37	1.45
18	B	830	CLA	MG-NA	4.29	2.16	2.06
18	O	204	CLA	C1C-C2C	-4.29	1.36	1.44
18	A	816	CLA	C1C-C2C	-4.29	1.36	1.44
18	B	805	CLA	C1C-C2C	-4.29	1.36	1.44
18	A	808	CLA	C1C-C2C	-4.29	1.36	1.44
18	S	215	CLA	C1C-C2C	-4.29	1.36	1.44
18	A	832	CLA	C1C-C2C	-4.29	1.36	1.44
18	Q	207	CLA	C1C-C2C	-4.29	1.36	1.44
18	S	206	CLA	C4C-C3C	-4.28	1.37	1.45
18	B	816	CLA	MG-NA	4.28	2.16	2.06
18	A	828	CLA	MG-NA	4.28	2.16	2.06
18	B	844	CLA	C4C-C3C	-4.28	1.37	1.45
18	A	849	CLA	MG-NA	4.28	2.16	2.06
18	J	103	CLA	C1C-C2C	-4.28	1.36	1.44
18	A	812	CLA	C1C-C2C	-4.28	1.36	1.44
18	Q	211	CLA	C1C-C2C	-4.28	1.36	1.44
18	P	313	CLA	C1C-C2C	-4.28	1.36	1.44
18	Q	211	CLA	C4C-C3C	-4.28	1.37	1.45
18	B	843	CLA	C1C-C2C	-4.27	1.36	1.44
18	S	214	CLA	C1C-C2C	-4.27	1.36	1.44
18	B	830	CLA	C1C-C2C	-4.27	1.36	1.44
18	Q	216	CLA	C1C-C2C	-4.27	1.36	1.44
18	A	820	CLA	C4C-C3C	-4.27	1.37	1.45
18	B	807	CLA	C1C-C2C	-4.27	1.36	1.44
18	U	208	CLA	C1C-C2C	-4.27	1.36	1.44
18	Q	203	CLA	C4C-C3C	-4.27	1.37	1.45
18	A	817	CLA	C1C-C2C	-4.27	1.36	1.44
18	F	803	CLA	C1C-C2C	-4.27	1.36	1.44
18	B	814	CLA	C4C-C3C	-4.27	1.37	1.45
18	T	206	CLA	C1C-C2C	-4.26	1.36	1.44
18	O	209	CLA	C1C-C2C	-4.26	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	804	CLA	C4C-C3C	-4.26	1.37	1.45
18	B	845	CLA	C1C-C2C	-4.26	1.36	1.44
18	A	826	CLA	C4C-C3C	-4.26	1.37	1.45
18	A	829	CLA	MG-NA	4.26	2.16	2.06
18	P	315	CLA	C1C-C2C	-4.26	1.36	1.44
18	T	202	CLA	C1C-C2C	-4.26	1.36	1.44
18	B	810	CLA	C1C-C2C	-4.26	1.36	1.44
18	O	206	CLA	C1C-C2C	-4.25	1.36	1.44
18	B	829	CLA	C1C-C2C	-4.25	1.36	1.44
18	R	205	CLA	C1C-C2C	-4.25	1.36	1.44
18	B	830	CLA	C4C-C3C	-4.25	1.37	1.45
28	P	302	KC1	C4A-C3A	-4.25	1.36	1.44
18	A	851	CLA	MG-NA	4.25	2.16	2.06
24	S	203	DD6	C5-C6	4.25	1.41	1.35
18	Q	204	CLA	C4C-C3C	-4.24	1.37	1.45
18	A	853	CLA	C1C-C2C	-4.24	1.36	1.44
18	A	806	CLA	C1C-C2C	-4.24	1.36	1.44
28	T	209	KC1	C4C-C3C	-4.24	1.37	1.45
18	A	814	CLA	C1C-C2C	-4.24	1.36	1.44
18	B	832	CLA	C1C-C2C	-4.24	1.36	1.44
18	P	312	CLA	C4C-C3C	-4.23	1.37	1.45
18	A	821	CLA	C1C-C2C	-4.23	1.36	1.44
18	B	801	CLA	C1C-C2C	-4.23	1.36	1.44
18	B	813	CLA	MG-NA	4.23	2.16	2.06
18	O	208	CLA	C4C-C3C	-4.23	1.37	1.45
18	J	103	CLA	MG-NA	4.23	2.16	2.06
18	U	209	CLA	MG-NA	4.23	2.16	2.06
18	B	817	CLA	C1C-C2C	-4.23	1.36	1.44
18	Q	208	CLA	C1C-C2C	-4.22	1.36	1.44
18	A	811	CLA	C4C-C3C	-4.22	1.37	1.45
18	B	812	CLA	C1C-C2C	-4.22	1.36	1.44
18	U	209	CLA	C1C-C2C	-4.22	1.36	1.44
18	B	826	CLA	C1C-C2C	-4.22	1.36	1.44
18	O	207	CLA	C4C-C3C	-4.22	1.37	1.45
18	B	821	CLA	C1C-C2C	-4.22	1.36	1.44
18	B	823	CLA	MG-NA	4.22	2.16	2.06
18	A	805	CLA	C1C-C2C	-4.22	1.36	1.44
18	B	801	CLA	MG-NA	4.21	2.16	2.06
18	B	814	CLA	MG-NC	4.21	2.16	2.06
18	A	828	CLA	C1C-C2C	-4.21	1.36	1.44
18	B	829	CLA	C4C-C3C	-4.21	1.37	1.45
18	A	822	CLA	C1C-C2C	-4.21	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	846	CLA	C1C-C2C	-4.21	1.36	1.44
18	B	827	CLA	MG-NA	4.20	2.16	2.06
18	T	207	CLA	C1C-C2C	-4.20	1.36	1.44
18	A	815	CLA	C1C-C2C	-4.20	1.36	1.44
18	P	310	CLA	C1C-C2C	-4.20	1.36	1.44
18	B	833	CLA	MG-NA	4.19	2.16	2.06
18	R	202	CLA	C1C-C2C	-4.19	1.36	1.44
18	S	207	CLA	C1C-C2C	-4.19	1.36	1.44
18	A	836	CLA	C1C-C2C	-4.19	1.36	1.44
18	B	823	CLA	C1C-C2C	-4.19	1.36	1.44
28	S	210	KC1	C4D-ND	-4.19	1.31	1.37
18	B	818	CLA	C1C-C2C	-4.19	1.36	1.44
18	F	802	CLA	C1C-C2C	-4.19	1.36	1.44
28	U	213	KC1	C1C-C2C	-4.19	1.36	1.44
18	B	806	CLA	C1C-C2C	-4.18	1.36	1.44
29	P	303	A86	C2-C1	4.18	1.41	1.35
24	P	317	DD6	C10-C11	4.18	1.41	1.35
18	A	802	CLA	C1C-C2C	-4.18	1.36	1.44
18	L	204	CLA	C1C-C2C	-4.18	1.36	1.44
18	B	807	CLA	MG-NA	4.17	2.16	2.06
18	Q	207	CLA	MG-NA	4.17	2.16	2.06
18	A	853	CLA	MG-NA	4.17	2.16	2.06
18	A	835	CLA	C1C-C2C	-4.17	1.36	1.44
18	A	807	CLA	MG-NA	4.17	2.16	2.06
18	B	831	CLA	C1C-C2C	-4.16	1.36	1.44
28	P	305	KC1	C4D-ND	-4.16	1.32	1.37
18	B	804	CLA	C1C-C2C	-4.16	1.36	1.44
29	Q	201	A86	C5-C6	4.15	1.41	1.35
24	P	316	DD6	C10-C11	4.15	1.41	1.35
18	T	202	CLA	MG-NA	4.15	2.16	2.06
18	T	210	CLA	C1C-C2C	-4.14	1.36	1.44
18	B	825	CLA	C1C-C2C	-4.14	1.36	1.44
24	T	213	DD6	C10-C11	4.14	1.41	1.35
28	P	311	KC1	C4C-C3C	-4.14	1.37	1.45
24	S	213	DD6	C26-C27	4.13	1.45	1.37
28	P	305	KC1	C4C-C3C	-4.13	1.37	1.45
24	O	201	DD6	C10-C11	4.13	1.41	1.35
18	U	211	CLA	MG-NA	4.12	2.16	2.06
24	U	203	DD6	C5-C6	4.12	1.41	1.35
18	Q	206	CLA	MG-NA	4.12	2.16	2.06
18	B	802	CLA	MG-NC	4.11	2.16	2.06
18	B	802	CLA	C1C-C2C	-4.11	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	O	201	DD6	C5-C6	4.11	1.41	1.35
18	A	809	CLA	MG-NA	4.10	2.16	2.06
28	S	210	KC1	C4C-C3C	-4.10	1.38	1.45
28	Q	210	KC1	C4A-C3A	-4.10	1.36	1.44
18	A	846	CLA	MG-NC	4.10	2.16	2.06
24	S	203	DD6	C2-C1	4.10	1.41	1.35
18	B	843	CLA	C4C-C3C	-4.09	1.38	1.45
24	U	203	DD6	C10-C11	4.09	1.41	1.35
18	U	208	CLA	C4C-C3C	-4.09	1.38	1.45
18	S	201	CLA	C1C-C2C	-4.08	1.36	1.44
28	P	302	KC1	MG-NA	4.07	2.15	2.06
24	U	212	DD6	C2-C1	4.07	1.41	1.35
18	P	315	CLA	MG-NA	4.07	2.15	2.06
18	L	202	CLA	MG-NA	4.06	2.15	2.06
18	O	203	CLA	MG-NA	4.05	2.15	2.06
28	S	208	KC1	C4A-C3A	-4.04	1.36	1.44
28	S	210	KC1	C4A-C3A	-4.03	1.36	1.44
18	B	835	CLA	C1C-C2C	-4.03	1.36	1.44
18	A	816	CLA	MG-NA	4.02	2.15	2.06
29	Q	201	A86	C26-C27	4.02	1.41	1.35
18	A	845	CLA	MG-NA	4.02	2.15	2.06
24	P	317	DD6	C5-C6	4.01	1.41	1.35
28	S	210	KC1	C3B-C4B	-4.01	1.38	1.46
18	A	824	CLA	C1C-C2C	-4.00	1.36	1.44
28	O	210	KC1	C3B-C4B	-4.00	1.38	1.46
24	S	213	DD6	C5-C6	4.00	1.41	1.35
28	P	302	KC1	C4C-C3C	-4.00	1.38	1.45
28	P	302	KC1	C4D-ND	-3.99	1.32	1.37
24	O	214	DD6	C10-C11	3.99	1.41	1.35
24	S	213	DD6	C2-C1	3.99	1.41	1.35
24	O	215	DD6	C10-C11	3.98	1.41	1.35
18	A	817	CLA	MG-NA	3.98	2.15	2.06
18	B	808	CLA	MG-NA	3.98	2.15	2.06
18	O	207	CLA	MG-NA	3.98	2.15	2.06
18	P	306	CLA	MG-NA	3.98	2.15	2.06
18	T	208	CLA	C1C-C2C	-3.97	1.36	1.44
18	A	808	CLA	MG-NA	3.97	2.15	2.06
24	S	213	DD6	C10-C11	3.97	1.41	1.35
24	O	201	DD6	C2-C1	3.97	1.41	1.35
18	O	205	CLA	MG-NA	3.97	2.15	2.06
18	T	211	CLA	C4C-C3C	-3.97	1.38	1.45
24	J	101	DD6	C10-C11	3.97	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	O	211	CLA	MG-NA	3.96	2.15	2.06
18	L	204	CLA	MG-NA	3.96	2.15	2.06
18	A	845	CLA	C1C-C2C	-3.95	1.36	1.44
18	A	824	CLA	MG-NA	3.95	2.15	2.06
28	P	302	KC1	C1B-C2B	-3.94	1.37	1.45
28	P	311	KC1	C1B-C2B	-3.94	1.37	1.45
18	O	202	CLA	MG-NA	3.94	2.15	2.06
28	U	213	KC1	C3B-C4B	-3.94	1.39	1.46
24	O	214	DD6	C2-C1	3.94	1.41	1.35
18	B	809	CLA	MG-NA	3.93	2.15	2.06
24	U	214	DD6	C2-C1	3.93	1.41	1.35
18	A	852	CLA	MG-NA	3.91	2.15	2.06
28	P	305	KC1	C3B-C4B	-3.90	1.39	1.46
18	B	818	CLA	MG-NA	3.89	2.15	2.06
18	B	831	CLA	MG-NA	3.89	2.15	2.06
18	B	820	CLA	MG-NA	3.89	2.15	2.06
28	S	208	KC1	C1B-C2B	-3.88	1.37	1.45
18	P	307	CLA	MG-NA	3.88	2.15	2.06
24	U	212	DD6	C5-C6	3.87	1.40	1.35
18	B	848	CLA	MG-NA	3.86	2.15	2.06
29	Q	214	A86	C2-C1	3.85	1.40	1.35
24	Q	202	DD6	C10-C11	3.85	1.40	1.35
18	Q	204	CLA	MG-NA	3.85	2.15	2.06
18	O	209	CLA	MG-NA	3.85	2.15	2.06
29	T	201	A86	C5-C6	3.84	1.40	1.35
29	P	303	A86	C5-C6	3.83	1.40	1.35
24	U	203	DD6	C2-C1	3.82	1.40	1.35
28	P	305	KC1	MG-ND	3.82	2.13	2.05
28	T	209	KC1	C4A-C3A	-3.82	1.37	1.44
24	Q	215	DD6	C10-C11	3.82	1.40	1.35
24	Q	202	DD6	C5-C6	3.81	1.40	1.35
18	A	814	CLA	MG-NA	3.81	2.15	2.06
18	A	827	CLA	MG-NC	3.81	2.15	2.06
18	O	204	CLA	MG-NA	3.79	2.15	2.06
18	F	803	CLA	MG-NA	3.79	2.15	2.06
18	A	830	CLA	MG-NA	3.78	2.15	2.06
29	T	201	A86	C2-C1	3.78	1.40	1.35
18	T	211	CLA	MG-NA	3.77	2.15	2.06
18	U	204	CLA	MG-NA	3.77	2.15	2.06
18	A	819	CLA	MG-NA	3.77	2.15	2.06
28	P	302	KC1	C3B-C4B	-3.77	1.39	1.46
28	S	208	KC1	C3B-C4B	-3.76	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	209	KC1	C3B-C4B	-3.76	1.39	1.46
18	A	847	CLA	MG-NA	3.76	2.15	2.06
28	Q	210	KC1	C3B-C4B	-3.75	1.39	1.46
28	Q	210	KC1	C1B-C2B	-3.75	1.37	1.45
28	P	311	KC1	C3B-C4B	-3.75	1.39	1.46
18	U	208	CLA	MG-NA	3.75	2.15	2.06
24	J	101	DD6	C2-C1	3.74	1.40	1.35
18	A	836	CLA	MG-NA	3.74	2.15	2.06
24	Q	202	DD6	C2-C1	3.74	1.40	1.35
18	Q	213	CLA	MG-NA	3.74	2.15	2.06
24	S	212	DD6	C10-C11	3.74	1.40	1.35
24	O	212	DD6	C2-C1	3.74	1.40	1.35
28	U	213	KC1	C4A-C3A	-3.73	1.37	1.44
18	A	801	CLA	MG-NA	3.73	2.15	2.06
28	T	209	KC1	C1B-C2B	-3.73	1.38	1.45
18	T	212	CLA	MG-NA	3.73	2.15	2.06
18	P	308	CLA	MG-NA	3.73	2.15	2.06
18	S	204	CLA	MG-NA	3.73	2.15	2.06
24	Q	215	DD6	C2-C1	3.73	1.40	1.35
18	B	823	CLA	MG-NC	3.72	2.15	2.06
18	U	206	CLA	MG-NA	3.72	2.15	2.06
24	U	212	DD6	C10-C11	3.72	1.40	1.35
24	Q	215	DD6	C5-C6	3.71	1.40	1.35
18	B	834	CLA	MG-NA	3.71	2.15	2.06
18	B	819	CLA	MG-NA	3.71	2.15	2.06
24	U	203	DD6	C26-C27	3.71	1.44	1.37
18	Q	208	CLA	MG-NA	3.71	2.15	2.06
24	O	201	DD6	C26-C27	3.70	1.44	1.37
18	R	202	CLA	MG-NA	3.69	2.15	2.06
29	P	303	A86	C26-C27	3.69	1.40	1.35
24	A	854	DD6	C10-C11	3.69	1.40	1.35
18	B	805	CLA	MG-NA	3.68	2.15	2.06
18	B	826	CLA	MG-NC	3.66	2.15	2.06
24	O	212	DD6	C10-C11	3.66	1.40	1.35
28	S	210	KC1	C1B-C2B	-3.66	1.38	1.45
18	B	829	CLA	MG-NA	3.65	2.14	2.06
18	A	810	CLA	MG-NA	3.64	2.14	2.06
18	A	818	CLA	MG-NA	3.64	2.14	2.06
28	O	210	KC1	C1B-C2B	-3.64	1.38	1.45
24	T	213	DD6	C2-C1	3.63	1.40	1.35
24	S	202	DD6	C5-C6	3.62	1.40	1.35
18	T	207	CLA	MG-NA	3.62	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	214	DD6	C10-C11	3.62	1.40	1.35
28	U	213	KC1	MG-NA	3.62	2.14	2.06
24	O	215	DD6	C5-C6	3.61	1.40	1.35
18	B	834	CLA	MG-NC	3.61	2.14	2.06
24	S	202	DD6	C2-C1	3.61	1.40	1.35
18	T	205	CLA	MG-NA	3.60	2.14	2.06
24	O	213	DD6	C5-C6	3.60	1.40	1.35
18	B	811	CLA	MG-NA	3.60	2.14	2.06
29	U	202	A86	C2-C1	3.60	1.40	1.35
24	O	212	DD6	C26-C27	3.58	1.44	1.37
18	S	214	CLA	MG-NA	3.58	2.14	2.06
18	Q	211	CLA	MG-NA	3.58	2.14	2.06
18	Q	216	CLA	MG-NA	3.58	2.14	2.06
18	P	309	CLA	MG-NA	3.56	2.14	2.06
18	B	843	CLA	MG-NC	3.55	2.14	2.06
18	U	205	CLA	MG-NA	3.55	2.14	2.06
24	S	202	DD6	C10-C11	3.55	1.40	1.35
18	Q	203	CLA	MG-NA	3.55	2.14	2.06
29	R	206	A86	C2-C1	3.54	1.40	1.35
18	T	206	CLA	MG-NA	3.53	2.14	2.06
18	P	310	CLA	MG-NA	3.53	2.14	2.06
18	P	312	CLA	MG-NA	3.53	2.14	2.06
29	U	202	A86	C5-C6	3.53	1.40	1.35
18	A	804	CLA	MG-NA	3.52	2.14	2.06
18	A	826	CLA	MG-NC	3.51	2.14	2.06
18	B	815	CLA	MG-NA	3.50	2.14	2.06
29	R	204	A86	C26-C27	3.50	1.40	1.35
29	Q	214	A86	C5-C6	3.50	1.40	1.35
24	O	215	DD6	C2-C1	3.49	1.40	1.35
18	S	215	CLA	MG-NA	3.49	2.14	2.06
24	O	214	DD6	C5-C6	3.48	1.40	1.35
24	S	212	DD6	C5-C6	3.48	1.40	1.35
24	J	101	DD6	C5-C6	3.48	1.40	1.35
18	O	206	CLA	MG-NA	3.48	2.14	2.06
18	T	210	CLA	MG-NA	3.47	2.14	2.06
24	S	209	DD6	C10-C11	3.47	1.40	1.35
24	S	212	DD6	C2-C1	3.46	1.40	1.35
28	U	213	KC1	C1B-C2B	-3.45	1.38	1.45
24	S	209	DD6	C5-C6	3.45	1.40	1.35
24	O	212	DD6	C5-C6	3.44	1.40	1.35
18	S	207	CLA	MG-NA	3.44	2.14	2.06
24	A	854	DD6	C5-C6	3.43	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	209	CLA	MG-NA	3.42	2.14	2.06
29	R	206	A86	C5-C6	3.42	1.40	1.35
18	B	817	CLA	MG-NA	3.41	2.14	2.06
28	P	305	KC1	C1B-C2B	-3.41	1.38	1.45
18	U	210	CLA	MG-NA	3.40	2.14	2.06
24	P	304	DD6	C10-C11	3.40	1.40	1.35
18	T	203	CLA	MG-NA	3.40	2.14	2.06
18	A	831	CLA	MG-NA	3.39	2.14	2.06
18	B	846	CLA	MG-NA	3.39	2.14	2.06
24	S	203	DD6	C26-C27	3.38	1.44	1.37
18	L	203	CLA	MG-NA	3.36	2.14	2.06
18	A	806	CLA	MG-NA	3.35	2.14	2.06
18	S	201	CLA	MG-NA	3.34	2.14	2.06
28	O	210	KC1	MG-NA	3.34	2.14	2.06
28	P	311	KC1	MG-NA	3.33	2.14	2.06
24	P	304	DD6	C5-C6	3.33	1.40	1.35
24	U	214	DD6	C8-C6	-3.33	1.41	1.50
18	A	838	CLA	MG-NA	3.31	2.14	2.06
18	B	803	CLA	MG-NA	3.31	2.14	2.06
18	Q	205	CLA	MG-NA	3.29	2.14	2.06
18	T	208	CLA	MG-NA	3.28	2.14	2.06
21	B	837	BCR	C1-C6	-3.28	1.49	1.53
21	R	203	BCR	C30-C25	-3.28	1.49	1.53
24	O	213	DD6	C10-C11	3.27	1.40	1.35
18	A	803	CLA	MG-NA	3.27	2.14	2.06
27	P	301	LMG	C4-C5	3.27	1.59	1.53
18	B	844	CLA	MG-NC	3.26	2.14	2.06
18	O	208	CLA	MG-NA	3.26	2.14	2.06
18	A	828	CLA	MG-NC	3.26	2.14	2.06
18	A	835	CLA	MG-NC	3.25	2.14	2.06
18	S	206	CLA	MG-NA	3.23	2.13	2.06
24	A	854	DD6	C2-C1	3.22	1.40	1.35
18	B	825	CLA	MG-NC	3.22	2.13	2.06
21	R	203	BCR	C1-C6	-3.21	1.49	1.53
18	B	830	CLA	MG-NC	3.18	2.13	2.06
24	U	214	DD6	C26-C27	3.18	1.43	1.37
28	S	208	KC1	MG-NA	3.17	2.13	2.06
18	B	810	CLA	MG-NC	3.16	2.13	2.06
24	S	209	DD6	C2-C1	3.16	1.40	1.35
18	A	802	CLA	MG-NC	3.14	2.13	2.06
24	T	214	DD6	C26-C27	3.14	1.43	1.37
29	T	201	A86	C26-C27	3.14	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	808	CLA	MG-NC	3.13	2.13	2.06
21	A	844	BCR	C1-C6	-3.12	1.49	1.53
18	A	822	CLA	MG-NA	3.12	2.13	2.06
24	P	316	DD6	C26-C27	3.11	1.43	1.37
24	P	314	DD6	C26-C27	3.11	1.43	1.37
24	O	213	DD6	C2-C1	3.08	1.39	1.35
28	S	210	KC1	MG-NA	3.08	2.13	2.06
24	P	304	DD6	C2-C1	3.07	1.39	1.35
21	J	104	BCR	C30-C25	-3.06	1.49	1.53
29	Q	214	A86	C26-C27	3.05	1.39	1.35
24	Q	215	DD6	C26-C27	3.04	1.43	1.37
24	O	213	DD6	C24-C1	-3.03	1.39	1.45
24	T	214	DD6	C2-C1	3.02	1.39	1.35
18	A	833	CLA	MG-NC	3.02	2.13	2.06
24	Q	202	DD6	C26-C27	3.01	1.43	1.37
18	A	812	CLA	MG-NC	3.00	2.13	2.06
26	B	847	SQD	O48-C23	3.00	1.42	1.33
26	M	102	SQD	O48-C23	3.00	1.42	1.33
28	T	209	KC1	MG-NC	2.98	2.13	2.06
18	A	821	CLA	MG-NC	2.98	2.13	2.06
21	B	838	BCR	C1-C6	-2.96	1.49	1.53
18	B	806	CLA	MG-NC	2.96	2.13	2.06
18	B	821	CLA	MG-NA	2.95	2.13	2.06
28	Q	210	KC1	MG-NA	2.93	2.13	2.06
18	B	817	CLA	C1B-C2B	-2.93	1.36	1.43
21	L	201	BCR	C1-C6	-2.92	1.49	1.53
18	A	811	CLA	MG-NC	2.92	2.13	2.06
18	A	805	CLA	MG-NC	2.90	2.13	2.06
24	S	202	DD6	C26-C27	2.90	1.43	1.37
21	L	205	BCR	C30-C25	-2.89	1.49	1.53
18	A	849	CLA	MG-NC	2.88	2.13	2.06
24	T	213	DD6	C26-C27	2.85	1.43	1.37
27	B	849	LMG	O1-C7	-2.85	1.38	1.43
21	I	101	BCR	C1-C6	-2.84	1.49	1.53
18	Q	212	CLA	MG-NC	2.84	2.13	2.06
21	B	841	BCR	C30-C25	-2.83	1.49	1.53
21	A	842	BCR	C30-C25	-2.83	1.49	1.53
21	A	843	BCR	C1-C6	-2.83	1.49	1.53
18	A	820	CLA	MG-NC	2.82	2.13	2.06
18	B	831	CLA	MG-NC	2.82	2.13	2.06
18	R	205	CLA	MG-NC	2.82	2.13	2.06
18	A	808	CLA	MG-NC	2.81	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	204	CLA	MG-NC	2.81	2.13	2.06
24	P	317	DD6	C3-C4	2.81	1.39	1.32
21	A	842	BCR	C1-C6	-2.79	1.49	1.53
26	M	102	SQD	O47-C7	2.78	1.42	1.34
24	P	304	DD6	C26-C27	2.78	1.42	1.37
21	L	201	BCR	C30-C25	-2.76	1.50	1.53
18	B	845	CLA	MG-NC	2.76	2.12	2.06
24	A	854	DD6	C26-C27	2.75	1.42	1.37
18	B	844	CLA	C3D-C4D	-2.74	1.38	1.44
18	B	817	CLA	C1D-C2D	-2.73	1.39	1.45
25	B	842	DGD	O1G-C1G	-2.73	1.38	1.45
18	F	802	CLA	MG-NC	2.73	2.12	2.06
18	A	816	CLA	MG-NC	2.73	2.12	2.06
21	B	839	BCR	C1-C6	-2.73	1.50	1.53
18	R	205	CLA	C3D-C4D	-2.73	1.38	1.44
18	B	824	CLA	MG-NC	2.73	2.12	2.06
24	P	304	DD6	C13-C11	-2.73	1.40	1.45
18	A	824	CLA	MG-NC	2.72	2.12	2.06
18	B	807	CLA	MG-NC	2.72	2.12	2.06
18	Q	211	CLA	C3D-C4D	-2.72	1.38	1.44
18	B	813	CLA	MG-NC	2.72	2.12	2.06
24	T	214	DD6	C8-C6	-2.72	1.40	1.45
18	P	313	CLA	MG-NC	2.71	2.12	2.06
28	P	302	KC1	C2A-C3A	2.71	1.42	1.37
21	L	205	BCR	C1-C6	-2.71	1.50	1.53
18	P	307	CLA	C3D-C4D	-2.71	1.38	1.44
24	O	215	DD6	C26-C27	2.71	1.42	1.37
18	B	812	CLA	MG-NC	2.71	2.12	2.06
18	B	817	CLA	C1B-NB	-2.71	1.34	1.37
29	U	202	A86	C24-C1	-2.70	1.40	1.45
18	A	816	CLA	C1B-C2B	-2.70	1.36	1.43
18	B	821	CLA	C3D-C4D	-2.70	1.38	1.44
18	P	315	CLA	MG-NC	2.70	2.12	2.06
18	A	822	CLA	C3D-C4D	-2.70	1.38	1.44
24	T	213	DD6	C24-C1	-2.69	1.40	1.45
24	S	209	DD6	C8-C6	-2.69	1.40	1.45
18	B	828	CLA	MG-NC	2.69	2.12	2.06
24	O	215	DD6	C24-C1	-2.69	1.40	1.45
26	B	847	SQD	O47-C7	2.69	1.41	1.34
24	S	212	DD6	C26-C27	2.69	1.42	1.37
24	O	213	DD6	C8-C6	-2.69	1.40	1.45
21	M	101	BCR	C1-C6	-2.68	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	S	214	CLA	C3D-C4D	-2.67	1.38	1.44
18	B	820	CLA	C1B-NB	-2.67	1.34	1.37
18	A	803	CLA	C3D-C4D	-2.67	1.38	1.44
18	B	832	CLA	MG-NC	2.66	2.12	2.06
24	S	212	DD6	C24-C1	-2.66	1.40	1.45
18	O	205	CLA	C3D-C4D	-2.66	1.38	1.44
18	B	804	CLA	MG-NC	2.66	2.12	2.06
18	B	846	CLA	C3D-C4D	-2.65	1.38	1.44
18	A	816	CLA	C3D-C4D	-2.65	1.38	1.44
28	U	213	KC1	MG-NC	2.65	2.12	2.06
24	S	209	DD6	C24-C1	-2.65	1.40	1.45
18	O	209	CLA	C1D-C2D	-2.64	1.40	1.45
18	A	836	CLA	MG-NC	2.64	2.12	2.06
18	S	204	CLA	C3D-C4D	-2.64	1.38	1.44
24	P	304	DD6	C24-C1	-2.63	1.40	1.45
29	U	202	A86	C8-C6	-2.63	1.40	1.45
29	R	206	A86	C26-C27	2.63	1.39	1.35
18	A	806	CLA	C3D-C4D	-2.62	1.38	1.44
18	B	817	CLA	C3D-C4D	-2.62	1.38	1.44
29	R	206	A86	C24-C1	-2.62	1.40	1.45
18	S	205	CLA	MG-NC	2.61	2.12	2.06
18	T	210	CLA	C1B-C2B	-2.61	1.37	1.43
18	B	803	CLA	C1B-NB	-2.61	1.34	1.37
24	S	209	DD6	C13-C11	-2.61	1.40	1.45
24	A	854	DD6	C24-C1	-2.61	1.40	1.45
18	B	807	CLA	C3D-C4D	-2.60	1.38	1.44
18	Q	216	CLA	C3D-C4D	-2.60	1.38	1.44
18	S	207	CLA	C3D-C4D	-2.60	1.38	1.44
18	R	205	CLA	MG-NB	2.60	2.10	2.05
18	A	818	CLA	C1B-NB	-2.60	1.34	1.37
28	S	208	KC1	C2A-C3A	2.60	1.42	1.37
18	B	805	CLA	MG-NC	2.59	2.12	2.06
21	B	841	BCR	C1-C6	-2.59	1.50	1.53
18	B	814	CLA	C3D-C4D	-2.59	1.38	1.44
18	B	810	CLA	C3D-C4D	-2.59	1.38	1.44
18	A	820	CLA	C3D-C4D	-2.59	1.38	1.44
18	B	815	CLA	C3D-C4D	-2.59	1.38	1.44
18	B	835	CLA	C1B-C2B	-2.58	1.37	1.43
18	Q	206	CLA	C3D-C4D	-2.58	1.38	1.44
21	I	102	BCR	C1-C6	-2.58	1.50	1.53
21	F	801	BCR	C30-C25	-2.58	1.50	1.53
18	U	210	CLA	C3D-C4D	-2.58	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	827	CLA	C3D-C4D	-2.57	1.38	1.44
21	B	838	BCR	C30-C25	-2.57	1.50	1.53
18	S	201	CLA	C3D-C4D	-2.57	1.38	1.44
18	A	815	CLA	MG-NC	2.57	2.12	2.06
24	S	202	DD6	C24-C1	-2.57	1.40	1.45
18	A	815	CLA	C3D-C4D	-2.57	1.38	1.44
18	R	202	CLA	C1B-C2B	-2.57	1.37	1.43
18	A	832	CLA	C1B-NB	-2.57	1.34	1.37
18	T	211	CLA	C3D-C4D	-2.57	1.38	1.44
21	M	101	BCR	C30-C25	-2.56	1.50	1.53
28	P	302	KC1	MG-NC	2.56	2.12	2.06
18	B	827	CLA	C1B-C2B	-2.56	1.37	1.43
18	B	828	CLA	C1D-C2D	-2.56	1.40	1.45
24	A	854	DD6	C13-C11	-2.56	1.40	1.45
18	L	203	CLA	MG-NB	2.56	2.10	2.05
18	B	822	CLA	C3D-C4D	-2.56	1.38	1.44
18	B	825	CLA	C3D-C4D	-2.56	1.38	1.44
24	J	101	DD6	C24-C1	-2.56	1.40	1.45
18	B	810	CLA	MG-NB	2.55	2.10	2.05
18	B	812	CLA	C3D-C4D	-2.55	1.38	1.44
18	A	836	CLA	C3D-C4D	-2.55	1.38	1.44
18	L	202	CLA	MG-NC	2.55	2.12	2.06
18	B	819	CLA	C3D-C4D	-2.55	1.38	1.44
27	P	301	LMG	C4-C3	2.55	1.58	1.52
28	P	302	KC1	C1B-NB	-2.55	1.34	1.37
18	A	825	CLA	C3D-C4D	-2.55	1.38	1.44
24	O	214	DD6	C24-C1	-2.54	1.40	1.45
18	A	849	CLA	C3D-C4D	-2.54	1.38	1.44
18	A	828	CLA	C3D-C4D	-2.54	1.38	1.44
18	A	853	CLA	C3D-C4D	-2.54	1.38	1.44
18	B	834	CLA	C3D-C4D	-2.54	1.38	1.44
18	A	832	CLA	MG-NC	2.54	2.12	2.06
18	O	203	CLA	C3D-C4D	-2.54	1.38	1.44
18	B	806	CLA	C3D-C4D	-2.54	1.38	1.44
18	B	801	CLA	MG-NC	2.54	2.12	2.06
18	O	211	CLA	MG-NC	2.53	2.12	2.06
21	A	843	BCR	C30-C25	-2.53	1.50	1.53
18	A	830	CLA	MG-NC	2.53	2.12	2.06
18	A	826	CLA	C3D-C4D	-2.53	1.38	1.44
18	B	824	CLA	C3D-C4D	-2.53	1.38	1.44
18	O	204	CLA	C1D-C2D	-2.53	1.40	1.45
18	B	819	CLA	MG-NC	2.53	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	854	DD6	C8-C6	-2.53	1.40	1.45
24	O	212	DD6	C8-C6	-2.53	1.40	1.45
18	A	819	CLA	C3D-C4D	-2.53	1.38	1.44
18	A	809	CLA	C3D-C4D	-2.53	1.38	1.44
18	Q	213	CLA	C3D-C4D	-2.52	1.38	1.44
18	A	818	CLA	C3D-C4D	-2.52	1.38	1.44
18	A	835	CLA	C3D-C4D	-2.52	1.38	1.44
18	A	847	CLA	C3D-C4D	-2.52	1.38	1.44
18	U	208	CLA	C3D-C4D	-2.52	1.38	1.44
18	A	801	CLA	C1B-NB	-2.52	1.34	1.37
24	P	304	DD6	C8-C6	-2.52	1.40	1.45
18	A	825	CLA	MG-NC	2.52	2.12	2.06
18	S	206	CLA	C3D-C4D	-2.52	1.38	1.44
21	B	840	BCR	C1-C6	-2.52	1.50	1.53
18	B	809	CLA	C1B-NB	-2.52	1.34	1.37
18	A	824	CLA	C3D-C4D	-2.52	1.38	1.44
18	B	833	CLA	C3D-C4D	-2.51	1.38	1.44
18	L	204	CLA	C3D-C4D	-2.51	1.38	1.44
21	B	839	BCR	C30-C25	-2.51	1.50	1.53
21	J	104	BCR	C1-C6	-2.51	1.50	1.53
18	B	818	CLA	C3D-C4D	-2.51	1.38	1.44
18	B	813	CLA	C3D-C4D	-2.51	1.38	1.44
18	T	206	CLA	C3D-C4D	-2.51	1.38	1.44
18	A	808	CLA	C3D-C4D	-2.51	1.38	1.44
18	A	807	CLA	C3D-C4D	-2.51	1.38	1.44
18	B	832	CLA	C3D-C4D	-2.51	1.38	1.44
18	L	203	CLA	C3D-C4D	-2.51	1.38	1.44
18	T	203	CLA	C3D-C4D	-2.51	1.38	1.44
18	P	315	CLA	C3D-C4D	-2.51	1.38	1.44
18	A	810	CLA	C3D-C4D	-2.51	1.38	1.44
18	B	820	CLA	C3D-C4D	-2.50	1.38	1.44
18	A	802	CLA	C3D-C4D	-2.50	1.38	1.44
18	O	202	CLA	C3D-C4D	-2.50	1.38	1.44
18	U	204	CLA	C3D-C4D	-2.50	1.38	1.44
28	T	209	KC1	C2A-C3A	2.50	1.42	1.37
18	A	813	CLA	MG-NC	2.50	2.12	2.06
18	J	103	CLA	MG-NC	2.50	2.12	2.06
18	U	205	CLA	C1D-C2D	-2.50	1.40	1.45
18	O	209	CLA	C3D-C4D	-2.50	1.38	1.44
18	A	852	CLA	C3D-C4D	-2.50	1.38	1.44
18	U	207	CLA	C3D-C4D	-2.50	1.38	1.44
18	A	847	CLA	MG-NC	2.50	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	837	BCR	C30-C25	-2.50	1.50	1.53
18	B	805	CLA	C3D-C4D	-2.49	1.38	1.44
24	S	212	DD6	C8-C6	-2.49	1.40	1.45
18	P	310	CLA	C3D-C4D	-2.49	1.38	1.44
18	B	808	CLA	C1D-C2D	-2.49	1.40	1.45
18	B	826	CLA	C3D-C4D	-2.49	1.38	1.44
18	U	206	CLA	C3D-C4D	-2.49	1.38	1.44
18	B	809	CLA	C3D-C4D	-2.49	1.38	1.44
18	B	829	CLA	C3D-C4D	-2.49	1.38	1.44
18	A	831	CLA	C1B-C2B	-2.49	1.37	1.43
18	B	818	CLA	C1B-C2B	-2.49	1.37	1.43
18	A	825	CLA	C1D-C2D	-2.49	1.40	1.45
29	R	206	A86	C8-C6	-2.49	1.40	1.45
18	Q	206	CLA	MG-NC	2.49	2.12	2.06
18	U	204	CLA	MG-NC	2.49	2.12	2.06
29	Q	214	A86	C8-C6	-2.49	1.40	1.45
18	B	815	CLA	C1B-C2B	-2.49	1.37	1.43
18	B	835	CLA	C1D-C2D	-2.49	1.40	1.45
29	T	201	A86	C8-C6	-2.48	1.40	1.45
18	A	804	CLA	C3D-C4D	-2.48	1.38	1.44
21	A	841	BCR	C1-C6	-2.48	1.50	1.53
29	U	202	A86	C26-C27	2.48	1.39	1.35
18	A	815	CLA	C1B-C2B	-2.48	1.37	1.43
18	A	805	CLA	C3D-C4D	-2.48	1.38	1.44
18	A	811	CLA	C3D-C4D	-2.48	1.38	1.44
18	B	819	CLA	C1D-C2D	-2.48	1.40	1.45
18	A	832	CLA	C1B-C2B	-2.48	1.37	1.43
18	A	813	CLA	C3D-C4D	-2.48	1.38	1.44
21	F	801	BCR	C1-C6	-2.48	1.50	1.53
18	S	204	CLA	C1B-C2B	-2.48	1.37	1.43
24	O	214	DD6	C26-C27	2.48	1.42	1.37
18	U	211	CLA	C3D-C4D	-2.48	1.38	1.44
24	J	101	DD6	C26-C27	2.47	1.42	1.37
18	B	835	CLA	C3D-C4D	-2.47	1.38	1.44
18	B	824	CLA	MG-NB	2.47	2.10	2.05
18	P	306	CLA	C3D-C4D	-2.47	1.38	1.44
18	A	846	CLA	C3D-C4D	-2.47	1.38	1.44
18	Q	212	CLA	C1D-C2D	-2.47	1.40	1.45
18	A	823	CLA	C1D-C2D	-2.47	1.40	1.45
18	Q	205	CLA	C3D-C4D	-2.47	1.38	1.44
21	B	840	BCR	C30-C25	-2.47	1.50	1.53
18	B	827	CLA	C3D-C4D	-2.47	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	846	CLA	C1D-C2D	-2.47	1.40	1.45
18	B	813	CLA	MG-NB	2.47	2.10	2.05
18	B	830	CLA	C1B-NB	-2.47	1.34	1.37
18	U	205	CLA	C3D-C4D	-2.47	1.38	1.44
18	Q	207	CLA	C3D-C4D	-2.47	1.38	1.44
18	T	207	CLA	C3D-C4D	-2.46	1.38	1.44
18	B	830	CLA	C3D-C4D	-2.46	1.38	1.44
18	B	811	CLA	C3D-C4D	-2.46	1.38	1.44
18	B	816	CLA	C3D-C4D	-2.46	1.38	1.44
18	O	208	CLA	C3D-C4D	-2.46	1.38	1.44
18	U	209	CLA	MG-NC	2.46	2.12	2.06
18	O	211	CLA	C3D-C4D	-2.46	1.38	1.44
18	A	813	CLA	C1B-C2B	-2.45	1.37	1.43
24	S	202	DD6	C13-C11	-2.45	1.40	1.45
18	B	822	CLA	C1D-C2D	-2.45	1.40	1.45
18	B	845	CLA	C1D-C2D	-2.45	1.40	1.45
18	A	846	CLA	C1D-C2D	-2.45	1.40	1.45
18	O	202	CLA	C1B-C2B	-2.45	1.37	1.43
18	O	204	CLA	C3D-C4D	-2.45	1.38	1.44
18	B	845	CLA	C3D-C4D	-2.44	1.38	1.44
18	B	848	CLA	C3D-C4D	-2.44	1.38	1.44
18	A	823	CLA	MG-NC	2.44	2.12	2.06
18	A	817	CLA	MG-NC	2.44	2.12	2.06
18	A	803	CLA	MG-NB	2.44	2.10	2.05
29	Q	214	A86	C24-C1	-2.44	1.40	1.45
18	O	204	CLA	MG-NC	2.44	2.12	2.06
18	B	822	CLA	MG-NC	2.44	2.12	2.06
18	U	206	CLA	C1B-C2B	-2.44	1.37	1.43
21	F	804	BCR	C30-C25	-2.44	1.50	1.53
18	Q	203	CLA	C3D-C4D	-2.44	1.38	1.44
18	A	832	CLA	C3D-C4D	-2.44	1.38	1.44
18	B	828	CLA	C1B-NB	-2.43	1.34	1.37
18	R	202	CLA	C3D-C4D	-2.43	1.38	1.44
18	Q	212	CLA	C3D-C4D	-2.43	1.38	1.44
18	U	204	CLA	C1D-C2D	-2.43	1.40	1.45
18	B	814	CLA	MG-NB	2.43	2.10	2.05
18	B	804	CLA	C1B-NB	-2.43	1.34	1.37
18	T	204	CLA	C3D-C4D	-2.43	1.38	1.44
18	Q	211	CLA	MG-NC	2.43	2.12	2.06
18	S	215	CLA	C3D-C4D	-2.43	1.38	1.44
24	J	101	DD6	C13-C11	-2.43	1.40	1.45
18	B	803	CLA	C1D-C2D	-2.42	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	O	213	DD6	C13-C11	-2.42	1.40	1.45
18	A	846	CLA	MG-NB	2.42	2.10	2.05
18	A	829	CLA	C3D-C4D	-2.42	1.38	1.44
18	A	831	CLA	C3D-C4D	-2.42	1.38	1.44
21	I	102	BCR	C30-C25	-2.42	1.50	1.53
18	A	821	CLA	C1D-C2D	-2.42	1.40	1.45
24	Q	202	DD6	C8-C6	-2.42	1.40	1.45
21	A	841	BCR	C30-C25	-2.42	1.50	1.53
18	P	309	CLA	C3D-C4D	-2.42	1.38	1.44
18	A	838	CLA	C1D-C2D	-2.42	1.40	1.45
18	B	844	CLA	C1D-C2D	-2.42	1.40	1.45
18	A	853	CLA	MG-NC	2.42	2.12	2.06
18	P	312	CLA	C3D-C4D	-2.42	1.38	1.44
18	O	206	CLA	C3D-C4D	-2.42	1.38	1.44
18	O	207	CLA	C1B-C2B	-2.42	1.37	1.43
24	S	212	DD6	C13-C11	-2.42	1.40	1.45
18	A	803	CLA	C1B-NB	-2.42	1.34	1.37
18	A	801	CLA	C1B-C2B	-2.41	1.37	1.43
18	B	825	CLA	C1D-C2D	-2.41	1.40	1.45
27	S	211	LMG	O7-C8	-2.41	1.40	1.46
18	F	803	CLA	C3D-C4D	-2.41	1.38	1.44
22	A	848	CL0	C3D-C4D	-2.41	1.38	1.44
18	T	207	CLA	C1D-C2D	-2.41	1.40	1.45
18	A	821	CLA	C3D-C4D	-2.41	1.38	1.44
18	Q	208	CLA	C3D-C4D	-2.41	1.38	1.44
18	B	832	CLA	C1B-NB	-2.41	1.34	1.37
24	S	202	DD6	C8-C6	-2.41	1.40	1.45
24	S	209	DD6	C26-C27	2.41	1.42	1.37
18	B	843	CLA	C3D-C4D	-2.41	1.38	1.44
18	A	802	CLA	C1D-C2D	-2.41	1.40	1.45
27	B	849	LMG	C4-C3	2.41	1.58	1.52
18	Q	213	CLA	C1D-C2D	-2.41	1.40	1.45
18	B	804	CLA	C3D-C4D	-2.41	1.38	1.44
18	A	829	CLA	MG-NC	2.41	2.12	2.06
18	A	804	CLA	MG-NC	2.41	2.12	2.06
24	O	212	DD6	C13-C11	-2.41	1.40	1.45
18	Q	209	CLA	C3D-C4D	-2.40	1.38	1.44
18	A	847	CLA	C1B-C2B	-2.40	1.37	1.43
24	S	213	DD6	C25-C26	-2.40	1.36	1.43
18	B	803	CLA	C3D-C4D	-2.40	1.38	1.44
28	S	208	KC1	C1A-CHA	2.40	1.47	1.40
18	B	805	CLA	C1B-NB	-2.40	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	U	209	CLA	C1B-C2B	-2.40	1.37	1.43
18	A	833	CLA	C3D-C4D	-2.40	1.38	1.44
18	O	207	CLA	C3D-C4D	-2.40	1.38	1.44
18	A	816	CLA	C1B-NB	-2.40	1.34	1.37
24	U	212	DD6	C8-C6	-2.40	1.40	1.45
18	B	814	CLA	C1D-C2D	-2.40	1.40	1.45
18	R	202	CLA	C1D-C2D	-2.40	1.40	1.45
18	B	828	CLA	C3D-C4D	-2.40	1.38	1.44
24	J	101	DD6	C8-C6	-2.40	1.40	1.45
18	A	823	CLA	C3D-C4D	-2.40	1.38	1.44
18	U	207	CLA	MG-NA	2.39	2.12	2.06
18	Q	208	CLA	MG-NC	2.39	2.12	2.06
18	A	830	CLA	C3D-C4D	-2.39	1.38	1.44
18	A	814	CLA	C1B-C2B	-2.39	1.37	1.43
18	B	831	CLA	C3D-C4D	-2.39	1.38	1.44
18	A	801	CLA	C1D-C2D	-2.39	1.40	1.45
18	B	810	CLA	C1D-C2D	-2.39	1.40	1.45
18	T	212	CLA	C3D-C4D	-2.39	1.38	1.44
22	A	848	CL0	C1D-C2D	-2.39	1.40	1.45
18	A	826	CLA	C1B-NB	-2.39	1.34	1.37
18	B	833	CLA	C1B-C2B	-2.39	1.37	1.43
21	A	844	BCR	C30-C25	-2.38	1.50	1.53
18	A	818	CLA	C1D-C2D	-2.38	1.40	1.45
18	B	823	CLA	C3D-C4D	-2.38	1.38	1.44
18	R	205	CLA	C1D-C2D	-2.38	1.40	1.45
18	Q	204	CLA	C3D-C4D	-2.38	1.38	1.44
18	A	814	CLA	C3D-C4D	-2.38	1.38	1.44
18	Q	208	CLA	C1D-C2D	-2.38	1.40	1.45
18	A	838	CLA	C3D-C4D	-2.38	1.38	1.44
18	A	815	CLA	C1D-C2D	-2.38	1.40	1.45
20	R	201	LHG	O7-C5	-2.38	1.40	1.46
18	B	823	CLA	C1D-C2D	-2.38	1.40	1.45
18	B	809	CLA	C1B-C2B	-2.38	1.37	1.43
18	B	802	CLA	C1D-C2D	-2.38	1.40	1.45
18	B	816	CLA	MG-NC	2.38	2.11	2.06
18	A	801	CLA	C3D-C4D	-2.37	1.38	1.44
18	T	208	CLA	C3D-C4D	-2.37	1.38	1.44
18	A	812	CLA	C3D-C4D	-2.37	1.38	1.44
18	A	828	CLA	C1D-C2D	-2.37	1.40	1.45
18	S	205	CLA	C1D-C2D	-2.37	1.40	1.45
18	T	210	CLA	C3D-C4D	-2.37	1.38	1.44
18	Q	211	CLA	C1D-C2D	-2.37	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	835	CLA	C1B-C2B	-2.37	1.37	1.43
18	P	308	CLA	C3D-C4D	-2.36	1.38	1.44
18	R	205	CLA	C1B-NB	-2.36	1.34	1.37
24	Q	215	DD6	C13-C11	-2.36	1.40	1.45
18	A	817	CLA	C3D-C4D	-2.36	1.38	1.44
18	A	817	CLA	C1B-C2B	-2.36	1.37	1.43
24	Q	215	DD6	C8-C6	-2.36	1.40	1.45
18	A	812	CLA	C1B-NB	-2.36	1.34	1.37
18	A	845	CLA	C3D-C4D	-2.36	1.38	1.44
18	A	807	CLA	C1B-NB	-2.36	1.34	1.37
24	Q	215	DD6	C24-C1	-2.36	1.40	1.45
18	A	851	CLA	C3D-C4D	-2.36	1.38	1.44
18	A	818	CLA	C1B-C2B	-2.36	1.37	1.43
18	O	203	CLA	C1B-C2B	-2.36	1.37	1.43
18	A	845	CLA	C1B-C2B	-2.36	1.37	1.43
18	S	205	CLA	C3D-C4D	-2.36	1.38	1.44
18	T	211	CLA	C1B-C2B	-2.35	1.37	1.43
29	T	201	A86	C24-C1	-2.35	1.40	1.45
18	A	827	CLA	C1D-C2D	-2.35	1.40	1.45
28	P	302	KC1	C1A-CHA	2.35	1.46	1.40
18	A	806	CLA	C1B-NB	-2.35	1.34	1.37
18	A	852	CLA	C1B-NB	-2.35	1.34	1.37
18	U	209	CLA	C1D-C2D	-2.35	1.40	1.45
27	B	849	LMG	O4-C4	-2.35	1.37	1.43
18	B	804	CLA	C1D-C2D	-2.35	1.40	1.45
24	S	213	DD6	C8-C6	-2.35	1.40	1.45
18	S	204	CLA	C1D-C2D	-2.35	1.40	1.45
18	B	830	CLA	C1B-C2B	-2.34	1.37	1.43
24	T	214	DD6	C13-C11	-2.34	1.40	1.45
18	B	834	CLA	MG-NB	2.34	2.10	2.05
18	A	819	CLA	C1B-C2B	-2.34	1.37	1.43
18	A	810	CLA	C1B-C2B	-2.34	1.37	1.43
18	A	832	CLA	C1D-C2D	-2.34	1.40	1.45
18	O	203	CLA	C1D-C2D	-2.34	1.40	1.45
18	L	202	CLA	C1B-NB	-2.34	1.34	1.37
18	B	809	CLA	C1D-C2D	-2.33	1.40	1.45
18	Q	207	CLA	C1B-C2B	-2.33	1.37	1.43
18	S	215	CLA	C1D-C2D	-2.33	1.40	1.45
18	A	819	CLA	MG-NC	2.33	2.11	2.06
18	T	208	CLA	C1D-C2D	-2.33	1.40	1.45
18	A	807	CLA	C1D-C2D	-2.33	1.40	1.45
18	O	204	CLA	C1B-NB	-2.33	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	103	CLA	C1B-C2B	-2.32	1.37	1.43
24	U	214	DD6	C5-C6	2.32	1.40	1.35
18	B	820	CLA	MG-NC	2.32	2.11	2.06
18	F	803	CLA	C1B-C2B	-2.32	1.37	1.43
18	B	822	CLA	C1B-C2B	-2.32	1.37	1.43
28	P	311	KC1	C1B-NB	-2.32	1.34	1.37
18	A	853	CLA	C1B-C2B	-2.32	1.37	1.43
24	O	212	DD6	C24-C1	-2.32	1.41	1.45
18	J	103	CLA	C3D-C4D	-2.32	1.38	1.44
18	A	804	CLA	C1B-NB	-2.32	1.34	1.37
18	B	811	CLA	C1D-C2D	-2.32	1.40	1.45
24	S	212	DD6	C25-C26	-2.32	1.36	1.43
18	B	821	CLA	C1B-NB	-2.31	1.34	1.37
18	B	843	CLA	C1B-C2B	-2.31	1.37	1.43
18	B	827	CLA	C1B-NB	-2.31	1.34	1.37
18	T	202	CLA	C3D-C4D	-2.31	1.39	1.44
18	L	204	CLA	C1B-NB	-2.31	1.34	1.37
18	B	848	CLA	C1B-C2B	-2.31	1.37	1.43
18	A	834	CLA	MG-NB	2.31	2.10	2.05
18	L	202	CLA	C1D-C2D	-2.31	1.40	1.45
18	P	307	CLA	MG-NC	2.31	2.11	2.06
18	A	808	CLA	C1D-C2D	-2.31	1.40	1.45
18	T	202	CLA	C1D-C2D	-2.31	1.40	1.45
18	B	808	CLA	C3D-C4D	-2.31	1.39	1.44
18	A	820	CLA	C1B-C2B	-2.31	1.37	1.43
18	A	809	CLA	C1B-NB	-2.31	1.34	1.37
28	O	210	KC1	MG-NC	2.31	2.11	2.06
18	J	103	CLA	C1D-C2D	-2.31	1.40	1.45
24	S	209	DD6	C25-C26	-2.31	1.36	1.43
18	B	803	CLA	C1B-C2B	-2.31	1.37	1.43
18	B	808	CLA	C1B-C2B	-2.31	1.37	1.43
18	A	808	CLA	MG-NB	2.31	2.10	2.05
18	T	211	CLA	MG-NC	2.31	2.11	2.06
18	A	819	CLA	C1B-NB	-2.31	1.34	1.37
18	B	846	CLA	C1B-C2B	-2.31	1.37	1.43
18	U	205	CLA	C1B-C2B	-2.31	1.37	1.43
18	A	814	CLA	C1D-C2D	-2.30	1.40	1.45
18	P	306	CLA	C1D-C2D	-2.30	1.40	1.45
18	T	205	CLA	C3D-C4D	-2.30	1.39	1.44
18	T	211	CLA	MG-NB	2.30	2.10	2.05
18	B	821	CLA	C1D-C2D	-2.30	1.40	1.45
18	A	803	CLA	C1B-C2B	-2.30	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	806	CLA	C1D-C2D	-2.30	1.40	1.45
18	A	851	CLA	C1D-C2D	-2.30	1.40	1.45
24	O	215	DD6	C25-C26	-2.30	1.36	1.43
20	R	201	LHG	P-O6	2.30	1.68	1.59
24	P	314	DD6	C13-C11	-2.30	1.41	1.45
18	B	818	CLA	MG-NC	2.30	2.11	2.06
18	B	802	CLA	C3D-C4D	-2.30	1.39	1.44
18	A	845	CLA	C1D-C2D	-2.30	1.40	1.45
18	P	310	CLA	C1D-C2D	-2.30	1.40	1.45
24	T	213	DD6	C8-C6	-2.30	1.41	1.45
18	U	211	CLA	MG-NC	2.30	2.11	2.06
21	F	804	BCR	C1-C6	-2.29	1.50	1.53
28	O	210	KC1	C1B-NB	-2.29	1.35	1.37
18	A	849	CLA	C1D-C2D	-2.29	1.40	1.45
18	B	825	CLA	C1B-NB	-2.29	1.35	1.37
18	L	204	CLA	MG-NC	2.29	2.11	2.06
28	U	213	KC1	C1A-CHA	2.29	1.46	1.40
18	F	802	CLA	C3D-C4D	-2.29	1.39	1.44
18	B	825	CLA	C1B-C2B	-2.29	1.37	1.43
18	T	204	CLA	C1D-C2D	-2.28	1.40	1.45
18	L	203	CLA	C1D-C2D	-2.28	1.40	1.45
18	B	801	CLA	C1B-C2B	-2.28	1.37	1.43
18	A	817	CLA	C1D-C2D	-2.28	1.40	1.45
18	A	805	CLA	MG-NB	2.28	2.10	2.05
18	A	845	CLA	MG-NC	2.28	2.11	2.06
18	A	838	CLA	C1B-NB	-2.28	1.35	1.37
28	T	209	KC1	C1A-CHA	2.28	1.46	1.40
18	T	202	CLA	C1B-C2B	-2.28	1.37	1.43
18	B	805	CLA	MG-NB	2.28	2.10	2.05
18	A	809	CLA	MG-NC	2.28	2.11	2.06
18	O	206	CLA	C1D-C2D	-2.28	1.40	1.45
24	O	215	DD6	C8-C6	-2.27	1.41	1.45
28	S	210	KC1	C1A-CHA	2.27	1.46	1.40
18	A	816	CLA	C1D-C2D	-2.27	1.40	1.45
18	P	313	CLA	C3D-C4D	-2.27	1.39	1.44
18	B	805	CLA	C1D-C2D	-2.27	1.40	1.45
18	B	829	CLA	C1B-C2B	-2.27	1.37	1.43
18	A	836	CLA	C1D-C2D	-2.27	1.40	1.45
18	P	315	CLA	C1D-C2D	-2.27	1.40	1.45
18	T	207	CLA	C1B-C2B	-2.27	1.37	1.43
18	T	208	CLA	C1B-C2B	-2.26	1.37	1.43
24	O	213	DD6	C25-C26	-2.26	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	U	211	CLA	C1B-C2B	-2.26	1.37	1.43
18	A	807	CLA	MG-NC	2.26	2.11	2.06
24	T	213	DD6	C25-C26	-2.26	1.36	1.43
18	P	312	CLA	MG-NC	2.26	2.11	2.06
18	A	826	CLA	C1B-C2B	-2.26	1.37	1.43
24	O	214	DD6	C25-C26	-2.26	1.36	1.43
18	U	208	CLA	C1B-C2B	-2.26	1.37	1.43
18	B	801	CLA	C3D-C4D	-2.26	1.39	1.44
18	A	825	CLA	C1B-NB	-2.26	1.35	1.37
18	B	816	CLA	C1B-NB	-2.26	1.35	1.37
18	A	847	CLA	MG-NB	2.26	2.10	2.05
18	B	845	CLA	C1B-C2B	-2.26	1.37	1.43
28	Q	210	KC1	C1B-NB	-2.26	1.35	1.37
24	P	314	DD6	C8-C6	-2.26	1.41	1.45
18	T	212	CLA	C1B-C2B	-2.25	1.37	1.43
18	A	834	CLA	C3D-C4D	-2.25	1.39	1.44
24	P	304	DD6	C25-C26	-2.25	1.36	1.43
18	A	814	CLA	C1B-NB	-2.25	1.35	1.37
18	Q	213	CLA	MG-NC	2.25	2.11	2.06
18	L	202	CLA	C3D-C4D	-2.25	1.39	1.44
27	B	849	LMG	C4-C5	2.25	1.57	1.53
18	A	809	CLA	C1D-C2D	-2.25	1.40	1.45
18	Q	209	CLA	C1D-C2D	-2.25	1.40	1.45
24	A	854	DD6	C25-C26	-2.25	1.36	1.43
18	A	806	CLA	C1B-C2B	-2.25	1.38	1.43
18	Q	204	CLA	MG-NC	2.24	2.11	2.06
18	T	206	CLA	MG-NC	2.24	2.11	2.06
18	B	846	CLA	MG-NC	2.24	2.11	2.06
24	U	214	DD6	C24-C1	-2.24	1.41	1.45
18	A	834	CLA	C1B-NB	-2.24	1.35	1.37
18	A	852	CLA	C1D-C2D	-2.24	1.40	1.45
18	L	203	CLA	C1B-NB	-2.23	1.35	1.37
18	B	834	CLA	C1B-C2B	-2.23	1.38	1.43
18	Q	216	CLA	C1D-C2D	-2.23	1.40	1.45
18	P	307	CLA	C1D-C2D	-2.23	1.40	1.45
26	B	847	SQD	O3-C3	-2.23	1.37	1.43
18	B	830	CLA	C1D-C2D	-2.23	1.40	1.45
27	B	849	LMG	C3-C2	2.23	1.58	1.52
28	S	208	KC1	C1B-NB	-2.23	1.35	1.37
24	O	214	DD6	C8-C6	-2.23	1.41	1.45
18	B	826	CLA	C1B-C2B	-2.23	1.38	1.43
18	A	851	CLA	MG-NC	2.23	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	813	CLA	C1D-C2D	-2.23	1.40	1.45
24	P	317	DD6	C13-C11	-2.23	1.41	1.45
18	B	835	CLA	MG-NC	2.23	2.11	2.06
24	O	212	DD6	C25-C26	-2.22	1.36	1.43
24	U	212	DD6	C26-C27	2.22	1.41	1.37
18	B	827	CLA	C1D-C2D	-2.22	1.40	1.45
18	O	204	CLA	C1B-C2B	-2.22	1.38	1.43
18	B	806	CLA	C1B-C2B	-2.22	1.38	1.43
24	P	314	DD6	C24-C1	-2.22	1.41	1.45
18	O	207	CLA	MG-NC	2.22	2.11	2.06
18	A	821	CLA	C1B-NB	-2.22	1.35	1.37
18	A	830	CLA	C1B-NB	-2.22	1.35	1.37
18	B	814	CLA	C1B-C2B	-2.22	1.38	1.43
18	A	831	CLA	C1B-NB	-2.22	1.35	1.37
18	B	831	CLA	C1D-C2D	-2.22	1.40	1.45
18	A	829	CLA	C1B-C2B	-2.22	1.38	1.43
18	O	207	CLA	C1D-C2D	-2.22	1.40	1.45
18	B	833	CLA	C1B-NB	-2.22	1.35	1.37
18	A	847	CLA	C1B-NB	-2.22	1.35	1.37
18	A	802	CLA	C1B-C2B	-2.21	1.38	1.43
18	B	804	CLA	C1B-C2B	-2.21	1.38	1.43
24	S	203	DD6	C13-C11	-2.21	1.41	1.45
29	P	303	A86	C8-C6	-2.21	1.41	1.45
18	A	820	CLA	C1D-C2D	-2.21	1.41	1.45
18	U	207	CLA	C1D-C2D	-2.21	1.41	1.45
18	B	809	CLA	MG-NC	2.21	2.11	2.06
18	A	853	CLA	C1D-C2D	-2.21	1.41	1.45
18	B	829	CLA	MG-NC	2.21	2.11	2.06
18	O	205	CLA	C1D-C2D	-2.21	1.41	1.45
27	P	301	LMG	O8-C9	-2.21	1.40	1.45
18	B	846	CLA	MG-NB	2.21	2.10	2.05
18	Q	206	CLA	C1D-C2D	-2.21	1.41	1.45
18	S	207	CLA	C1B-C2B	-2.20	1.38	1.43
28	O	210	KC1	C1A-CHA	2.20	1.46	1.40
18	B	816	CLA	C1B-C2B	-2.20	1.38	1.43
18	R	205	CLA	C1B-C2B	-2.20	1.38	1.43
18	O	209	CLA	C1B-C2B	-2.20	1.38	1.43
18	L	204	CLA	C1D-C2D	-2.20	1.41	1.45
18	T	205	CLA	C1D-C2D	-2.20	1.41	1.45
24	P	316	DD6	C24-C1	-2.20	1.41	1.45
18	A	814	CLA	MG-NC	2.20	2.11	2.06
18	A	813	CLA	C1D-C2D	-2.20	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Q	210	KC1	C1A-CHA	2.20	1.46	1.40
18	A	824	CLA	C1D-C2D	-2.20	1.41	1.45
18	U	210	CLA	C1D-C2D	-2.20	1.41	1.45
18	A	825	CLA	C1B-C2B	-2.19	1.38	1.43
18	B	824	CLA	C1B-C2B	-2.19	1.38	1.43
18	B	845	CLA	MG-NB	2.19	2.10	2.05
18	B	831	CLA	C1B-NB	-2.19	1.35	1.37
24	U	203	DD6	C13-C11	-2.19	1.41	1.45
18	Q	203	CLA	C1D-C2D	-2.19	1.41	1.45
18	O	202	CLA	MG-NC	2.19	2.11	2.06
18	T	212	CLA	C1D-C2D	-2.19	1.41	1.45
18	B	816	CLA	C1D-C2D	-2.19	1.41	1.45
18	B	834	CLA	C1D-C2D	-2.19	1.41	1.45
18	A	819	CLA	C1D-C2D	-2.19	1.41	1.45
18	A	845	CLA	C1B-NB	-2.19	1.35	1.37
18	S	215	CLA	C1B-NB	-2.18	1.35	1.37
18	O	206	CLA	MG-NC	2.18	2.11	2.06
18	B	820	CLA	C1D-C2D	-2.18	1.41	1.45
18	P	313	CLA	C1B-C2B	-2.18	1.38	1.43
18	O	209	CLA	C1B-NB	-2.18	1.35	1.37
18	A	836	CLA	CHB-C1B	2.18	1.44	1.39
18	A	822	CLA	C1B-C2B	-2.18	1.38	1.43
18	B	813	CLA	C1B-C2B	-2.18	1.38	1.43
18	F	802	CLA	C1D-C2D	-2.18	1.41	1.45
18	S	214	CLA	C1D-C2D	-2.18	1.41	1.45
24	O	214	DD6	C13-C11	-2.18	1.41	1.45
18	S	214	CLA	C1B-C2B	-2.18	1.38	1.43
24	S	202	DD6	C25-C26	-2.18	1.36	1.43
18	A	804	CLA	C1B-C2B	-2.18	1.38	1.43
18	A	835	CLA	C1D-C2D	-2.17	1.41	1.45
18	P	315	CLA	C1B-NB	-2.17	1.35	1.37
18	B	815	CLA	MG-NB	2.17	2.10	2.05
18	B	843	CLA	C1D-C2D	-2.17	1.41	1.45
18	B	812	CLA	C1B-C2B	-2.17	1.38	1.43
18	R	202	CLA	C1B-NB	-2.17	1.35	1.37
18	A	852	CLA	C1B-C2B	-2.17	1.38	1.43
18	S	205	CLA	C1B-C2B	-2.17	1.38	1.43
18	U	205	CLA	C1B-NB	-2.17	1.35	1.37
18	U	211	CLA	C1D-C2D	-2.17	1.41	1.45
18	A	830	CLA	C1D-C2D	-2.17	1.41	1.45
18	O	211	CLA	C1D-C2D	-2.17	1.41	1.45
18	Q	206	CLA	MG-NB	2.17	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	207	CLA	C1D-C2D	-2.17	1.41	1.45
18	A	806	CLA	C1D-C2D	-2.17	1.41	1.45
18	A	827	CLA	C1B-C2B	-2.16	1.38	1.43
18	A	812	CLA	C1D-C2D	-2.16	1.41	1.45
18	A	826	CLA	C1D-C2D	-2.16	1.41	1.45
24	O	201	DD6	C24-C1	-2.16	1.41	1.45
18	A	851	CLA	C1B-NB	-2.16	1.35	1.37
18	O	206	CLA	C1B-NB	-2.16	1.35	1.37
28	S	210	KC1	C1B-NB	-2.16	1.35	1.37
18	A	807	CLA	C1B-C2B	-2.16	1.38	1.43
18	S	201	CLA	MG-NC	2.16	2.11	2.06
18	P	306	CLA	C1B-C2B	-2.16	1.38	1.43
24	S	213	DD6	C13-C11	-2.16	1.41	1.45
18	B	807	CLA	C1D-C2D	-2.16	1.41	1.45
29	Q	201	A86	C25-C24	2.16	1.40	1.34
24	Q	202	DD6	C13-C11	-2.16	1.41	1.45
28	P	311	KC1	C1A-CHA	2.15	1.46	1.40
18	O	205	CLA	C1B-NB	-2.15	1.35	1.37
18	A	833	CLA	C1D-C2D	-2.15	1.41	1.45
24	U	203	DD6	C24-C1	-2.15	1.41	1.45
18	R	202	CLA	MG-NC	2.15	2.11	2.06
24	Q	202	DD6	C24-C1	-2.15	1.41	1.45
26	M	102	SQD	O2-C2	-2.15	1.37	1.43
18	B	806	CLA	C1B-NB	-2.15	1.35	1.37
18	B	810	CLA	CAB-C3B	-2.15	1.46	1.50
18	P	309	CLA	C1D-C2D	-2.15	1.41	1.45
18	B	833	CLA	MG-NC	2.15	2.11	2.06
18	T	204	CLA	C1B-C2B	-2.15	1.38	1.43
18	B	833	CLA	C1D-C2D	-2.15	1.41	1.45
18	P	307	CLA	C1B-C2B	-2.15	1.38	1.43
18	Q	205	CLA	C1D-C2D	-2.15	1.41	1.45
18	A	830	CLA	C1B-C2B	-2.14	1.38	1.43
18	B	826	CLA	C1D-C2D	-2.14	1.41	1.45
18	B	821	CLA	MG-NC	2.14	2.11	2.06
18	T	206	CLA	C1D-C2D	-2.14	1.41	1.45
18	T	202	CLA	MG-NC	2.14	2.11	2.06
18	T	203	CLA	C1D-C2D	-2.14	1.41	1.45
24	U	203	DD6	C8-C6	-2.14	1.41	1.45
18	A	808	CLA	C1B-C2B	-2.14	1.38	1.43
18	Q	207	CLA	MG-NC	2.14	2.11	2.06
18	B	810	CLA	C1B-C2B	-2.14	1.38	1.43
18	A	803	CLA	MG-NC	2.13	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	824	CLA	C1B-C2B	-2.13	1.38	1.43
18	B	811	CLA	C1B-C2B	-2.13	1.38	1.43
18	B	848	CLA	C1D-C2D	-2.13	1.41	1.45
18	O	208	CLA	C1B-C2B	-2.13	1.38	1.43
18	O	205	CLA	C1B-C2B	-2.13	1.38	1.43
18	B	805	CLA	C1B-C2B	-2.13	1.38	1.43
24	J	101	DD6	C25-C26	-2.13	1.36	1.43
18	S	215	CLA	C1B-C2B	-2.13	1.38	1.43
18	B	818	CLA	C1B-NB	-2.13	1.35	1.37
18	B	848	CLA	C1B-NB	-2.13	1.35	1.37
18	A	804	CLA	C1D-C2D	-2.12	1.41	1.45
18	O	204	CLA	CHB-C1B	2.12	1.44	1.39
18	B	811	CLA	C1B-NB	-2.12	1.35	1.37
24	U	212	DD6	C13-C11	-2.12	1.41	1.45
18	B	820	CLA	C1B-C2B	-2.12	1.38	1.43
18	P	310	CLA	C1B-C2B	-2.12	1.38	1.43
18	A	823	CLA	C1B-NB	-2.12	1.35	1.37
24	S	203	DD6	C24-C1	-2.12	1.41	1.45
18	O	207	CLA	C1B-NB	-2.12	1.35	1.37
18	P	308	CLA	C1B-NB	-2.12	1.35	1.37
18	A	851	CLA	C1B-C2B	-2.12	1.38	1.43
24	S	203	DD6	C8-C6	-2.12	1.41	1.45
18	S	206	CLA	C1B-C2B	-2.11	1.38	1.43
18	B	843	CLA	C1B-NB	-2.11	1.35	1.37
24	P	317	DD6	C8-C6	-2.11	1.41	1.45
24	O	201	DD6	C8-C6	-2.11	1.41	1.45
18	A	823	CLA	C1B-C2B	-2.11	1.38	1.43
18	Q	209	CLA	C1B-C2B	-2.11	1.38	1.43
18	P	308	CLA	C1D-C2D	-2.11	1.41	1.45
26	B	847	SQD	O4-C4	-2.11	1.38	1.43
18	B	801	CLA	C1B-NB	-2.11	1.35	1.37
18	B	829	CLA	C1D-C2D	-2.11	1.41	1.45
18	B	807	CLA	C1B-C2B	-2.11	1.38	1.43
18	U	210	CLA	C1B-C2B	-2.11	1.38	1.43
18	U	207	CLA	C1B-C2B	-2.10	1.38	1.43
18	A	829	CLA	C1B-NB	-2.10	1.35	1.37
18	A	829	CLA	C1D-C2D	-2.10	1.41	1.45
18	B	822	CLA	C1B-NB	-2.10	1.35	1.37
18	B	828	CLA	C1B-C2B	-2.10	1.38	1.43
18	O	208	CLA	C1B-NB	-2.10	1.35	1.37
18	B	844	CLA	C1B-C2B	-2.10	1.38	1.43
18	Q	203	CLA	MG-NC	2.10	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	P	305	KC1	C1A-CHA	2.10	1.46	1.40
18	O	211	CLA	C1B-C2B	-2.10	1.38	1.43
18	Q	205	CLA	C1B-NB	-2.10	1.35	1.37
18	F	802	CLA	C1B-C2B	-2.10	1.38	1.43
18	B	832	CLA	C1B-C2B	-2.10	1.38	1.43
18	O	203	CLA	MG-NC	2.10	2.11	2.06
18	A	821	CLA	C1B-C2B	-2.10	1.38	1.43
18	S	201	CLA	C1B-C2B	-2.10	1.38	1.43
26	B	847	SQD	O47-C45	-2.10	1.41	1.46
21	I	101	BCR	C30-C25	-2.10	1.50	1.53
18	B	808	CLA	C1B-NB	-2.09	1.35	1.37
26	B	847	SQD	O2-C2	-2.09	1.38	1.43
18	B	834	CLA	C1B-NB	-2.09	1.35	1.37
18	O	202	CLA	C1D-C2D	-2.09	1.41	1.45
24	S	213	DD6	C24-C1	-2.09	1.41	1.45
18	B	848	CLA	MG-NC	2.09	2.11	2.06
18	U	210	CLA	C1B-NB	-2.09	1.35	1.37
28	S	210	KC1	C3B-C2B	2.09	1.41	1.37
24	O	201	DD6	C13-C11	-2.09	1.41	1.45
18	S	204	CLA	C1B-NB	-2.09	1.35	1.37
18	A	811	CLA	C1B-NB	-2.09	1.35	1.37
18	T	205	CLA	C1B-NB	-2.09	1.35	1.37
18	B	807	CLA	C1B-NB	-2.08	1.35	1.37
18	P	308	CLA	C1B-C2B	-2.08	1.38	1.43
18	T	203	CLA	C1B-C2B	-2.08	1.38	1.43
18	A	838	CLA	C1B-C2B	-2.08	1.38	1.43
26	M	102	SQD	O4-C4	-2.08	1.38	1.43
18	A	834	CLA	C1D-C2D	-2.08	1.41	1.45
18	Q	216	CLA	C1B-NB	-2.08	1.35	1.37
18	A	836	CLA	C1B-NB	-2.08	1.35	1.37
18	T	208	CLA	MG-NC	2.08	2.11	2.06
18	A	834	CLA	C1B-C2B	-2.08	1.38	1.43
18	A	811	CLA	C1D-C2D	-2.08	1.41	1.45
24	U	203	DD6	C25-C24	2.08	1.39	1.34
18	L	204	CLA	C1B-C2B	-2.08	1.38	1.43
28	U	213	KC1	C3B-C2B	2.08	1.41	1.37
24	O	215	DD6	C13-C11	-2.08	1.41	1.45
18	B	801	CLA	C1D-C2D	-2.07	1.41	1.45
18	S	206	CLA	C1D-C2D	-2.07	1.41	1.45
20	A	840	LHG	O7-C5	-2.07	1.41	1.46
18	A	810	CLA	C1D-C2D	-2.07	1.41	1.45
18	A	827	CLA	C1B-NB	-2.07	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	802	CLA	CHB-C1B	2.07	1.44	1.39
18	B	821	CLA	C1B-C2B	-2.07	1.38	1.43
18	A	828	CLA	C1B-NB	-2.07	1.35	1.37
18	P	309	CLA	C1B-C2B	-2.07	1.38	1.43
18	A	836	CLA	C1B-C2B	-2.07	1.38	1.43
18	B	832	CLA	C1D-C2D	-2.07	1.41	1.45
18	P	315	CLA	C1B-C2B	-2.06	1.38	1.43
18	A	802	CLA	C1B-NB	-2.06	1.35	1.37
24	U	214	DD6	C25-C26	-2.06	1.37	1.43
18	A	817	CLA	C1B-NB	-2.06	1.35	1.37
18	O	208	CLA	MG-NC	2.06	2.11	2.06
18	P	309	CLA	C1B-NB	-2.06	1.35	1.37
18	B	812	CLA	C1D-C2D	-2.06	1.41	1.45
18	A	838	CLA	MG-NC	2.06	2.11	2.06
18	U	208	CLA	C1D-C2D	-2.06	1.41	1.45
18	B	813	CLA	C1B-NB	-2.06	1.35	1.37
24	T	214	DD6	C24-C1	-2.06	1.41	1.45
18	U	209	CLA	C3D-C4D	-2.06	1.39	1.44
18	S	207	CLA	C1D-C2D	-2.06	1.41	1.45
18	A	847	CLA	C1D-C2D	-2.06	1.41	1.45
18	O	206	CLA	CHB-C1B	2.06	1.44	1.39
18	B	815	CLA	C1D-C2D	-2.06	1.41	1.45
18	Q	212	CLA	C1B-C2B	-2.06	1.38	1.43
18	A	833	CLA	MG-NB	2.05	2.09	2.05
18	U	204	CLA	C1B-C2B	-2.05	1.38	1.43
29	P	303	A86	C24-C1	-2.05	1.41	1.45
18	P	306	CLA	MG-NC	2.05	2.11	2.06
18	F	803	CLA	MG-NC	2.05	2.11	2.06
18	O	208	CLA	C1D-C2D	-2.05	1.41	1.45
18	Q	208	CLA	CHB-C1B	2.05	1.44	1.39
18	S	207	CLA	MG-NC	2.05	2.11	2.06
18	Q	211	CLA	CHB-C1B	2.05	1.44	1.39
18	B	819	CLA	C1B-C2B	-2.05	1.38	1.43
18	Q	216	CLA	C1B-C2B	-2.05	1.38	1.43
18	S	201	CLA	C1B-NB	-2.05	1.35	1.37
18	A	824	CLA	C1B-NB	-2.05	1.35	1.37
18	L	202	CLA	C1B-C2B	-2.04	1.38	1.43
18	B	818	CLA	C1D-C2D	-2.04	1.41	1.45
18	A	811	CLA	C1B-C2B	-2.04	1.38	1.43
18	B	812	CLA	MG-NB	2.04	2.09	2.05
18	B	826	CLA	MG-NB	2.04	2.09	2.05
18	A	808	CLA	C1B-NB	-2.04	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	P	310	CLA	CHB-C1B	2.04	1.44	1.39
24	O	201	DD6	C25-C26	-2.04	1.37	1.43
18	Q	213	CLA	C1B-C2B	-2.04	1.38	1.43
18	B	824	CLA	C1B-NB	-2.04	1.35	1.37
18	B	823	CLA	CHB-C1B	2.04	1.44	1.39
24	P	316	DD6	C8-C6	-2.04	1.41	1.45
18	A	805	CLA	C1B-C2B	-2.04	1.38	1.43
18	B	831	CLA	C1B-C2B	-2.04	1.38	1.43
18	A	846	CLA	C1B-NB	-2.04	1.35	1.37
18	Q	212	CLA	C1B-NB	-2.04	1.35	1.37
18	Q	205	CLA	C1B-C2B	-2.03	1.38	1.43
18	Q	208	CLA	C1B-NB	-2.03	1.35	1.37
18	A	812	CLA	C1B-C2B	-2.03	1.38	1.43
18	A	831	CLA	C1D-C2D	-2.03	1.41	1.45
18	F	803	CLA	C1D-C2D	-2.03	1.41	1.45
18	Q	205	CLA	MG-NC	2.03	2.11	2.06
18	B	824	CLA	C1D-C2D	-2.03	1.41	1.45
18	L	203	CLA	C1B-C2B	-2.03	1.38	1.43
18	P	307	CLA	C1B-NB	-2.03	1.35	1.37
18	A	833	CLA	C1B-NB	-2.02	1.35	1.37
18	P	312	CLA	C1D-C2D	-2.02	1.41	1.45
18	A	805	CLA	C1D-C2D	-2.02	1.41	1.45
18	A	805	CLA	C1B-NB	-2.02	1.35	1.37
24	U	212	DD6	C24-C1	-2.02	1.41	1.45
18	A	809	CLA	C1B-C2B	-2.02	1.38	1.43
18	T	206	CLA	CHB-C1B	2.02	1.43	1.39
18	U	210	CLA	CHB-C1B	2.02	1.43	1.39
18	B	829	CLA	C1B-NB	-2.02	1.35	1.37
18	S	205	CLA	C1B-NB	-2.02	1.35	1.37
18	Q	211	CLA	C1B-NB	-2.02	1.35	1.37
18	A	846	CLA	C1B-C2B	-2.02	1.38	1.43
18	P	312	CLA	C1B-NB	-2.01	1.35	1.37
18	B	827	CLA	MG-NC	2.01	2.11	2.06
18	U	206	CLA	C1D-C2D	-2.01	1.41	1.45
27	J	102	LMG	C1-C2	2.01	1.58	1.52
18	T	206	CLA	C1B-C2B	-2.01	1.38	1.43
18	A	852	CLA	MG-NC	2.01	2.11	2.06
18	U	208	CLA	C1B-NB	-2.01	1.35	1.37
18	Q	204	CLA	C1B-C2B	-2.01	1.38	1.43
28	T	209	KC1	C1B-NB	-2.01	1.35	1.37
18	Q	216	CLA	MG-NC	2.01	2.11	2.06
18	B	844	CLA	C1B-NB	-2.01	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	845	CLA	C1B-NB	-2.01	1.35	1.37
18	T	203	CLA	MG-NC	2.01	2.11	2.06
18	A	833	CLA	C1B-C2B	-2.00	1.38	1.43
18	P	309	CLA	MG-NC	2.00	2.11	2.06
24	P	317	DD6	C4-C5	-2.00	1.38	1.45
24	Q	202	DD6	C25-C26	-2.00	1.37	1.43
18	T	205	CLA	C1B-C2B	-2.00	1.38	1.43
27	Q	217	LMG	C3-C2	2.00	1.57	1.52
24	S	203	DD6	C25-C26	-2.00	1.37	1.43
18	Q	208	CLA	C1B-C2B	-2.00	1.38	1.43
18	A	810	CLA	C1B-NB	-2.00	1.35	1.37

All (1224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	824	CLA	C1-O2A-CGA	7.98	137.38	116.44
24	U	212	DD6	C3-C4-C5	7.17	138.16	123.47
18	B	824	CLA	C5-C3-C2	6.10	133.46	121.12
24	P	317	DD6	C3-C4-C5	5.90	131.04	123.25
24	S	203	DD6	C3-C4-C5	5.84	135.44	123.47
24	P	314	DD6	C4-C3-C2	5.64	135.04	123.47
18	U	207	CLA	CHD-C1D-ND	-5.24	119.64	124.45
24	T	214	DD6	C4-C3-C2	5.23	134.18	123.47
24	U	203	DD6	C4-C3-C2	5.09	133.91	123.47
18	L	202	CLA	O2A-C1-C2	-5.06	97.14	108.97
18	A	808	CLA	O2A-C1-C2	-5.05	95.35	108.64
18	O	209	CLA	C5-C3-C2	5.03	131.30	121.12
24	T	213	DD6	C12-C11-C10	-5.01	115.90	122.92
24	P	314	DD6	C8-C6-C5	4.98	126.58	118.94
29	T	201	A86	C17-C16-C15	4.92	114.18	109.16
18	A	833	CLA	O2A-C1-C2	4.87	121.44	108.64
18	S	201	CLA	CHD-C1D-ND	-4.87	119.98	124.45
29	R	206	A86	C17-C16-C15	4.78	114.04	109.16
29	U	202	A86	C17-C16-C15	4.76	114.02	109.16
18	B	824	CLA	O2A-C1-C2	-4.72	96.24	108.64
24	T	213	DD6	C13-C11-C10	4.70	126.15	118.94
24	P	316	DD6	C12-C11-C10	-4.69	116.36	122.92
29	Q	201	A86	C3-C4-C5	4.63	132.96	123.47
29	R	204	A86	C4-C3-C2	4.59	132.87	123.47
18	A	803	CLA	CHD-C1D-ND	-4.58	120.25	124.45
29	P	303	A86	C17-C16-C15	4.56	113.82	109.16
18	B	824	CLA	C4-C3-C2	-4.51	112.10	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	314	DD6	C10-C9-C8	4.46	137.14	123.22
24	O	212	DD6	C3-C4-C5	4.45	132.58	123.47
24	O	212	DD6	C4-C3-C2	4.41	132.51	123.47
24	O	214	DD6	C12-C11-C10	-4.40	116.75	122.92
24	P	316	DD6	C8-C6-C5	4.40	125.69	118.94
24	O	215	DD6	C12-C11-C10	-4.39	116.77	122.92
24	T	213	DD6	C3-C4-C5	4.39	132.47	123.47
26	B	847	SQD	O8-S-C6	4.39	112.73	105.74
24	P	314	DD6	C12-C11-C10	-4.39	116.78	122.92
18	A	822	CLA	CHD-C1D-ND	-4.39	120.42	124.45
18	L	202	CLA	C1-O2A-CGA	4.38	127.93	116.44
24	T	214	DD6	C-C1-C2	-4.37	116.80	122.92
24	Q	202	DD6	C12-C11-C10	-4.37	116.80	122.92
18	Q	207	CLA	C4D-CHA-C1A	4.37	126.56	121.25
24	J	101	DD6	C12-C11-C10	-4.36	116.81	122.92
24	P	304	DD6	C12-C11-C10	-4.33	116.86	122.92
24	S	213	DD6	C4-C3-C2	4.32	132.33	123.47
18	B	815	CLA	CHD-C1D-ND	-4.32	120.49	124.45
24	Q	202	DD6	C3-C4-C5	4.30	132.27	123.47
18	T	210	CLA	CHD-C1D-ND	-4.29	120.51	124.45
24	S	203	DD6	C12-C11-C10	-4.28	116.93	122.92
27	P	301	LMG	C1-C2-C3	-4.28	101.08	110.00
24	T	214	DD6	C12-C11-C10	-4.25	116.96	122.92
24	T	214	DD6	C10-C9-C8	4.25	136.47	123.22
18	B	846	CLA	C1-O2A-CGA	4.24	127.58	116.44
24	S	209	DD6	C3-C4-C5	4.24	132.15	123.47
24	S	203	DD6	C4-C3-C2	4.22	132.12	123.47
18	S	207	CLA	CHD-C1D-ND	-4.22	120.58	124.45
24	S	212	DD6	C12-C11-C10	-4.21	117.02	122.92
18	A	805	CLA	CHD-C1D-ND	-4.21	120.58	124.45
24	U	212	DD6	C12-C11-C10	-4.21	117.03	122.92
24	O	212	DD6	C12-C11-C10	-4.19	117.06	122.92
24	P	314	DD6	C7-C6-C5	-4.18	117.06	122.92
18	L	203	CLA	CHD-C1D-ND	-4.18	120.61	124.45
29	R	204	A86	C3-C4-C5	4.17	132.02	123.47
24	P	316	DD6	C7-C6-C5	-4.17	117.09	122.92
24	Q	215	DD6	C12-C11-C10	-4.16	117.10	122.92
24	J	101	DD6	C3-C4-C5	4.16	131.99	123.47
24	U	203	DD6	C-C1-C2	-4.15	117.11	122.92
18	B	818	CLA	CHD-C1D-ND	-4.15	120.64	124.45
18	B	832	CLA	CHD-C1D-ND	-4.14	120.65	124.45
24	S	202	DD6	C12-C11-C10	-4.13	117.13	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	O	213	DD6	C4-C3-C2	4.13	131.94	123.47
24	S	202	DD6	C3-C4-C5	4.13	131.94	123.47
24	U	203	DD6	C24-C1-C2	4.13	125.28	118.94
24	A	854	DD6	C12-C11-C10	-4.12	117.15	122.92
18	S	214	CLA	CHD-C1D-ND	-4.12	120.67	124.45
24	U	203	DD6	C12-C11-C10	-4.11	117.16	122.92
20	A	840	LHG	O4-P-O5	4.11	132.53	112.24
18	A	847	CLA	CHD-C1D-ND	-4.10	120.68	124.45
24	Q	215	DD6	C4-C3-C2	4.10	131.87	123.47
18	B	807	CLA	CHD-C1D-ND	-4.08	120.71	124.45
18	B	824	CLA	CHD-C1D-ND	-4.08	120.71	124.45
20	A	839	LHG	O4-P-O5	4.07	132.37	112.24
24	O	201	DD6	C12-C11-C10	-4.07	117.22	122.92
24	P	314	DD6	C3-C4-C5	4.07	131.80	123.47
24	P	317	DD6	C12-C11-C10	-4.05	117.24	122.92
29	R	204	A86	C28-C27-C26	-4.05	117.24	122.92
18	A	824	CLA	CHD-C1D-ND	-4.05	120.73	124.45
29	P	303	A86	C3-C4-C5	4.04	131.75	123.47
18	F	803	CLA	CHD-C1D-ND	-4.03	120.75	124.45
18	U	206	CLA	CHD-C1D-ND	-4.03	120.75	124.45
29	R	204	A86	C17-C16-C15	4.03	113.27	109.16
29	Q	201	A86	C17-C16-C15	4.02	113.27	109.16
18	U	210	CLA	CHD-C1D-ND	-4.02	120.76	124.45
18	B	826	CLA	CHD-C1D-ND	-4.02	120.76	124.45
18	B	801	CLA	C4D-CHA-C1A	3.99	126.11	121.25
20	R	201	LHG	O4-P-O5	3.98	131.91	112.24
24	T	214	DD6	C8-C6-C5	3.97	125.04	118.94
26	M	102	SQD	O47-C7-C8	3.97	120.06	111.50
24	S	213	DD6	C12-C11-C10	-3.97	117.37	122.92
18	A	831	CLA	CHD-C1D-ND	-3.95	120.82	124.45
18	A	838	CLA	C4D-CHA-C1A	3.95	126.06	121.25
18	Q	207	CLA	CHD-C1D-ND	-3.95	120.83	124.45
29	Q	201	A86	C4-C3-C2	3.94	131.55	123.47
24	U	212	DD6	C8-C6-C5	3.94	124.98	118.94
18	T	211	CLA	CHD-C1D-ND	-3.93	120.84	124.45
24	S	212	DD6	C3-C4-C5	3.93	131.52	123.47
18	O	205	CLA	CHD-C1D-ND	-3.92	120.85	124.45
26	M	102	SQD	O9-S-C6	3.92	111.60	106.94
29	U	202	A86	C4-C3-C2	3.92	131.50	123.47
24	O	201	DD6	C4-C3-C2	3.92	131.50	123.47
18	B	830	CLA	C4D-CHA-C1A	3.92	126.02	121.25
24	S	209	DD6	C12-C11-C10	-3.92	117.44	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	807	CLA	C4D-CHA-C1A	3.91	126.01	121.25
24	O	214	DD6	C3-C4-C5	3.91	131.49	123.47
24	T	214	DD6	C3-C4-C5	3.91	131.48	123.47
24	J	101	DD6	C13-C11-C10	3.91	124.94	118.94
18	Q	216	CLA	CHD-C1D-ND	-3.91	120.86	124.45
18	A	801	CLA	CHD-C1D-ND	-3.90	120.87	124.45
24	O	201	DD6	C3-C4-C5	3.90	131.46	123.47
29	Q	201	A86	C7-C6-C5	-3.89	117.47	122.92
18	B	827	CLA	CHD-C1D-ND	-3.89	120.88	124.45
24	S	203	DD6	C24-C1-C2	3.88	124.90	118.94
18	T	212	CLA	CHD-C1D-ND	-3.87	120.89	124.45
18	B	848	CLA	CHD-C1D-ND	-3.87	120.90	124.45
18	A	829	CLA	CHD-C1D-ND	-3.87	120.90	124.45
24	U	212	DD6	C7-C6-C5	-3.86	117.51	122.92
18	B	826	CLA	C4D-CHA-C1A	3.85	125.94	121.25
18	P	307	CLA	CHD-C1D-ND	-3.85	120.92	124.45
21	M	101	BCR	C2-C1-C6	3.85	116.41	110.48
24	S	203	DD6	C-C1-C2	-3.82	117.56	122.92
18	A	830	CLA	CHD-C1D-ND	-3.82	120.94	124.45
18	B	829	CLA	CHD-C1D-ND	-3.82	120.94	124.45
24	U	203	DD6	C26-C25-C24	3.82	135.13	123.22
18	B	818	CLA	C4D-CHA-C1A	3.82	125.89	121.25
18	A	810	CLA	CHD-C1D-ND	-3.81	120.95	124.45
18	Q	205	CLA	CHD-C1D-ND	-3.80	120.96	124.45
24	O	212	DD6	C-C1-C2	-3.80	117.60	122.92
18	B	831	CLA	CHD-C1D-ND	-3.80	120.96	124.45
18	L	203	CLA	C4D-CHA-C1A	3.79	125.86	121.25
18	A	822	CLA	C4D-CHA-C1A	3.79	125.86	121.25
24	S	203	DD6	C7-C6-C5	-3.79	117.61	122.92
24	U	214	DD6	C4-C3-C2	3.79	131.23	123.47
18	B	812	CLA	CHD-C1D-ND	-3.78	120.98	124.45
18	A	806	CLA	CHD-C1D-ND	-3.78	120.98	124.45
24	J	101	DD6	C7-C6-C5	-3.78	117.63	122.92
18	A	811	CLA	C4D-CHA-C1A	3.78	125.84	121.25
18	B	816	CLA	C4D-CHA-C1A	3.77	125.84	121.25
18	P	313	CLA	CHD-C1D-ND	-3.77	120.99	124.45
18	P	308	CLA	CHD-C1D-ND	-3.76	121.00	124.45
18	A	819	CLA	CHD-C1D-ND	-3.76	121.00	124.45
18	P	312	CLA	CHD-C1D-ND	-3.75	121.00	124.45
18	A	829	CLA	C4D-CHA-C1A	3.74	125.80	121.25
18	A	833	CLA	C4D-CHA-C1A	3.74	125.80	121.25
24	J	101	DD6	C8-C6-C5	3.74	124.68	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	208	CLA	C4D-CHA-C1A	3.74	125.80	121.25
18	P	306	CLA	C4D-CHA-C1A	3.74	125.80	121.25
26	M	102	SQD	O9-S-O7	-3.73	101.03	113.95
24	O	213	DD6	C12-C11-C10	-3.73	117.69	122.92
18	A	816	CLA	CHD-C1D-ND	-3.73	121.03	124.45
18	P	308	CLA	C4D-CHA-C1A	3.73	125.79	121.25
24	S	203	DD6	C8-C6-C5	3.72	124.66	118.94
24	O	215	DD6	C4-C3-C2	3.72	131.10	123.47
18	T	203	CLA	CHD-C1D-ND	-3.72	121.03	124.45
29	R	204	A86	C-C1-C2	-3.72	117.71	122.92
24	S	213	DD6	C-C1-C2	-3.72	117.72	122.92
18	B	814	CLA	C4D-CHA-C1A	3.71	125.77	121.25
18	L	202	CLA	C4D-CHA-C1A	3.71	125.77	121.25
21	F	801	BCR	C3-C4-C5	-3.70	107.47	114.08
18	B	846	CLA	CHD-C1D-ND	-3.70	121.06	124.45
24	A	854	DD6	C-C1-C2	-3.70	117.74	122.92
21	A	841	BCR	C2-C1-C6	3.70	116.17	110.48
18	T	212	CLA	C4D-CHA-C1A	3.70	125.75	121.25
24	T	214	DD6	C24-C1-C2	3.69	124.61	118.94
18	T	203	CLA	C4D-CHA-C1A	3.69	125.74	121.25
18	B	805	CLA	CHD-C1D-ND	-3.69	121.06	124.45
18	A	804	CLA	CHD-C1D-ND	-3.69	121.06	124.45
29	Q	201	A86	C8-C6-C5	3.69	124.60	118.94
18	B	843	CLA	C4D-CHA-C1A	3.68	125.73	121.25
18	P	306	CLA	CHD-C1D-ND	-3.68	121.07	124.45
28	P	311	KC1	C2A-C3A-C4A	3.68	109.22	106.49
24	T	213	DD6	C4-C3-C2	3.68	131.01	123.47
24	P	316	DD6	C4-C3-C2	3.68	131.01	123.47
24	P	314	DD6	C-C1-C2	-3.67	117.78	122.92
18	A	853	CLA	CHD-C1D-ND	-3.66	121.09	124.45
18	S	201	CLA	C4D-CHA-C1A	3.66	125.70	121.25
29	Q	214	A86	C3-C4-C5	3.66	130.97	123.47
18	U	211	CLA	CHD-C1D-ND	-3.65	121.10	124.45
18	A	831	CLA	C4D-CHA-C1A	3.65	125.69	121.25
18	Q	203	CLA	C4D-CHA-C1A	3.65	125.69	121.25
21	I	101	BCR	C2-C1-C6	3.65	116.10	110.48
18	A	819	CLA	C4D-CHA-C1A	3.65	125.69	121.25
18	F	803	CLA	C4D-CHA-C1A	3.64	125.68	121.25
24	O	212	DD6	C24-C1-C2	3.64	124.52	118.94
18	O	208	CLA	CHD-C1D-ND	-3.64	121.11	124.45
24	P	314	DD6	C13-C11-C10	3.64	124.52	118.94
18	U	204	CLA	C4D-CHA-C1A	3.63	125.67	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	832	CLA	C4D-CHA-C1A	3.63	125.67	121.25
18	Q	205	CLA	C4D-CHA-C1A	3.63	125.67	121.25
18	O	211	CLA	C4D-CHA-C1A	3.63	125.67	121.25
18	P	310	CLA	CHD-C1D-ND	-3.63	121.12	124.45
24	P	304	DD6	C4-C3-C2	3.63	130.91	123.47
18	A	816	CLA	C4D-CHA-C1A	3.63	125.66	121.25
29	R	204	A86	C24-C1-C2	3.62	124.50	118.94
26	B	847	SQD	O47-C7-C8	3.62	119.30	111.50
29	T	201	A86	C4-C3-C2	3.62	130.89	123.47
18	P	309	CLA	CHD-C1D-ND	-3.62	121.13	124.45
18	R	202	CLA	CHD-C1D-ND	-3.61	121.13	124.45
24	P	316	DD6	C13-C11-C10	3.61	124.49	118.94
18	B	821	CLA	CHD-C1D-ND	-3.61	121.14	124.45
18	T	206	CLA	CHD-C1D-ND	-3.61	121.14	124.45
18	T	202	CLA	C4D-CHA-C1A	3.61	125.64	121.25
18	U	211	CLA	C4D-CHA-C1A	3.60	125.64	121.25
18	L	204	CLA	C4D-CHA-C1A	3.60	125.63	121.25
18	S	205	CLA	C4D-CHA-C1A	3.60	125.63	121.25
18	A	813	CLA	CHD-C1D-ND	-3.60	121.15	124.45
18	B	813	CLA	CHD-C1D-ND	-3.60	121.15	124.45
18	T	210	CLA	C4D-CHA-C1A	3.59	125.62	121.25
18	B	831	CLA	C4D-CHA-C1A	3.59	125.62	121.25
18	P	313	CLA	C4D-CHA-C1A	3.59	125.61	121.25
29	R	206	A86	C3-C4-C5	3.59	130.82	123.47
24	U	214	DD6	C3-C4-C5	3.58	130.81	123.47
18	A	803	CLA	C4D-CHA-C1A	3.57	125.60	121.25
18	B	816	CLA	CHD-C1D-ND	-3.57	121.17	124.45
18	B	846	CLA	C4D-CHA-C1A	3.57	125.59	121.25
18	O	202	CLA	CHD-C1D-ND	-3.57	121.17	124.45
29	U	202	A86	C3-C4-C5	3.57	130.78	123.47
18	A	828	CLA	C4D-CHA-C1A	3.57	125.59	121.25
18	A	805	CLA	C4D-CHA-C1A	3.57	125.59	121.25
29	R	204	A86	C7-C6-C5	-3.56	117.94	122.92
18	B	833	CLA	CHD-C1D-ND	-3.55	121.19	124.45
18	A	815	CLA	C4D-CHA-C1A	3.55	125.57	121.25
18	A	820	CLA	C4D-CHA-C1A	3.55	125.57	121.25
24	Q	202	DD6	C-C1-C2	-3.55	117.95	122.92
24	U	212	DD6	C-C1-C2	-3.55	117.95	122.92
24	U	214	DD6	C-C1-C2	-3.55	117.96	122.92
18	S	214	CLA	C4D-CHA-C1A	3.54	125.56	121.25
18	Q	203	CLA	CHD-C1D-ND	-3.54	121.20	124.45
24	A	854	DD6	C24-C1-C2	3.53	124.36	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	853	CLA	C4D-CHA-C1A	3.53	125.55	121.25
18	R	202	CLA	C4D-CHA-C1A	3.53	125.55	121.25
18	S	207	CLA	C4D-CHA-C1A	3.53	125.55	121.25
18	A	834	CLA	C4D-CHA-C1A	3.52	125.54	121.25
24	P	314	DD6	C24-C1-C2	3.52	124.35	118.94
18	L	204	CLA	CHD-C1D-ND	-3.52	121.22	124.45
18	O	206	CLA	C4D-CHA-C1A	3.52	125.53	121.25
18	A	835	CLA	CHD-C1D-ND	-3.52	121.22	124.45
24	S	212	DD6	C7-C6-C5	-3.52	118.00	122.92
18	B	845	CLA	C4D-CHA-C1A	3.51	125.53	121.25
18	Q	209	CLA	C4D-CHA-C1A	3.51	125.53	121.25
18	P	315	CLA	C4D-CHA-C1A	3.51	125.52	121.25
18	B	811	CLA	C4D-CHA-C1A	3.51	125.52	121.25
18	S	206	CLA	CHD-C1D-ND	-3.51	121.23	124.45
24	S	213	DD6	C24-C1-C2	3.51	124.32	118.94
24	O	212	DD6	C7-C6-C5	-3.50	118.02	122.92
18	B	815	CLA	C4D-CHA-C1A	3.50	125.50	121.25
18	A	827	CLA	C4D-CHA-C1A	3.49	125.49	121.25
21	L	205	BCR	C2-C1-C6	3.48	115.84	110.48
18	A	833	CLA	CHD-C1D-ND	-3.48	121.25	124.45
20	A	840	LHG	O8-C23-C24	3.48	120.51	111.38
21	F	801	BCR	C2-C1-C6	3.48	115.84	110.48
24	A	854	DD6	C7-C6-C5	-3.48	118.05	122.92
18	F	802	CLA	C4D-CHA-C1A	3.48	125.48	121.25
18	T	208	CLA	CHD-C1D-ND	-3.48	121.26	124.45
24	O	214	DD6	C7-C6-C5	-3.48	118.06	122.92
18	S	204	CLA	C4D-CHA-C1A	3.47	125.48	121.25
24	O	215	DD6	C-C1-C2	-3.47	118.06	122.92
28	Q	210	KC1	C1A-C2A-C3A	-3.47	104.36	107.11
24	P	304	DD6	C-C1-C2	-3.47	118.06	122.92
18	O	211	CLA	CHD-C1D-ND	-3.47	121.27	124.45
18	A	845	CLA	C4D-CHA-C1A	3.47	125.47	121.25
18	B	801	CLA	CHD-C1D-ND	-3.46	121.27	124.45
18	A	824	CLA	C4D-CHA-C1A	3.46	125.46	121.25
18	T	206	CLA	C4D-CHA-C1A	3.46	125.46	121.25
18	A	832	CLA	C4D-CHA-C1A	3.46	125.46	121.25
24	S	202	DD6	C7-C6-C5	-3.46	118.08	122.92
24	U	203	DD6	C3-C4-C5	3.46	130.55	123.47
18	O	207	CLA	CHD-C1D-ND	-3.45	121.28	124.45
24	Q	202	DD6	C7-C6-C5	-3.45	118.09	122.92
18	A	836	CLA	C4D-CHA-C1A	3.45	125.45	121.25
18	A	830	CLA	C4D-CHA-C1A	3.44	125.44	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	O	201	DD6	C7-C6-C5	-3.44	118.10	122.92
29	Q	201	A86	C28-C27-C26	-3.44	118.10	122.92
18	U	205	CLA	C4D-CHA-C1A	3.44	125.43	121.25
18	P	310	CLA	C4D-CHA-C1A	3.44	125.43	121.25
18	A	852	CLA	CHD-C1D-ND	-3.44	121.30	124.45
18	P	315	CLA	C4A-NA-C1A	3.43	108.25	106.71
26	M	102	SQD	O7-S-C6	3.43	111.02	106.94
24	Q	215	DD6	C7-C6-C5	-3.43	118.12	122.92
18	B	848	CLA	C4D-CHA-C1A	3.43	125.42	121.25
29	T	201	A86	C3-C4-C5	3.43	130.49	123.47
18	B	825	CLA	CHD-C1D-ND	-3.42	121.31	124.45
18	O	204	CLA	C4D-CHA-C1A	3.42	125.41	121.25
29	Q	201	A86	C-C1-C2	-3.42	118.14	122.92
18	B	828	CLA	C4D-CHA-C1A	3.41	125.41	121.25
18	B	834	CLA	C4D-CHA-C1A	3.41	125.40	121.25
18	O	209	CLA	C4-C3-C2	-3.41	114.93	123.68
18	B	848	CLA	O2A-C1-C2	3.41	117.60	108.64
28	O	210	KC1	C2A-C3A-C4A	3.41	109.02	106.49
18	Q	204	CLA	CHD-C1D-ND	-3.41	121.32	124.45
18	A	811	CLA	CHD-C1D-ND	-3.41	121.32	124.45
24	O	215	DD6	C24-C1-C2	3.40	124.16	118.94
24	P	317	DD6	C7-C6-C5	-3.40	118.16	122.92
18	S	204	CLA	CHD-C1D-ND	-3.40	121.33	124.45
18	O	209	CLA	O2A-C1-C2	-3.40	99.70	108.64
26	B	847	SQD	O9-S-O7	-3.40	102.19	113.95
18	U	208	CLA	C4D-CHA-C1A	3.39	125.38	121.25
29	R	206	A86	C4-C3-C2	3.39	130.42	123.47
18	Q	213	CLA	C4D-CHA-C1A	3.39	125.38	121.25
18	B	829	CLA	C4D-CHA-C1A	3.39	125.38	121.25
18	U	208	CLA	CHD-C1D-ND	-3.39	121.34	124.45
28	P	302	KC1	CHC-C4B-NB	-3.39	121.34	124.45
24	P	316	DD6	C-C1-C2	-3.39	118.17	122.92
18	O	207	CLA	C4D-CHA-C1A	3.39	125.37	121.25
24	S	202	DD6	C-C1-C2	-3.39	118.18	122.92
18	B	846	CLA	O2A-C1-C2	-3.38	99.76	108.64
24	O	201	DD6	C-C1-C2	-3.37	118.20	122.92
18	B	824	CLA	C4D-CHA-C1A	3.37	125.35	121.25
24	O	215	DD6	C7-C6-C5	-3.37	118.21	122.92
18	A	809	CLA	CHD-C1D-ND	-3.36	121.36	124.45
18	P	315	CLA	CHD-C1D-ND	-3.36	121.37	124.45
28	P	311	KC1	CHC-C4B-NB	-3.36	121.37	124.45
18	A	808	CLA	C4D-CHA-C1A	3.36	125.33	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	815	CLA	CHD-C1D-ND	-3.35	121.37	124.45
24	U	212	DD6	C24-C1-C2	3.35	124.09	118.94
29	P	303	A86	C7-C6-C5	-3.35	118.23	122.92
26	M	102	SQD	O6-C1-C2	3.35	113.53	108.30
18	B	819	CLA	CHD-C1D-ND	-3.34	121.38	124.45
18	O	208	CLA	C4D-CHA-C1A	3.34	125.32	121.25
18	T	211	CLA	CAC-C3C-C4C	3.34	129.15	124.81
24	Q	215	DD6	C-C1-C2	-3.34	118.24	122.92
29	R	206	A86	C7-C6-C5	-3.34	118.25	122.92
29	Q	214	A86	C35-C34-C33	3.34	115.70	109.88
18	Q	204	CLA	C4D-CHA-C1A	3.34	125.31	121.25
18	A	852	CLA	C4D-CHA-C1A	3.33	125.31	121.25
18	A	845	CLA	CHD-C1D-ND	-3.33	121.39	124.45
18	A	838	CLA	CHD-C1D-ND	-3.33	121.39	124.45
29	T	201	A86	C-C1-C2	-3.33	118.26	122.92
18	O	206	CLA	CHD-C1D-ND	-3.33	121.40	124.45
18	Q	209	CLA	CHD-C1D-ND	-3.33	121.40	124.45
21	B	840	BCR	C15-C16-C17	-3.33	116.66	123.47
24	O	212	DD6	C8-C6-C5	3.32	124.04	118.94
18	Q	206	CLA	CHD-C1D-ND	-3.32	121.40	124.45
18	U	207	CLA	C4D-CHA-C1A	3.32	125.29	121.25
18	A	820	CLA	CHD-C1D-ND	-3.32	121.40	124.45
18	B	827	CLA	C4D-CHA-C1A	3.32	125.29	121.25
24	U	203	DD6	C7-C6-C5	-3.31	118.28	122.92
18	R	205	CLA	CHD-C1D-ND	-3.31	121.41	124.45
29	T	201	A86	C7-C6-C5	-3.31	118.29	122.92
18	Q	208	CLA	C4D-CHA-C1A	3.30	125.27	121.25
18	P	312	CLA	C4D-CHA-C1A	3.30	125.26	121.25
18	A	817	CLA	CHD-C1D-ND	-3.30	121.42	124.45
18	B	835	CLA	C4D-CHA-C1A	3.30	125.26	121.25
18	B	814	CLA	CHD-C1D-ND	-3.29	121.43	124.45
18	A	810	CLA	C4D-CHA-C1A	3.29	125.26	121.25
18	B	805	CLA	C4D-CHA-C1A	3.29	125.26	121.25
18	U	207	CLA	CAA-C2A-C3A	-3.29	103.76	112.78
28	Q	210	KC1	CHC-C4B-NB	-3.29	121.43	124.45
21	L	205	BCR	C3-C4-C5	-3.29	108.21	114.08
18	A	851	CLA	CHD-C1D-ND	-3.29	121.44	124.45
29	R	204	A86	C8-C6-C5	3.28	123.97	118.94
18	B	812	CLA	C4D-CHA-C1A	3.28	125.23	121.25
21	J	104	BCR	C2-C1-C6	3.27	115.52	110.48
24	A	854	DD6	C3-C4-C5	3.27	130.18	123.47
18	A	832	CLA	CHD-C1D-ND	-3.27	121.45	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	808	CLA	CHD-C1D-ND	-3.27	121.45	124.45
18	B	803	CLA	CHD-C1D-ND	-3.27	121.45	124.45
24	T	213	DD6	C8-C6-C5	3.27	123.95	118.94
18	A	835	CLA	C4D-CHA-C1A	3.26	125.22	121.25
18	Q	213	CLA	CHD-C1D-ND	-3.26	121.45	124.45
24	S	212	DD6	C8-C6-C5	3.26	123.94	118.94
18	Q	206	CLA	C4D-CHA-C1A	3.26	125.21	121.25
18	A	847	CLA	C4D-CHA-C1A	3.25	125.21	121.25
24	T	213	DD6	C7-C6-C5	-3.25	118.37	122.92
18	A	813	CLA	C4D-CHA-C1A	3.24	125.20	121.25
18	U	206	CLA	C4D-CHA-C1A	3.24	125.19	121.25
18	A	827	CLA	CHD-C1D-ND	-3.24	121.48	124.45
24	Q	202	DD6	C4-C3-C2	3.24	130.11	123.47
18	A	817	CLA	C4D-CHA-C1A	3.24	125.19	121.25
18	B	844	CLA	C4D-CHA-C1A	3.24	125.19	121.25
18	A	851	CLA	C4D-CHA-C1A	3.24	125.19	121.25
29	U	202	A86	C7-C6-C5	-3.24	118.39	122.92
28	P	305	KC1	CAA-C2A-C1A	3.24	139.62	124.75
28	O	210	KC1	CAA-C2A-C1A	3.23	139.61	124.75
18	Q	212	CLA	CHD-C1D-ND	-3.23	121.48	124.45
24	P	316	DD6	C24-C1-C2	3.23	123.90	118.94
18	B	824	CLA	C1-C2-C3	3.22	131.62	126.04
18	B	833	CLA	C4D-CHA-C1A	3.22	125.17	121.25
18	B	806	CLA	CHD-C1D-ND	-3.22	121.50	124.45
18	B	813	CLA	C4D-CHA-C1A	3.22	125.16	121.25
18	A	836	CLA	O2A-C1-C2	-3.21	100.19	108.64
29	Q	214	A86	C7-C6-C5	-3.21	118.42	122.92
29	Q	214	A86	C4-C3-C2	3.21	130.05	123.47
24	U	214	DD6	C24-C1-C2	3.21	123.86	118.94
24	Q	215	DD6	C3-C4-C5	3.21	130.04	123.47
18	B	845	CLA	CHD-C1D-ND	-3.21	121.51	124.45
24	A	854	DD6	C4-C3-C2	3.20	130.04	123.47
18	A	846	CLA	C4D-CHA-C1A	3.20	125.15	121.25
18	B	822	CLA	C4D-CHA-C1A	3.20	125.14	121.25
18	S	205	CLA	CHD-C1D-ND	-3.20	121.52	124.45
18	U	205	CLA	CHD-C1D-ND	-3.19	121.52	124.45
18	A	825	CLA	CHD-C1D-ND	-3.18	121.53	124.45
18	O	202	CLA	C4D-CHA-C1A	3.18	125.12	121.25
24	O	215	DD6	C14-C13-C11	3.18	130.46	125.53
18	B	817	CLA	C4D-CHA-C1A	3.18	125.11	121.25
18	B	843	CLA	CHD-C1D-ND	-3.17	121.54	124.45
24	Q	202	DD6	C24-C1-C2	3.17	123.81	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R	206	A86	C-C1-C2	-3.17	118.48	122.92
18	B	834	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	Q	214	A86	C-C1-C2	-3.16	118.50	122.92
18	B	809	CLA	C4D-CHA-C1A	3.16	125.09	121.25
24	P	304	DD6	C7-C6-C5	-3.15	118.51	122.92
24	S	202	DD6	C4-C3-C2	3.15	129.92	123.47
24	Q	202	DD6	C8-C6-C5	3.14	123.76	118.94
18	A	849	CLA	CHD-C1D-ND	-3.14	121.57	124.45
18	B	819	CLA	C4D-CHA-C1A	3.13	125.06	121.25
18	T	205	CLA	CHD-C1D-ND	-3.13	121.58	124.45
26	B	847	SQD	C4-C3-C2	3.13	116.28	110.82
24	T	214	DD6	C7-C6-C5	-3.12	118.55	122.92
24	Q	202	DD6	C15-C14-C13	3.12	132.59	125.99
18	T	207	CLA	C4D-CHA-C1A	3.12	125.05	121.25
18	B	835	CLA	CHD-C1D-ND	-3.12	121.59	124.45
24	J	101	DD6	C10-C9-C8	3.11	132.94	123.22
18	B	823	CLA	C4D-CHA-C1A	3.11	125.04	121.25
18	A	807	CLA	C4D-CHA-C1A	3.11	125.04	121.25
21	B	840	BCR	C15-C14-C13	-3.11	122.87	127.31
24	O	201	DD6	C24-C1-C2	3.11	123.71	118.94
24	O	215	DD6	C3-C4-C5	3.10	129.83	123.47
29	R	204	A86	C20-C19-C18	-3.10	106.61	112.75
24	P	317	DD6	C8-C6-C5	3.10	123.69	118.94
26	M	102	SQD	C4-C3-C2	3.10	116.23	110.82
24	A	854	DD6	C26-C25-C24	3.10	132.88	123.22
21	R	203	BCR	C19-C18-C17	-3.09	117.92	124.81
29	P	303	A86	C-C1-C2	-3.09	118.59	122.92
18	A	828	CLA	CHD-C1D-ND	-3.09	121.62	124.45
24	O	201	DD6	C8-C6-C5	3.09	123.68	118.94
18	A	802	CLA	CHD-C1D-ND	-3.08	121.62	124.45
18	Q	208	CLA	CHD-C1D-ND	-3.08	121.62	124.45
18	B	828	CLA	C4A-NA-C1A	3.08	108.09	106.71
18	B	809	CLA	CHD-C1D-ND	-3.08	121.62	124.45
18	U	209	CLA	CHD-C1D-ND	-3.08	121.62	124.45
24	S	212	DD6	C-C1-C2	-3.08	118.61	122.92
27	J	102	LMG	O6-C1-O1	-3.07	102.69	109.97
18	P	309	CLA	C4D-CHA-C1A	3.07	124.99	121.25
24	Q	215	DD6	C8-C6-C5	3.07	123.65	118.94
18	A	824	CLA	O2A-C1-C2	3.07	116.70	108.64
18	A	836	CLA	CHD-C1D-ND	-3.07	121.64	124.45
18	U	207	CLA	O2A-C1-C2	3.07	116.69	108.64
18	A	812	CLA	C4D-CHA-C1A	3.07	124.98	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	O	203	CLA	CHD-C1D-ND	-3.07	121.64	124.45
18	A	821	CLA	CHA-C1A-NA	-3.07	119.38	126.40
18	B	820	CLA	CHD-C1D-ND	-3.06	121.64	124.45
24	S	213	DD6	C7-C6-C5	-3.06	118.63	122.92
18	J	103	CLA	C4D-CHA-C1A	3.06	124.98	121.25
18	O	203	CLA	C4D-CHA-C1A	3.06	124.97	121.25
18	U	209	CLA	C4D-CHA-C1A	3.06	124.97	121.25
18	L	202	CLA	CHD-C1D-ND	-3.06	121.64	124.45
18	R	205	CLA	C4D-CHA-C1A	3.06	124.97	121.25
18	A	818	CLA	CHD-C1D-ND	-3.06	121.64	124.45
24	A	854	DD6	C8-C6-C5	3.06	123.63	118.94
18	B	828	CLA	CHD-C1D-ND	-3.05	121.65	124.45
18	B	806	CLA	C4D-CHA-C1A	3.05	124.96	121.25
18	A	804	CLA	C4D-CHA-C1A	3.05	124.96	121.25
24	P	304	DD6	C24-C1-C2	3.04	123.61	118.94
18	Q	216	CLA	C4D-CHA-C1A	3.04	124.95	121.25
18	Q	212	CLA	CAA-C2A-C1A	3.04	121.92	111.97
18	T	207	CLA	CHD-C1D-ND	-3.03	121.67	124.45
28	S	208	KC1	CHC-C4B-NB	-3.03	121.67	124.45
24	S	213	DD6	C3-C4-C5	3.03	129.68	123.47
18	T	205	CLA	C4D-CHA-C1A	3.03	124.94	121.25
18	A	825	CLA	C4D-CHA-C1A	3.03	124.93	121.25
28	P	311	KC1	CAA-C2A-C1A	3.03	138.65	124.75
24	P	314	DD6	C23-C16-C17	-3.02	103.73	108.98
29	P	303	A86	C4-C3-C2	3.02	129.67	123.47
26	M	102	SQD	O8-S-C6	3.02	110.56	105.74
18	A	849	CLA	C4D-CHA-C1A	3.02	124.93	121.25
18	Q	212	CLA	CHA-C1A-NA	-3.02	119.48	126.40
21	I	102	BCR	C27-C26-C25	3.02	127.12	122.73
18	A	834	CLA	CHD-C1D-ND	-3.02	121.68	124.45
18	B	804	CLA	CHD-C1D-ND	-3.02	121.68	124.45
18	B	820	CLA	CHA-C1A-NA	-3.02	119.49	126.40
24	P	304	DD6	C3-C4-C5	3.02	129.65	123.47
18	U	210	CLA	C4D-CHA-C1A	3.01	124.92	121.25
18	A	809	CLA	C4D-CHA-C1A	3.01	124.91	121.25
24	J	101	DD6	C-C1-C2	-3.01	118.71	122.92
24	O	201	DD6	C13-C11-C10	3.00	123.55	118.94
18	B	810	CLA	CHD-C1D-ND	-3.00	121.69	124.45
18	S	201	CLA	CMD-C2D-C1D	3.00	130.00	124.71
24	O	214	DD6	C-C1-C2	-3.00	118.72	122.92
24	T	213	DD6	C-C1-C2	-3.00	118.73	122.92
18	S	215	CLA	C4D-CHA-C1A	2.99	124.89	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	807	CLA	C4A-NA-C1A	2.99	108.05	106.71
18	B	844	CLA	CHD-C1D-ND	-2.99	121.70	124.45
18	O	205	CLA	C4D-CHA-C1A	2.99	124.89	121.25
18	P	307	CLA	O2A-C1-C2	2.99	116.49	108.64
24	O	214	DD6	C8-C6-C5	2.99	123.53	118.94
18	T	202	CLA	CHD-C1D-ND	-2.99	121.71	124.45
18	B	811	CLA	CHD-C1D-ND	-2.98	121.71	124.45
24	S	202	DD6	C24-C1-C2	2.98	123.52	118.94
18	B	810	CLA	C4D-CHA-C1A	2.98	124.88	121.25
18	T	211	CLA	C4D-CHA-C1A	2.98	124.87	121.25
24	S	203	DD6	C26-C25-C24	2.98	132.51	123.22
24	O	213	DD6	C28-C27-C29	2.98	122.74	116.84
24	T	214	DD6	C26-C25-C24	2.98	132.50	123.22
18	A	818	CLA	C4D-CHA-C1A	2.97	124.87	121.25
21	F	804	BCR	C2-C1-C6	2.97	115.06	110.48
26	B	847	SQD	C44-O6-C1	2.97	119.55	113.74
24	S	209	DD6	C7-C6-C5	-2.97	118.76	122.92
26	B	847	SQD	O9-S-C6	2.97	110.47	106.94
24	O	213	DD6	C-C1-C2	-2.97	118.77	122.92
24	Q	215	DD6	C24-C1-C2	2.97	123.49	118.94
18	A	821	CLA	CHD-C1D-ND	-2.97	121.73	124.45
29	R	204	A86	C26-C25-C24	2.96	132.46	123.22
29	P	303	A86	C8-C6-C5	2.96	123.48	118.94
18	A	826	CLA	CHD-C1D-ND	-2.96	121.74	124.45
18	A	814	CLA	CHD-C1D-ND	-2.95	121.74	124.45
21	A	843	BCR	C2-C1-C6	2.95	115.02	110.48
29	T	201	A86	C20-C19-C18	-2.94	106.93	112.75
18	A	812	CLA	CHD-C1D-ND	-2.93	121.76	124.45
24	S	212	DD6	C4-C3-C2	2.93	129.48	123.47
18	A	846	CLA	CHD-C1D-ND	-2.92	121.77	124.45
18	A	821	CLA	C4D-CHA-C1A	2.92	124.81	121.25
18	P	313	CLA	CHA-C1A-NA	-2.92	119.71	126.40
18	U	204	CLA	CHD-C1D-ND	-2.92	121.77	124.45
18	L	202	CLA	CHA-C1A-NA	-2.92	119.72	126.40
18	A	812	CLA	CHA-C1A-NA	-2.92	119.72	126.40
29	R	204	A86	C23-C16-C17	-2.92	103.92	108.98
18	S	215	CLA	CHD-C1D-ND	-2.91	121.78	124.45
21	R	203	BCR	C19-C20-C21	-2.91	117.52	123.47
18	T	204	CLA	CHD-C1D-ND	-2.91	121.78	124.45
28	P	305	KC1	CAA-CBA-CGA	-2.90	112.33	127.26
18	A	814	CLA	C4A-NA-C1A	2.90	108.01	106.71
26	B	847	SQD	O7-S-C6	2.90	110.39	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	830	CLA	CHD-C1D-ND	-2.90	121.79	124.45
29	P	303	A86	C25-C26-C27	2.89	131.44	127.31
29	Q	214	A86	C28-C27-C26	-2.89	118.88	122.92
18	A	823	CLA	C4D-CHA-C1A	2.89	124.76	121.25
18	B	828	CLA	CHA-C1A-NA	-2.89	119.79	126.40
24	U	203	DD6	C8-C6-C5	2.88	123.36	118.94
18	T	202	CLA	CHA-C1A-NA	-2.88	119.80	126.40
24	S	202	DD6	C8-C6-C5	2.88	123.35	118.94
18	Q	211	CLA	CHD-C1D-ND	-2.87	121.81	124.45
18	A	802	CLA	C4D-CHA-C1A	2.87	124.74	121.25
18	A	807	CLA	CHD-C1D-ND	-2.87	121.82	124.45
18	A	834	CLA	CHA-C1A-NA	-2.87	119.83	126.40
28	U	213	KC1	CHD-C1D-ND	-2.87	121.22	124.26
27	Q	217	LMG	O6-C1-O1	-2.86	103.19	109.97
21	F	804	BCR	C35-C13-C14	-2.86	118.91	122.92
18	F	802	CLA	C1-O2A-CGA	2.86	123.95	116.44
18	P	315	CLA	CHA-C1A-NA	-2.86	119.86	126.40
29	T	201	A86	C28-C27-C26	-2.85	118.92	122.92
24	P	304	DD6	C13-C11-C10	2.85	123.32	118.94
18	B	825	CLA	C4D-CHA-C1A	2.85	124.72	121.25
18	A	806	CLA	C4D-CHA-C1A	2.85	124.72	121.25
20	R	201	LHG	O8-C23-C24	2.85	120.85	111.91
18	B	835	CLA	O2A-C1-C2	2.84	116.10	108.64
18	F	802	CLA	CHA-C1A-NA	-2.84	119.89	126.40
18	A	821	CLA	C4A-NA-C1A	2.84	107.98	106.71
18	F	802	CLA	C4A-NA-C1A	2.84	107.98	106.71
29	R	206	A86	C8-C6-C5	2.83	123.29	118.94
18	Q	211	CLA	O2D-CGD-CBD	2.83	116.30	111.27
29	T	201	A86	C8-C6-C5	2.83	123.29	118.94
18	A	828	CLA	CHA-C1A-NA	-2.83	119.91	126.40
18	B	803	CLA	C4D-CHA-C1A	2.83	124.69	121.25
24	O	213	DD6	C7-C6-C5	-2.83	118.96	122.92
18	O	203	CLA	CHA-C1A-NA	-2.83	119.92	126.40
24	T	213	DD6	C34-C35-C36	2.83	117.49	111.85
29	U	202	A86	C25-C26-C27	2.82	131.34	127.31
24	T	213	DD6	C9-C10-C11	2.82	131.34	127.31
18	A	802	CLA	CHA-C1A-NA	-2.82	119.94	126.40
18	B	823	CLA	CHA-C1A-NA	-2.82	119.94	126.40
24	S	209	DD6	C-C1-C2	-2.82	118.98	122.92
18	A	807	CLA	CHA-C1A-NA	-2.82	119.95	126.40
24	U	203	DD6	C20-C19-C18	2.81	118.32	112.75
18	T	212	CLA	CHA-C1A-NA	-2.81	119.96	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	J	103	CLA	CHA-C1A-NA	-2.81	119.96	126.40
18	B	802	CLA	CHA-C1A-NA	-2.81	119.97	126.40
22	A	848	CL0	CHA-C1A-NA	-2.81	119.97	126.40
21	R	203	BCR	C40-C30-C25	2.81	114.85	110.30
18	B	835	CLA	CHA-C1A-NA	-2.81	119.97	126.40
18	Q	208	CLA	O2A-C1-C2	2.81	116.01	108.64
28	Q	210	KC1	CAB-C3B-C4B	2.80	131.67	124.90
18	A	817	CLA	CHA-C1A-NA	-2.80	119.98	126.40
29	U	202	A86	C-C1-C2	-2.80	119.00	122.92
18	B	819	CLA	CHA-C1A-NA	-2.80	119.98	126.40
18	A	814	CLA	CHA-C1A-NA	-2.80	119.98	126.40
18	A	815	CLA	CHA-C1A-NA	-2.80	119.98	126.40
24	P	316	DD6	C3-C4-C5	2.80	129.21	123.47
28	Q	210	KC1	CBA-CAA-C2A	2.80	135.95	125.27
21	M	101	BCR	C3-C4-C5	-2.80	109.08	114.08
18	B	808	CLA	C4D-CHA-C1A	2.80	124.66	121.25
21	L	201	BCR	C15-C14-C13	-2.80	123.32	127.31
18	B	801	CLA	CHA-C1A-NA	-2.80	119.99	126.40
18	B	834	CLA	CHA-C1A-NA	-2.80	119.99	126.40
18	J	103	CLA	CHD-C1D-ND	-2.80	121.89	124.45
18	A	812	CLA	C4A-NA-C1A	2.79	107.96	106.71
24	O	215	DD6	C8-C6-C5	2.79	123.22	118.94
18	A	845	CLA	CHA-C1A-NA	-2.79	120.01	126.40
18	O	204	CLA	CHD-C1D-ND	-2.79	121.89	124.45
18	U	209	CLA	CHA-C1A-NA	-2.79	120.01	126.40
18	B	825	CLA	CHA-C1A-NA	-2.79	120.02	126.40
18	B	827	CLA	CHA-C1A-NA	-2.78	120.02	126.40
18	O	204	CLA	CHA-C1A-NA	-2.78	120.02	126.40
18	B	804	CLA	CHA-C1A-NA	-2.78	120.02	126.40
21	B	840	BCR	C2-C1-C6	2.78	114.76	110.48
21	L	205	BCR	C11-C10-C9	-2.78	123.34	127.31
18	B	845	CLA	CHA-C1A-NA	-2.78	120.04	126.40
18	B	803	CLA	CHA-C1A-NA	-2.77	120.05	126.40
18	B	848	CLA	CHA-C1A-NA	-2.77	120.05	126.40
18	A	832	CLA	CHA-C1A-NA	-2.77	120.06	126.40
18	A	825	CLA	CHA-C1A-NA	-2.76	120.07	126.40
29	U	202	A86	C8-C6-C5	2.76	123.18	118.94
21	M	101	BCR	C11-C10-C9	-2.76	123.36	127.31
18	A	813	CLA	CHA-C1A-NA	-2.76	120.07	126.40
29	R	206	A86	C24-C1-C2	2.76	123.18	118.94
18	O	209	CLA	C7-C6-C5	2.76	120.86	113.36
18	Q	212	CLA	C4A-NA-C1A	2.76	107.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	814	CLA	C4D-CHA-C1A	2.76	124.61	121.25
18	Q	208	CLA	CHA-C1A-NA	-2.76	120.08	126.40
18	R	205	CLA	CHA-C1A-NA	-2.76	120.08	126.40
29	T	201	A86	C24-C1-C2	2.76	123.17	118.94
18	B	809	CLA	CHA-C1A-NA	-2.76	120.09	126.40
18	O	209	CLA	CHA-C1A-NA	-2.75	120.09	126.40
18	B	832	CLA	CHA-C1A-NA	-2.75	120.09	126.40
25	B	842	DGD	O5D-C6D-C5D	-2.75	103.95	109.05
27	B	849	LMG	O1-C1-C2	-2.75	104.01	108.30
28	P	305	KC1	CHD-C1D-ND	-2.75	121.34	124.26
25	B	842	DGD	CDB-CCB-CBB	-2.75	100.46	114.42
24	P	316	DD6	C26-C25-C24	2.75	131.80	123.22
18	P	307	CLA	C4D-CHA-C1A	2.75	124.59	121.25
18	B	806	CLA	CHA-C1A-NA	-2.75	120.11	126.40
18	S	215	CLA	CHA-C1A-NA	-2.75	120.11	126.40
24	S	203	DD6	C13-C11-C10	2.74	123.15	118.94
21	J	104	BCR	C24-C23-C22	-2.74	122.09	126.23
18	U	207	CLA	CHD-C4C-NC	2.74	128.52	124.20
29	R	204	A86	C10-C9-C8	2.74	131.77	123.22
29	Q	214	A86	C40-C32-C31	2.74	112.92	110.47
18	O	207	CLA	CHA-C1A-NA	-2.74	120.13	126.40
18	B	821	CLA	C4D-CHA-C1A	2.74	124.58	121.25
18	A	834	CLA	C4A-NA-C1A	2.73	107.94	106.71
18	F	802	CLA	CHD-C1D-ND	-2.73	121.94	124.45
18	A	847	CLA	CHA-C1A-NA	-2.73	120.14	126.40
18	B	822	CLA	CHD-C1D-ND	-2.73	121.94	124.45
29	Q	214	A86	C8-C6-C5	2.73	123.13	118.94
18	B	844	CLA	CHA-C1A-NA	-2.73	120.15	126.40
18	Q	204	CLA	CHA-C1A-NA	-2.73	120.15	126.40
18	O	211	CLA	CAA-C2A-C3A	-2.73	109.73	116.10
18	A	811	CLA	CHA-C1A-NA	-2.73	120.15	126.40
18	A	826	CLA	CHA-C1A-NA	-2.73	120.16	126.40
18	A	801	CLA	CHA-C1A-NA	-2.73	120.16	126.40
18	O	202	CLA	CHA-C1A-NA	-2.72	120.16	126.40
18	A	823	CLA	CHA-C1A-NA	-2.72	120.16	126.40
28	S	210	KC1	CAC-C3C-C4C	2.72	128.34	124.81
18	T	212	CLA	C4A-NA-C1A	2.72	107.93	106.71
18	U	204	CLA	CHA-C1A-NA	-2.72	120.17	126.40
18	B	818	CLA	CHA-C1A-NA	-2.72	120.17	126.40
18	B	835	CLA	C3B-C4B-NB	-2.72	107.99	110.52
18	A	818	CLA	CHA-C1A-NA	-2.72	120.17	126.40
18	T	204	CLA	CHA-C1A-NA	-2.72	120.17	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Q	216	CLA	CHA-C1A-NA	-2.72	120.17	126.40
18	O	211	CLA	CHA-C1A-NA	-2.72	120.18	126.40
18	T	204	CLA	C4D-CHA-C1A	2.72	124.55	121.25
18	P	309	CLA	CHA-C1A-NA	-2.71	120.18	126.40
18	B	829	CLA	CHA-C1A-NA	-2.71	120.19	126.40
18	A	808	CLA	C1-O2A-CGA	2.71	123.56	116.44
18	A	849	CLA	CHA-C1A-NA	-2.71	120.19	126.40
18	A	852	CLA	CHA-C1A-NA	-2.71	120.19	126.40
18	T	210	CLA	C3B-C4B-NB	-2.71	108.00	110.52
18	B	822	CLA	CHA-C1A-NA	-2.71	120.19	126.40
18	B	820	CLA	C4A-NA-C1A	2.71	107.92	106.71
18	O	209	CLA	CHD-C1D-ND	-2.70	121.97	124.45
18	B	843	CLA	CHA-C1A-NA	-2.70	120.21	126.40
18	L	204	CLA	CHA-C1A-NA	-2.70	120.21	126.40
28	P	311	KC1	CAB-C3B-C4B	2.70	131.42	124.90
28	Q	210	KC1	C2A-C3A-C4A	2.70	108.49	106.49
29	Q	201	A86	C26-C25-C24	2.70	131.65	123.22
18	T	211	CLA	CHA-C1A-NA	-2.70	120.22	126.40
18	A	826	CLA	C4D-CHA-C1A	2.70	124.53	121.25
18	A	846	CLA	CHA-C1A-NA	-2.70	120.22	126.40
24	T	214	DD6	C37-C36-C31	-2.70	120.69	124.35
18	Q	207	CLA	CHA-C1A-NA	-2.70	120.23	126.40
18	B	833	CLA	CHA-C1A-NA	-2.69	120.23	126.40
18	B	802	CLA	C4D-CHA-C1A	2.69	124.53	121.25
18	T	205	CLA	CHA-C1A-NA	-2.69	120.23	126.40
18	Q	211	CLA	CHA-C1A-NA	-2.69	120.24	126.40
18	A	801	CLA	C4D-CHA-C1A	2.69	124.52	121.25
18	U	205	CLA	CHA-C1A-NA	-2.69	120.24	126.40
24	J	101	DD6	C4-C3-C2	2.69	128.98	123.47
18	P	312	CLA	CHA-C1A-NA	-2.69	120.25	126.40
18	U	208	CLA	CHA-C1A-NA	-2.69	120.25	126.40
18	R	202	CLA	CHA-C1A-NA	-2.69	120.25	126.40
18	T	206	CLA	CHA-C1A-NA	-2.69	120.25	126.40
18	A	824	CLA	CHA-C1A-NA	-2.68	120.26	126.40
18	B	816	CLA	CHA-C1A-NA	-2.68	120.26	126.40
18	A	831	CLA	CHA-C1A-NA	-2.68	120.27	126.40
28	S	208	KC1	CAB-C3B-C4B	2.68	131.36	124.90
21	B	839	BCR	C24-C23-C22	-2.68	122.19	126.23
18	S	205	CLA	CHA-C1A-NA	-2.67	120.27	126.40
18	T	202	CLA	C4A-NA-C1A	2.67	107.91	106.71
18	A	851	CLA	CHA-C1A-NA	-2.67	120.28	126.40
18	T	207	CLA	CHA-C1A-NA	-2.67	120.28	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	836	CLA	CHA-C1A-NA	-2.67	120.28	126.40
18	P	306	CLA	CHA-C1A-NA	-2.67	120.28	126.40
18	B	830	CLA	CHA-C1A-NA	-2.67	120.28	126.40
18	B	822	CLA	C4A-NA-C1A	2.67	107.91	106.71
18	A	847	CLA	C4A-NA-C1A	2.67	107.91	106.71
18	A	853	CLA	CHA-C1A-NA	-2.66	120.30	126.40
28	P	305	KC1	CHB-C4A-NA	2.66	128.39	124.20
18	A	830	CLA	CHA-C1A-NA	-2.66	120.31	126.40
18	A	827	CLA	CHA-C1A-NA	-2.66	120.31	126.40
29	Q	214	A86	C24-C1-C2	2.66	123.02	118.94
18	A	810	CLA	CHA-C1A-NA	-2.66	120.31	126.40
28	T	209	KC1	CAB-C3B-C4B	2.66	131.31	124.90
18	B	813	CLA	CHA-C1A-NA	-2.65	120.32	126.40
21	L	205	BCR	C27-C26-C25	2.65	126.58	122.73
27	U	201	LMG	O6-C1-O1	-2.65	103.69	109.97
20	R	201	LHG	C11-C10-C9	-2.65	100.96	114.42
24	U	203	DD6	C13-C11-C10	2.65	123.01	118.94
18	A	833	CLA	CHA-C1A-NA	-2.65	120.33	126.40
18	T	210	CLA	CHA-C1A-NA	-2.65	120.33	126.40
18	A	816	CLA	CHA-C1A-NA	-2.65	120.33	126.40
18	B	845	CLA	C4A-NA-C1A	2.65	107.90	106.71
18	A	820	CLA	CHA-C1A-NA	-2.65	120.33	126.40
18	B	817	CLA	CHA-C1A-NA	-2.65	120.34	126.40
18	Q	205	CLA	CHA-C1A-NA	-2.65	120.34	126.40
18	B	804	CLA	C4D-CHA-C1A	2.64	124.47	121.25
18	Q	213	CLA	CHA-C1A-NA	-2.64	120.35	126.40
18	T	203	CLA	CHA-C1A-NA	-2.64	120.35	126.40
18	B	823	CLA	CHD-C1D-ND	-2.64	122.03	124.45
18	A	819	CLA	CHA-C1A-NA	-2.63	120.36	126.40
22	A	848	CL0	C4D-CHA-C1A	2.63	124.45	121.25
18	S	204	CLA	CHA-C1A-NA	-2.63	120.37	126.40
18	A	838	CLA	CHA-C1A-NA	-2.63	120.37	126.40
18	A	805	CLA	CHA-C1A-NA	-2.63	120.38	126.40
29	Q	201	A86	C24-C1-C2	2.63	122.97	118.94
18	S	206	CLA	CHA-C1A-NA	-2.63	120.38	126.40
18	U	211	CLA	CHA-C1A-NA	-2.62	120.39	126.40
18	B	810	CLA	CHA-C1A-NA	-2.62	120.40	126.40
18	O	209	CLA	C4D-CHA-C1A	2.62	124.44	121.25
18	B	812	CLA	CHA-C1A-NA	-2.62	120.40	126.40
18	P	307	CLA	CHA-C1A-NA	-2.62	120.40	126.40
24	O	214	DD6	C4-C3-C2	2.62	128.83	123.47
21	B	838	BCR	C33-C5-C6	-2.61	121.59	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	835	CLA	CHA-C1A-NA	-2.61	120.42	126.40
18	B	807	CLA	CHA-C1A-NA	-2.61	120.42	126.40
18	S	207	CLA	CHA-C1A-NA	-2.61	120.42	126.40
18	A	809	CLA	CHA-C1A-NA	-2.61	120.42	126.40
18	S	201	CLA	CHA-C1A-NA	-2.61	120.42	126.40
18	B	805	CLA	CHA-C1A-NA	-2.61	120.43	126.40
18	U	210	CLA	CHA-C1A-NA	-2.60	120.43	126.40
29	R	206	A86	C28-C27-C26	-2.60	119.28	122.92
18	A	829	CLA	CHA-C1A-NA	-2.60	120.44	126.40
18	P	308	CLA	CHA-C1A-NA	-2.60	120.44	126.40
29	R	206	A86	C20-C19-C18	-2.60	107.60	112.75
18	S	214	CLA	CHA-C1A-NA	-2.60	120.45	126.40
18	O	206	CLA	CHA-C1A-NA	-2.60	120.45	126.40
21	B	837	BCR	C29-C30-C25	2.59	114.47	110.48
28	P	305	KC1	C2A-C3A-C4A	2.59	108.41	106.49
18	B	811	CLA	CHA-C1A-NA	-2.59	120.46	126.40
18	U	210	CLA	C4A-NA-C1A	2.59	107.87	106.71
21	A	844	BCR	C27-C26-C25	2.59	126.49	122.73
18	B	814	CLA	CHA-C1A-NA	-2.58	120.48	126.40
24	S	212	DD6	C24-C1-C2	2.58	122.91	118.94
18	B	808	CLA	CHA-C1A-NA	-2.58	120.49	126.40
24	P	316	DD6	C4-C5-C6	2.58	130.99	127.31
18	B	818	CLA	CHC-C4B-NB	-2.58	121.53	124.26
18	S	206	CLA	C4D-CHA-C1A	2.58	124.39	121.25
21	L	201	BCR	C15-C16-C17	-2.58	118.20	123.47
18	Q	213	CLA	C1-O2A-CGA	2.58	123.20	116.44
18	Q	212	CLA	C4D-CHA-C1A	2.57	124.38	121.25
18	F	803	CLA	CHA-C1A-NA	-2.57	120.50	126.40
27	Q	217	LMG	O1-C1-C2	-2.57	104.29	108.30
29	P	303	A86	C24-C1-C2	2.57	122.88	118.94
18	A	803	CLA	CHD-C1D-C2D	2.57	130.87	125.48
27	Q	217	LMG	O3-C3-C2	-2.57	104.42	110.35
24	S	209	DD6	O1-C20-C19	-2.57	111.45	113.38
18	O	208	CLA	CHA-C1A-NA	-2.57	120.52	126.40
18	Q	203	CLA	C1-O2A-CGA	2.57	123.18	116.44
18	B	846	CLA	CHA-C1A-NA	-2.57	120.52	126.40
18	A	808	CLA	CHA-C1A-NA	-2.56	120.53	126.40
27	P	301	LMG	C1-O6-C5	-2.56	108.66	113.69
29	R	204	A86	C28-C27-C29	-2.56	112.99	118.93
20	A	839	LHG	O8-C23-C24	2.56	119.94	111.91
29	P	303	A86	C20-C19-C18	-2.56	107.69	112.75
18	A	804	CLA	CHA-C1A-NA	-2.56	120.54	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Q	203	CLA	CHA-C1A-NA	-2.55	120.55	126.40
28	P	305	KC1	C4D-C3D-CAD	2.55	109.14	107.42
18	B	834	CLA	C4A-NA-C1A	2.55	107.85	106.71
18	L	202	CLA	C4A-NA-C1A	2.55	107.85	106.71
28	P	302	KC1	CAB-C3B-C4B	2.55	131.05	124.90
18	S	201	CLA	CHD-C1D-C2D	2.55	130.82	125.48
18	B	826	CLA	CHA-C1A-NA	-2.54	120.58	126.40
18	O	205	CLA	CHA-C1A-NA	-2.54	120.58	126.40
24	S	213	DD6	C29-C30-C31	-2.54	169.00	175.43
24	Q	202	DD6	C13-C11-C10	2.54	122.83	118.94
26	M	102	SQD	O5-C5-C4	2.53	114.30	109.69
21	F	801	BCR	C24-C23-C22	-2.53	122.41	126.23
18	A	823	CLA	CHD-C1D-ND	-2.53	122.13	124.45
18	S	207	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
18	P	310	CLA	CHA-C1A-NA	-2.53	120.61	126.40
24	O	213	DD6	C24-C1-C2	2.53	122.82	118.94
24	P	304	DD6	C8-C6-C5	2.53	122.82	118.94
18	A	806	CLA	CHA-C1A-NA	-2.53	120.61	126.40
24	O	215	DD6	C23-C16-C17	-2.52	104.60	108.98
28	S	210	KC1	O2D-CGD-CBD	2.52	115.75	111.27
18	B	831	CLA	CHA-C1A-NA	-2.52	120.62	126.40
24	T	213	DD6	C24-C1-C2	2.52	122.81	118.94
18	A	831	CLA	CHC-C4B-NB	-2.52	121.59	124.26
18	A	813	CLA	CHC-C4B-NB	-2.52	121.59	124.26
18	Q	206	CLA	CHA-C1A-NA	-2.52	120.63	126.40
18	Q	204	CLA	C4A-NA-C1A	2.52	107.84	106.71
24	O	215	DD6	C37-C36-C31	-2.52	120.93	124.35
24	O	214	DD6	C13-C11-C10	2.51	122.80	118.94
21	M	101	BCR	C15-C14-C13	-2.51	123.73	127.31
18	L	203	CLA	CHA-C1A-NA	-2.51	120.66	126.40
18	T	208	CLA	CHA-C1A-NA	-2.50	120.67	126.40
29	R	206	A86	C23-C16-C17	-2.50	104.64	108.98
21	I	102	BCR	C2-C1-C6	2.50	114.33	110.48
18	J	103	CLA	CHC-C4B-NB	-2.50	121.61	124.26
18	A	808	CLA	CAA-CBA-CGA	-2.50	105.96	113.25
24	Q	215	DD6	C13-C11-C10	2.49	122.77	118.94
21	R	203	BCR	C39-C30-C25	-2.49	106.25	110.30
18	Q	211	CLA	C4D-CHA-C1A	2.49	124.28	121.25
28	S	208	KC1	C4D-C3D-CAD	2.49	109.10	107.42
18	B	824	CLA	CHA-C1A-NA	-2.49	120.70	126.40
21	I	101	BCR	C3-C4-C5	-2.49	109.64	114.08
24	O	213	DD6	C12-C11-C13	2.48	121.99	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	848	CLA	CHC-C4B-NB	-2.48	121.63	124.26
18	S	207	CLA	CHD-C1D-C2D	2.48	130.68	125.48
24	O	214	DD6	C24-C1-C2	2.47	122.74	118.94
18	U	206	CLA	CHA-C1A-NA	-2.47	120.73	126.40
28	S	210	KC1	CGD-CBD-CAD	-2.47	102.72	110.73
18	A	810	CLA	CHC-C4B-NB	-2.47	121.64	124.26
24	U	212	DD6	C26-C25-C24	2.47	130.93	123.22
18	O	211	CLA	C4A-NA-C1A	2.47	107.82	106.71
18	P	312	CLA	CAA-C2A-C3A	-2.46	110.36	116.10
18	B	809	CLA	C4A-NA-C1A	2.46	107.81	106.71
24	U	212	DD6	C14-C13-C11	2.46	129.34	125.53
18	B	815	CLA	CHA-C1A-NA	-2.46	120.77	126.40
21	A	842	BCR	C27-C26-C25	2.46	126.30	122.73
21	J	104	BCR	C27-C26-C25	2.46	126.30	122.73
24	O	215	DD6	O1-C20-C19	-2.45	111.54	113.38
18	B	824	CLA	CAA-CBA-CGA	-2.45	106.08	113.25
28	P	311	KC1	CHC-C4B-C3B	2.45	129.45	125.26
18	B	821	CLA	CHA-C1A-NA	-2.45	120.78	126.40
24	S	213	DD6	C8-C6-C5	2.45	122.70	118.94
21	F	804	BCR	C27-C26-C25	2.45	126.28	122.73
18	B	815	CLA	CHD-C1D-C2D	2.45	130.61	125.48
18	F	803	CLA	CHC-C4B-NB	-2.44	121.67	124.26
18	S	204	CLA	CHC-C4B-NB	-2.44	121.68	124.26
18	Q	209	CLA	CHA-C1A-NA	-2.44	120.82	126.40
21	A	843	BCR	C29-C30-C25	2.44	114.23	110.48
18	B	802	CLA	CHD-C1D-ND	-2.44	122.22	124.45
18	B	820	CLA	C4D-CHA-C1A	2.44	124.21	121.25
18	T	210	CLA	CHD-C1D-C2D	2.43	130.58	125.48
24	U	212	DD6	O1-C20-C19	-2.43	111.56	113.38
18	A	803	CLA	CHA-C1A-NA	-2.43	120.83	126.40
20	A	840	LHG	C11-C10-C9	-2.43	102.10	114.42
24	P	316	DD6	C37-C36-C31	-2.43	121.05	124.35
18	A	817	CLA	CHC-C4B-NB	-2.42	121.69	124.26
18	T	210	CLA	CHC-C4B-NB	-2.42	121.70	124.26
24	J	101	DD6	C24-C1-C2	2.42	122.65	118.94
18	B	808	CLA	CHD-C1D-ND	-2.42	122.23	124.45
24	Q	202	DD6	O1-C20-C19	-2.41	111.57	113.38
18	R	202	CLA	C1D-ND-C4D	2.41	108.05	106.33
28	Q	210	KC1	CHD-C1D-ND	-2.41	121.71	124.26
18	B	846	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
21	A	841	BCR	C28-C27-C26	-2.40	109.78	114.08
18	B	825	CLA	C4A-NA-C1A	2.40	107.79	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L	201	BCR	C27-C26-C25	2.40	126.22	122.73
28	P	311	KC1	CHB-C4A-NA	2.40	127.99	124.20
27	B	849	LMG	O6-C1-O1	-2.40	104.29	109.97
18	B	813	CLA	O2A-C1-C2	-2.40	103.36	108.97
24	O	212	DD6	C10-C9-C8	2.40	130.70	123.22
24	S	203	DD6	C33-C32-C31	2.40	114.48	109.62
18	A	817	CLA	C4A-NA-C1A	2.39	107.78	106.71
21	B	837	BCR	C33-C5-C6	-2.39	121.84	124.53
27	S	211	LMG	C6-C5-C4	-2.39	107.40	113.00
21	B	839	BCR	C27-C26-C25	2.39	126.20	122.73
18	B	815	CLA	CHC-C4B-NB	-2.39	121.73	124.26
18	B	846	CLA	CHC-C4B-NB	-2.39	121.73	124.26
21	B	838	BCR	C15-C14-C13	-2.39	123.90	127.31
24	U	203	DD6	C33-C32-C31	2.39	114.46	109.62
18	B	835	CLA	CHC-C4B-NB	-2.39	121.73	124.26
18	T	208	CLA	CHC-C4B-NB	-2.39	121.73	124.26
18	B	827	CLA	CHC-C4B-NB	-2.38	121.73	124.26
18	A	836	CLA	C1-O2A-CGA	2.38	122.70	116.44
18	B	832	CLA	C4A-NA-C1A	2.38	107.78	106.71
21	R	203	BCR	C33-C5-C6	-2.38	121.85	124.53
28	P	302	KC1	CHC-C4B-C3B	2.38	129.33	125.26
21	B	837	BCR	C28-C27-C26	-2.38	109.83	114.08
18	A	820	CLA	O2A-C1-C2	2.38	114.88	108.64
24	P	317	DD6	C22-C16-C17	-2.38	104.86	108.98
18	S	214	CLA	CHD-C1D-C2D	2.37	130.46	125.48
24	S	213	DD6	C26-C25-C24	2.37	130.62	123.22
21	F	801	BCR	C16-C15-C14	-2.37	118.61	123.47
18	B	822	CLA	CHC-C4B-NB	-2.37	121.75	124.26
27	Q	217	LMG	O1-C7-C8	-2.37	105.19	110.90
25	B	842	DGD	CFB-CEB-CDB	-2.37	102.41	114.42
28	S	208	KC1	CHC-C4B-C3B	2.37	129.31	125.26
18	A	832	CLA	C4A-NA-C1A	2.36	107.77	106.71
18	A	847	CLA	CHC-C4B-NB	-2.36	121.75	124.26
18	A	814	CLA	CHC-C4B-NB	-2.36	121.75	124.26
18	S	201	CLA	CGD-CBD-CAD	-2.36	103.08	110.73
26	B	847	SQD	C1-C2-C3	2.36	114.91	110.00
18	T	208	CLA	C4B-CHC-C1C	2.36	131.94	126.34
29	T	201	A86	C22-C16-C17	-2.36	104.88	108.98
21	A	842	BCR	C2-C1-C6	2.36	114.11	110.48
25	B	842	DGD	O6D-C1D-O3G	-2.36	104.39	109.97
18	U	207	CLA	CHA-C1A-NA	-2.35	121.01	126.40
18	A	822	CLA	CHD-C1D-C2D	2.35	130.41	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	U	207	CLA	CHD-C1D-C2D	2.34	130.39	125.48
18	O	203	CLA	CHC-C4B-NB	-2.34	121.78	124.26
21	L	201	BCR	C7-C8-C9	-2.34	122.70	126.23
21	R	203	BCR	C24-C23-C22	-2.34	122.70	126.23
24	P	316	DD6	C22-C16-C17	-2.34	104.92	108.98
18	A	852	CLA	C4A-NA-C1A	2.34	107.76	106.71
18	A	847	CLA	CHD-C1D-C2D	2.34	130.39	125.48
18	T	212	CLA	CHC-C4B-NB	-2.34	121.78	124.26
24	P	304	DD6	C41-C32-C31	-2.33	106.76	110.47
18	B	824	CLA	CHD-C1D-C2D	2.33	130.37	125.48
18	P	313	CLA	C4A-NA-C1A	2.33	107.75	106.71
18	Q	211	CLA	CAA-C2A-C3A	-2.33	110.66	116.10
18	B	833	CLA	C4A-NA-C1A	2.33	107.75	106.71
18	B	835	CLA	C4A-NA-C1A	2.33	107.75	106.71
18	Q	208	CLA	C4A-NA-C1A	2.33	107.75	106.71
28	P	311	KC1	C4D-C3D-CAD	2.32	108.99	107.42
21	A	844	BCR	C2-C1-C6	2.32	114.06	110.48
27	Q	217	LMG	O2-C2-C1	-2.32	104.41	110.05
18	A	822	CLA	CHA-C1A-NA	-2.32	121.08	126.40
27	Q	217	LMG	C40-C39-C38	-2.32	102.67	114.42
18	U	206	CLA	CHC-C4B-NB	-2.32	121.81	124.26
18	T	202	CLA	CHC-C4B-NB	-2.32	121.81	124.26
18	B	817	CLA	CHD-C1D-ND	-2.31	122.33	124.45
21	B	839	BCR	C2-C1-C6	2.31	114.04	110.48
21	R	203	BCR	C29-C30-C25	2.31	114.04	110.48
24	U	214	DD6	C26-C25-C24	2.31	130.41	123.22
21	I	101	BCR	C28-C27-C26	-2.31	109.96	114.08
28	P	311	KC1	CAC-C3C-C4C	2.30	127.80	124.81
21	R	203	BCR	C40-C30-C39	-2.30	101.47	108.53
28	Q	210	KC1	CHC-C4B-C3B	2.30	129.19	125.26
24	P	317	DD6	C13-C11-C10	2.30	122.47	118.94
20	R	201	LHG	C20-C19-C18	-2.29	102.79	114.42
18	O	203	CLA	C4A-NA-C1A	2.29	107.73	106.71
18	A	815	CLA	C3B-C4B-NB	-2.29	108.39	110.52
21	I	101	BCR	C15-C14-C13	-2.28	124.05	127.31
29	P	303	A86	C28-C27-C26	-2.28	119.73	122.92
21	B	838	BCR	C11-C10-C9	-2.28	124.06	127.31
18	O	207	CLA	CHC-C4B-NB	-2.28	121.84	124.26
24	P	304	DD6	C33-C32-C31	2.28	114.23	109.62
18	U	209	CLA	CHC-C4B-NB	-2.27	121.85	124.26
18	A	804	CLA	C1-O2A-CGA	2.27	122.41	116.44
21	B	841	BCR	C27-C26-C25	2.27	126.03	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Q	205	CLA	CHD-C1D-C2D	2.27	130.24	125.48
18	T	208	CLA	O2A-C1-C2	2.27	114.60	108.64
18	F	803	CLA	CHD-C1D-C2D	2.27	130.24	125.48
28	P	302	KC1	CHB-C4A-C3A	-2.27	121.43	124.98
18	A	846	CLA	C4A-NA-C1A	2.27	107.73	106.71
18	Q	213	CLA	C4A-NA-C1A	2.27	107.73	106.71
18	B	833	CLA	CHD-C1D-C2D	2.27	130.24	125.48
21	B	838	BCR	C29-C30-C25	2.26	113.97	110.48
21	B	838	BCR	C28-C27-C26	-2.26	110.04	114.08
24	O	212	DD6	C13-C11-C10	2.26	122.41	118.94
18	P	312	CLA	CHD-C1D-C2D	2.26	130.22	125.48
24	T	213	DD6	C37-C36-C31	-2.26	121.28	124.35
18	T	208	CLA	CMC-C2C-C1C	2.26	128.48	125.04
21	A	844	BCR	C15-C14-C13	-2.26	124.09	127.31
24	O	213	DD6	C3-C4-C5	2.25	128.09	123.47
28	O	210	KC1	CBA-CAA-C2A	2.25	133.86	125.27
18	B	818	CLA	CHD-C1D-C2D	2.25	130.21	125.48
21	A	842	BCR	C15-C16-C17	-2.25	118.87	123.47
18	T	207	CLA	CHC-C4B-NB	-2.25	121.88	124.26
21	M	101	BCR	C15-C16-C17	-2.25	118.87	123.47
18	B	826	CLA	CHD-C1D-C2D	2.25	130.19	125.48
29	U	202	A86	C28-C27-C26	-2.24	119.78	122.92
18	B	832	CLA	CHD-C1D-C2D	2.24	130.18	125.48
18	Q	207	CLA	C1-O2A-CGA	2.24	123.49	116.11
18	A	831	CLA	CHD-C1D-C2D	2.24	130.18	125.48
26	B	847	SQD	O48-C23-C24	2.24	118.93	111.91
18	Q	216	CLA	CHD-C1D-C2D	2.24	130.18	125.48
24	O	213	DD6	C37-C36-C31	-2.24	121.31	124.35
24	S	212	DD6	C10-C9-C8	2.24	130.19	123.22
21	B	840	BCR	C27-C26-C25	2.24	125.98	122.73
18	Q	204	CLA	O2A-C1-C2	2.23	114.50	108.64
21	F	801	BCR	C27-C26-C25	2.23	125.97	122.73
18	A	805	CLA	CHD-C1D-C2D	2.23	130.16	125.48
29	Q	214	A86	C17-C16-C15	2.23	111.44	109.16
27	Q	217	LMG	C38-C37-C36	-2.23	103.11	114.42
27	Q	217	LMG	C42-C41-C40	-2.23	103.11	114.42
28	U	213	KC1	C2A-C3A-C4A	2.23	108.14	106.49
18	U	206	CLA	CHD-C1D-C2D	2.22	130.15	125.48
18	A	804	CLA	CAA-CBA-CGA	2.22	119.75	113.25
18	A	853	CLA	CMD-C2D-C1D	2.22	128.62	124.71
29	R	204	A86	C12-C11-C10	-2.22	118.06	123.42
18	B	806	CLA	C4A-NA-C1A	2.22	107.70	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	841	BCR	C10-C11-C12	-2.22	116.30	123.22
18	B	801	CLA	C1D-ND-C4D	2.22	107.91	106.33
18	Q	212	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
18	A	815	CLA	CHC-C4B-NB	-2.21	121.91	124.26
18	A	829	CLA	CHD-C1D-C2D	2.21	130.12	125.48
24	S	203	DD6	C10-C9-C8	2.21	130.11	123.22
18	P	307	CLA	C1-O2A-CGA	2.21	122.24	116.44
18	B	807	CLA	CHD-C1D-C2D	2.21	130.11	125.48
18	B	812	CLA	CHD-C1D-C2D	2.21	130.11	125.48
18	T	206	CLA	C1-O2A-CGA	2.20	123.36	116.11
18	B	819	CLA	C2A-C1A-CHA	2.20	127.71	123.86
21	M	101	BCR	C27-C26-C25	2.20	125.92	122.73
18	O	204	CLA	C4A-NA-C1A	2.20	107.69	106.71
21	I	102	BCR	C15-C16-C17	-2.20	118.97	123.47
18	A	816	CLA	CHD-C1D-C2D	2.20	130.09	125.48
18	A	824	CLA	CHD-C1D-C2D	2.20	130.09	125.48
18	B	823	CLA	O2A-C1-C2	-2.20	102.86	108.64
18	B	817	CLA	C3B-C4B-NB	-2.20	108.48	110.52
28	U	213	KC1	CAA-C2A-C1A	2.19	134.83	124.75
28	S	210	KC1	C2A-C3A-C4A	2.19	108.11	106.49
18	A	804	CLA	CHD-C1D-C2D	2.19	130.08	125.48
24	T	213	DD6	C33-C34-C35	2.19	113.30	110.30
18	O	202	CLA	CHC-C4B-NB	-2.19	121.94	124.26
28	O	210	KC1	C4D-C3D-CAD	2.19	108.90	107.42
18	A	823	CLA	C4A-NA-C1A	2.19	107.69	106.71
18	A	827	CLA	C4A-NA-C1A	2.19	107.69	106.71
24	U	212	DD6	C4-C3-C2	2.19	127.95	123.47
21	R	203	BCR	C27-C26-C25	2.19	125.90	122.73
24	U	203	DD6	C28-C27-C29	-2.18	112.51	116.84
18	A	836	CLA	CAA-C2A-C1A	2.18	119.13	111.97
18	U	210	CLA	CHD-C1D-C2D	2.18	130.06	125.48
18	B	829	CLA	CHD-C1D-C2D	2.18	130.06	125.48
25	B	842	DGD	CBB-CAB-C9B	-2.18	103.34	114.42
18	P	306	CLA	CHD-C1D-C2D	2.18	130.06	125.48
18	A	830	CLA	CHD-C1D-C2D	2.18	130.06	125.48
25	B	842	DGD	O2D-C2D-C1D	-2.18	104.75	110.05
20	A	839	LHG	C11-C10-C9	-2.18	103.35	114.42
21	B	837	BCR	C7-C8-C9	-2.18	122.94	126.23
21	A	843	BCR	C28-C27-C26	-2.18	110.18	114.08
18	T	211	CLA	CHC-C4B-NB	-2.18	121.95	124.26
18	O	202	CLA	CHD-C1D-C2D	2.18	130.05	125.48
18	B	833	CLA	CHC-C4B-NB	-2.17	121.96	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	O	213	DD6	C34-C35-C36	2.17	116.18	111.85
28	P	302	KC1	C1A-C2A-C3A	-2.17	105.39	107.11
18	O	208	CLA	CHD-C1D-C2D	2.17	130.03	125.48
24	S	213	DD6	C34-C35-C36	2.16	116.17	111.85
18	Q	212	CLA	C2A-C1A-CHA	2.16	127.64	123.86
18	B	817	CLA	CHC-C4B-NB	-2.16	121.97	124.26
18	B	845	CLA	CHC-C4B-NB	-2.16	121.97	124.26
21	F	801	BCR	C7-C8-C9	-2.16	122.97	126.23
21	I	101	BCR	C29-C30-C25	2.16	113.80	110.48
21	R	203	BCR	C16-C15-C14	-2.16	119.06	123.47
18	S	214	CLA	CMD-C2D-C1D	2.15	128.51	124.71
24	S	209	DD6	C8-C6-C5	2.15	122.25	118.94
28	P	305	KC1	CMD-C2D-C1D	2.15	128.65	125.37
18	O	205	CLA	CHD-C1D-C2D	2.15	130.00	125.48
18	A	821	CLA	C2A-C1A-CHA	2.15	127.62	123.86
18	U	208	CLA	CHD-C1D-C2D	2.15	129.99	125.48
28	T	209	KC1	C1A-C2A-C3A	-2.15	105.41	107.11
24	O	214	DD6	O1-C20-C19	-2.15	111.77	113.38
21	A	841	BCR	C29-C30-C25	2.15	113.79	110.48
18	P	315	CLA	CAA-C2A-C1A	2.15	119.02	111.97
20	A	839	LHG	C18-C17-C16	-2.15	103.52	114.42
18	R	205	CLA	CAA-C2A-C1A	2.15	119.01	111.97
21	B	838	BCR	C15-C16-C17	-2.15	119.08	123.47
18	B	830	CLA	C4A-NA-C1A	2.15	107.67	106.71
18	P	308	CLA	CHD-C1D-C2D	2.15	129.98	125.48
18	U	208	CLA	CHC-C4B-NB	-2.15	121.98	124.26
18	T	212	CLA	CHD-C1D-C2D	2.15	129.98	125.48
18	Q	204	CLA	CHD-C1D-C2D	2.14	129.98	125.48
18	A	821	CLA	C1D-ND-C4D	2.14	107.86	106.33
28	Q	210	KC1	C4D-C3D-CAD	2.14	108.87	107.42
24	S	209	DD6	C22-C16-C17	-2.14	105.27	108.98
24	T	214	DD6	C13-C11-C10	2.14	122.22	118.94
24	S	213	DD6	C13-C11-C10	2.14	122.22	118.94
18	R	202	CLA	CHD-C1D-C2D	2.14	129.96	125.48
24	S	213	DD6	C20-C19-C18	-2.14	108.52	112.75
18	B	819	CLA	CHD-C1D-C2D	2.14	129.96	125.48
18	B	844	CLA	C2D-C1D-ND	-2.13	108.53	110.10
27	J	102	LMG	O3-C3-C2	-2.13	105.42	110.35
21	A	844	BCR	C15-C16-C17	-2.13	119.10	123.47
18	A	813	CLA	C4A-NA-C1A	2.13	107.67	106.71
18	T	203	CLA	CHD-C1D-C2D	2.13	129.95	125.48
24	S	202	DD6	C13-C11-C10	2.13	122.21	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	848	CL0	CHC-C4B-NB	2.13	126.51	124.26
18	P	307	CLA	CHD-C1D-C2D	2.13	129.94	125.48
18	A	806	CLA	CHD-C1D-C2D	2.13	129.94	125.48
18	B	848	CLA	CHD-C1D-C2D	2.13	129.94	125.48
18	A	819	CLA	CHD-C1D-C2D	2.12	129.94	125.48
18	A	853	CLA	CHC-C4B-NB	-2.12	122.01	124.26
21	B	840	BCR	C8-C7-C6	-2.12	121.24	127.20
18	T	211	CLA	CHD-C1D-C2D	2.12	129.93	125.48
18	P	308	CLA	C4A-NA-C1A	2.12	107.66	106.71
24	S	212	DD6	C28-C27-C29	2.12	121.04	116.84
21	A	842	BCR	C15-C14-C13	-2.12	124.28	127.31
29	Q	201	A86	C25-C24-C1	2.12	132.37	126.42
21	J	104	BCR	C15-C16-C17	-2.12	119.13	123.47
27	S	211	LMG	O6-C1-O1	-2.12	104.96	109.97
18	A	853	CLA	CHD-C1D-C2D	2.12	129.92	125.48
27	B	849	LMG	C1-O6-C5	-2.12	109.53	113.69
18	B	814	CLA	CAC-C3C-C4C	2.11	127.55	124.81
18	B	809	CLA	C1D-ND-C4D	2.11	107.84	106.33
20	R	201	LHG	C27-C26-C25	-2.11	103.70	114.42
18	A	835	CLA	C3B-C4B-NB	-2.11	108.56	110.52
18	B	817	CLA	CHB-C1B-NB	2.11	126.49	124.26
24	O	214	DD6	C25-C26-C27	2.11	132.71	126.58
18	L	204	CLA	CHD-C1D-C2D	2.11	129.90	125.48
18	U	209	CLA	C2A-C1A-CHA	2.11	127.55	123.86
27	S	211	LMG	C38-C37-C36	-2.11	103.73	114.42
18	B	820	CLA	C2A-C1A-CHA	2.11	127.54	123.86
24	T	213	DD6	C28-C27-C29	2.11	121.01	116.84
18	B	827	CLA	CHD-C1D-C2D	2.10	129.90	125.48
18	Q	207	CLA	CHD-C1D-C2D	2.10	129.90	125.48
21	M	101	BCR	C35-C13-C14	-2.10	119.98	122.92
24	O	215	DD6	C12-C11-C13	2.10	121.39	118.08
18	Q	203	CLA	CHD-C1D-C2D	2.10	129.89	125.48
18	T	206	CLA	CHD-C1D-C2D	2.10	129.88	125.48
18	T	205	CLA	O2A-C1-C2	2.10	114.15	108.64
29	T	201	A86	C26-C25-C24	2.10	129.77	123.22
29	U	202	A86	C24-C1-C2	2.10	122.16	118.94
18	B	803	CLA	C4A-NA-C1A	2.10	107.65	106.71
21	I	101	BCR	C10-C11-C12	-2.09	116.68	123.22
18	B	816	CLA	CHD-C1D-C2D	2.09	129.87	125.48
18	U	204	CLA	CAA-CBA-CGA	2.09	119.37	113.25
26	M	102	SQD	C44-O6-C1	2.09	117.83	113.74
18	A	807	CLA	C1D-ND-C4D	2.09	107.82	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	830	CLA	CAC-C3C-C4C	2.09	127.52	124.81
18	A	813	CLA	C1-O2A-CGA	2.09	121.93	116.44
18	S	201	CLA	C4A-NA-C1A	2.09	107.65	106.71
18	P	309	CLA	CHD-C1D-C2D	2.09	129.87	125.48
18	B	835	CLA	C1D-ND-C4D	2.09	107.82	106.33
18	B	824	CLA	C6-C5-C3	2.09	118.93	113.45
21	B	841	BCR	C8-C7-C6	-2.09	121.34	127.20
22	A	848	CL0	C5-C3-C2	2.09	125.34	121.12
18	B	805	CLA	CHD-C1D-C2D	2.09	129.86	125.48
27	B	849	LMG	O3-C3-C2	-2.09	105.53	110.35
18	B	802	CLA	C2A-C1A-CHA	2.08	127.50	123.86
18	P	313	CLA	CHD-C1D-C2D	2.08	129.85	125.48
18	A	828	CLA	C4A-NA-C1A	2.08	107.64	106.71
18	B	817	CLA	O2A-C1-C2	2.08	114.11	108.64
18	A	810	CLA	CHD-C1D-C2D	2.08	129.85	125.48
18	O	211	CLA	CHD-C1D-C2D	2.08	129.84	125.48
18	A	820	CLA	O2D-CGD-CBD	2.08	114.96	111.27
18	B	833	CLA	C2D-C1D-ND	-2.08	108.57	110.10
20	A	839	LHG	C27-C26-C25	-2.08	103.88	114.42
18	L	203	CLA	CHD-C1D-C2D	2.08	129.84	125.48
25	B	842	DGD	O3E-C3E-C2E	-2.08	105.55	110.35
24	O	214	DD6	C10-C9-C8	2.07	129.69	123.22
28	P	302	KC1	CHB-C4A-NA	2.07	127.47	124.20
18	T	211	CLA	C1C-C2C-C3C	2.07	109.14	106.96
29	U	202	A86	C20-C19-C18	-2.07	108.65	112.75
18	O	208	CLA	CAA-CBA-CGA	2.07	119.31	113.25
21	B	840	BCR	C35-C13-C14	-2.07	120.02	122.92
18	U	211	CLA	C4A-NA-C1A	2.07	107.64	106.71
18	B	815	CLA	C3B-C4B-NB	-2.07	108.59	110.52
21	F	804	BCR	C16-C15-C14	-2.07	119.24	123.47
24	S	212	DD6	C13-C11-C10	2.07	122.11	118.94
28	O	210	KC1	CHB-C4A-NA	2.07	127.46	124.20
18	B	821	CLA	CHD-C1D-C2D	2.07	129.81	125.48
21	I	101	BCR	C16-C15-C14	-2.07	119.24	123.47
18	S	206	CLA	CHD-C1D-C2D	2.06	129.81	125.48
27	S	211	LMG	O3-C3-C2	-2.06	105.58	110.35
18	A	820	CLA	CHD-C1D-C2D	2.06	129.80	125.48
18	B	803	CLA	C2A-C1A-CHA	2.06	127.45	123.86
21	R	203	BCR	C17-C16-C15	-2.06	120.23	124.81
18	B	829	CLA	CHC-C4B-NB	-2.06	122.08	124.26
28	S	210	KC1	CAA-C2A-C1A	2.05	134.18	124.75
18	O	204	CLA	C1D-ND-C4D	2.05	107.79	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	833	CLA	C4A-NA-C1A	2.05	107.63	106.71
24	U	214	DD6	C33-C32-C31	2.05	113.78	109.62
24	O	201	DD6	C26-C25-C24	2.05	129.62	123.22
18	U	207	CLA	C3A-C2A-C1A	-2.05	98.27	101.34
24	Q	215	DD6	C22-C16-C17	-2.05	105.42	108.98
18	O	206	CLA	C4A-NA-C1A	2.05	107.63	106.71
21	I	101	BCR	C16-C17-C18	-2.05	124.39	127.31
18	B	829	CLA	C3B-C4B-NB	-2.05	108.61	110.52
21	B	838	BCR	C38-C26-C27	-2.05	109.68	113.62
18	B	825	CLA	CHD-C1D-C2D	2.05	129.77	125.48
21	B	841	BCR	C33-C5-C6	-2.05	122.23	124.53
18	A	810	CLA	C4A-NA-C1A	2.04	107.62	106.71
18	B	801	CLA	CHD-C1D-C2D	2.04	129.76	125.48
18	U	204	CLA	C4A-NA-C1A	2.04	107.62	106.71
18	T	210	CLA	CAA-C2A-C3A	-2.04	111.34	116.10
18	B	844	CLA	CHD-C1D-C2D	2.04	129.76	125.48
18	T	206	CLA	O2D-CGD-CBD	2.04	114.89	111.27
18	B	818	CLA	C3B-C4B-NB	-2.04	108.62	110.52
18	U	211	CLA	CHD-C1D-C2D	2.04	129.75	125.48
26	M	102	SQD	O48-C23-C24	2.04	118.30	111.91
27	B	849	LMG	O1-C7-C8	-2.04	105.99	110.90
28	U	213	KC1	CGD-CBD-CAD	-2.04	104.14	110.73
18	Q	211	CLA	CED-O2D-CGD	2.03	120.54	115.94
27	U	201	LMG	O3-C3-C2	-2.03	105.65	110.35
18	B	844	CLA	CGD-CBD-CAD	-2.03	104.15	110.73
28	T	209	KC1	CHC-C4B-NB	-2.03	122.59	124.45
18	A	801	CLA	C2A-C1A-CHA	2.03	127.41	123.86
21	I	102	BCR	C38-C26-C25	-2.03	122.25	124.53
24	S	203	DD6	O1-C20-C19	-2.03	111.86	113.38
18	A	811	CLA	CHD-C1D-C2D	2.03	129.74	125.48
24	A	854	DD6	C10-C9-C8	2.03	129.55	123.22
18	B	820	CLA	C1D-ND-C4D	2.03	107.78	106.33
24	S	209	DD6	C24-C1-C2	2.03	122.05	118.94
18	R	202	CLA	C3B-C4B-NB	-2.03	108.64	110.52
21	M	101	BCR	C24-C23-C22	-2.03	123.17	126.23
18	B	821	CLA	CMD-C2D-C1D	2.03	128.28	124.71
18	A	808	CLA	C5-C3-C2	2.03	125.22	121.12
21	B	839	BCR	C1-C6-C5	-2.03	119.76	122.61
18	A	852	CLA	CHD-C1D-C2D	2.02	129.73	125.48
27	U	201	LMG	C1-C2-C3	-2.02	105.78	110.00
18	B	817	CLA	C2D-C1D-ND	-2.02	108.61	110.10
27	U	201	LMG	O7-C10-O9	-2.02	118.81	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	207	CLA	C4A-NA-C1A	2.02	107.61	106.71
24	S	203	DD6	C22-C16-C17	-2.02	105.48	108.98
18	A	813	CLA	CHD-C1D-C2D	2.02	129.71	125.48
24	A	854	DD6	C37-C36-C31	-2.02	121.61	124.35
24	S	213	DD6	O1-C20-C19	-2.02	111.87	113.38
18	P	306	CLA	C1D-ND-C4D	2.01	107.77	106.33
18	L	204	CLA	O2D-CGD-CBD	2.01	114.84	111.27
24	O	213	DD6	C8-C6-C5	2.01	122.03	118.94
21	A	844	BCR	C33-C5-C6	-2.01	122.27	124.53
18	A	833	CLA	CHD-C1D-C2D	2.01	129.70	125.48
24	O	214	DD6	C37-C36-C31	-2.01	121.62	124.35
24	S	209	DD6	C12-C11-C13	2.01	121.24	118.08
21	A	841	BCR	C11-C10-C9	-2.00	124.45	127.31
18	S	206	CLA	C2A-C1A-CHA	2.00	127.36	123.86
18	A	853	CLA	C4A-NA-C1A	2.00	107.61	106.71
21	A	841	BCR	C3-C4-C5	-2.00	110.50	114.08
26	B	847	SQD	O3-C3-C2	-2.00	105.72	110.35
24	U	203	DD6	C22-C16-C17	-2.00	105.50	108.98
18	A	824	CLA	CMD-C2D-C1D	2.00	128.24	124.71
29	R	204	A86	C35-C34-C33	2.00	114.73	110.44
21	B	840	BCR	C29-C30-C25	2.00	113.56	110.48

There are no chirality outliers.

All (1386) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	808	CLA	CBA-CGA-O2A-C1
18	A	815	CLA	C1A-C2A-CAA-CBA
18	A	815	CLA	C3A-C2A-CAA-CBA
18	A	816	CLA	CHA-CBD-CGD-O1D
18	A	816	CLA	CHA-CBD-CGD-O2D
18	A	820	CLA	CBD-CGD-O2D-CED
18	A	820	CLA	O1D-CGD-O2D-CED
18	A	825	CLA	C2A-CAA-CBA-CGA
18	A	826	CLA	CHA-CBD-CGD-O1D
18	A	826	CLA	CHA-CBD-CGD-O2D
18	A	829	CLA	CHA-CBD-CGD-O1D
18	A	829	CLA	CHA-CBD-CGD-O2D
18	A	831	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	A	831	CLA	CHA-CBD-CGD-O2D
18	A	834	CLA	CHA-CBD-CGD-O1D
18	A	834	CLA	CHA-CBD-CGD-O2D
18	A	838	CLA	CBD-CGD-O2D-CED
18	A	838	CLA	O1D-CGD-O2D-CED
18	A	846	CLA	C6-C7-C8-C9
18	A	847	CLA	CHA-CBD-CGD-O1D
18	A	847	CLA	CHA-CBD-CGD-O2D
18	B	808	CLA	CHA-CBD-CGD-O2D
18	B	809	CLA	CHA-CBD-CGD-O1D
18	B	809	CLA	CHA-CBD-CGD-O2D
18	B	813	CLA	C1A-C2A-CAA-CBA
18	B	819	CLA	CHA-CBD-CGD-O1D
18	B	819	CLA	CHA-CBD-CGD-O2D
18	B	821	CLA	CHA-CBD-CGD-O1D
18	B	821	CLA	CHA-CBD-CGD-O2D
18	B	824	CLA	CBA-CGA-O2A-C1
18	B	824	CLA	O1A-CGA-O2A-C1
18	B	846	CLA	C1A-C2A-CAA-CBA
18	B	848	CLA	C1A-C2A-CAA-CBA
18	B	848	CLA	C3A-C2A-CAA-CBA
18	F	802	CLA	CBA-CGA-O2A-C1
18	F	802	CLA	O1A-CGA-O2A-C1
18	L	202	CLA	C1A-C2A-CAA-CBA
18	L	202	CLA	CBA-CGA-O2A-C1
18	L	202	CLA	O1A-CGA-O2A-C1
18	L	204	CLA	C1A-C2A-CAA-CBA
18	L	204	CLA	CBD-CGD-O2D-CED
18	L	204	CLA	O1D-CGD-O2D-CED
18	P	307	CLA	C1A-C2A-CAA-CBA
18	P	307	CLA	C3A-C2A-CAA-CBA
18	P	307	CLA	C2-C3-C5-C6
18	P	307	CLA	C4-C3-C5-C6
18	P	308	CLA	CHA-CBD-CGD-O1D
18	P	308	CLA	CHA-CBD-CGD-O2D
18	P	310	CLA	CBD-CGD-O2D-CED
18	P	310	CLA	O1D-CGD-O2D-CED
18	P	312	CLA	CBD-CGD-O2D-CED
18	P	312	CLA	O1D-CGD-O2D-CED
18	Q	203	CLA	CBA-CGA-O2A-C1
18	Q	203	CLA	O1A-CGA-O2A-C1
18	Q	205	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	Q	205	CLA	CHA-CBD-CGD-O2D
18	Q	207	CLA	C1A-C2A-CAA-CBA
18	Q	211	CLA	CBD-CGD-O2D-CED
18	Q	211	CLA	O1D-CGD-O2D-CED
18	Q	212	CLA	CHA-CBD-CGD-O2D
18	Q	212	CLA	C11-C12-C13-C14
18	Q	213	CLA	CBA-CGA-O2A-C1
18	Q	213	CLA	O1A-CGA-O2A-C1
18	R	205	CLA	CBD-CGD-O2D-CED
18	R	205	CLA	O1D-CGD-O2D-CED
18	R	205	CLA	C2-C3-C5-C6
18	R	205	CLA	C4-C3-C5-C6
18	S	205	CLA	CBD-CGD-O2D-CED
18	S	205	CLA	O1D-CGD-O2D-CED
18	U	204	CLA	CHA-CBD-CGD-O1D
18	U	204	CLA	CHA-CBD-CGD-O2D
18	U	206	CLA	CHA-CBD-CGD-O1D
18	U	206	CLA	CHA-CBD-CGD-O2D
18	T	205	CLA	C1A-C2A-CAA-CBA
18	T	205	CLA	C3A-C2A-CAA-CBA
18	T	206	CLA	CBD-CGD-O2D-CED
18	T	206	CLA	O1D-CGD-O2D-CED
18	T	208	CLA	CBD-CGD-O2D-CED
18	T	208	CLA	O1D-CGD-O2D-CED
18	T	208	CLA	C2-C3-C5-C6
18	T	208	CLA	C4-C3-C5-C6
18	T	211	CLA	CBD-CGD-O2D-CED
18	T	211	CLA	O1D-CGD-O2D-CED
20	A	839	LHG	C4-O6-P-O4
20	A	840	LHG	C3-O3-P-O5
20	R	201	LHG	C3-O3-P-O4
20	R	201	LHG	C4-O6-P-O3
20	R	201	LHG	C4-O6-P-O4
20	R	201	LHG	C4-O6-P-O5
21	A	841	BCR	C20-C21-C22-C37
21	A	841	BCR	C22-C23-C24-C25
21	A	841	BCR	C23-C24-C25-C30
21	A	842	BCR	C7-C8-C9-C34
21	A	842	BCR	C20-C21-C22-C23
21	A	842	BCR	C20-C21-C22-C37
21	A	842	BCR	C21-C22-C23-C24
21	A	842	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	A	844	BCR	C20-C21-C22-C23
21	A	844	BCR	C20-C21-C22-C37
21	A	844	BCR	C23-C24-C25-C30
21	B	837	BCR	C1-C6-C7-C8
21	B	837	BCR	C37-C22-C23-C24
21	B	838	BCR	C7-C8-C9-C10
21	B	838	BCR	C21-C22-C23-C24
21	B	838	BCR	C37-C22-C23-C24
21	B	840	BCR	C23-C24-C25-C30
21	B	841	BCR	C1-C6-C7-C8
21	F	801	BCR	C7-C8-C9-C10
21	F	801	BCR	C21-C22-C23-C24
21	F	801	BCR	C37-C22-C23-C24
21	F	804	BCR	C7-C8-C9-C34
21	F	804	BCR	C37-C22-C23-C24
21	I	101	BCR	C37-C22-C23-C24
21	I	102	BCR	C7-C8-C9-C10
21	I	102	BCR	C7-C8-C9-C34
21	I	102	BCR	C21-C22-C23-C24
21	I	102	BCR	C23-C24-C25-C26
21	I	102	BCR	C23-C24-C25-C30
21	J	104	BCR	C7-C8-C9-C10
21	J	104	BCR	C7-C8-C9-C34
21	J	104	BCR	C11-C12-C13-C14
21	J	104	BCR	C11-C12-C13-C35
21	J	104	BCR	C20-C21-C22-C37
21	J	104	BCR	C21-C22-C23-C24
21	J	104	BCR	C37-C22-C23-C24
21	L	201	BCR	C1-C6-C7-C8
21	L	201	BCR	C20-C21-C22-C23
21	L	201	BCR	C20-C21-C22-C37
21	L	201	BCR	C21-C22-C23-C24
21	L	201	BCR	C37-C22-C23-C24
21	L	205	BCR	C1-C6-C7-C8
21	L	205	BCR	C23-C24-C25-C30
21	M	101	BCR	C7-C8-C9-C10
21	M	101	BCR	C7-C8-C9-C34
21	M	101	BCR	C37-C22-C23-C24
21	R	203	BCR	C7-C8-C9-C34
21	R	203	BCR	C23-C24-C25-C30
24	A	854	DD6	C-C1-C24-C25
24	A	854	DD6	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
24	A	854	DD6	C10-C11-C13-C14
24	A	854	DD6	C12-C11-C13-C14
24	A	854	DD6	C5-C6-C8-C9
24	A	854	DD6	C7-C6-C8-C9
24	J	101	DD6	C24-C25-C26-C27
24	O	212	DD6	C-C1-C24-C25
24	O	212	DD6	C2-C1-C24-C25
24	O	212	DD6	C10-C11-C13-C14
24	O	212	DD6	C12-C11-C13-C14
24	O	212	DD6	C2-C3-C4-C5
24	O	212	DD6	C4-C5-C6-C7
24	O	212	DD6	C4-C5-C6-C8
24	O	214	DD6	C11-C13-C14-C15
24	O	214	DD6	C4-C5-C6-C7
24	O	214	DD6	C4-C5-C6-C8
24	O	215	DD6	C9-C10-C11-C12
24	O	215	DD6	C9-C10-C11-C13
24	O	215	DD6	C11-C13-C14-C15
24	O	215	DD6	C2-C3-C4-C5
24	O	215	DD6	C4-C5-C6-C7
24	O	215	DD6	C4-C5-C6-C8
24	O	215	DD6	C5-C6-C8-C9
24	O	215	DD6	C7-C6-C8-C9
24	P	304	DD6	C-C1-C24-C25
24	P	304	DD6	C9-C10-C11-C12
24	P	304	DD6	C9-C10-C11-C13
24	P	304	DD6	C11-C13-C14-C15
24	P	314	DD6	C10-C11-C13-C14
24	P	314	DD6	C12-C11-C13-C14
24	P	314	DD6	C13-C14-C15-O1
24	P	314	DD6	C2-C3-C4-C5
24	P	316	DD6	C9-C10-C11-C12
24	P	316	DD6	C9-C10-C11-C13
24	P	316	DD6	C10-C11-C13-C14
24	P	316	DD6	C12-C11-C13-C14
24	P	316	DD6	C11-C13-C14-C15
24	P	316	DD6	C13-C14-C15-O1
24	P	316	DD6	C2-C3-C4-C5
24	P	316	DD6	C5-C6-C8-C9
24	P	316	DD6	C7-C6-C8-C9
24	P	317	DD6	C11-C13-C14-C15
24	P	317	DD6	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	P	317	DD6	C4-C5-C6-C8
24	P	317	DD6	C5-C6-C8-C9
24	P	317	DD6	C7-C6-C8-C9
24	Q	215	DD6	C9-C10-C11-C12
24	Q	215	DD6	C9-C10-C11-C13
24	Q	215	DD6	C10-C11-C13-C14
24	Q	215	DD6	C12-C11-C13-C14
24	Q	215	DD6	C11-C13-C14-C15
24	S	202	DD6	C9-C10-C11-C12
24	S	202	DD6	C9-C10-C11-C13
24	S	203	DD6	C13-C14-C15-O1
24	S	209	DD6	C10-C11-C13-C14
24	S	209	DD6	C12-C11-C13-C14
24	S	209	DD6	C13-C14-C15-O1
24	S	212	DD6	C-C1-C24-C25
24	S	212	DD6	C2-C1-C24-C25
24	S	212	DD6	C9-C10-C11-C12
24	S	212	DD6	C9-C10-C11-C13
24	S	212	DD6	C10-C11-C13-C14
24	S	212	DD6	C12-C11-C13-C14
24	S	212	DD6	C11-C13-C14-C15
24	S	212	DD6	C1-C24-C25-C26
24	S	212	DD6	C5-C6-C8-C9
24	S	212	DD6	C7-C6-C8-C9
24	S	213	DD6	C2-C1-C24-C25
24	S	213	DD6	C9-C10-C11-C12
24	S	213	DD6	C9-C10-C11-C13
24	S	213	DD6	C10-C11-C13-C14
24	S	213	DD6	C12-C11-C13-C14
24	S	213	DD6	C11-C13-C14-C15
24	S	213	DD6	C1-C24-C25-C26
24	U	203	DD6	C-C1-C24-C25
24	U	203	DD6	C2-C1-C24-C25
24	U	203	DD6	C11-C13-C14-C15
24	U	203	DD6	C1-C24-C25-C26
24	U	203	DD6	C2-C3-C4-C5
24	U	203	DD6	C4-C5-C6-C7
24	U	203	DD6	C4-C5-C6-C8
24	U	203	DD6	C5-C6-C8-C9
24	U	203	DD6	C7-C6-C8-C9
24	U	212	DD6	C10-C11-C13-C14
24	U	212	DD6	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
24	U	212	DD6	C11-C13-C14-C15
24	U	212	DD6	C5-C6-C8-C9
24	U	214	DD6	C-C1-C24-C25
24	U	214	DD6	C2-C1-C24-C25
24	U	214	DD6	C24-C25-C26-C27
24	U	214	DD6	C2-C3-C4-C5
24	U	214	DD6	C3-C4-C5-C6
24	U	214	DD6	C4-C5-C6-C7
24	U	214	DD6	C4-C5-C6-C8
24	T	213	DD6	C9-C10-C11-C12
24	T	213	DD6	C9-C10-C11-C13
24	T	213	DD6	C13-C14-C15-O1
24	T	213	DD6	C3-C4-C5-C6
24	T	213	DD6	C4-C5-C6-C7
24	T	213	DD6	C4-C5-C6-C8
24	T	214	DD6	C9-C10-C11-C12
24	T	214	DD6	C9-C10-C11-C13
24	T	214	DD6	C11-C13-C14-C15
24	T	214	DD6	C1-C24-C25-C26
24	T	214	DD6	C24-C25-C26-C27
24	T	214	DD6	C3-C4-C5-C6
26	B	847	SQD	C5-C6-S-O7
26	B	847	SQD	C5-C6-S-O8
26	B	847	SQD	C5-C6-S-O9
26	M	102	SQD	O5-C1-O6-C44
26	M	102	SQD	O5-C5-C6-S
27	J	102	LMG	C2-C1-O1-C7
27	J	102	LMG	O6-C1-O1-C7
27	P	301	LMG	O7-C8-C9-O8
27	Q	217	LMG	C2-C1-O1-C7
27	Q	217	LMG	O6-C1-O1-C7
27	U	201	LMG	C2-C1-O1-C7
27	U	201	LMG	O6-C1-O1-C7
27	U	201	LMG	C11-C10-O7-C8
28	P	311	KC1	CAD-CBD-CGD-O2D
28	P	311	KC1	CHA-CBD-CGD-O2D
28	P	311	KC1	CBD-CGD-O2D-CED
28	Q	210	KC1	C2A-CAA-CBA-CGA
28	S	210	KC1	C3A-C2A-CAA-CBA
28	S	210	KC1	C2A-CAA-CBA-CGA
28	S	210	KC1	CBD-CGD-O2D-CED
28	S	210	KC1	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	P	303	A86	C-C1-C24-C25
29	P	303	A86	C2-C1-C24-C25
29	P	303	A86	C11-C10-C9-C8
29	P	303	A86	C1-C24-C25-C26
29	P	303	A86	C35-C34-O4-C38
29	P	303	A86	C39-C38-O4-C34
29	P	303	A86	C4-C5-C6-C7
29	P	303	A86	C4-C5-C6-C8
29	Q	201	A86	C-C1-C2-C3
29	Q	201	A86	C24-C1-C2-C3
29	Q	201	A86	C-C1-C24-C25
29	Q	201	A86	C2-C1-C24-C25
29	Q	201	A86	C9-C10-C11-C12
29	Q	201	A86	C9-C10-C11-C13
29	Q	201	A86	C10-C11-C13-O
29	Q	201	A86	C12-C11-C13-O
29	Q	201	A86	C1-C24-C25-C26
29	Q	201	A86	C6-C8-C9-C10
29	Q	214	A86	C39-C38-O4-C34
29	Q	214	A86	O5-C38-O4-C34
29	R	206	A86	C2-C3-C4-C5
29	R	206	A86	O5-C38-O4-C34
29	U	202	A86	C10-C11-C13-O
29	U	202	A86	C12-C11-C13-O
29	U	202	A86	C2-C3-C4-C5
29	U	202	A86	C4-C5-C6-C7
29	U	202	A86	C4-C5-C6-C8
29	U	202	A86	C5-C6-C8-C9
29	U	202	A86	C7-C6-C8-C9
29	T	201	A86	C9-C10-C11-C12
29	T	201	A86	C9-C10-C11-C13
29	T	201	A86	C1-C24-C25-C26
29	T	201	A86	C26-C27-C29-C30
29	T	201	A86	C39-C38-O4-C34
29	T	201	A86	C6-C8-C9-C10
29	Q	201	A86	C39-C38-O4-C34
29	R	206	A86	C39-C38-O4-C34
29	U	202	A86	C39-C38-O4-C34
18	A	808	CLA	O1A-CGA-O2A-C1
18	Q	207	CLA	O1A-CGA-O2A-C1
18	T	206	CLA	O1A-CGA-O2A-C1
29	P	303	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
29	Q	201	A86	O5-C38-O4-C34
20	A	840	LHG	O9-C7-O7-C5
27	J	102	LMG	O9-C10-O7-C8
27	U	201	LMG	O9-C10-O7-C8
18	Q	207	CLA	CBA-CGA-O2A-C1
18	T	206	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	C3-C5-C6-C7
18	B	815	CLA	C3-C5-C6-C7
18	P	307	CLA	C3-C5-C6-C7
18	Q	204	CLA	C3-C5-C6-C7
18	U	205	CLA	C3-C5-C6-C7
18	U	210	CLA	C3-C5-C6-C7
29	T	201	A86	O5-C38-O4-C34
18	A	845	CLA	C4-C3-C5-C6
18	A	847	CLA	C4-C3-C5-C6
18	O	209	CLA	C4-C3-C5-C6
18	B	846	CLA	C2-C3-C5-C6
18	B	813	CLA	C2A-CAA-CBA-CGA
18	B	833	CLA	C2A-CAA-CBA-CGA
18	B	848	CLA	C2A-CAA-CBA-CGA
18	A	846	CLA	C3-C5-C6-C7
18	B	806	CLA	C3-C5-C6-C7
18	B	833	CLA	C3-C5-C6-C7
18	T	208	CLA	C3-C5-C6-C7
20	R	201	LHG	C32-C33-C34-C35
29	U	202	A86	O5-C38-O4-C34
24	A	854	DD6	C24-C25-C26-C27
24	O	215	DD6	C24-C25-C26-C27
24	U	203	DD6	C1-C2-C3-C4
24	U	203	DD6	C24-C25-C26-C27
20	R	201	LHG	O2-C2-C3-O3
18	Q	205	CLA	C3-C5-C6-C7
18	Q	216	CLA	C3-C5-C6-C7
27	B	849	LMG	O6-C5-C6-O5
24	U	212	DD6	C2-C3-C4-C5
27	S	211	LMG	O6-C5-C6-O5
18	Q	213	CLA	C3-C5-C6-C7
27	J	102	LMG	O6-C5-C6-O5
18	F	802	CLA	O2A-C1-C2-C3
18	B	814	CLA	C4-C3-C5-C6
18	P	306	CLA	C4-C3-C5-C6
18	Q	206	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	A	845	CLA	C2-C3-C5-C6
18	A	847	CLA	C2-C3-C5-C6
18	B	814	CLA	C2-C3-C5-C6
18	P	306	CLA	C2-C3-C5-C6
18	Q	206	CLA	C2-C3-C5-C6
27	S	211	LMG	C4-C5-C6-O5
18	A	808	CLA	C1-C2-C3-C5
18	O	209	CLA	C1-C2-C3-C5
18	B	805	CLA	C3-C5-C6-C7
20	R	201	LHG	C24-C23-O8-C6
27	J	102	LMG	C29-C28-O8-C9
24	U	203	DD6	C3-C4-C5-C6
29	Q	201	A86	C11-C10-C9-C8
29	T	201	A86	C1-C2-C3-C4
18	B	845	CLA	C13-C15-C16-C17
18	Q	203	CLA	O2A-C1-C2-C3
18	B	806	CLA	C6-C7-C8-C9
18	U	204	CLA	C11-C10-C8-C9
21	B	837	BCR	C7-C8-C9-C34
21	F	801	BCR	C7-C8-C9-C34
21	I	102	BCR	C37-C22-C23-C24
24	J	101	DD6	C-C1-C24-C25
24	J	101	DD6	C12-C11-C13-C14
24	O	213	DD6	C12-C11-C13-C14
24	O	214	DD6	C12-C11-C13-C14
24	O	215	DD6	C12-C11-C13-C14
24	P	316	DD6	C-C1-C24-C25
24	P	317	DD6	C12-C11-C13-C14
24	S	202	DD6	C7-C6-C8-C9
24	S	203	DD6	C12-C11-C13-C14
24	S	213	DD6	C-C1-C24-C25
24	T	213	DD6	C-C1-C24-C25
24	T	213	DD6	C7-C6-C8-C9
24	T	214	DD6	C12-C11-C13-C14
29	P	303	A86	C7-C6-C8-C9
29	Q	201	A86	C7-C6-C8-C9
29	Q	214	A86	C-C1-C24-C25
21	B	837	BCR	C7-C8-C9-C10
21	R	203	BCR	C7-C8-C9-C10
24	J	101	DD6	C10-C11-C13-C14
24	O	214	DD6	C10-C11-C13-C14
24	O	215	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
24	P	317	DD6	C10-C11-C13-C14
24	S	202	DD6	C5-C6-C8-C9
24	S	203	DD6	C10-C11-C13-C14
24	T	213	DD6	C5-C6-C8-C9
24	T	214	DD6	C10-C11-C13-C14
29	P	303	A86	C5-C6-C8-C9
29	Q	201	A86	C5-C6-C8-C9
25	B	842	DGD	O6E-C5E-C6E-O5E
20	A	840	LHG	C8-C7-O7-C5
18	Q	205	CLA	C5-C6-C7-C8
18	U	205	CLA	C5-C6-C7-C8
18	B	846	CLA	C3-C5-C6-C7
18	A	811	CLA	C10-C11-C12-C13
18	A	821	CLA	C15-C16-C17-C18
18	A	823	CLA	C15-C16-C17-C18
18	B	806	CLA	C10-C11-C12-C13
18	Q	204	CLA	C10-C11-C12-C13
20	A	839	LHG	C23-C24-C25-C26
26	B	847	SQD	C23-C24-C25-C26
18	A	804	CLA	C8-C10-C11-C12
18	A	846	CLA	C5-C6-C7-C8
18	A	851	CLA	C8-C10-C11-C12
18	O	205	CLA	C15-C16-C17-C18
18	P	307	CLA	C5-C6-C7-C8
18	Q	216	CLA	C15-C16-C17-C18
18	S	201	CLA	C10-C11-C12-C13
26	M	102	SQD	C7-C8-C9-C10
18	A	809	CLA	C8-C10-C11-C12
18	A	828	CLA	C13-C15-C16-C17
18	B	817	CLA	C15-C16-C17-C18
18	U	207	CLA	C8-C10-C11-C12
27	P	301	LMG	C10-C11-C12-C13
18	Q	206	CLA	C3-C5-C6-C7
18	A	801	CLA	C10-C11-C12-C13
18	Q	212	CLA	C8-C10-C11-C12
18	O	209	CLA	C11-C12-C13-C15
18	Q	212	CLA	C6-C7-C8-C10
18	Q	212	CLA	C12-C13-C15-C16
18	U	207	CLA	C11-C12-C13-C15
18	A	834	CLA	C3-C5-C6-C7
18	B	834	CLA	C3-C5-C6-C7
18	S	215	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	S	202	DD6	C1-C2-C3-C4
24	S	202	DD6	C3-C4-C5-C6
24	S	212	DD6	C1-C2-C3-C4
24	S	213	DD6	C24-C25-C26-C27
24	T	214	DD6	C1-C2-C3-C4
29	T	201	A86	C3-C4-C5-C6
18	A	807	CLA	C2A-CAA-CBA-CGA
18	T	205	CLA	C2A-CAA-CBA-CGA
18	Q	212	CLA	C5-C6-C7-C8
27	J	102	LMG	O10-C28-O8-C9
24	O	212	DD6	C1-C24-C25-C26
29	Q	214	A86	C6-C8-C9-C10
18	A	822	CLA	C8-C10-C11-C12
18	A	828	CLA	C15-C16-C17-C18
18	B	833	CLA	C15-C16-C17-C18
18	A	833	CLA	C10-C11-C12-C13
18	A	846	CLA	C10-C11-C12-C13
18	A	851	CLA	C10-C11-C12-C13
18	B	817	CLA	C10-C11-C12-C13
18	B	828	CLA	C5-C6-C7-C8
18	B	830	CLA	C8-C10-C11-C12
18	B	843	CLA	C10-C11-C12-C13
18	O	204	CLA	C15-C16-C17-C18
18	Q	216	CLA	C13-C15-C16-C17
18	U	210	CLA	C15-C16-C17-C18
18	Q	209	CLA	C13-C15-C16-C17
18	U	210	CLA	C8-C10-C11-C12
19	B	836	PQN	C23-C25-C26-C27
20	R	201	LHG	C3-O3-P-O6
18	B	830	CLA	C5-C6-C7-C8
18	B	831	CLA	C13-C15-C16-C17
18	S	201	CLA	C8-C10-C11-C12
27	S	211	LMG	C10-C11-C12-C13
20	A	839	LHG	C28-C29-C30-C31
18	A	845	CLA	C2A-CAA-CBA-CGA
18	P	307	CLA	C2A-CAA-CBA-CGA
29	P	303	A86	C2-C3-C4-C5
18	Q	209	CLA	C15-C16-C17-C18
24	A	854	DD6	C1-C2-C3-C4
24	A	854	DD6	C3-C4-C5-C6
24	S	209	DD6	C24-C25-C26-C27
24	S	212	DD6	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
24	T	213	DD6	C24-C25-C26-C27
27	B	849	LMG	C4-C5-C6-O5
27	J	102	LMG	C11-C10-O7-C8
21	B	840	BCR	C16-C17-C18-C36
21	R	203	BCR	C20-C21-C22-C37
24	A	854	DD6	C9-C10-C11-C12
24	O	213	DD6	C9-C10-C11-C12
24	P	314	DD6	C9-C10-C11-C12
24	P	316	DD6	C4-C5-C6-C7
24	P	317	DD6	C9-C10-C11-C12
24	Q	202	DD6	C4-C5-C6-C7
24	S	202	DD6	C4-C5-C6-C7
24	S	203	DD6	C9-C10-C11-C12
29	Q	201	A86	C4-C5-C6-C7
29	Q	214	A86	C4-C5-C6-C7
29	U	202	A86	C-C1-C2-C3
18	B	821	CLA	C15-C16-C17-C18
27	J	102	LMG	C14-C15-C16-C17
27	P	301	LMG	C12-C13-C14-C15
28	P	305	KC1	C2A-CAA-CBA-CGA
18	P	310	CLA	C1-C2-C3-C5
20	A	839	LHG	C24-C25-C26-C27
25	B	842	DGD	C7A-C8A-C9A-CAA
26	B	847	SQD	C34-C35-C36-C37
27	S	211	LMG	C33-C34-C35-C36
27	J	102	LMG	C4-C5-C6-O5
18	Q	213	CLA	C5-C6-C7-C8
20	A	839	LHG	C27-C28-C29-C30
18	Q	209	CLA	C3-C5-C6-C7
18	Q	212	CLA	C3-C5-C6-C7
20	A	840	LHG	C7-C8-C9-C10
21	A	841	BCR	C20-C21-C22-C23
21	B	837	BCR	C11-C10-C9-C8
21	B	839	BCR	C20-C21-C22-C23
21	F	801	BCR	C11-C10-C9-C8
21	F	804	BCR	C12-C13-C14-C15
21	I	101	BCR	C20-C21-C22-C23
21	I	102	BCR	C20-C21-C22-C23
21	J	104	BCR	C20-C21-C22-C23
24	A	854	DD6	C9-C10-C11-C13
24	O	213	DD6	C9-C10-C11-C13
24	P	314	DD6	C9-C10-C11-C13

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Mol	Chain	Res	Type	Atoms
24	P	316	DD6	C4-C5-C6-C8
24	P	317	DD6	C9-C10-C11-C13
24	Q	202	DD6	C4-C5-C6-C8
24	S	202	DD6	C4-C5-C6-C8
24	S	203	DD6	C9-C10-C11-C13
26	B	847	SQD	C2-C1-O6-C44
29	Q	201	A86	C4-C5-C6-C8
29	U	202	A86	C24-C1-C2-C3
29	T	201	A86	C24-C1-C2-C3
20	A	839	LHG	C34-C35-C36-C37
25	B	842	DGD	C4A-C5A-C6A-C7A
25	B	842	DGD	C5A-C6A-C7A-C8A
27	J	102	LMG	C15-C16-C17-C18
18	B	816	CLA	C8-C10-C11-C12
18	A	806	CLA	C4-C3-C5-C6
26	B	847	SQD	C26-C27-C28-C29
18	A	849	CLA	C11-C10-C8-C9
18	O	204	CLA	C14-C13-C15-C16
18	Q	204	CLA	C11-C12-C13-C14
20	R	201	LHG	C14-C15-C16-C17
20	R	201	LHG	C30-C31-C32-C33
26	B	847	SQD	O10-C23-O48-C46
21	A	844	BCR	C37-C22-C23-C24
21	I	101	BCR	C11-C12-C13-C35
24	P	314	DD6	C-C1-C24-C25
24	Q	202	DD6	C12-C11-C13-C14
24	U	212	DD6	C7-C6-C8-C9
24	T	214	DD6	C-C1-C24-C25
29	T	201	A86	C-C1-C24-C25
26	M	102	SQD	C29-C30-C31-C32
20	R	201	LHG	O1-C1-C2-C3
21	A	844	BCR	C21-C22-C23-C24
24	P	304	DD6	C2-C1-C24-C25
24	Q	202	DD6	C10-C11-C13-C14
24	T	214	DD6	C2-C1-C24-C25
29	T	201	A86	C2-C1-C24-C25
20	A	839	LHG	C10-C11-C12-C13
20	R	201	LHG	C17-C18-C19-C20
26	B	847	SQD	C32-C33-C34-C35
27	Q	217	LMG	C38-C39-C40-C41
18	B	810	CLA	C6-C7-C8-C10
27	Q	217	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
27	S	211	LMG	C30-C31-C32-C33
18	T	205	CLA	C8-C10-C11-C12
20	A	840	LHG	C24-C23-O8-C6
25	B	842	DGD	C9B-CAB-CBB-CCB
18	A	851	CLA	C3A-C2A-CAA-CBA
18	B	813	CLA	C3A-C2A-CAA-CBA
18	F	803	CLA	C3A-C2A-CAA-CBA
18	O	202	CLA	C3A-C2A-CAA-CBA
18	P	309	CLA	C3A-C2A-CAA-CBA
18	Q	203	CLA	C3A-C2A-CAA-CBA
18	Q	207	CLA	C3A-C2A-CAA-CBA
18	T	204	CLA	C3A-C2A-CAA-CBA
18	O	209	CLA	C5-C6-C7-C8
27	J	102	LMG	C13-C14-C15-C16
27	P	301	LMG	C29-C30-C31-C32
18	B	810	CLA	C6-C7-C8-C9
20	R	201	LHG	C15-C16-C17-C18
26	M	102	SQD	C25-C26-C27-C28
26	M	102	SQD	C31-C32-C33-C34
27	S	211	LMG	C36-C37-C38-C39
24	J	101	DD6	C2-C3-C4-C5
24	Q	215	DD6	C2-C3-C4-C5
24	S	212	DD6	C2-C3-C4-C5
18	B	809	CLA	C3-C5-C6-C7
18	R	205	CLA	C3-C5-C6-C7
29	P	303	A86	C9-C10-C11-C13
18	A	806	CLA	C2-C3-C5-C6
25	B	842	DGD	CAB-CBB-CCB-CDB
27	S	211	LMG	C35-C36-C37-C38
18	A	818	CLA	C3-C5-C6-C7
25	B	842	DGD	CDB-CEB-CFB-CGB
25	B	842	DGD	CEB-CFB-CGB-CHB
18	B	803	CLA	C15-C16-C17-C18
20	A	839	LHG	C9-C10-C11-C12
20	R	201	LHG	O10-C23-O8-C6
21	A	841	BCR	C23-C24-C25-C26
21	A	844	BCR	C23-C24-C25-C26
21	B	837	BCR	C5-C6-C7-C8
21	B	838	BCR	C1-C6-C7-C8
21	B	838	BCR	C5-C6-C7-C8
21	B	840	BCR	C23-C24-C25-C26
21	B	841	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	L	201	BCR	C5-C6-C7-C8
21	L	205	BCR	C5-C6-C7-C8
21	L	205	BCR	C23-C24-C25-C26
21	R	203	BCR	C1-C6-C7-C8
21	R	203	BCR	C5-C6-C7-C8
21	R	203	BCR	C23-C24-C25-C26
27	S	211	LMG	C34-C35-C36-C37
27	P	301	LMG	C29-C28-O8-C9
18	A	807	CLA	C13-C15-C16-C17
18	A	815	CLA	C15-C16-C17-C18
18	A	833	CLA	C15-C16-C17-C18
18	A	851	CLA	C15-C16-C17-C18
18	B	846	CLA	C13-C15-C16-C17
18	T	208	CLA	C10-C11-C12-C13
18	B	815	CLA	C4-C3-C5-C6
18	B	846	CLA	C4-C3-C5-C6
18	A	823	CLA	C2-C3-C5-C6
18	A	824	CLA	C11-C12-C13-C15
18	A	846	CLA	C11-C10-C8-C7
18	B	806	CLA	C6-C7-C8-C10
18	B	823	CLA	C6-C7-C8-C10
18	B	843	CLA	C11-C10-C8-C7
18	Q	205	CLA	C11-C10-C8-C7
18	Q	212	CLA	C11-C12-C13-C15
24	Q	215	DD6	C24-C25-C26-C27
24	S	212	DD6	C3-C4-C5-C6
18	R	205	CLA	C16-C17-C18-C19
18	L	204	CLA	C2A-CAA-CBA-CGA
18	Q	213	CLA	C2A-CAA-CBA-CGA
18	A	801	CLA	C8-C10-C11-C12
25	B	842	DGD	C3B-C4B-C5B-C6B
27	U	201	LMG	C29-C30-C31-C32
27	Q	217	LMG	C14-C15-C16-C17
18	P	306	CLA	C8-C10-C11-C12
27	J	102	LMG	C19-C20-C21-C22
27	Q	217	LMG	C15-C16-C17-C18
26	B	847	SQD	O5-C1-O6-C44
20	R	201	LHG	C8-C7-O7-C5
21	J	104	BCR	C18-C19-C20-C21
24	O	214	DD6	C1-C24-C25-C26
28	P	302	KC1	C4B-C3B-CAB-CBB
18	B	820	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	B	824	CLA	C3-C5-C6-C7
25	B	842	DGD	C1B-C2B-C3B-C4B
27	Q	217	LMG	C29-C30-C31-C32
27	Q	217	LMG	C41-C42-C43-C44
25	B	842	DGD	O2G-C2G-C3G-O3G
27	J	102	LMG	O7-C8-C9-O8
27	U	201	LMG	O1-C7-C8-O7
27	S	211	LMG	C19-C20-C21-C22
18	T	205	CLA	C5-C6-C7-C8
18	O	209	CLA	C2-C3-C5-C6
18	S	201	CLA	C2-C3-C5-C6
24	P	314	DD6	C27-C29-C30-C31
24	P	316	DD6	C27-C29-C30-C31
24	S	213	DD6	C27-C29-C30-C31
24	U	203	DD6	C27-C29-C30-C31
24	T	214	DD6	C27-C29-C30-C31
18	B	823	CLA	C6-C7-C8-C9
18	B	843	CLA	C11-C10-C8-C9
18	Q	212	CLA	C14-C13-C15-C16
18	U	207	CLA	C11-C12-C13-C14
27	U	201	LMG	C30-C31-C32-C33
18	A	851	CLA	C3-C5-C6-C7
27	S	211	LMG	C38-C39-C40-C41
24	P	304	DD6	C12-C11-C13-C14
24	U	203	DD6	C12-C11-C13-C14
18	B	805	CLA	C15-C16-C17-C18
27	Q	217	LMG	C17-C18-C19-C20
27	Q	217	LMG	C23-C24-C25-C26
24	P	304	DD6	C10-C11-C13-C14
24	U	203	DD6	C10-C11-C13-C14
18	B	812	CLA	C1A-C2A-CAA-CBA
18	B	823	CLA	C1A-C2A-CAA-CBA
18	F	803	CLA	C1A-C2A-CAA-CBA
18	O	202	CLA	C1A-C2A-CAA-CBA
18	P	309	CLA	C1A-C2A-CAA-CBA
18	Q	204	CLA	C1A-C2A-CAA-CBA
18	T	204	CLA	C1A-C2A-CAA-CBA
18	T	208	CLA	C1A-C2A-CAA-CBA
24	O	214	DD6	C3-C4-C5-C6
18	A	836	CLA	C15-C16-C17-C18
26	B	847	SQD	C24-C25-C26-C27
18	A	835	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
18	A	823	CLA	C4-C3-C5-C6
18	A	824	CLA	C5-C6-C7-C8
18	B	817	CLA	C8-C10-C11-C12
18	B	817	CLA	C16-C17-C18-C20
18	S	201	CLA	C3-C5-C6-C7
26	B	847	SQD	O6-C44-C45-C46
26	B	847	SQD	C44-C45-C46-O48
27	Q	217	LMG	O1-C7-C8-C9
27	S	211	LMG	C7-C8-C9-O8
27	U	201	LMG	O1-C7-C8-C9
27	B	849	LMG	C8-C7-O1-C1
27	Q	217	LMG	C24-C25-C26-C27
27	U	201	LMG	C31-C32-C33-C34
27	S	211	LMG	C40-C41-C42-C43
18	S	201	CLA	C5-C6-C7-C8
27	B	849	LMG	C10-C11-C12-C13
25	B	842	DGD	C7B-C8B-C9B-CAB
27	S	211	LMG	C32-C33-C34-C35
18	B	845	CLA	C15-C16-C17-C18
21	J	104	BCR	C16-C17-C18-C36
24	O	212	DD6	C9-C10-C11-C12
24	S	212	DD6	C4-C5-C6-C7
18	A	818	CLA	C4-C3-C5-C6
18	S	215	CLA	C4-C3-C5-C6
20	A	839	LHG	C7-C8-C9-C10
18	A	823	CLA	C13-C15-C16-C17
18	A	833	CLA	C13-C15-C16-C17
18	P	307	CLA	C2-C1-O2A-CGA
18	S	215	CLA	C5-C6-C7-C8
18	R	205	CLA	C16-C17-C18-C20
18	O	209	CLA	C8-C10-C11-C12
18	Q	204	CLA	C8-C10-C11-C12
21	J	104	BCR	C16-C17-C18-C19
24	O	212	DD6	C9-C10-C11-C13
24	S	212	DD6	C4-C5-C6-C8
29	Q	214	A86	C4-C5-C6-C8
27	P	301	LMG	O1-C7-C8-O7
27	J	102	LMG	C29-C30-C31-C32
18	A	825	CLA	C4-C3-C5-C6
18	A	834	CLA	C4-C3-C5-C6
18	S	201	CLA	C4-C3-C5-C6
18	A	804	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
18	A	815	CLA	C12-C13-C15-C16
18	A	845	CLA	C12-C13-C15-C16
18	A	852	CLA	C11-C12-C13-C15
18	Q	204	CLA	C6-C7-C8-C10
18	Q	205	CLA	C6-C7-C8-C10
18	S	215	CLA	C2-C3-C5-C6
18	U	204	CLA	C11-C10-C8-C7
27	J	102	LMG	C20-C21-C22-C23
18	A	804	CLA	C11-C10-C8-C9
18	A	804	CLA	C11-C12-C13-C14
18	A	807	CLA	C11-C10-C8-C9
18	A	815	CLA	C11-C10-C8-C9
18	A	824	CLA	C11-C12-C13-C14
18	A	845	CLA	C14-C13-C15-C16
18	A	851	CLA	C11-C12-C13-C14
18	A	852	CLA	C11-C12-C13-C14
18	O	209	CLA	C11-C12-C13-C14
18	Q	205	CLA	C6-C7-C8-C9
18	Q	209	CLA	C14-C13-C15-C16
18	U	205	CLA	C6-C7-C8-C9
29	Q	201	A86	C2-C3-C4-C5
18	B	804	CLA	C2A-CAA-CBA-CGA
24	O	201	DD6	C12-C11-C13-C14
29	T	201	A86	C7-C6-C8-C9
18	U	205	CLA	C16-C17-C18-C19
24	O	201	DD6	C10-C11-C13-C14
18	B	808	CLA	C3-C5-C6-C7
18	B	816	CLA	C10-C11-C12-C13
26	B	847	SQD	C12-C13-C14-C15
26	B	847	SQD	C25-C26-C27-C28
20	R	201	LHG	O6-C4-C5-C6
24	A	854	DD6	C11-C13-C14-C15
18	B	807	CLA	C4-C3-C5-C6
18	U	204	CLA	C4-C3-C5-C6
18	A	818	CLA	C2-C3-C5-C6
18	A	825	CLA	C2-C3-C5-C6
18	B	819	CLA	C2-C3-C5-C6
18	R	205	CLA	C10-C11-C12-C13
27	J	102	LMG	C12-C13-C14-C15
18	B	834	CLA	C13-C15-C16-C17
27	Q	217	LMG	C20-C21-C22-C23
20	R	201	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
18	L	202	CLA	C3A-C2A-CAA-CBA
18	L	204	CLA	C3A-C2A-CAA-CBA
20	R	201	LHG	C9-C10-C11-C12
26	B	847	SQD	C11-C12-C13-C14
18	T	208	CLA	C16-C17-C18-C20
20	A	839	LHG	C24-C23-O8-C6
27	U	201	LMG	C29-C28-O8-C9
18	A	852	CLA	C15-C16-C17-C18
25	B	842	DGD	C1G-C2G-C3G-O3G
27	B	849	LMG	O1-C7-C8-C9
27	P	301	LMG	O1-C7-C8-C9
27	S	211	LMG	C39-C40-C41-C42
18	Q	216	CLA	C5-C6-C7-C8
18	A	835	CLA	C2A-CAA-CBA-CGA
20	R	201	LHG	O1-C1-C2-O2
18	U	204	CLA	C5-C6-C7-C8
28	P	305	KC1	C3A-C2A-CAA-CBA
18	A	834	CLA	C16-C17-C18-C19
20	R	201	LHG	C31-C32-C33-C34
18	A	808	CLA	C3-C5-C6-C7
18	A	851	CLA	C5-C6-C7-C8
29	Q	201	A86	C10-C11-C13-C14
29	U	202	A86	C10-C11-C13-C14
27	S	211	LMG	C20-C21-C22-C23
18	B	809	CLA	C2-C1-O2A-CGA
18	A	834	CLA	C2-C3-C5-C6
18	B	803	CLA	C6-C7-C8-C9
18	B	831	CLA	C14-C13-C15-C16
18	B	846	CLA	C11-C12-C13-C14
18	O	205	CLA	C14-C13-C15-C16
18	Q	204	CLA	C6-C7-C8-C9
18	Q	212	CLA	C6-C7-C8-C9
25	B	842	DGD	C6B-C7B-C8B-C9B
18	A	815	CLA	C2A-CAA-CBA-CGA
21	A	841	BCR	C5-C6-C7-C8
21	A	842	BCR	C5-C6-C7-C8
21	A	842	BCR	C23-C24-C25-C26
21	A	843	BCR	C5-C6-C7-C8
21	A	843	BCR	C23-C24-C25-C26
21	A	843	BCR	C23-C24-C25-C30
21	A	844	BCR	C1-C6-C7-C8
21	A	844	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	B	837	BCR	C23-C24-C25-C26
21	B	840	BCR	C5-C6-C7-C8
21	F	804	BCR	C5-C6-C7-C8
21	F	804	BCR	C23-C24-C25-C26
21	I	101	BCR	C1-C6-C7-C8
21	I	101	BCR	C5-C6-C7-C8
21	I	102	BCR	C5-C6-C7-C8
21	L	201	BCR	C23-C24-C25-C26
21	L	201	BCR	C23-C24-C25-C30
18	A	836	CLA	C8-C10-C11-C12
18	B	843	CLA	C8-C10-C11-C12
27	Q	217	LMG	C42-C43-C44-C45
21	L	205	BCR	C7-C8-C9-C34
21	B	837	BCR	C21-C22-C23-C24
21	M	101	BCR	C21-C22-C23-C24
24	J	101	DD6	C2-C1-C24-C25
24	O	213	DD6	C10-C11-C13-C14
24	P	314	DD6	C2-C1-C24-C25
24	P	316	DD6	C2-C1-C24-C25
24	T	213	DD6	C2-C1-C24-C25
29	Q	214	A86	C2-C1-C24-C25
24	Q	202	DD6	C2-C3-C4-C5
27	J	102	LMG	C11-C12-C13-C14
18	A	835	CLA	C16-C17-C18-C19
27	S	211	LMG	C31-C32-C33-C34
18	A	804	CLA	C11-C12-C13-C15
18	A	811	CLA	C11-C12-C13-C15
18	A	828	CLA	C12-C13-C15-C16
18	A	846	CLA	C6-C7-C8-C10
18	A	849	CLA	C11-C10-C8-C7
18	A	851	CLA	C11-C12-C13-C15
18	B	805	CLA	C11-C10-C8-C7
18	B	809	CLA	C6-C7-C8-C10
18	B	831	CLA	C12-C13-C15-C16
18	U	204	CLA	C2-C3-C5-C6
18	U	205	CLA	C6-C7-C8-C10
18	O	209	CLA	C1-C2-C3-C4
24	U	212	DD6	C24-C25-C26-C27
29	Q	201	A86	C1-C2-C3-C4
18	U	205	CLA	C16-C17-C18-C20
18	T	208	CLA	C16-C17-C18-C19
26	M	102	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
18	A	846	CLA	C8-C10-C11-C12
18	B	820	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C10-C11-C12-C13
21	B	841	BCR	C20-C21-C22-C37
24	U	212	DD6	C9-C10-C11-C12
24	U	212	DD6	C4-C5-C6-C7
29	T	201	A86	C-C1-C2-C3
29	P	303	A86	C9-C10-C11-C12
18	O	205	CLA	C16-C17-C18-C20
26	M	102	SQD	C24-C23-O48-C46
27	P	301	LMG	O10-C28-O8-C9
18	A	805	CLA	CAD-CBD-CGD-O2D
18	A	812	CLA	CAD-CBD-CGD-O2D
18	A	814	CLA	CAD-CBD-CGD-O2D
18	B	812	CLA	CAD-CBD-CGD-O2D
18	B	828	CLA	CAD-CBD-CGD-O2D
18	B	833	CLA	CAD-CBD-CGD-O2D
18	F	802	CLA	CAD-CBD-CGD-O2D
18	Q	211	CLA	CAD-CBD-CGD-O2D
18	S	201	CLA	CAD-CBD-CGD-O2D
18	U	209	CLA	CAD-CBD-CGD-O2D
27	J	102	LMG	C7-C8-O7-C10
28	T	209	KC1	CAD-CBD-CGD-O2D
29	T	201	A86	C28-C27-C29-C30
18	A	801	CLA	C13-C15-C16-C17
21	B	838	BCR	C6-C7-C8-C9
21	L	205	BCR	C22-C23-C24-C25
21	R	203	BCR	C22-C23-C24-C25
18	B	814	CLA	C6-C7-C8-C10
18	B	807	CLA	C2-C3-C5-C6
27	P	301	LMG	C7-C8-C9-O8
20	R	201	LHG	O6-C4-C5-O7
18	A	836	CLA	C13-C15-C16-C17
18	L	204	CLA	CAA-CBA-CGA-O2A
28	P	311	KC1	C4B-C3B-CAB-CBB
28	Q	210	KC1	C4B-C3B-CAB-CBB
28	S	208	KC1	C4B-C3B-CAB-CBB
28	T	209	KC1	C4B-C3B-CAB-CBB
27	U	201	LMG	C12-C13-C14-C15
18	A	847	CLA	C16-C17-C18-C20
18	B	817	CLA	C16-C17-C18-C19
18	A	803	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	A	803	CLA	CHA-CBD-CGD-O2D
18	A	806	CLA	CHA-CBD-CGD-O1D
18	A	849	CLA	CHA-CBD-CGD-O1D
18	A	849	CLA	CHA-CBD-CGD-O2D
18	A	851	CLA	CHA-CBD-CGD-O1D
18	A	851	CLA	CHA-CBD-CGD-O2D
18	B	808	CLA	CHA-CBD-CGD-O1D
18	B	820	CLA	CHA-CBD-CGD-O1D
18	B	820	CLA	CHA-CBD-CGD-O2D
18	J	103	CLA	CHA-CBD-CGD-O1D
18	Q	212	CLA	CHA-CBD-CGD-O1D
28	U	213	KC1	CHA-CBD-CGD-O1D
28	U	213	KC1	CHA-CBD-CGD-O2D
18	B	820	CLA	C5-C6-C7-C8
20	A	840	LHG	O10-C23-O8-C6
26	M	102	SQD	O6-C44-C45-O47
27	B	849	LMG	O1-C7-C8-O7
27	S	211	LMG	O7-C8-C9-O8
29	Q	201	A86	C13-C14-C15-O1
18	U	210	CLA	C2-C3-C5-C6
24	A	854	DD6	C27-C29-C30-C31
24	P	304	DD6	C27-C29-C30-C31
24	U	214	DD6	C27-C29-C30-C31
21	A	844	BCR	C7-C8-C9-C34
21	B	838	BCR	C7-C8-C9-C34
21	L	205	BCR	C7-C8-C9-C10
18	A	813	CLA	C1A-C2A-CAA-CBA
18	B	825	CLA	C1A-C2A-CAA-CBA
18	O	203	CLA	C1A-C2A-CAA-CBA
18	Q	206	CLA	CHA-CBD-CGD-O2D
18	Q	209	CLA	C1A-C2A-CAA-CBA
21	L	205	BCR	C9-C10-C11-C12
29	R	204	A86	C11-C10-C9-C8
18	T	208	CLA	C8-C10-C11-C12
18	A	804	CLA	C3-C5-C6-C7
25	B	842	DGD	C4E-C5E-C6E-O5E
20	R	201	LHG	C3-O3-P-O5
18	O	205	CLA	C16-C17-C18-C19
18	L	202	CLA	O2A-C1-C2-C3
25	B	842	DGD	C5B-C6B-C7B-C8B
26	B	847	SQD	C27-C28-C29-C30
18	A	803	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	J	103	CLA	CAD-CBD-CGD-O1D
18	Q	216	CLA	CAD-CBD-CGD-O1D
18	S	207	CLA	CAD-CBD-CGD-O1D
18	T	212	CLA	CAD-CBD-CGD-O1D
18	A	815	CLA	C10-C11-C12-C13
18	Q	212	CLA	C15-C16-C17-C18
20	A	839	LHG	O9-C7-O7-C5
18	B	819	CLA	C4-C3-C5-C6
18	T	205	CLA	C4-C3-C5-C6
18	A	823	CLA	C11-C12-C13-C15
18	A	825	CLA	C12-C13-C15-C16
18	O	209	CLA	C6-C7-C8-C10
18	R	205	CLA	C11-C12-C13-C15
18	U	204	CLA	C6-C7-C8-C10
19	A	837	PQN	C22-C23-C25-C26
20	A	839	LHG	C11-C10-C9-C8
26	B	847	SQD	C30-C31-C32-C33
27	Q	217	LMG	C35-C36-C37-C38
18	A	821	CLA	C8-C10-C11-C12
18	B	801	CLA	C2A-CAA-CBA-CGA
20	R	201	LHG	C10-C11-C12-C13
27	Q	217	LMG	C40-C41-C42-C43
18	B	815	CLA	CAA-CBA-CGA-O2A
27	J	102	LMG	O1-C7-C8-C9
27	J	102	LMG	C7-C8-C9-O8
18	A	802	CLA	C5-C6-C7-C8
20	R	201	LHG	C11-C12-C13-C14
18	A	811	CLA	C11-C12-C13-C14
18	A	825	CLA	C14-C13-C15-C16
18	A	828	CLA	C14-C13-C15-C16
18	A	846	CLA	C11-C10-C8-C9
18	B	805	CLA	C11-C10-C8-C9
18	P	306	CLA	C11-C12-C13-C14
18	O	209	CLA	C3-C5-C6-C7
27	J	102	LMG	C17-C18-C19-C20
18	U	207	CLA	C10-C11-C12-C13
27	Q	217	LMG	C37-C38-C39-C40
18	U	210	CLA	C4-C3-C5-C6
18	B	818	CLA	CAA-CBA-CGA-O2A
18	A	833	CLA	O1A-CGA-O2A-C1
18	A	833	CLA	CBA-CGA-O2A-C1
18	A	805	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
18	B	827	CLA	C1-C2-C3-C4
18	L	202	CLA	C1-C2-C3-C4
18	T	205	CLA	C3-C5-C6-C7
18	A	829	CLA	C15-C16-C17-C18
18	B	803	CLA	C13-C15-C16-C17
18	O	204	CLA	C13-C15-C16-C17
20	R	201	LHG	C1-C2-C3-O3
26	M	102	SQD	C26-C27-C28-C29
18	A	823	CLA	C2-C1-O2A-CGA
18	B	834	CLA	C2-C1-O2A-CGA
18	L	202	CLA	C2-C1-O2A-CGA
18	O	209	CLA	C2-C1-O2A-CGA
18	A	815	CLA	CAA-CBA-CGA-O2A
20	A	840	LHG	C10-C11-C12-C13
29	Q	201	A86	C12-C11-C13-C14
21	A	841	BCR	C1-C6-C7-C8
21	A	842	BCR	C1-C6-C7-C8
21	A	842	BCR	C23-C24-C25-C30
21	A	843	BCR	C1-C6-C7-C8
21	B	837	BCR	C23-C24-C25-C30
21	B	839	BCR	C5-C6-C7-C8
21	B	840	BCR	C1-C6-C7-C8
21	F	804	BCR	C1-C6-C7-C8
21	F	804	BCR	C23-C24-C25-C30
21	I	102	BCR	C1-C6-C7-C8
26	M	102	SQD	C23-C24-C25-C26
21	I	101	BCR	C16-C17-C18-C19
21	L	201	BCR	C11-C10-C9-C8
21	R	203	BCR	C20-C21-C22-C23
26	B	847	SQD	O47-C45-C46-O48
27	Q	217	LMG	O1-C7-C8-O7
20	A	839	LHG	C3-O3-P-O6
20	A	840	LHG	C3-O3-P-O6
18	B	809	CLA	C8-C10-C11-C12
18	A	823	CLA	C12-C13-C15-C16
18	O	204	CLA	C12-C13-C15-C16
18	Q	204	CLA	C11-C12-C13-C15
18	Q	216	CLA	C6-C7-C8-C10
19	A	837	PQN	C17-C18-C20-C21
26	M	102	SQD	O48-C23-C24-C25
18	B	809	CLA	C6-C7-C8-C9
18	Q	216	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
18	B	825	CLA	C16-C17-C18-C20
18	Q	216	CLA	C16-C17-C18-C19
26	B	847	SQD	C9-C10-C11-C12
22	A	848	CL0	CAA-CBA-CGA-O2A
18	A	821	CLA	C4-C3-C5-C6
18	A	833	CLA	C4-C3-C5-C6
18	A	834	CLA	C16-C17-C18-C20
20	A	839	LHG	C33-C34-C35-C36
24	O	212	DD6	C1-C2-C3-C4
24	O	213	DD6	C1-C2-C3-C4
24	P	314	DD6	C1-C2-C3-C4
25	B	842	DGD	C8B-C9B-CAB-CBB
18	A	815	CLA	C8-C10-C11-C12
18	B	825	CLA	C10-C11-C12-C13
29	U	202	A86	C6-C8-C9-C10
18	A	838	CLA	C4-C3-C5-C6
18	B	823	CLA	C4-C3-C5-C6
18	B	824	CLA	C4-C3-C5-C6
24	S	209	DD6	C2-C3-C4-C5
18	Q	216	CLA	C10-C11-C12-C13
20	R	201	LHG	C34-C35-C36-C37
18	A	847	CLA	C2-C1-O2A-CGA
18	O	208	CLA	C2-C1-O2A-CGA
18	P	308	CLA	C2-C1-O2A-CGA
27	J	102	LMG	C21-C22-C23-C24
18	B	805	CLA	C2A-CAA-CBA-CGA
18	A	802	CLA	C3A-C2A-CAA-CBA
18	B	846	CLA	C3A-C2A-CAA-CBA
18	U	207	CLA	C3A-C2A-CAA-CBA
27	U	201	LMG	C4-C5-C6-O5
24	P	314	DD6	C3-C4-C5-C6
18	O	208	CLA	C4-C3-C5-C6
18	B	823	CLA	C2-C3-C5-C6
24	Q	215	DD6	C27-C29-C30-C31
18	A	847	CLA	C11-C10-C8-C9
18	B	817	CLA	C11-C12-C13-C14
18	B	821	CLA	C14-C13-C15-C16
18	S	201	CLA	C6-C7-C8-C9
18	B	815	CLA	C5-C6-C7-C8
20	R	201	LHG	C33-C34-C35-C36
21	B	839	BCR	C20-C21-C22-C37
21	F	804	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
21	L	201	BCR	C11-C10-C9-C34
24	S	203	DD6	C-C1-C2-C3
29	Q	201	A86	C25-C26-C27-C28
29	T	201	A86	C25-C26-C27-C28
18	Q	206	CLA	C2A-CAA-CBA-CGA
18	T	206	CLA	C2A-CAA-CBA-CGA
18	Q	216	CLA	C16-C17-C18-C20
18	B	814	CLA	O2A-C1-C2-C3
18	B	819	CLA	O2A-C1-C2-C3
18	S	201	CLA	O2A-C1-C2-C3
29	T	201	A86	C5-C6-C8-C9
18	B	808	CLA	C4-C3-C5-C6
18	A	802	CLA	C1A-C2A-CAA-CBA
18	A	807	CLA	C1A-C2A-CAA-CBA
18	A	826	CLA	C1A-C2A-CAA-CBA
18	A	851	CLA	C1A-C2A-CAA-CBA
18	A	853	CLA	C1A-C2A-CAA-CBA
18	B	824	CLA	C1A-C2A-CAA-CBA
18	Q	203	CLA	C1A-C2A-CAA-CBA
26	B	847	SQD	C24-C23-O48-C46
26	M	102	SQD	C10-C11-C12-C13
18	A	815	CLA	C11-C12-C13-C15
18	A	824	CLA	C11-C10-C8-C7
18	B	815	CLA	C6-C7-C8-C10
18	B	825	CLA	C12-C13-C15-C16
18	O	208	CLA	C2-C3-C5-C6
27	S	211	LMG	C37-C38-C39-C40
18	S	206	CLA	CAA-CBA-CGA-O1A
18	U	206	CLA	CAA-CBA-CGA-O1A
20	R	201	LHG	C35-C36-C37-C38
24	Q	202	DD6	C24-C25-C26-C27
20	A	839	LHG	C26-C27-C28-C29
20	A	839	LHG	C4-O6-P-O3
27	S	211	LMG	C28-C29-C30-C31
18	A	814	CLA	C2A-CAA-CBA-CGA
19	A	837	PQN	C23-C25-C26-C27
20	A	839	LHG	C30-C31-C32-C33
25	B	842	DGD	C3A-C4A-C5A-C6A
18	A	847	CLA	C13-C15-C16-C17
24	S	203	DD6	C24-C1-C2-C3
29	T	201	A86	C25-C26-C27-C29
24	S	203	DD6	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
18	A	815	CLA	C13-C15-C16-C17
18	B	824	CLA	C2A-CAA-CBA-CGA
21	R	203	BCR	C19-C20-C21-C22
25	B	842	DGD	C2B-C3B-C4B-C5B
18	A	849	CLA	C4-C3-C5-C6
18	B	832	CLA	C2-C1-O2A-CGA
18	A	807	CLA	C2-C1-O2A-CGA
18	B	802	CLA	C2-C1-O2A-CGA
18	B	808	CLA	C2-C3-C5-C6
18	B	824	CLA	C2-C3-C5-C6
18	A	834	CLA	C13-C15-C16-C17
18	A	801	CLA	C6-C7-C8-C9
18	B	823	CLA	C11-C10-C8-C9
18	O	206	CLA	C11-C12-C13-C14
18	A	804	CLA	C10-C11-C12-C13
18	B	803	CLA	C3-C5-C6-C7
18	S	206	CLA	CAA-CBA-CGA-O2A
18	B	803	CLA	C2A-CAA-CBA-CGA
18	U	206	CLA	CAA-CBA-CGA-O2A
21	B	839	BCR	C1-C6-C7-C8
21	B	841	BCR	C23-C24-C25-C30
21	F	801	BCR	C1-C6-C7-C8
21	F	801	BCR	C23-C24-C25-C26
21	F	801	BCR	C23-C24-C25-C30
21	J	104	BCR	C23-C24-C25-C26
21	J	104	BCR	C23-C24-C25-C30
18	P	306	CLA	C10-C11-C12-C13
27	S	211	LMG	C14-C15-C16-C17
25	B	842	DGD	O1G-C1G-C2G-C3G
24	O	201	DD6	C24-C25-C26-C27
24	T	213	DD6	C1-C2-C3-C4
18	A	821	CLA	C2-C3-C5-C6
18	A	838	CLA	C2-C3-C5-C6
18	B	828	CLA	C3-C5-C6-C7
18	Q	212	CLA	C13-C15-C16-C17
18	A	804	CLA	C4-C3-C5-C6
18	B	834	CLA	C4-C3-C5-C6
26	M	102	SQD	O10-C23-C24-C25
18	A	849	CLA	C2-C3-C5-C6
18	B	815	CLA	C2-C3-C5-C6
18	B	834	CLA	C12-C13-C15-C16
18	P	306	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	Q	209	CLA	C12-C13-C15-C16
18	A	808	CLA	C1-C2-C3-C4
18	B	827	CLA	O2A-C1-C2-C3
20	R	201	LHG	O7-C7-C8-C9
27	P	301	LMG	O7-C10-C11-C12
27	S	211	LMG	C29-C30-C31-C32
24	P	314	DD6	C4-C5-C6-C7
24	P	317	DD6	C3-C4-C5-C6
27	B	849	LMG	O7-C10-C11-C12
18	B	809	CLA	C4-C3-C5-C6
18	B	817	CLA	C4-C3-C5-C6
18	Q	212	CLA	C4-C3-C5-C6
18	A	828	CLA	C2-C3-C5-C6
18	S	207	CLA	C2-C3-C5-C6
18	B	831	CLA	C16-C17-C18-C20
18	A	815	CLA	C14-C13-C15-C16
18	B	806	CLA	C11-C10-C8-C9
18	B	825	CLA	C14-C13-C15-C16
18	P	306	CLA	C14-C13-C15-C16
18	U	204	CLA	C6-C7-C8-C9
18	U	205	CLA	C11-C12-C13-C14
19	A	837	PQN	C24-C23-C25-C26
18	A	814	CLA	CAA-CBA-CGA-O2A
18	A	853	CLA	C3A-C2A-CAA-CBA
18	B	805	CLA	C3A-C2A-CAA-CBA
20	A	839	LHG	C29-C30-C31-C32
18	A	811	CLA	CAA-CBA-CGA-O2A
18	U	208	CLA	CAA-CBA-CGA-O2A
18	A	804	CLA	CAD-CBD-CGD-O2D
18	A	810	CLA	CAD-CBD-CGD-O2D
18	A	811	CLA	CAD-CBD-CGD-O2D
18	A	819	CLA	CAD-CBD-CGD-O2D
18	A	822	CLA	CAD-CBD-CGD-O2D
18	A	823	CLA	CAD-CBD-CGD-O2D
18	A	827	CLA	CAD-CBD-CGD-O2D
18	A	835	CLA	CAD-CBD-CGD-O2D
18	L	202	CLA	CAD-CBD-CGD-O2D
18	U	207	CLA	CAD-CBD-CGD-O2D
18	T	205	CLA	CAD-CBD-CGD-O2D
18	T	207	CLA	CAD-CBD-CGD-O2D
28	P	305	KC1	CAD-CBD-CGD-O2D
18	B	825	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	A	803	CLA	C2A-CAA-CBA-CGA
18	A	806	CLA	C2A-CAA-CBA-CGA
18	P	308	CLA	C2A-CAA-CBA-CGA
18	T	208	CLA	C2A-CAA-CBA-CGA
18	A	821	CLA	CAA-CBA-CGA-O2A
18	Q	216	CLA	CAA-CBA-CGA-O2A
21	F	804	BCR	C21-C22-C23-C24
27	S	211	LMG	O1-C7-C8-C9
27	U	201	LMG	C7-C8-C9-O8
18	B	804	CLA	CAA-CBA-CGA-O2A
18	T	211	CLA	C2C-C3C-CAC-CBC
19	A	837	PQN	C18-C20-C21-C22
18	B	844	CLA	CAA-CBA-CGA-O2A
18	B	804	CLA	CAA-CBA-CGA-O1A
18	A	821	CLA	O2A-C1-C2-C3
18	A	824	CLA	O2A-C1-C2-C3
18	A	827	CLA	O2A-C1-C2-C3
18	Q	204	CLA	O2A-C1-C2-C3
18	Q	208	CLA	O2A-C1-C2-C3
20	R	201	LHG	C7-C8-C9-C10
18	A	801	CLA	CHA-CBD-CGD-O2D
18	A	813	CLA	CHA-CBD-CGD-O2D
18	A	821	CLA	CHA-CBD-CGD-O1D
18	A	821	CLA	CHA-CBD-CGD-O2D
18	B	802	CLA	CHA-CBD-CGD-O1D
18	B	802	CLA	CHA-CBD-CGD-O2D
18	B	804	CLA	CHA-CBD-CGD-O1D
18	B	813	CLA	CHA-CBD-CGD-O2D
18	B	818	CLA	CHA-CBD-CGD-O2D
18	B	848	CLA	CHA-CBD-CGD-O2D
18	J	103	CLA	CHA-CBD-CGD-O2D
18	O	204	CLA	CHA-CBD-CGD-O2D
18	O	205	CLA	CHA-CBD-CGD-O1D
18	O	205	CLA	CHA-CBD-CGD-O2D
18	Q	209	CLA	CHA-CBD-CGD-O1D
18	Q	216	CLA	CHA-CBD-CGD-O1D
18	S	207	CLA	CHA-CBD-CGD-O1D
18	U	209	CLA	CHA-CBD-CGD-O2D
18	U	210	CLA	CHA-CBD-CGD-O2D
18	T	203	CLA	CHA-CBD-CGD-O2D
18	B	848	CLA	CAA-CBA-CGA-O2A
27	P	301	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
24	P	314	DD6	C4-C5-C6-C8
24	U	212	DD6	C9-C10-C11-C13
24	U	212	DD6	C4-C5-C6-C8
29	Q	201	A86	C25-C26-C27-C29
18	A	814	CLA	CAA-CBA-CGA-O1A
18	B	806	CLA	CAA-CBA-CGA-O2A
18	U	211	CLA	CAA-CBA-CGA-O2A
27	U	201	LMG	O7-C8-C9-O8
18	B	834	CLA	C5-C6-C7-C8
29	Q	214	A86	C13-C14-C15-O1
29	R	206	A86	C13-C14-C15-O1
29	U	202	A86	C13-C14-C15-O1
27	U	201	LMG	C11-C12-C13-C14
18	A	804	CLA	C2-C3-C5-C6
18	A	807	CLA	C11-C10-C8-C7
18	Q	212	CLA	C11-C10-C8-C7
18	F	803	CLA	CAA-CBA-CGA-O2A
18	P	307	CLA	CAA-CBA-CGA-O2A
18	A	823	CLA	C11-C12-C13-C14
18	O	209	CLA	C6-C7-C8-C9
18	R	205	CLA	C11-C12-C13-C14
19	A	837	PQN	C19-C18-C20-C21
24	O	215	DD6	C1-C2-C3-C4
18	A	807	CLA	C2B-C3B-CAB-CBB
18	A	809	CLA	C2B-C3B-CAB-CBB
18	A	834	CLA	C2B-C3B-CAB-CBB
18	A	838	CLA	C2B-C3B-CAB-CBB
18	A	845	CLA	C2B-C3B-CAB-CBB
18	A	852	CLA	C2B-C3B-CAB-CBB
18	B	805	CLA	C2B-C3B-CAB-CBB
18	B	819	CLA	C2B-C3B-CAB-CBB
18	B	824	CLA	C2B-C3B-CAB-CBB
18	B	832	CLA	C2B-C3B-CAB-CBB
18	F	802	CLA	C2B-C3B-CAB-CBB
18	L	204	CLA	C2B-C3B-CAB-CBB
18	P	307	CLA	C2B-C3B-CAB-CBB
18	P	310	CLA	C2B-C3B-CAB-CBB
18	P	315	CLA	C2B-C3B-CAB-CBB
18	Q	208	CLA	C2B-C3B-CAB-CBB
18	Q	211	CLA	C2B-C3B-CAB-CBB
18	Q	213	CLA	C2B-C3B-CAB-CBB
18	R	205	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	S	205	CLA	C2B-C3B-CAB-CBB
18	S	207	CLA	C2B-C3B-CAB-CBB
18	S	214	CLA	C2B-C3B-CAB-CBB
18	U	204	CLA	C2B-C3B-CAB-CBB
18	U	205	CLA	C2B-C3B-CAB-CBB
18	U	207	CLA	C2B-C3B-CAB-CBB
18	U	210	CLA	C2B-C3B-CAB-CBB
18	U	211	CLA	C2B-C3B-CAB-CBB
18	T	203	CLA	C2B-C3B-CAB-CBB
18	T	208	CLA	C2B-C3B-CAB-CBB
24	O	214	DD6	C2-C3-C4-C5
27	Q	217	LMG	C19-C20-C21-C22
18	P	306	CLA	C2A-CAA-CBA-CGA
18	T	205	CLA	CAA-CBA-CGA-O2A
27	Q	217	LMG	C21-C22-C23-C24
18	U	204	CLA	C3-C5-C6-C7
27	J	102	LMG	O9-C10-C11-C12
18	A	829	CLA	C16-C17-C18-C20
27	Q	217	LMG	C33-C34-C35-C36
18	A	803	CLA	CAA-CBA-CGA-O2A
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	843	CLA	C1A-C2A-CAA-CBA
18	S	205	CLA	C1A-C2A-CAA-CBA
18	U	204	CLA	C2-C1-O2A-CGA
18	A	811	CLA	CAA-CBA-CGA-O1A
27	Q	217	LMG	O10-C28-C29-C30
18	B	803	CLA	CAA-CBA-CGA-O2A
18	T	212	CLA	CAA-CBA-CGA-O2A
18	Q	209	CLA	C2A-CAA-CBA-CGA
18	A	849	CLA	C16-C17-C18-C20
27	B	849	LMG	O9-C10-C11-C12
27	P	301	LMG	O9-C10-C11-C12
18	A	847	CLA	C10-C11-C12-C13
18	S	207	CLA	C4-C3-C5-C6
18	P	307	CLA	CAA-CBA-CGA-O1A
18	Q	216	CLA	CAA-CBA-CGA-O1A
26	M	102	SQD	O49-C7-C8-C9
18	B	834	CLA	C2-C3-C5-C6
18	T	205	CLA	C2-C3-C5-C6
18	B	829	CLA	C4B-C3B-CAB-CBB
18	B	848	CLA	C4B-C3B-CAB-CBB
18	O	207	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	T	202	CLA	C4B-C3B-CAB-CBB
18	T	212	CLA	C4B-C3B-CAB-CBB
18	A	821	CLA	CAA-CBA-CGA-O1A
18	B	848	CLA	CAA-CBA-CGA-O1A
21	B	841	BCR	C23-C24-C25-C26
24	S	209	DD6	C11-C13-C14-C15
18	B	806	CLA	CAA-CBA-CGA-O1A
18	U	208	CLA	CAA-CBA-CGA-O1A
18	Q	204	CLA	C5-C6-C7-C8
21	L	201	BCR	C18-C19-C20-C21
18	F	803	CLA	CAA-CBA-CGA-O1A
18	T	205	CLA	CAA-CBA-CGA-O1A
27	S	211	LMG	O9-C10-C11-C12
27	S	211	LMG	O10-C28-C29-C30
18	B	844	CLA	CAA-CBA-CGA-O1A
18	U	211	CLA	CAA-CBA-CGA-O1A
18	B	835	CLA	C4-C3-C5-C6
18	B	805	CLA	CAD-CBD-CGD-O1D
18	B	825	CLA	CAD-CBD-CGD-O1D
18	B	830	CLA	CAD-CBD-CGD-O1D
18	U	207	CLA	CAD-CBD-CGD-O1D
28	U	213	KC1	CAD-CBD-CGD-O1D
27	U	201	LMG	O10-C28-O8-C9
18	Q	206	CLA	CAA-CBA-CGA-O2A
20	A	839	LHG	O8-C23-C24-C25
18	B	815	CLA	C6-C7-C8-C9
18	B	833	CLA	C11-C12-C13-C14
18	L	203	CLA	C11-C12-C13-C14
18	Q	216	CLA	C6-C7-C8-C9
18	S	205	CLA	CAA-CBA-CGA-O2A
27	Q	217	LMG	O8-C28-C29-C30
27	S	211	LMG	O7-C10-C11-C12
27	S	211	LMG	O8-C28-C29-C30
18	P	308	CLA	CAA-CBA-CGA-O2A
18	T	204	CLA	CAA-CBA-CGA-O2A
27	J	102	LMG	O7-C10-C11-C12
20	R	201	LHG	O9-C7-O7-C5
18	A	828	CLA	C4-C3-C5-C6
18	A	846	CLA	C4-C3-C5-C6
18	P	308	CLA	C4-C3-C5-C6
18	A	821	CLA	C11-C10-C8-C7
18	A	824	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	B	806	CLA	C11-C10-C8-C7
18	B	815	CLA	C11-C10-C8-C7
18	B	819	CLA	C3A-C2A-CAA-CBA
18	L	204	CLA	CAA-CBA-CGA-O1A
18	T	211	CLA	CAA-CBA-CGA-O1A
26	B	847	SQD	O49-C7-C8-C9
18	A	820	CLA	CAA-CBA-CGA-O2A
18	T	211	CLA	CAA-CBA-CGA-O2A
26	B	847	SQD	O47-C7-C8-C9
21	A	842	BCR	C7-C8-C9-C10
18	P	308	CLA	CAA-CBA-CGA-O1A
18	T	204	CLA	CAA-CBA-CGA-O1A
18	T	212	CLA	CAA-CBA-CGA-O1A
26	M	102	SQD	O47-C7-C8-C9
18	B	824	CLA	C5-C6-C7-C8
18	P	306	CLA	C15-C16-C17-C18
19	A	837	PQN	C20-C21-C22-C23
18	B	819	CLA	C5-C6-C7-C8
27	U	201	LMG	O6-C5-C6-O5
18	U	210	CLA	C13-C15-C16-C17
18	O	207	CLA	CAA-CBA-CGA-O2A
18	B	823	CLA	C13-C15-C16-C17
18	B	827	CLA	C2A-CAA-CBA-CGA
20	A	839	LHG	C14-C15-C16-C17
18	Q	206	CLA	CAA-CBA-CGA-O1A
18	A	801	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

151 monomers are involved in 253 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	840	BCR	1	0
18	B	834	CLA	3	0
21	J	104	BCR	1	0
18	A	820	CLA	1	0
18	Q	212	CLA	1	0
18	T	202	CLA	2	0
18	Q	207	CLA	1	0
18	A	826	CLA	2	0
18	A	846	CLA	1	0
18	B	843	CLA	3	0
29	R	204	A86	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	848	CLA	3	0
18	A	845	CLA	3	0
18	B	819	CLA	5	0
18	L	202	CLA	2	0
18	U	209	CLA	1	0
26	M	102	SQD	3	0
18	B	810	CLA	1	0
18	A	847	CLA	3	0
18	A	808	CLA	1	0
18	T	208	CLA	3	0
28	O	210	KC1	1	0
20	A	839	LHG	1	0
18	A	821	CLA	1	0
18	B	835	CLA	8	0
18	B	831	CLA	3	0
18	L	203	CLA	2	0
18	A	828	CLA	2	0
18	B	830	CLA	2	0
18	Q	206	CLA	2	0
18	Q	216	CLA	2	0
21	A	841	BCR	1	0
18	A	835	CLA	3	0
18	A	825	CLA	1	0
18	A	823	CLA	3	0
18	O	208	CLA	2	0
21	A	842	BCR	1	0
18	U	207	CLA	3	0
21	L	201	BCR	2	0
18	S	201	CLA	4	0
18	A	810	CLA	1	0
18	A	833	CLA	5	0
18	Q	208	CLA	5	0
18	B	820	CLA	3	0
21	I	101	BCR	2	0
18	P	313	CLA	1	0
25	B	842	DGD	5	0
18	Q	205	CLA	1	0
21	F	801	BCR	1	0
27	J	102	LMG	2	0
18	B	846	CLA	7	0
20	A	840	LHG	1	0
18	R	202	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	T	211	CLA	2	0
18	O	207	CLA	2	0
18	Q	209	CLA	1	0
18	A	851	CLA	1	0
18	A	815	CLA	2	0
27	S	211	LMG	6	0
18	S	204	CLA	2	0
18	T	210	CLA	1	0
18	A	807	CLA	2	0
18	B	818	CLA	1	0
18	B	816	CLA	2	0
18	B	845	CLA	1	0
18	P	307	CLA	1	0
18	B	802	CLA	2	0
21	B	841	BCR	2	0
18	A	803	CLA	2	0
18	B	815	CLA	3	0
18	B	825	CLA	1	0
18	B	808	CLA	4	0
27	Q	217	LMG	6	0
18	S	214	CLA	4	0
18	T	212	CLA	1	0
18	A	814	CLA	2	0
21	I	102	BCR	2	0
18	P	306	CLA	1	0
18	U	206	CLA	2	0
18	B	821	CLA	4	0
21	R	203	BCR	3	0
18	A	853	CLA	2	0
18	A	838	CLA	1	0
21	F	804	BCR	3	0
18	A	849	CLA	1	0
28	T	209	KC1	2	0
18	B	817	CLA	2	0
18	S	207	CLA	2	0
18	B	803	CLA	3	0
21	M	101	BCR	4	0
18	A	817	CLA	1	0
18	O	209	CLA	2	0
18	O	202	CLA	2	0
24	P	304	DD6	1	0
18	S	206	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	U	205	CLA	1	0
18	A	804	CLA	1	0
19	A	837	PQN	2	0
21	A	843	BCR	2	0
21	B	839	BCR	1	0
18	A	836	CLA	2	0
18	A	834	CLA	3	0
18	A	824	CLA	3	0
21	B	837	BCR	2	0
18	A	811	CLA	2	0
18	U	211	CLA	3	0
18	U	208	CLA	1	0
21	B	838	BCR	1	0
18	O	204	CLA	1	0
18	B	801	CLA	1	0
18	A	822	CLA	1	0
18	O	203	CLA	1	0
18	A	801	CLA	4	0
27	P	301	LMG	1	0
27	B	849	LMG	2	0
18	B	827	CLA	4	0
18	J	103	CLA	2	0
18	B	824	CLA	3	0
18	B	822	CLA	1	0
18	P	315	CLA	1	0
18	Q	203	CLA	1	0
18	B	806	CLA	1	0
26	B	847	SQD	3	0
18	O	206	CLA	1	0
21	A	844	BCR	1	0
29	R	206	A86	1	0
18	T	205	CLA	2	0
18	A	831	CLA	2	0
18	B	828	CLA	1	0
18	B	807	CLA	4	0
18	A	852	CLA	4	0
18	B	844	CLA	2	0
21	L	205	BCR	4	0
18	B	812	CLA	1	0
18	A	813	CLA	1	0
20	R	201	LHG	2	0
18	B	829	CLA	2	0

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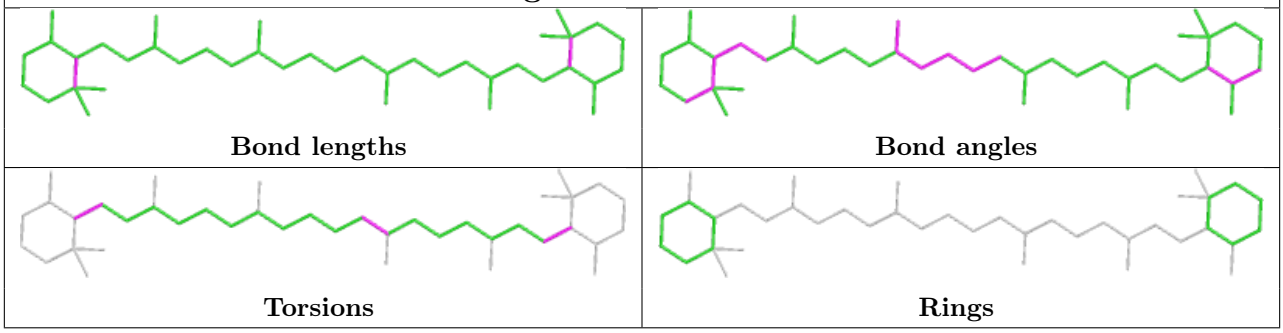
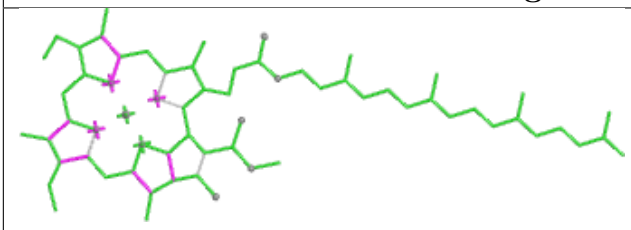
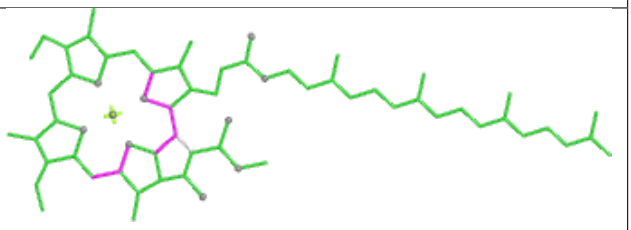
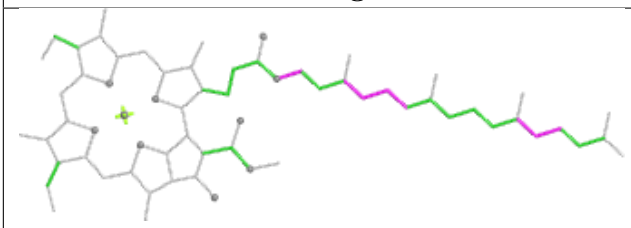
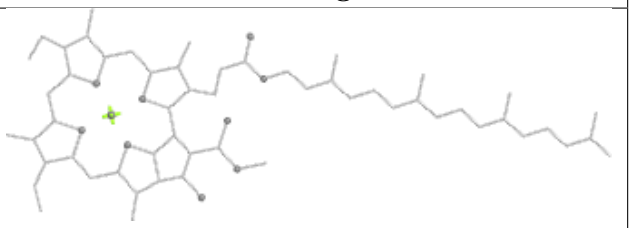
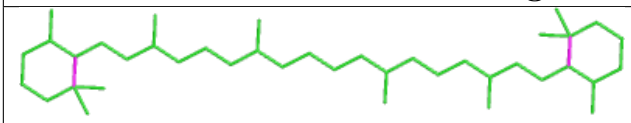
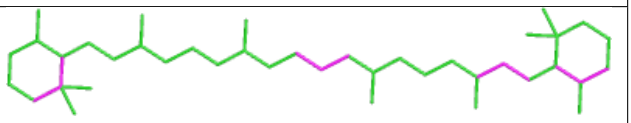
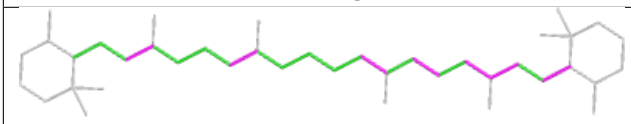
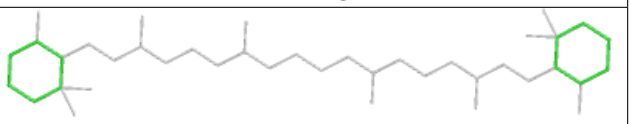
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	R	205	CLA	3	0
27	U	201	LMG	2	0
29	U	202	A86	1	0
18	U	210	CLA	4	0
18	T	207	CLA	2	0
22	A	848	CL0	3	0
18	S	215	CLA	2	0
18	A	830	CLA	1	0
18	F	803	CLA	1	0
18	O	205	CLA	2	0
18	A	818	CLA	2	0
18	B	833	CLA	2	0
19	B	836	PQN	1	0
18	A	816	CLA	2	0

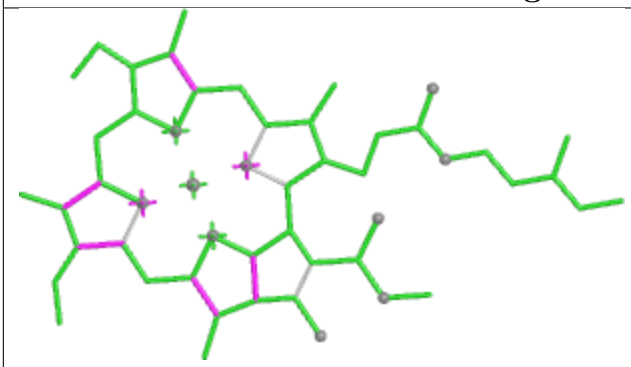
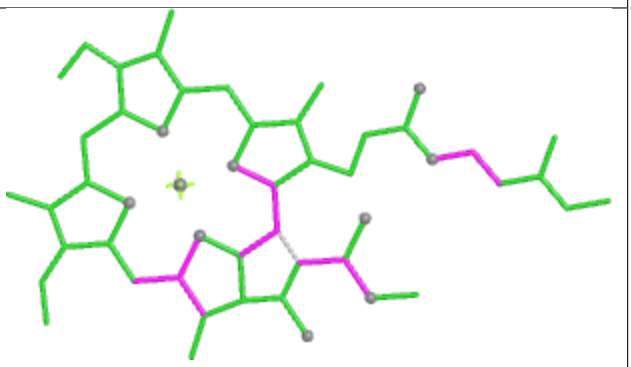
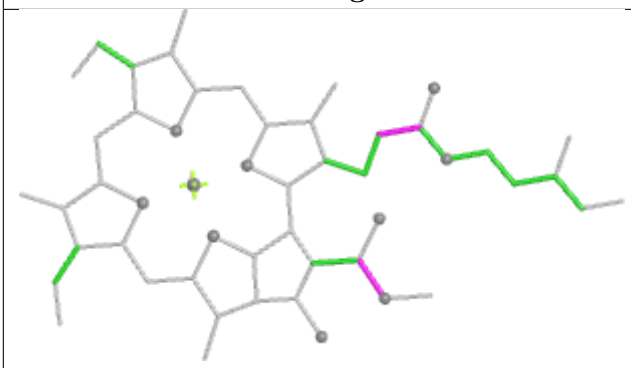
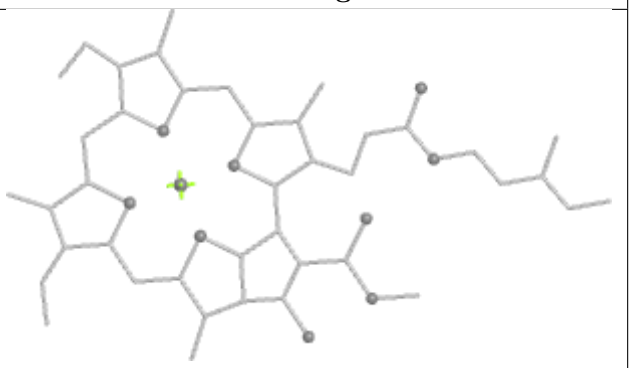
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

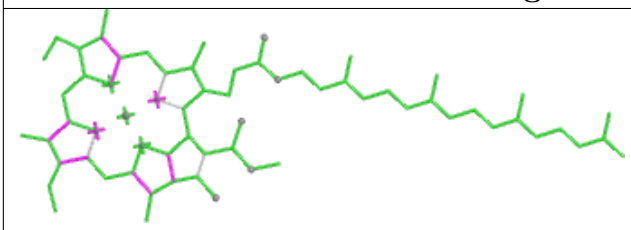
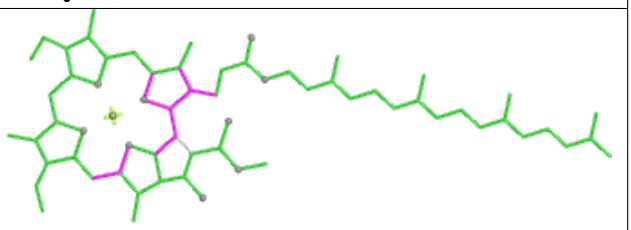
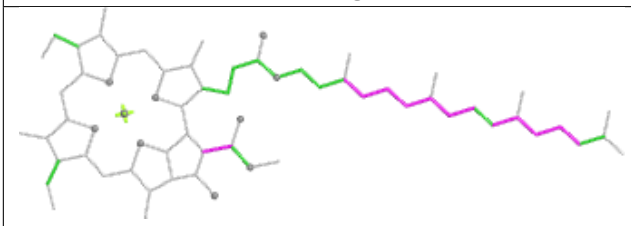
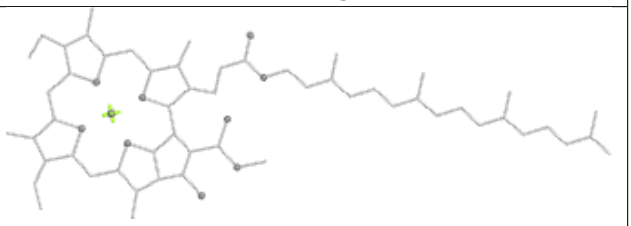
Ligand BCR B 840



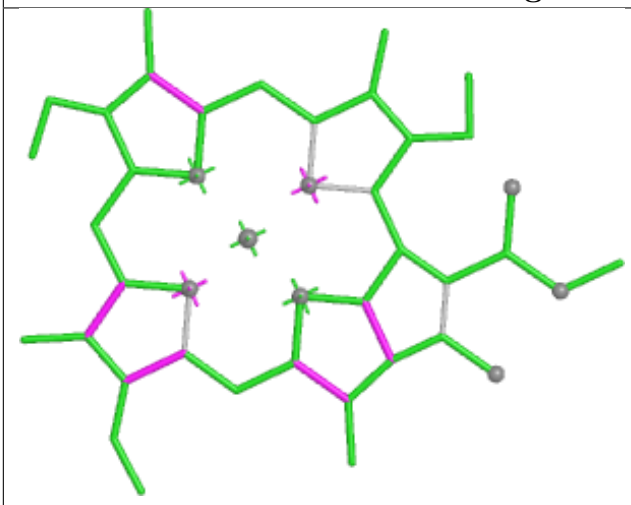
Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR J 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

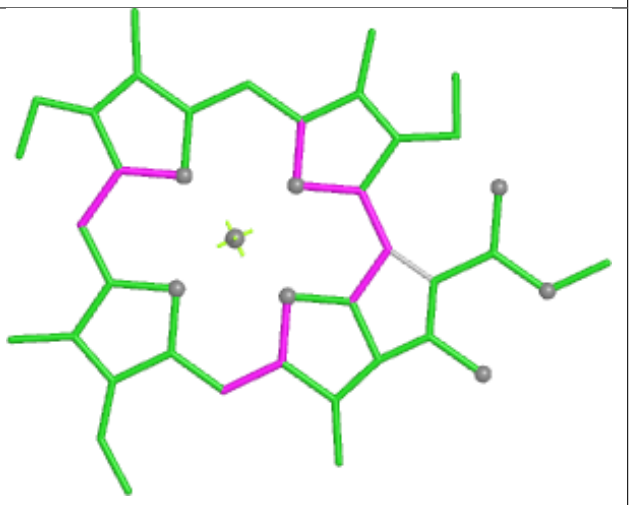
Ligand CLA A 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 212	
 Bond lengths	 Bond angles
 Torsions	 Rings

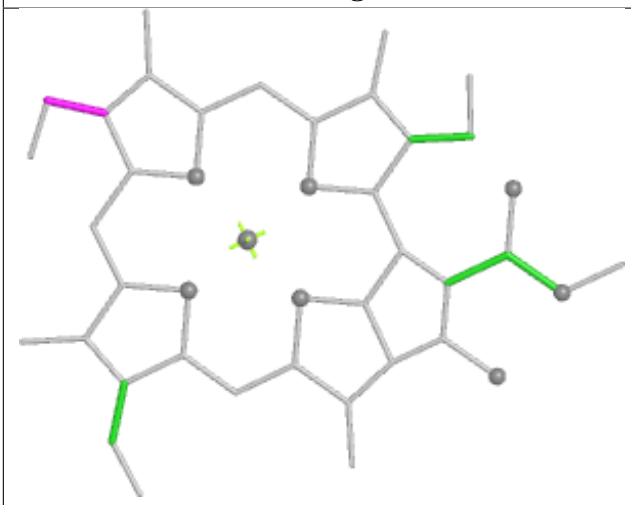
Ligand CLA T 202



Bond lengths



Bond angles



Torsions

Rings

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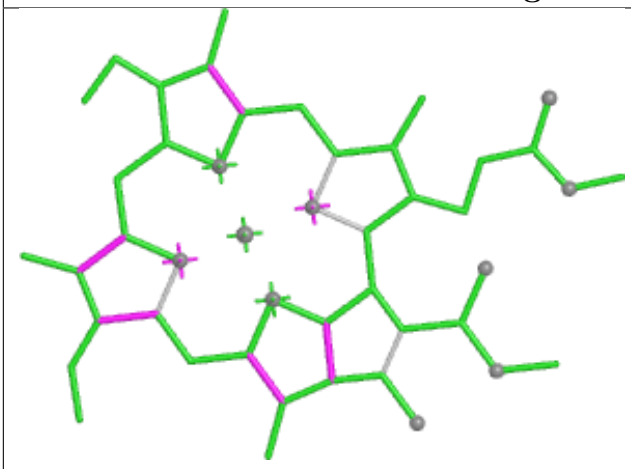

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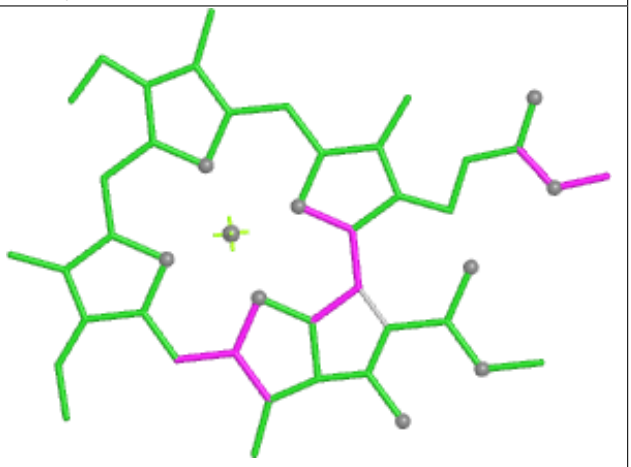

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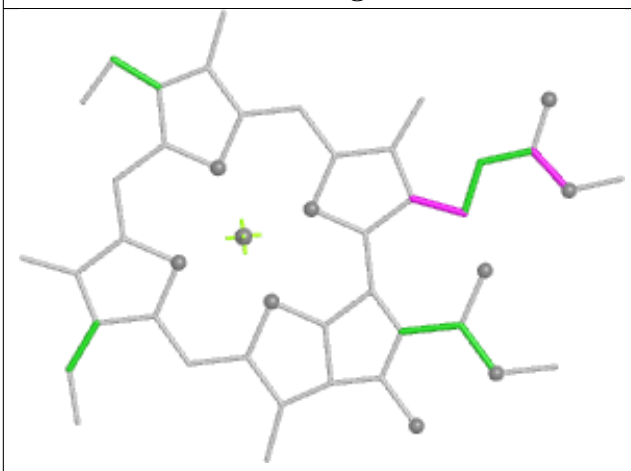

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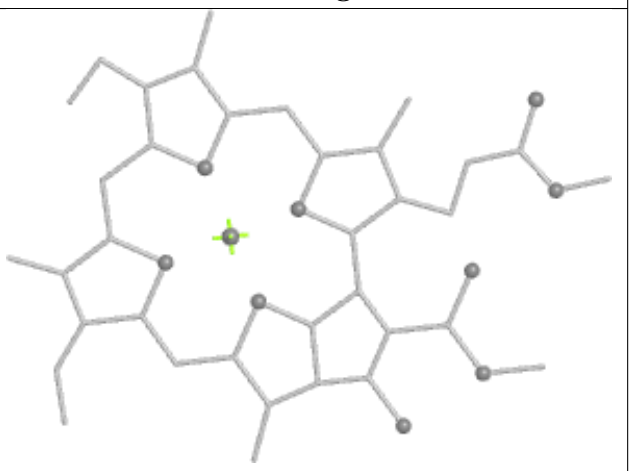
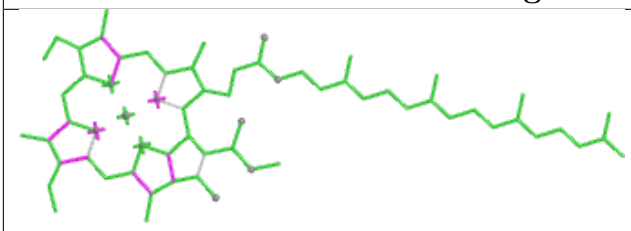


Rings

Ligand CLA A 826



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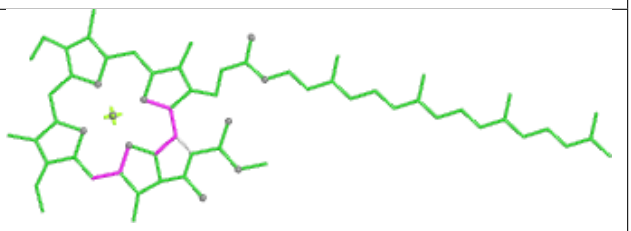

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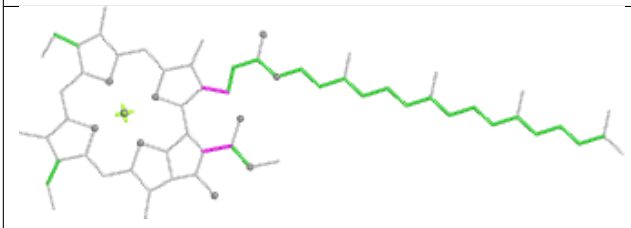

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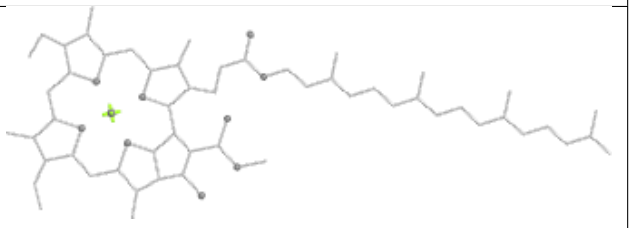
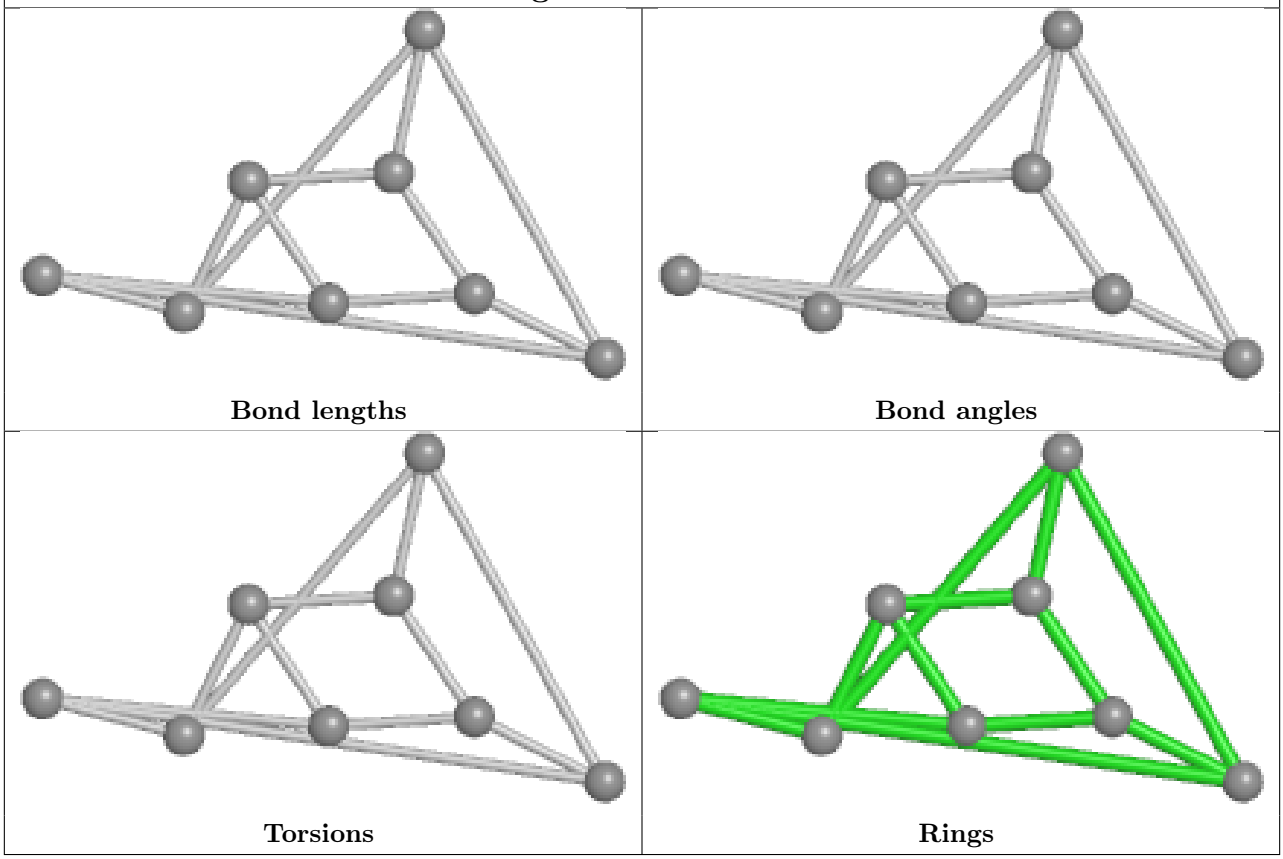
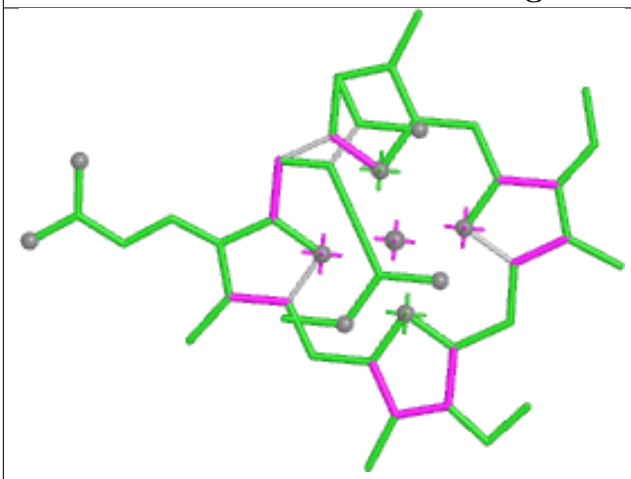


Rings

Ligand SF4 A 850



Ligand KC1 U 213



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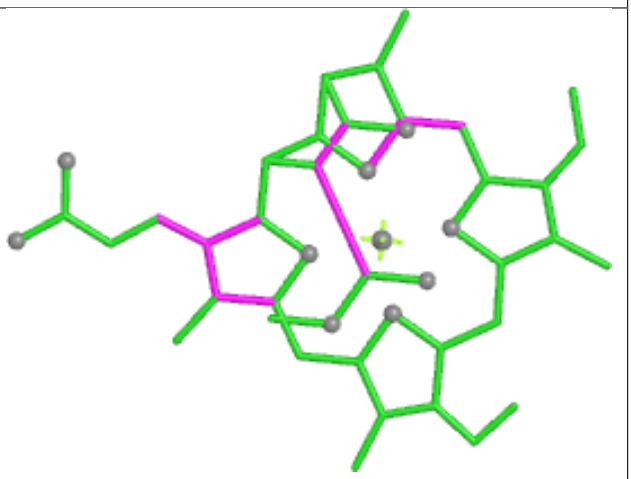
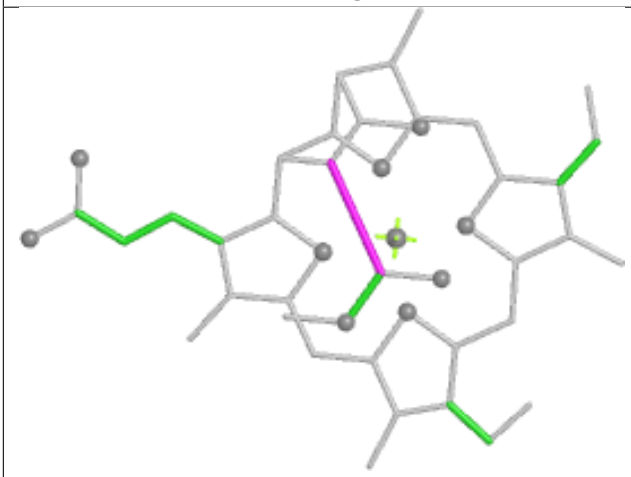


Bond angles



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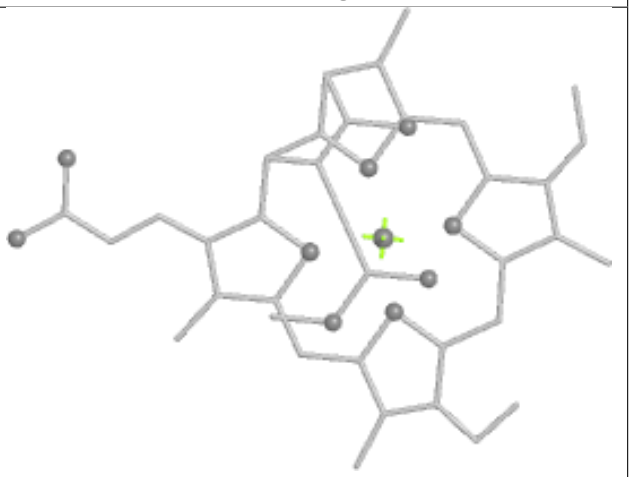
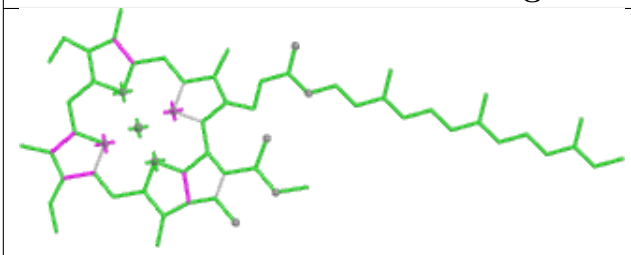


Rings

Ligand CLA Q 204



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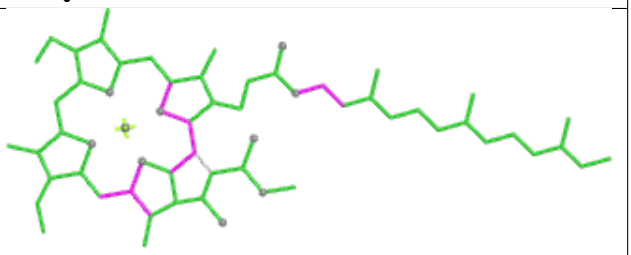
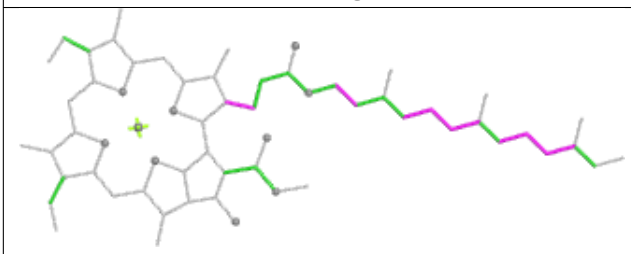
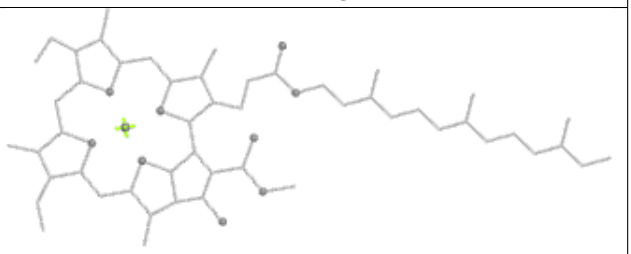


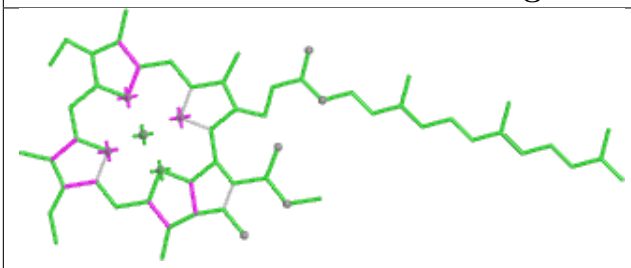
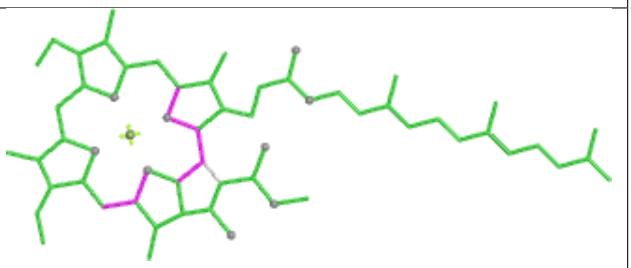
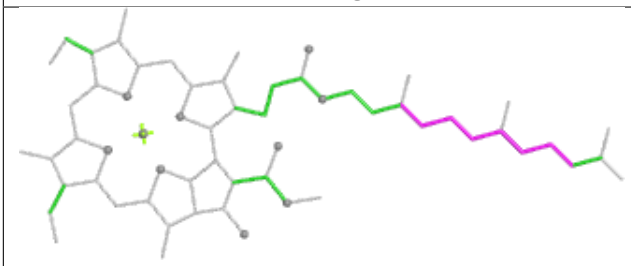
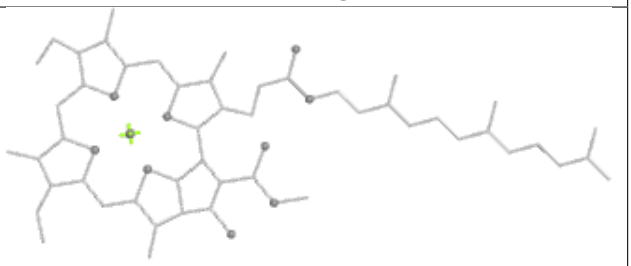
Bond angles



Torsions



Rings

Ligand CLA A 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

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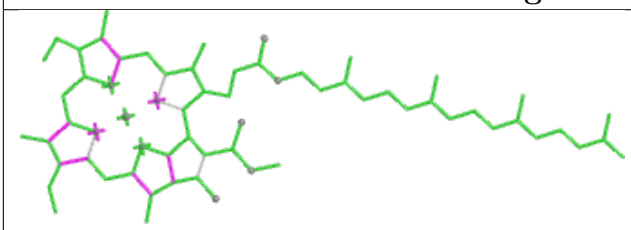
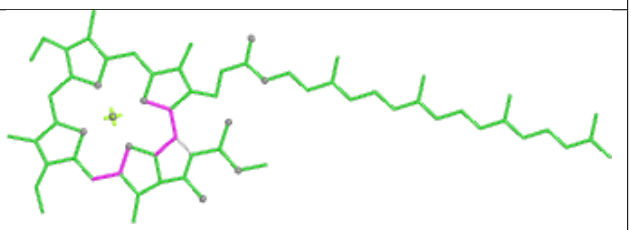
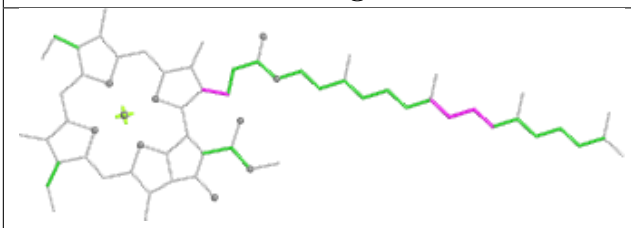
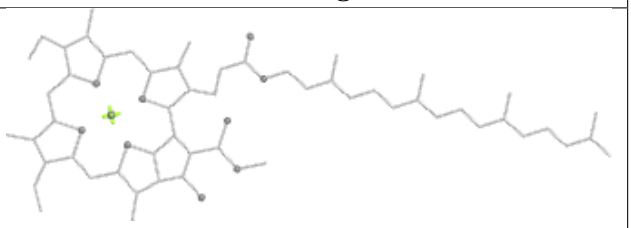
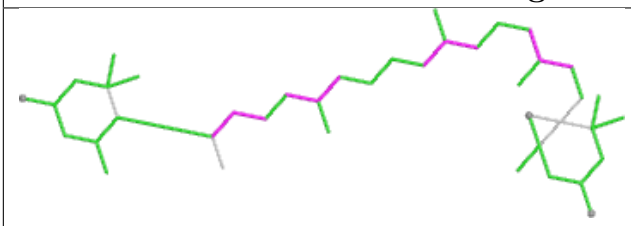
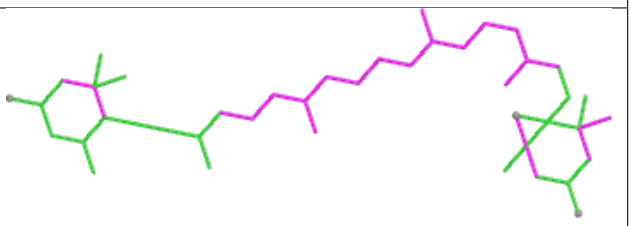
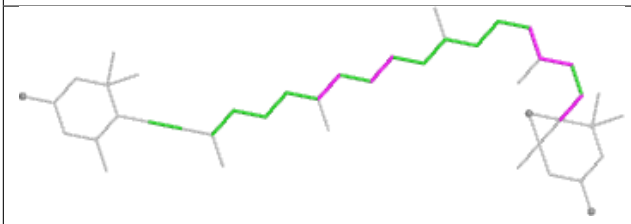
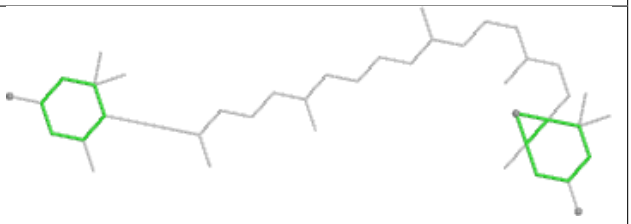
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 S 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

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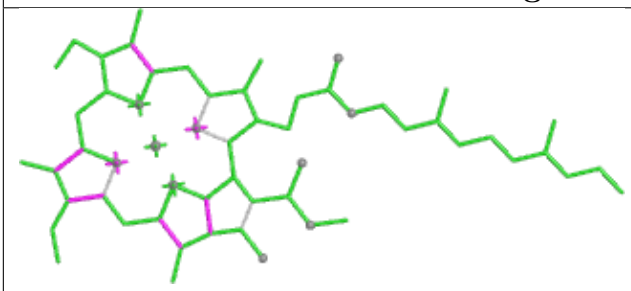
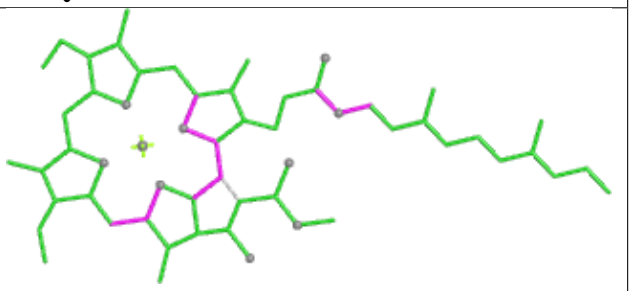
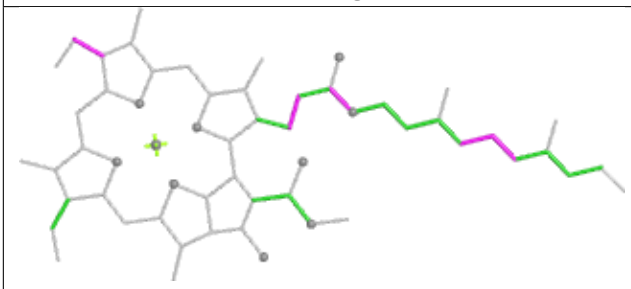
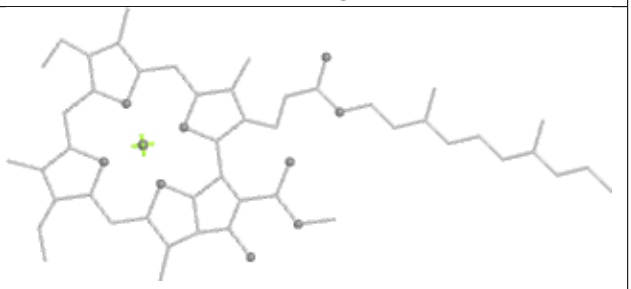
 Bond lengths	 Bond angles
 Torsions	 Rings

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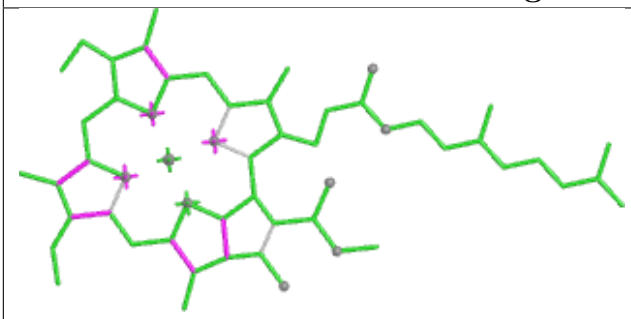
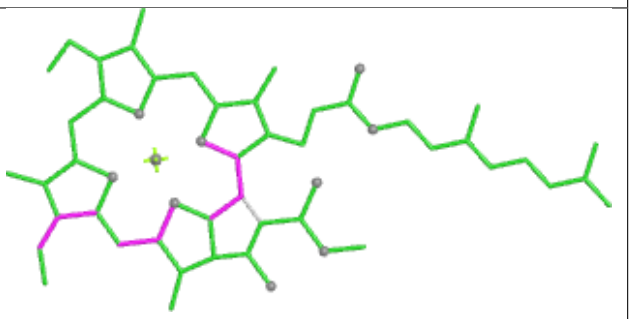
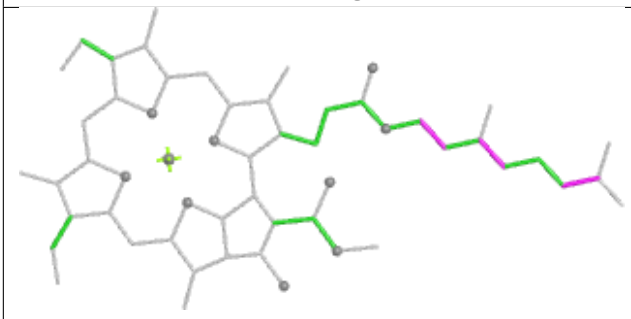
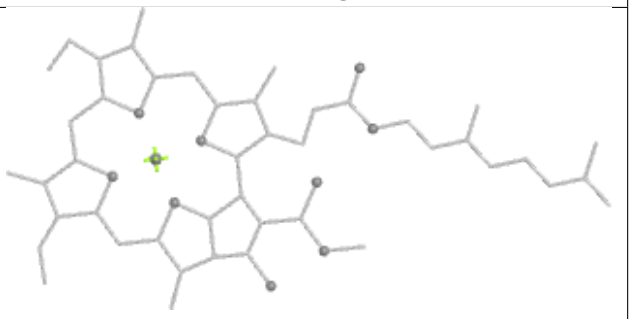
 Bond lengths	 Bond angles
 Torsions	 Rings

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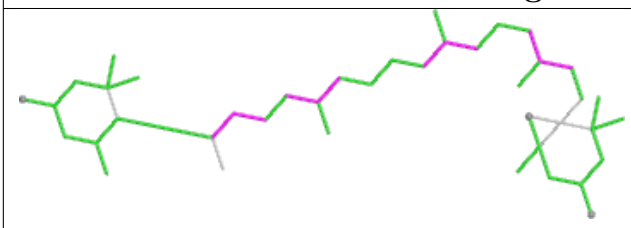
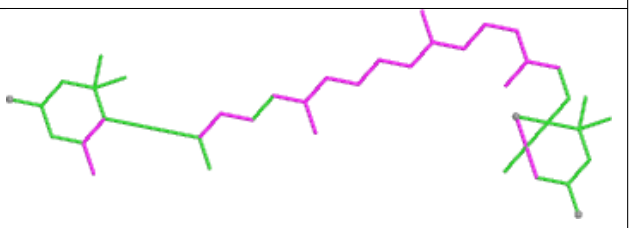
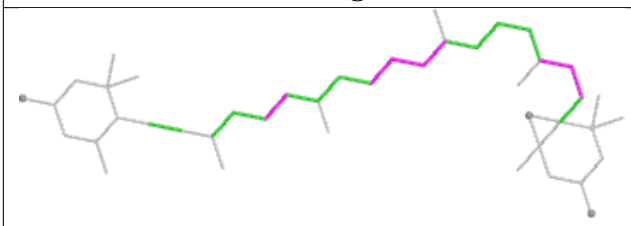
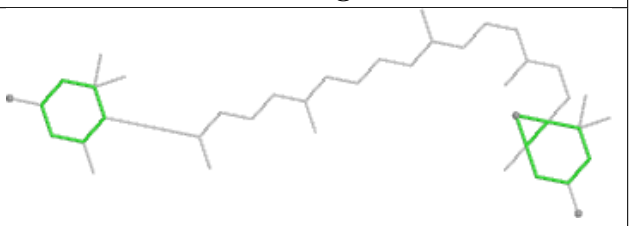
 Bond lengths	 Bond angles
 Torsions	 Rings

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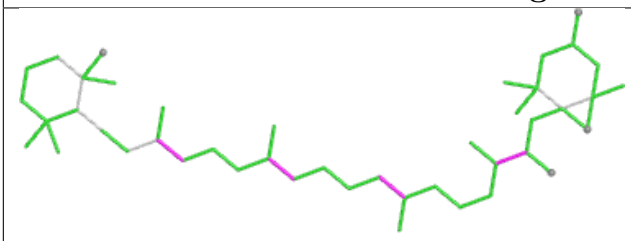
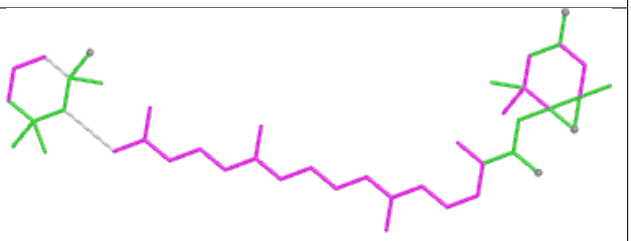
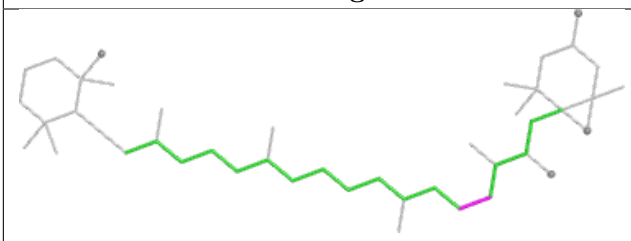
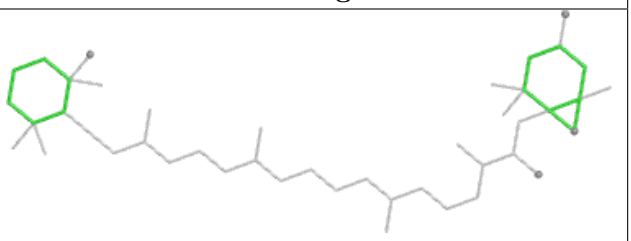
 Bond lengths	 Bond angles
 Torsions	 Rings

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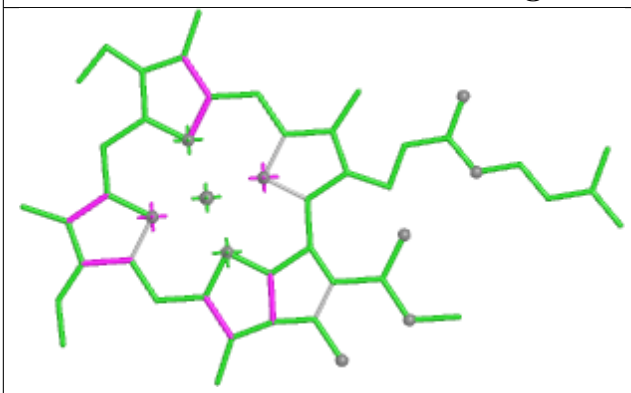
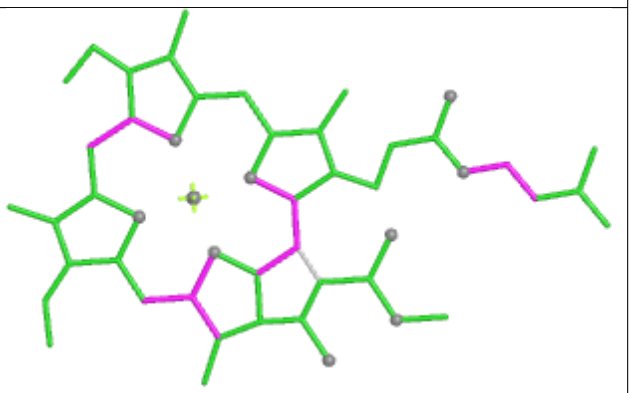
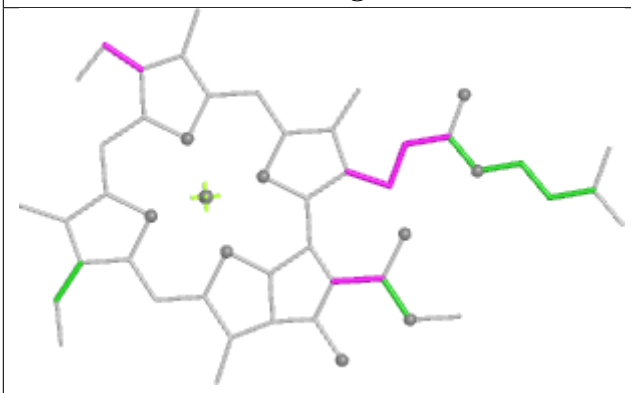
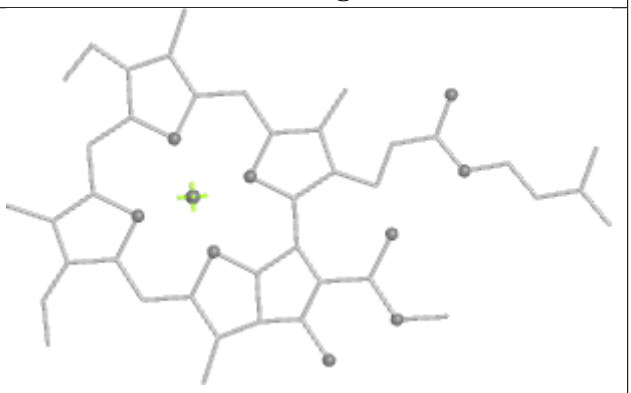
 Bond lengths	 Bond angles
 Torsions	 Rings

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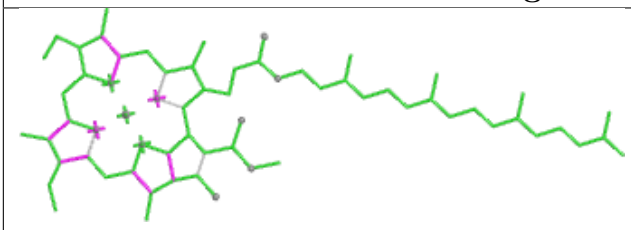
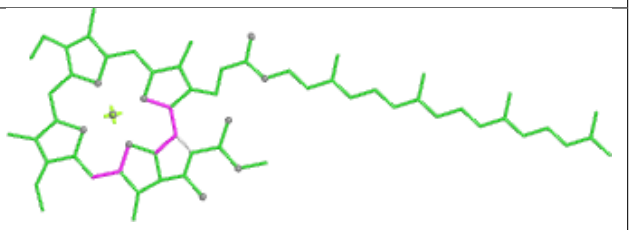
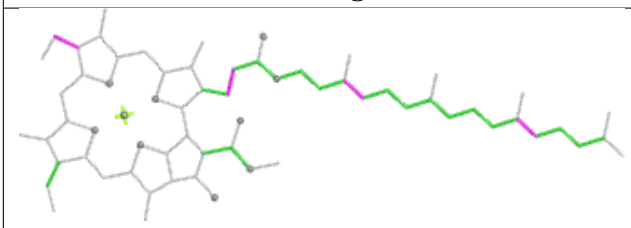
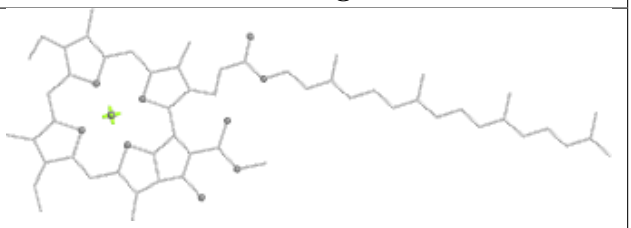
 Bond lengths	 Bond angles
 Torsions	 Rings

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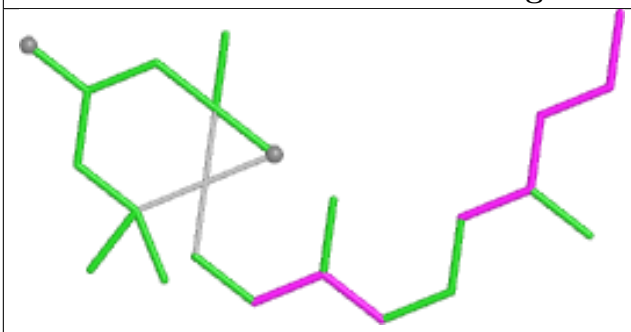
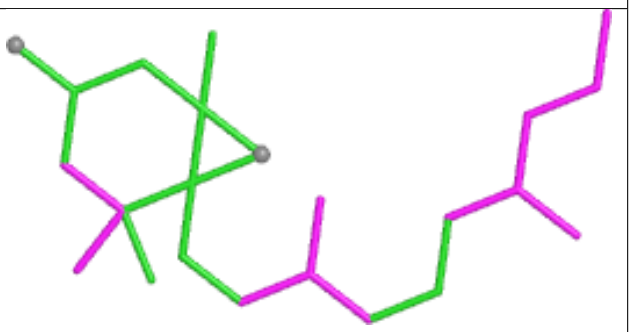
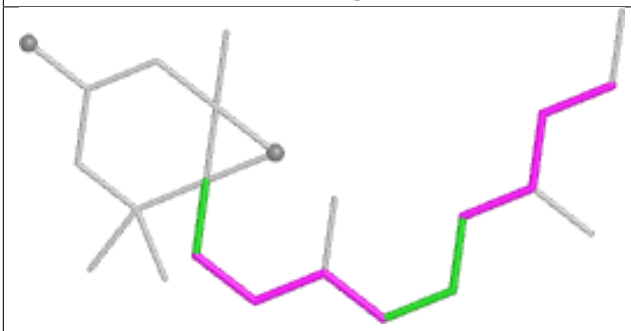
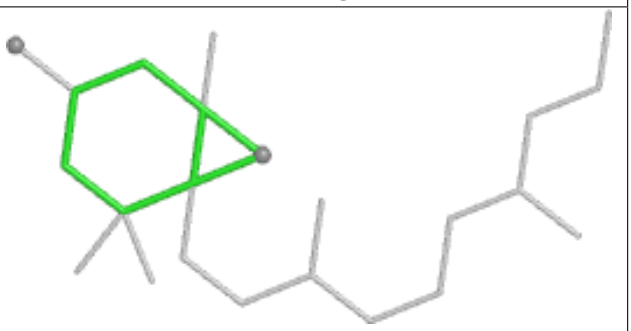
 Bond lengths	 Bond angles
 Torsions	 Rings

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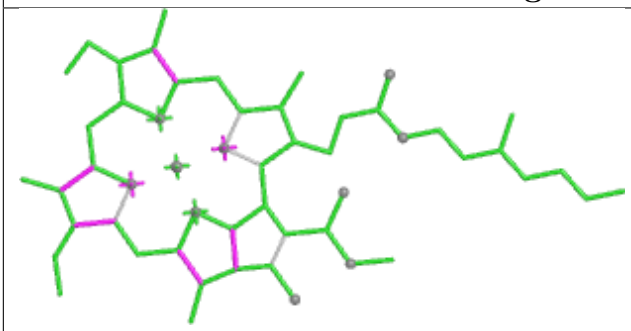
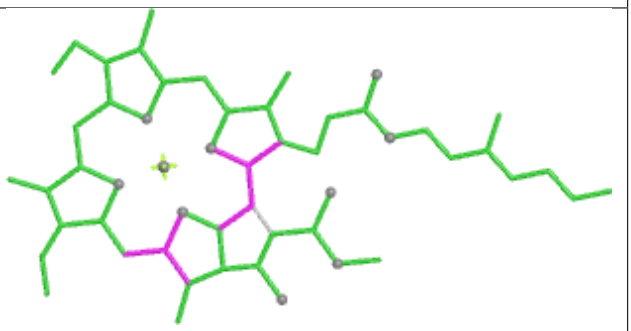
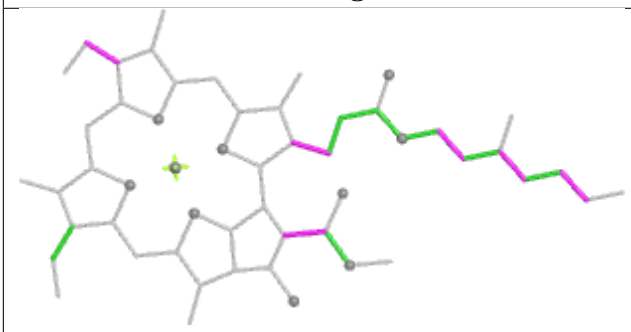
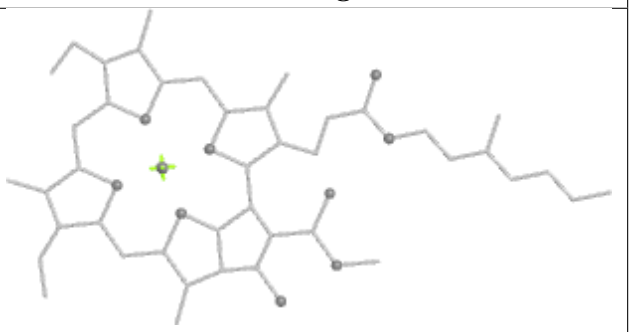
 Bond lengths	 Bond angles
 Torsions	 Rings

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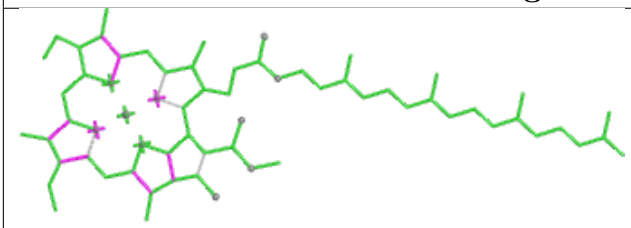
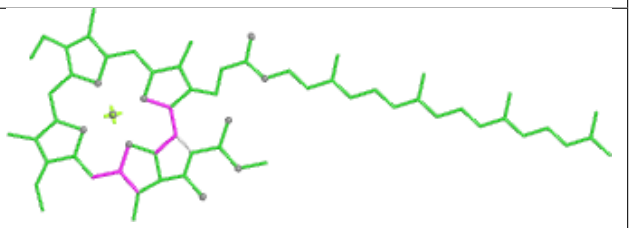
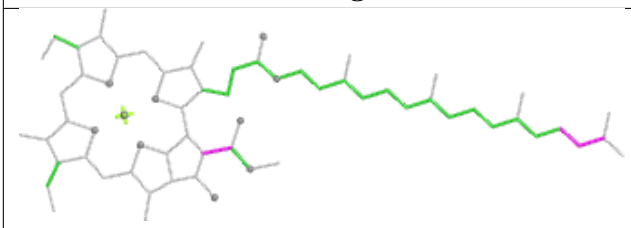
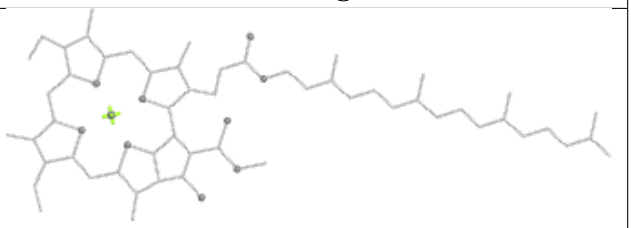
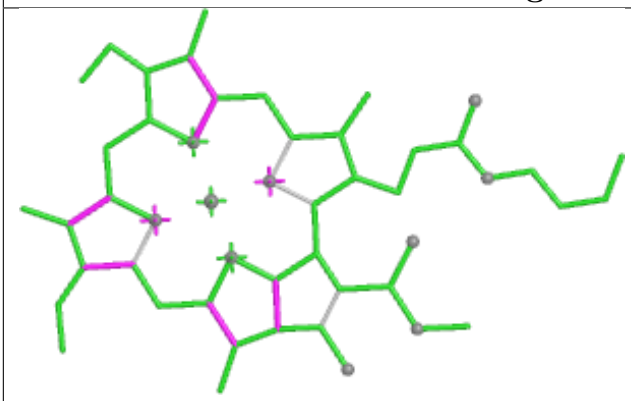
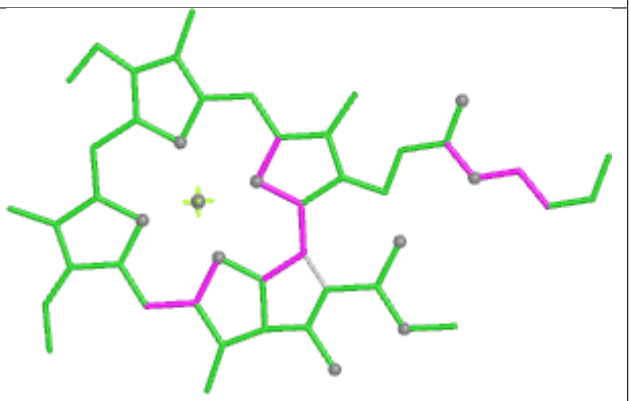
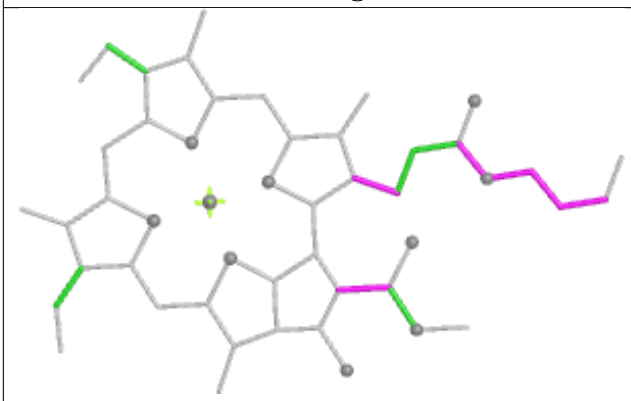
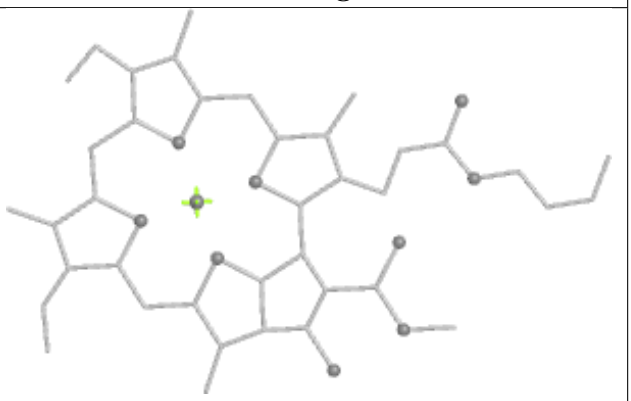
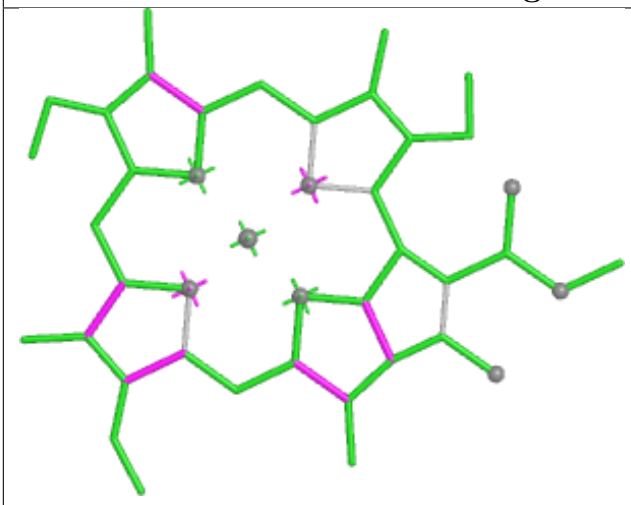
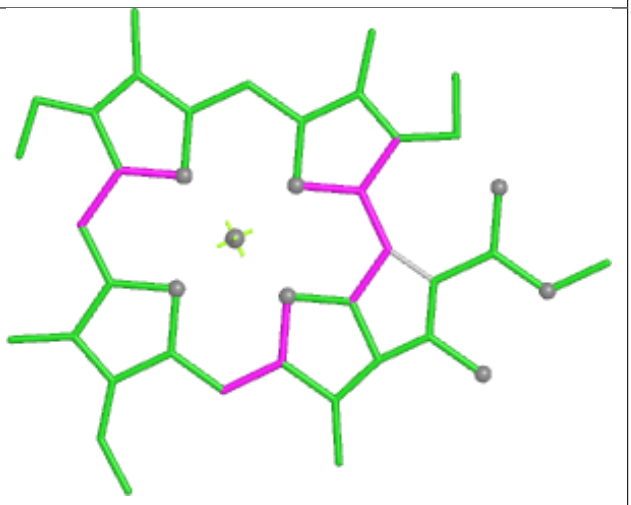
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

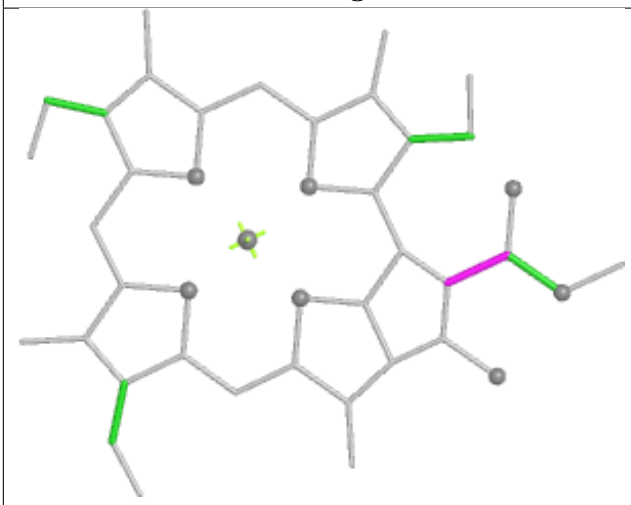
Ligand CLA U 209



Bond lengths



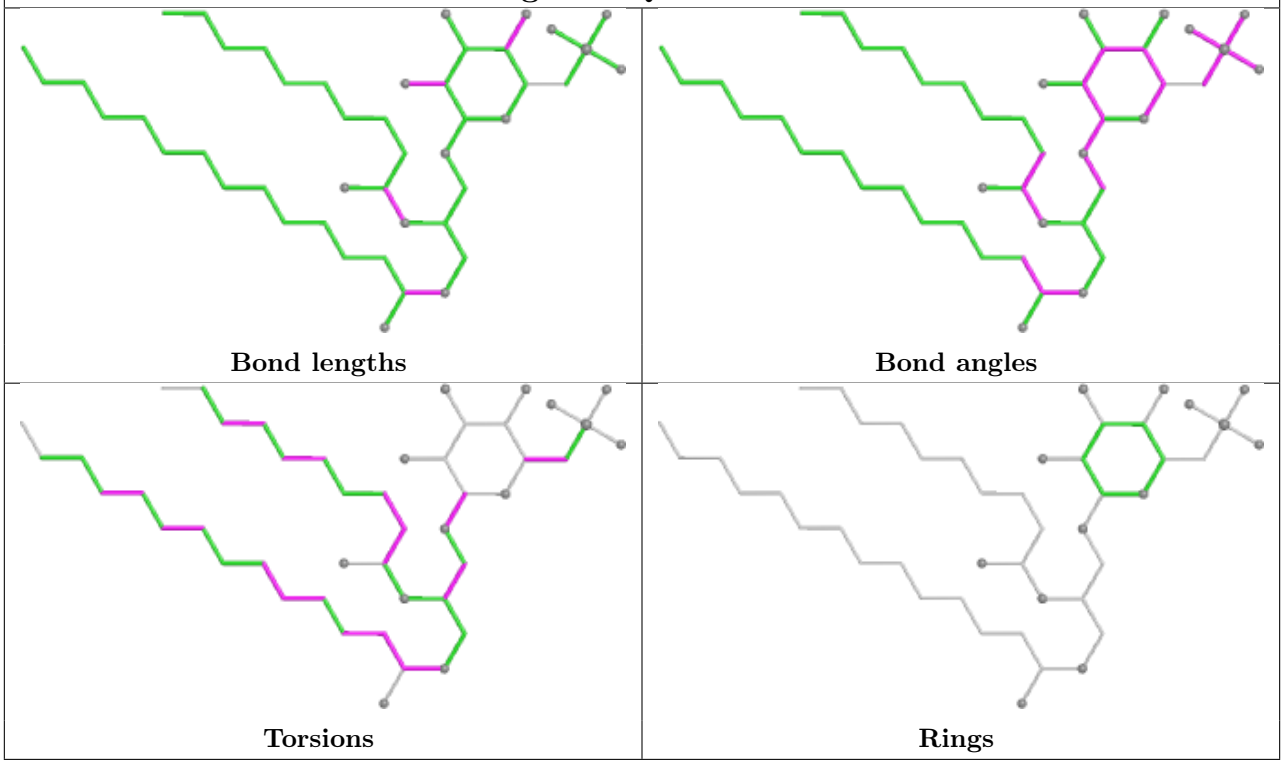
Bond angles



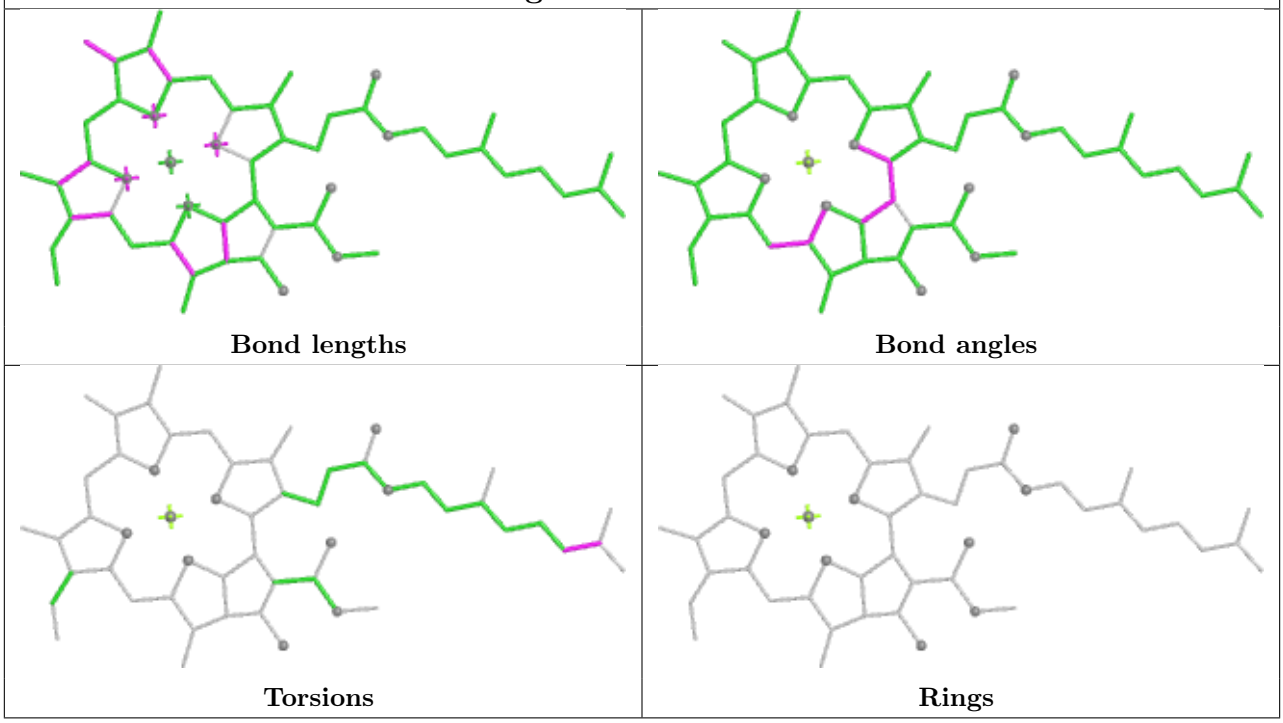
Torsions

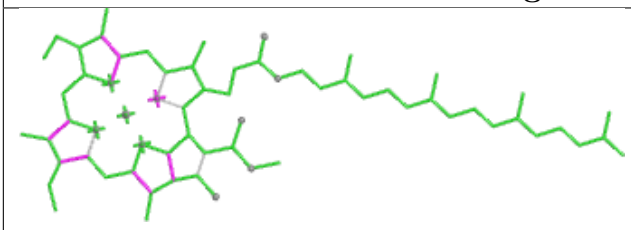
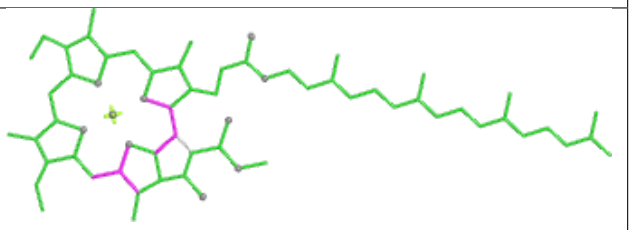
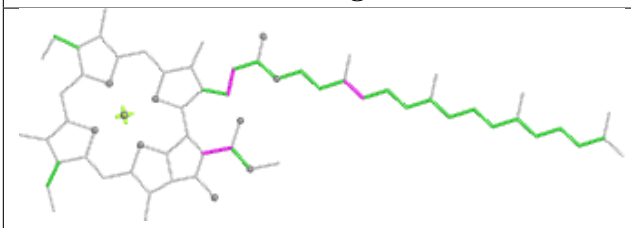
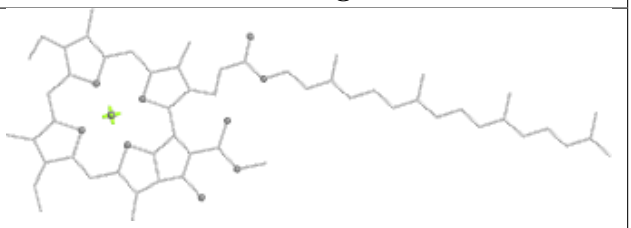
Rings

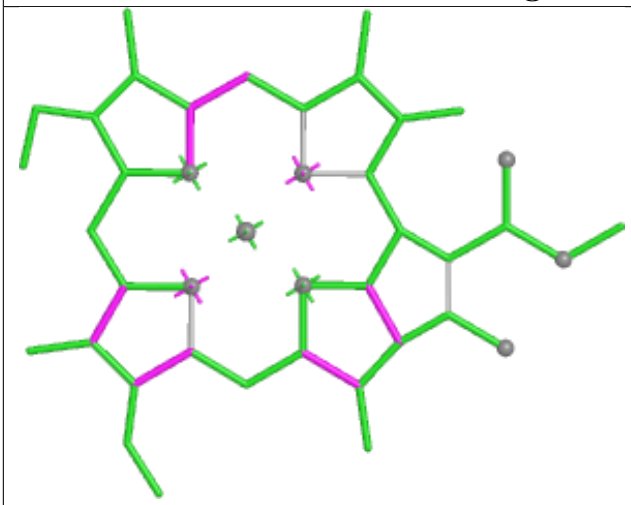
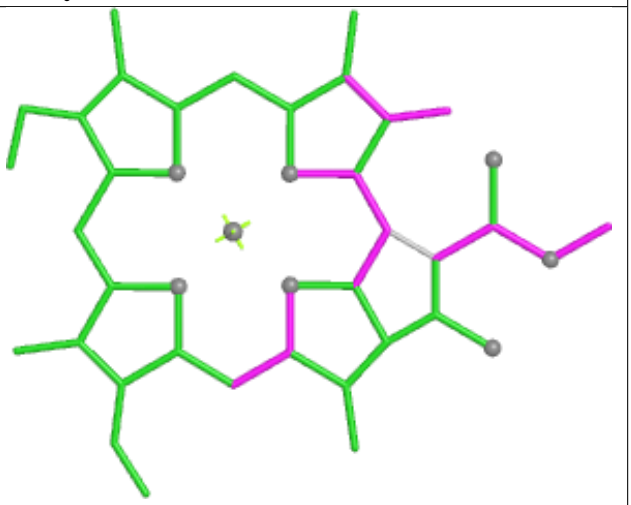
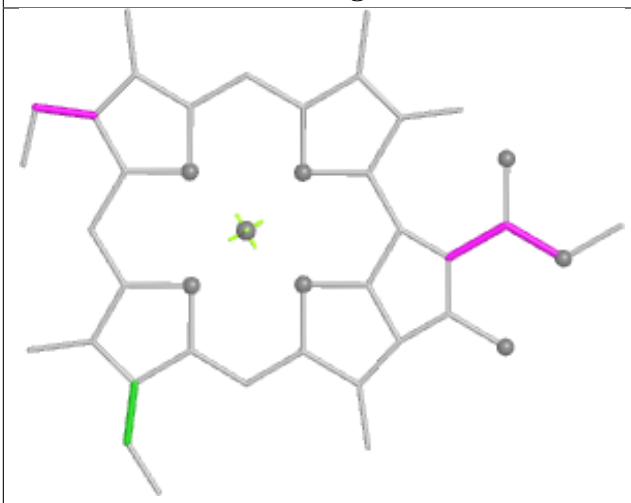
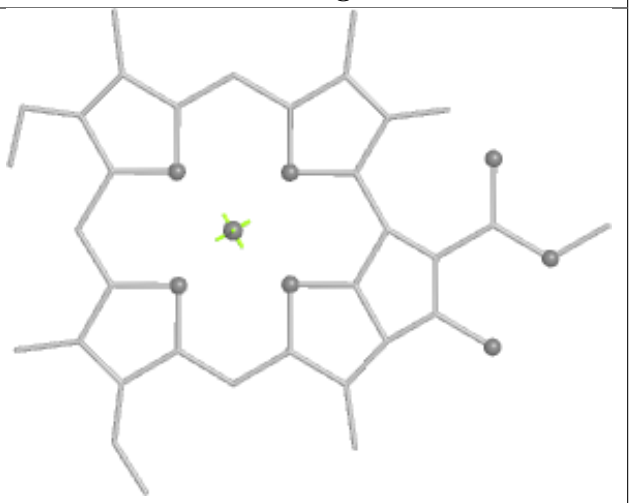
Ligand SQD M 102

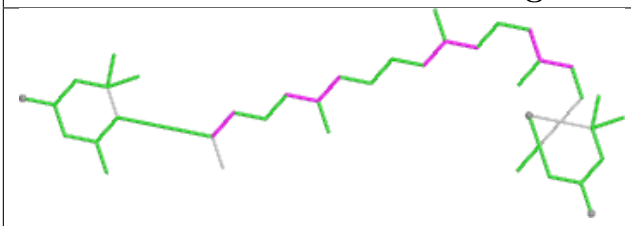
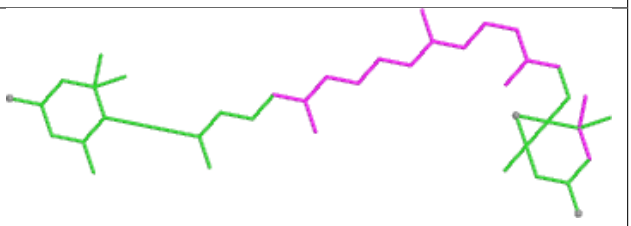
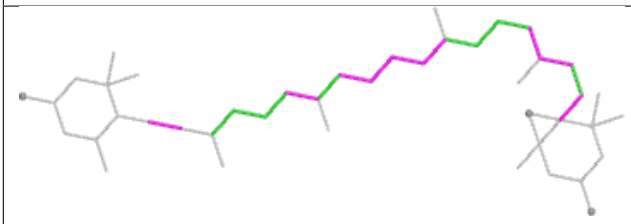
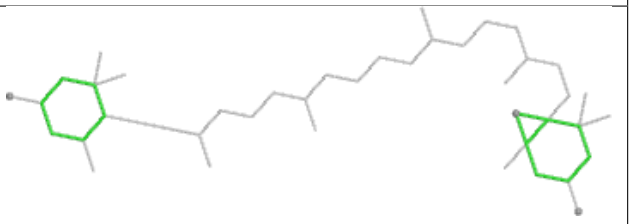


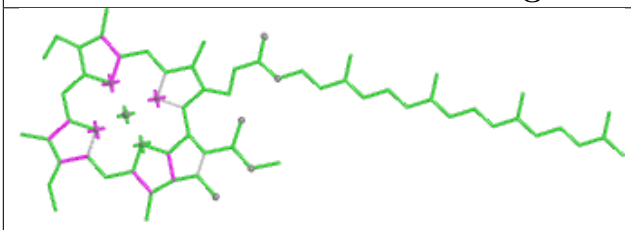
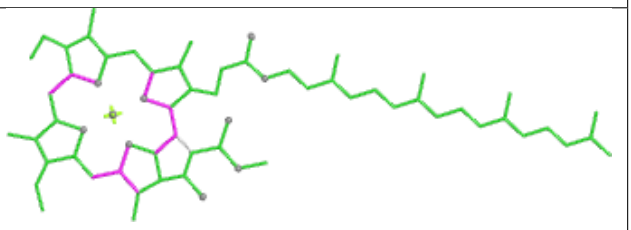
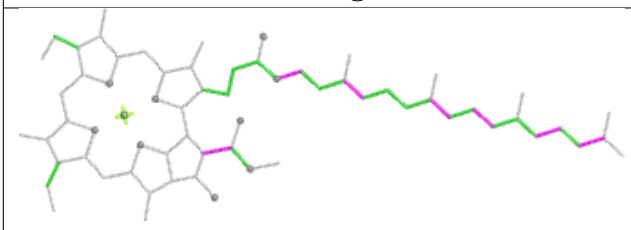
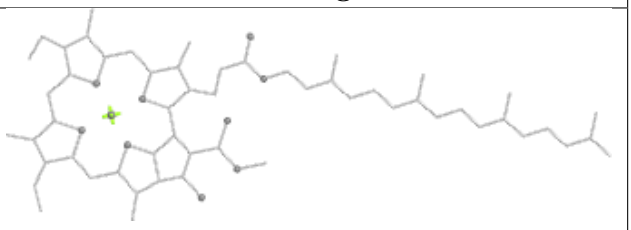
Ligand CLA B 810



Ligand CLA A 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 211	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 P 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

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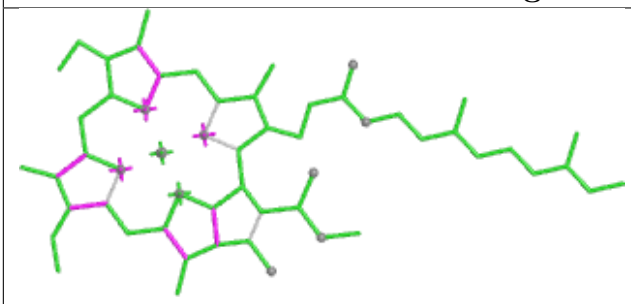
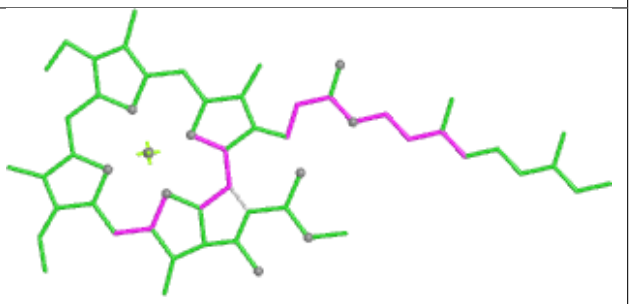
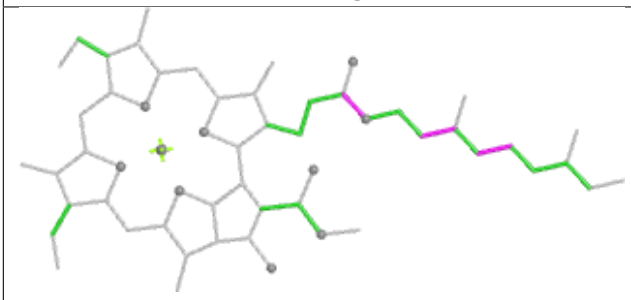
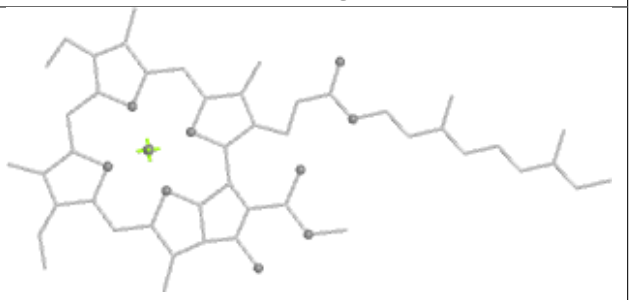
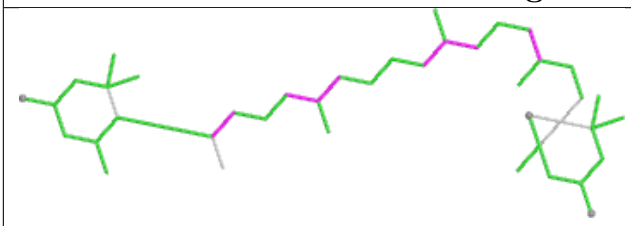
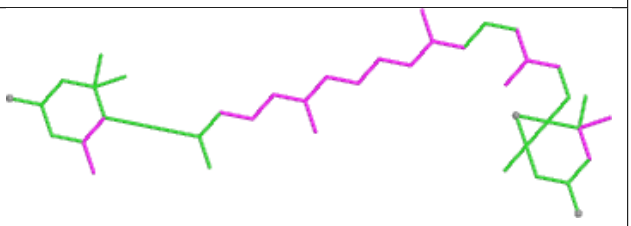
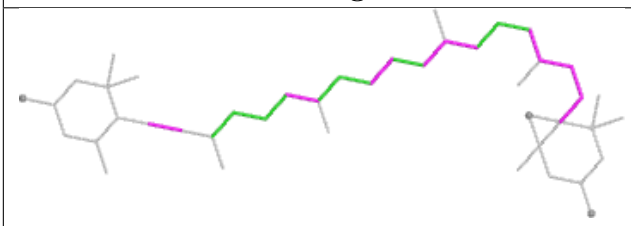
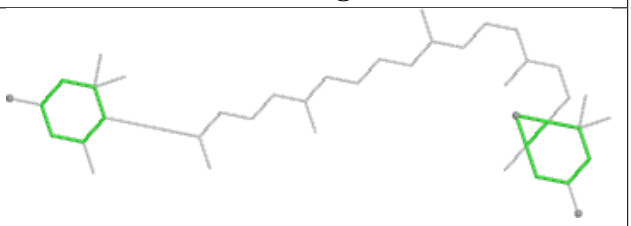
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 P 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

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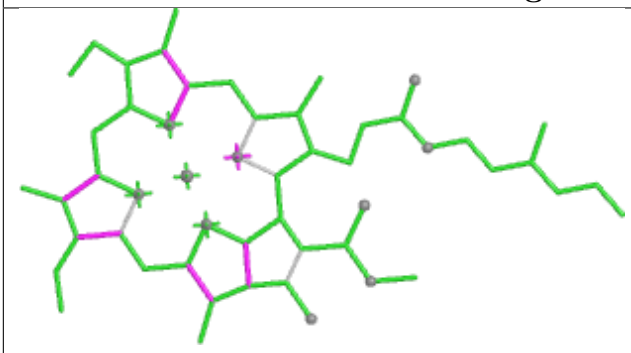
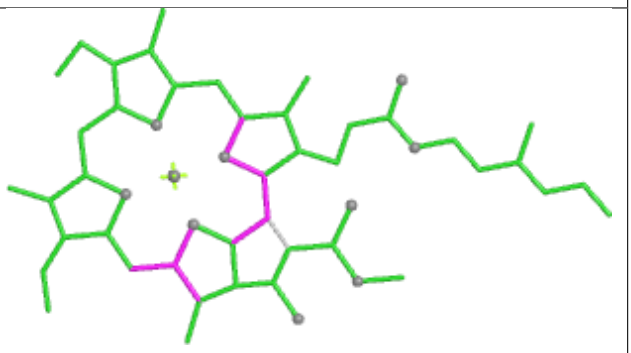
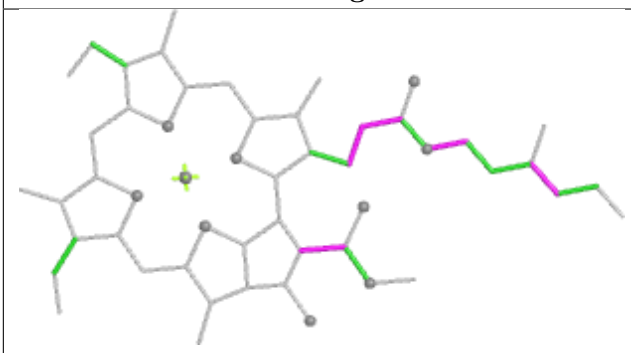
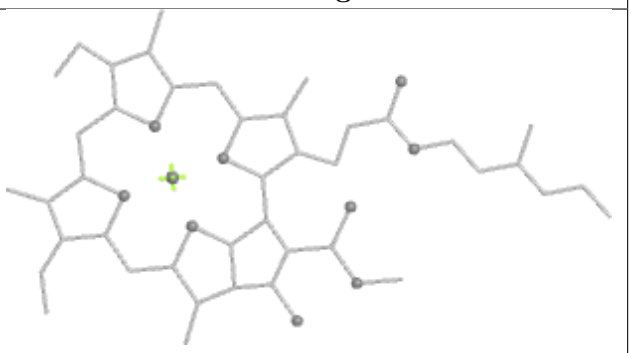
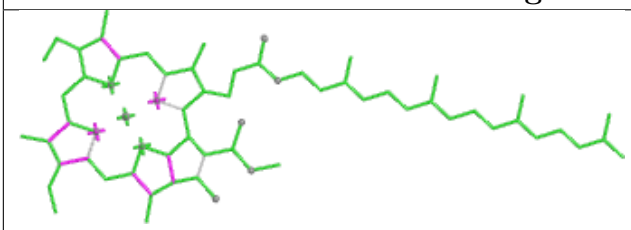
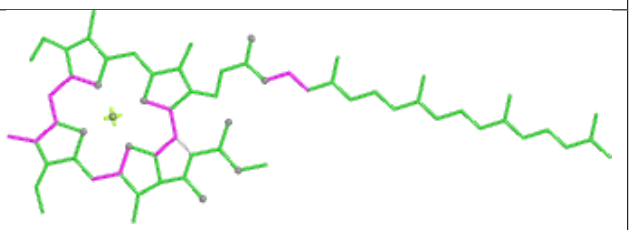
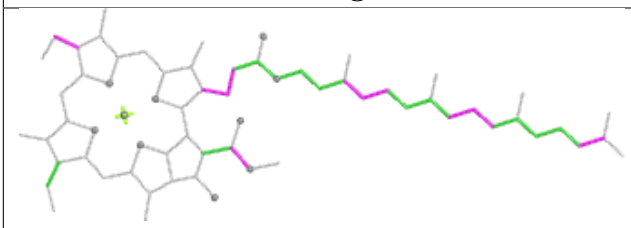
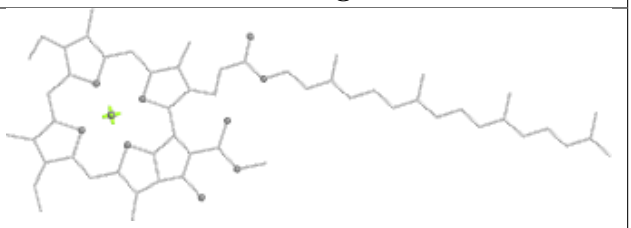
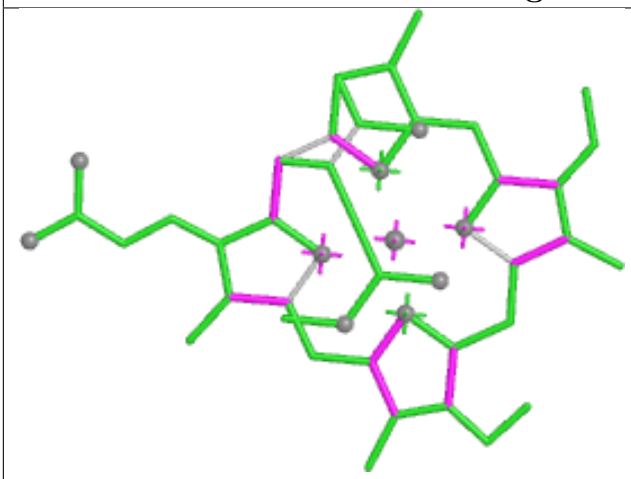
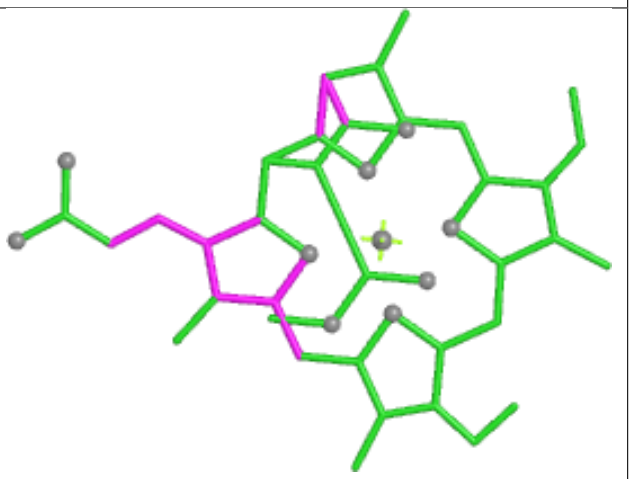
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA T 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

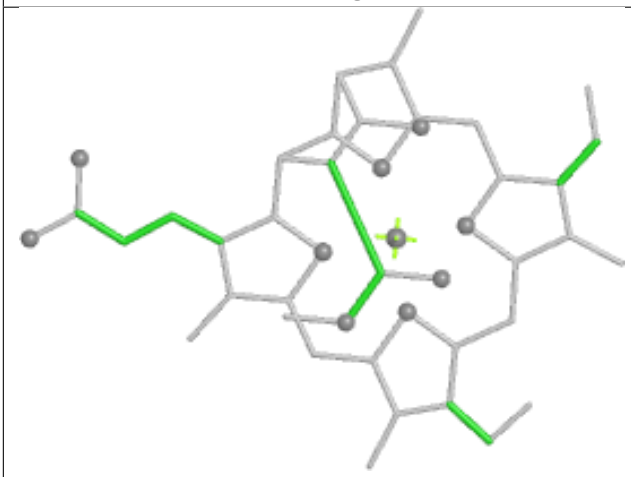
Ligand KC1 O 210



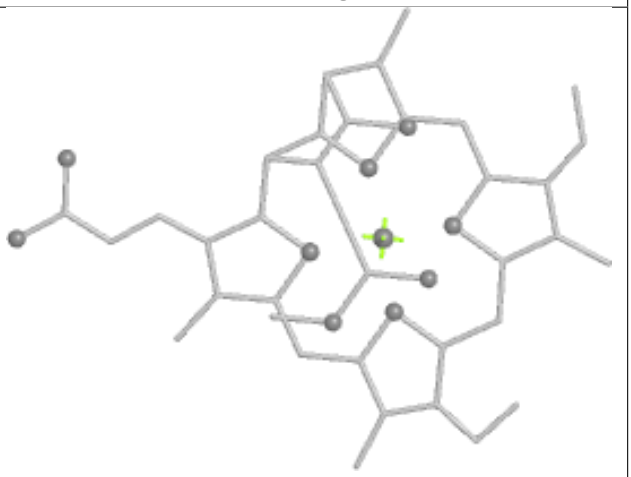
Bond lengths



Bond angles

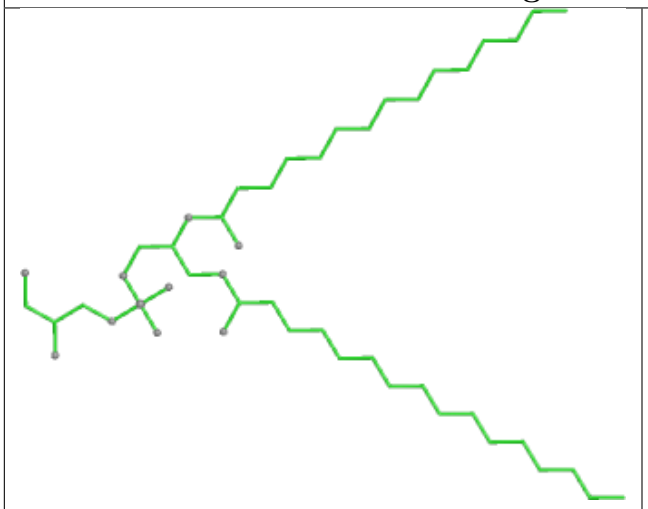


Torsions



Rings

Ligand LHG A 839



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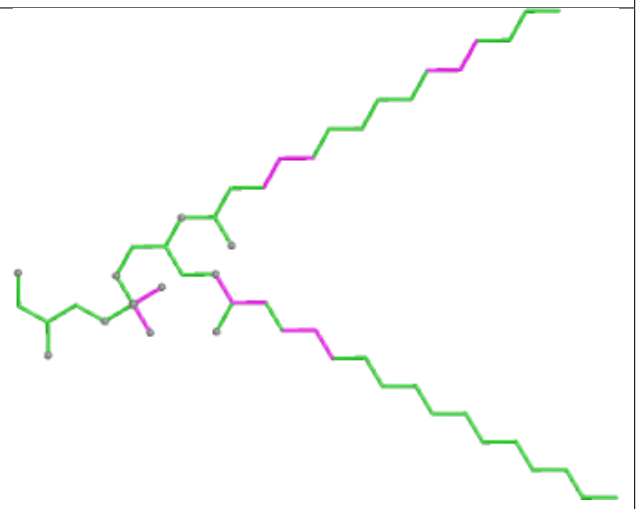
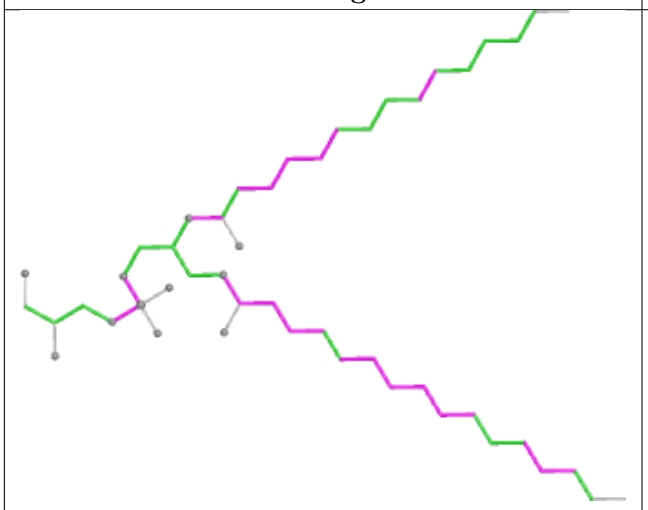


Bond angles



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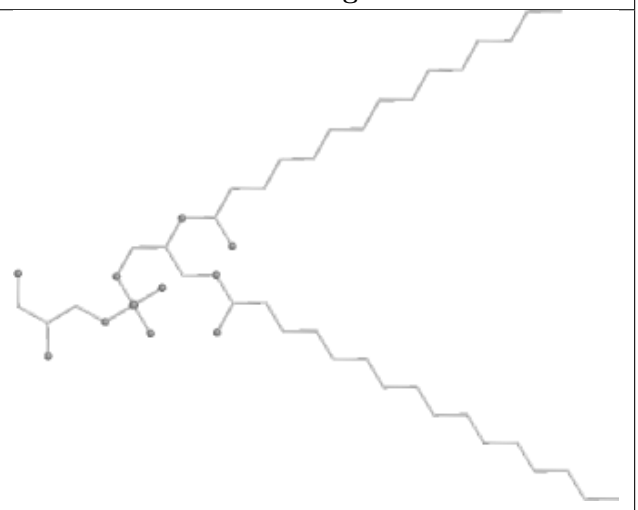
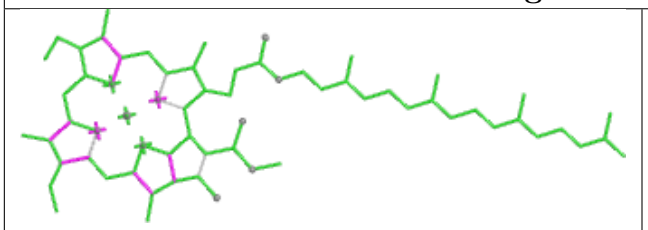


Rings

Ligand CLA A 821



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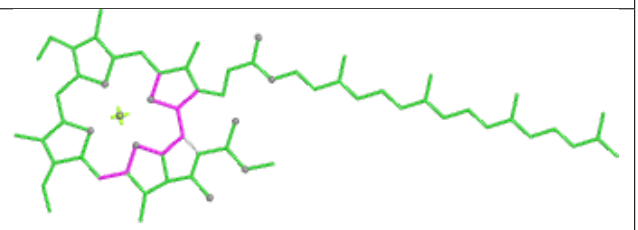
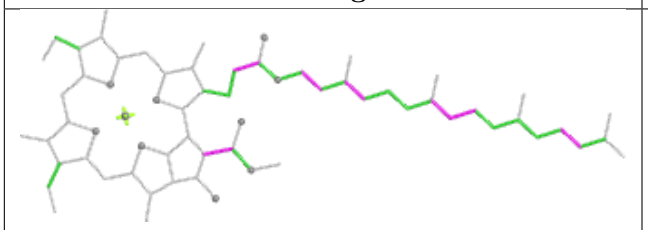


Bond angles



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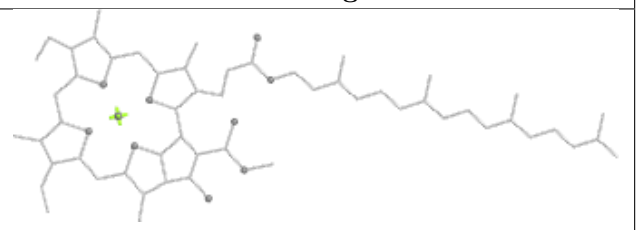
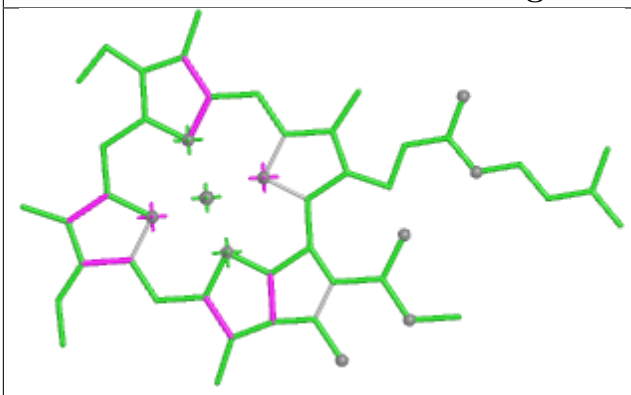
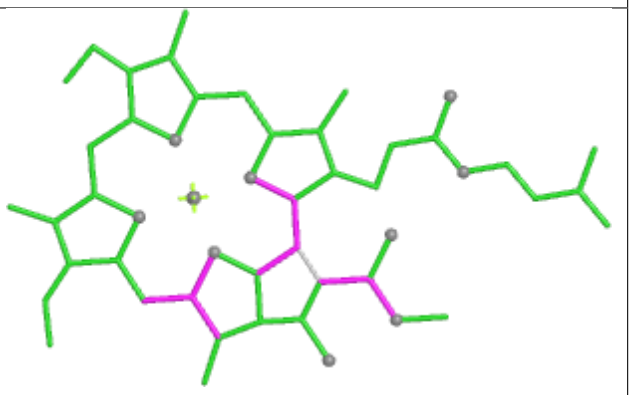
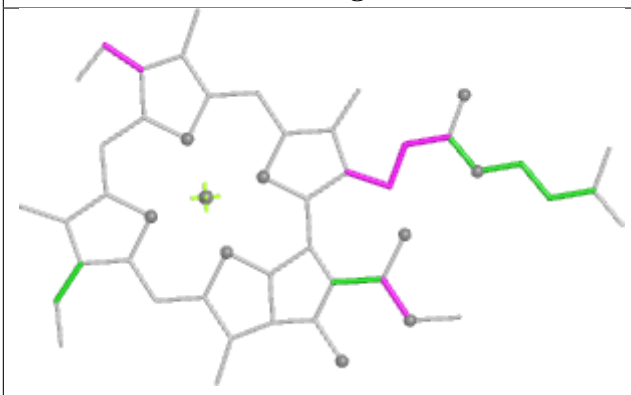
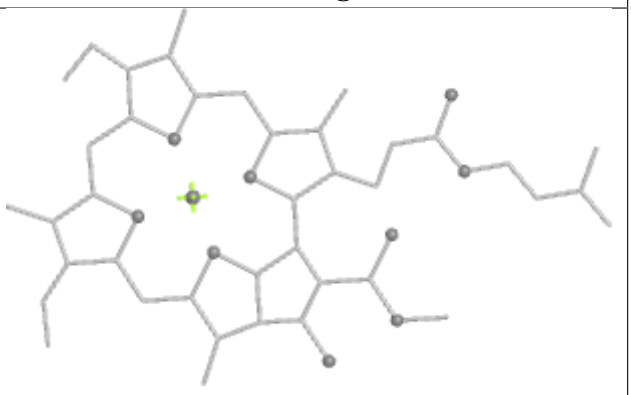
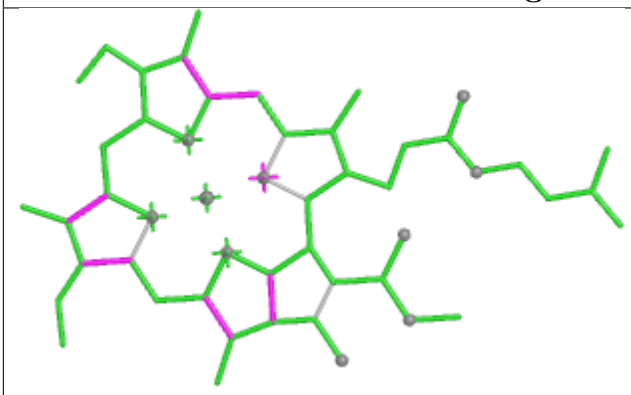


Rings

Ligand CLA L 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA P 310



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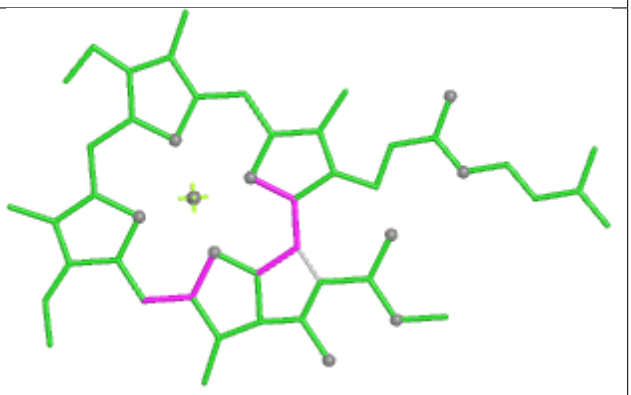
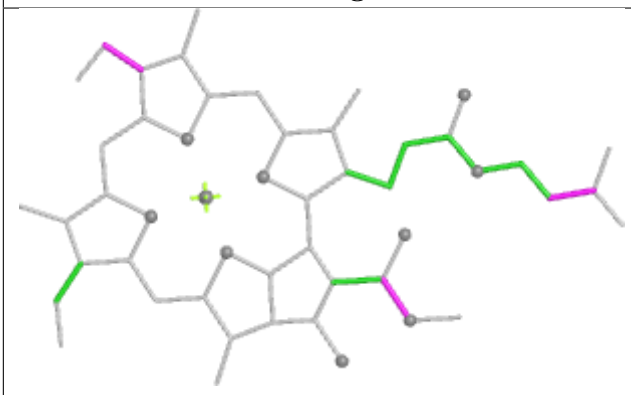


Bond angles



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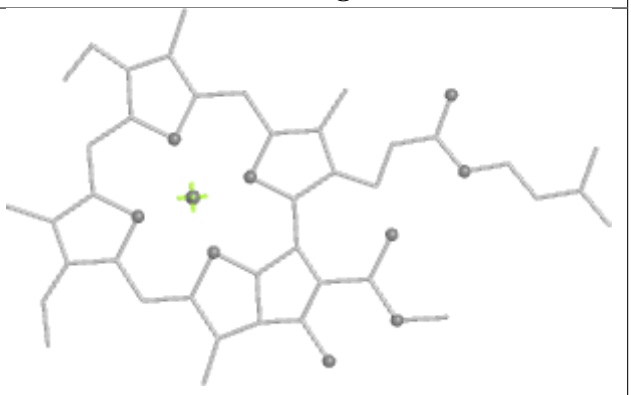
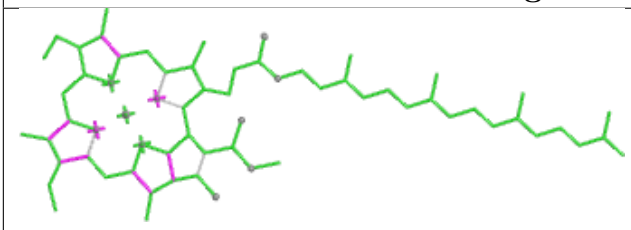
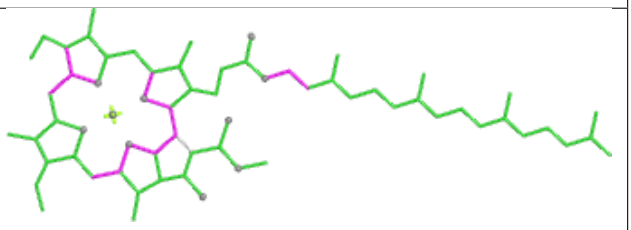


Rings

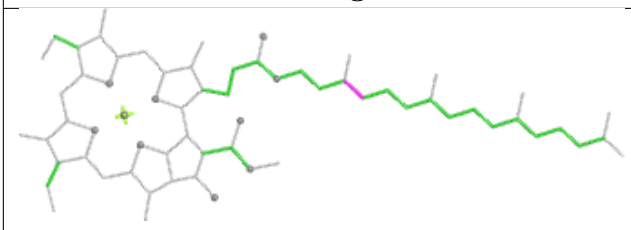
Ligand CLA B 835



Bond lengths



Bond angles



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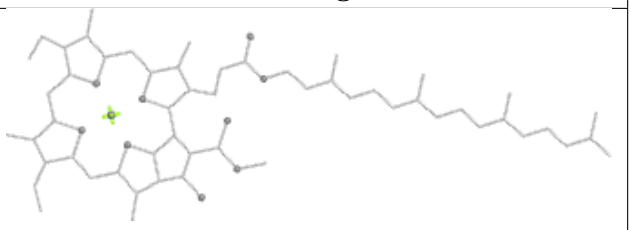
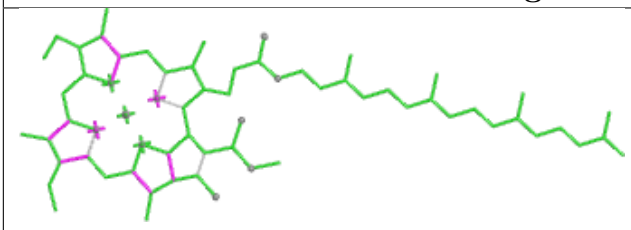
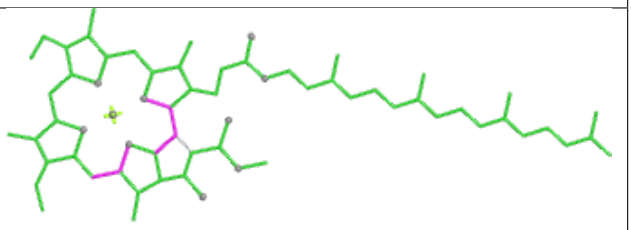
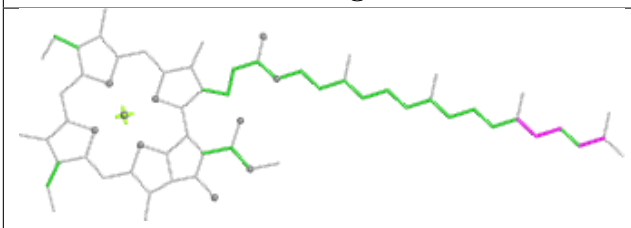
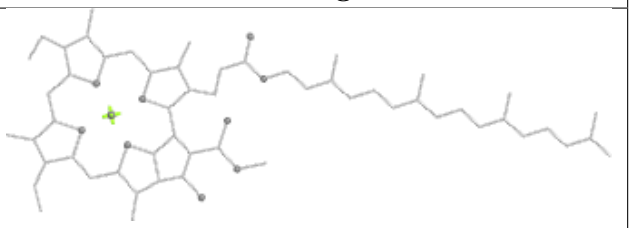
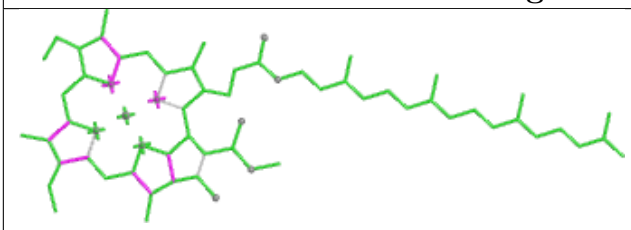
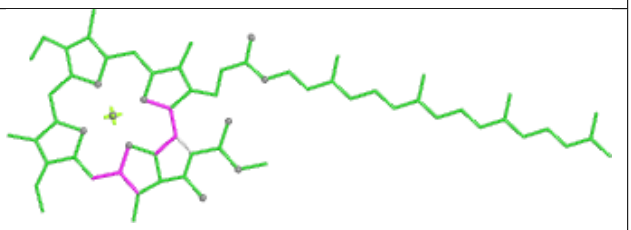
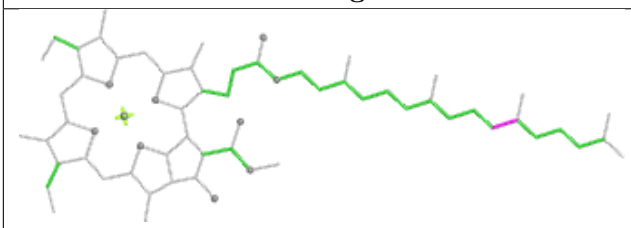
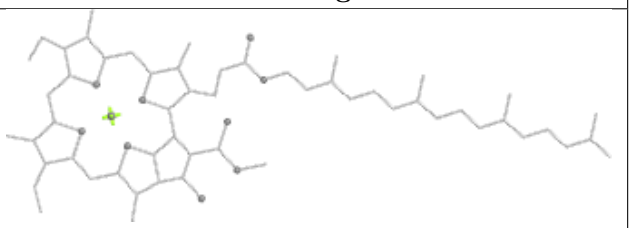


Rings

Ligand CLA B 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

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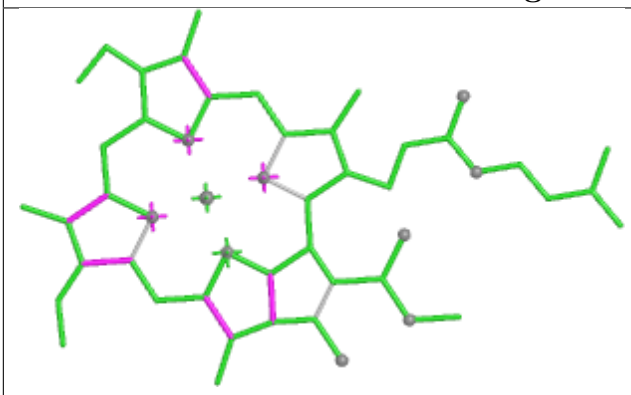
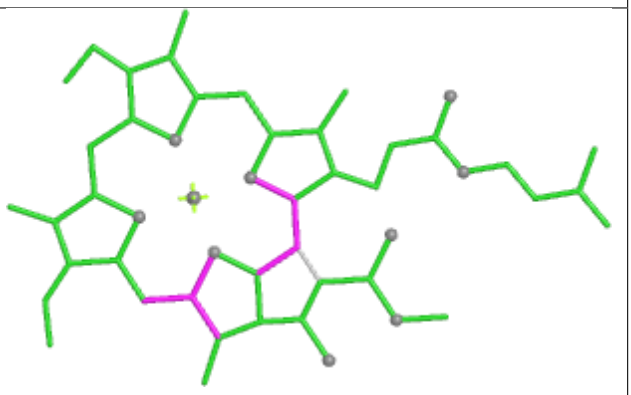
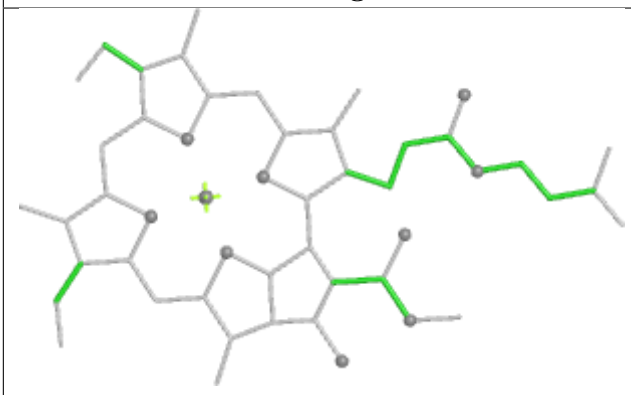
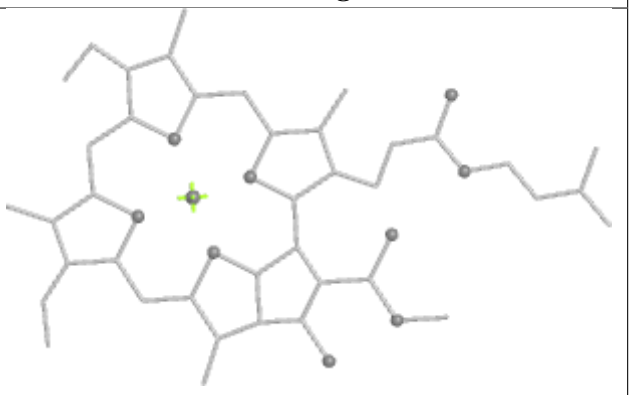
 Bond lengths	 Bond angles
 Torsions	 Rings

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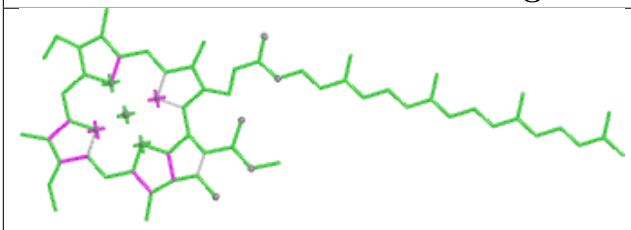
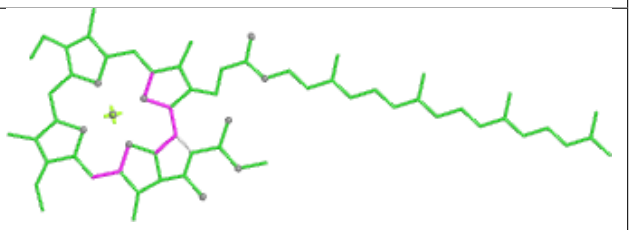
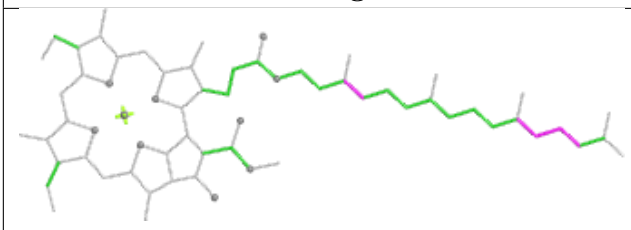
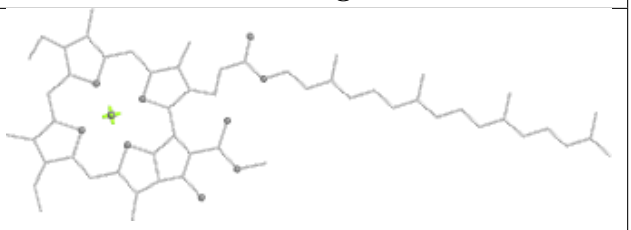
 Bond lengths	 Bond angles
 Torsions	 Rings

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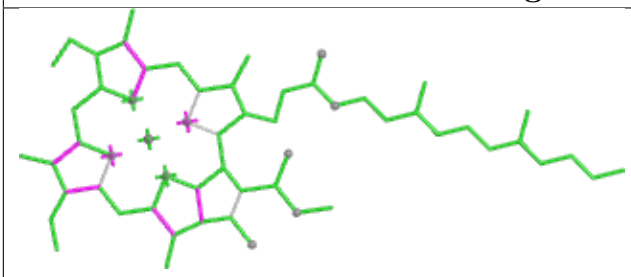
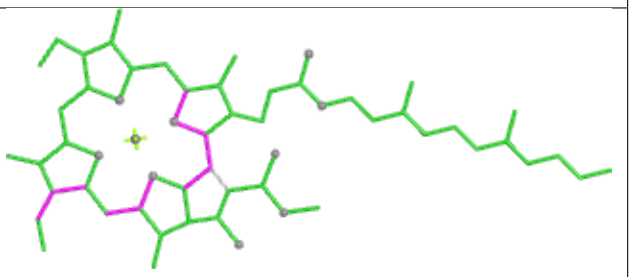
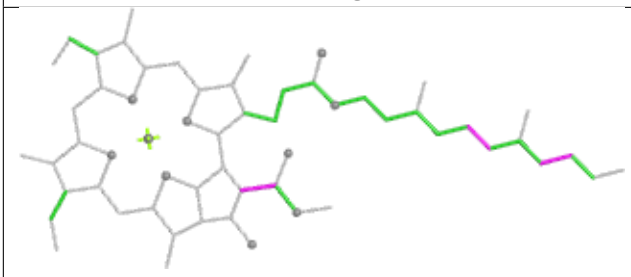
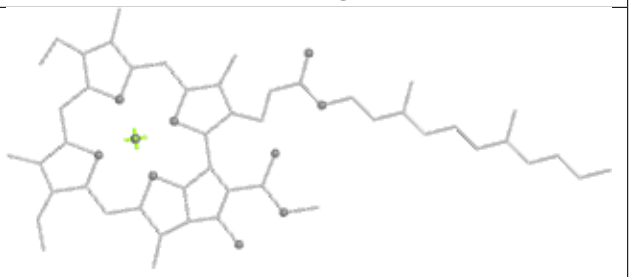
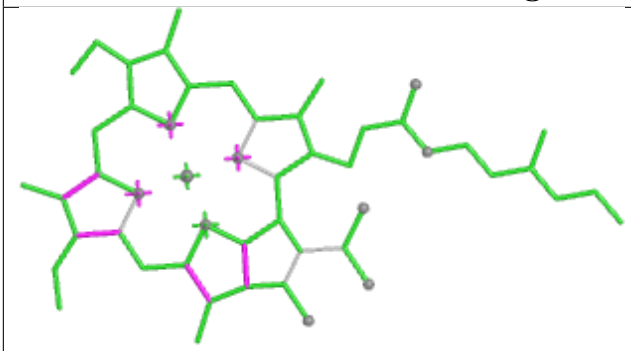
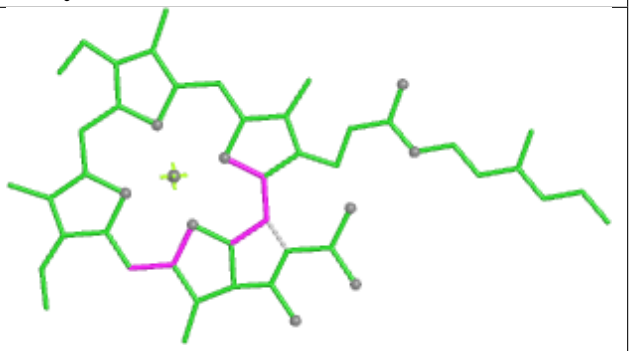
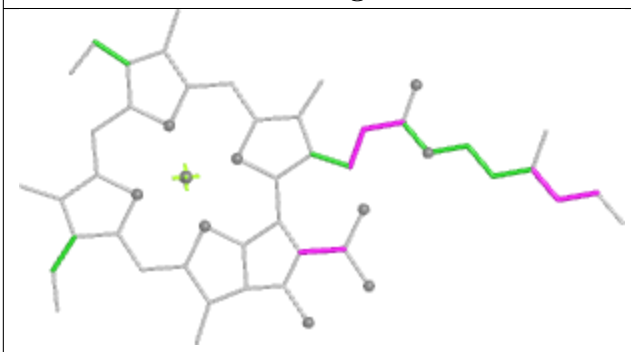
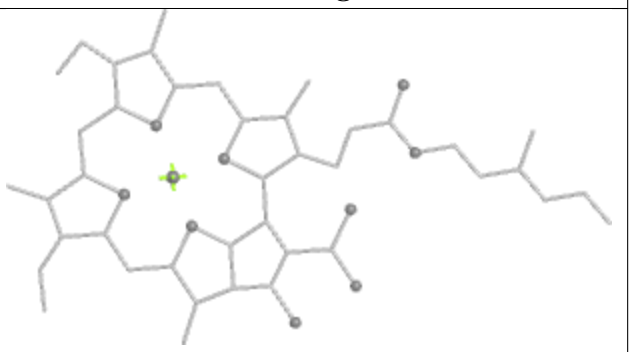
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

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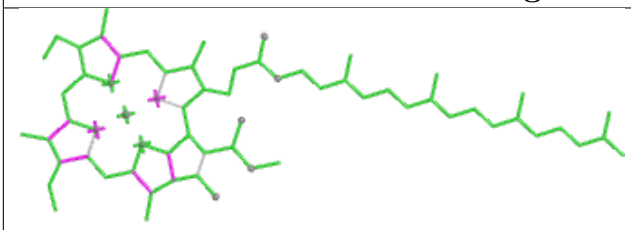
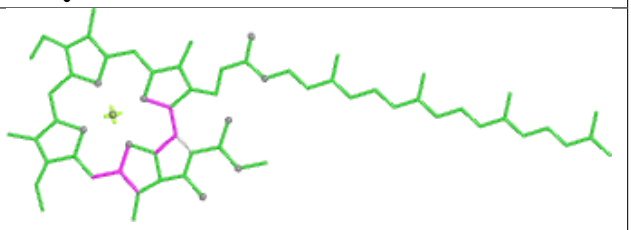
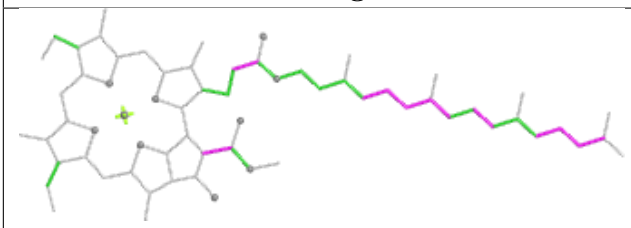
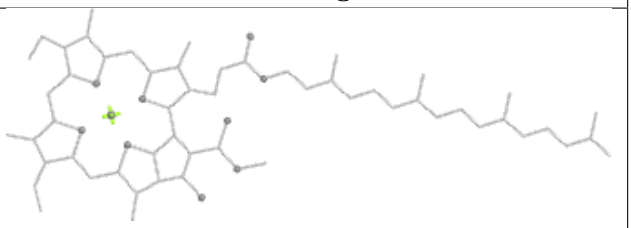
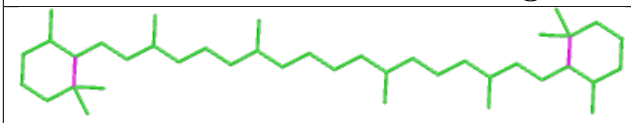
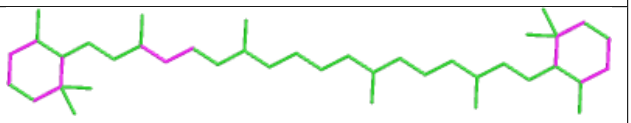
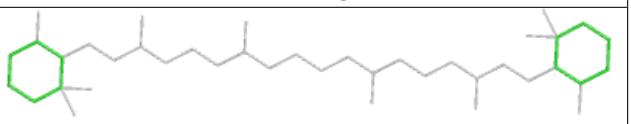
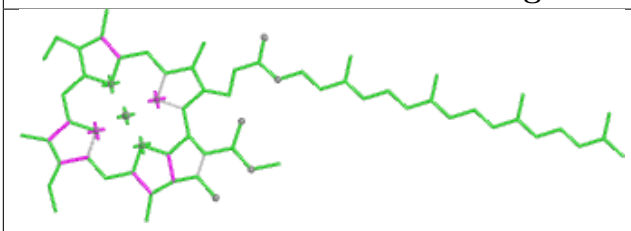
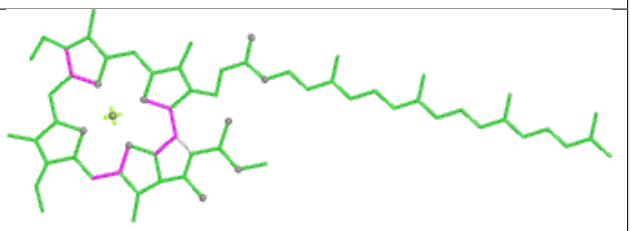
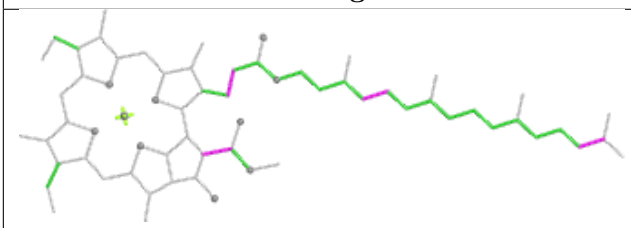
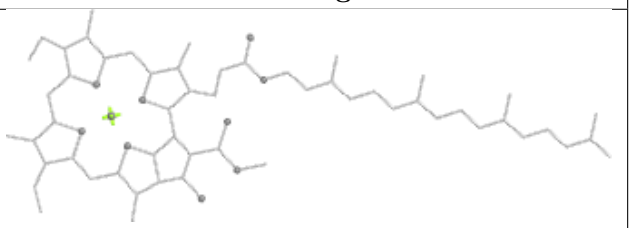
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 841	
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand CLA A 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

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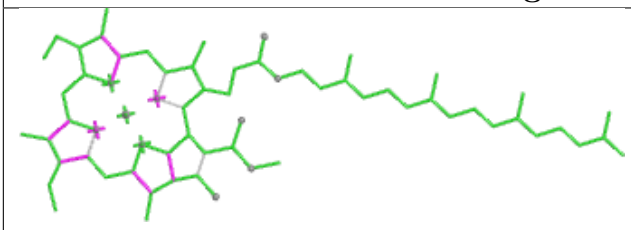
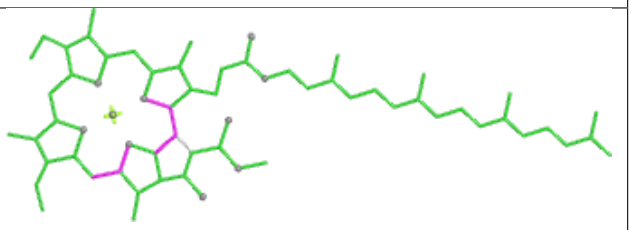
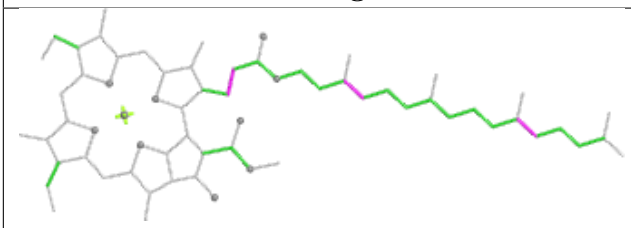
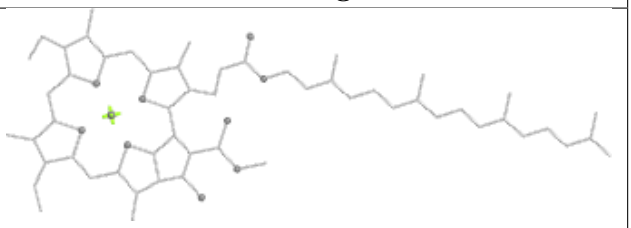
 Bond lengths	 Bond angles
 Torsions	 Rings

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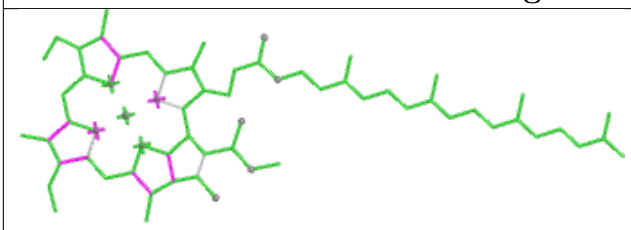
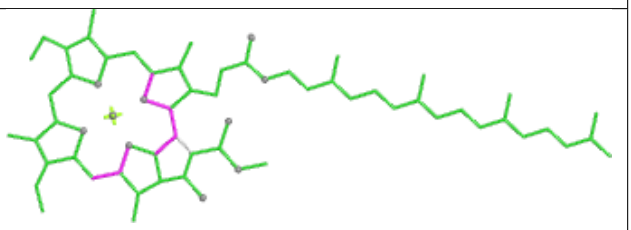
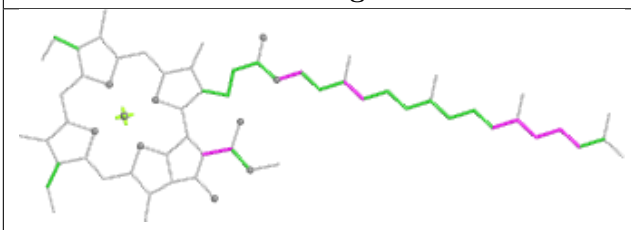
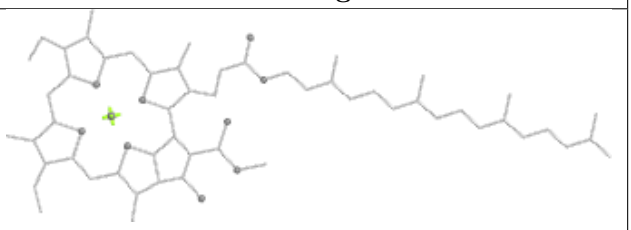
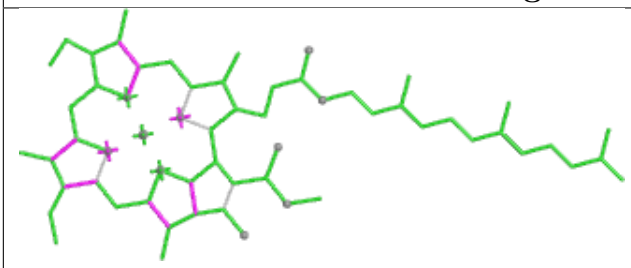
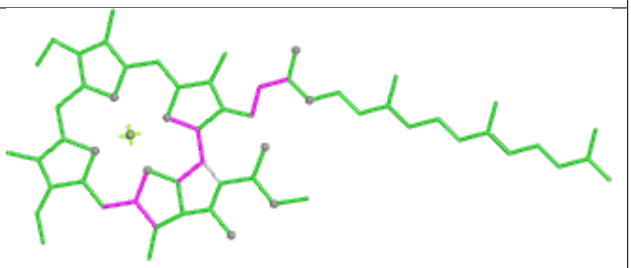
 Bond lengths	 Bond angles
 Torsions	 Rings

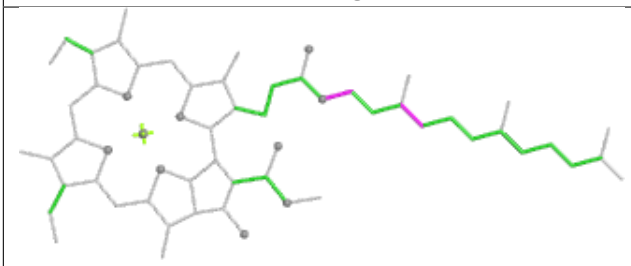
Ligand CLA O 208



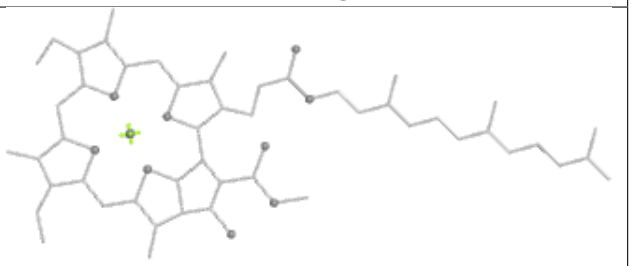
Bond lengths



Bond angles

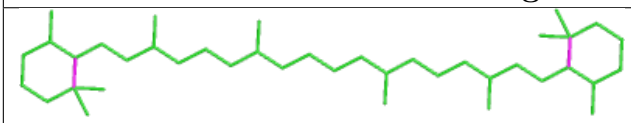


Torsions

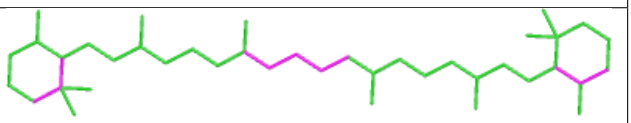


Rings

Ligand BCR A 842

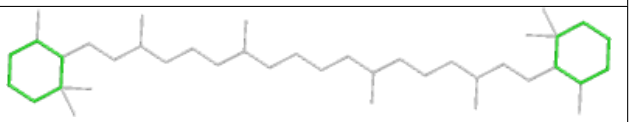


Bond lengths



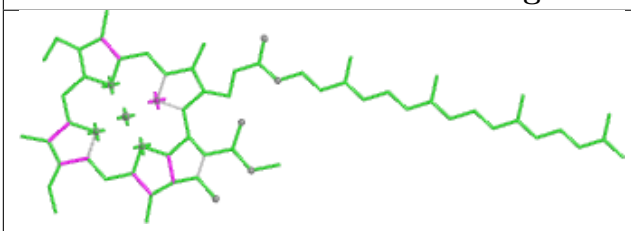
Bond angles

Torsions

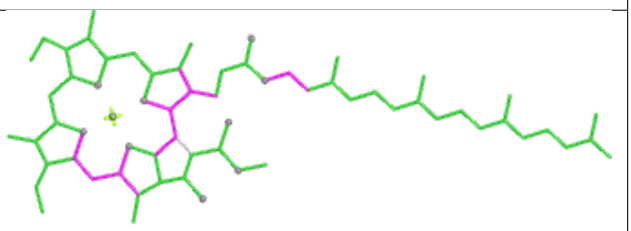


Rings

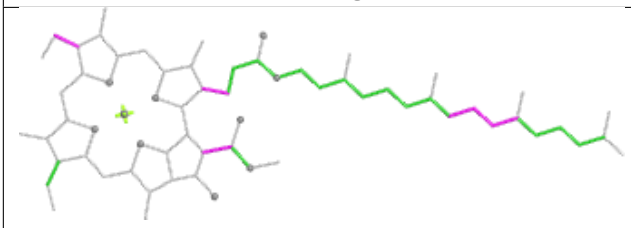
Ligand CLA U 207



Bond lengths



Bond angles



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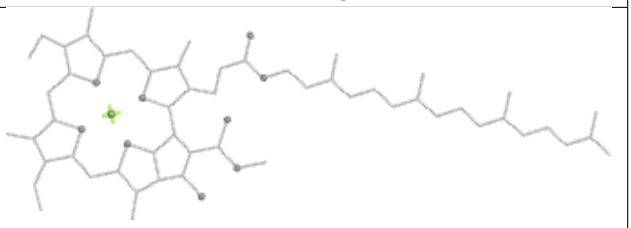
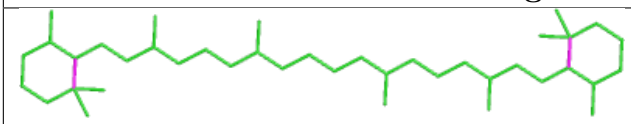
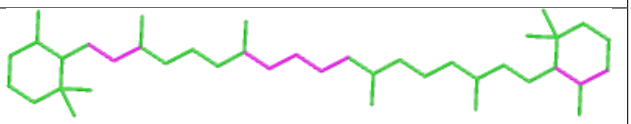


Rings

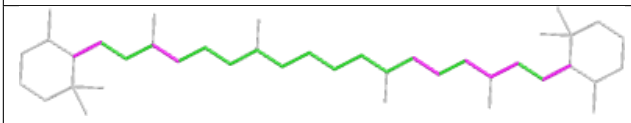
Ligand BCR L 201



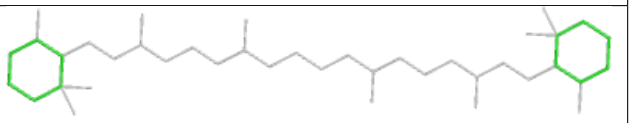
Bond lengths



Bond angles

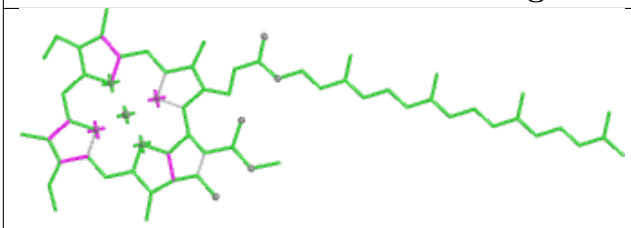


Torsions

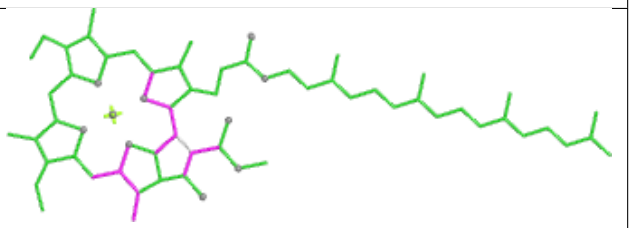


Rings

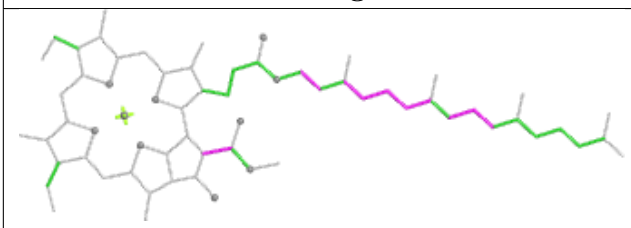
Ligand CLA S 201



Bond lengths



Bond angles



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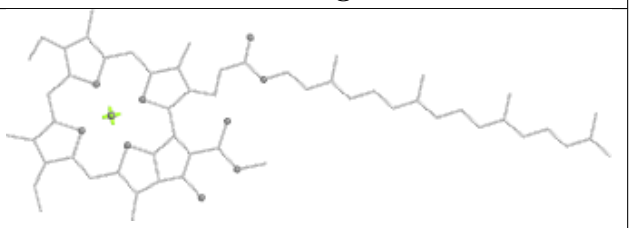
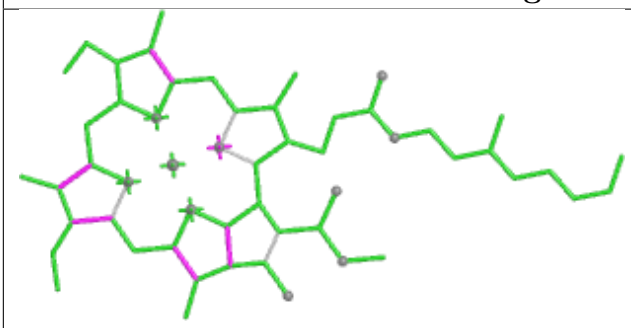
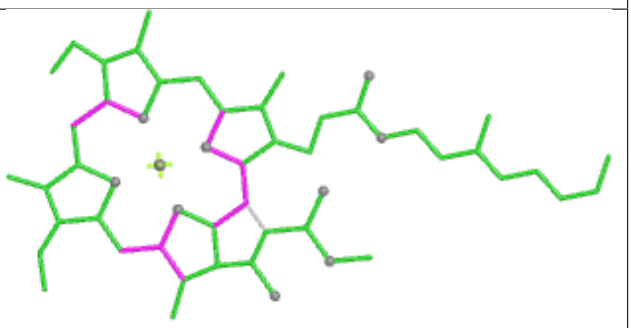


Rings

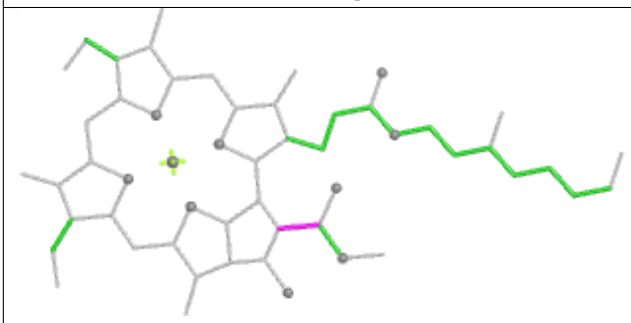
Ligand CLA A 810



Bond lengths



Bond angles



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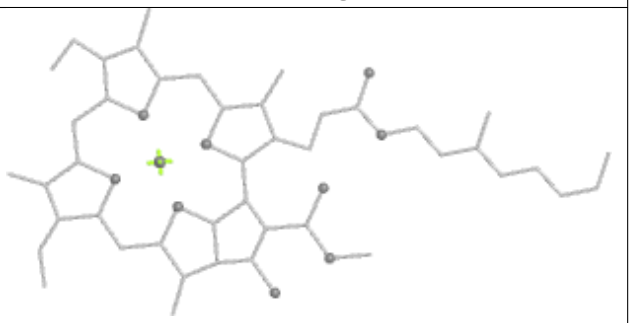
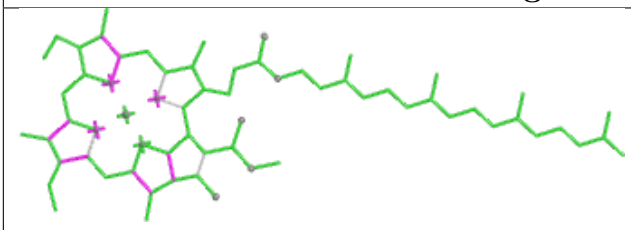
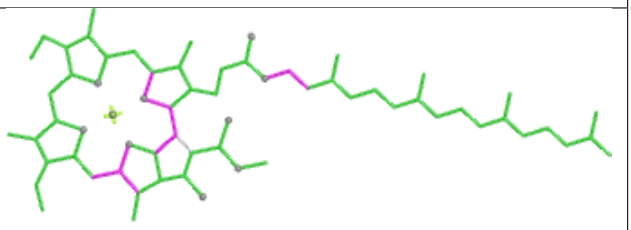
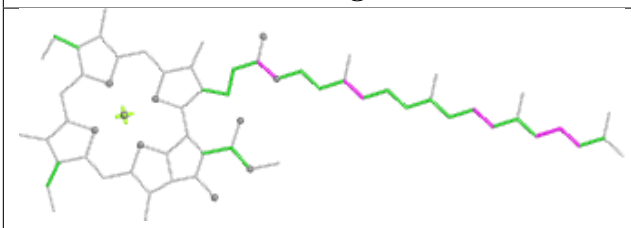
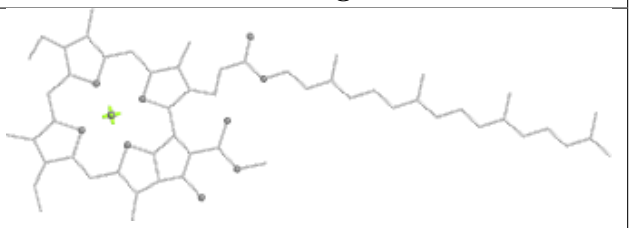
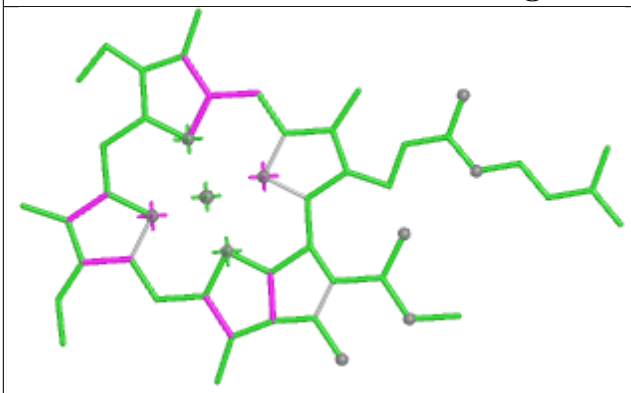
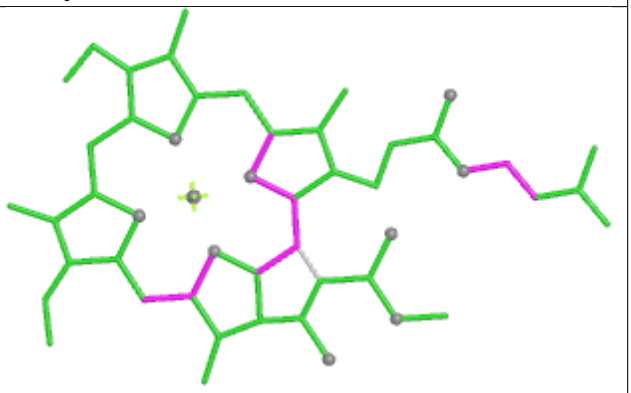
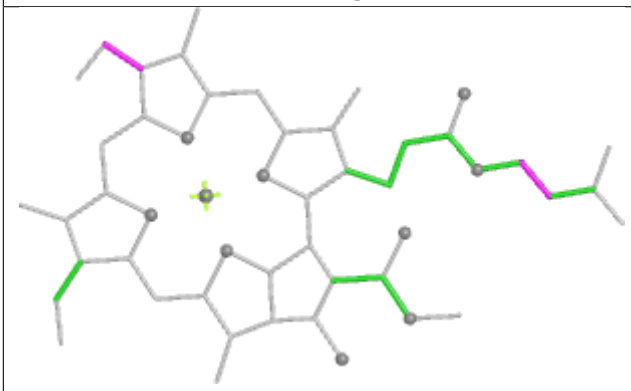
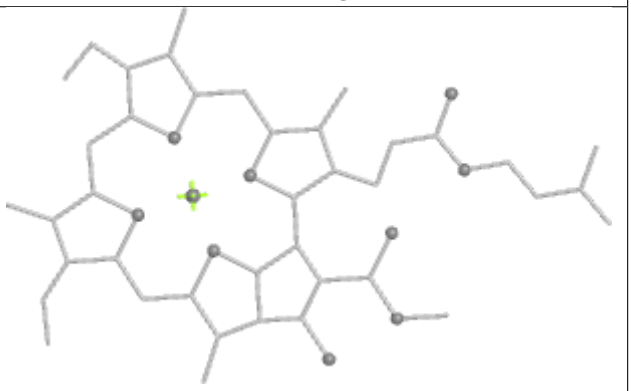
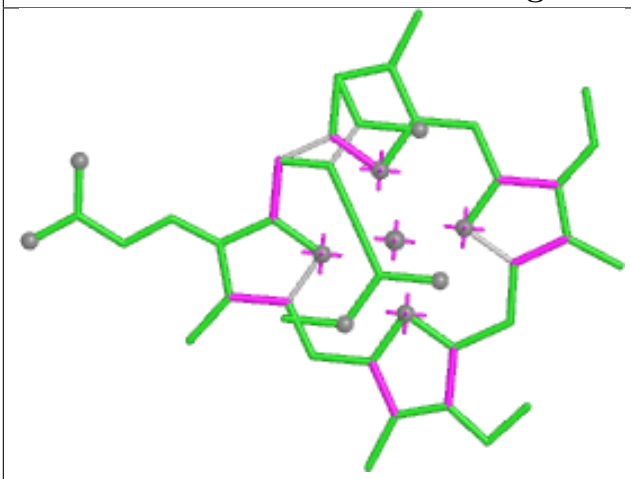


Rings

Ligand CLA A 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 P 305



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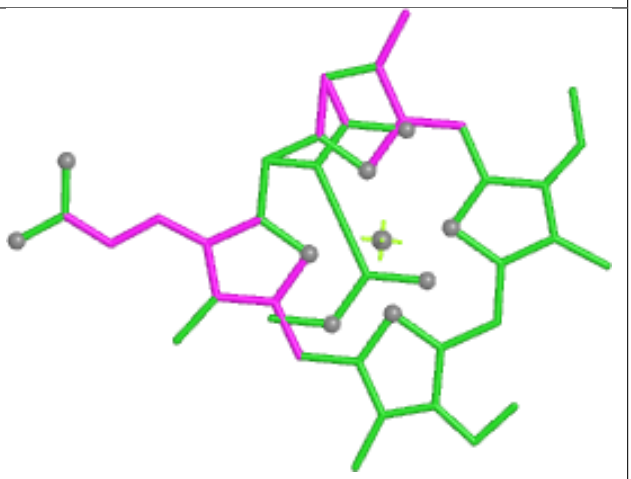
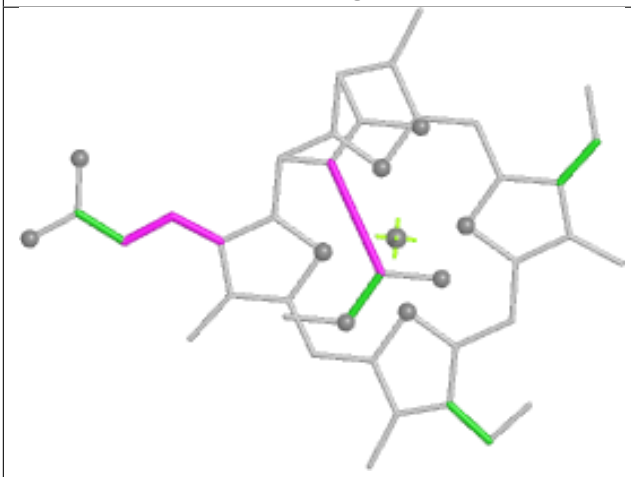


Bond angles



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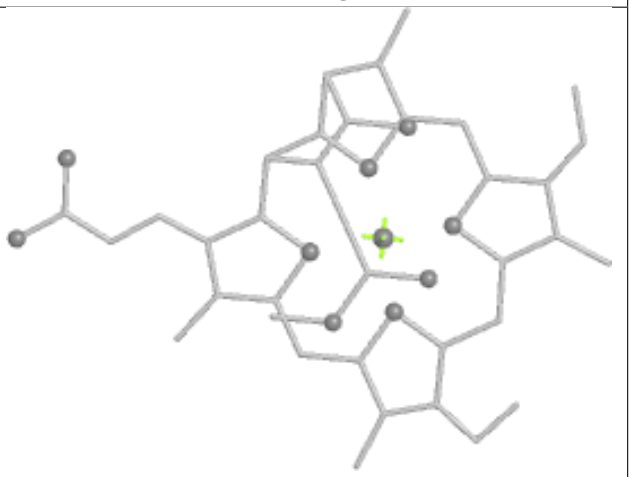
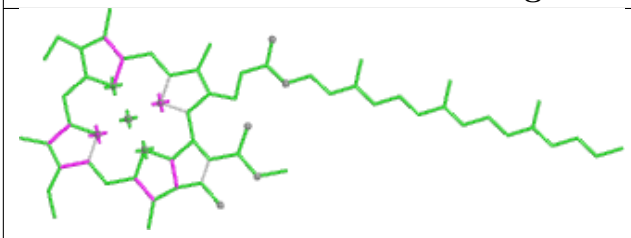


Rings

Ligand CLA B 820



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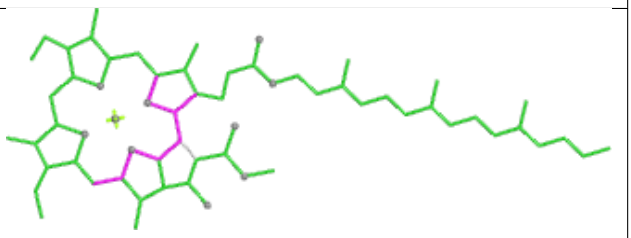
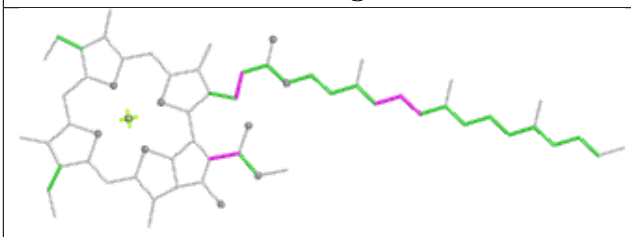


Bond angles



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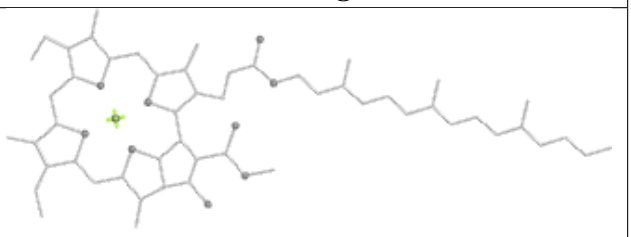
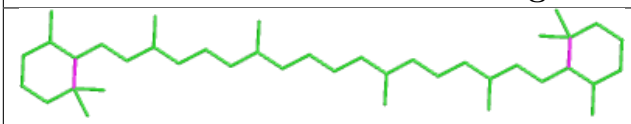
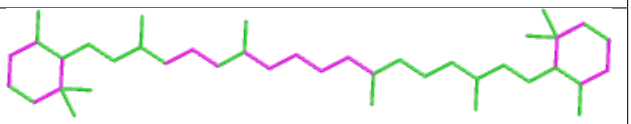
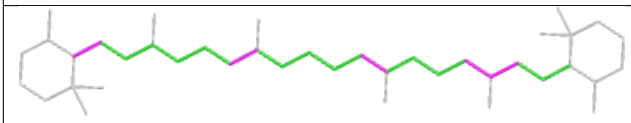
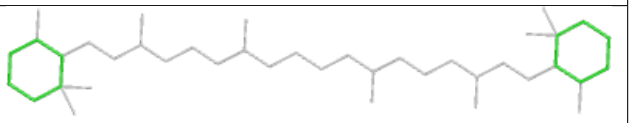
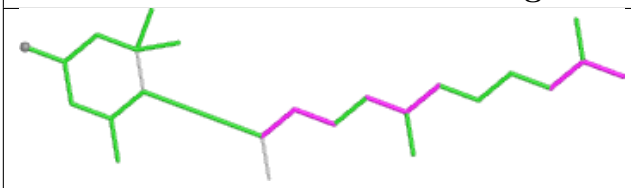
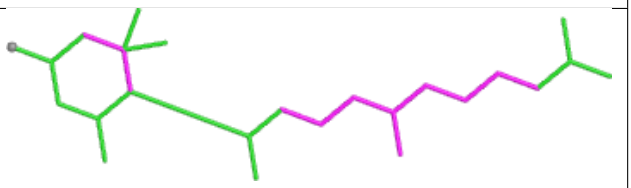
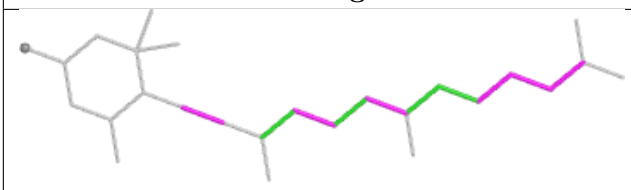
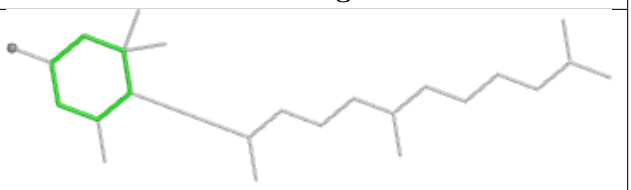
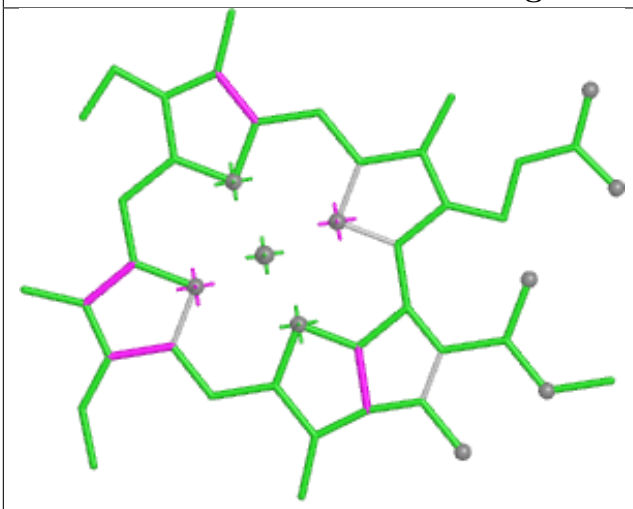


Rings

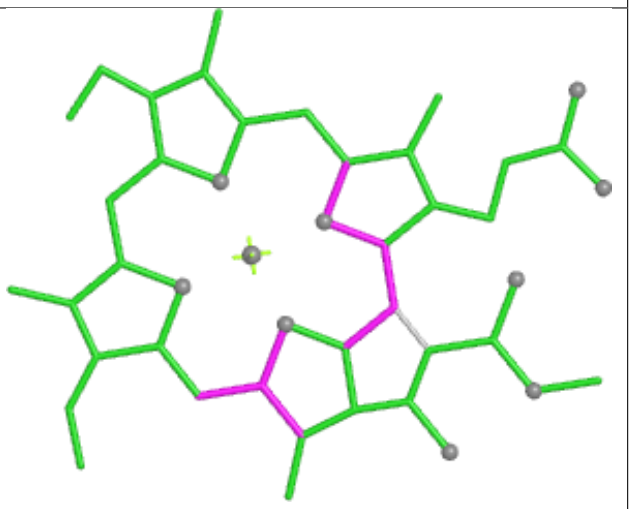
Ligand BCR I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 U 214	
 Bond lengths	 Bond angles
 Torsions	 Rings

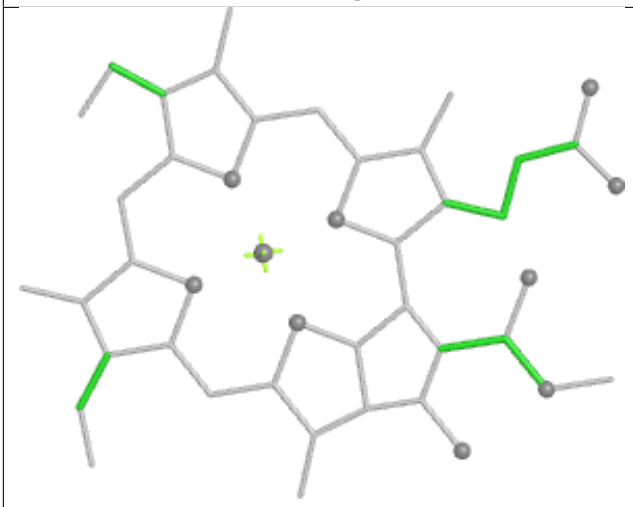
Ligand CLA P 313



Bond lengths



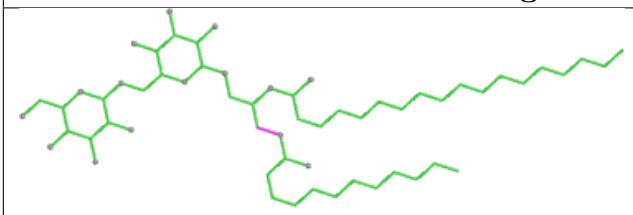
Bond angles



Torsions

Rings

Ligand DGD B 842



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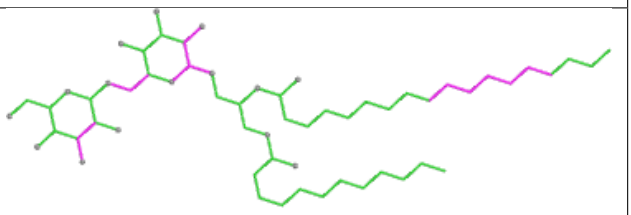
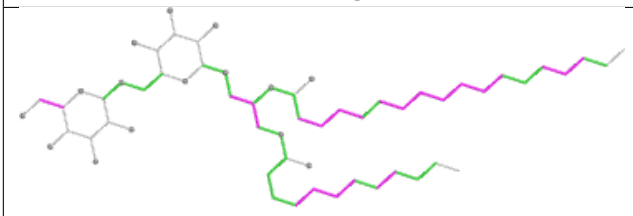
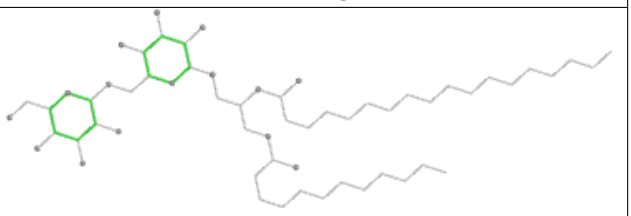


Bond angles

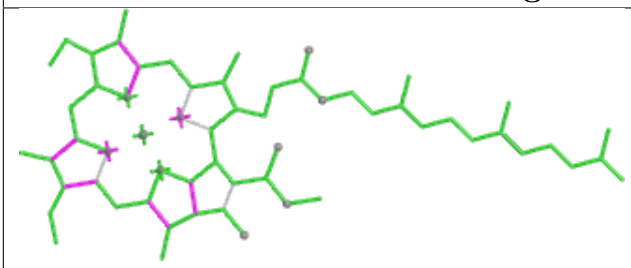


Torsions



Rings

Ligand CLA Q 205



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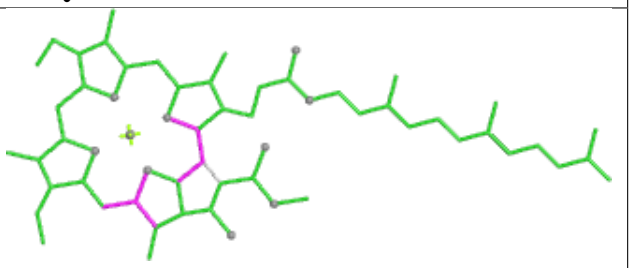
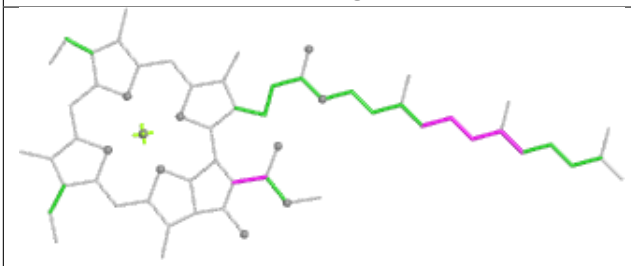
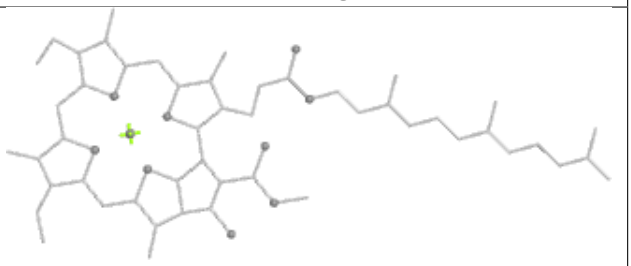


Bond angles

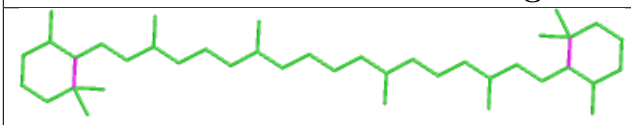


Torsions



Rings

Ligand BCR F 801



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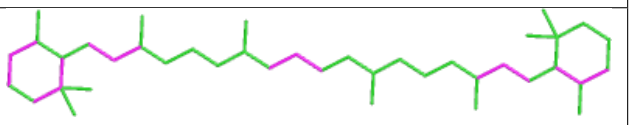
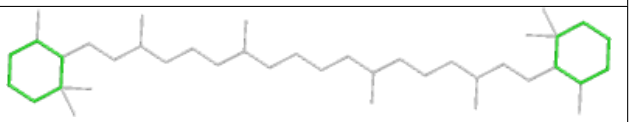


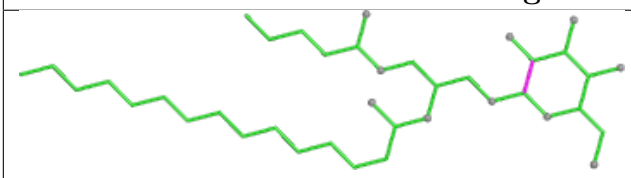
Bond angles

Torsions

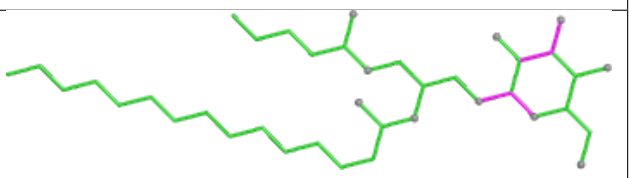


Rings

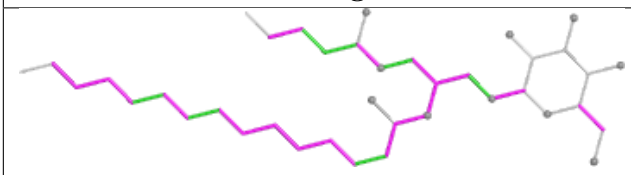
Ligand LMG J 102



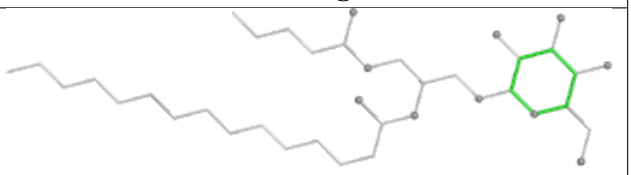
Bond lengths



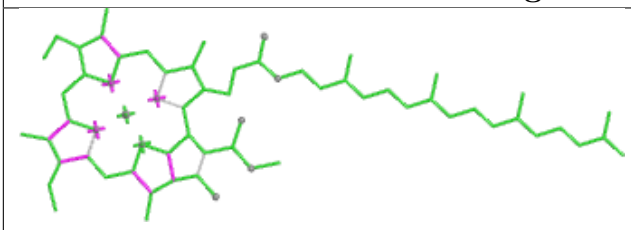
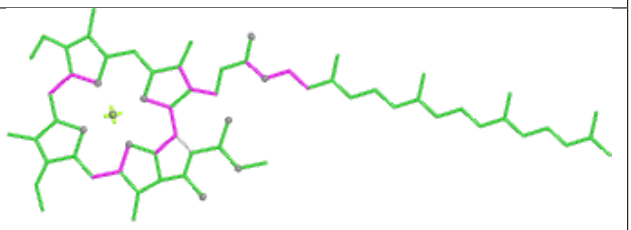
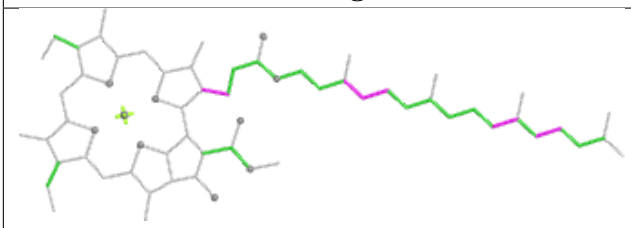
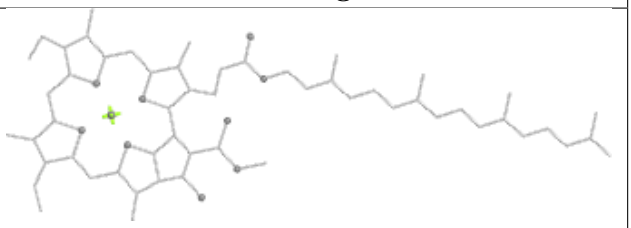
Bond angles

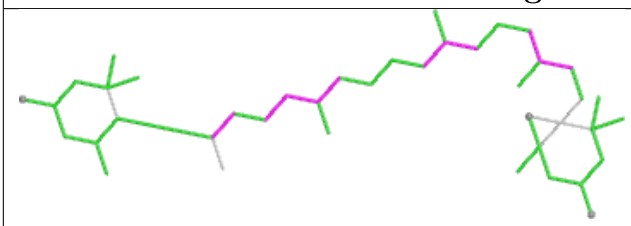
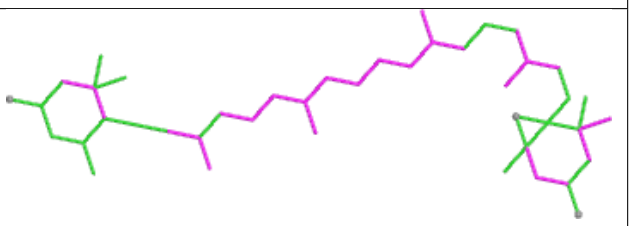
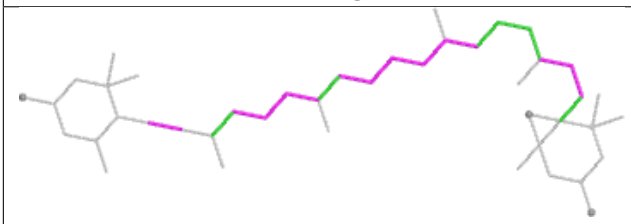


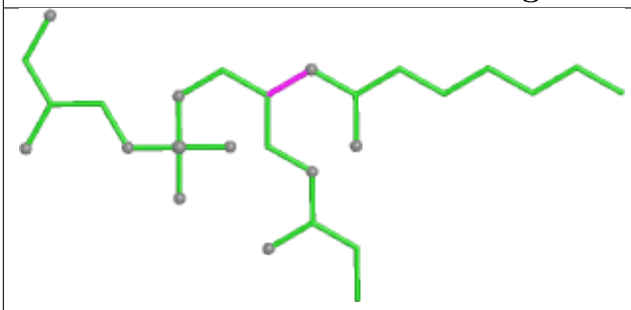
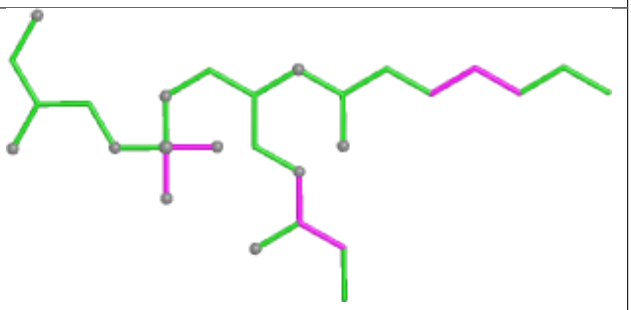
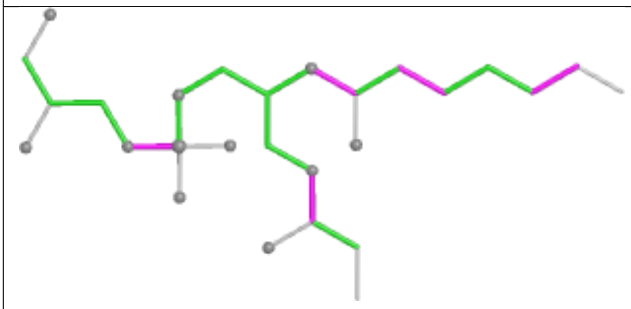
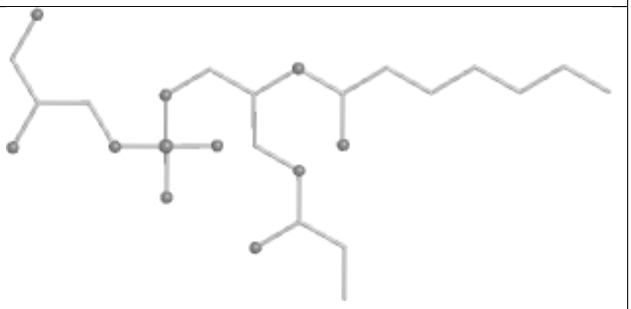
Torsions



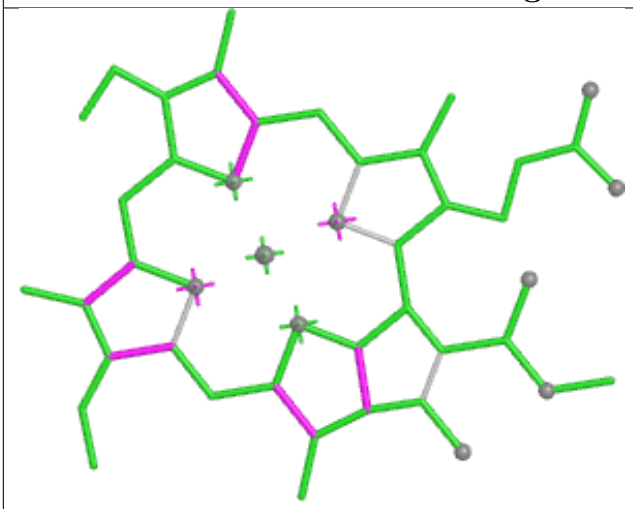
Rings

Ligand CLA B 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

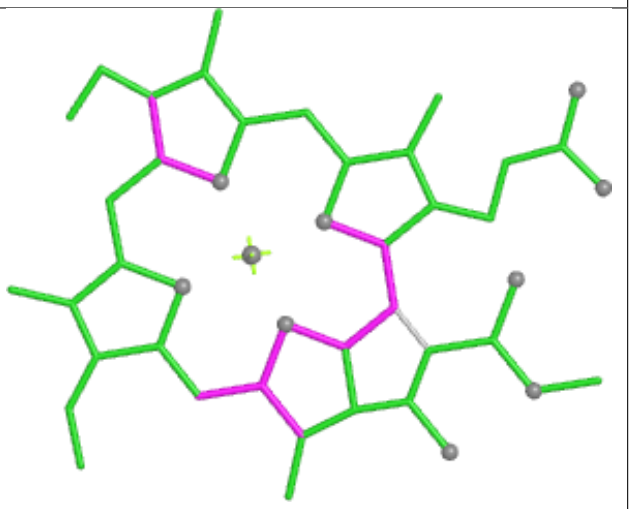
Ligand DD6 U 203	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LHG A 840	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

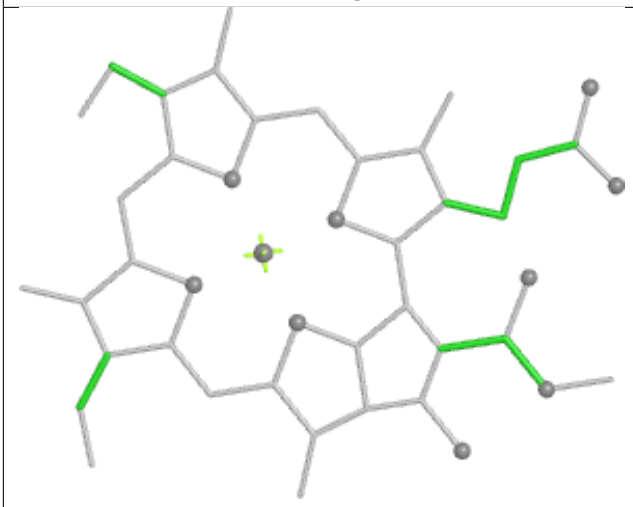
Ligand CLA R 202



Bond lengths

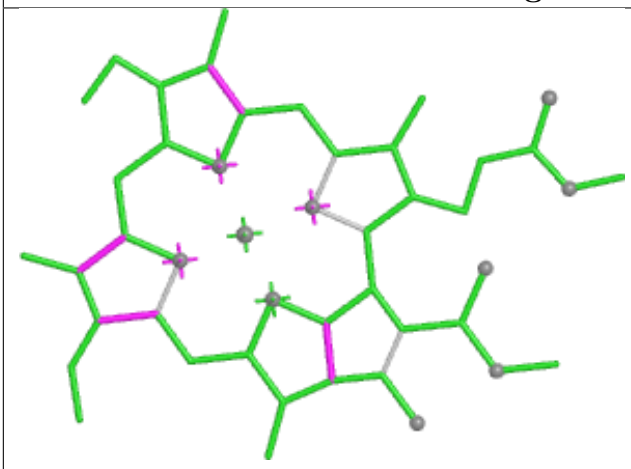
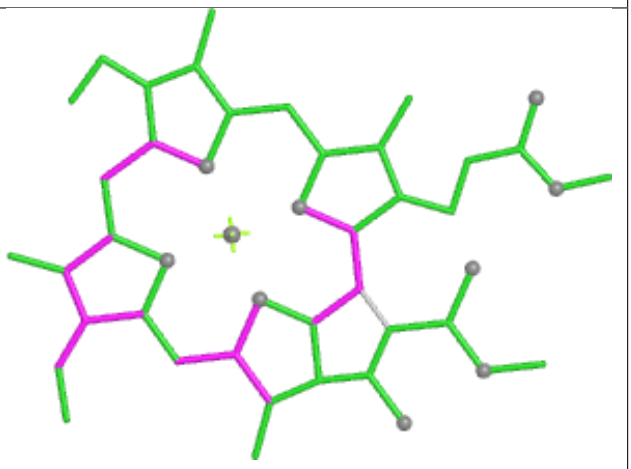
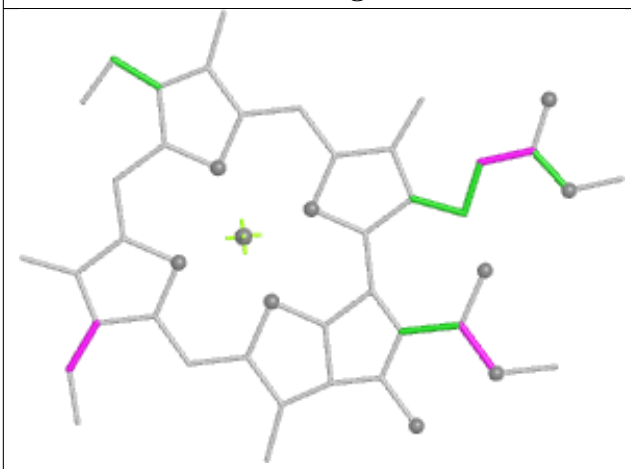
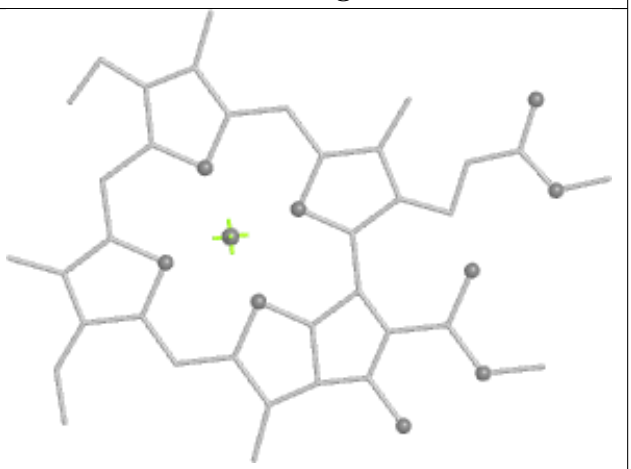


Bond angles

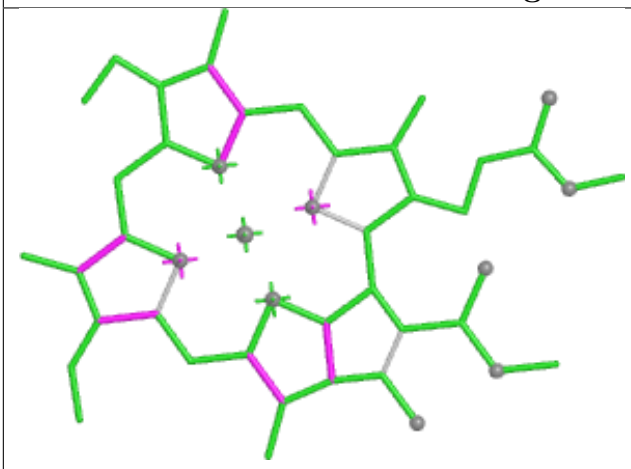


Torsions

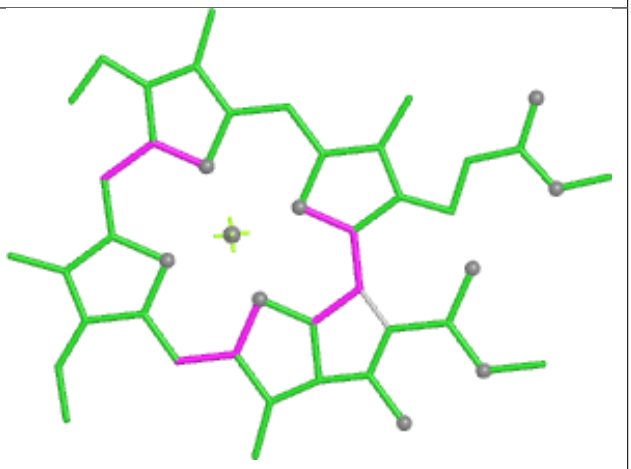
Rings

Ligand CLA T 211	
 Bond lengths	 Bond angles
 Torsions	 Rings

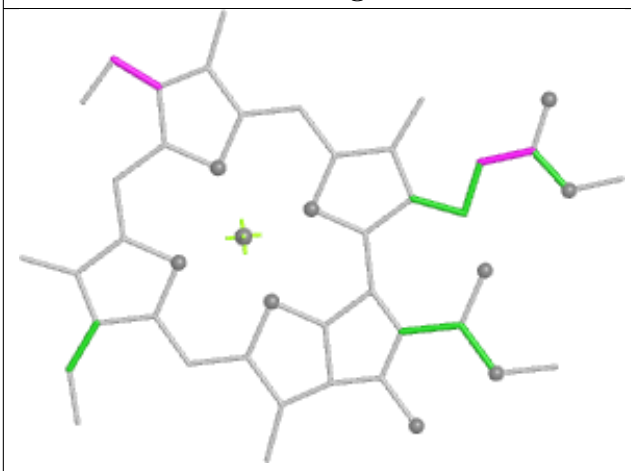
Ligand CLA O 207



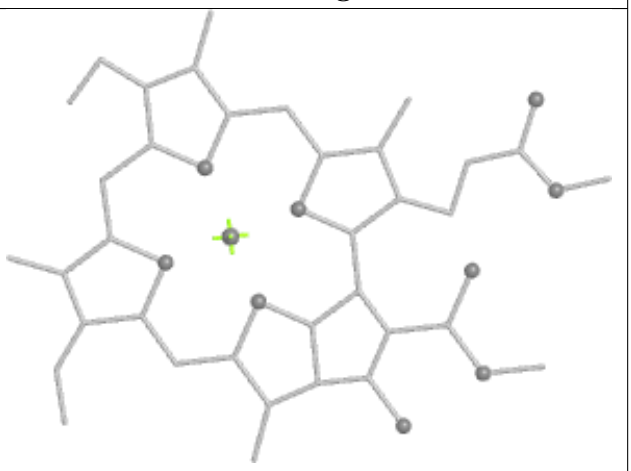
Bond lengths



Bond angles

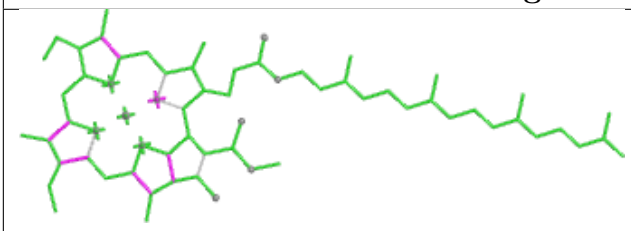


Torsions



Rings

Ligand CLA Q 209



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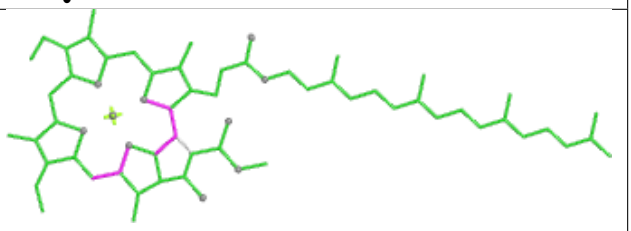

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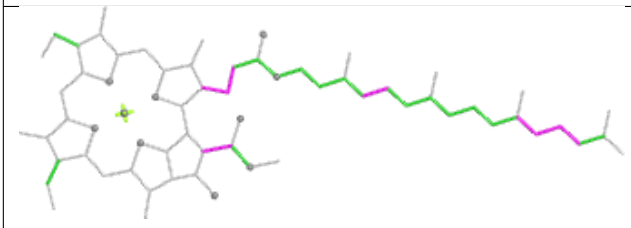

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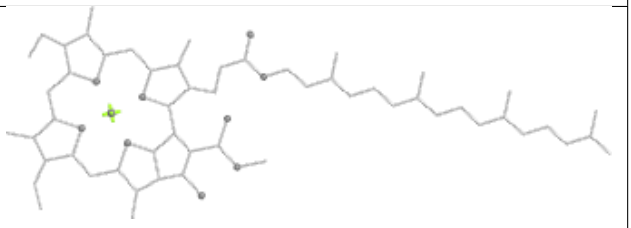
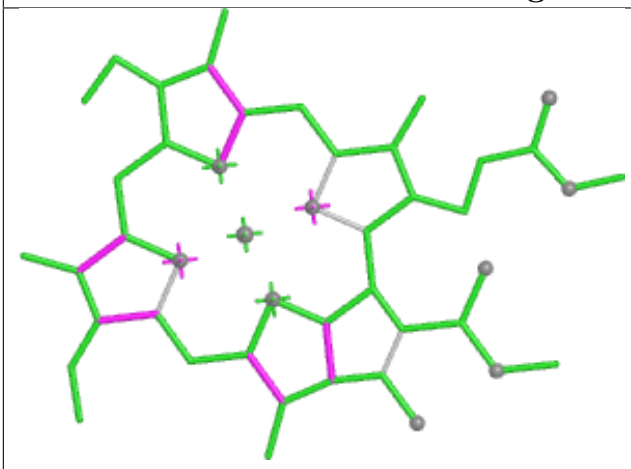


Rings

Ligand CLA S 205



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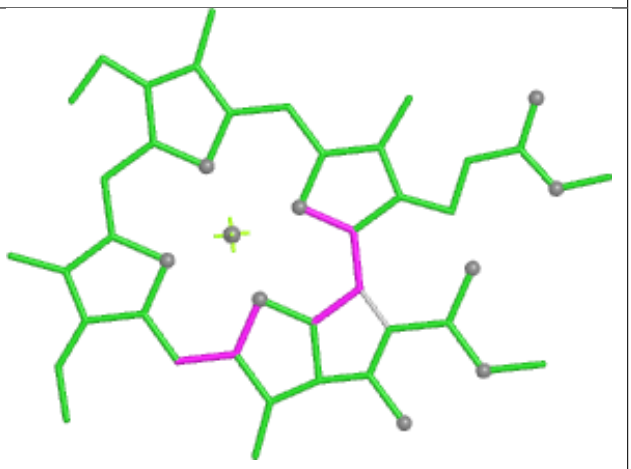

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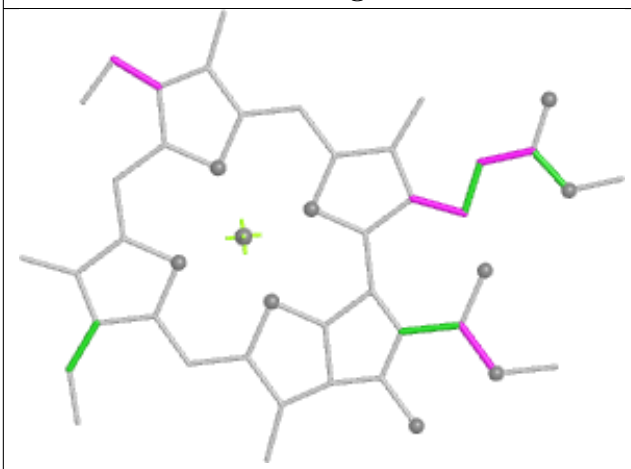

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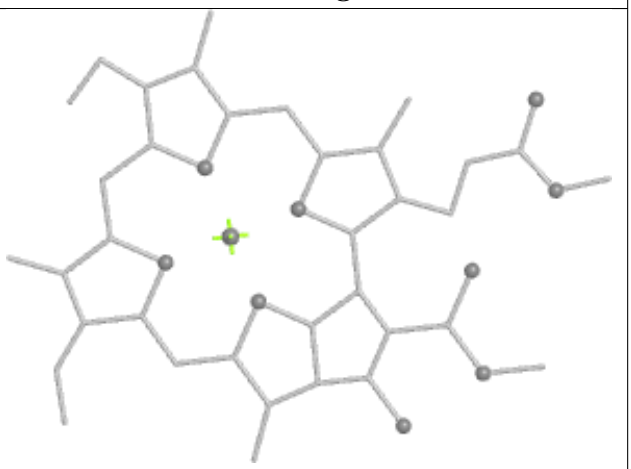
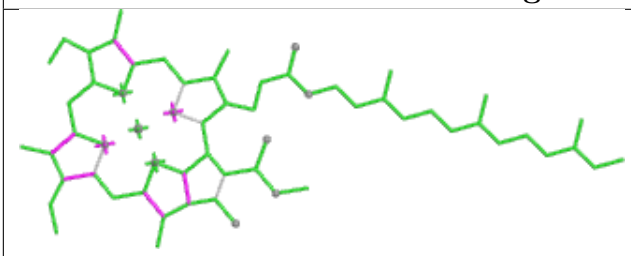


Rings

Ligand CLA U 204



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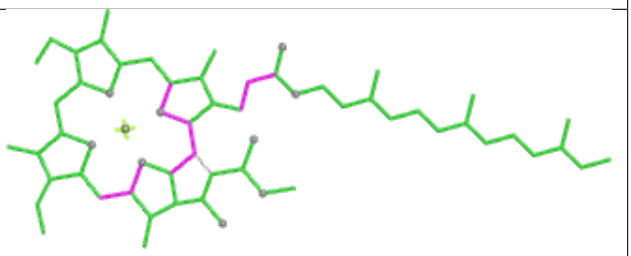
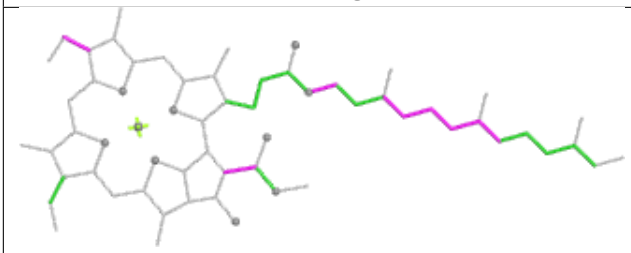


Bond angles



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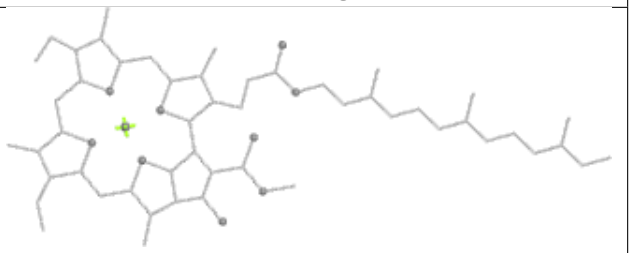
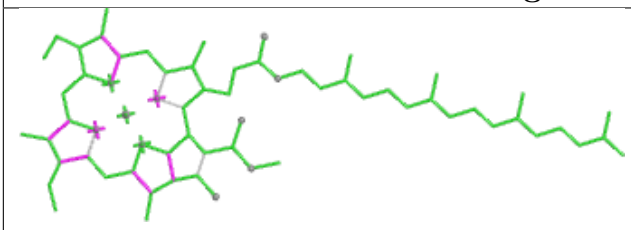
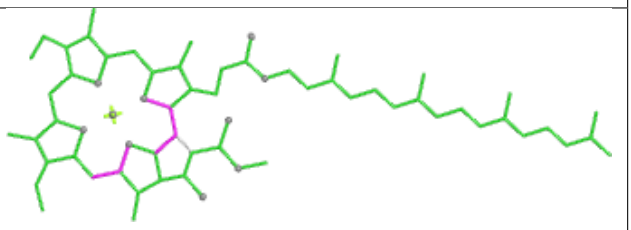
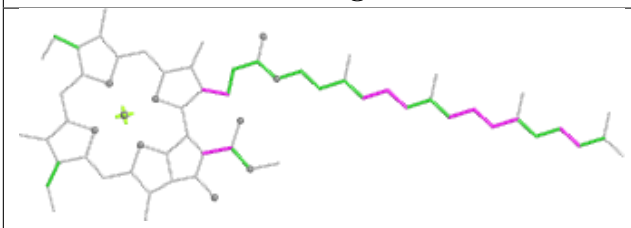
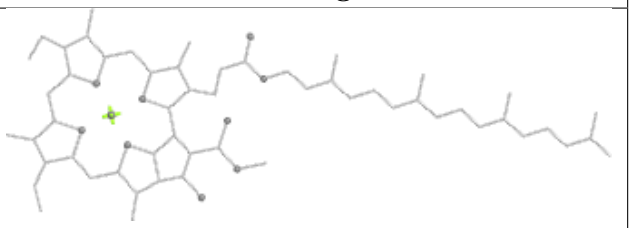


Rings

Ligand CLA A 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

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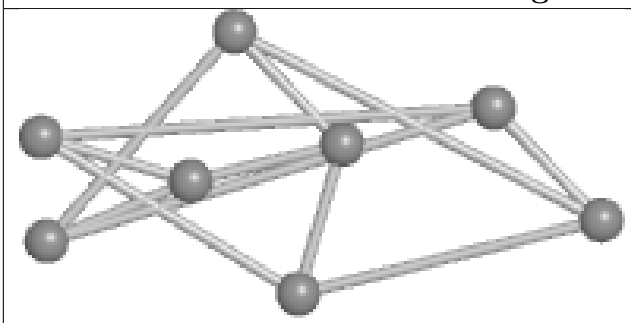
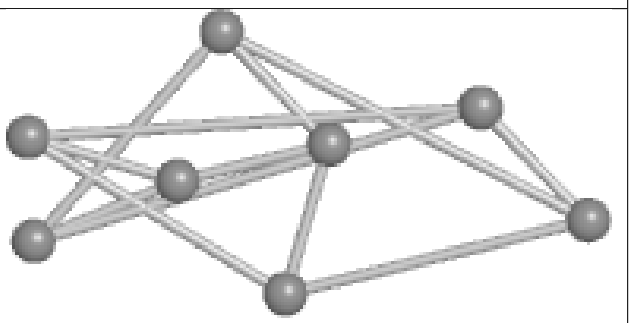
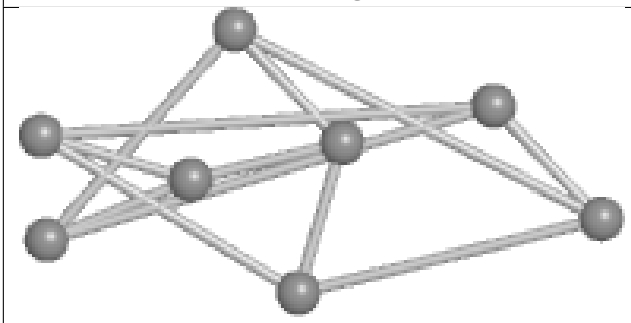
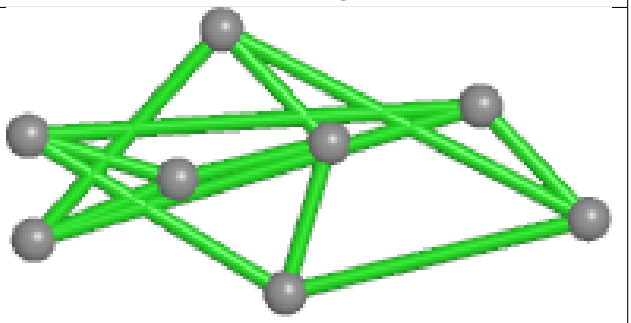
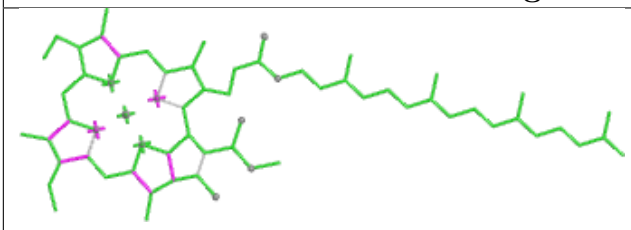
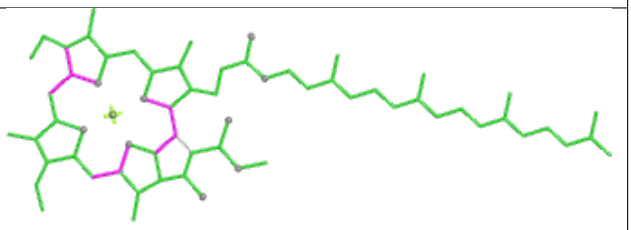
 Bond lengths	 Bond angles
 Torsions	 Rings

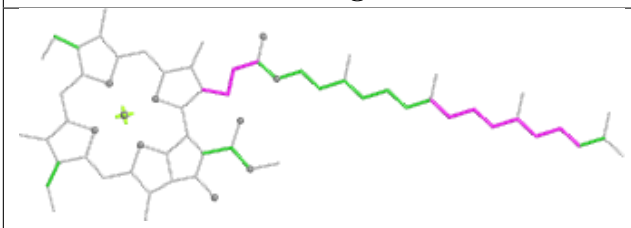
Ligand CLA A 815



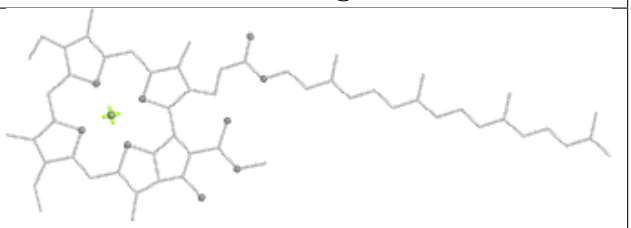
Bond lengths



Bond angles

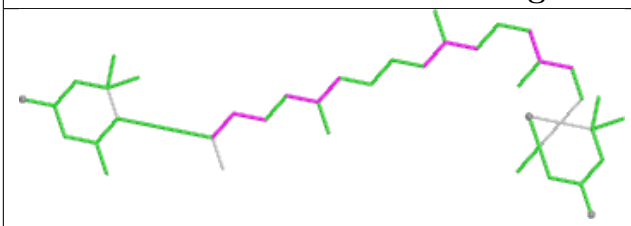


Torsions

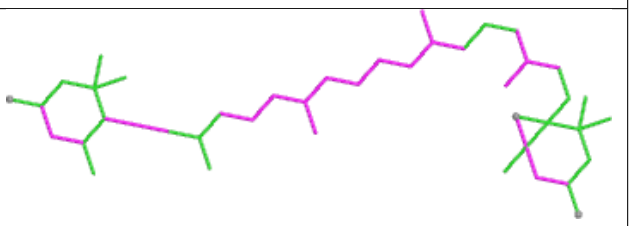


Rings

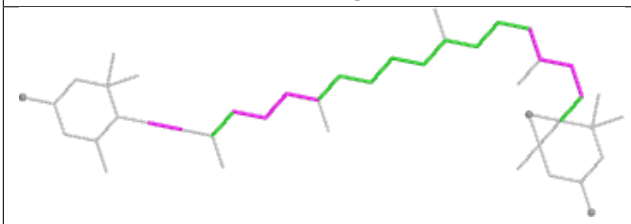
Ligand DD6 S 213



Bond lengths



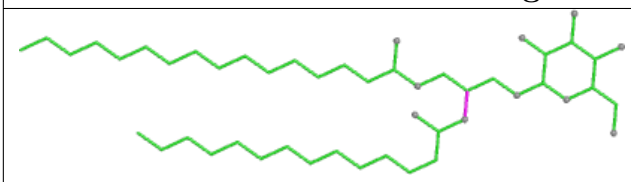
Bond angles



Torsions

Rings

Ligand LMG S 211



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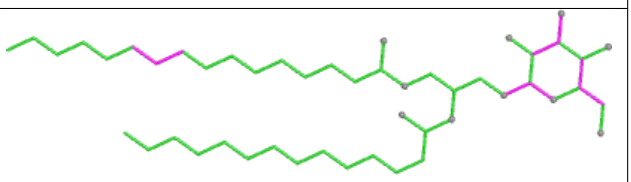
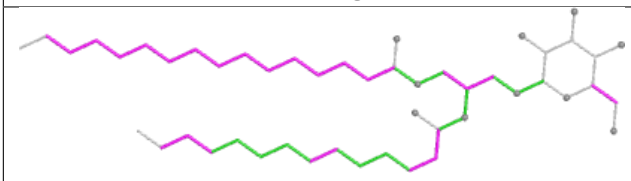
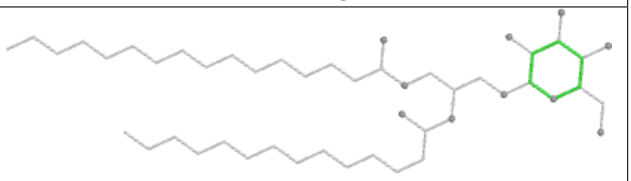


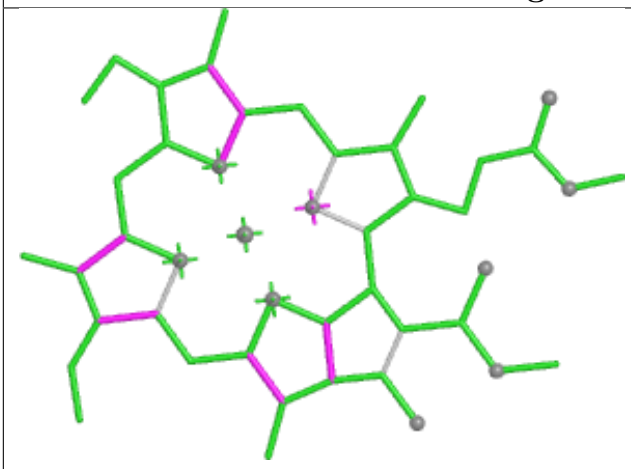
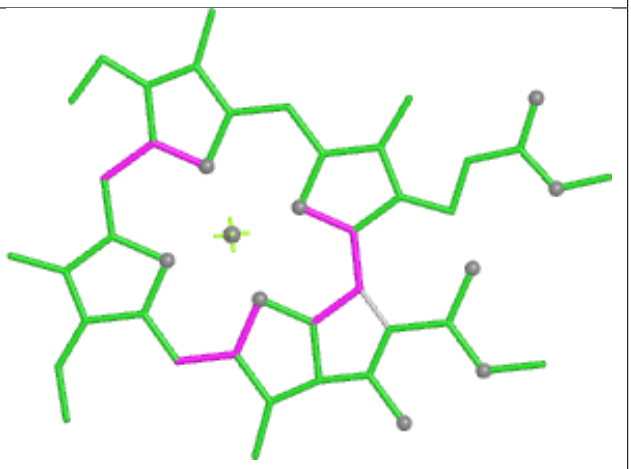
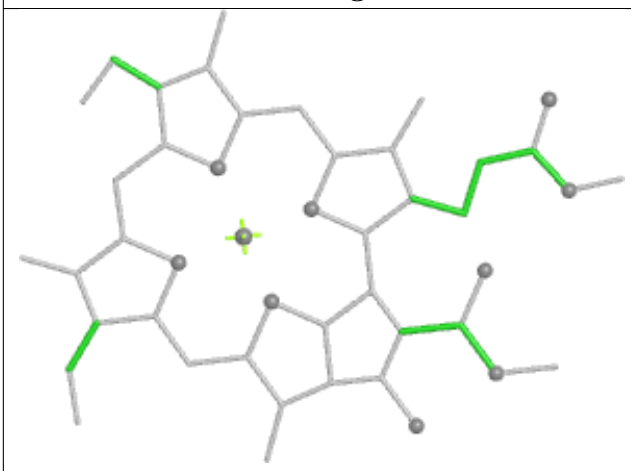
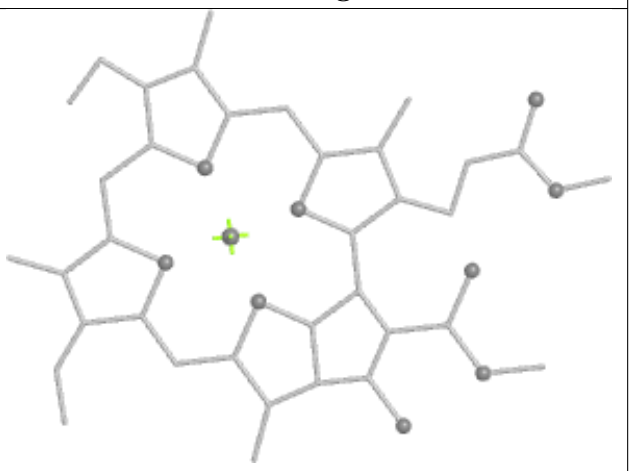
Bond angles



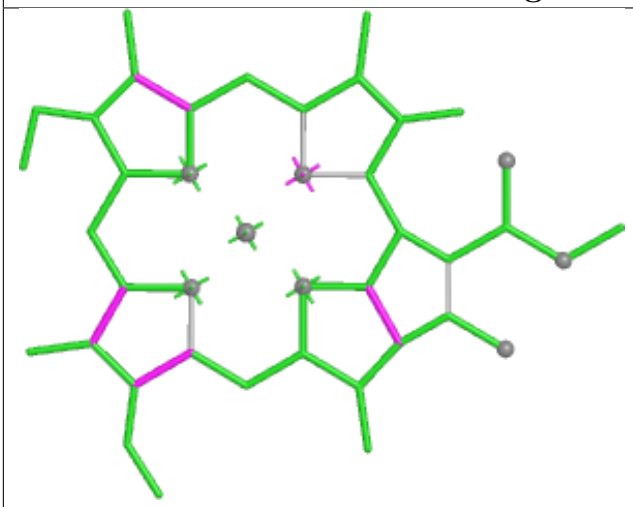
Torsions



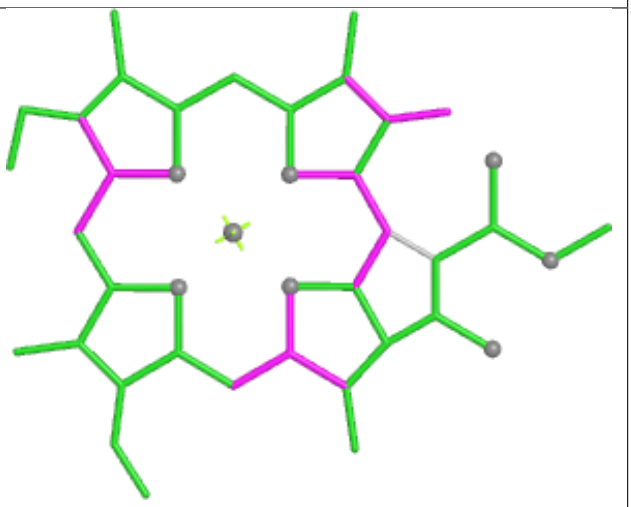
Rings

Ligand CLA S 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

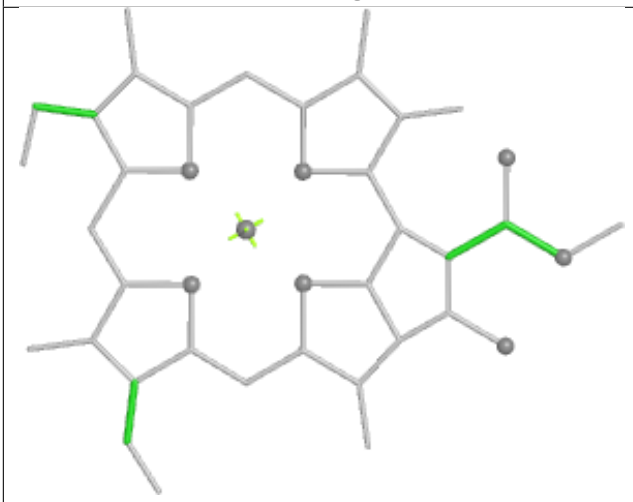
Ligand CLA T 210



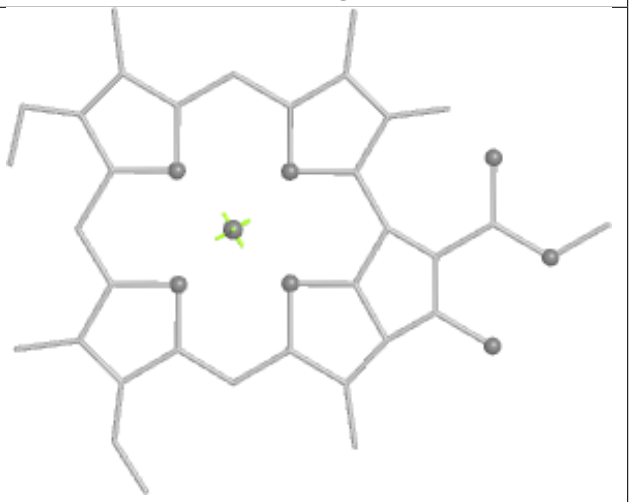
Bond lengths



Bond angles

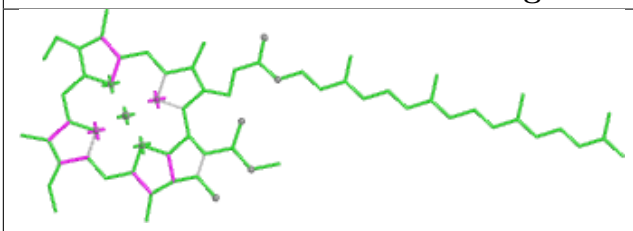


Torsions



Rings

Ligand CLA A 807



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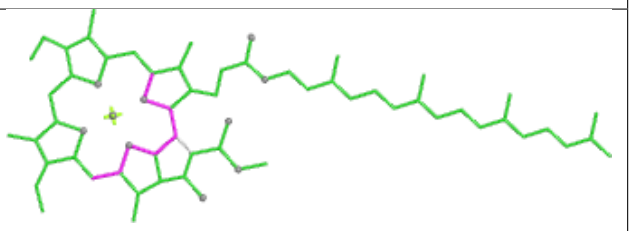
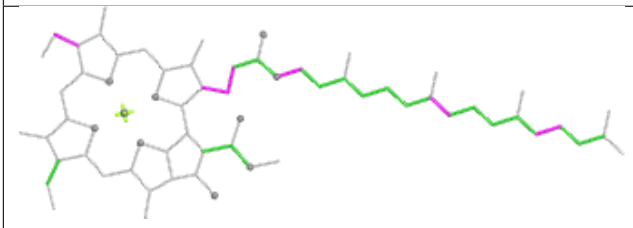


Bond angles



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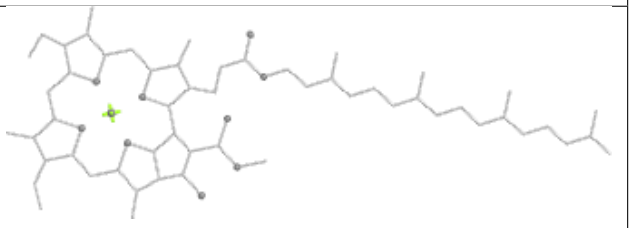
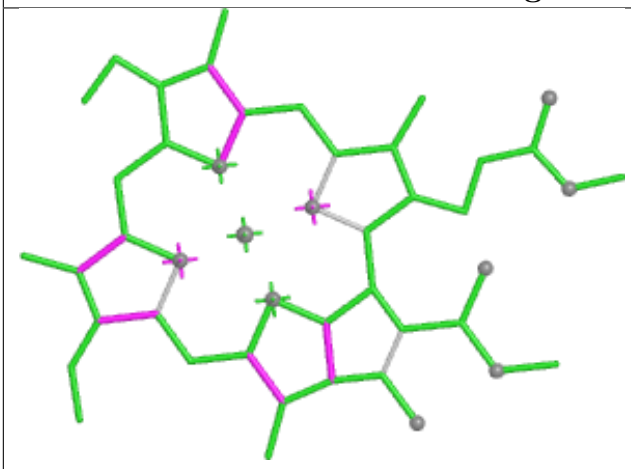
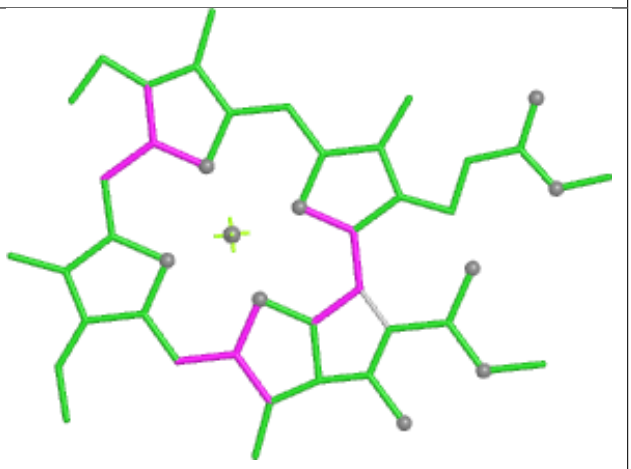
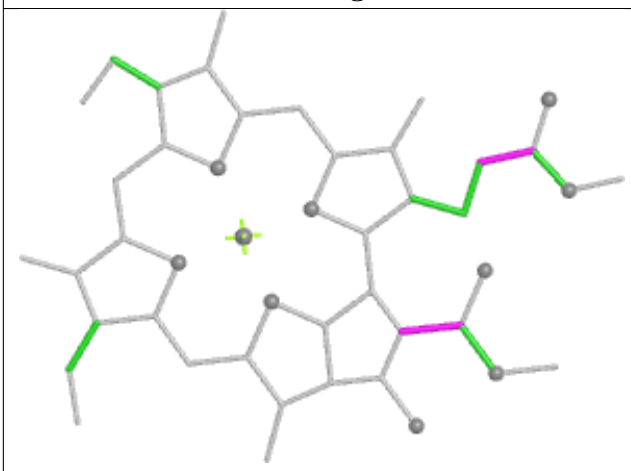
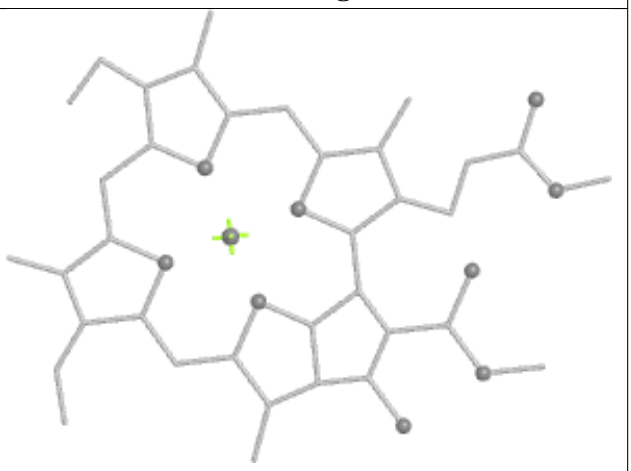
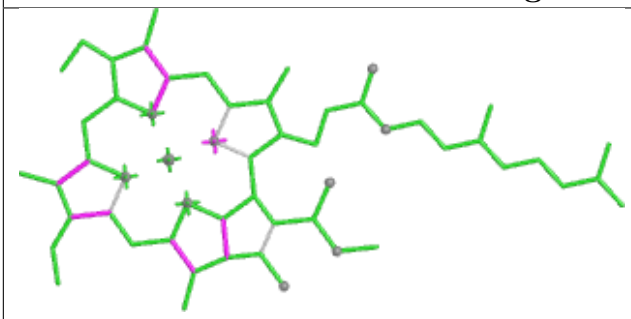
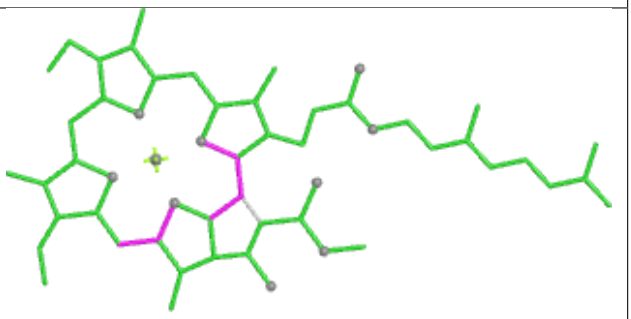
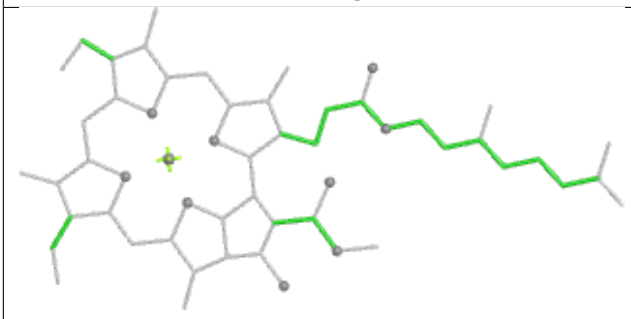
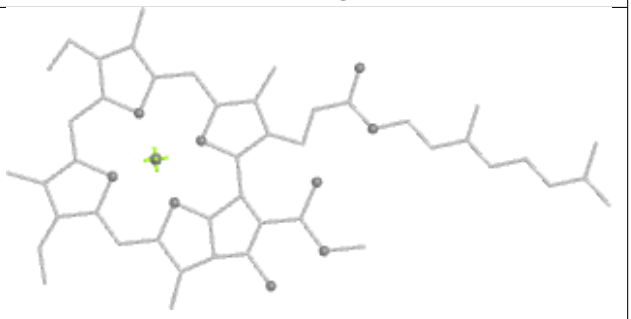
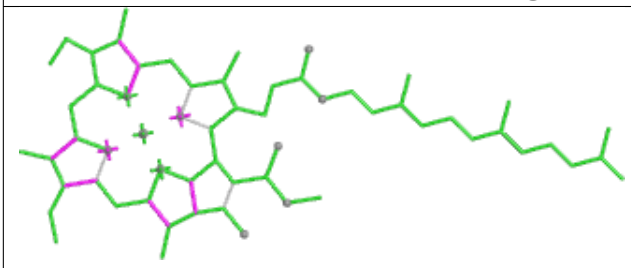
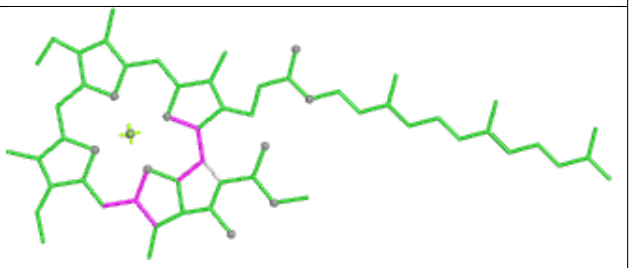
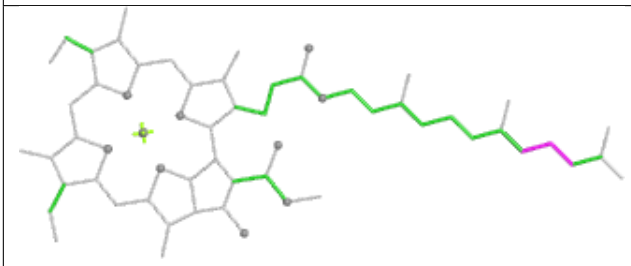
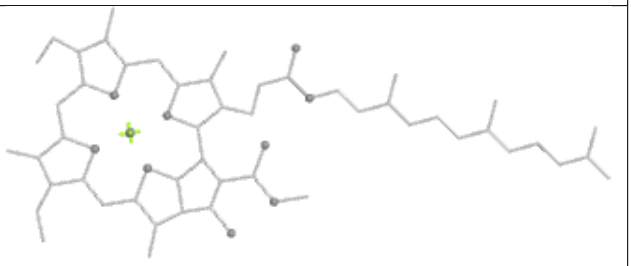


Rings

Ligand CLA B 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

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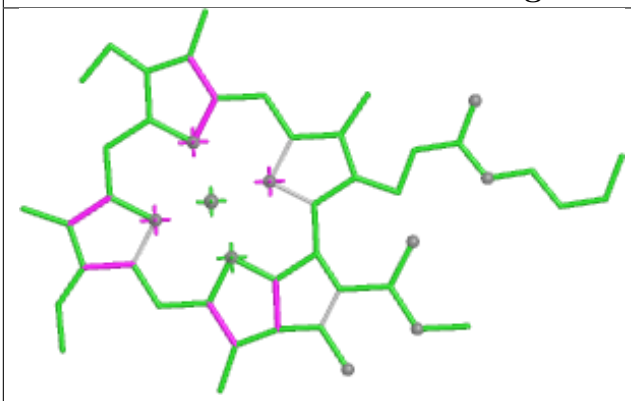
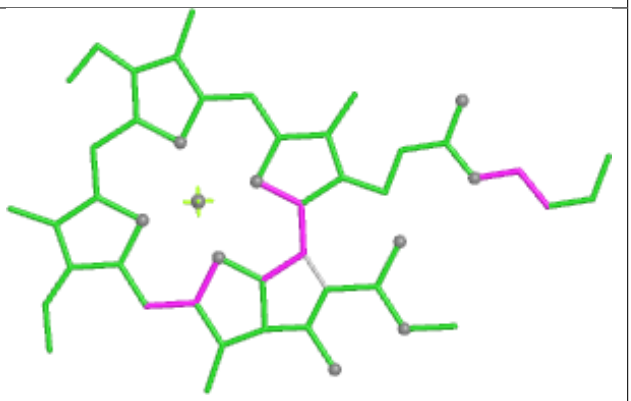
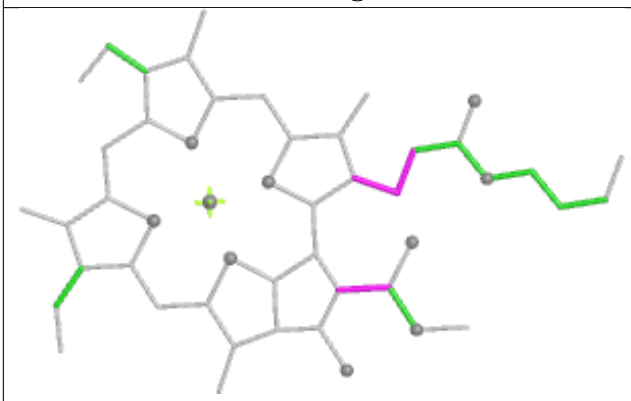
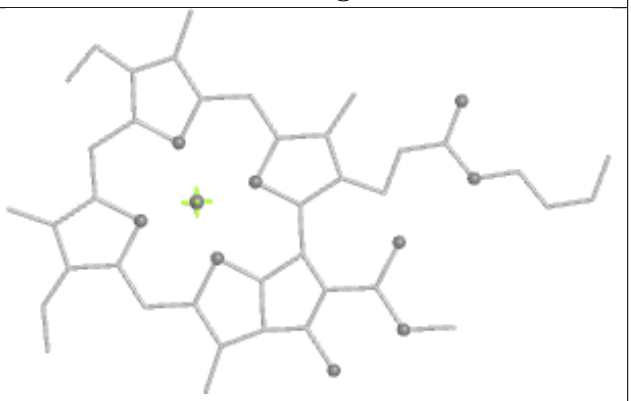
 Bond lengths	 Bond angles
 Torsions	 Rings

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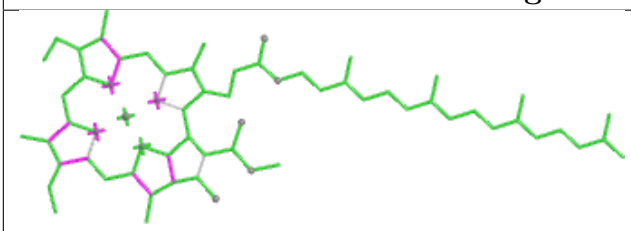
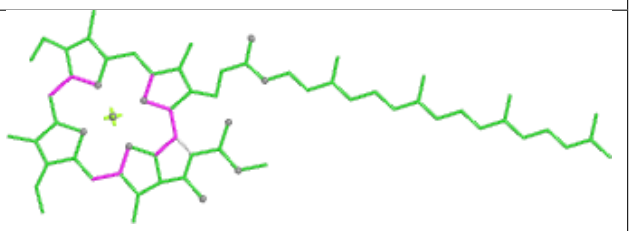
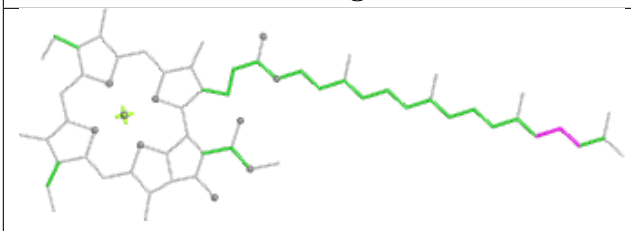
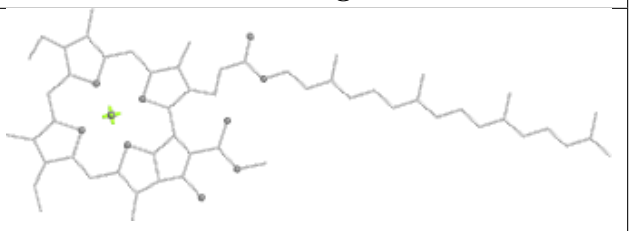
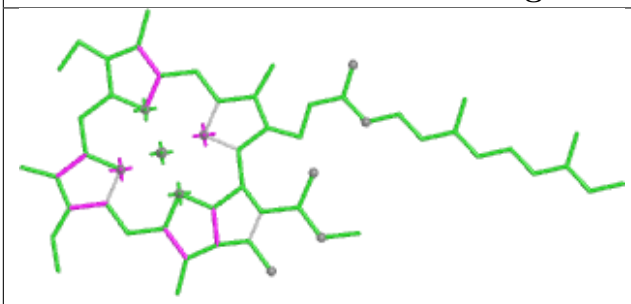
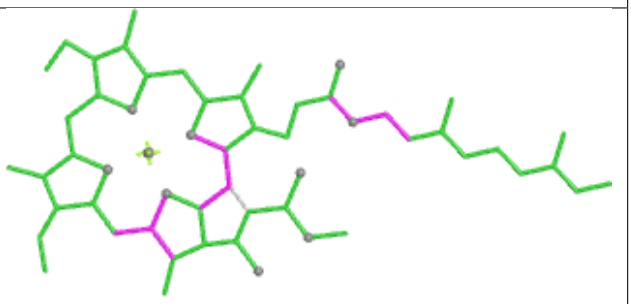
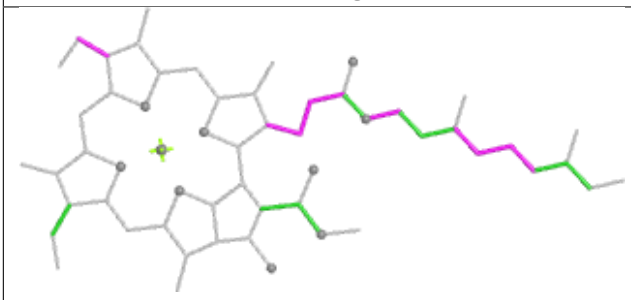
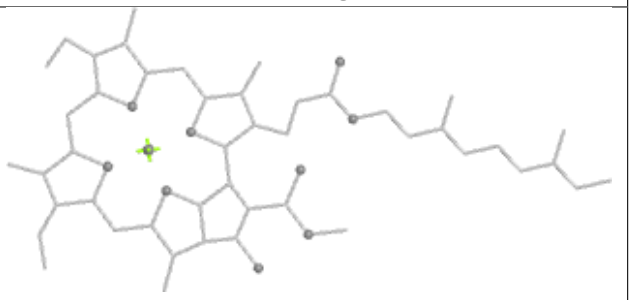
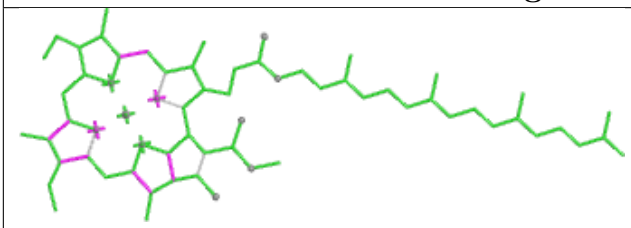
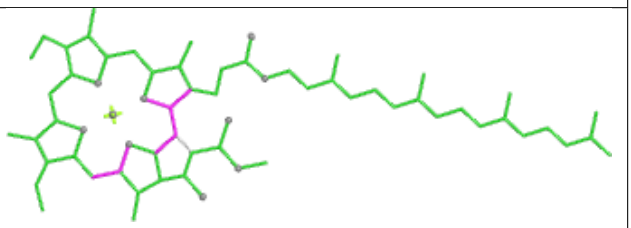
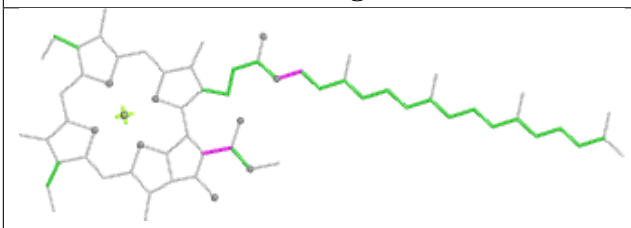
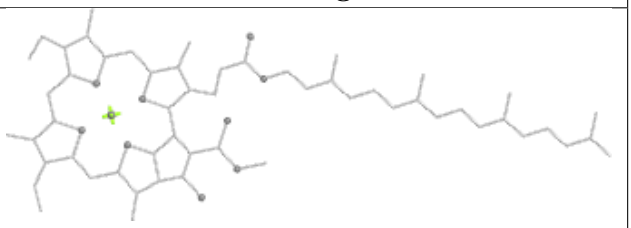
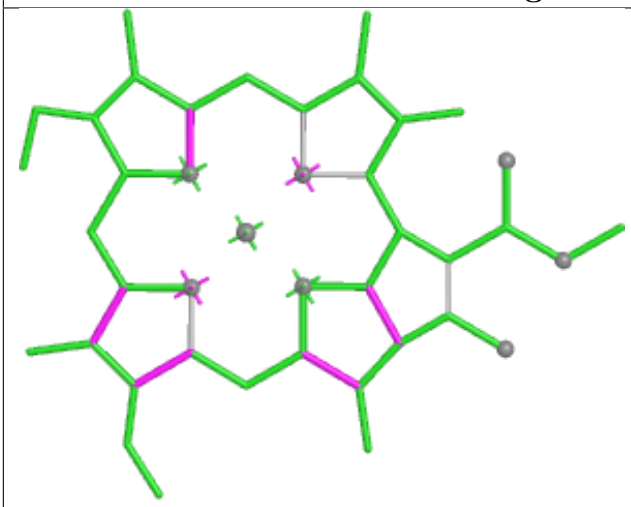
 Bond lengths	 Bond angles
 Torsions	 Rings

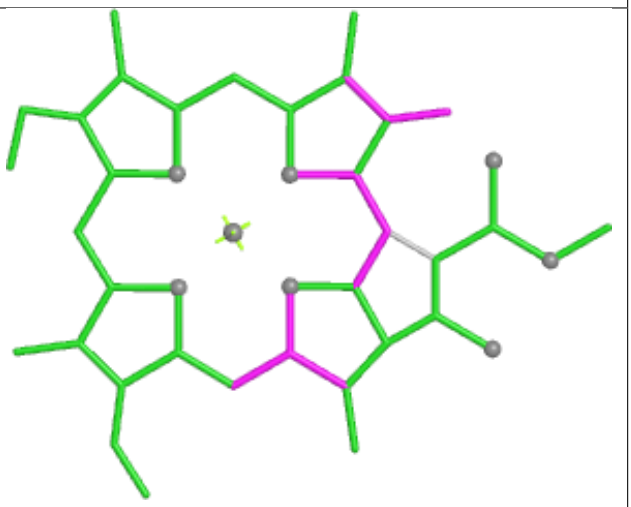
Ligand CLA P 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

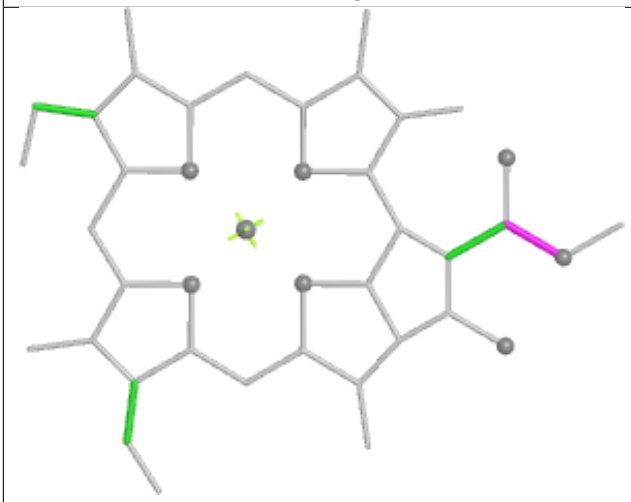
Ligand CLA P 312



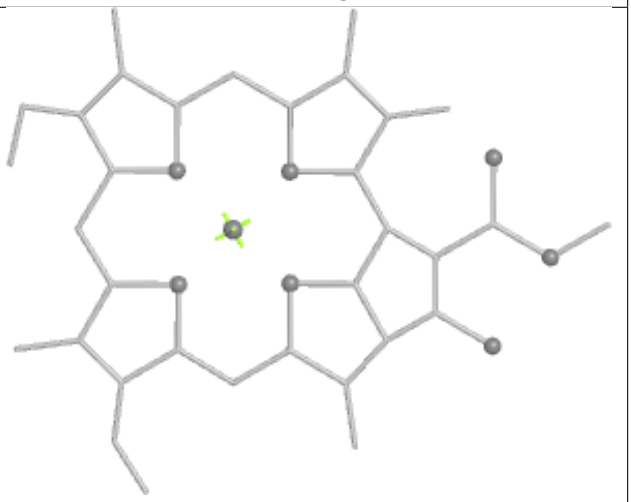
Bond lengths



Bond angles

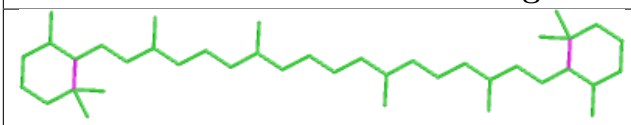


Torsions

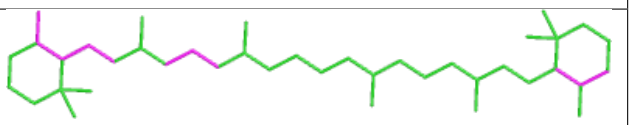


Rings

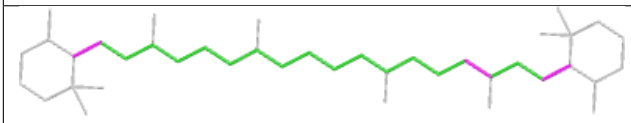
Ligand BCR B 841



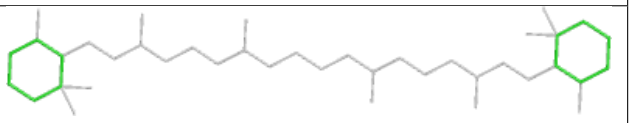
Bond lengths



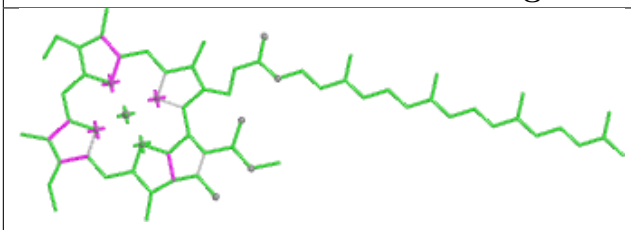
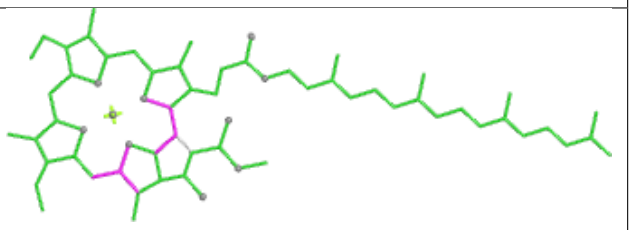
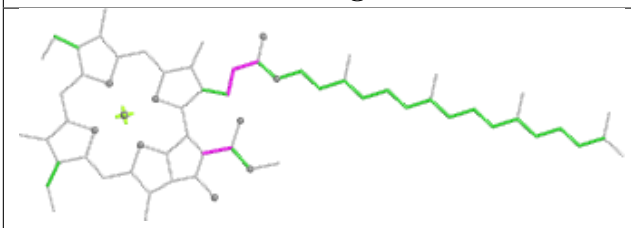
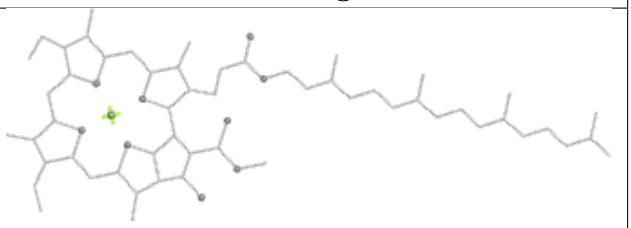
Bond angles

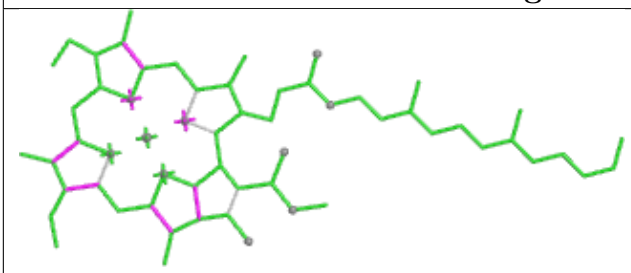
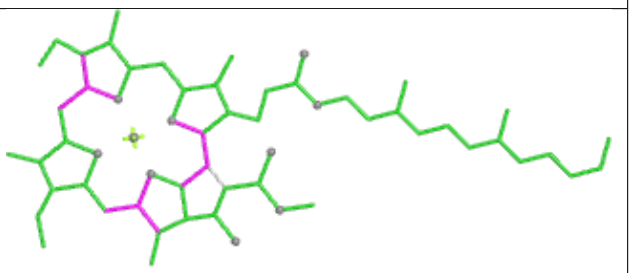
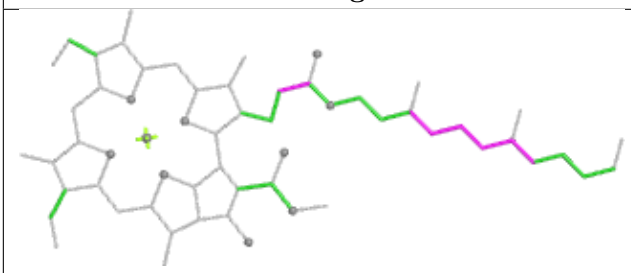
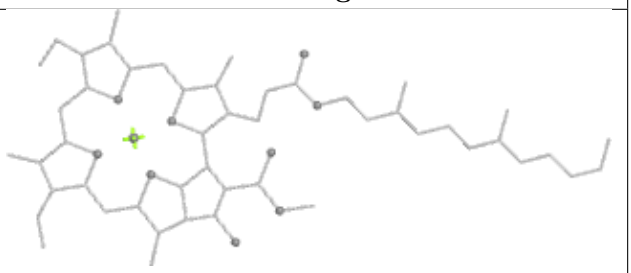


Torsions

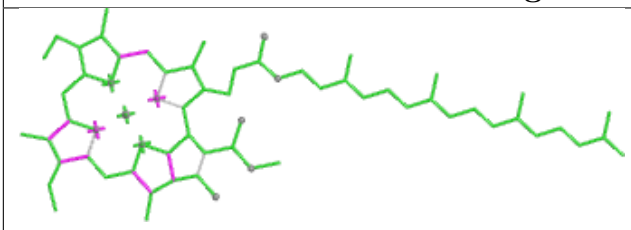


Rings

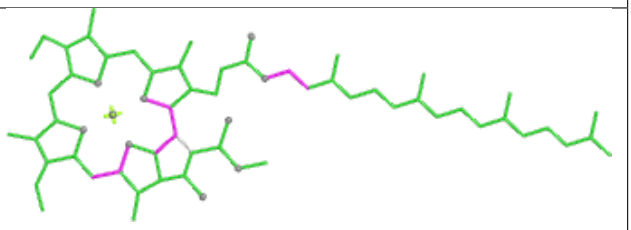
Ligand CLA A 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

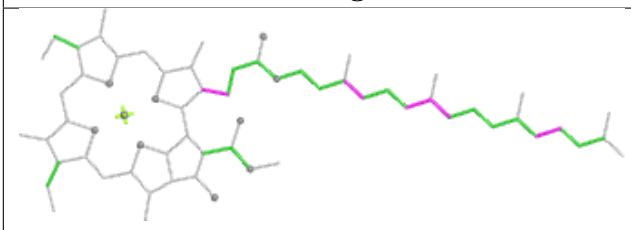
Ligand CLA B 823



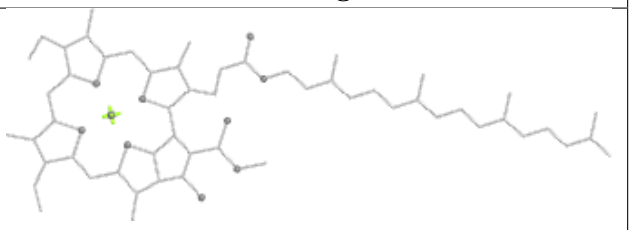
Bond lengths



Bond angles

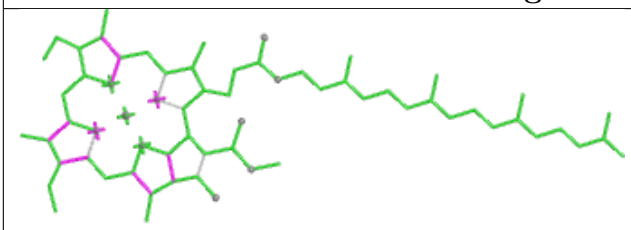


Torsions

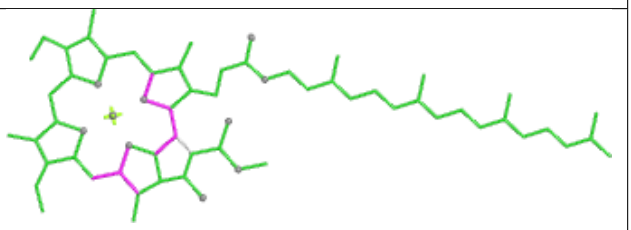


Rings

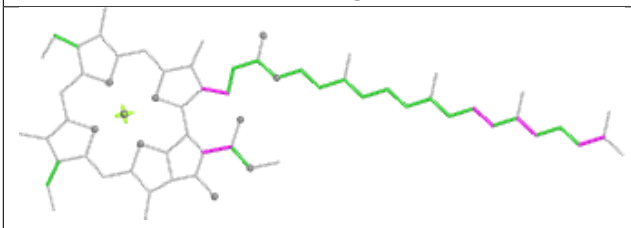
Ligand CLA B 825



Bond lengths



Bond angles



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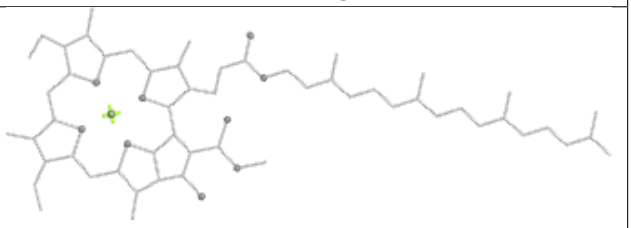
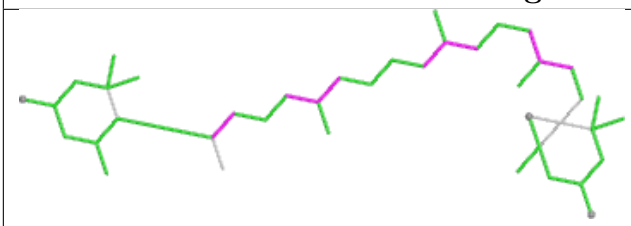
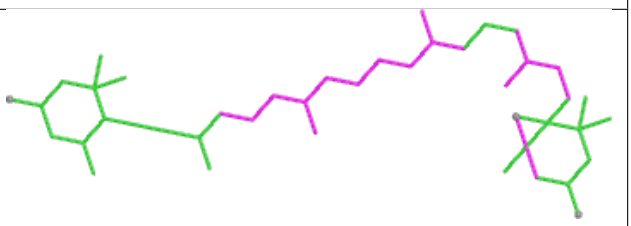


Rings

Ligand DD6 U 212



Bond lengths



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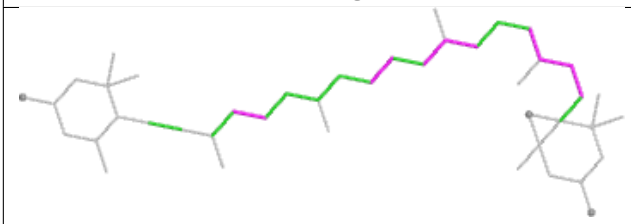
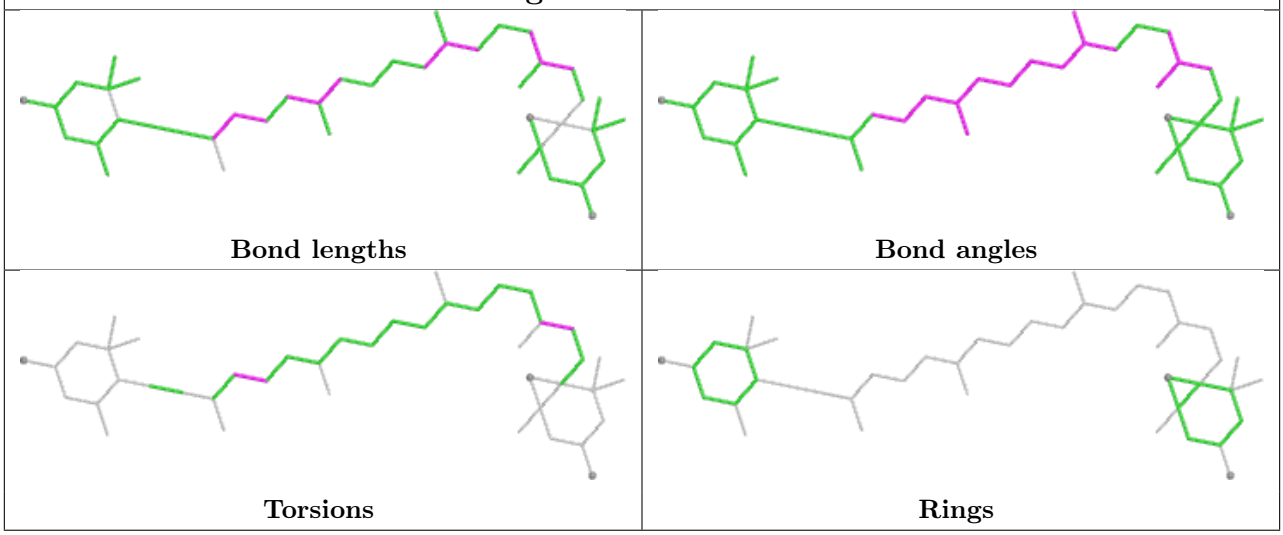


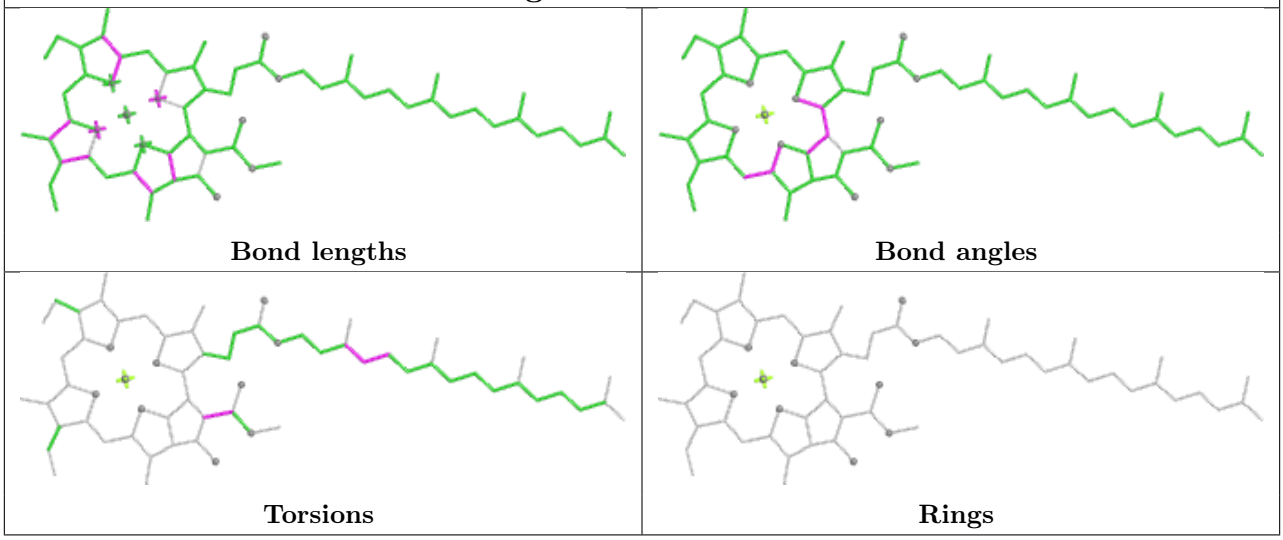
Torsions

Rings

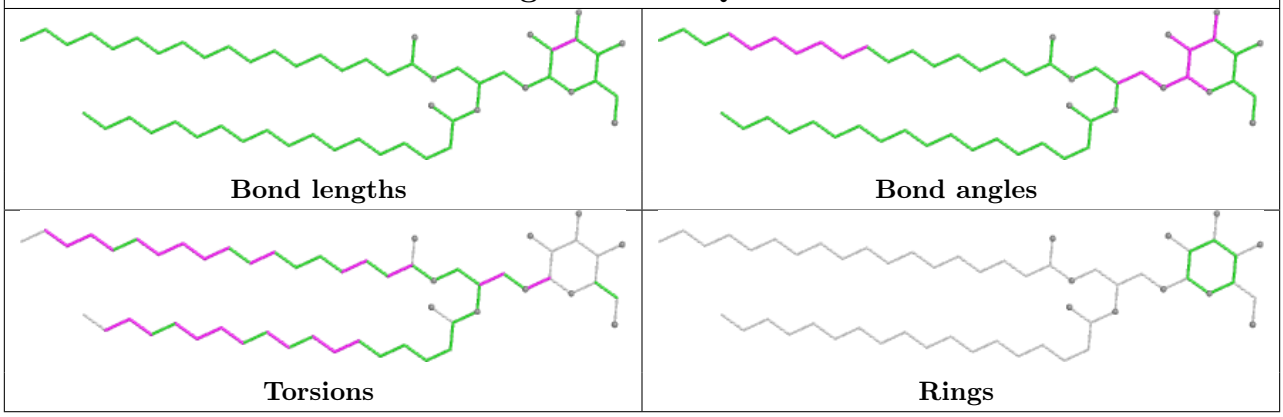
Ligand DD6 O 201

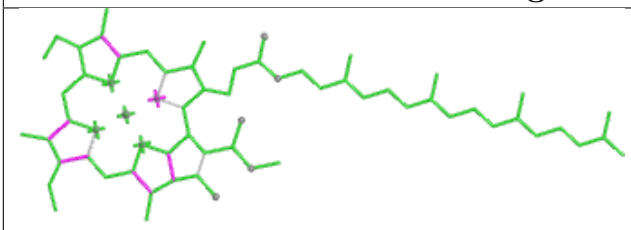
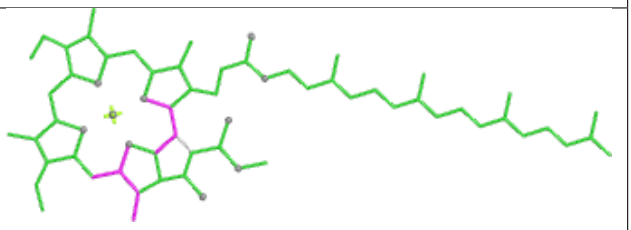
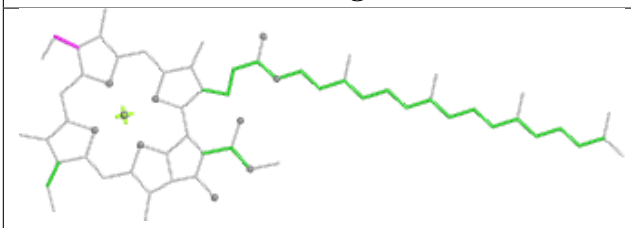
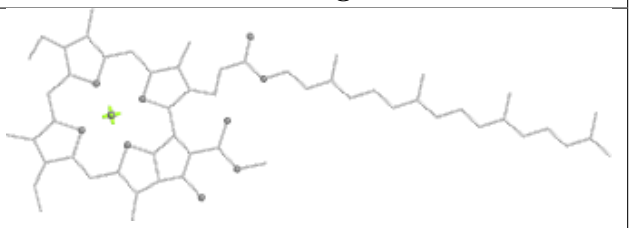


Ligand CLA B 808



Ligand LMG Q 217



Ligand CLA S 214	
 Bond lengths	 Bond angles
 Torsions	 Rings

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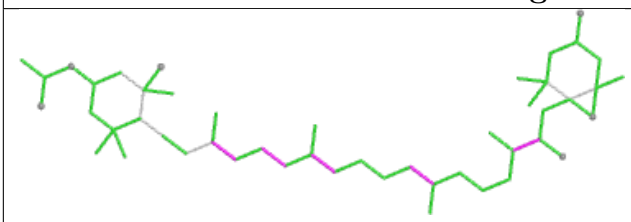
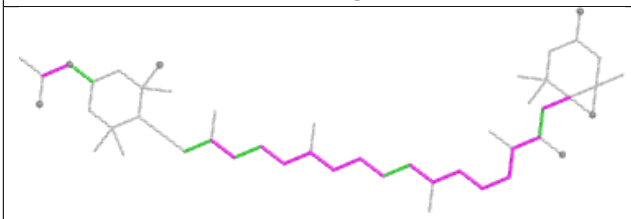
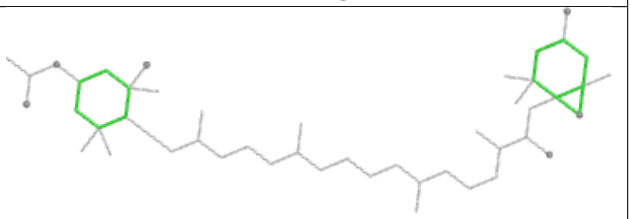
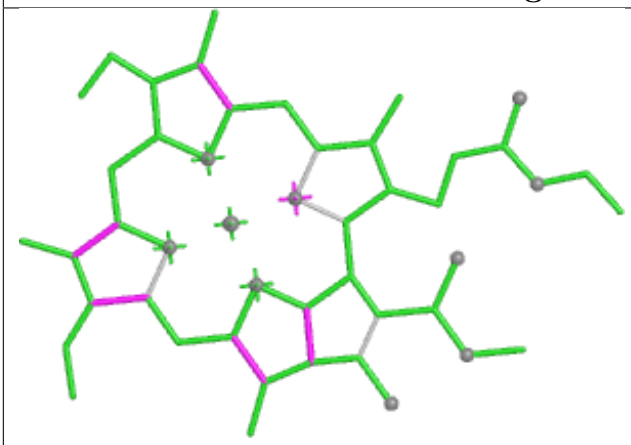
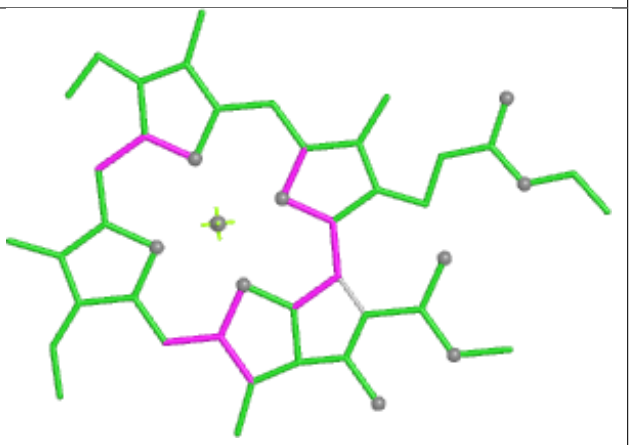
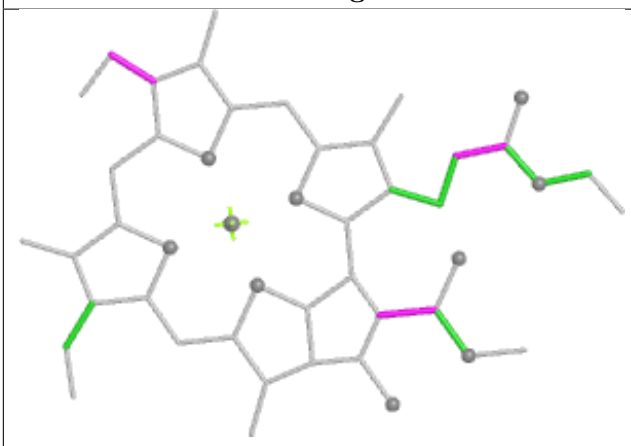
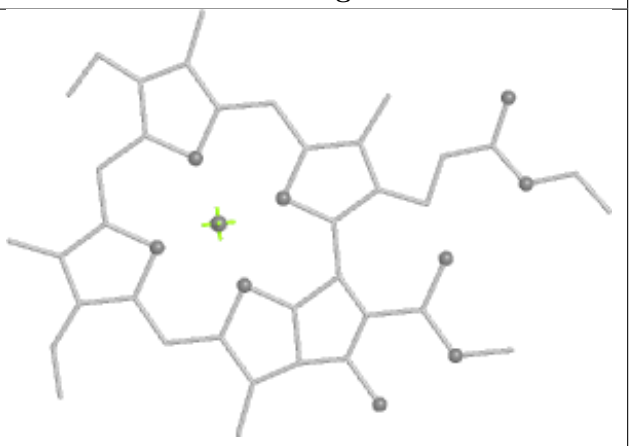
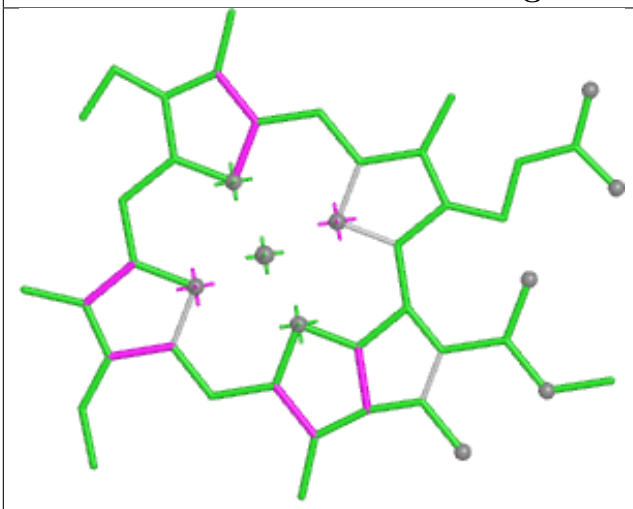
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand CLA T 212	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A 814



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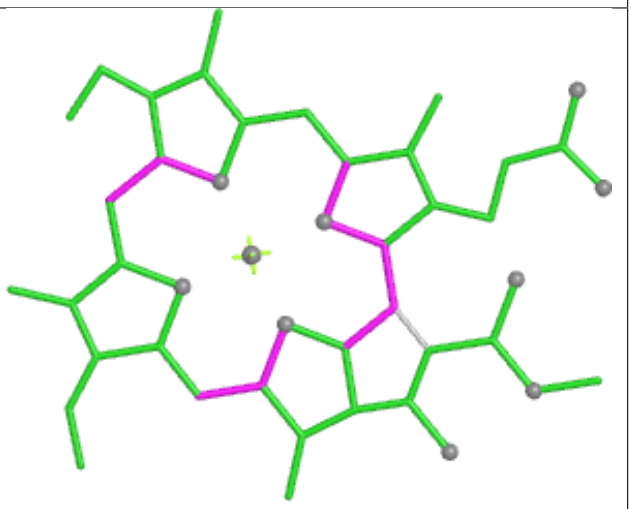
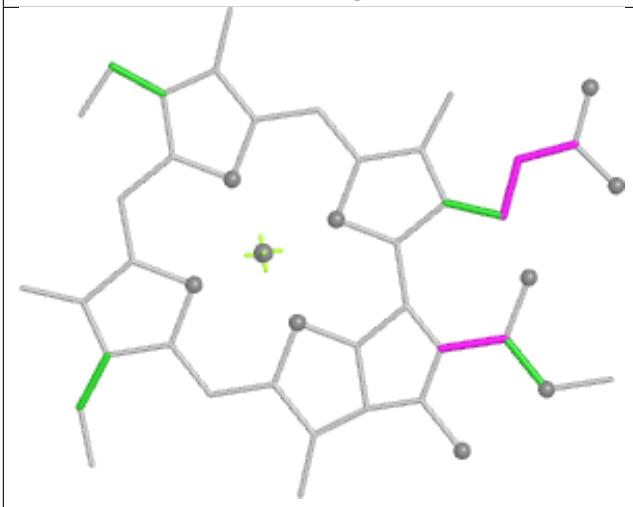


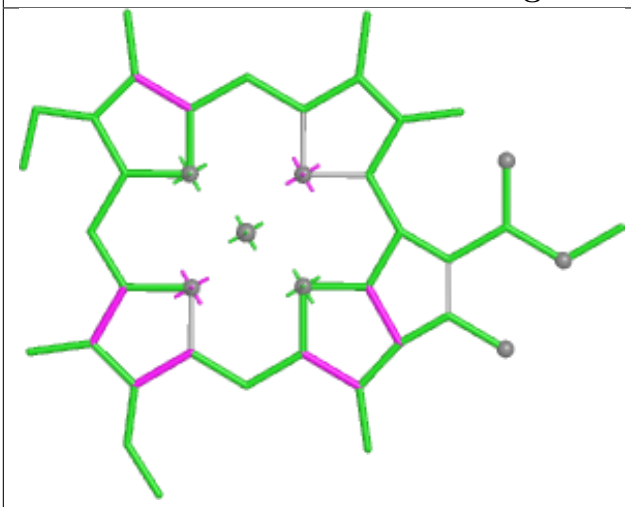
Bond angles



Torsions

Rings

Ligand CLA O 211



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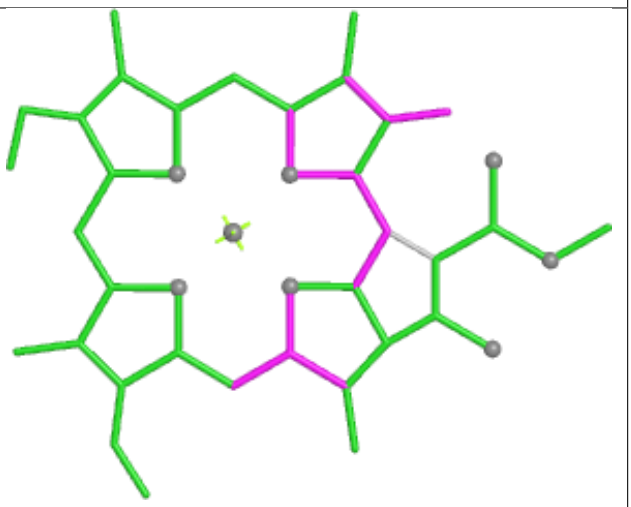
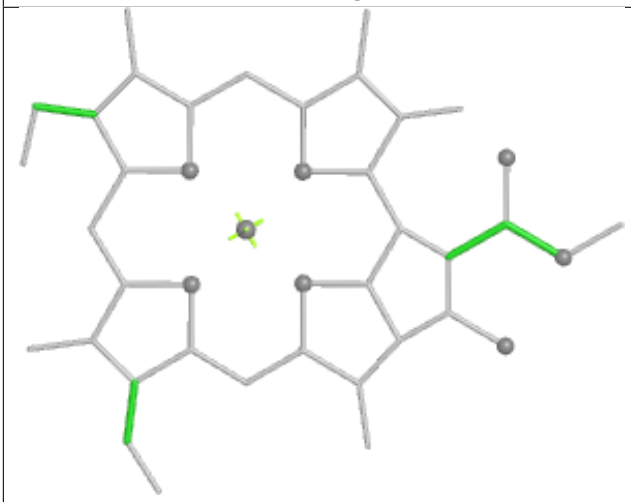
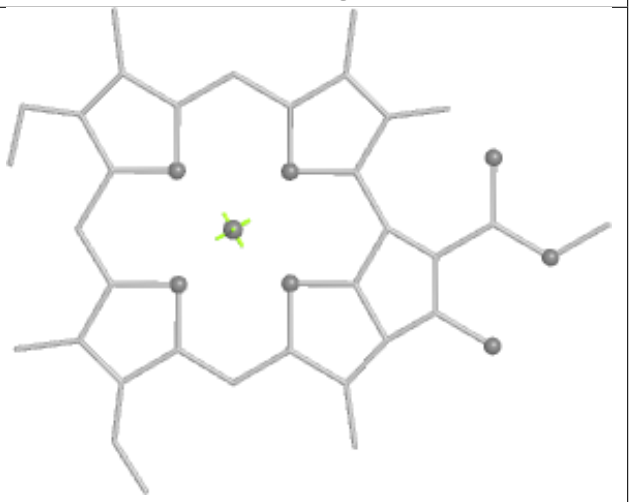


Bond angles

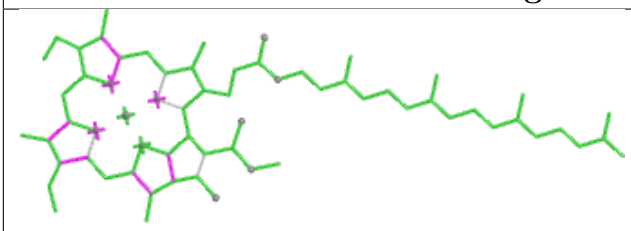


Torsions



Rings

Ligand CLA B 805



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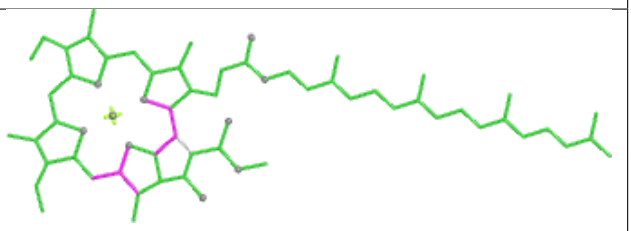
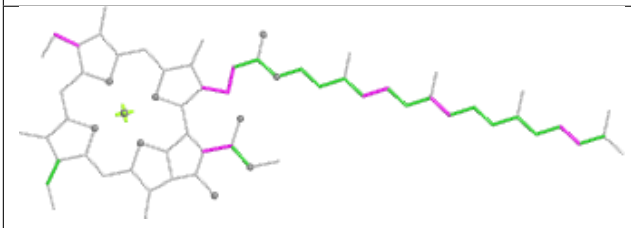
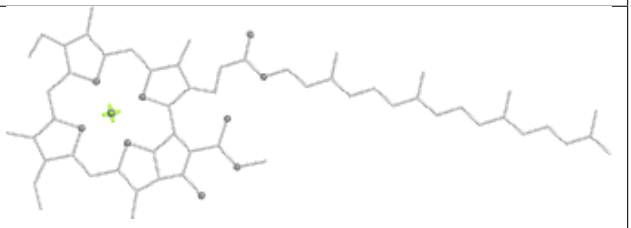


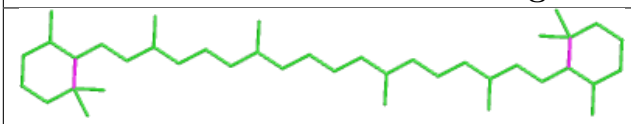
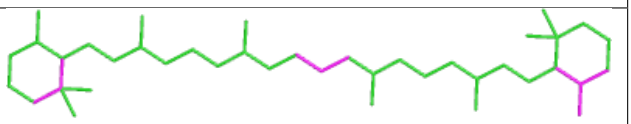
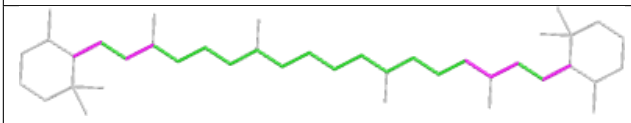
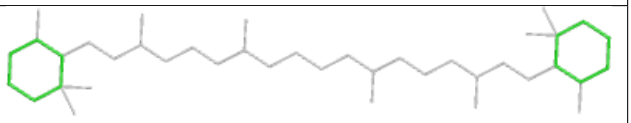
Bond angles

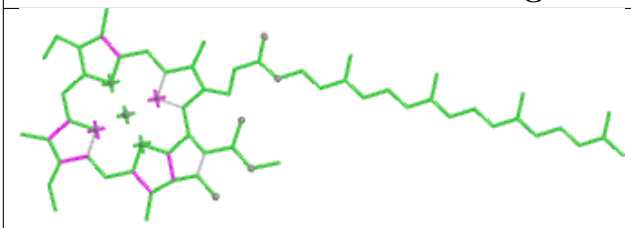
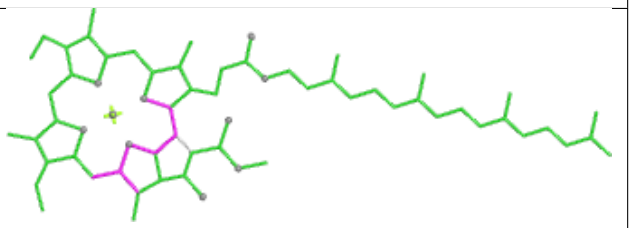
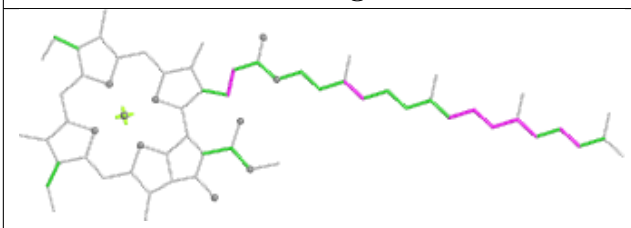
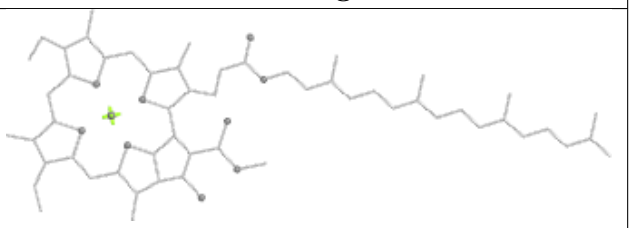


Torsions

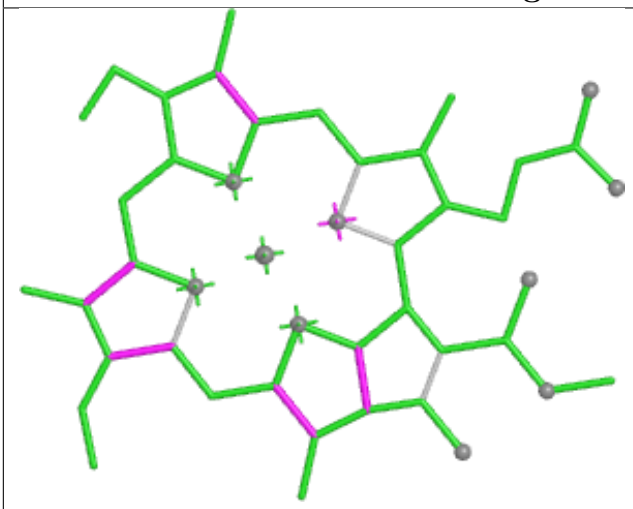


Rings

Ligand BCR I 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA P 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 206



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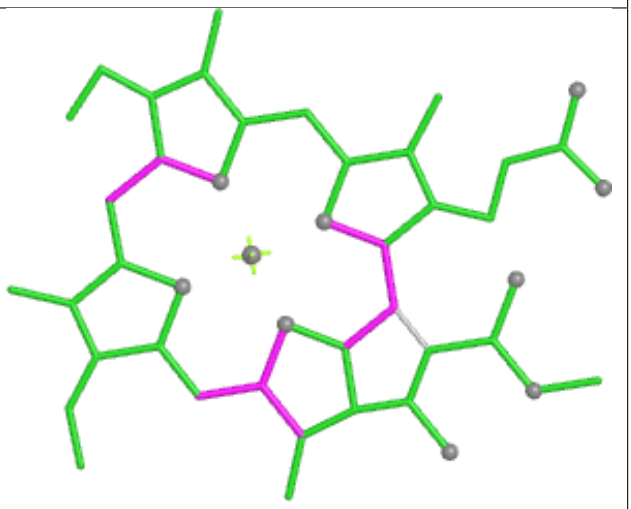
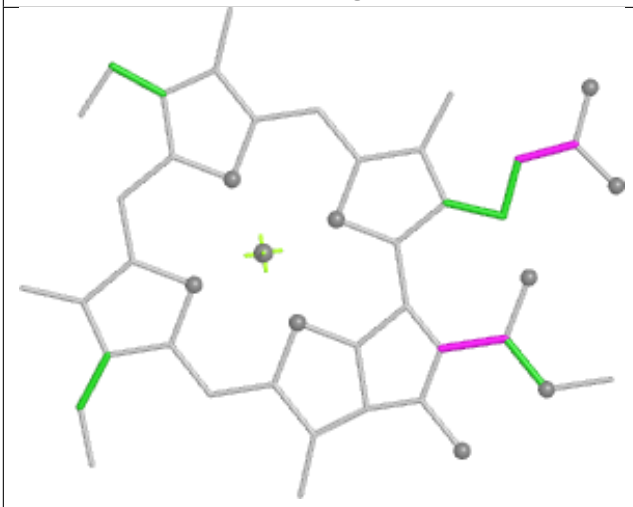


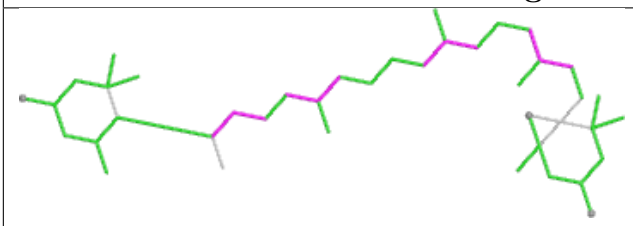
Bond angles



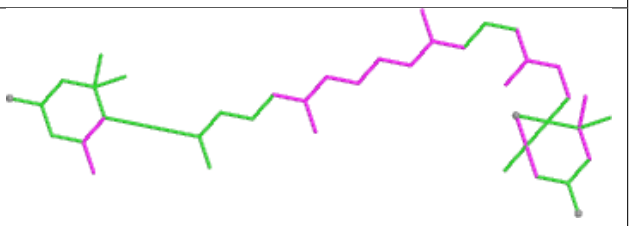
Torsions

Rings

Ligand DD6 O 215



Bond lengths



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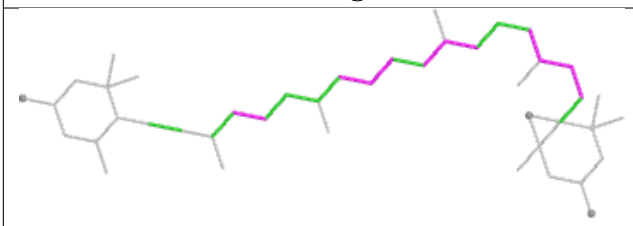

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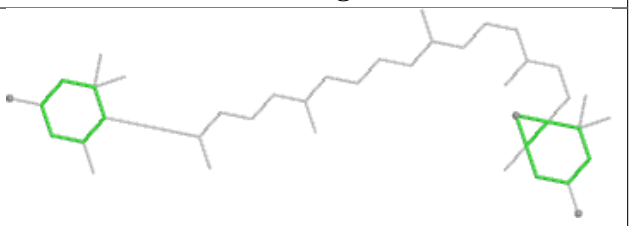
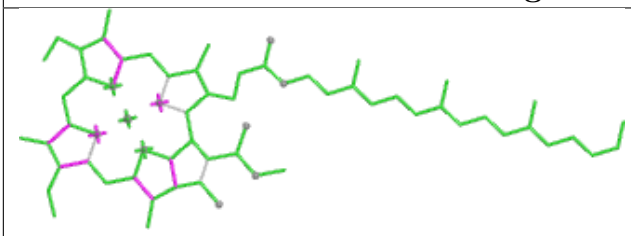
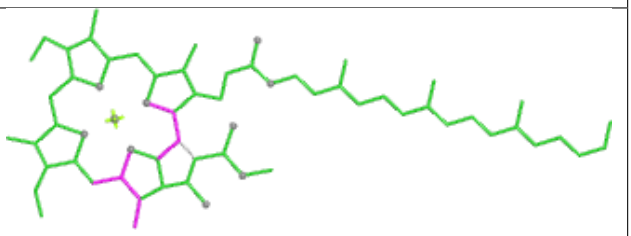
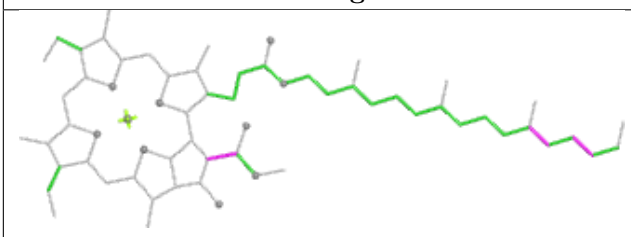
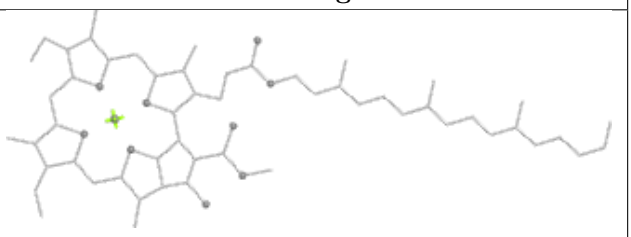
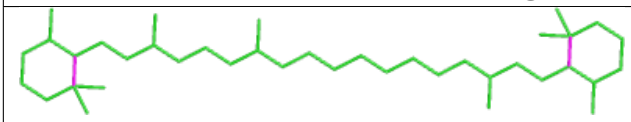
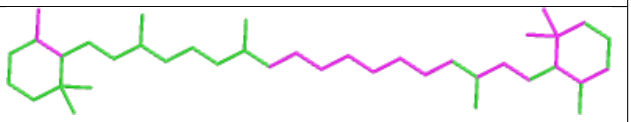
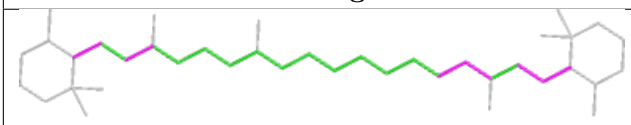
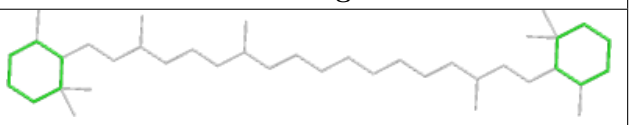
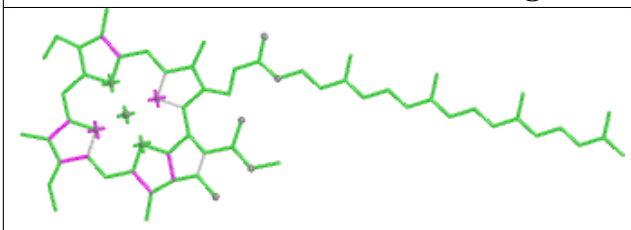
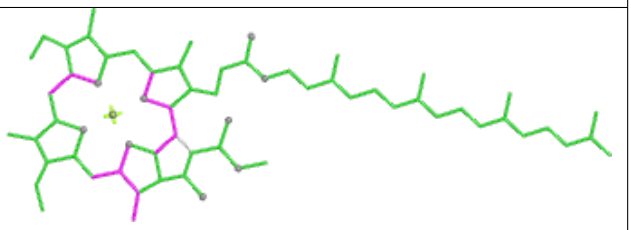
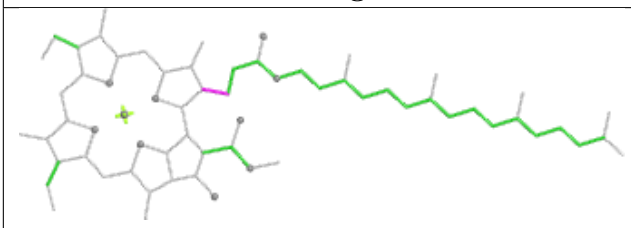
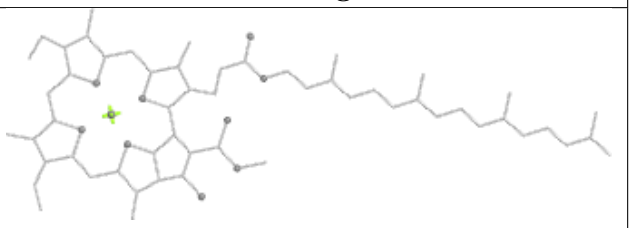
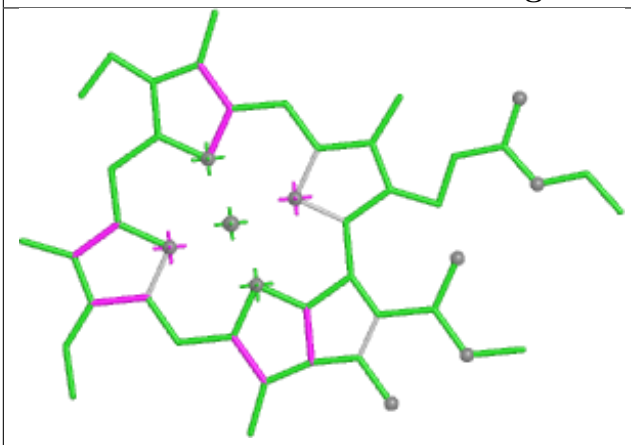
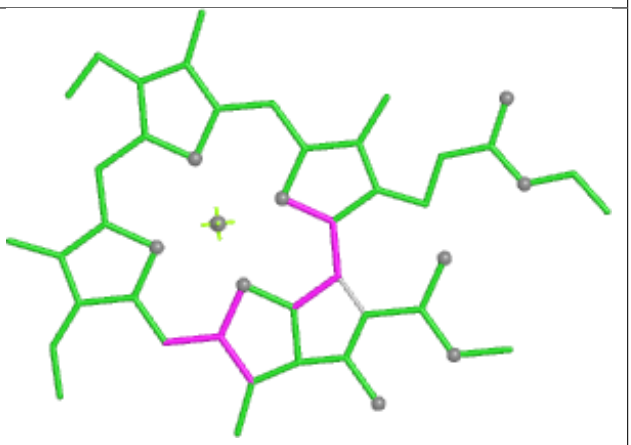


Rings

Ligand CLA B 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR R 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 853	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA P 309	
	
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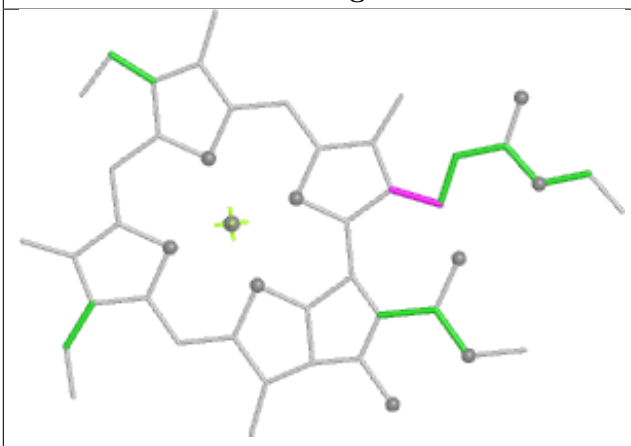
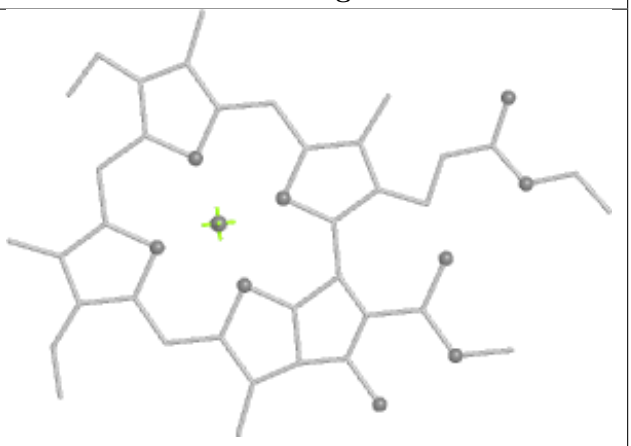
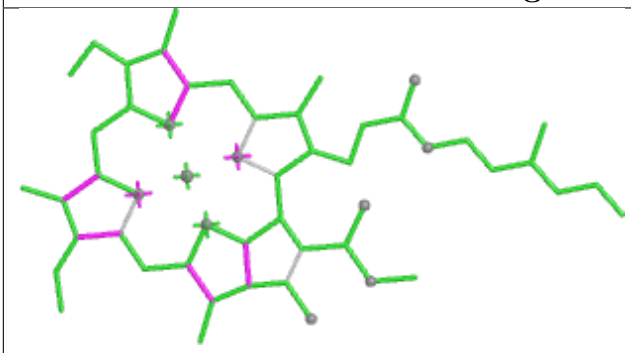
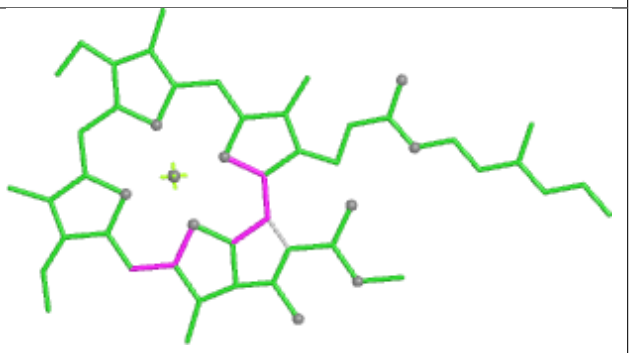
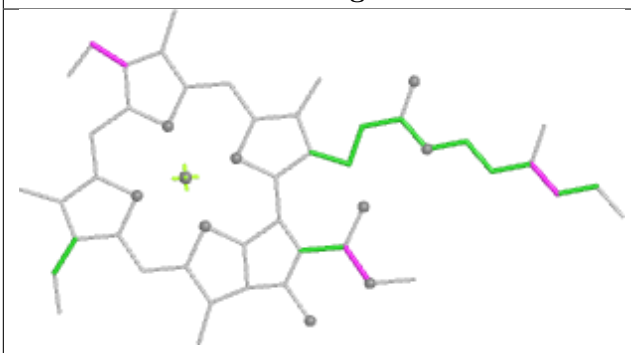
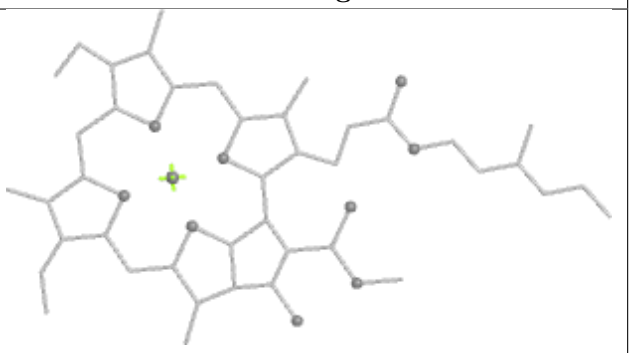
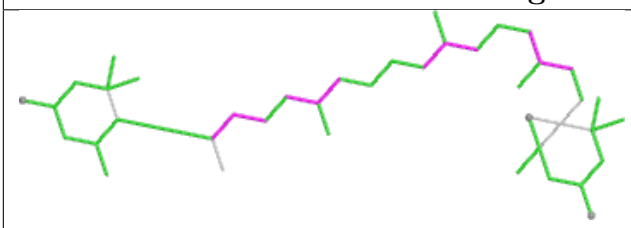
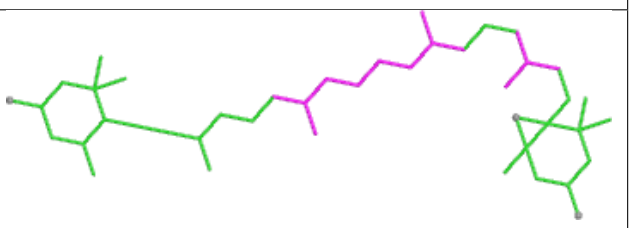
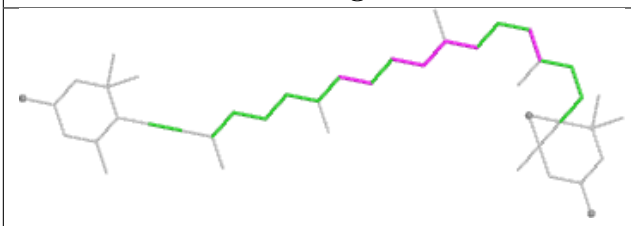
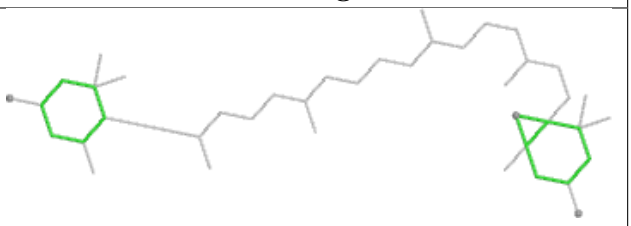
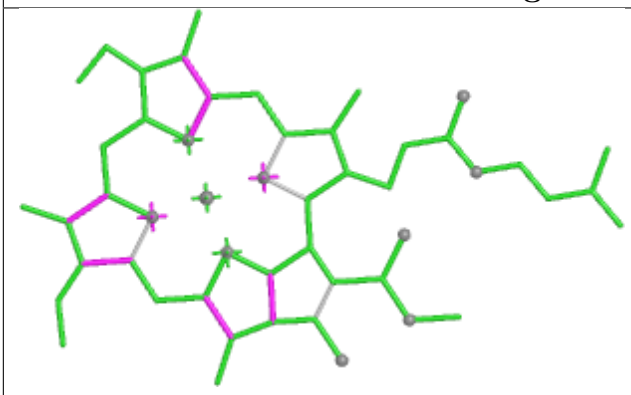
	
Torsions	**Rings**

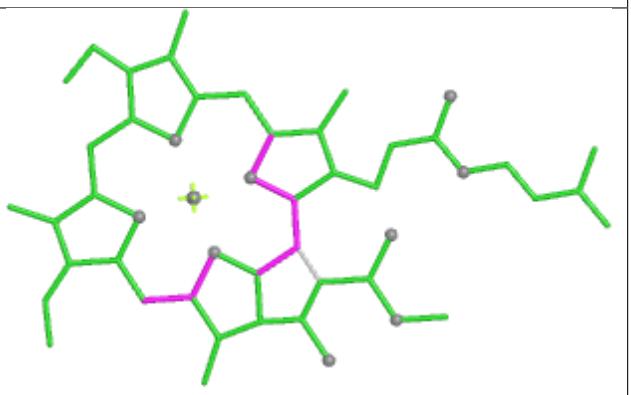
Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 S 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

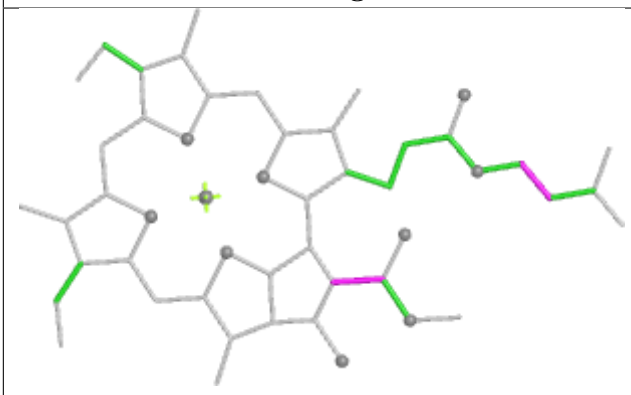
Ligand CLA A 827



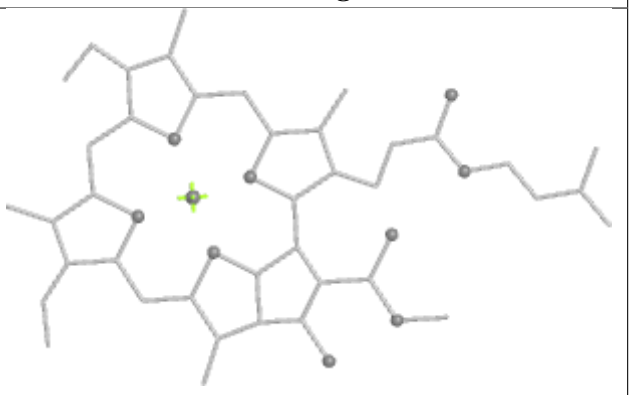
Bond lengths



Bond angles

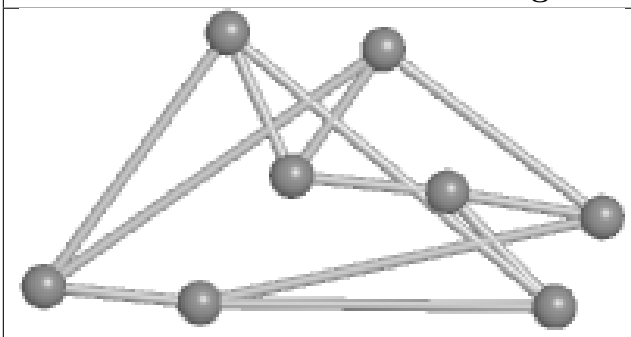


Torsions

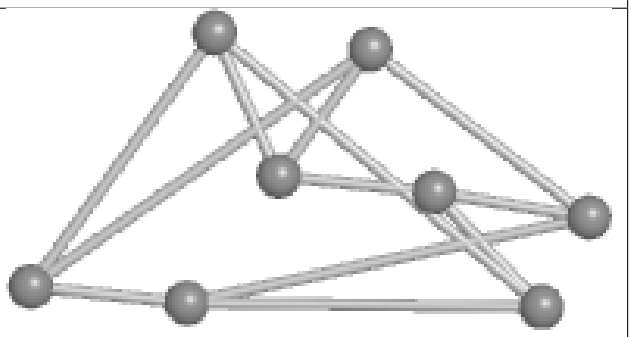


Rings

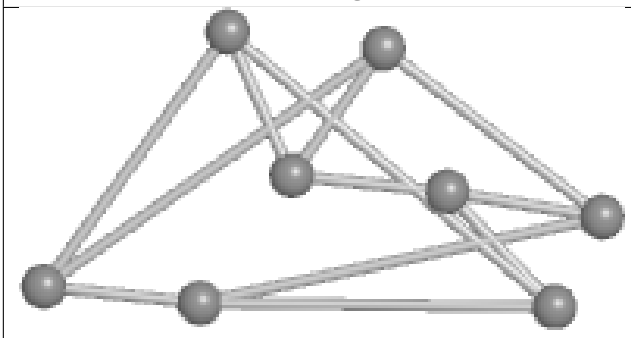
Ligand SF4 C 102



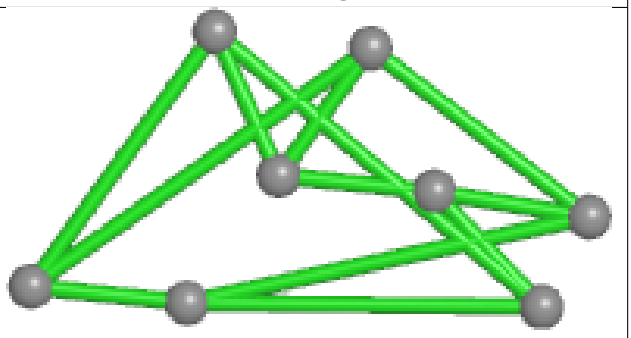
Bond lengths



Bond angles

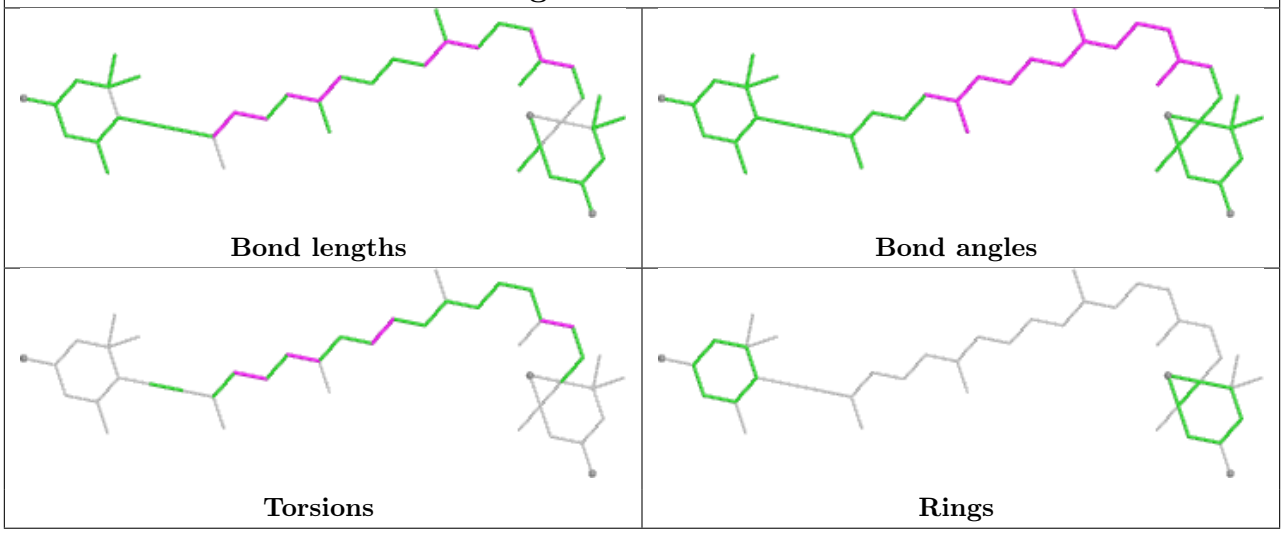


Torsions

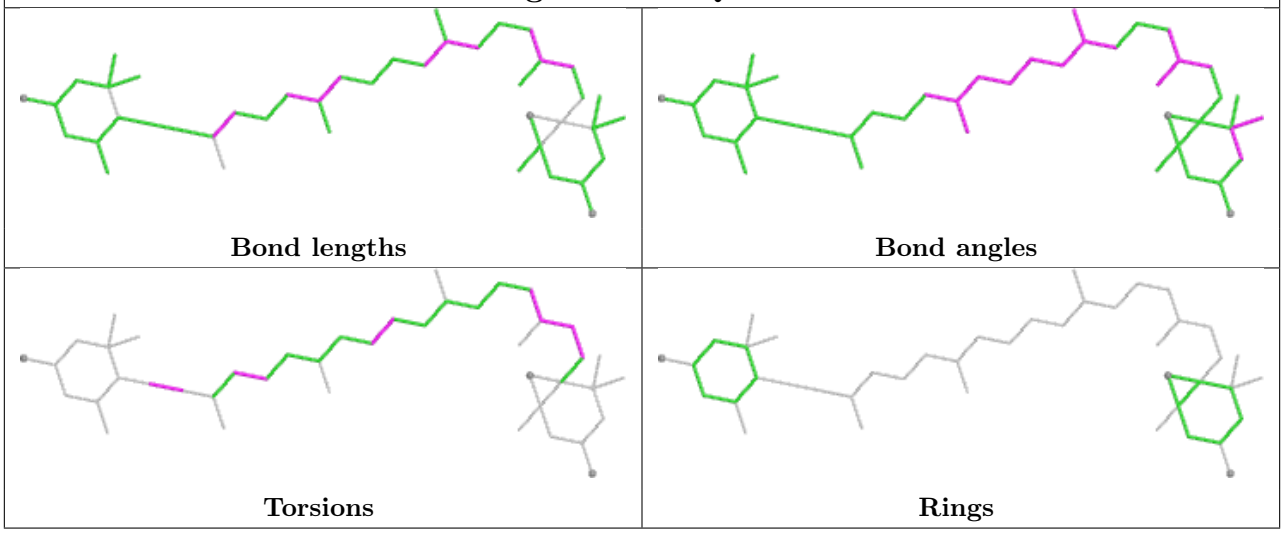


Rings

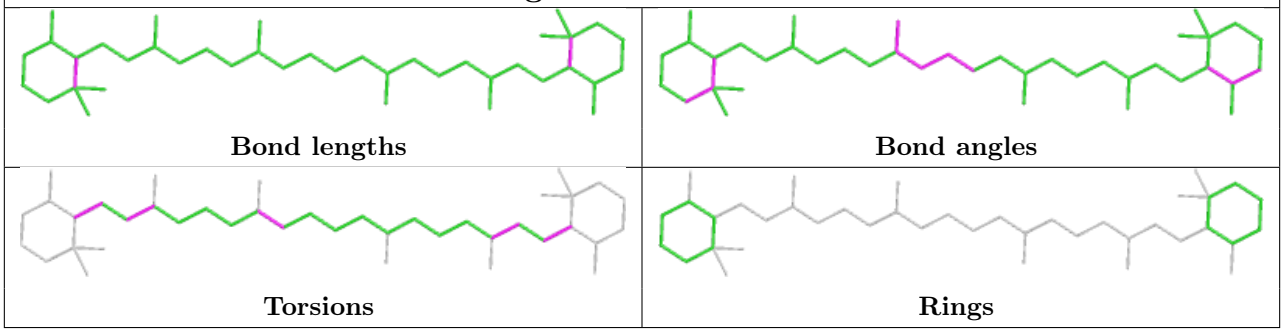
Ligand DD6 J 101

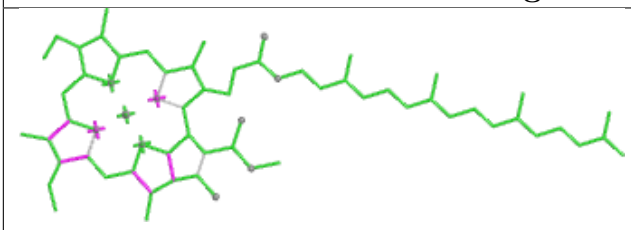
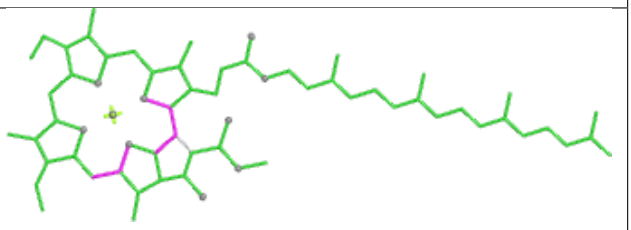
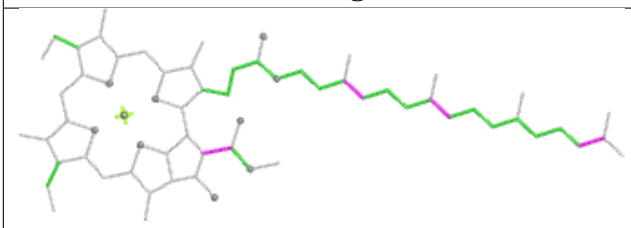
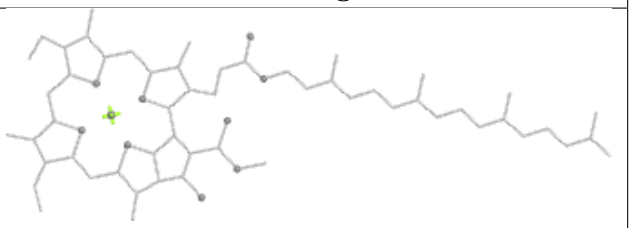


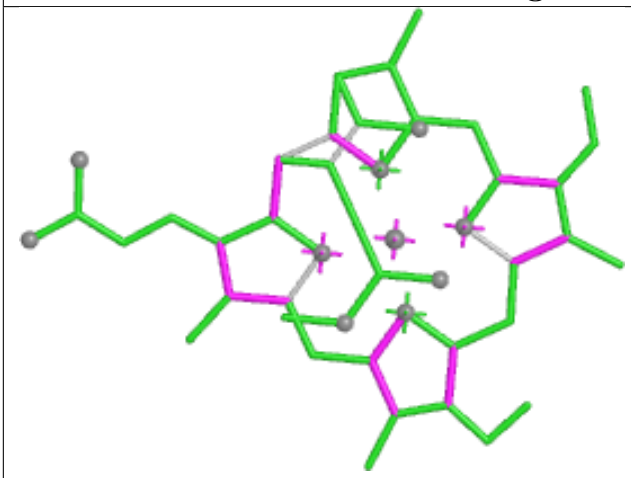
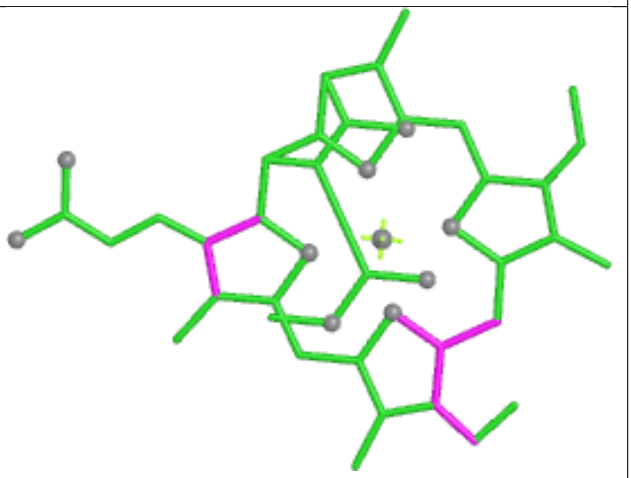
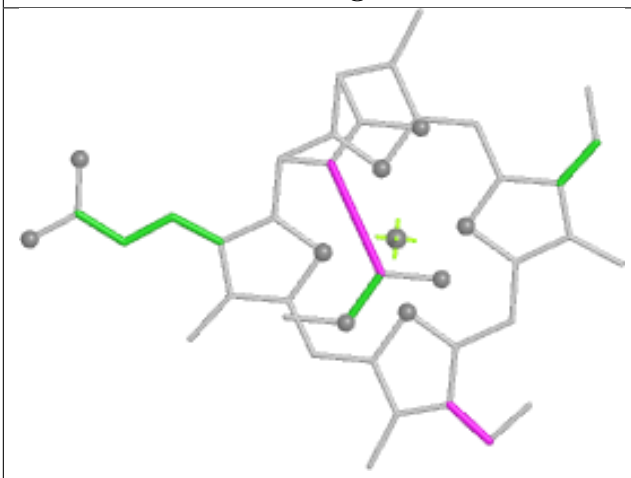
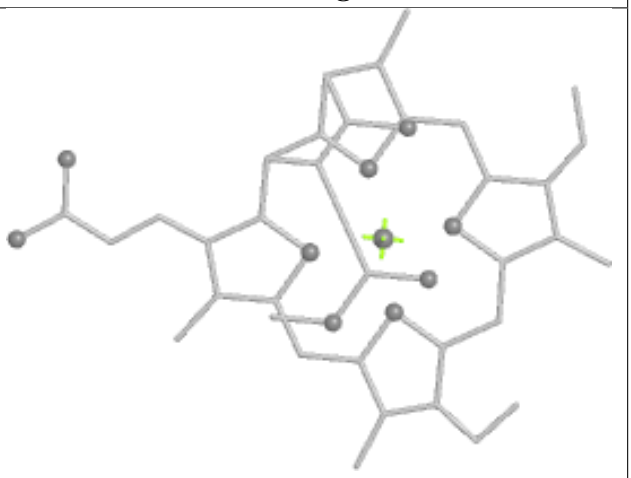
Ligand DD6 Q 215

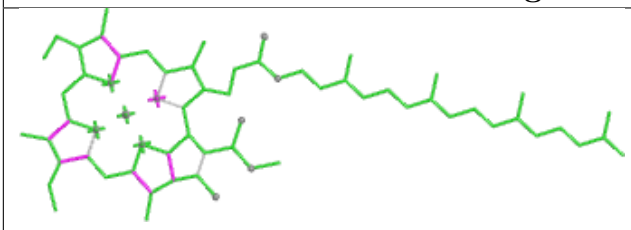
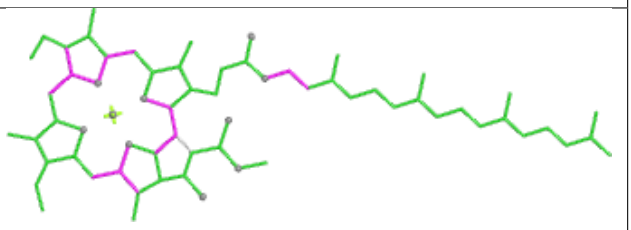
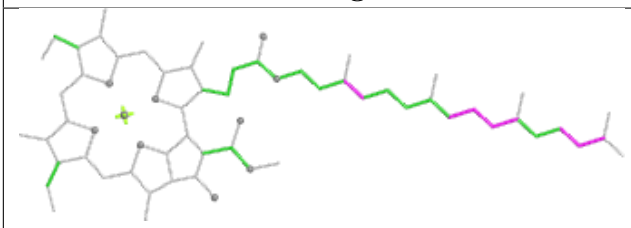
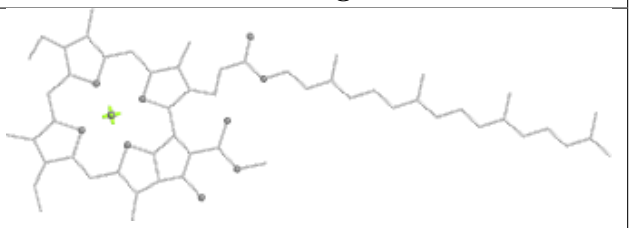


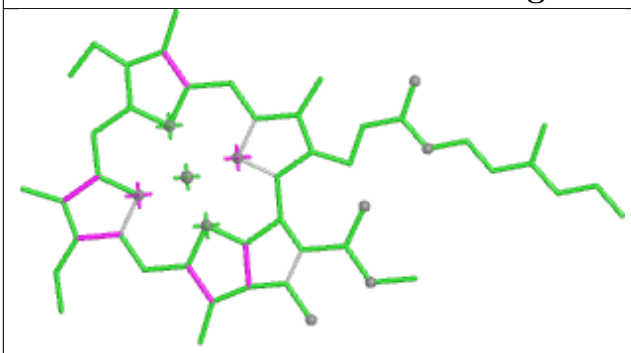
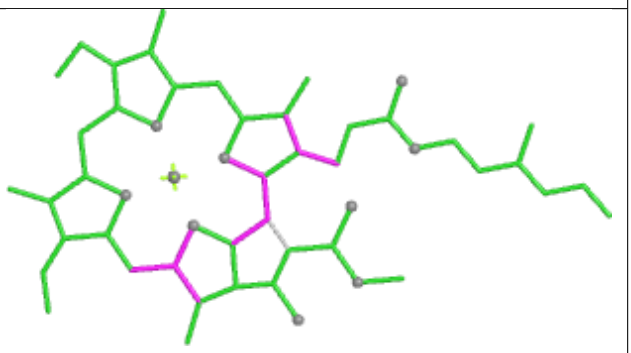
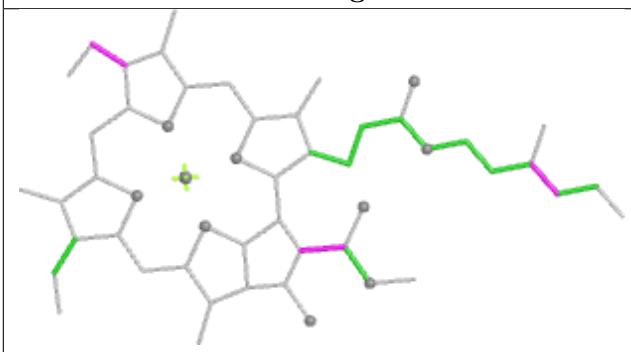
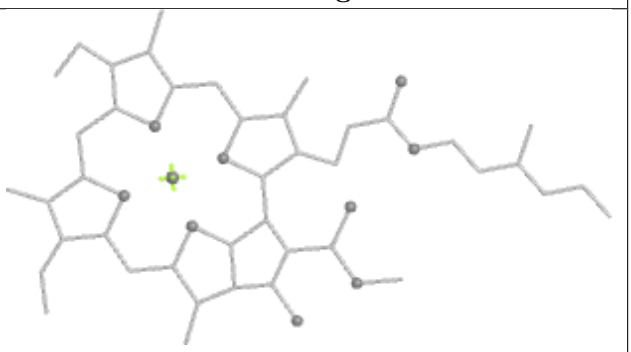
Ligand BCR F 804

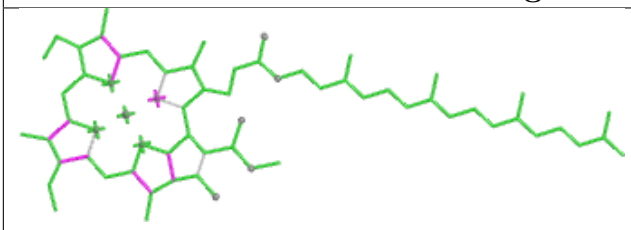
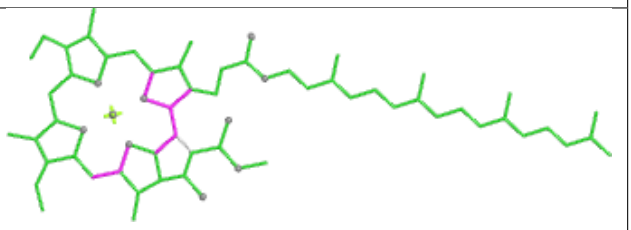
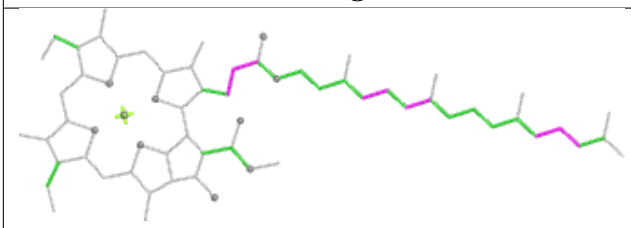
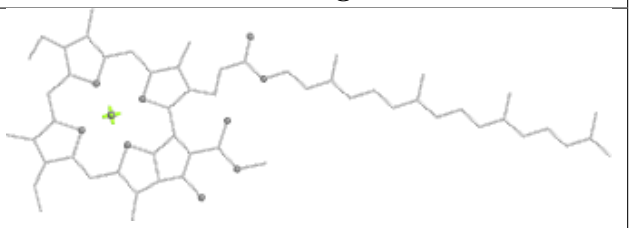


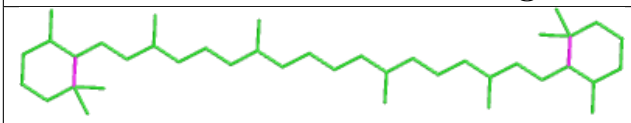
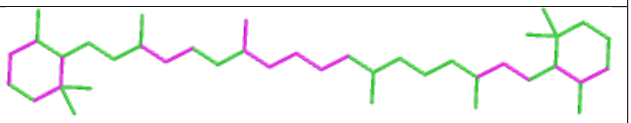
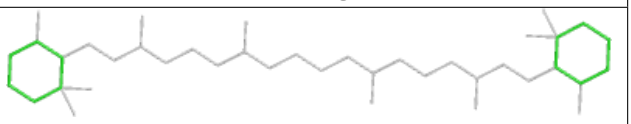
Ligand CLA A 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 T 209	
 Bond lengths	 Bond angles
 Torsions	 Rings

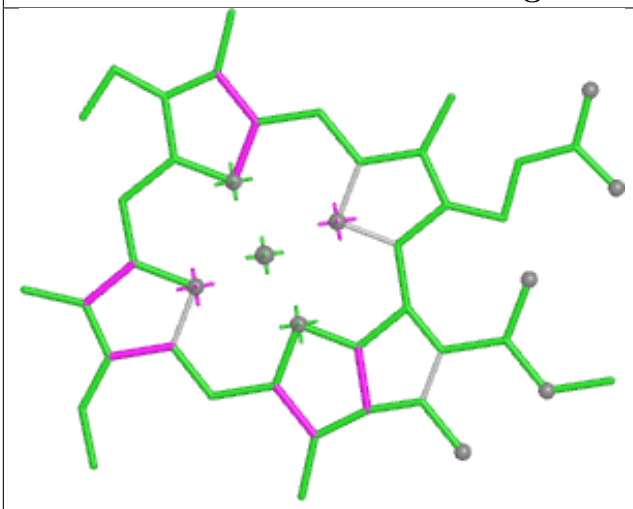
Ligand CLA B 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 207	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR M 101	
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand CLA A 817



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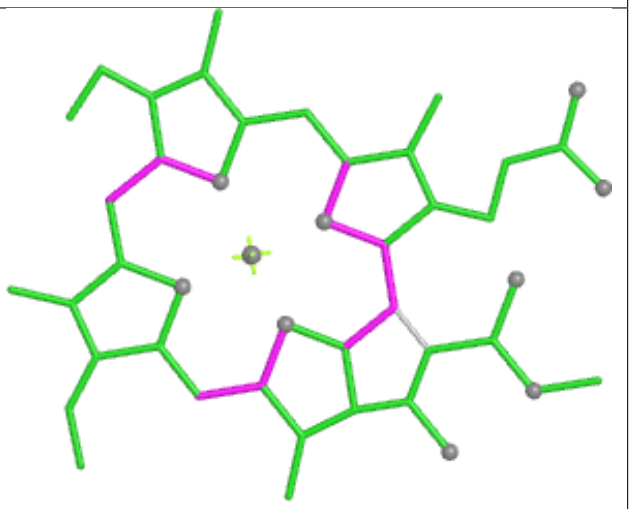

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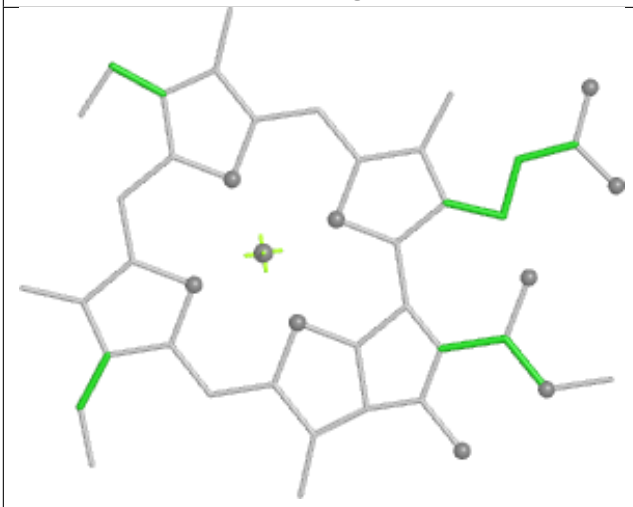
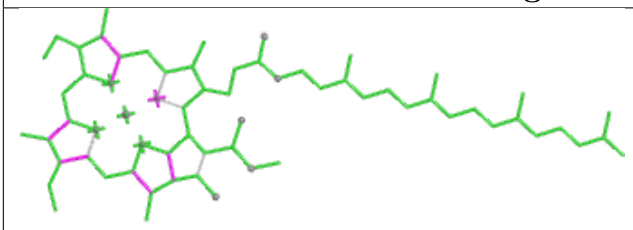


Torsions

Rings

Ligand CLA O 209



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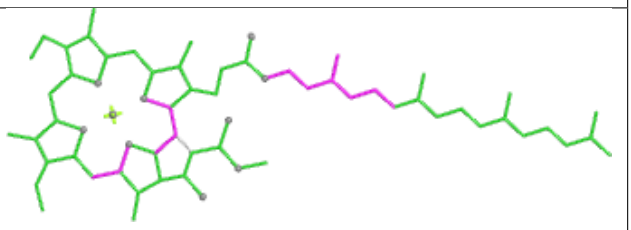

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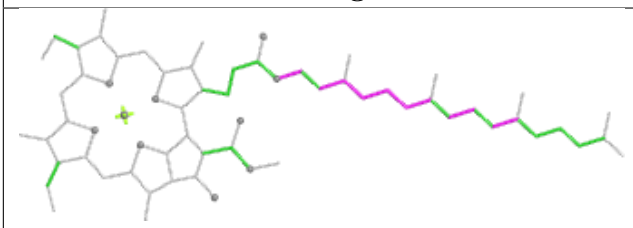

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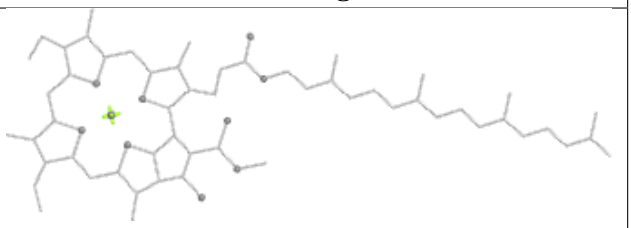
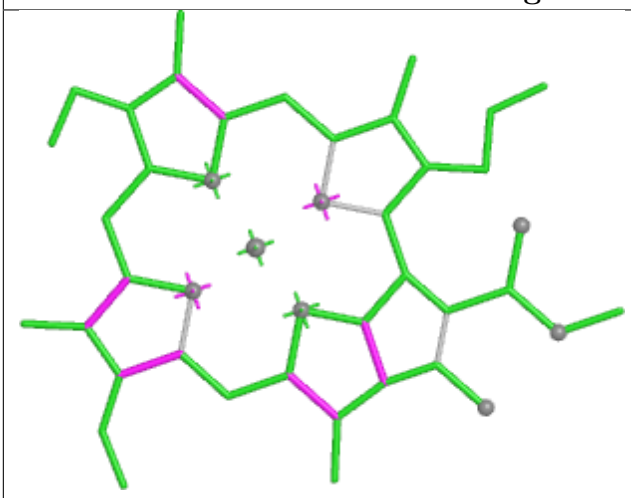


Rings

Ligand CLA O 202



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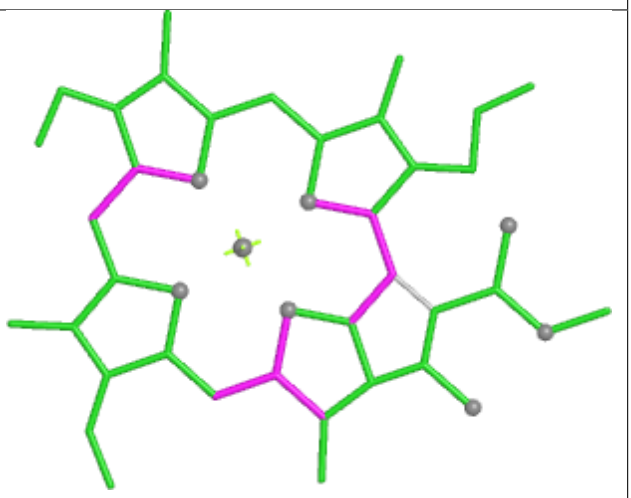

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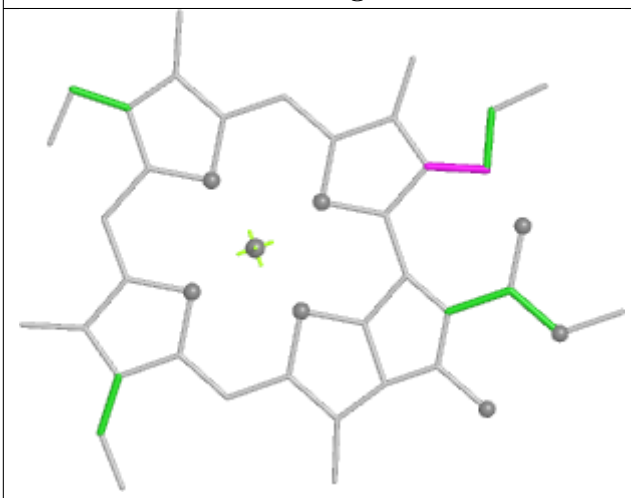

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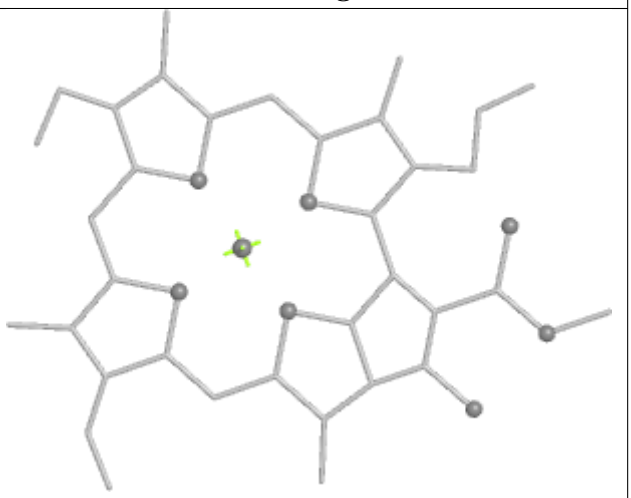
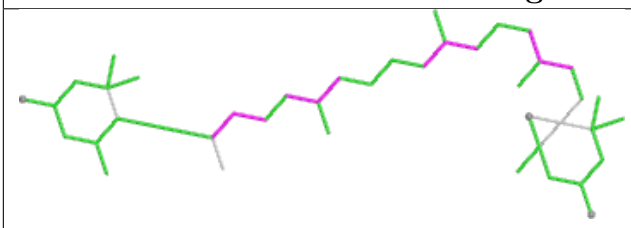


Rings

Ligand DD6 P 304



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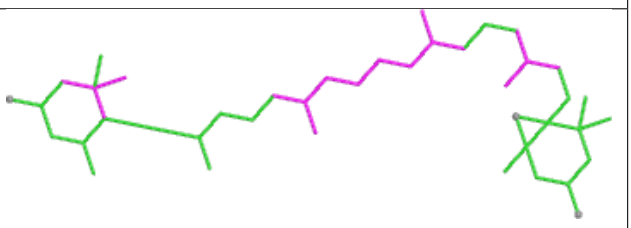

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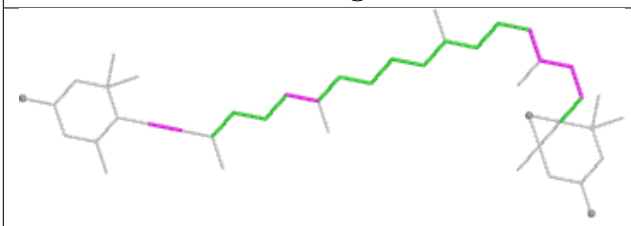

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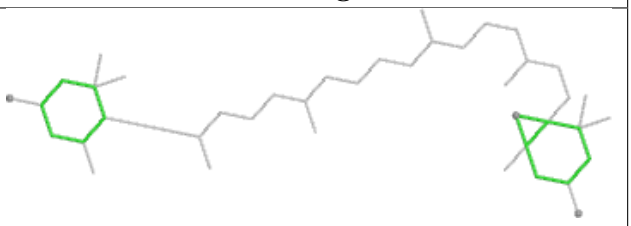
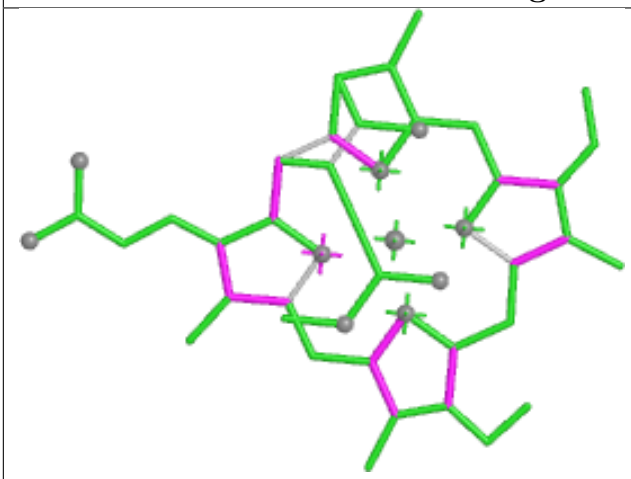


Rings

Ligand KC1 S 208



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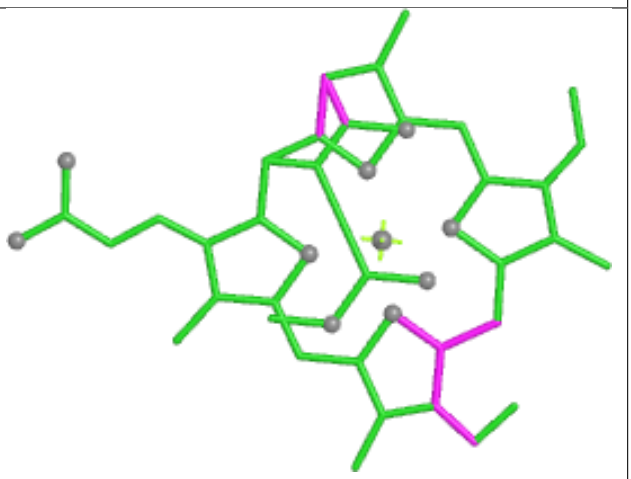

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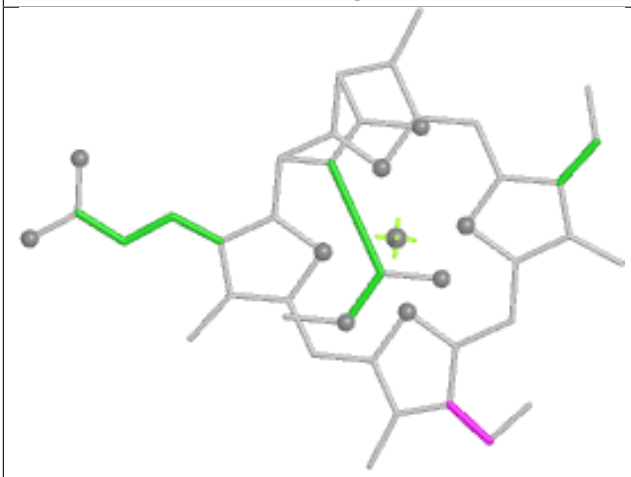

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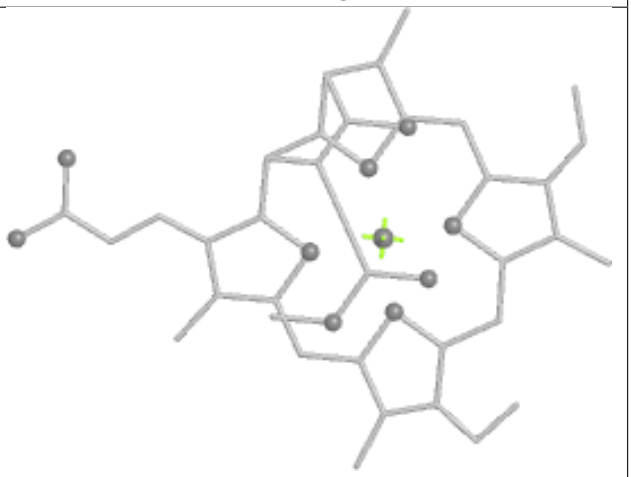
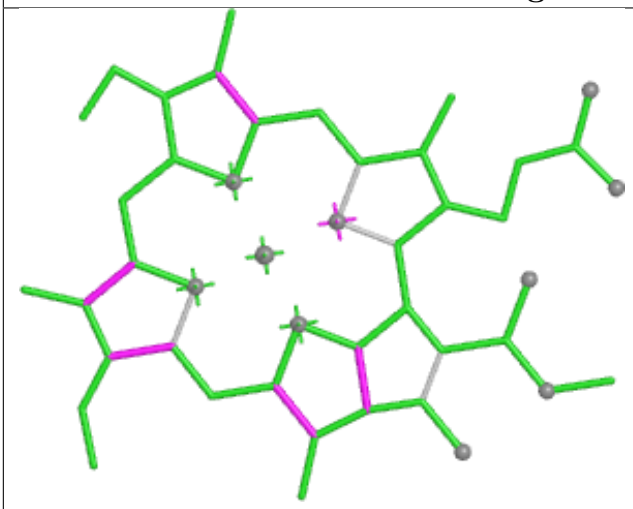


Rings

Ligand CLA S 206



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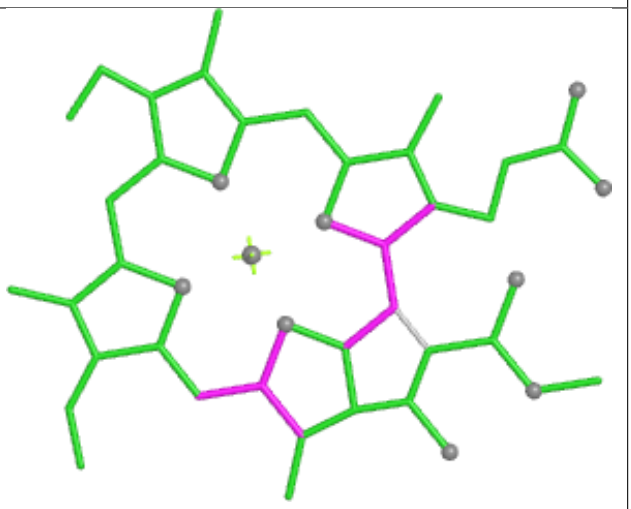

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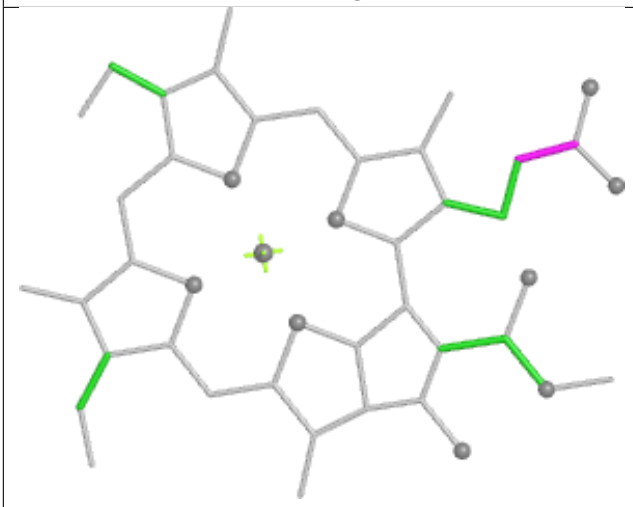
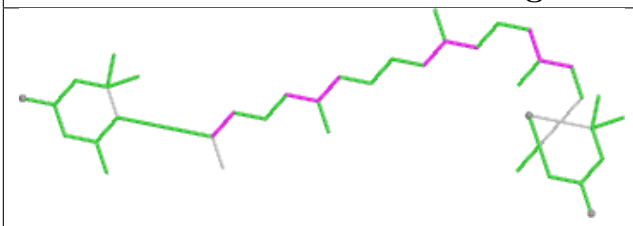


Torsions

Rings

Ligand DD6 T 214



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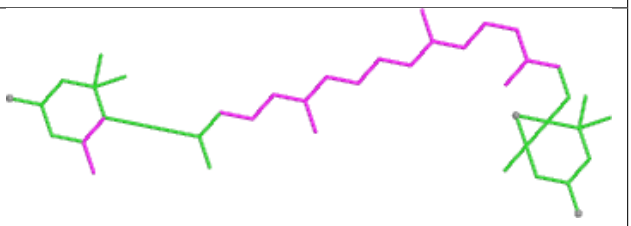

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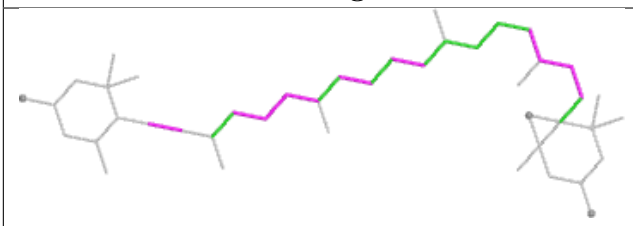

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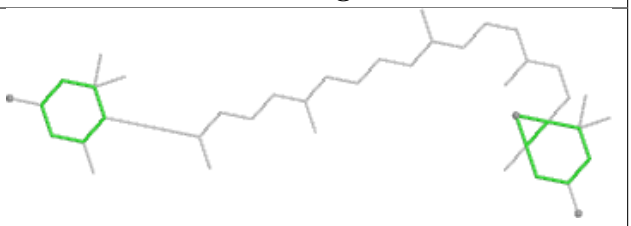
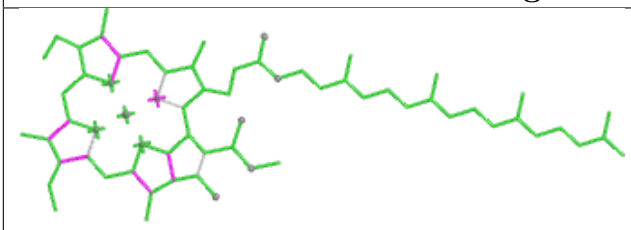


Rings

Ligand CLA U 205



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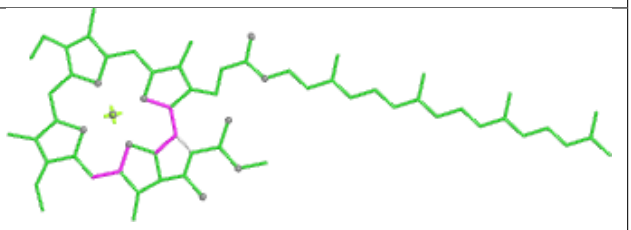

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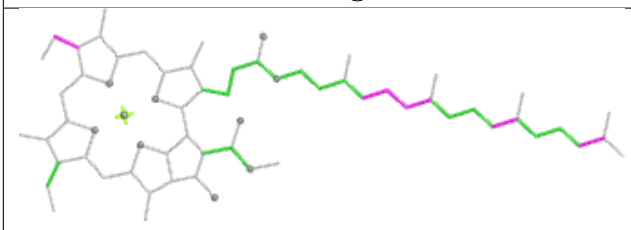

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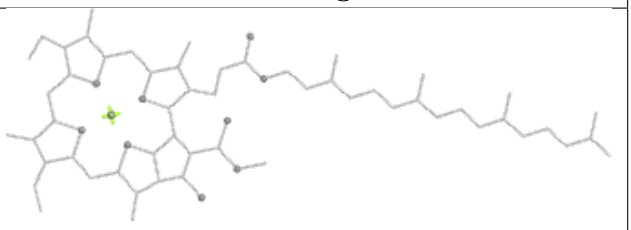
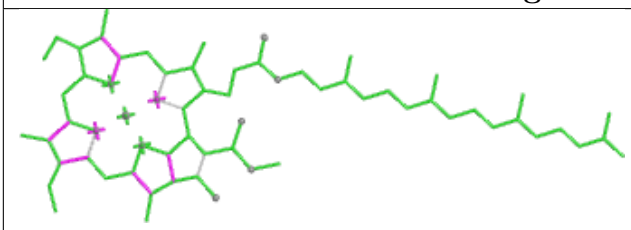


Rings

Ligand CLA A 804



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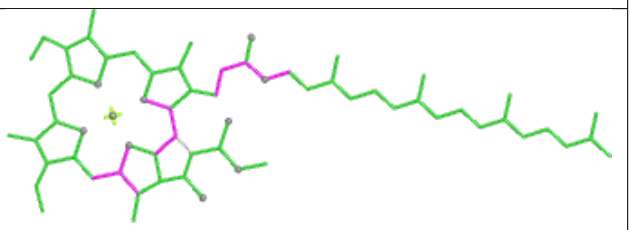

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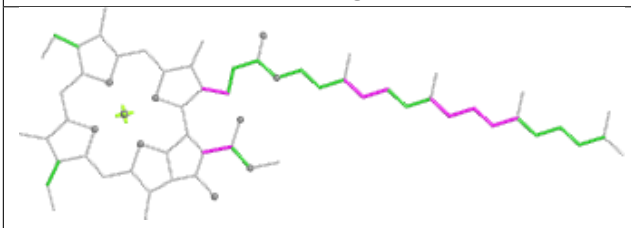

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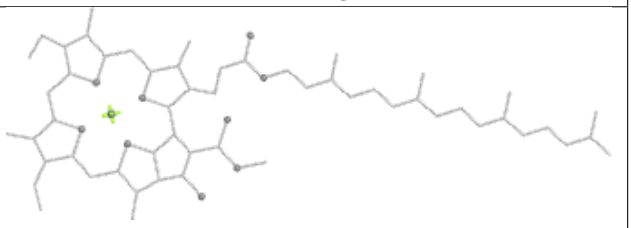
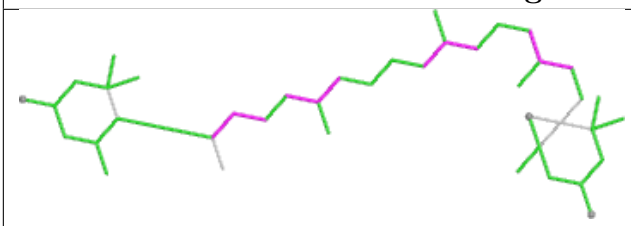


Rings

Ligand DD6 Q 202



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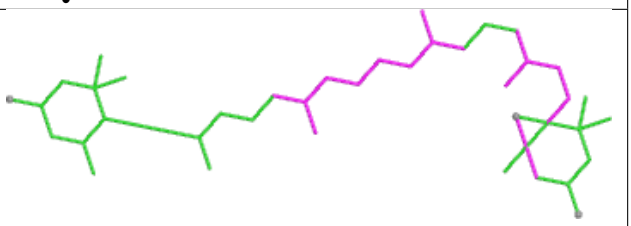
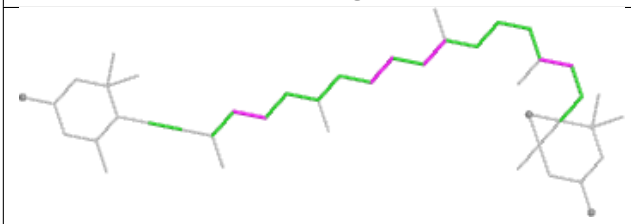


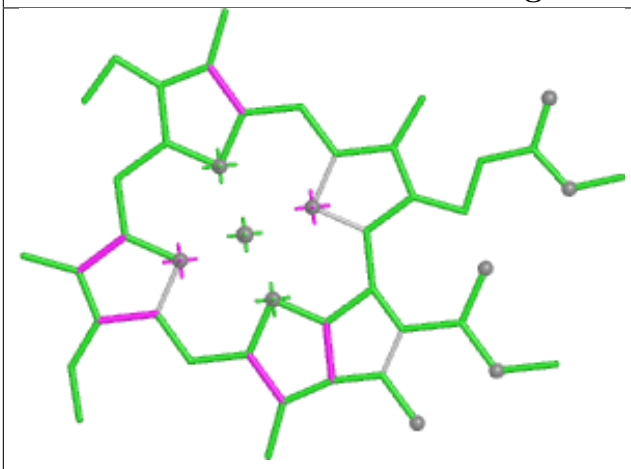
Bond angles



Torsions

Rings

Ligand CLA T 204



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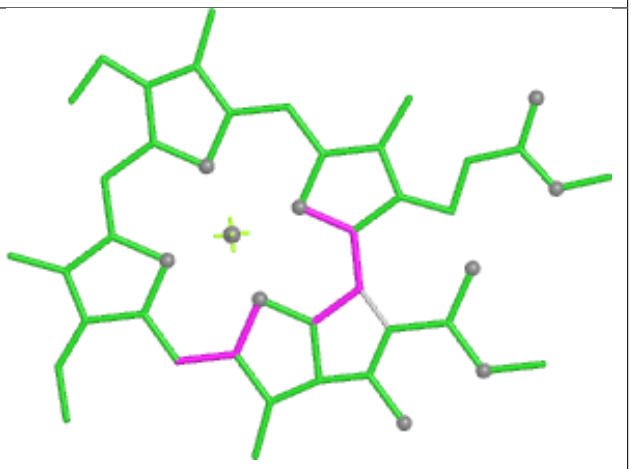
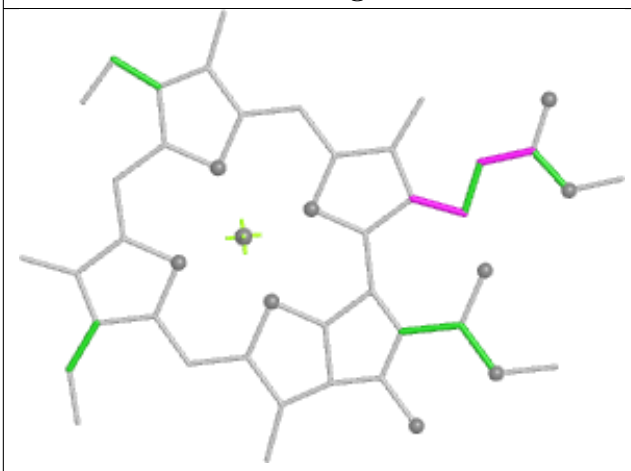


Bond angles



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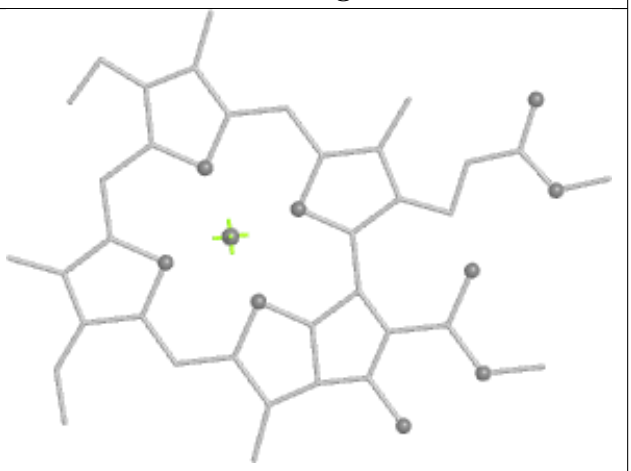
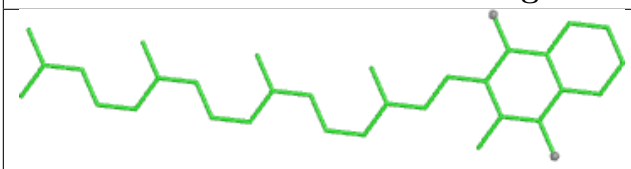


Rings

Ligand PQN A 837



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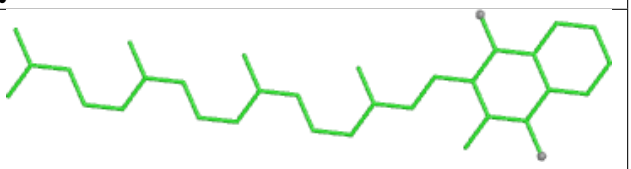
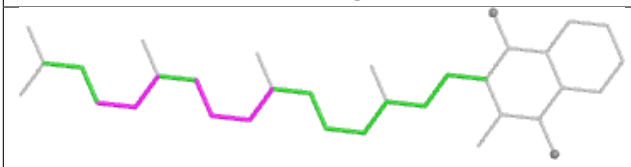


Bond angles



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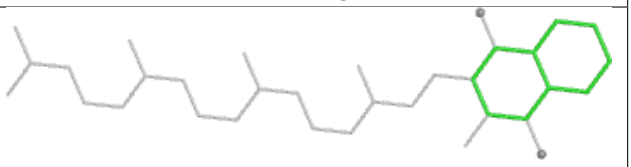
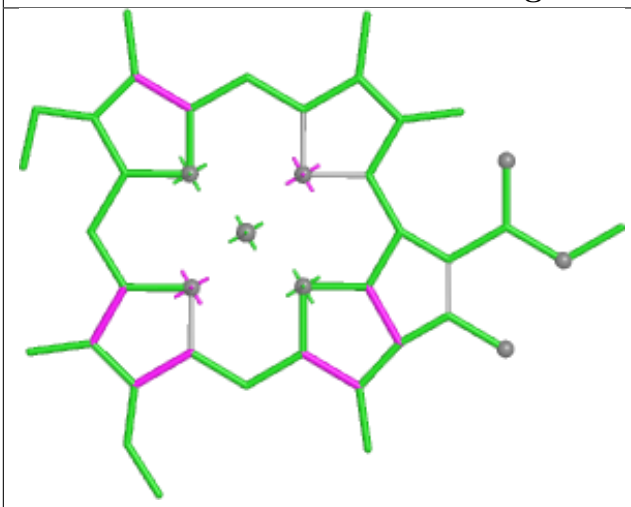
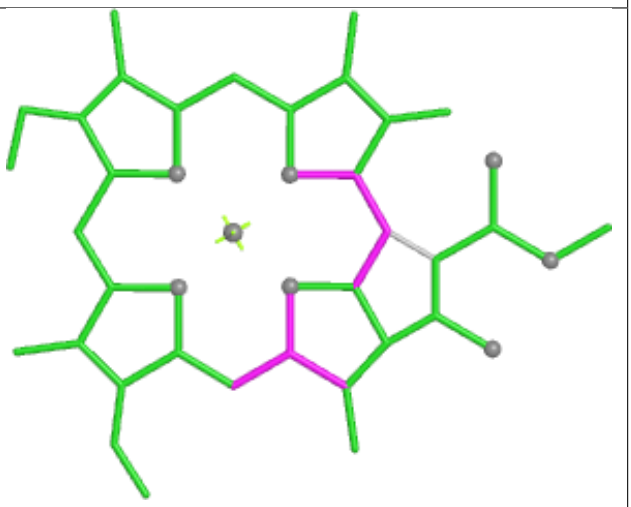


Rings

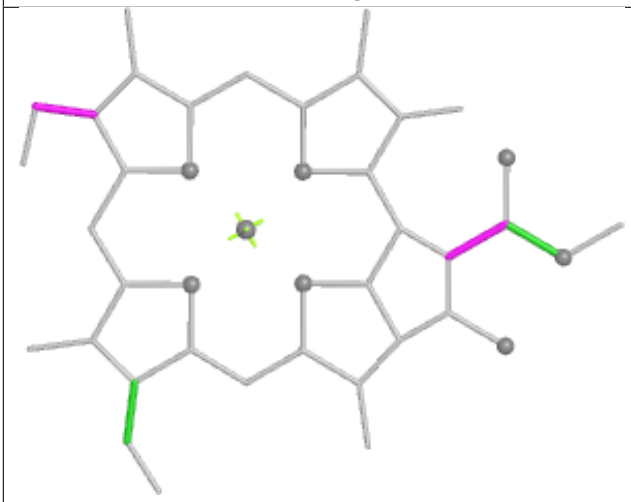
Ligand CLA T 203



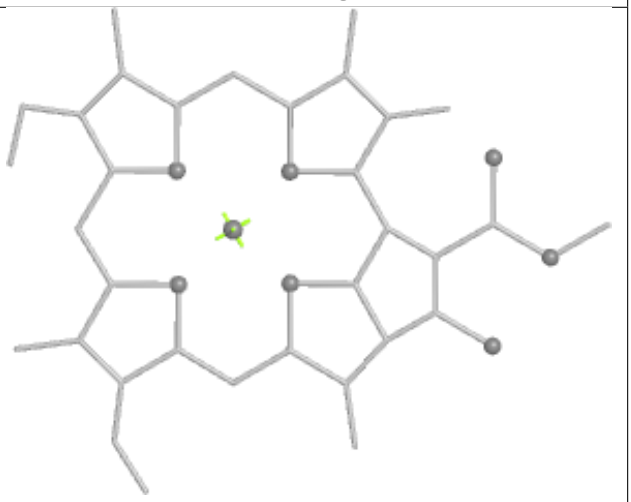
Bond lengths



Bond angles

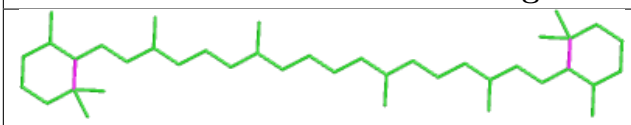


Torsions

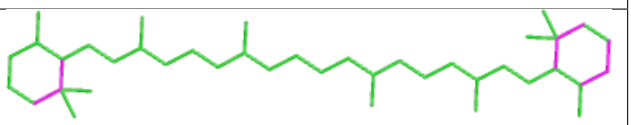


Rings

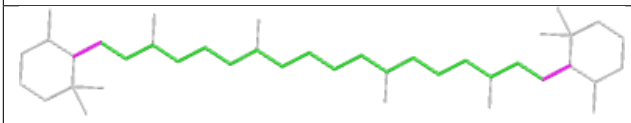
Ligand BCR A 843



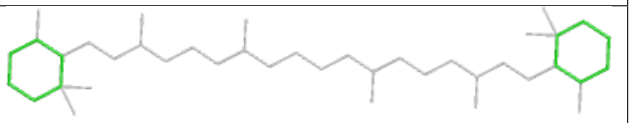
Bond lengths



Bond angles

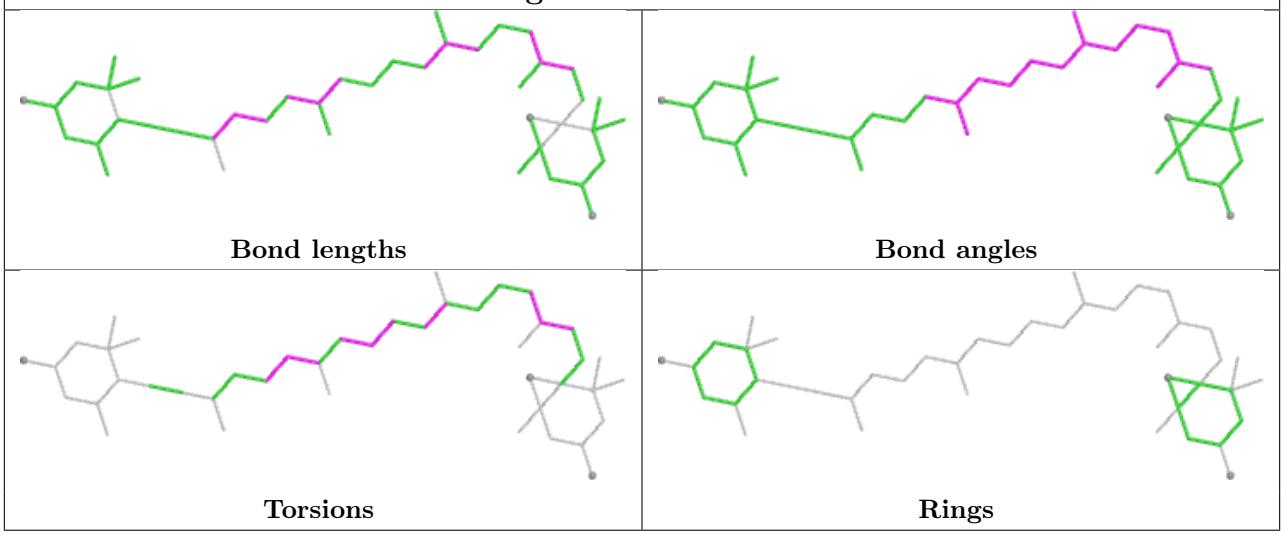


Torsions

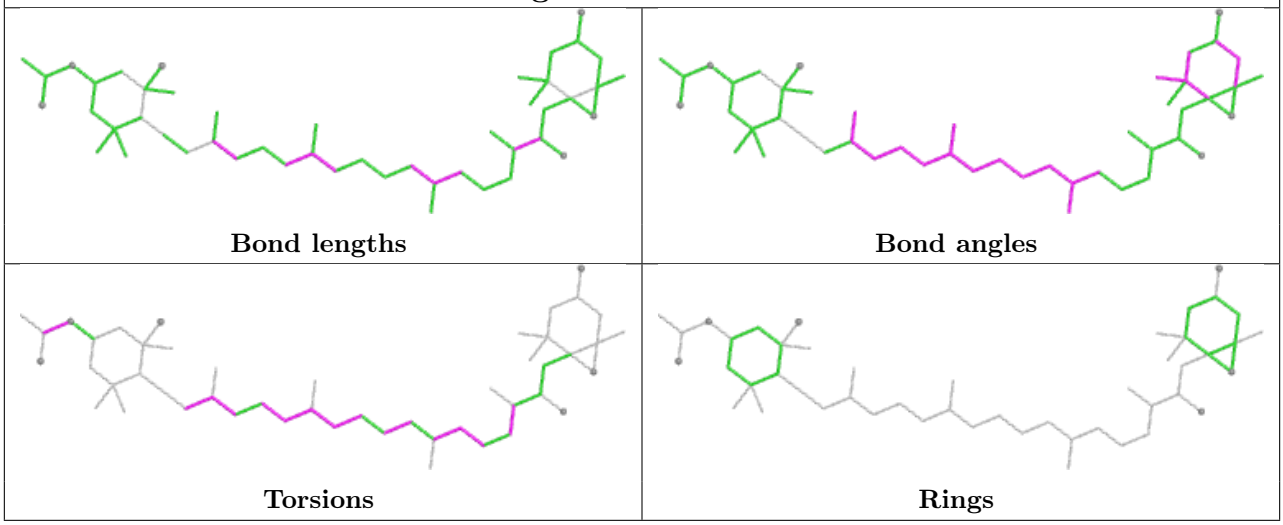


Rings

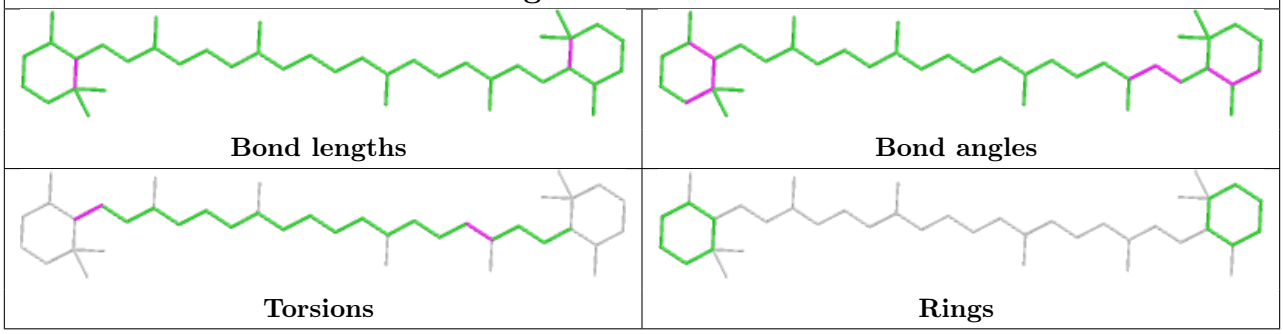
Ligand DD6 O 212



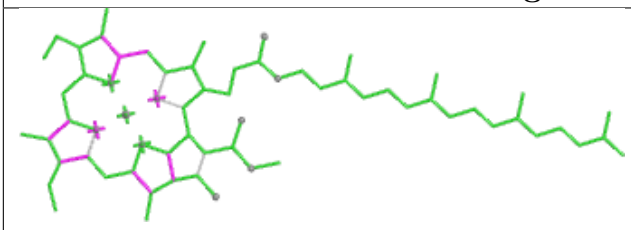
Ligand A86 T 201



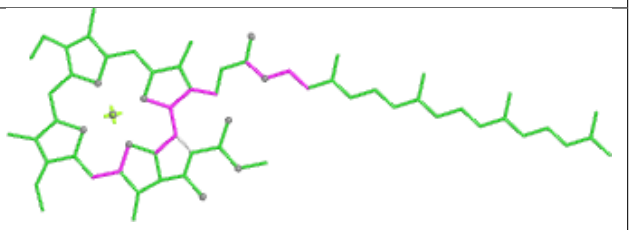
Ligand BCR B 839



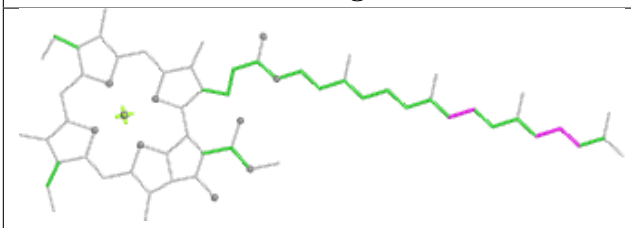
Ligand CLA A 836



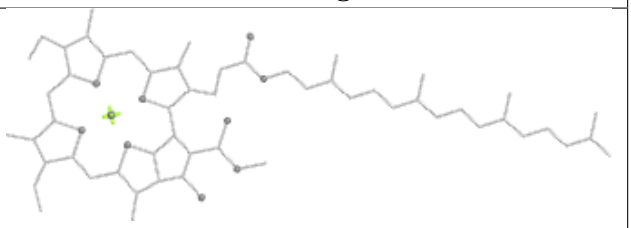
Bond lengths



Bond angles

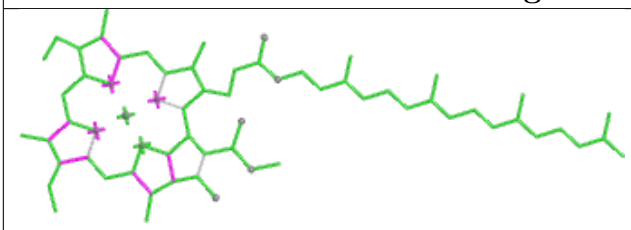


Torsions

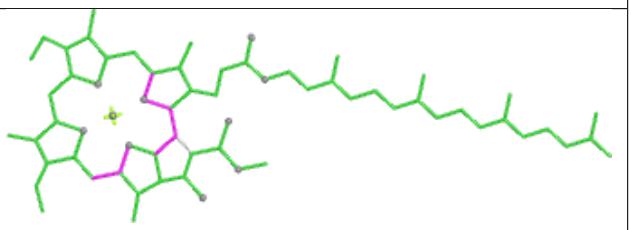


Rings

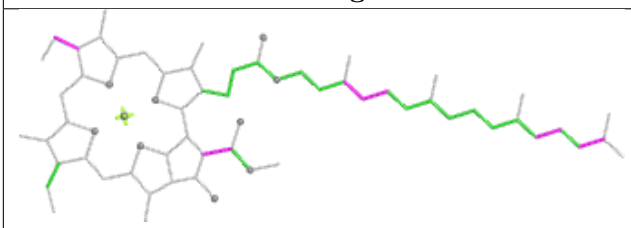
Ligand CLA A 834



Bond lengths



Bond angles



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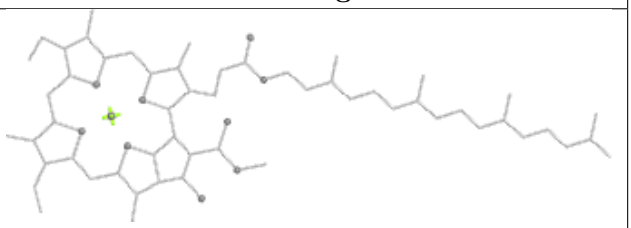
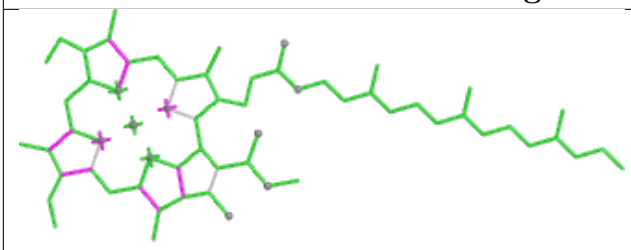
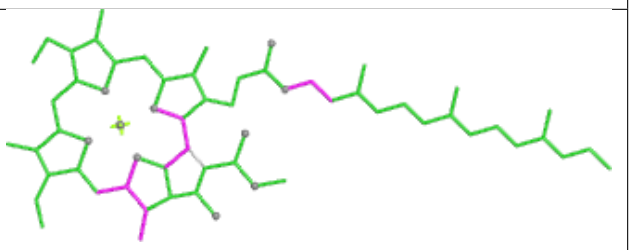


Rings

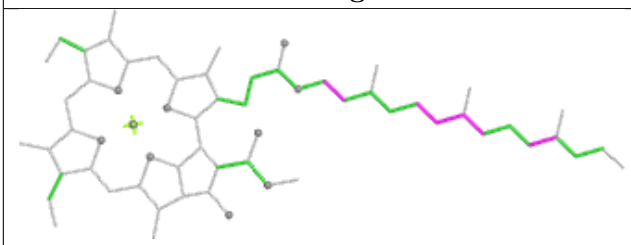
Ligand CLA A 824



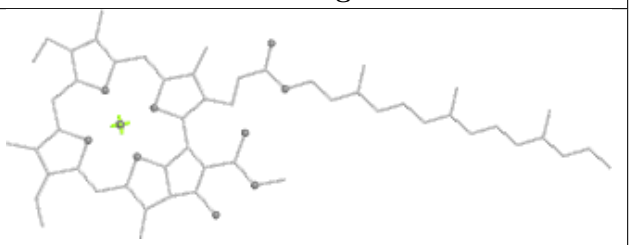
Bond lengths



Bond angles

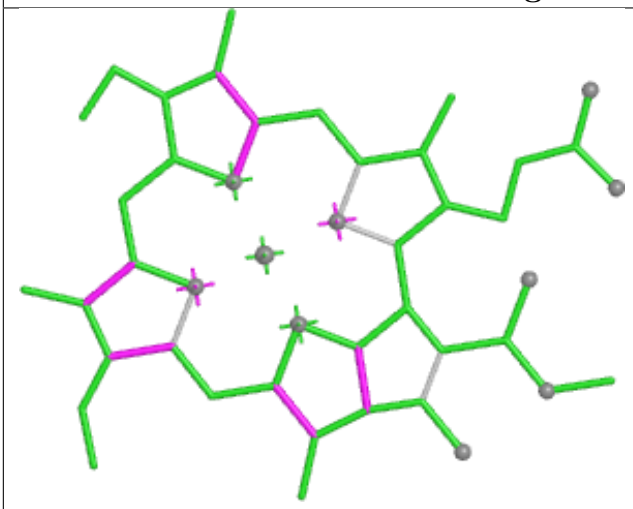


Torsions

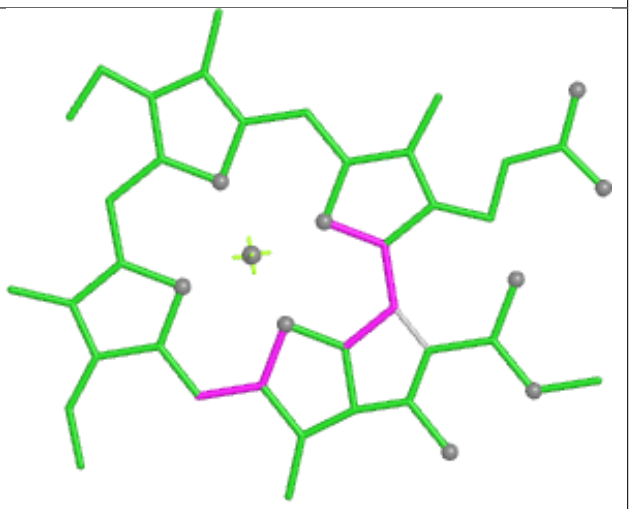


Rings

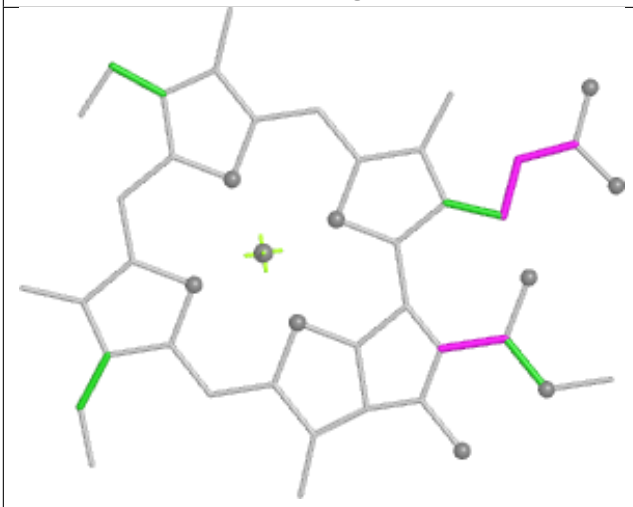
Ligand CLA B 804



Bond lengths



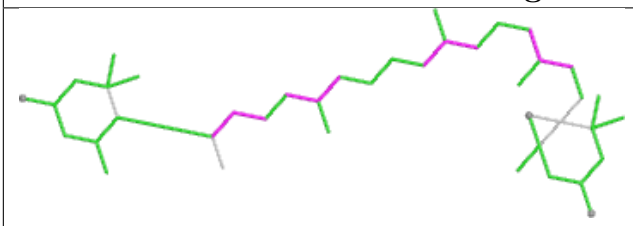
Bond angles



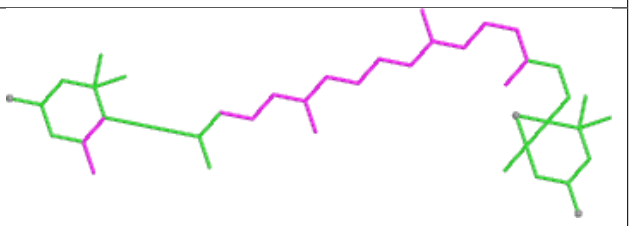
Torsions

Rings

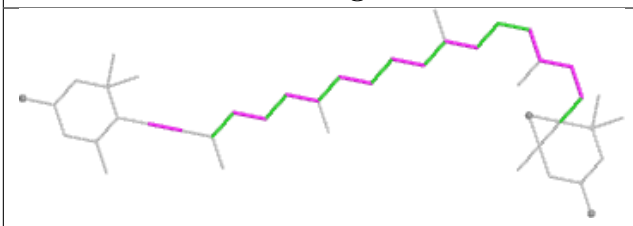
Ligand DD6 A 854



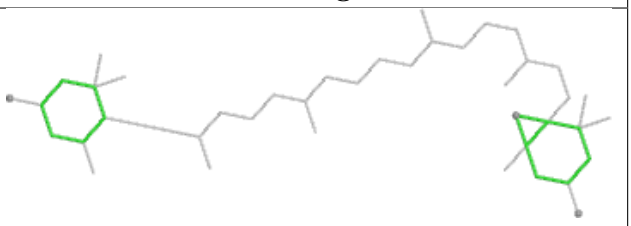
Bond lengths



Bond angles

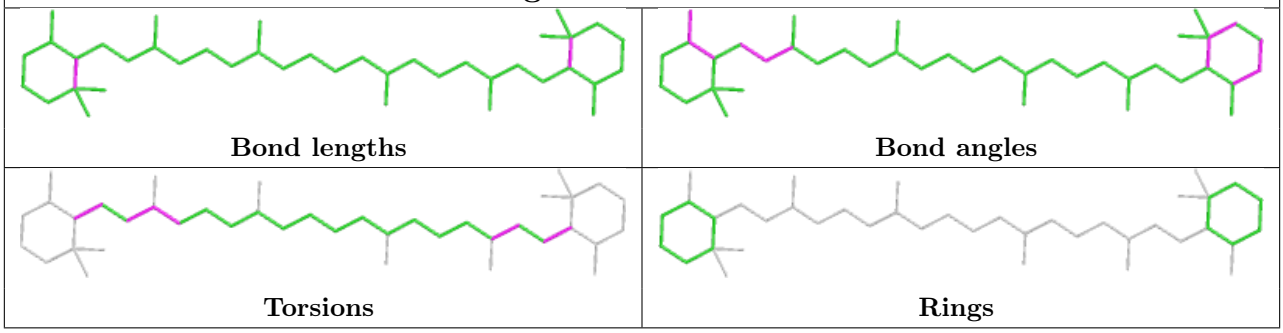


Torsions

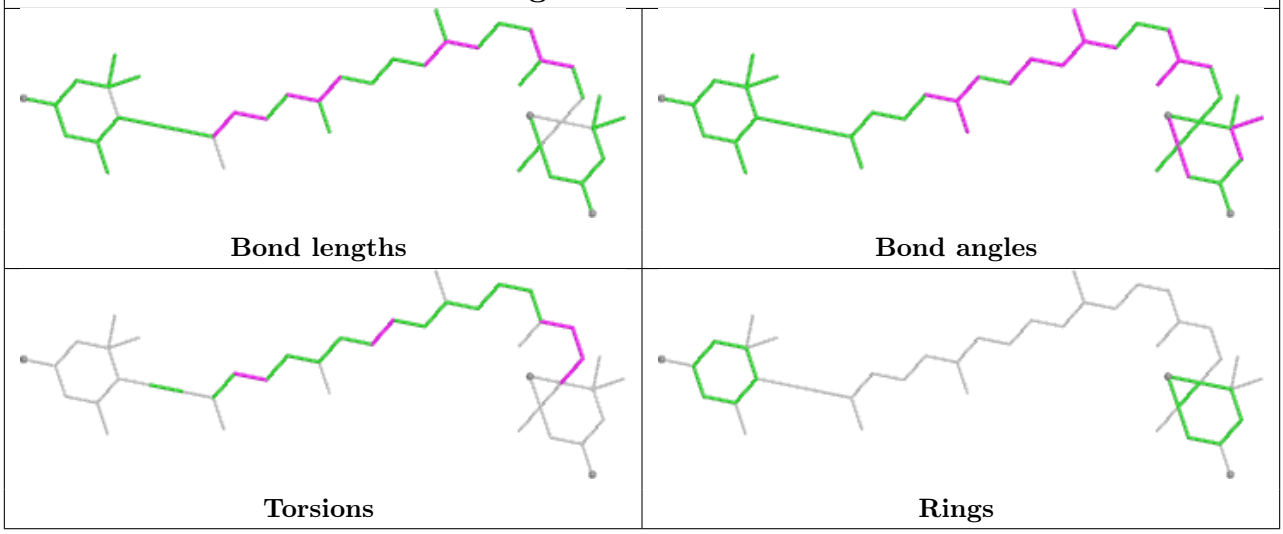


Rings

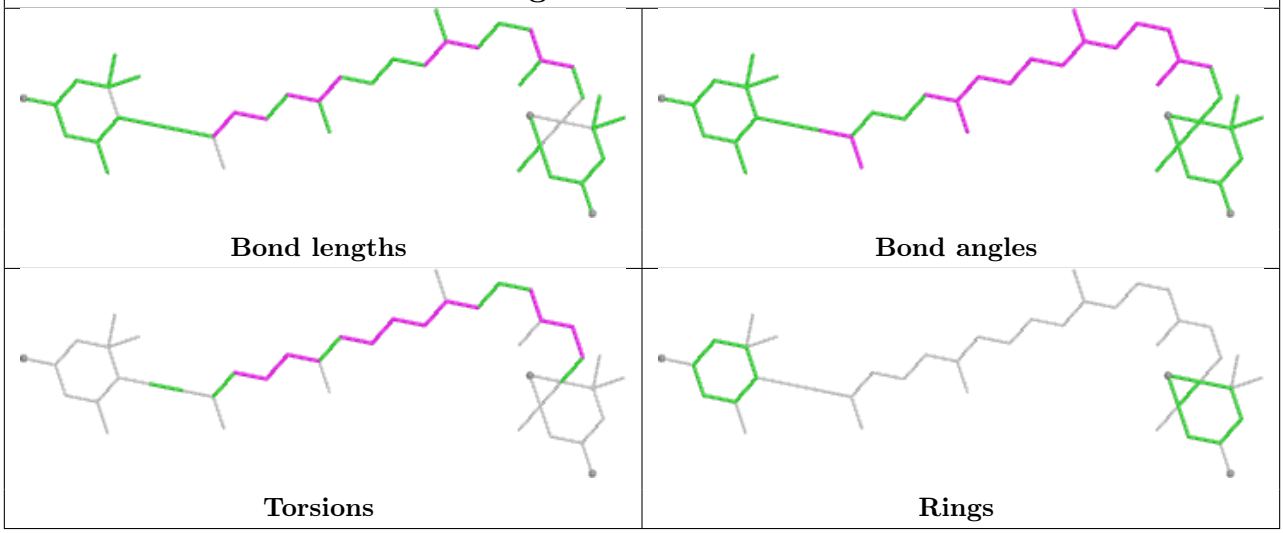
Ligand BCR B 837

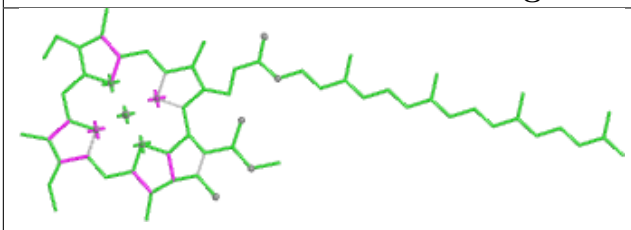
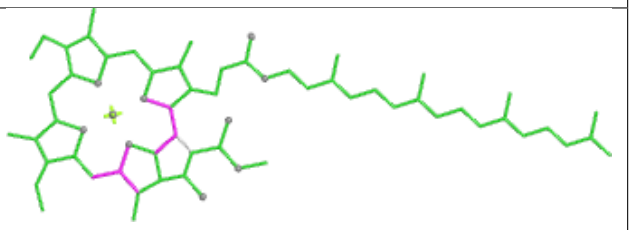
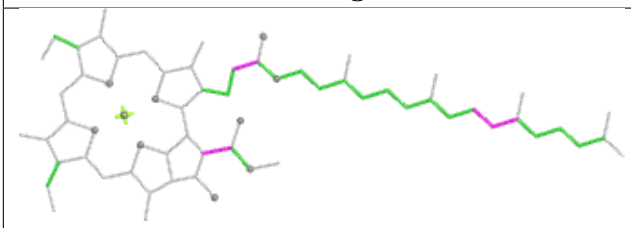
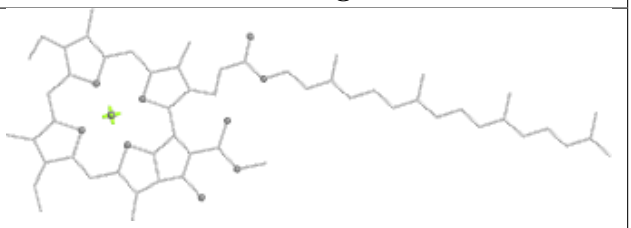


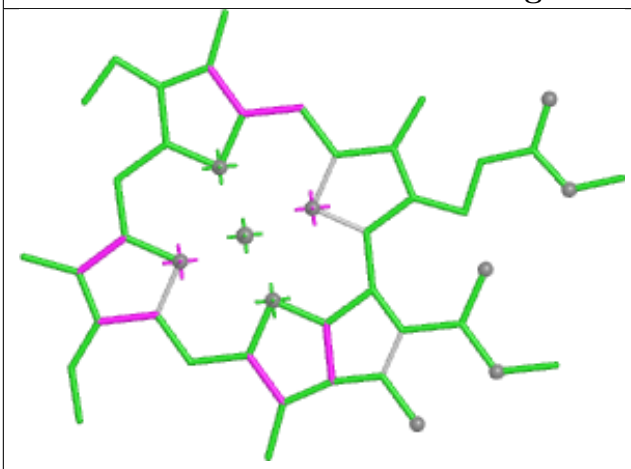
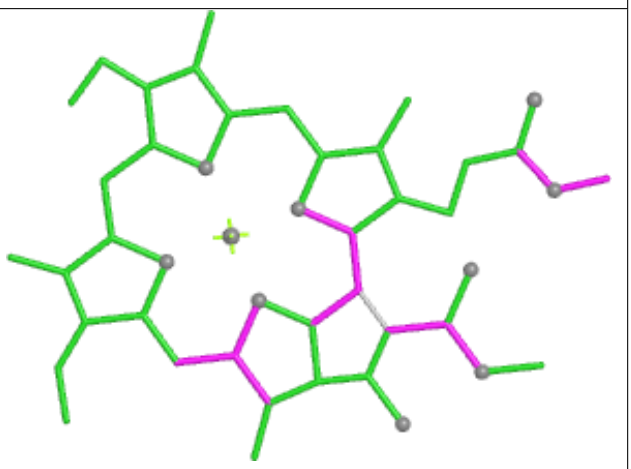
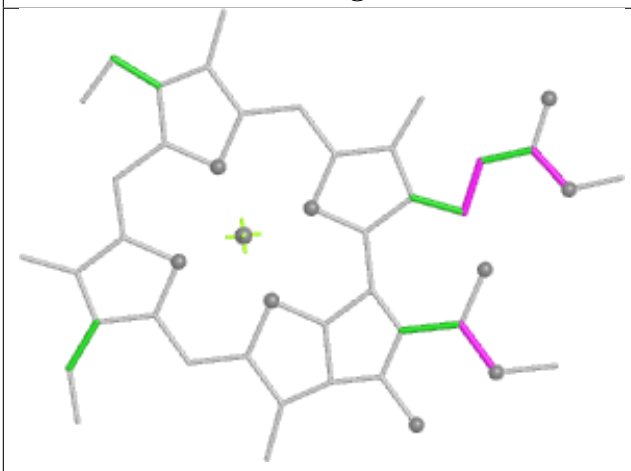
Ligand DD6 S 209

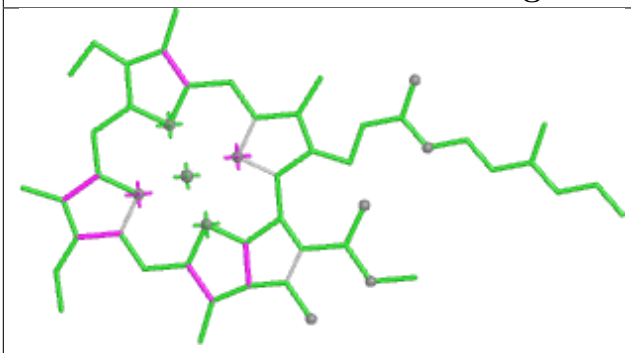
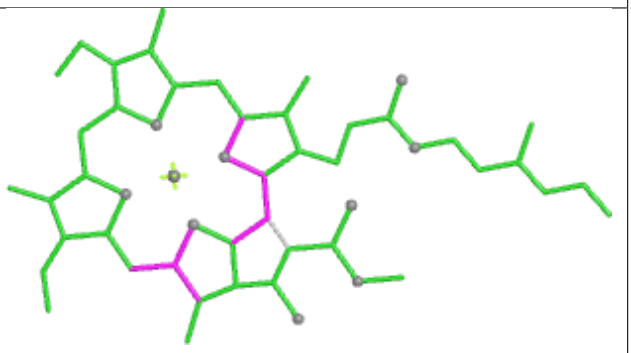
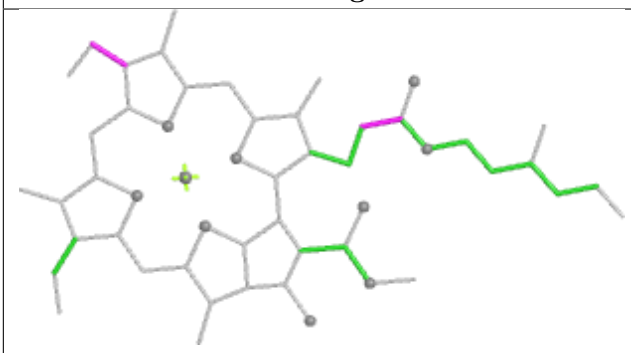
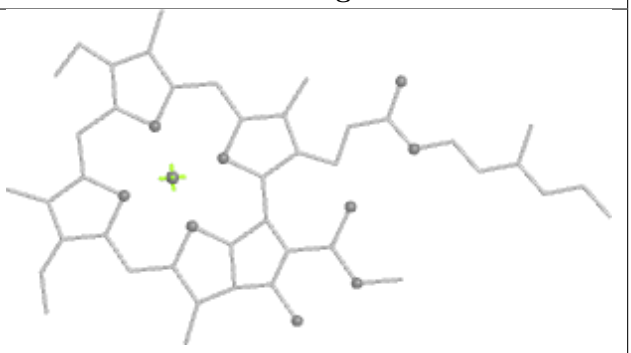


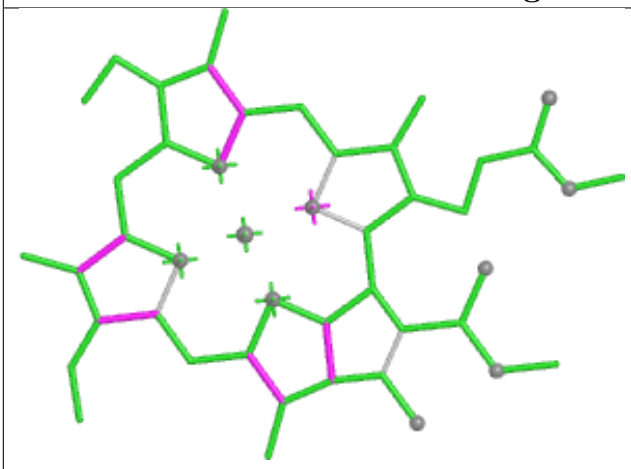
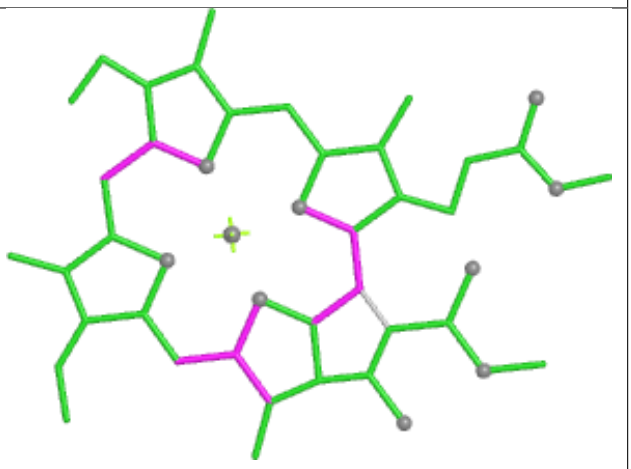
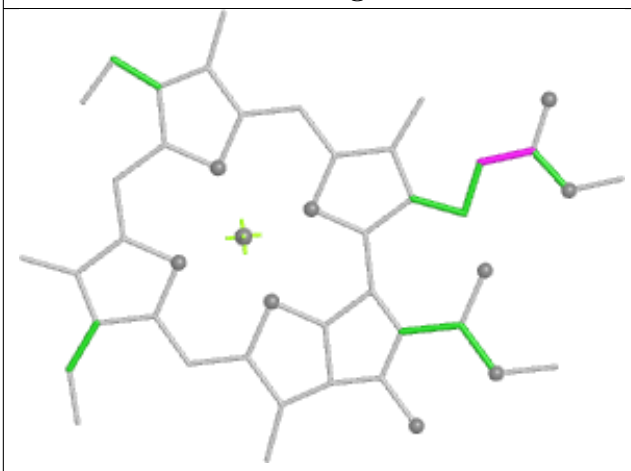
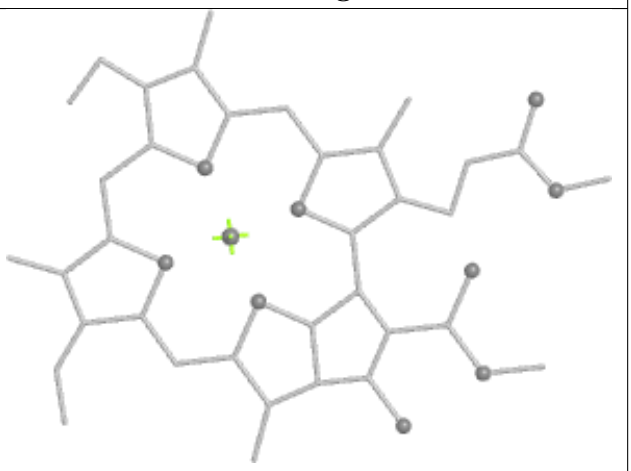
Ligand DD6 S 212



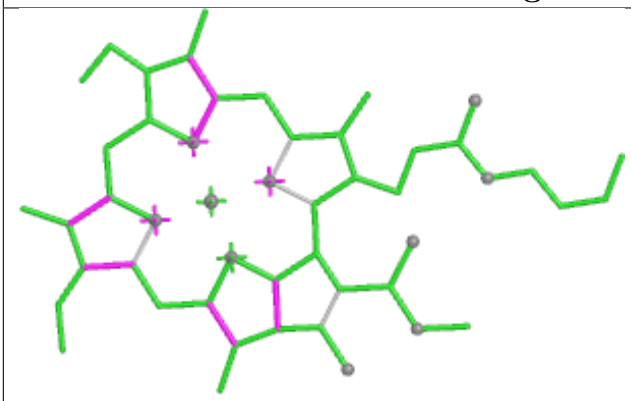
Ligand CLA A 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA T 206	
 Bond lengths	 Bond angles
 Torsions	Rings

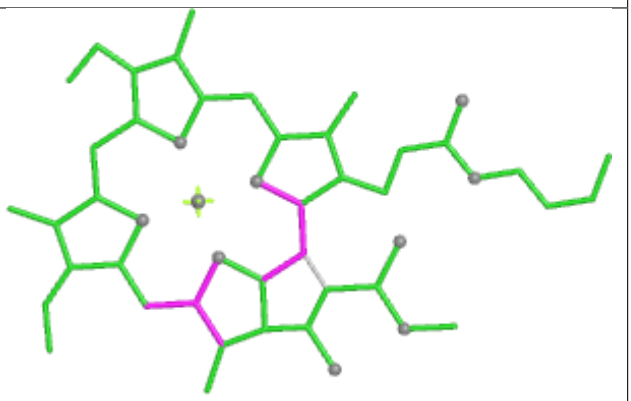
Ligand CLA U 211	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

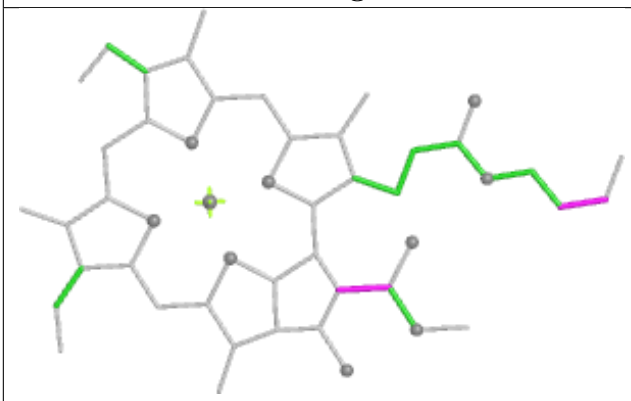
Ligand CLA A 805



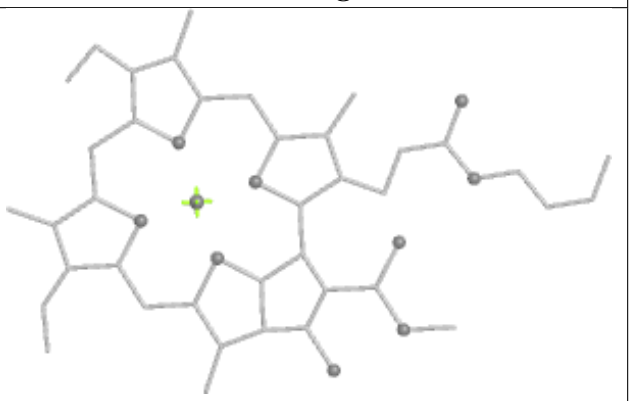
Bond lengths



Bond angles



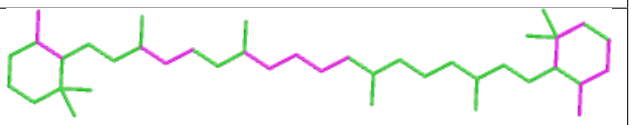
Torsions



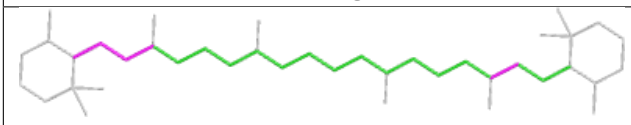
Rings

Ligand BCR B 838

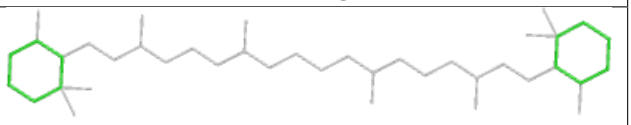
Bond lengths



Bond angles

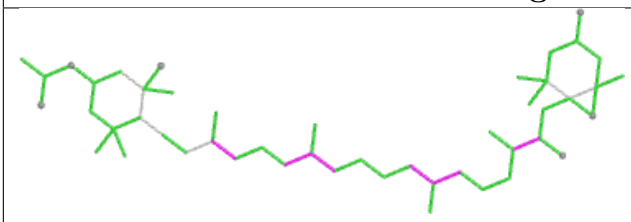


Torsions

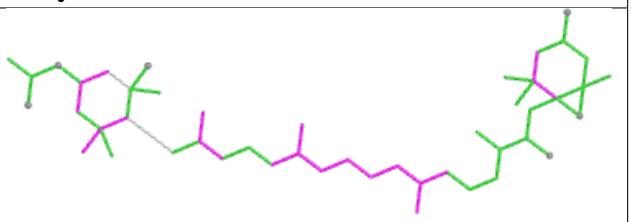


Rings

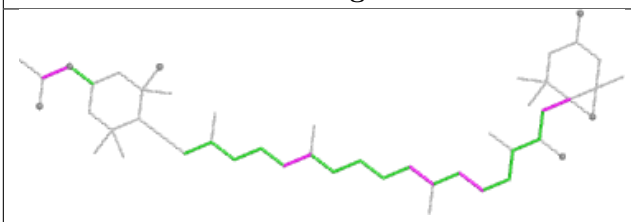
Ligand A86 Q 214



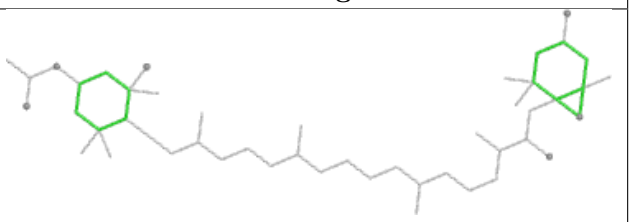
Bond lengths



Bond angles

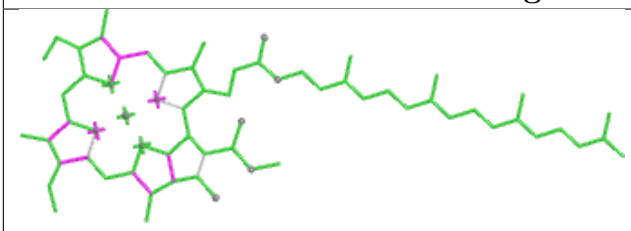


Torsions

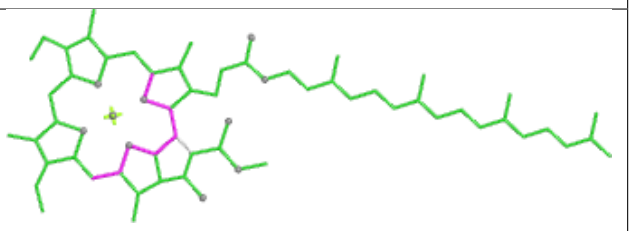


Rings

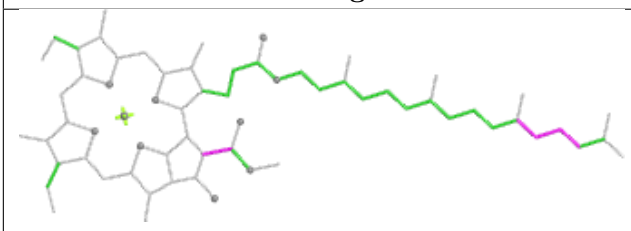
Ligand CLA O 204



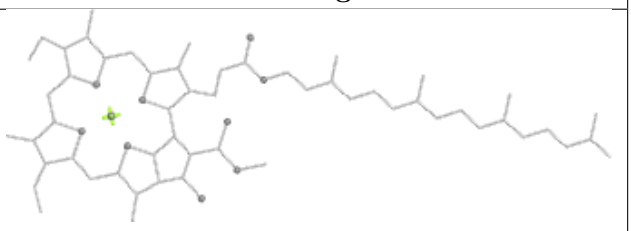
Bond lengths



Bond angles

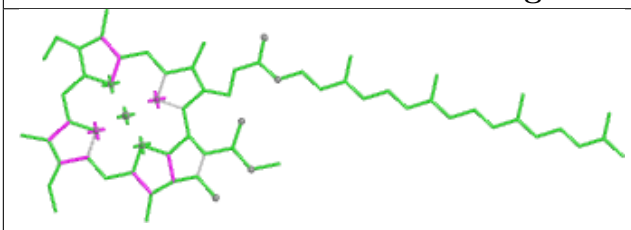


Torsions

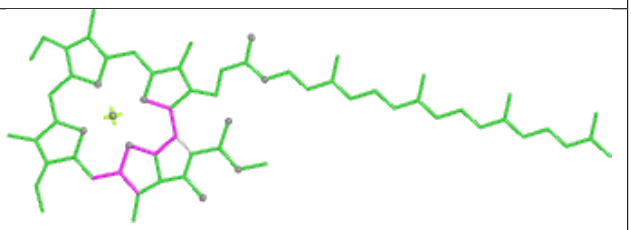


Rings

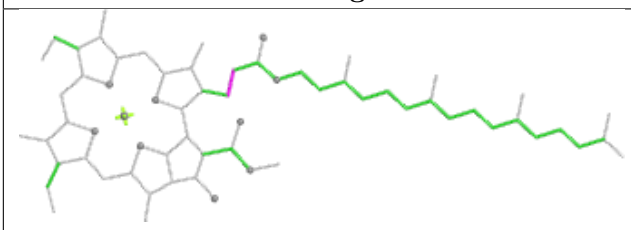
Ligand CLA B 801



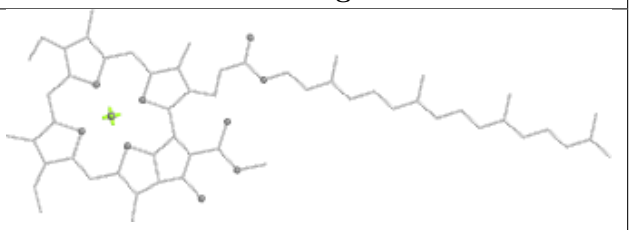
Bond lengths



Bond angles

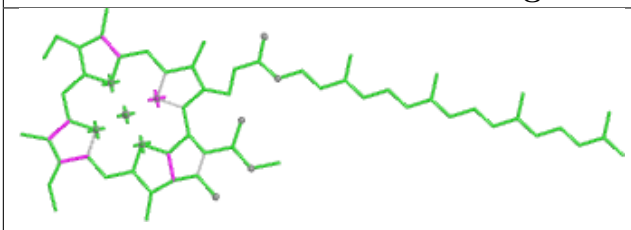


Torsions

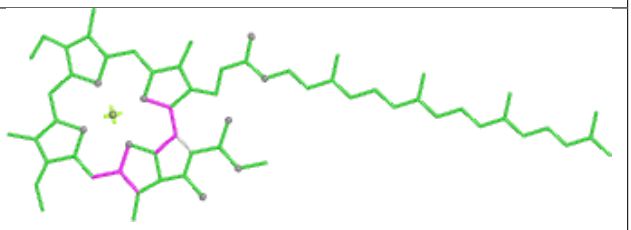


Rings

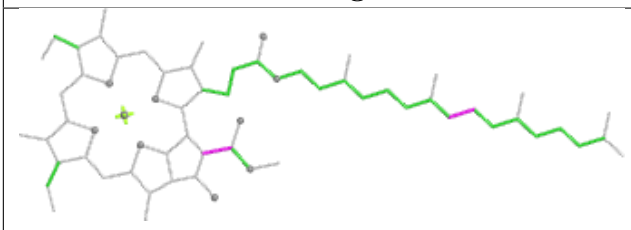
Ligand CLA A 822



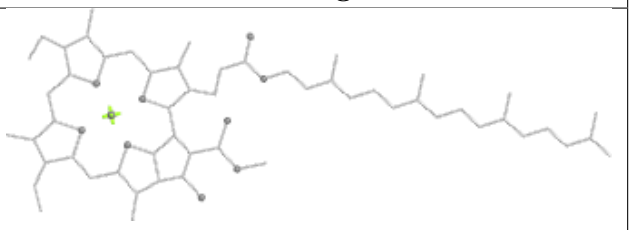
Bond lengths



Bond angles

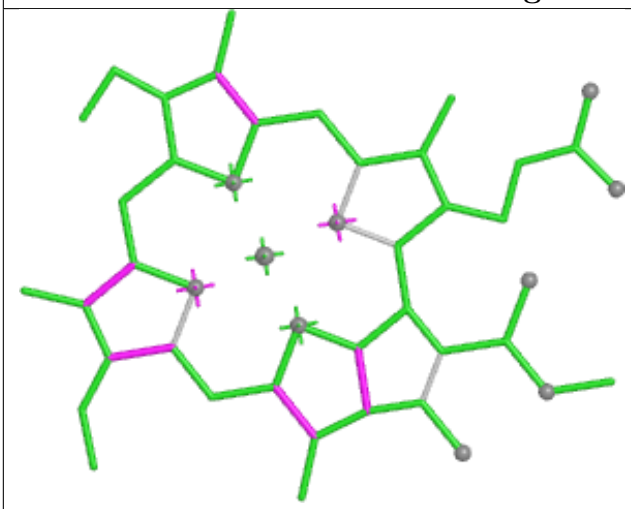


Torsions

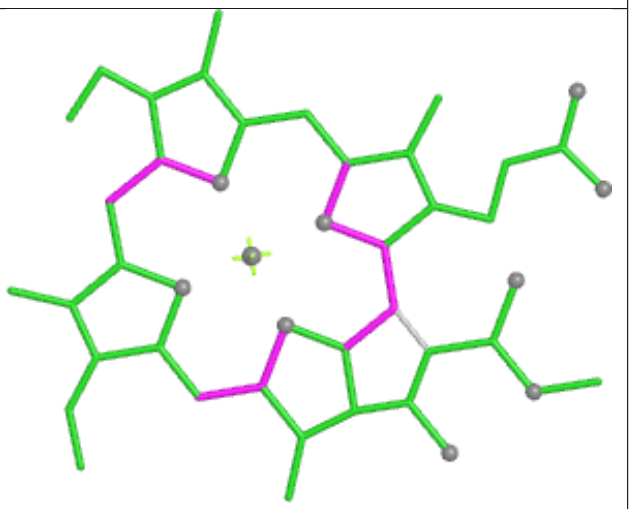


Rings

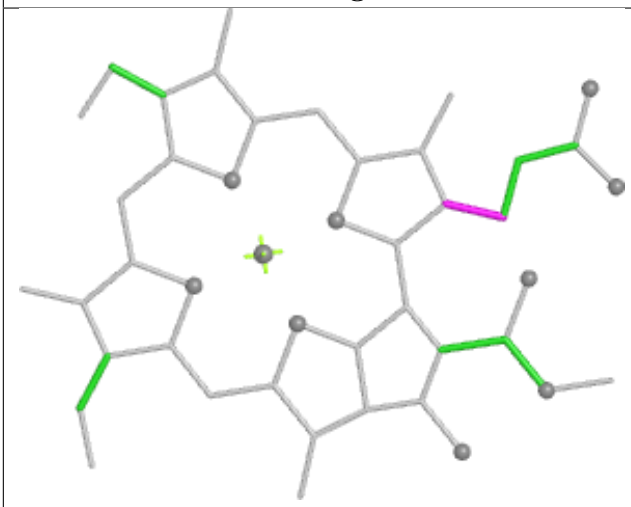
Ligand CLA O 203



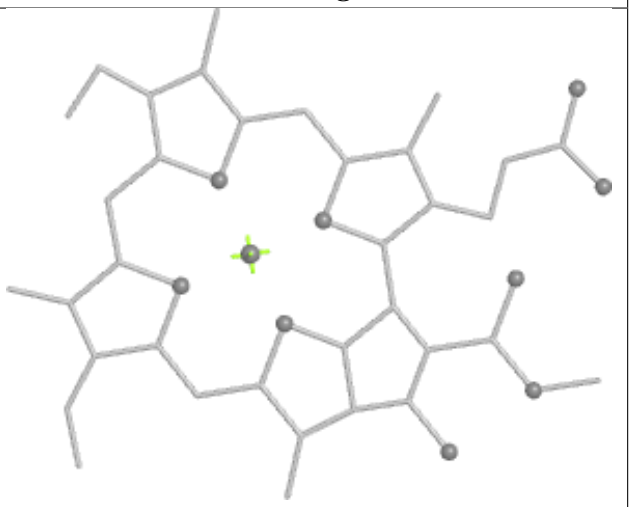
Bond lengths



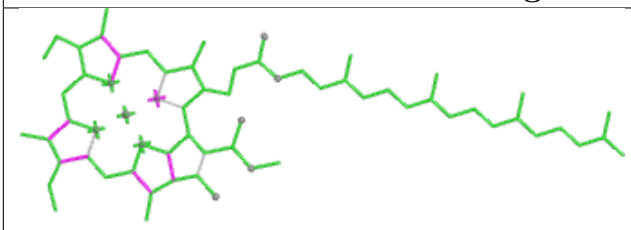
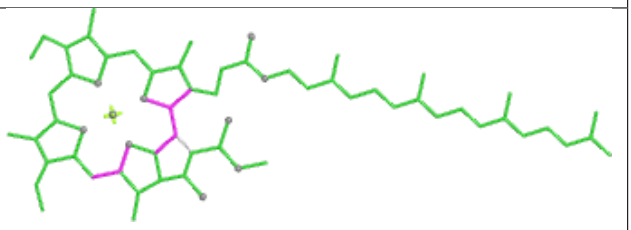
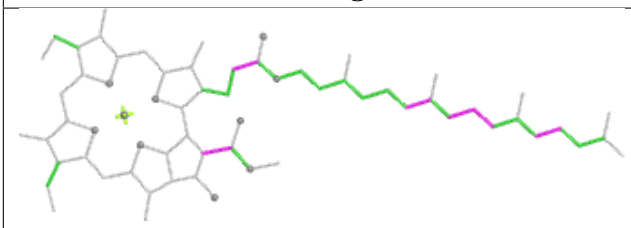
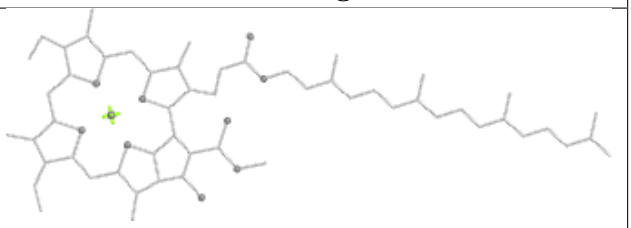
Bond angles

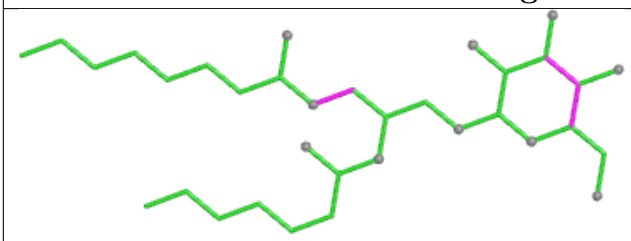
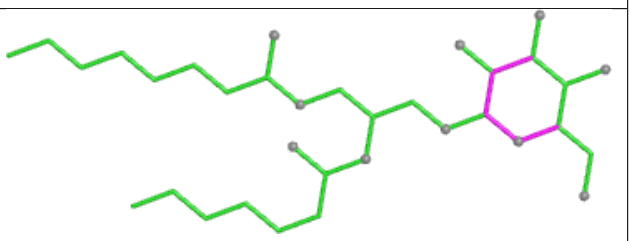
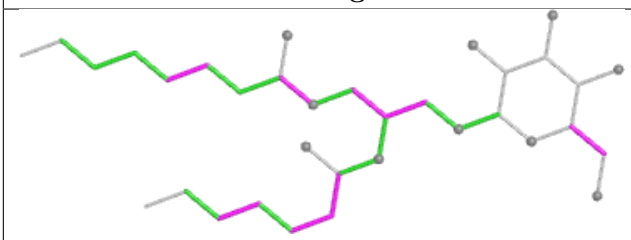
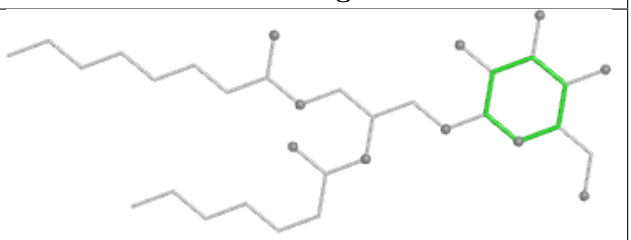


Torsions

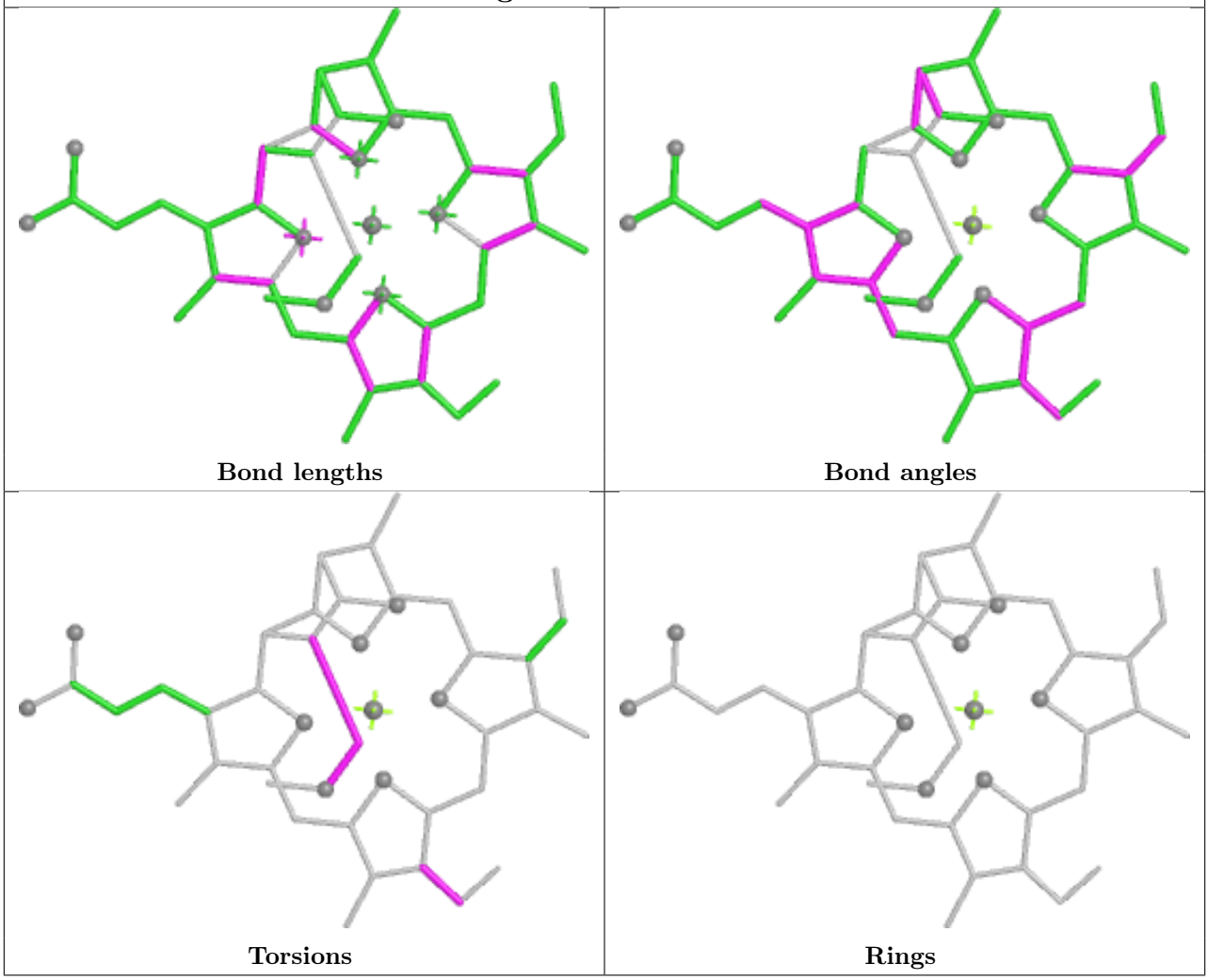


Rings

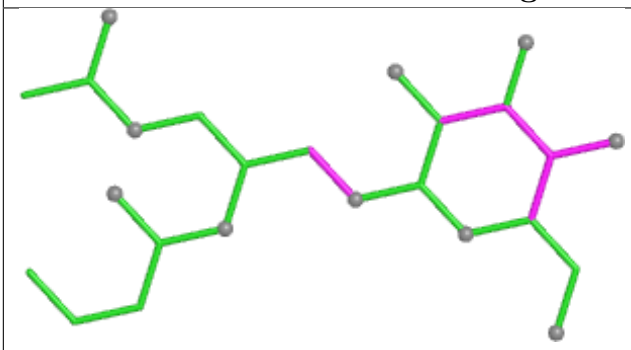
Ligand CLA A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG P 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

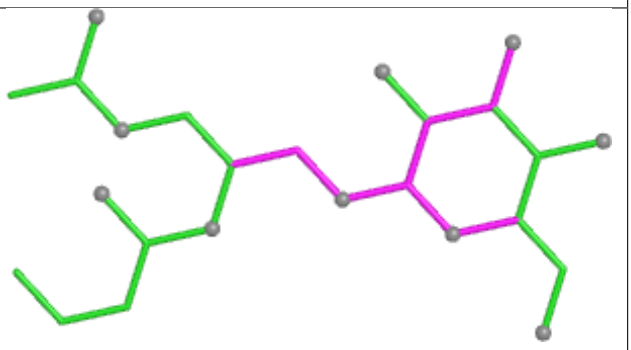
Ligand KC1 P 311



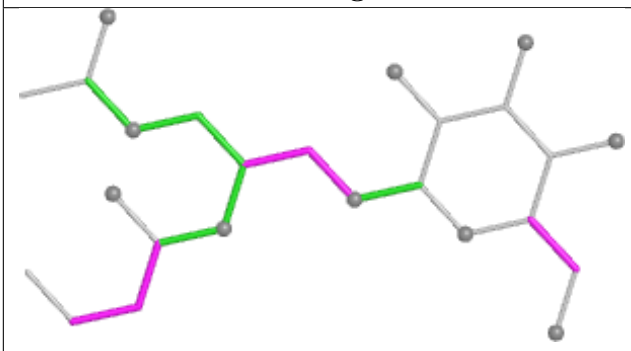
Ligand LMG B 849



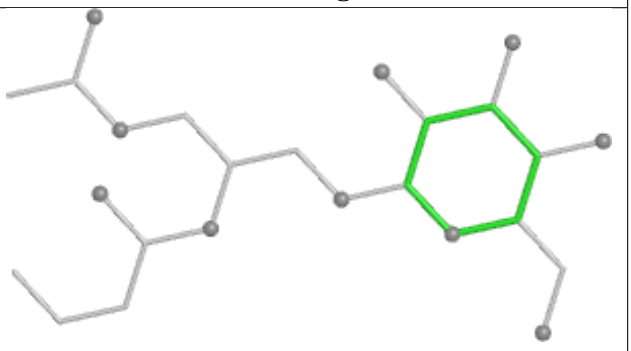
Bond lengths



Bond angles

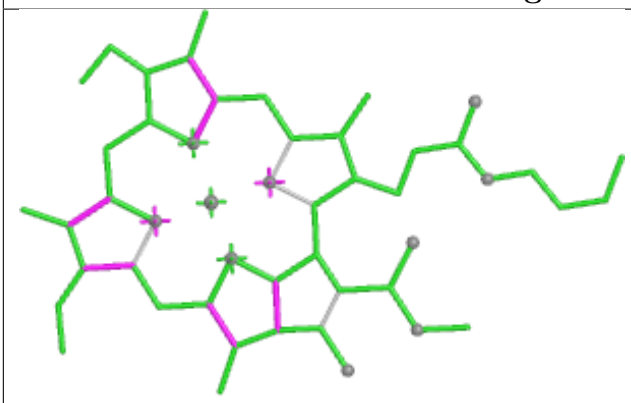


Torsions

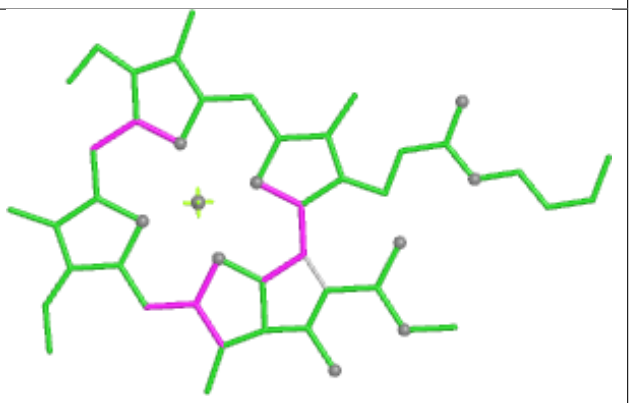


Rings

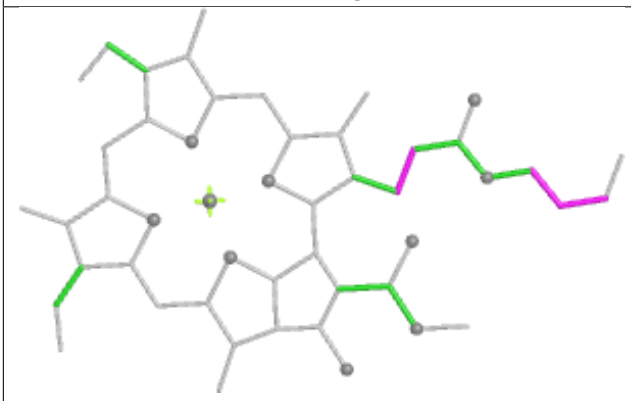
Ligand CLA B 827



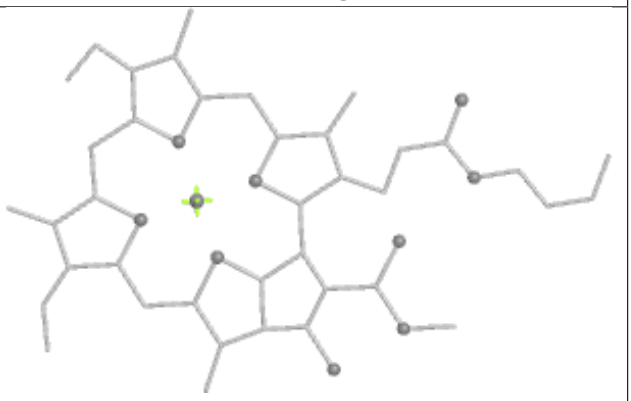
Bond lengths



Bond angles

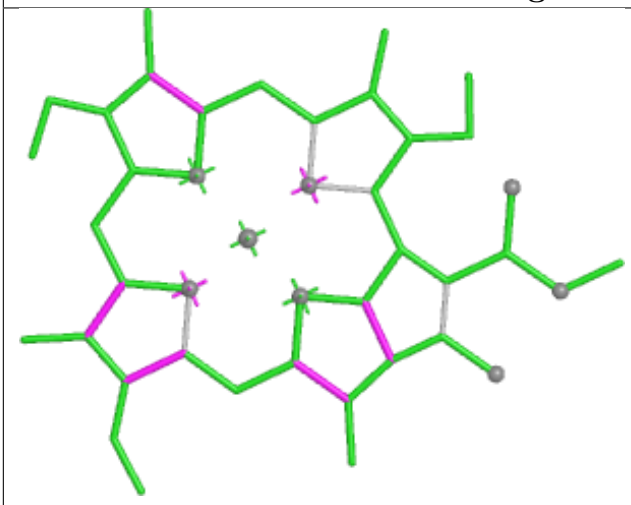


Torsions

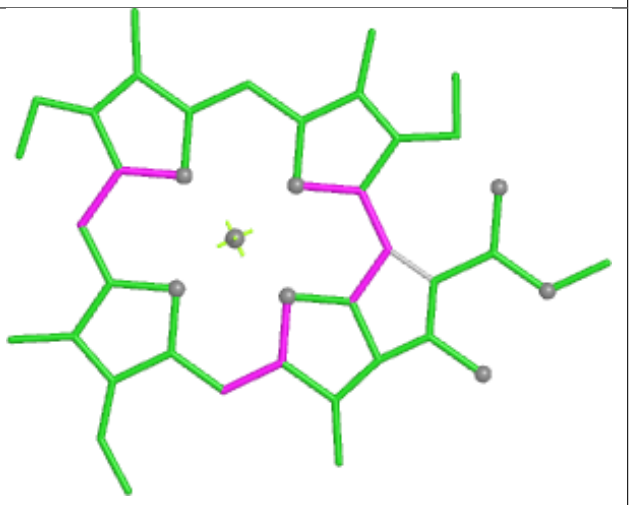


Rings

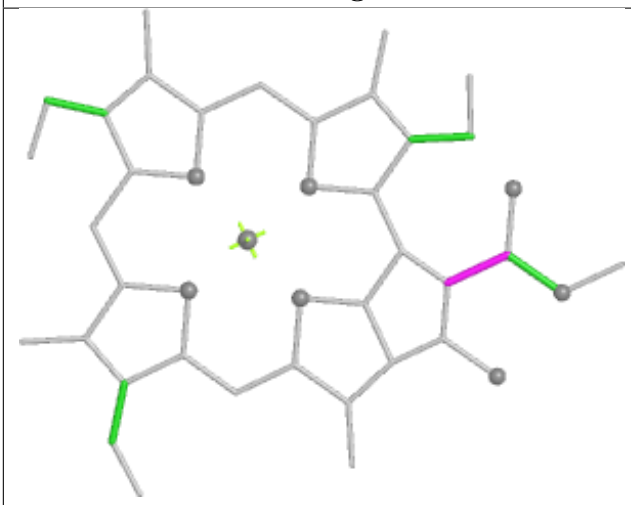
Ligand CLA J 103



Bond lengths



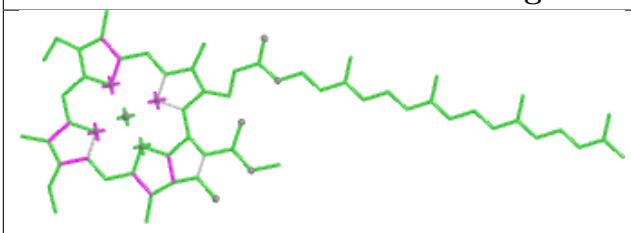
Bond angles



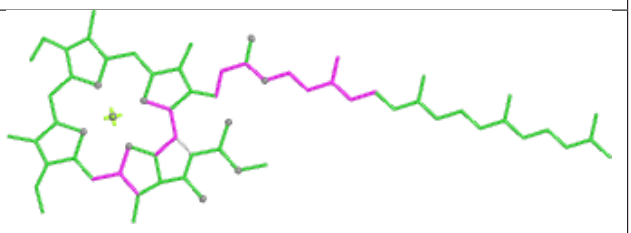
Torsions

Rings

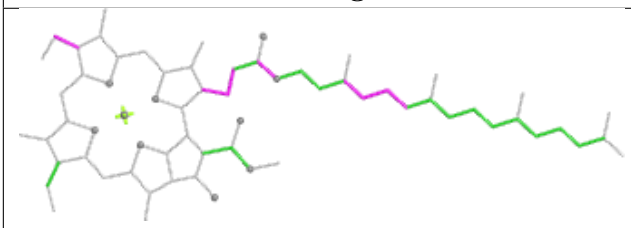
Ligand CLA B 824



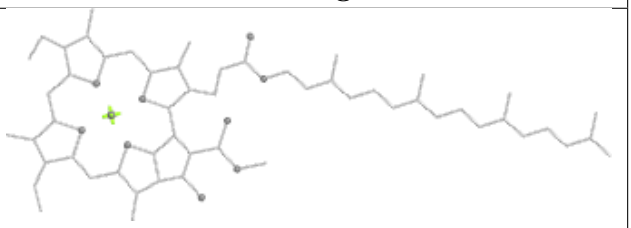
Bond lengths



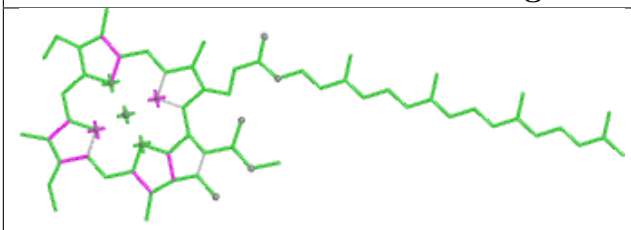
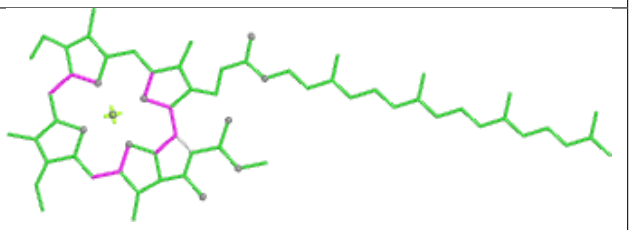
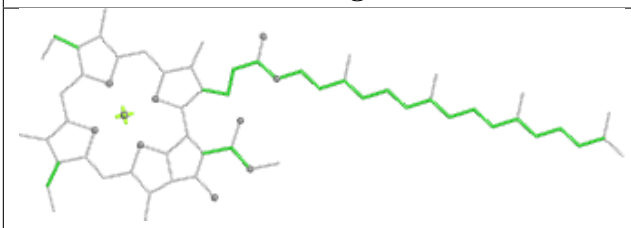
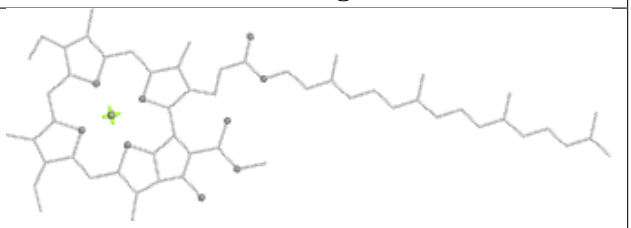
Bond angles

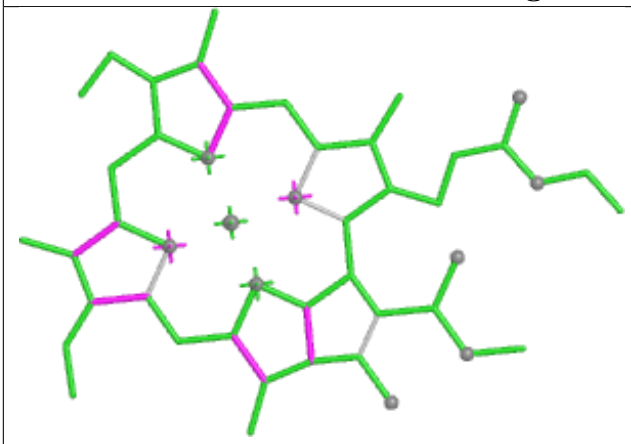
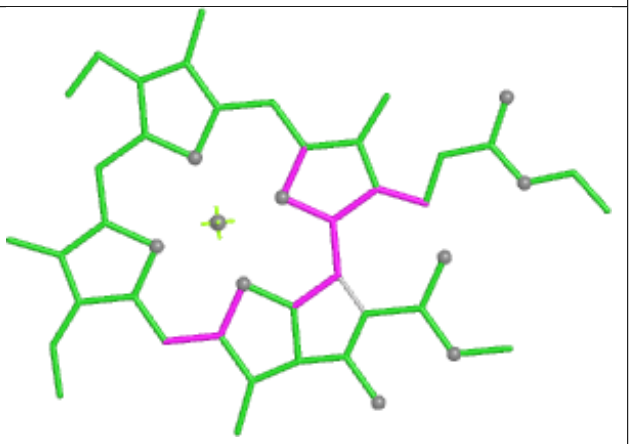
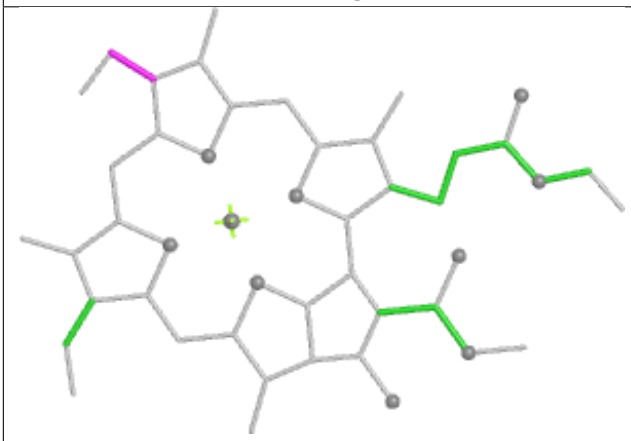
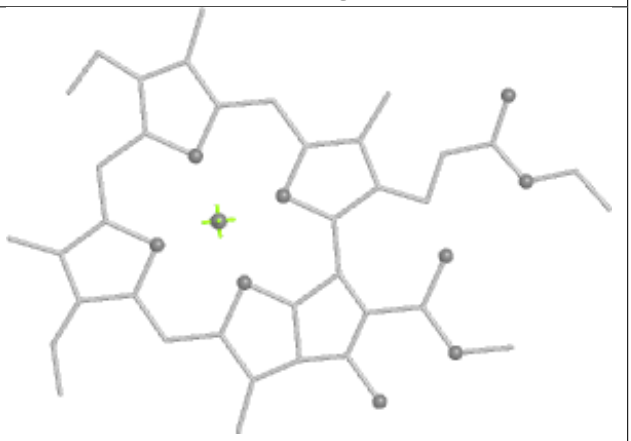


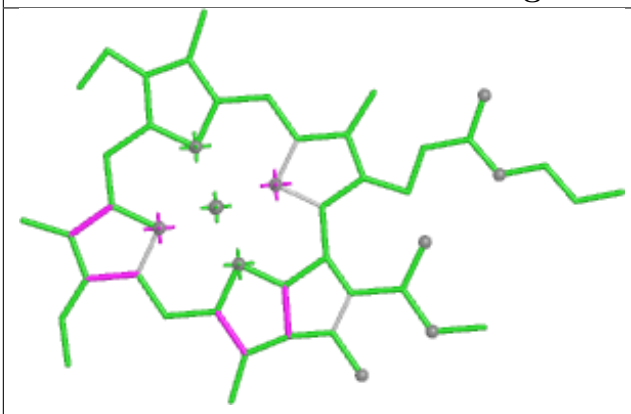
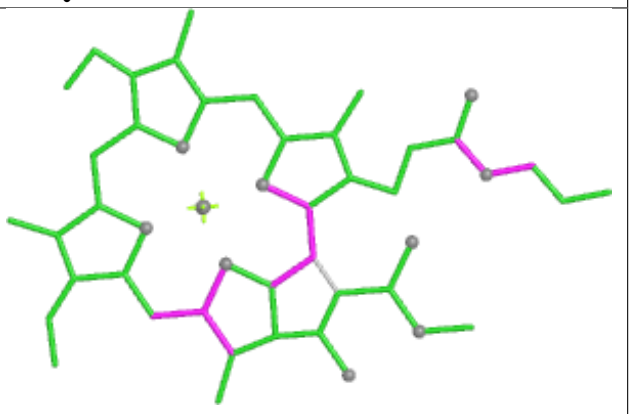
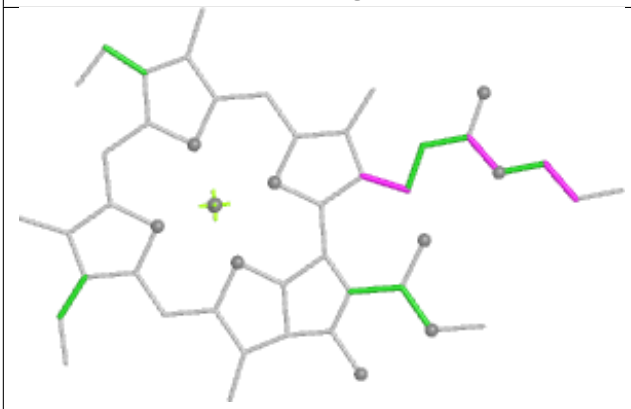
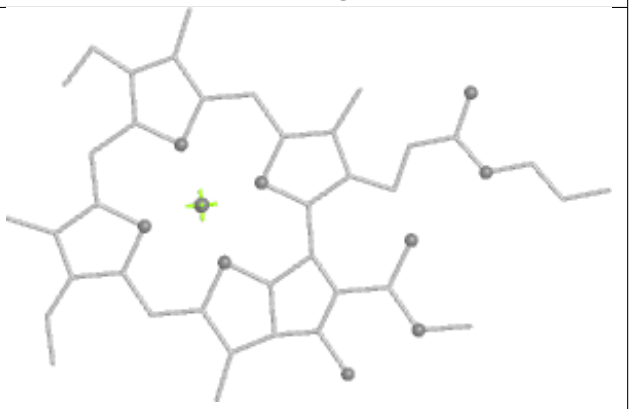
Torsions

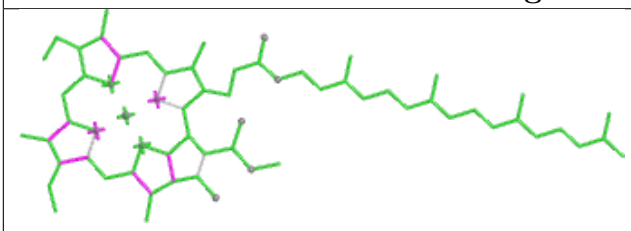
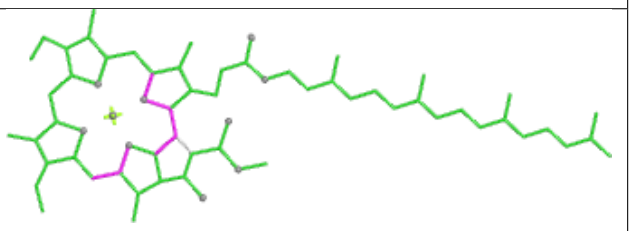
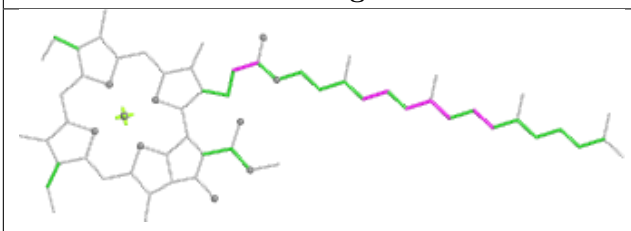
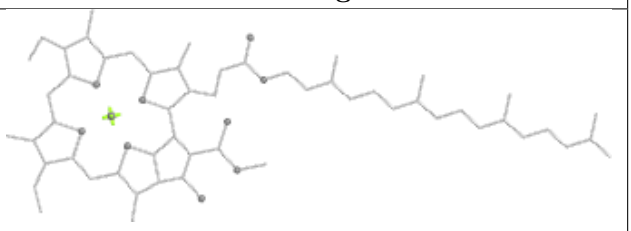


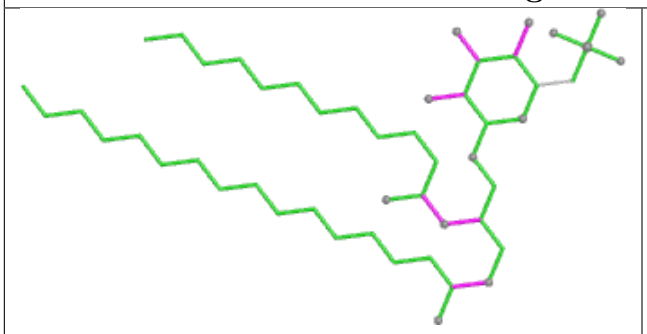
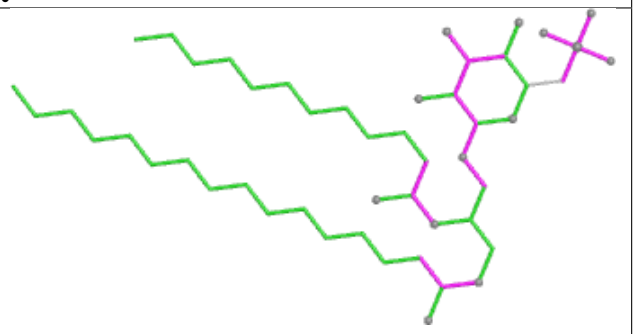
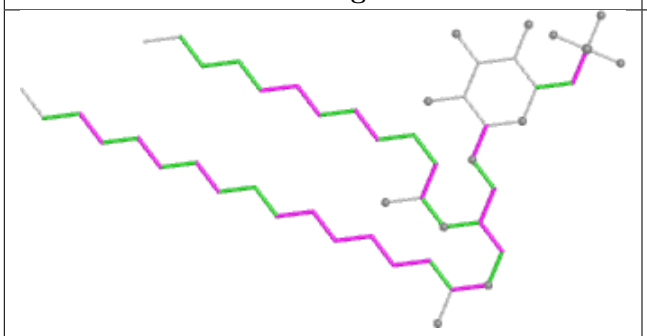
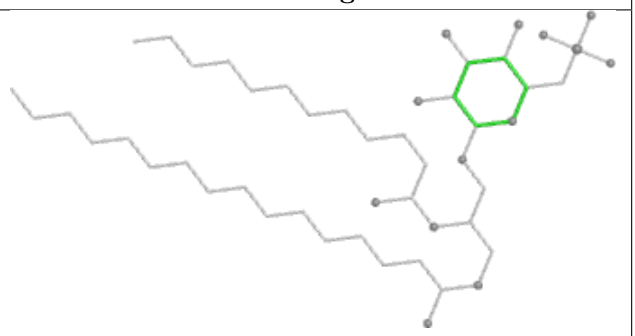
Rings

Ligand CLA B 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

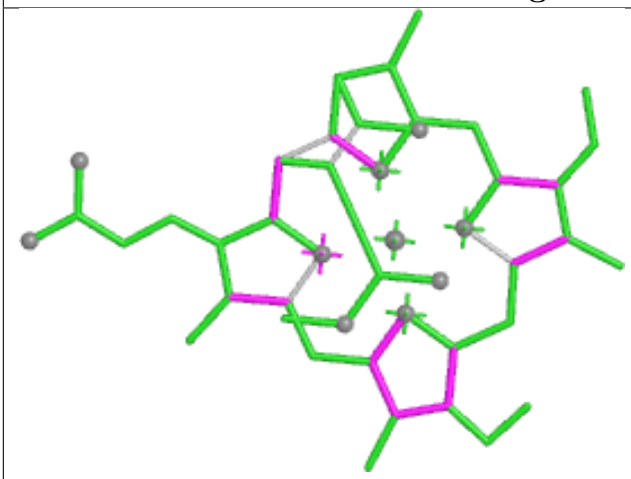
Ligand CLA P 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

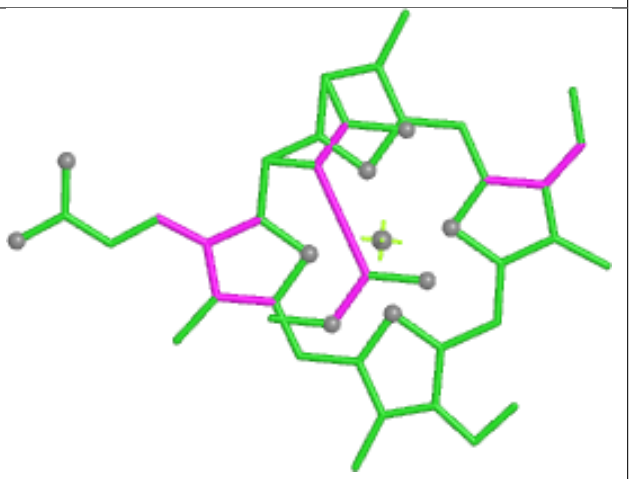
Ligand CLA B 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD B 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

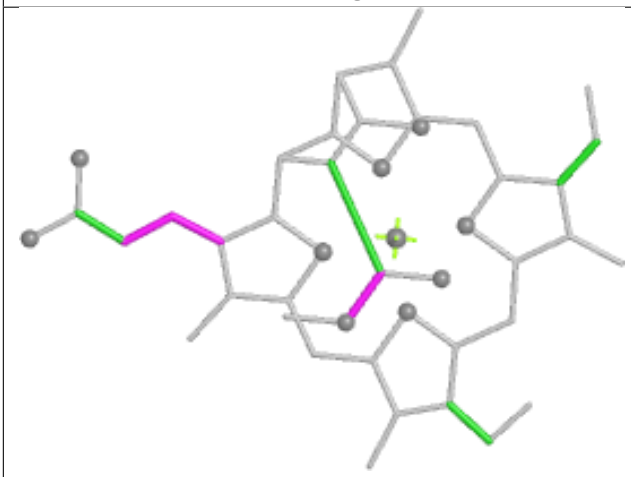
Ligand KC1 S 210



Bond lengths



Bond angles



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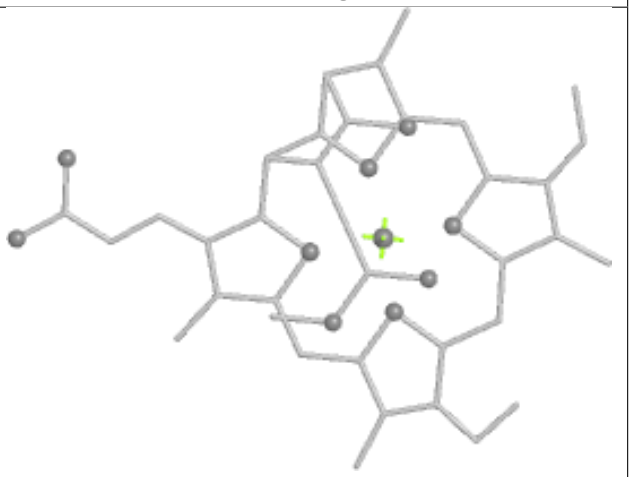
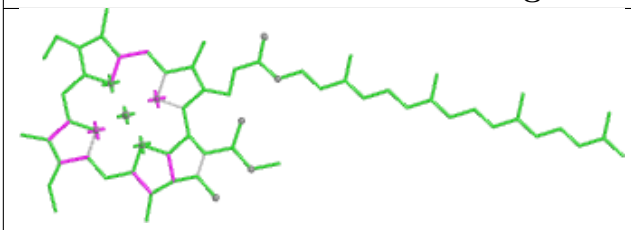


Rings

Ligand CLA O 206



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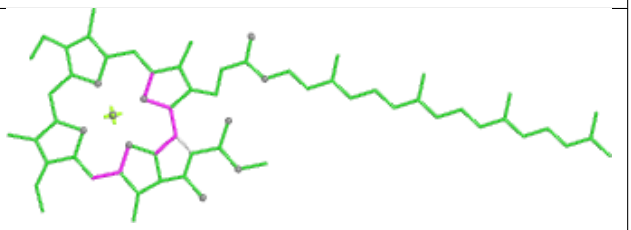

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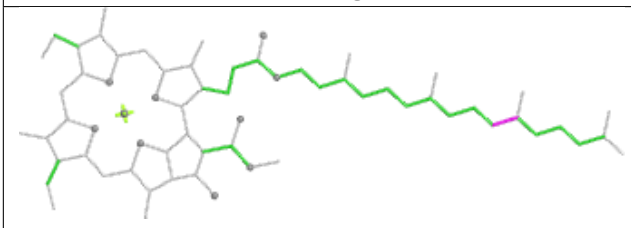

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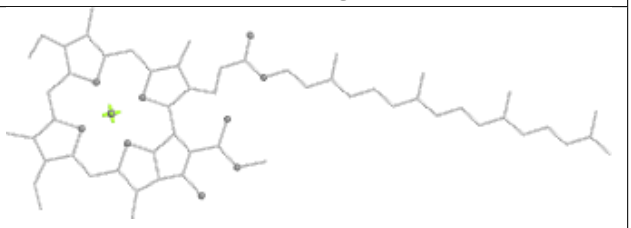
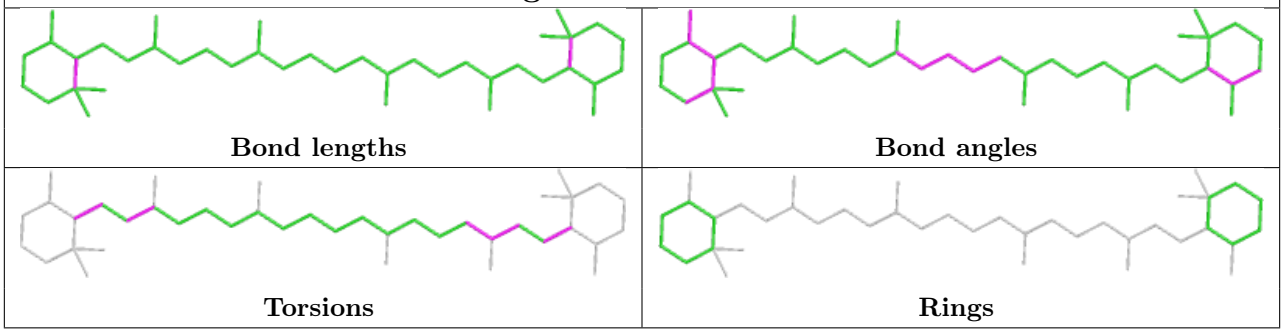
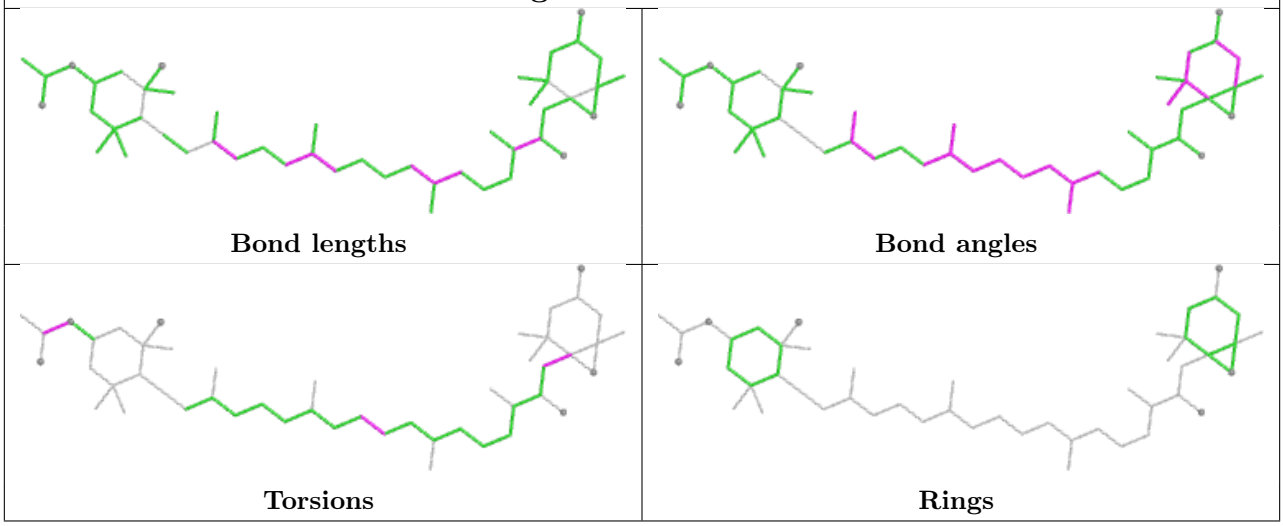


Rings

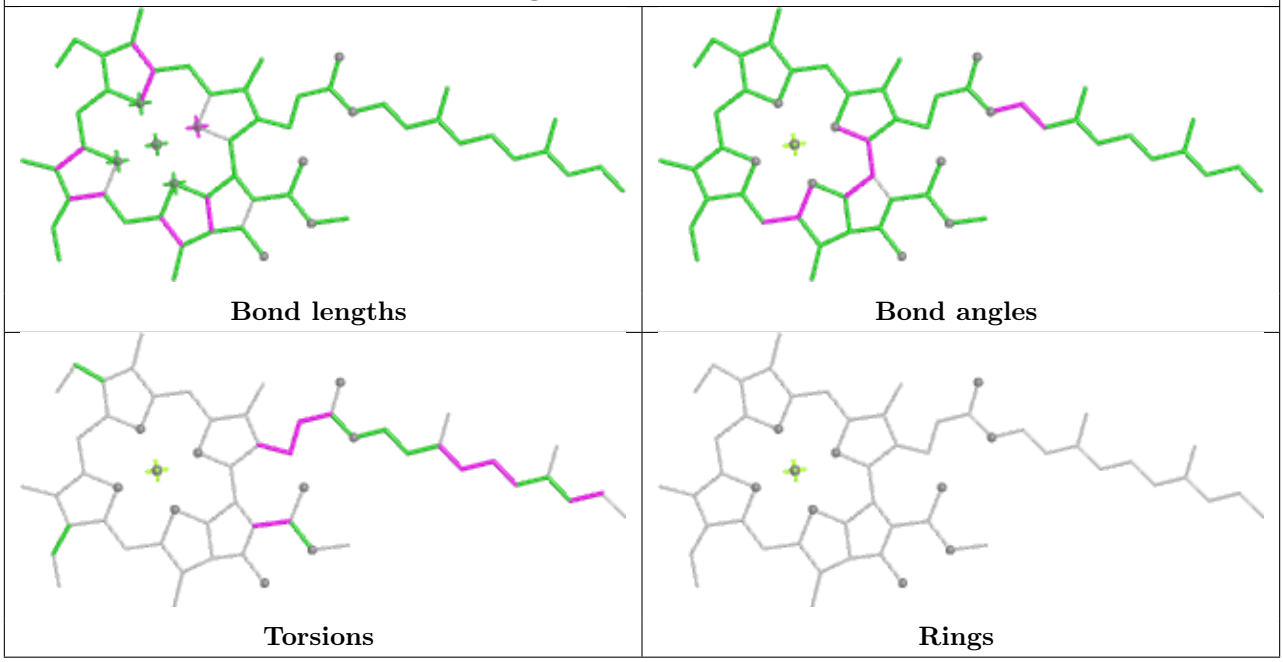
Ligand BCR A 844



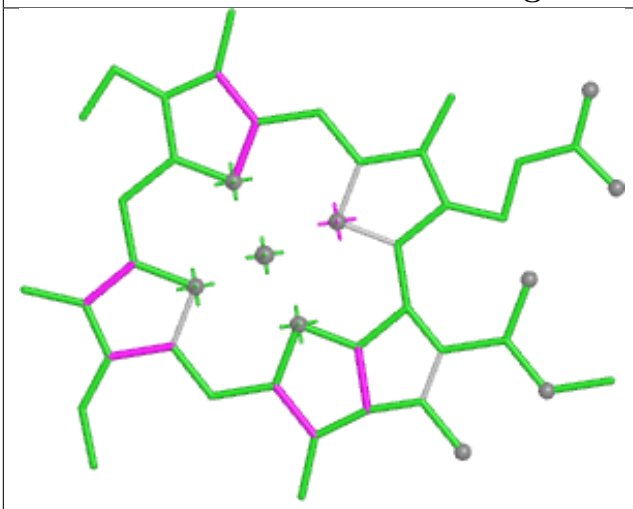
Ligand A86 R 206



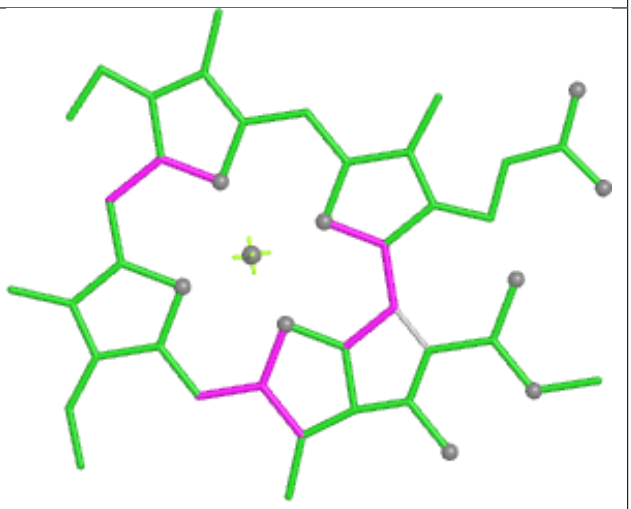
Ligand CLA T 205



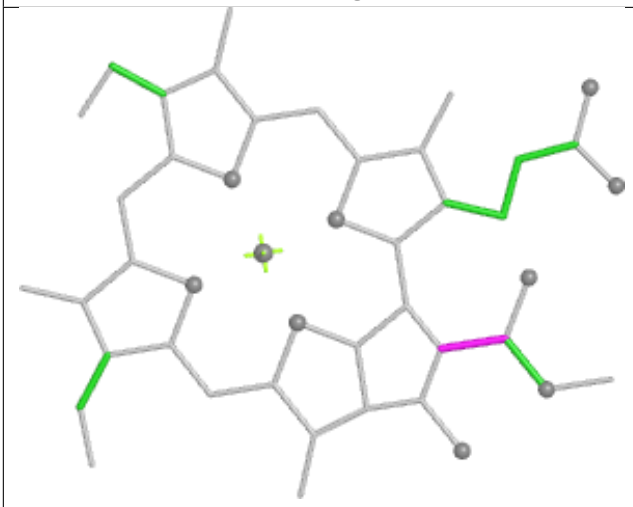
Ligand CLA A 831



Bond lengths



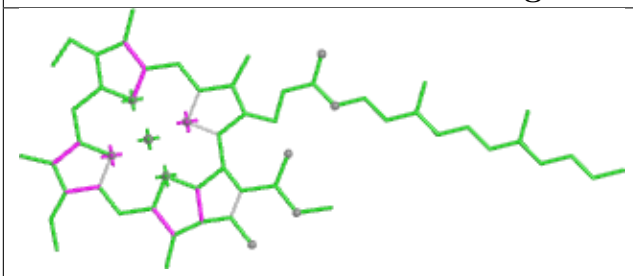
Bond angles



Torsions

Rings

Ligand CLA B 828



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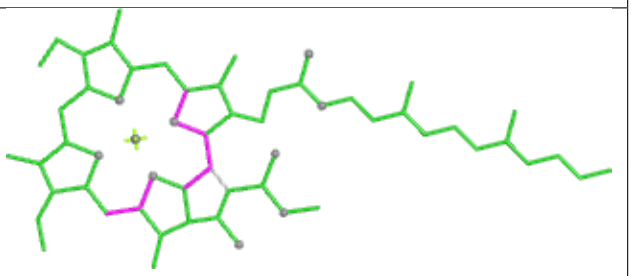

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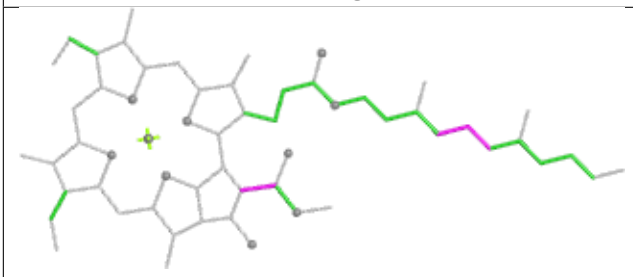

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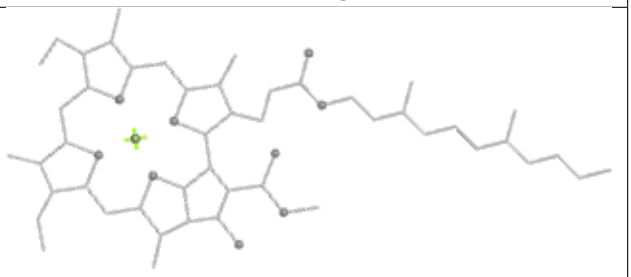

Rings

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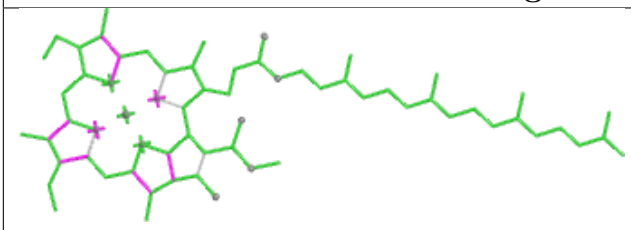
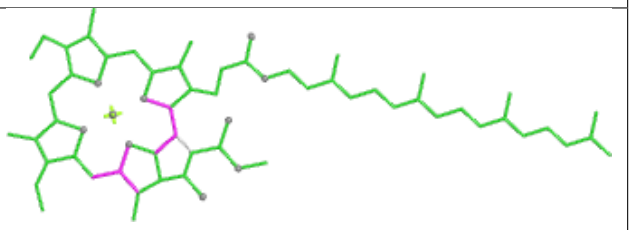
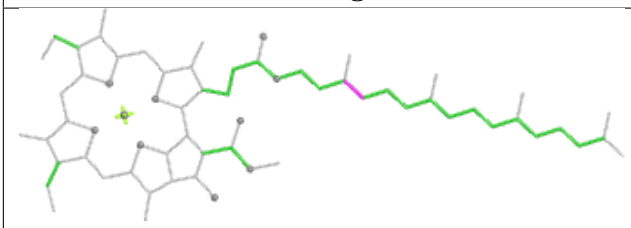
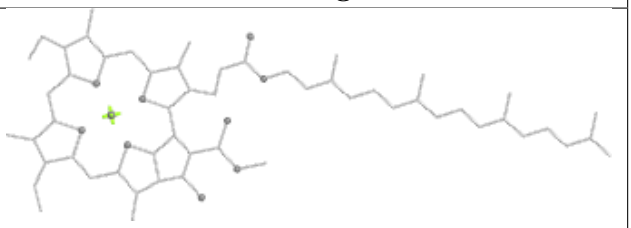
 Bond lengths	 Bond angles
 Torsions	 Rings

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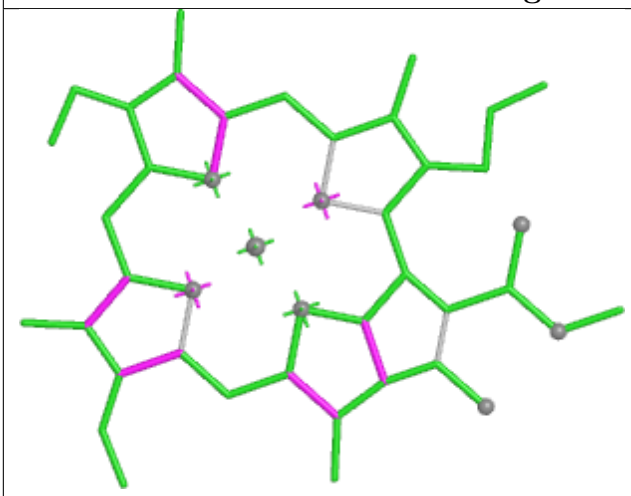
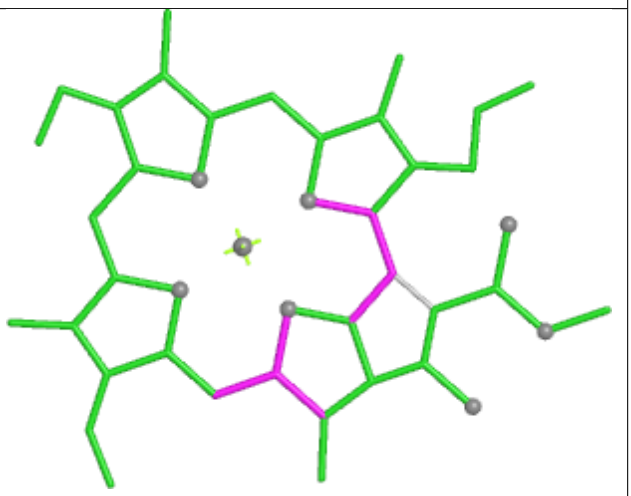
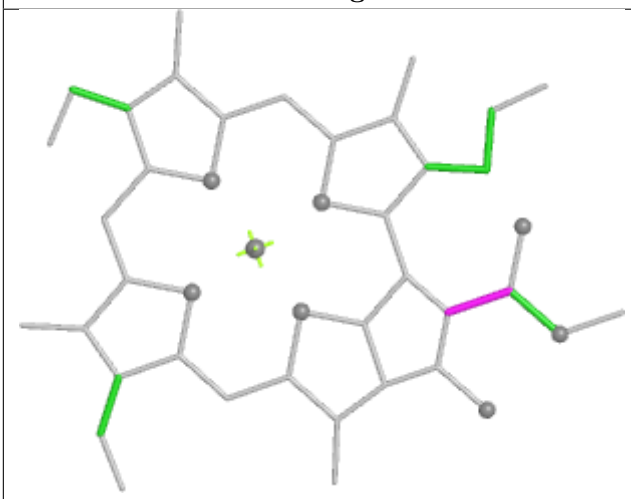
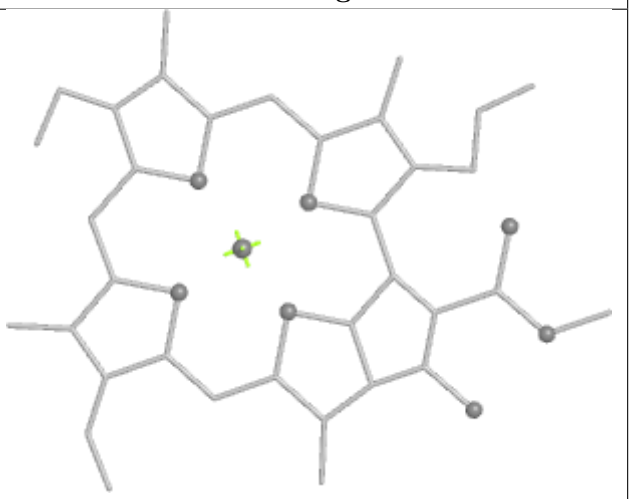
 Bond lengths	 Bond angles
 Torsions	 Rings

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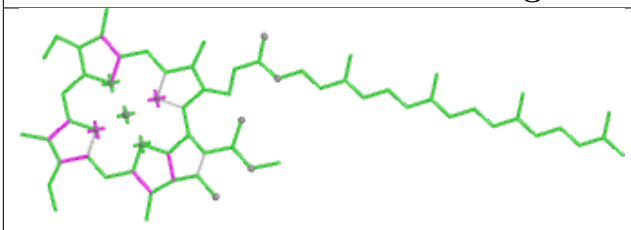
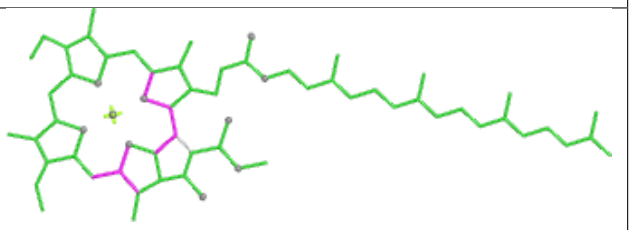
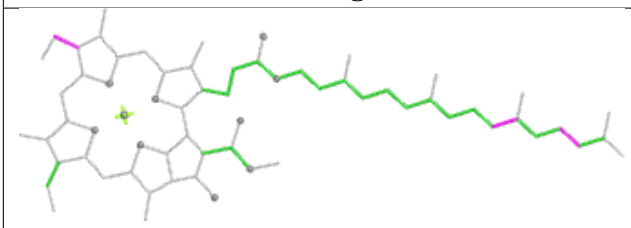
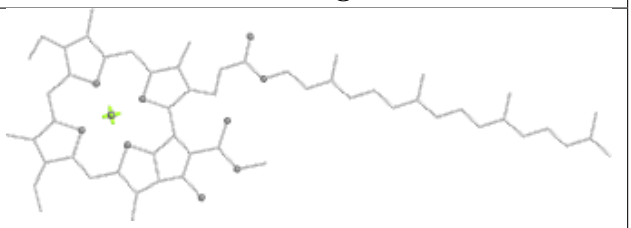
 Bond lengths	 Bond angles
 Torsions	 Rings

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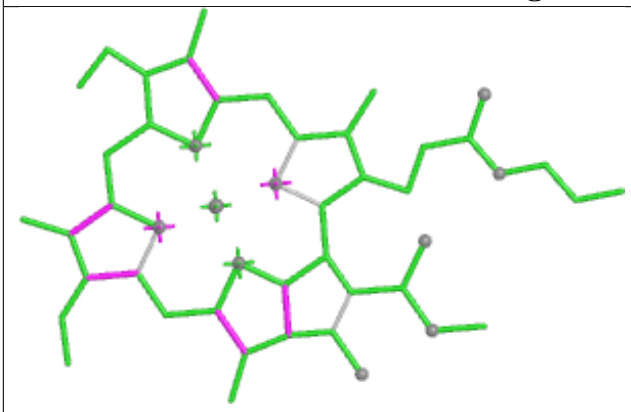
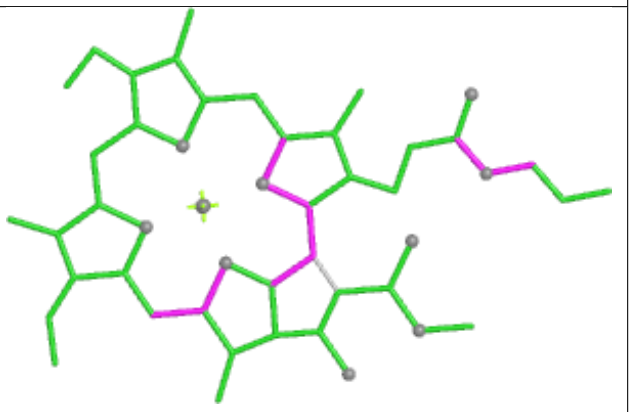
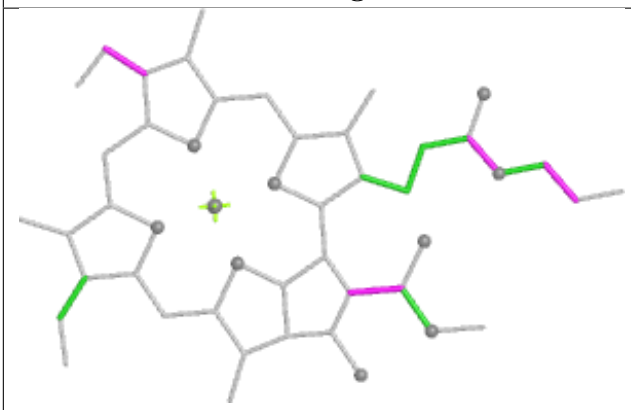
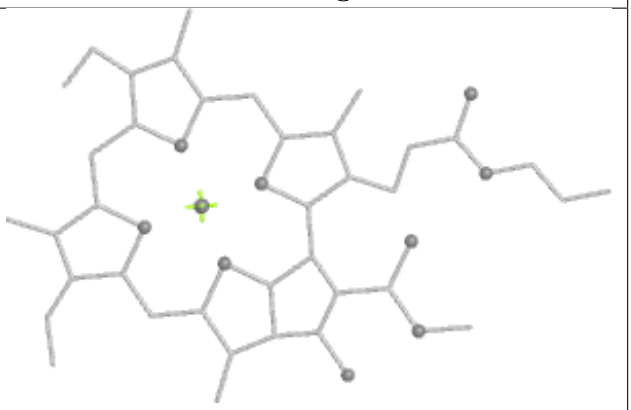
 Bond lengths	 Bond angles
 Torsions	 Rings

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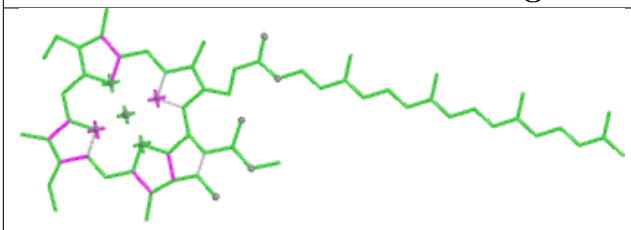
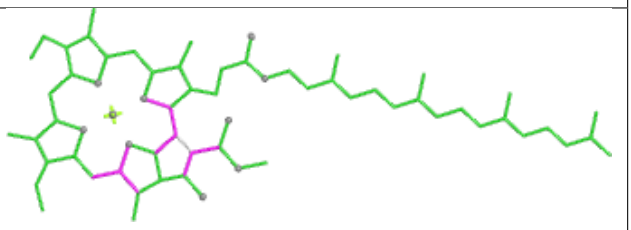
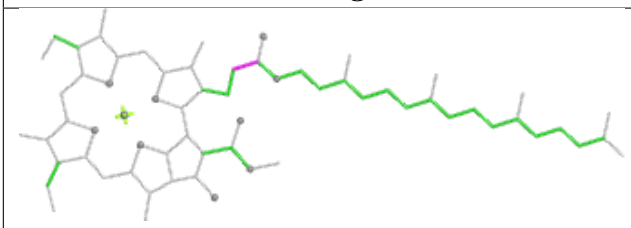
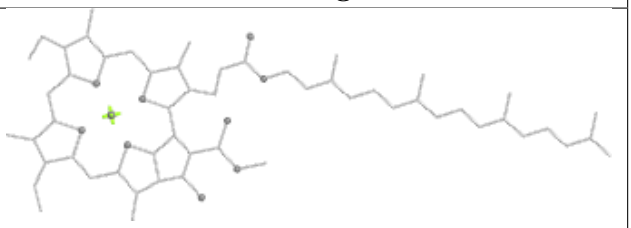
 Bond lengths	 Bond angles
 Torsions	 Rings

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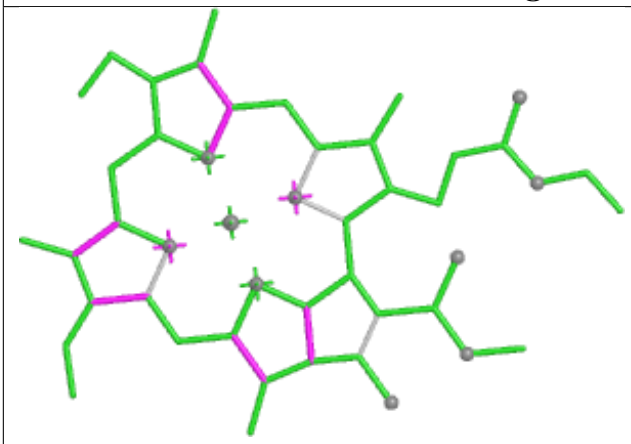
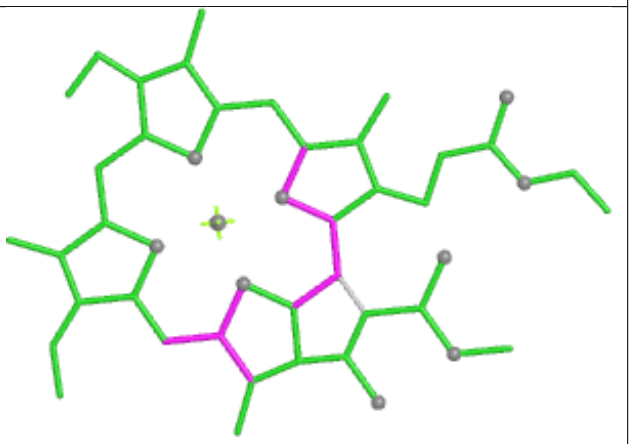
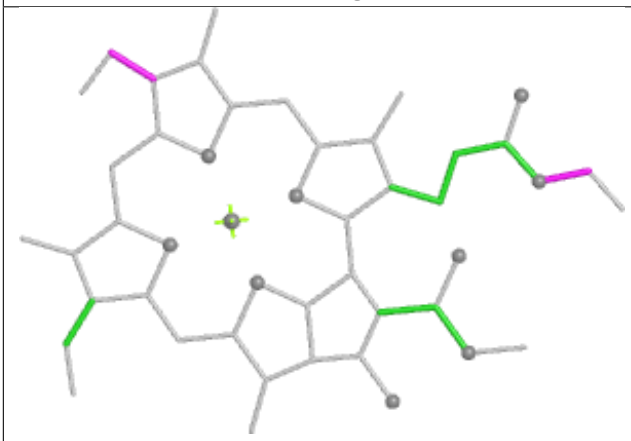
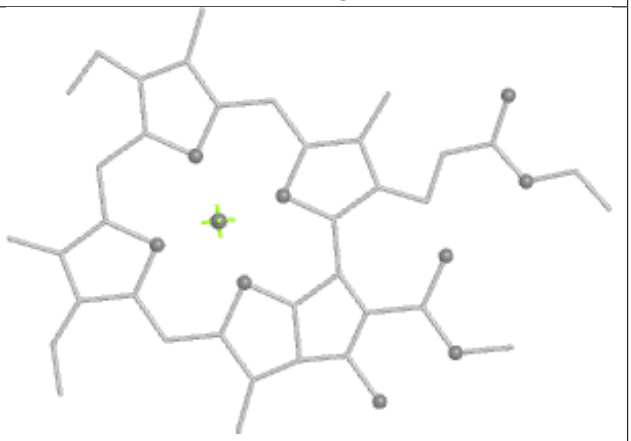
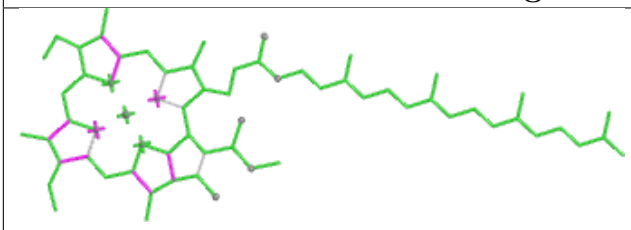
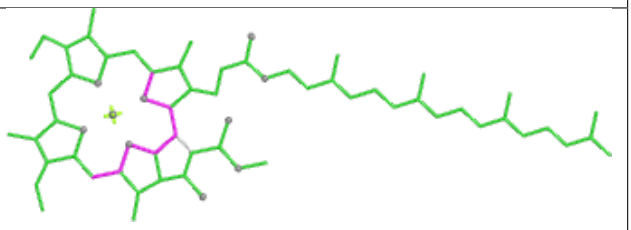
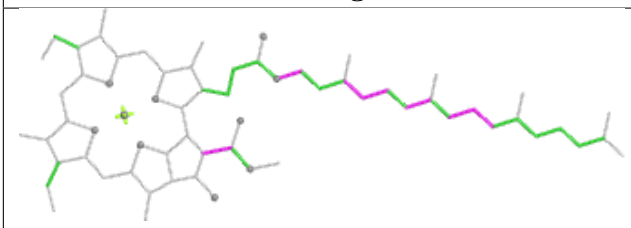
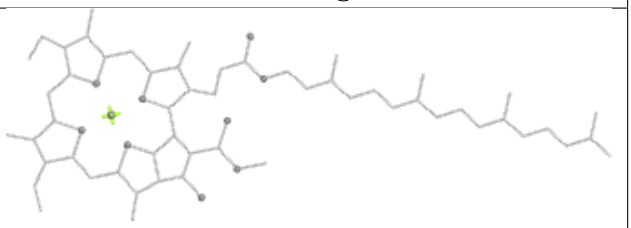
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

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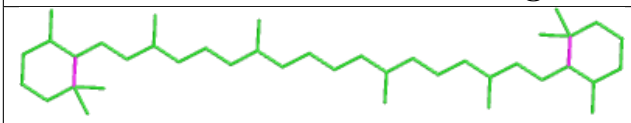
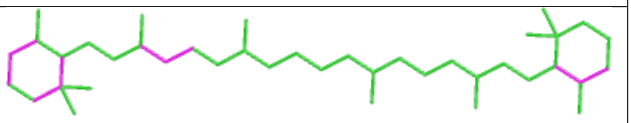
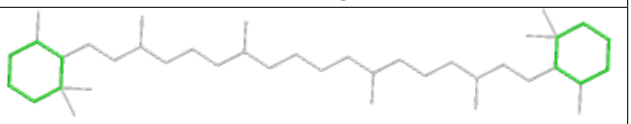
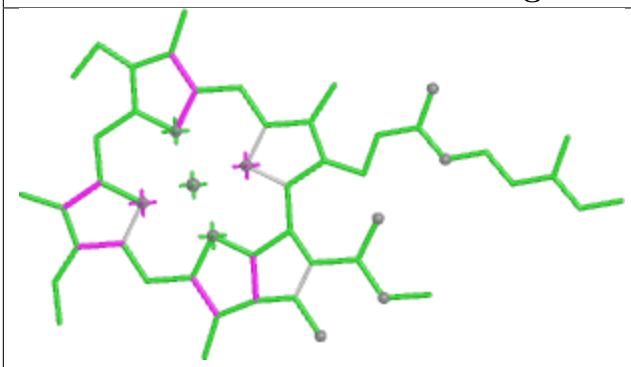
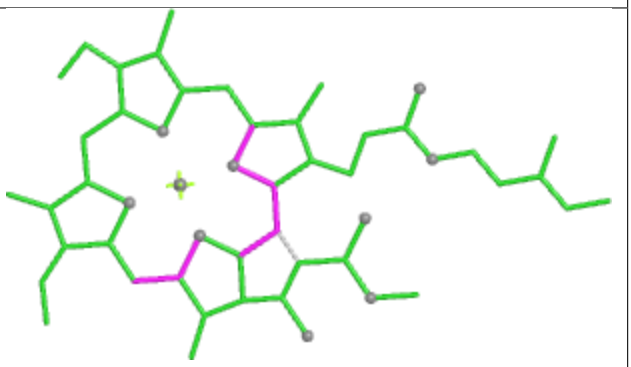
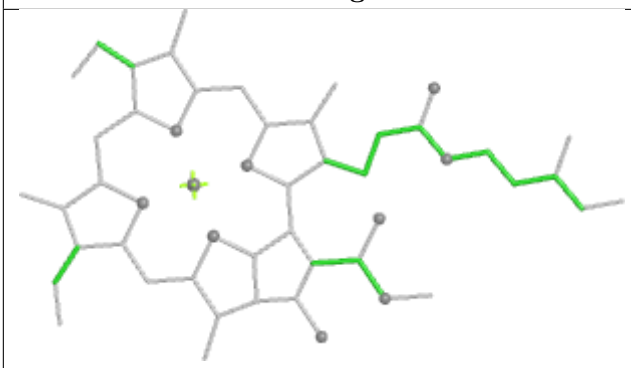
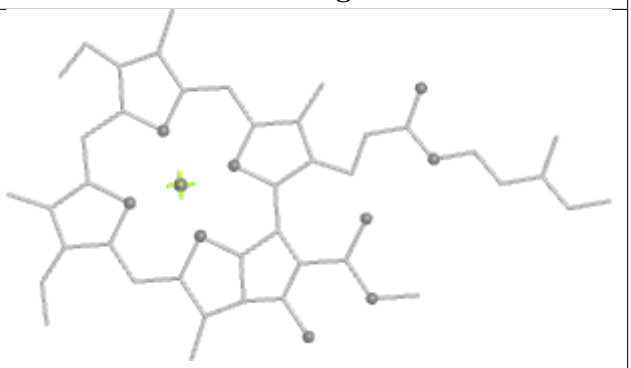
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand CLA A 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

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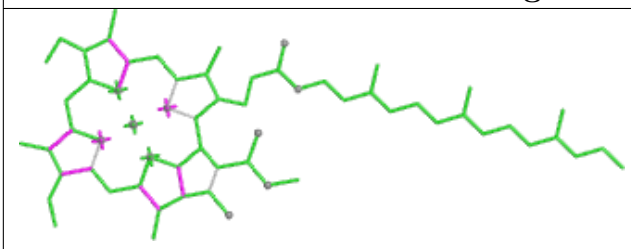
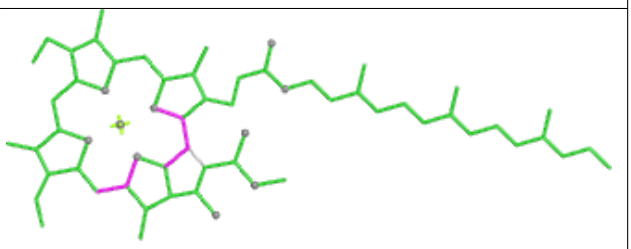
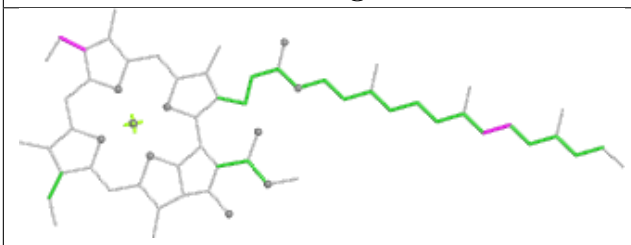
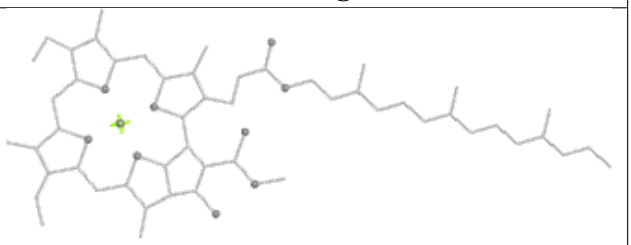
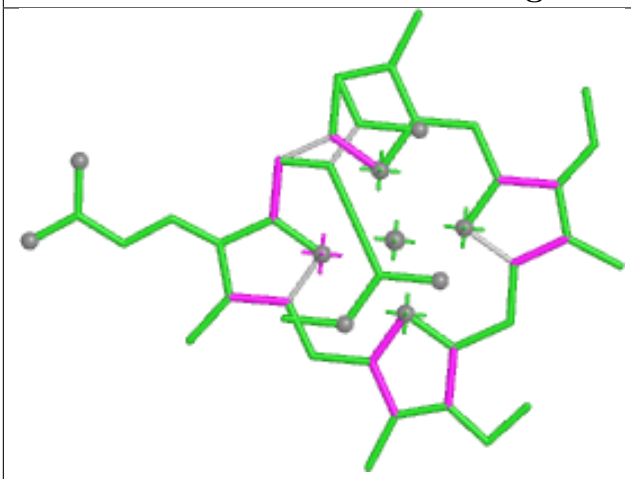
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 Q 210



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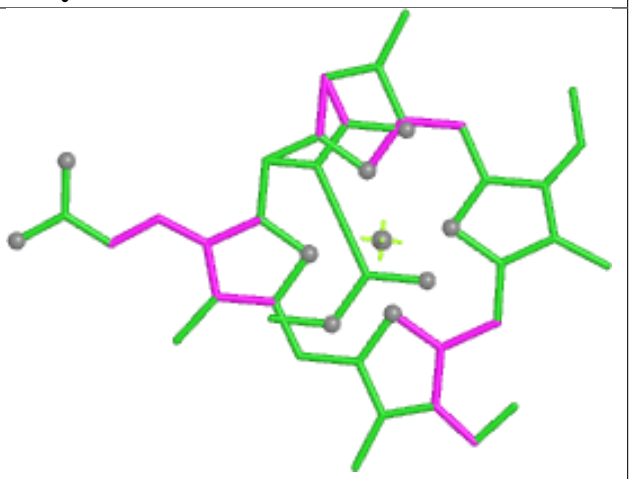

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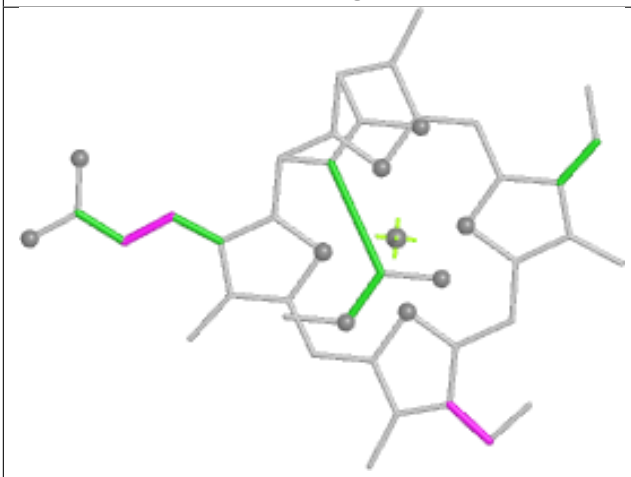

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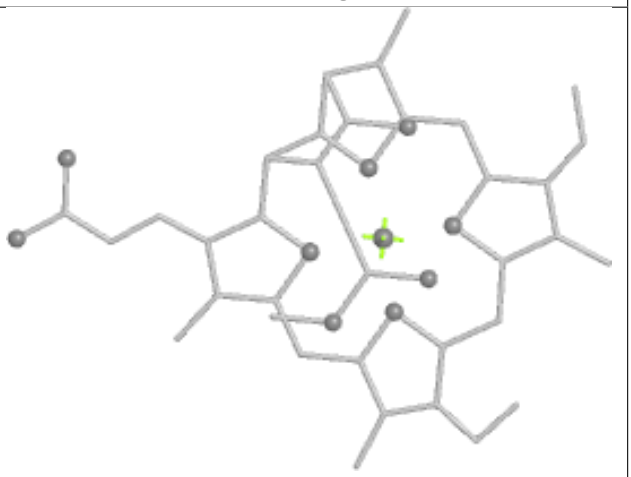
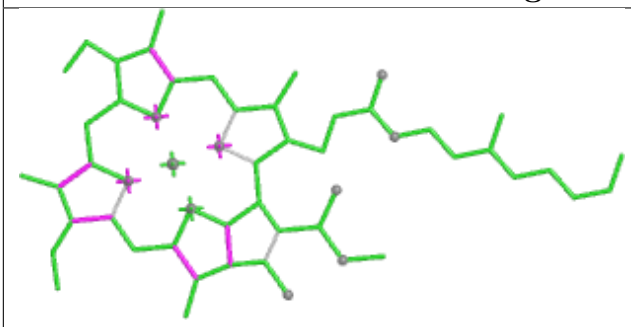


Rings

Ligand CLA B 812



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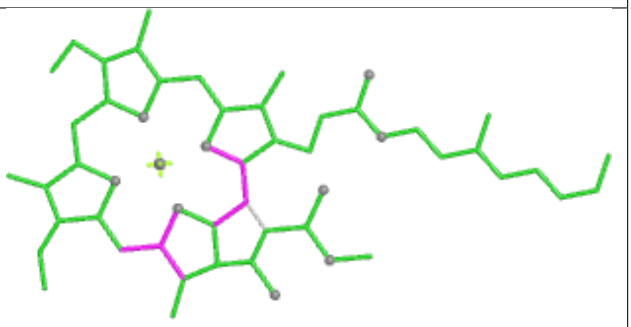

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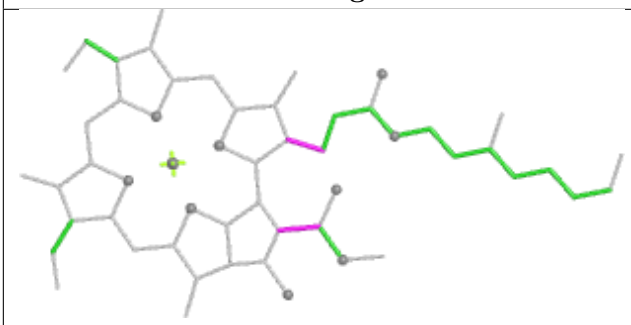

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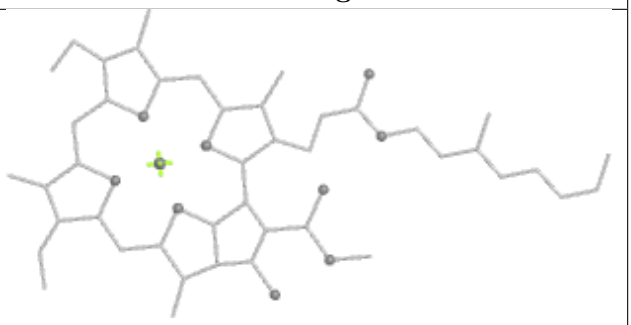
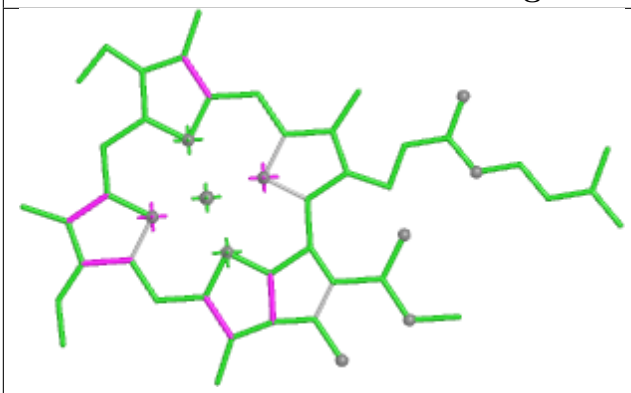


Rings

Ligand CLA A 813



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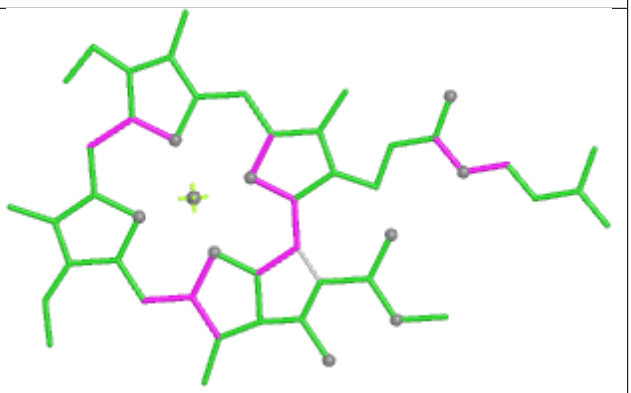

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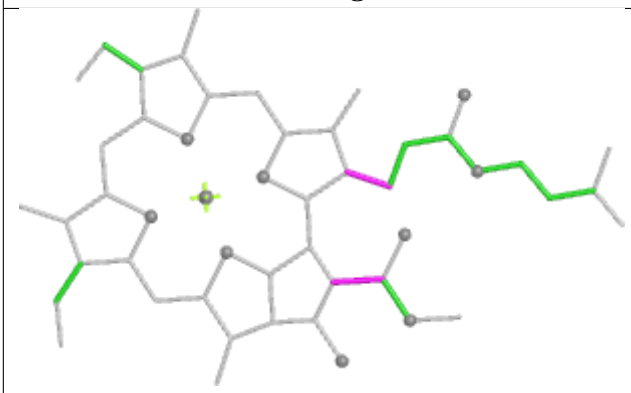

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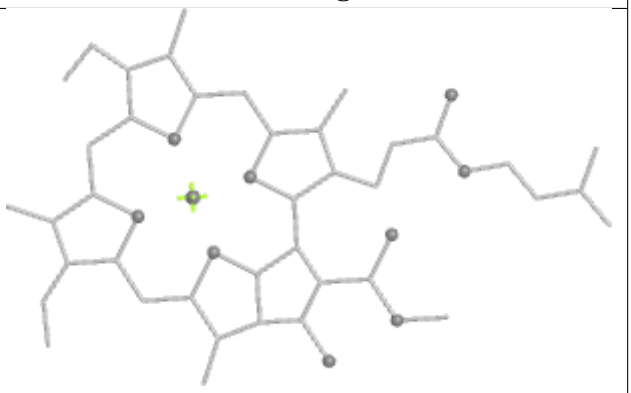
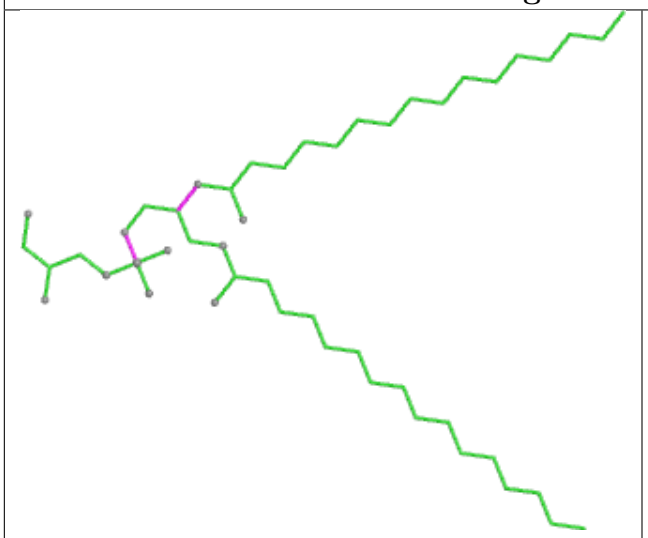


Rings

Ligand LHG R 201



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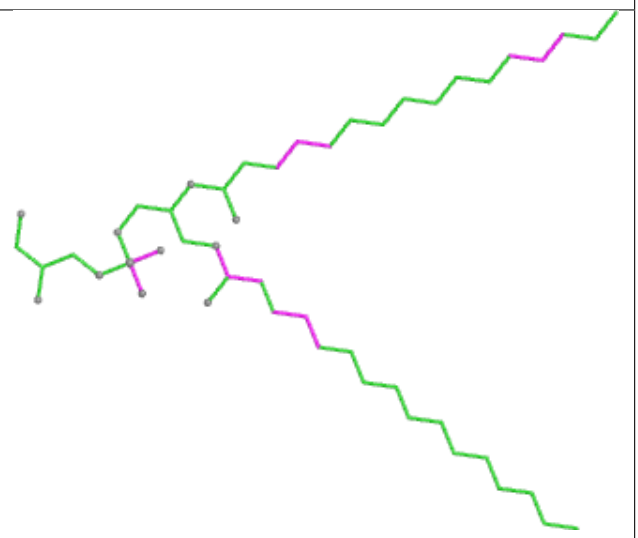

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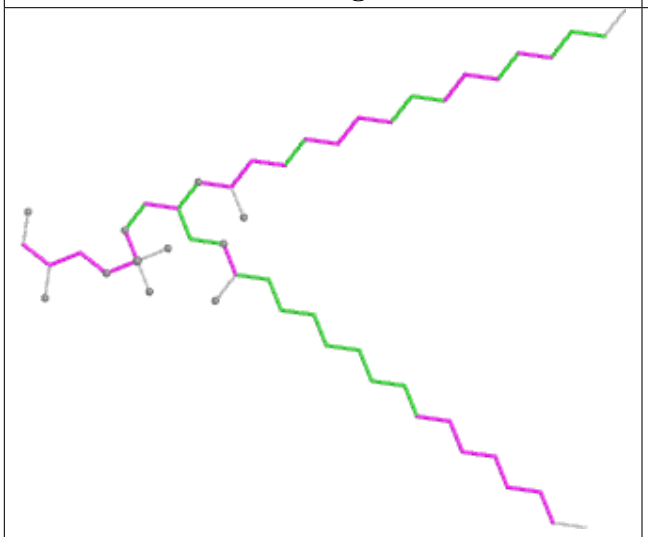

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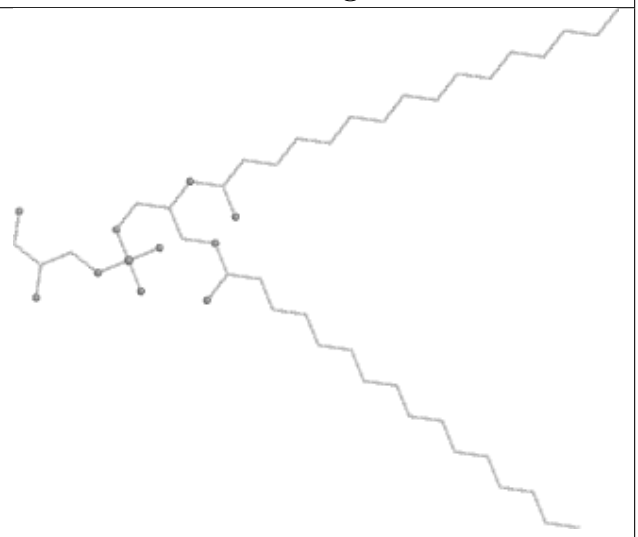
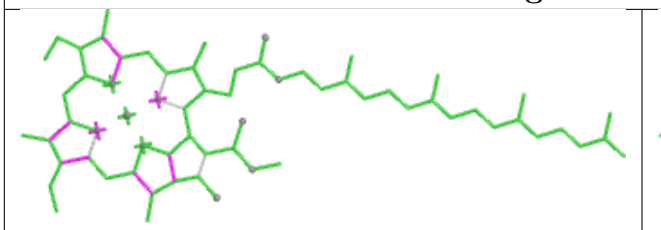


Rings

Ligand CLA B 829



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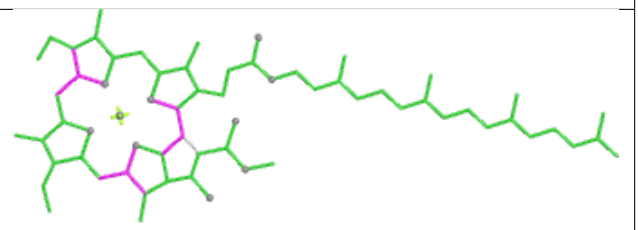

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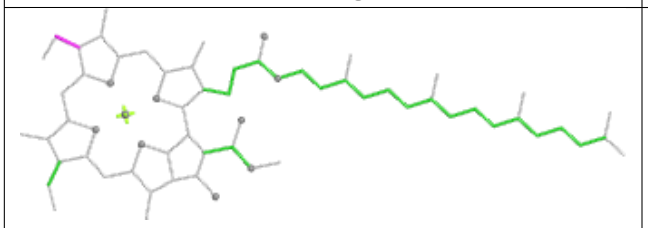

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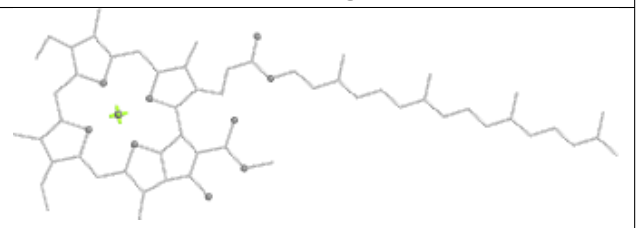
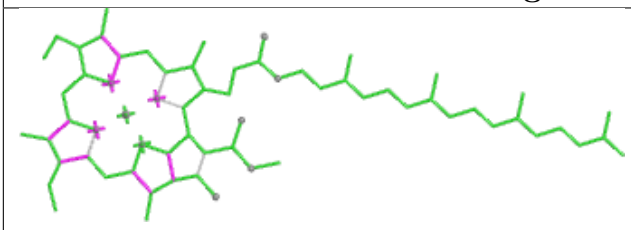
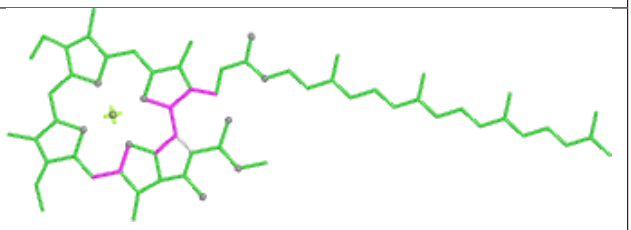
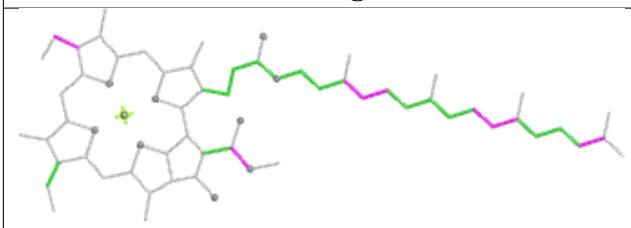
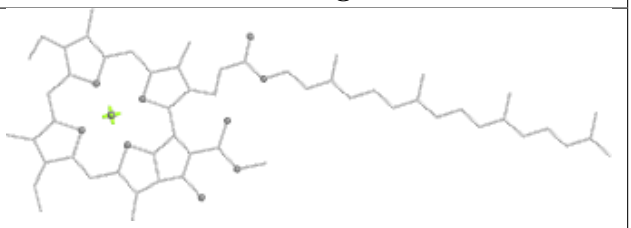
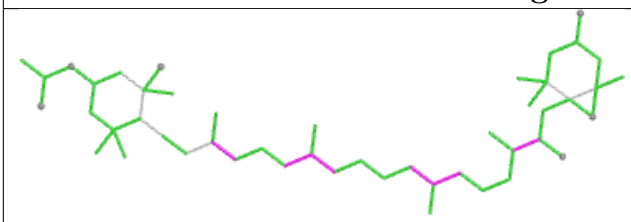
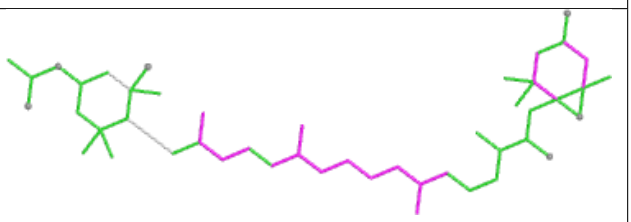
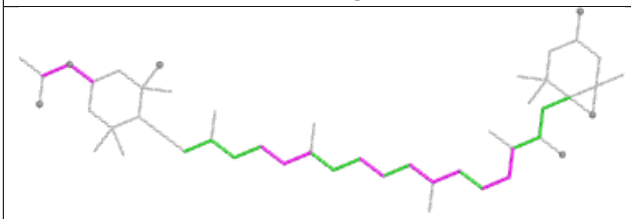
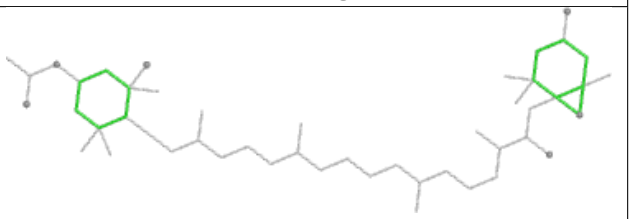
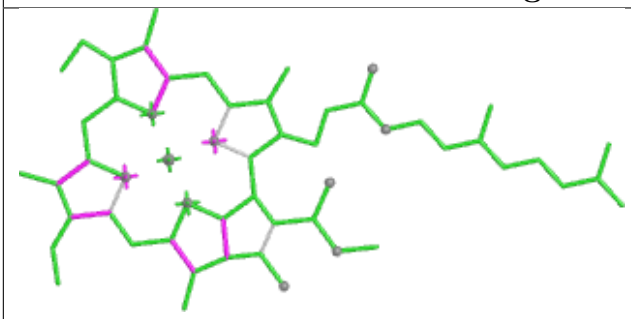
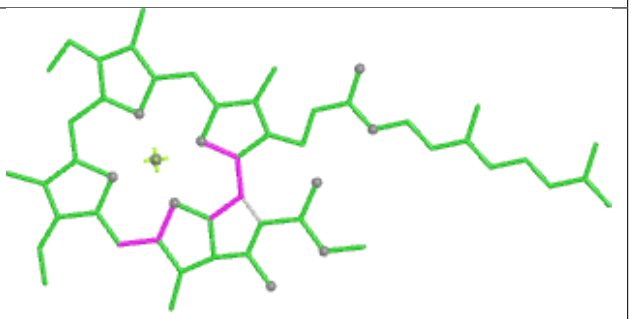
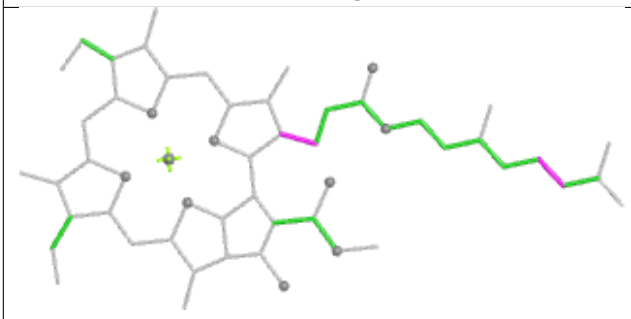
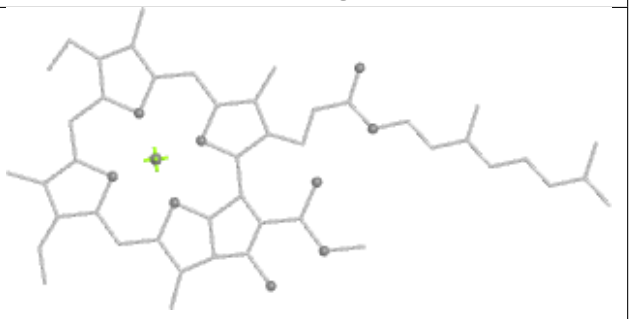
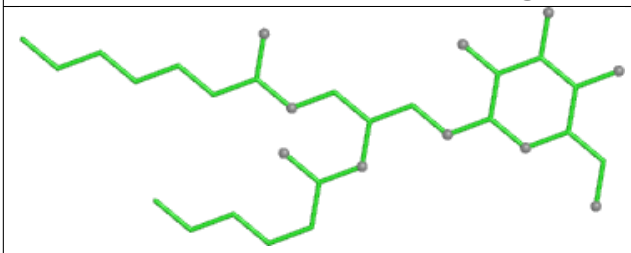
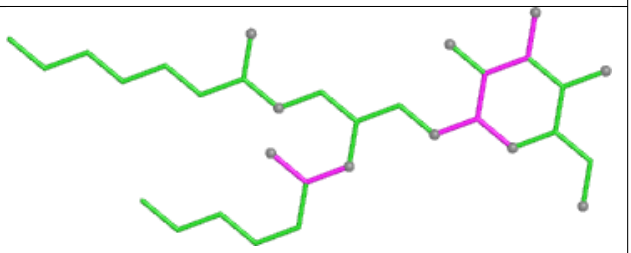
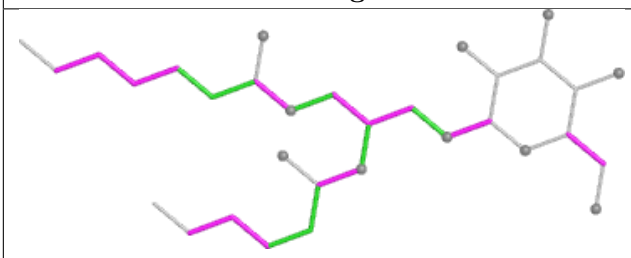
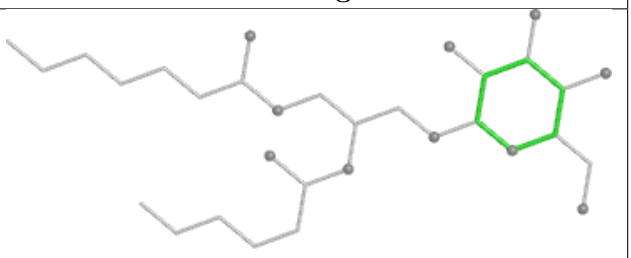


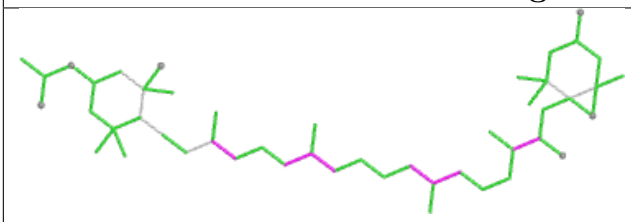
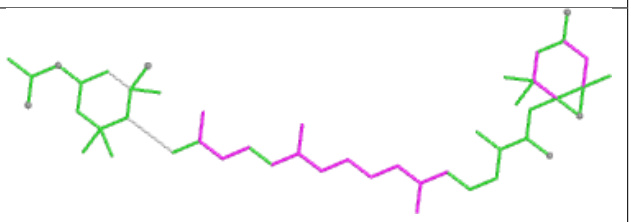
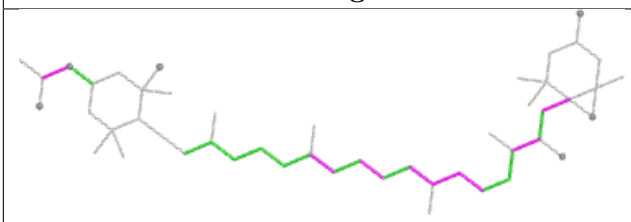
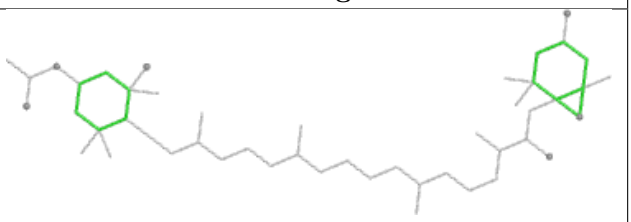
Rings

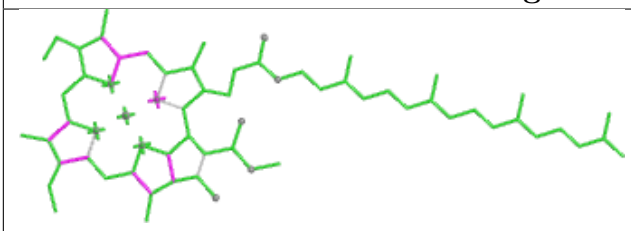
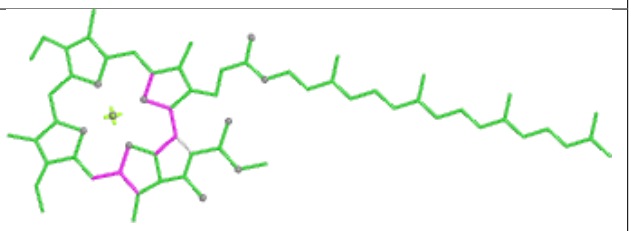
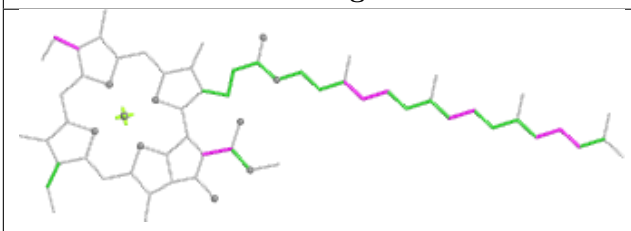
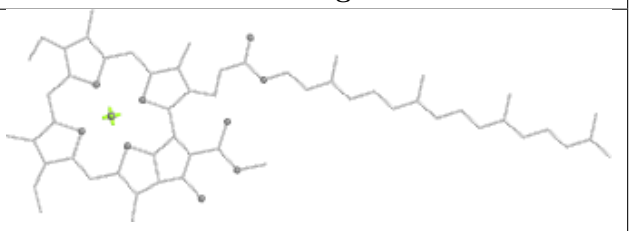
Ligand CLA R 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 P 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

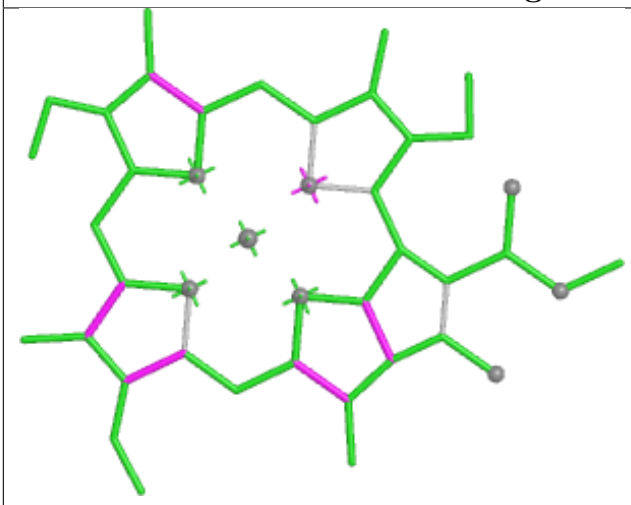
Ligand CLA A 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG U 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

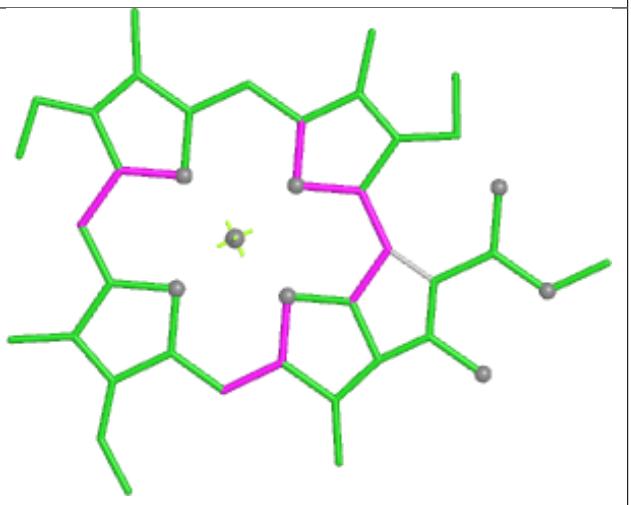
Ligand A86 U 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 210	
 Bond lengths	 Bond angles
 Torsions	 Rings

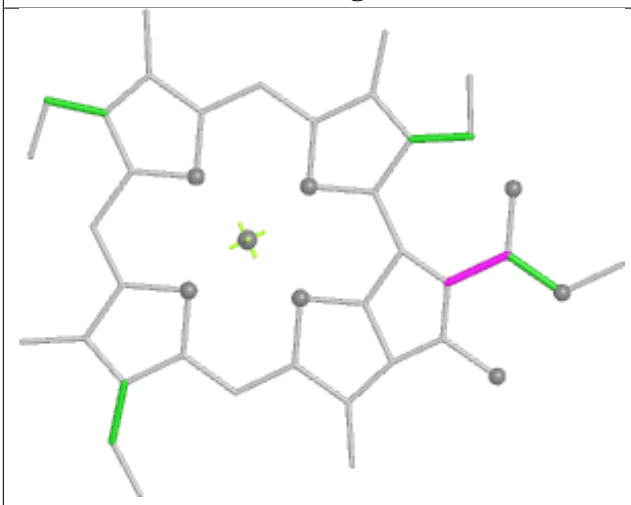
Ligand CLA T 207



Bond lengths



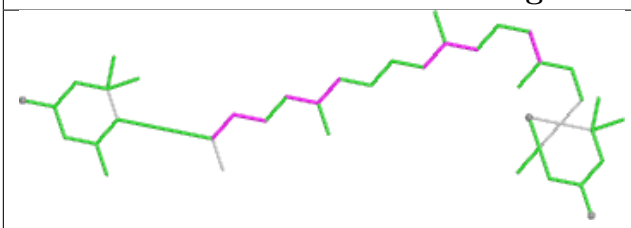
Bond angles



Torsions

Rings

Ligand DD6 T 213



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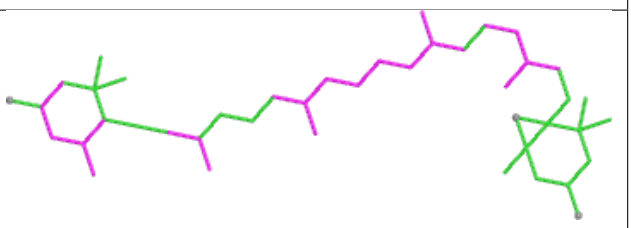

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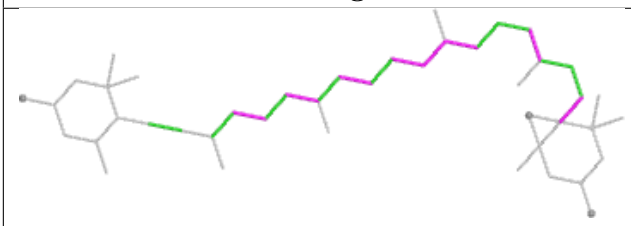

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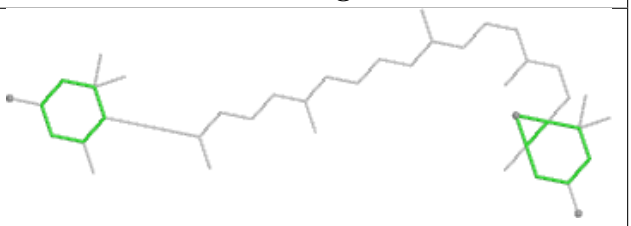
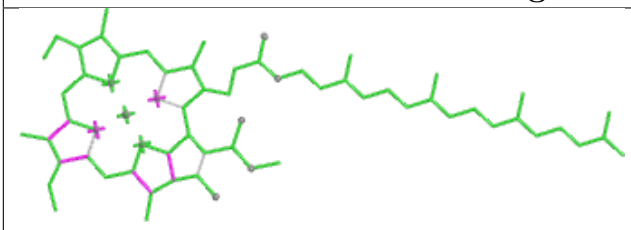
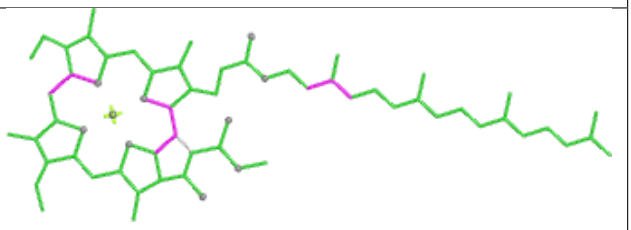
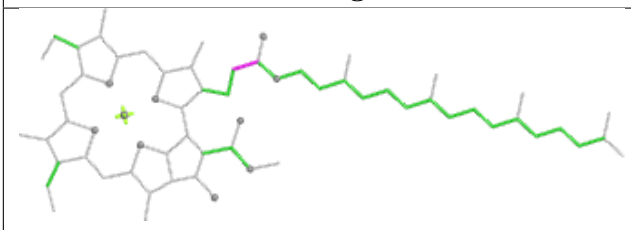
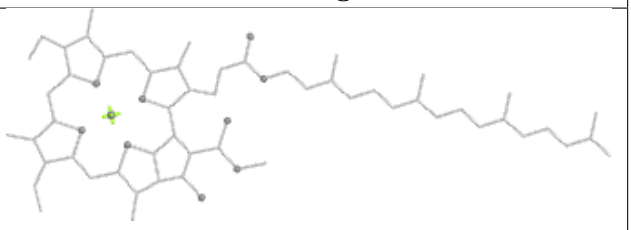
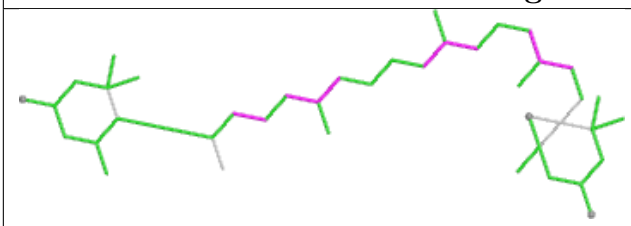
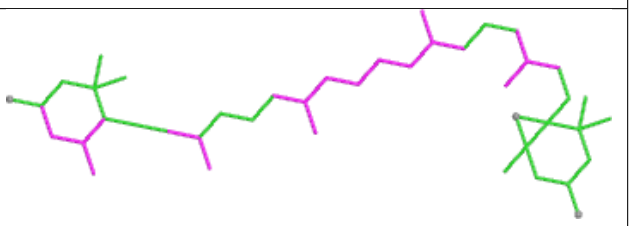
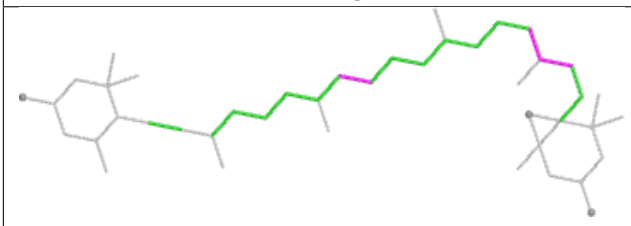
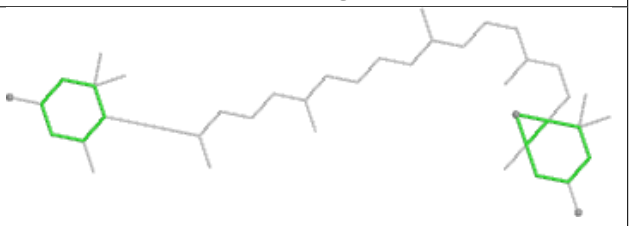
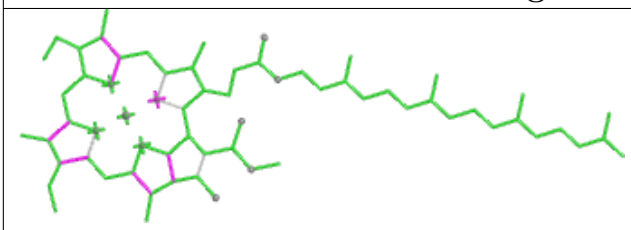
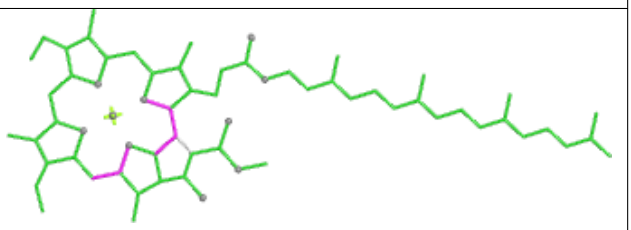
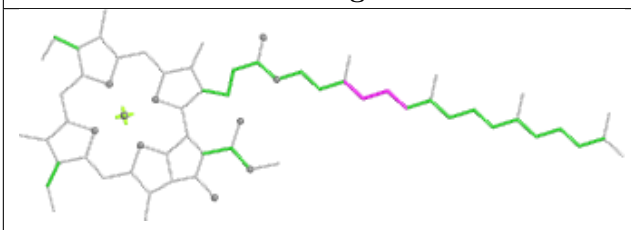
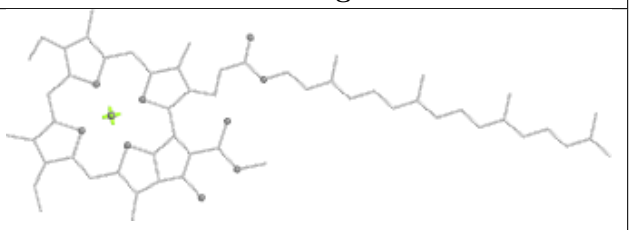
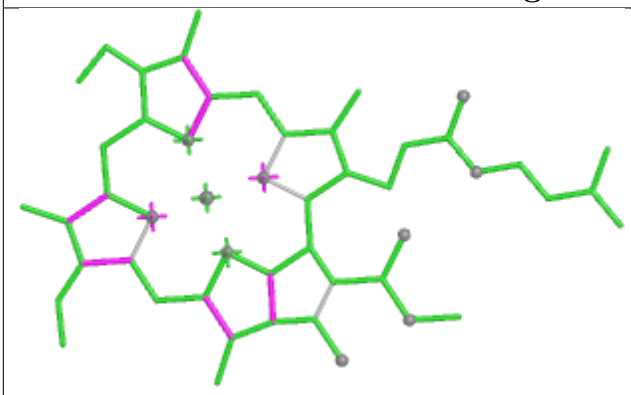
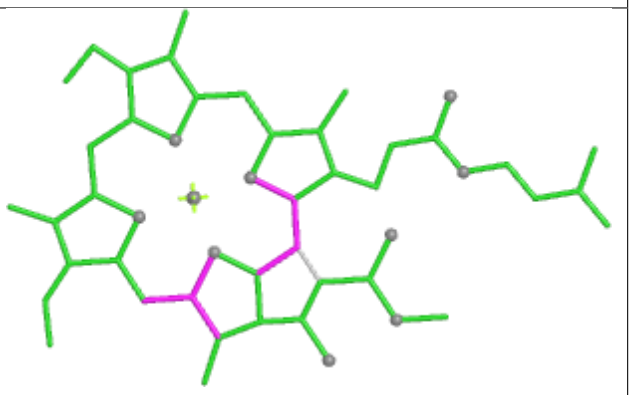
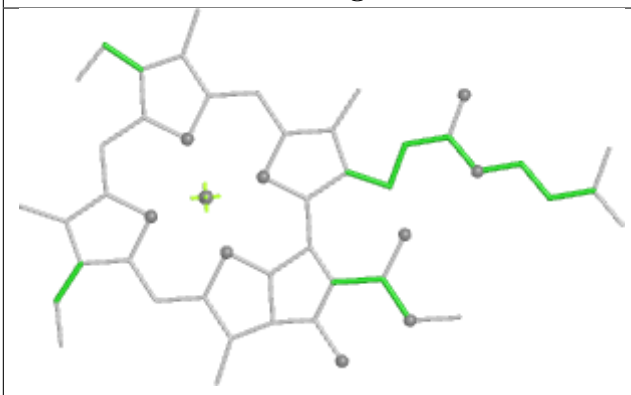
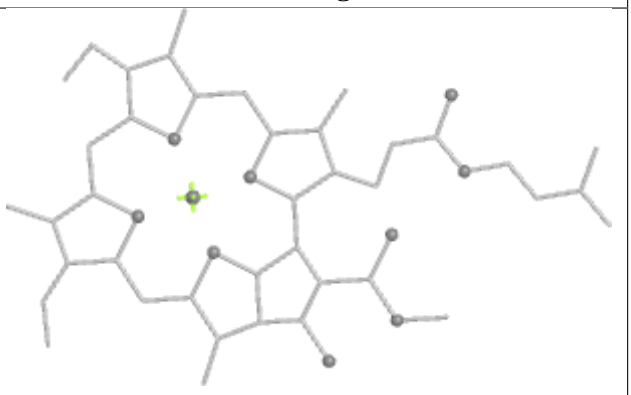


Rings

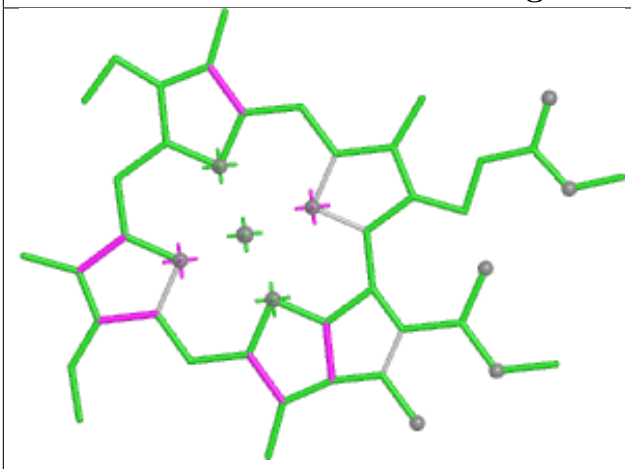
Ligand CL0 A 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 O 213	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 215	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 803



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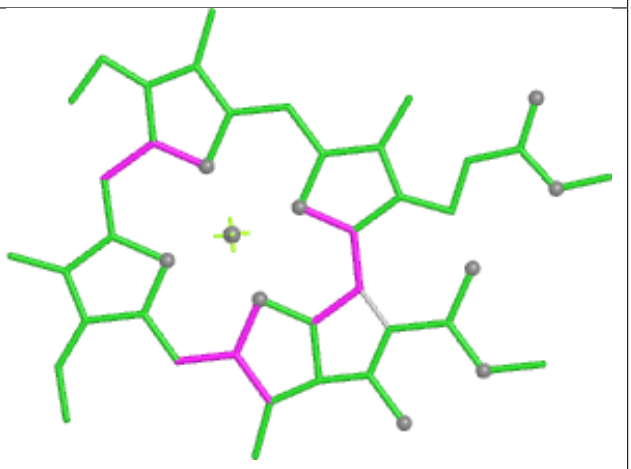

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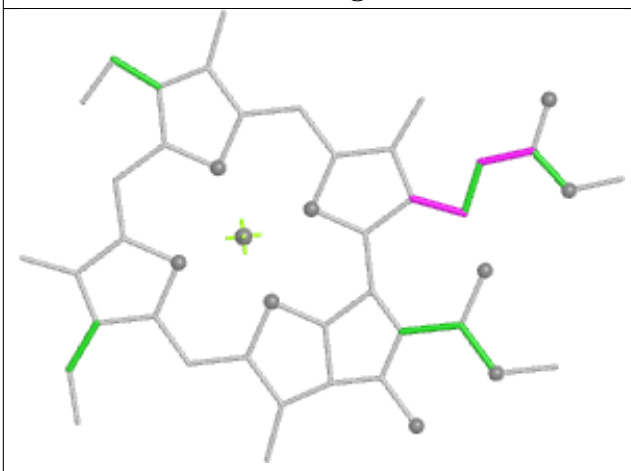

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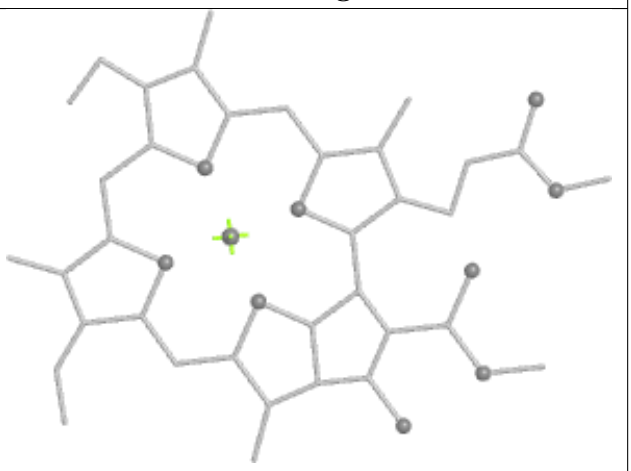
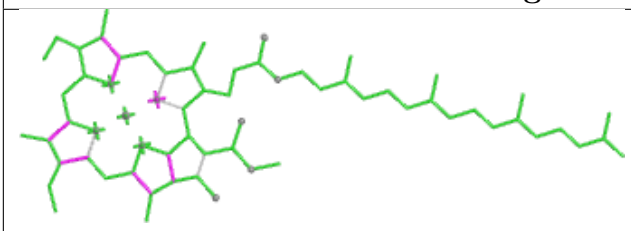


Rings

Ligand CLA O 205



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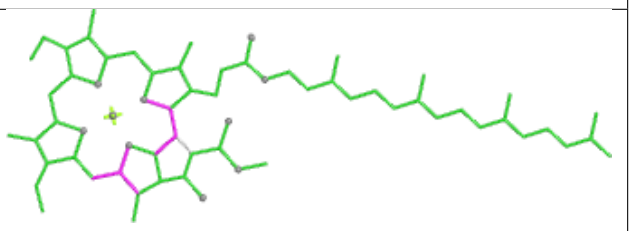

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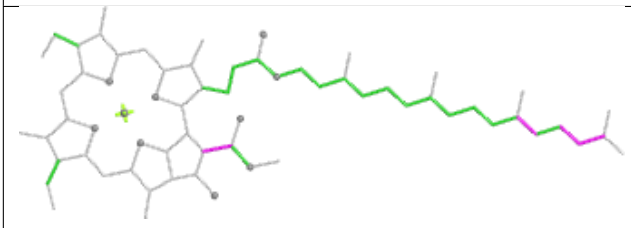

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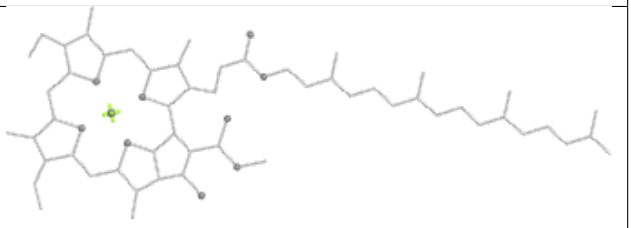
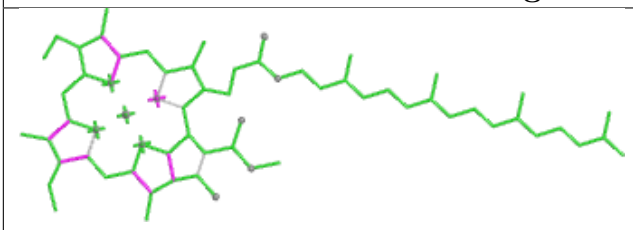


Rings

Ligand CLA A 818



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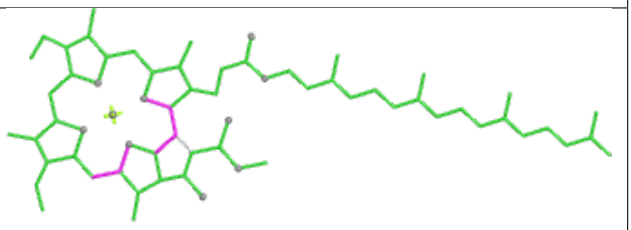

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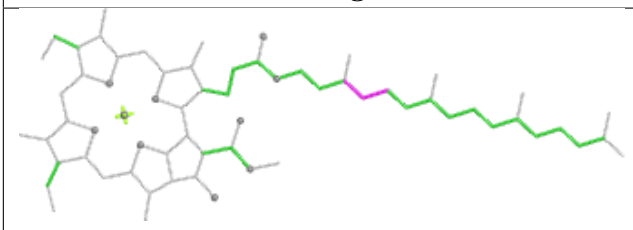

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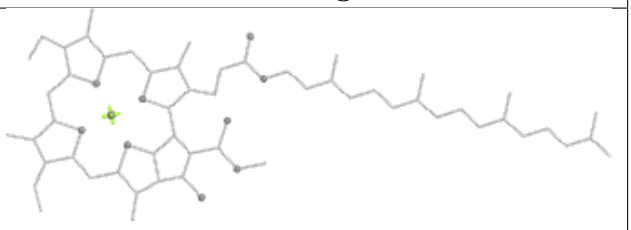
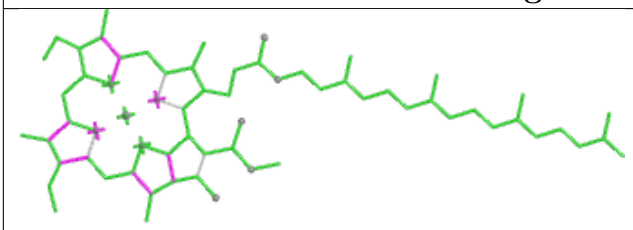


Rings

Ligand CLA B 833



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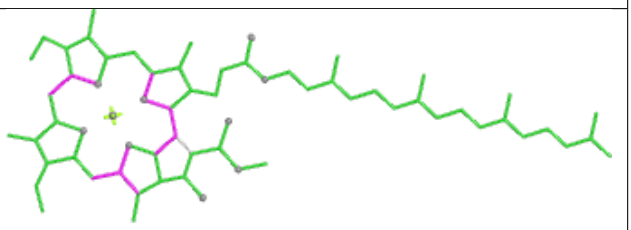
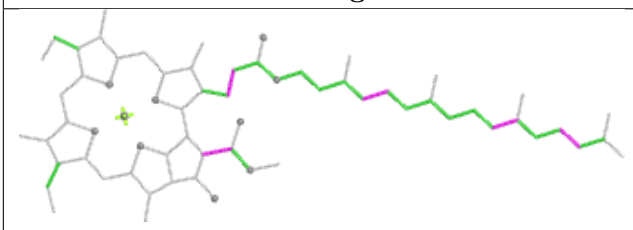


Bond angles



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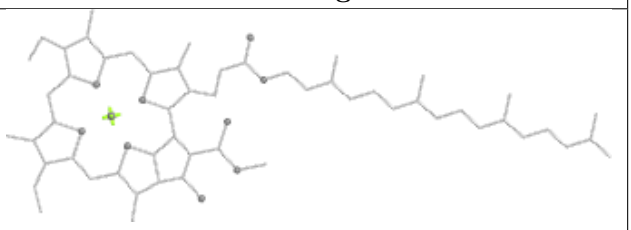
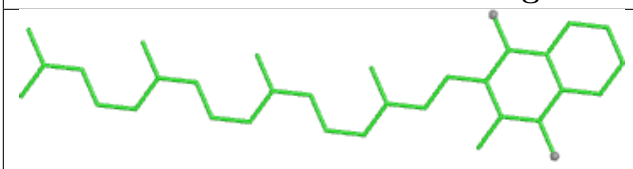


Rings

Ligand PQN B 836



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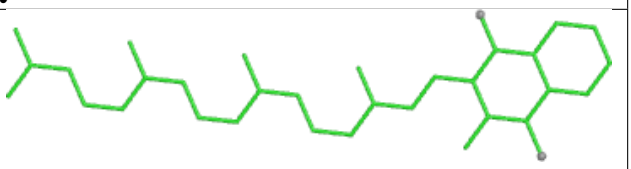
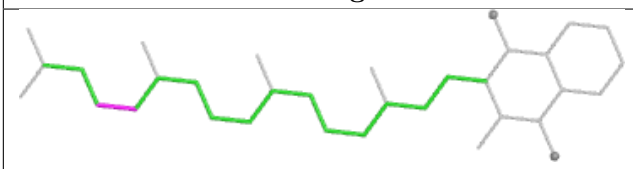


Bond angles



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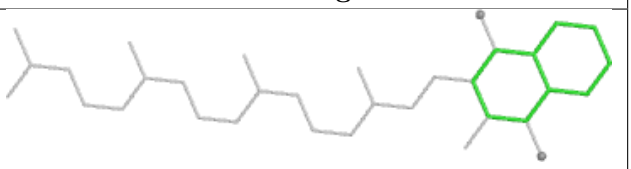
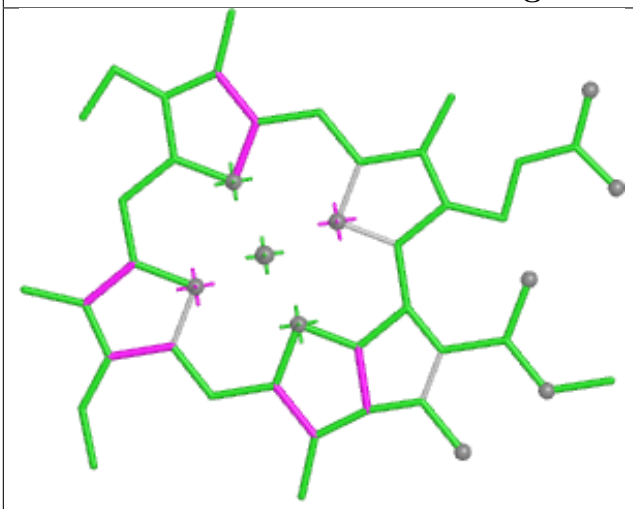


Rings

Ligand CLA A 812



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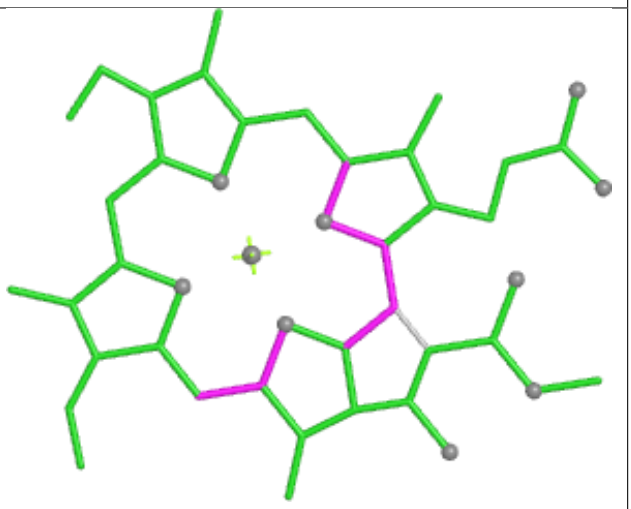
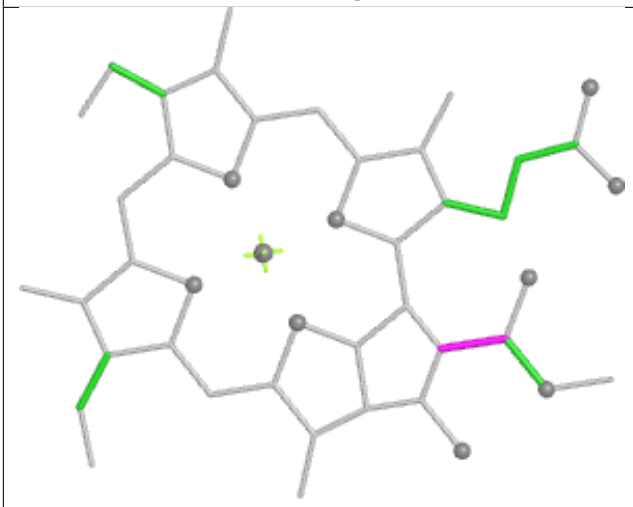


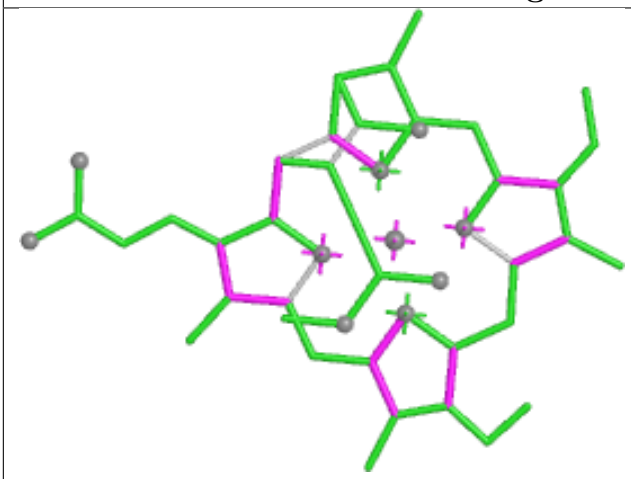
Bond angles



Torsions

Rings

Ligand KC1 P 302



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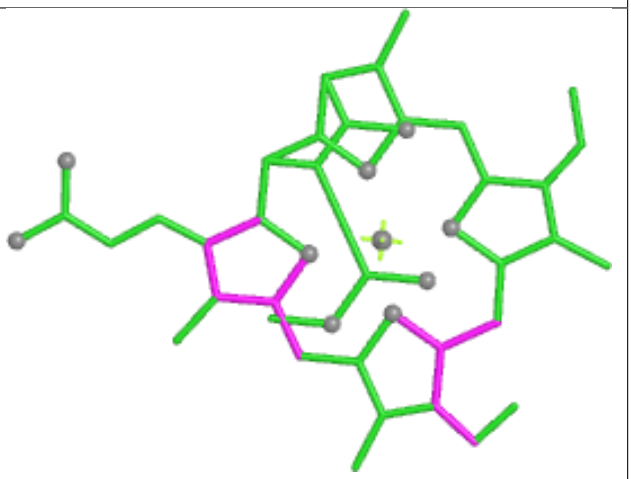
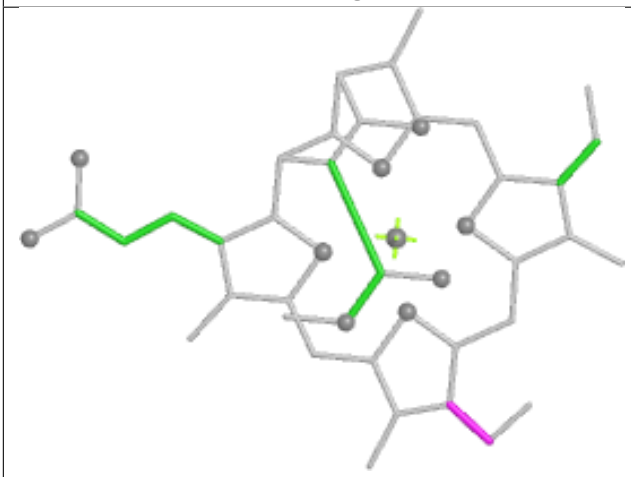


Bond angles



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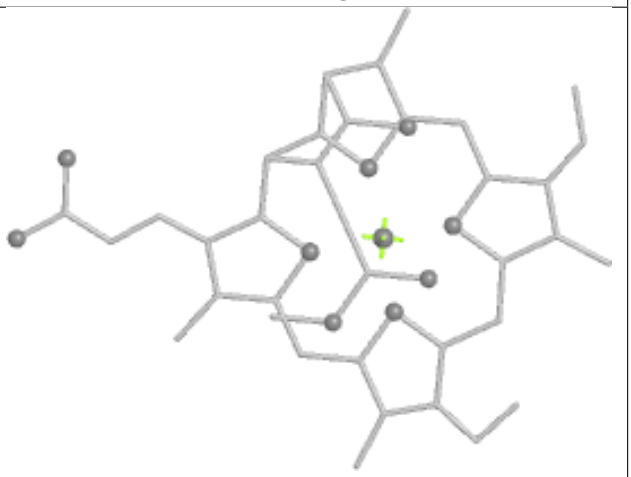
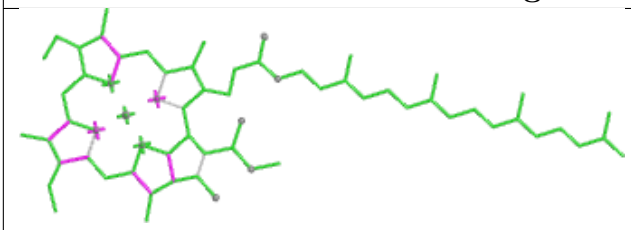


Rings

Ligand CLA A 816



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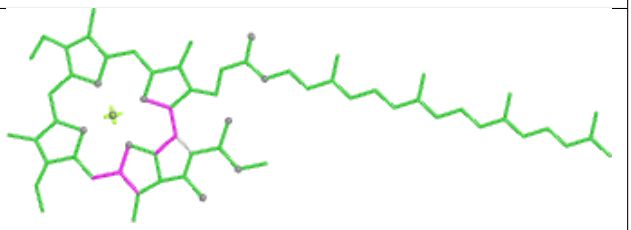

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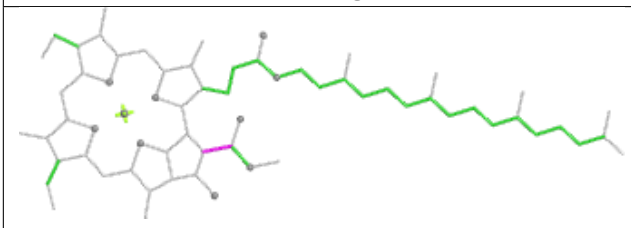
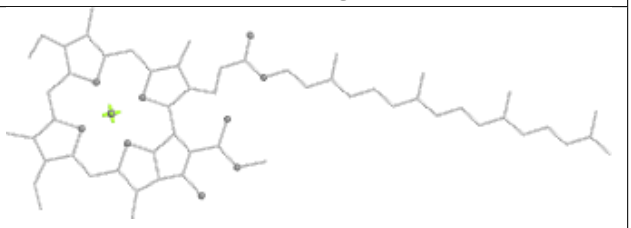


Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

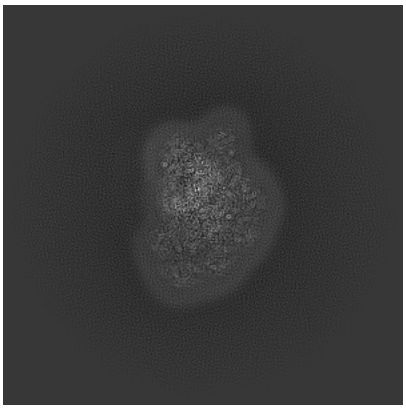
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-64378. These allow visual inspection of the internal detail of the map and identification of artifacts.

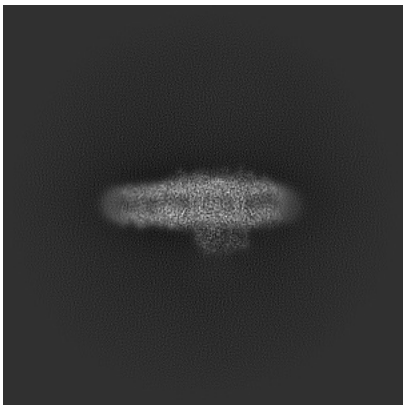
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

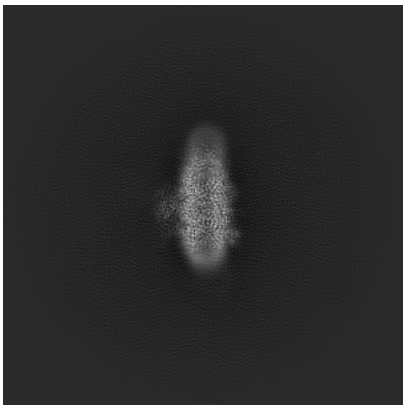
6.1.1 Primary map



X

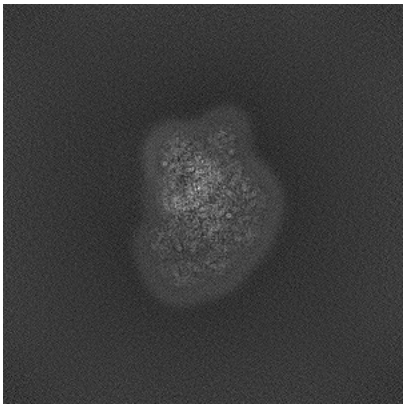


Y

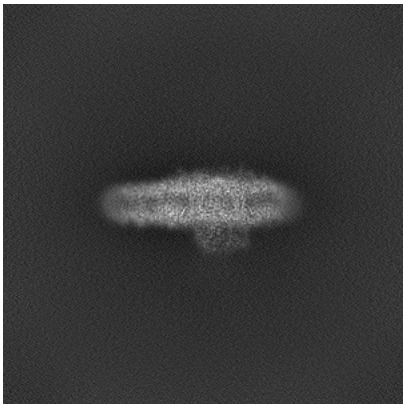


Z

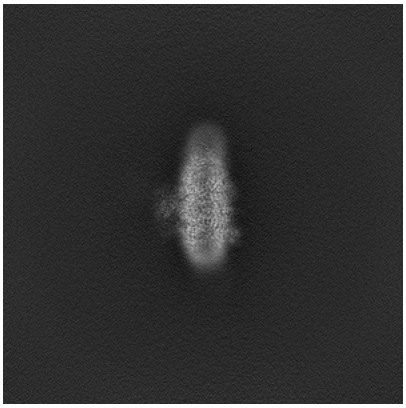
6.1.2 Raw map



X



Y

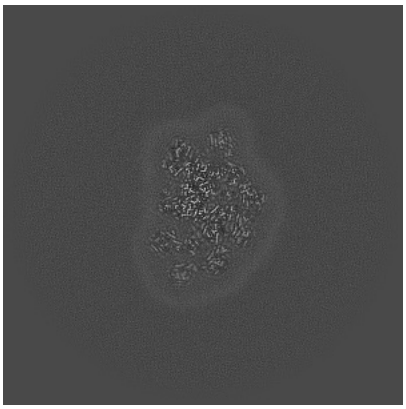


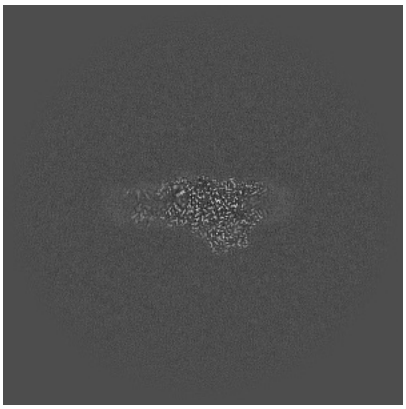
Z

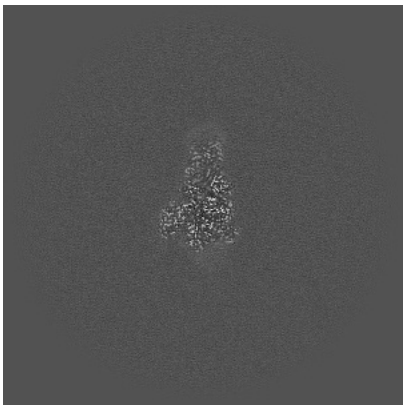
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

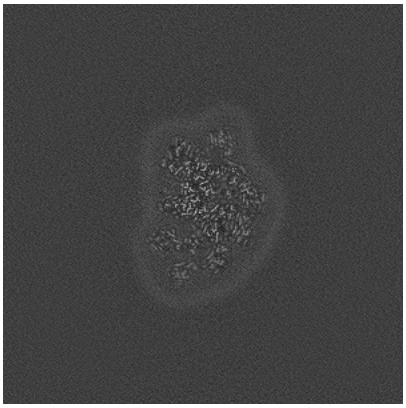
6.2.1 Primary map

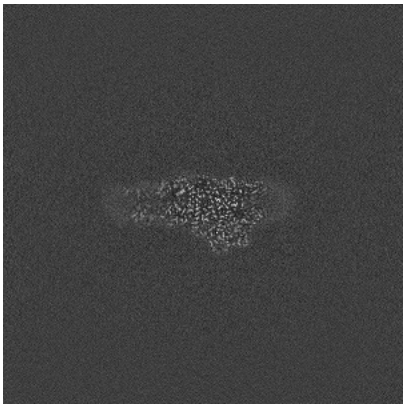

X Index: 300

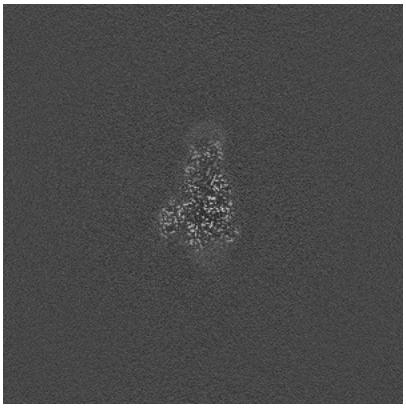

Y Index: 300


Z Index: 300

6.2.2 Raw map


X Index: 300

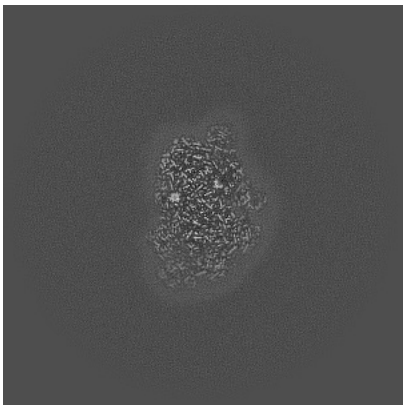

Y Index: 300

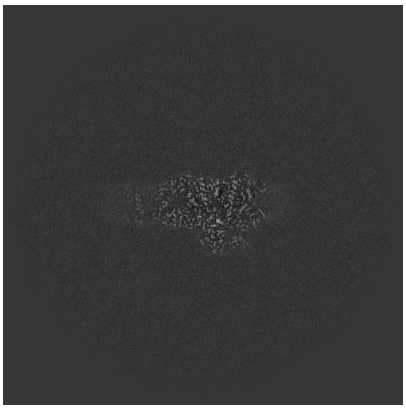

Z Index: 300

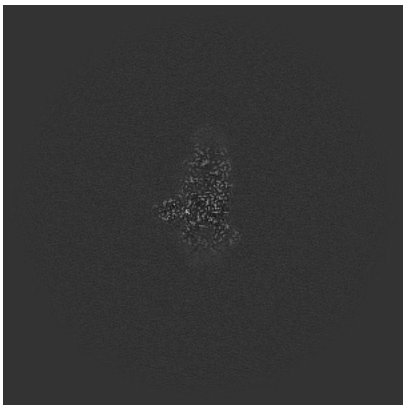
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

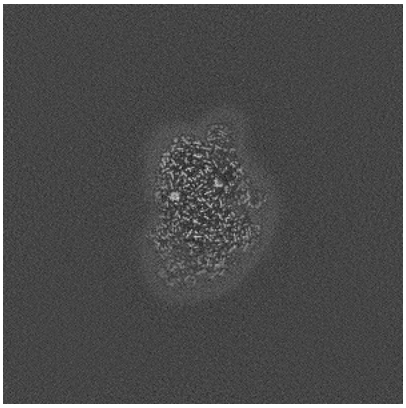
6.3.1 Primary map

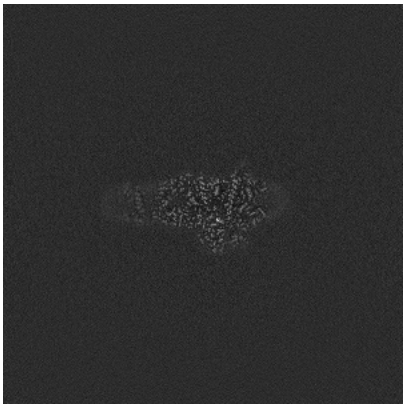

X Index: 284

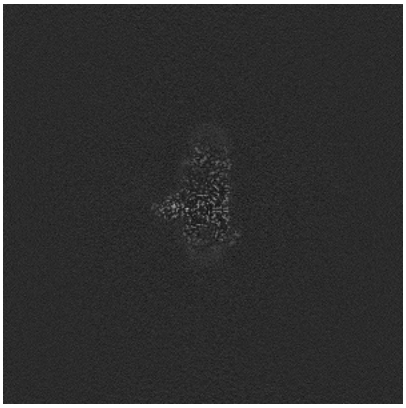

Y Index: 289


Z Index: 320

6.3.2 Raw map


X Index: 284

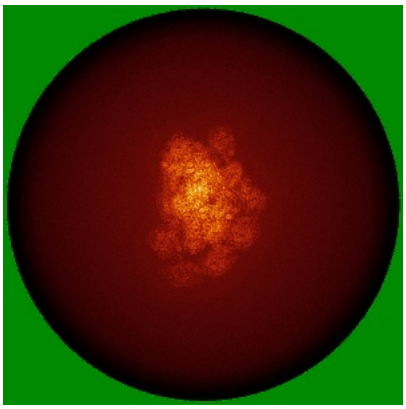

Y Index: 289

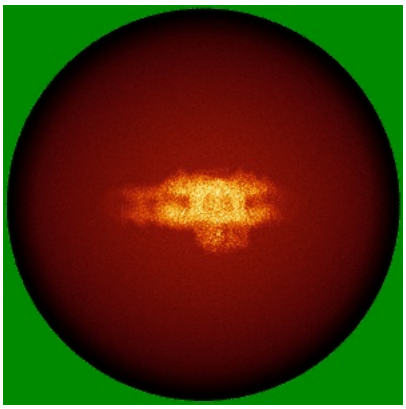

Z Index: 322

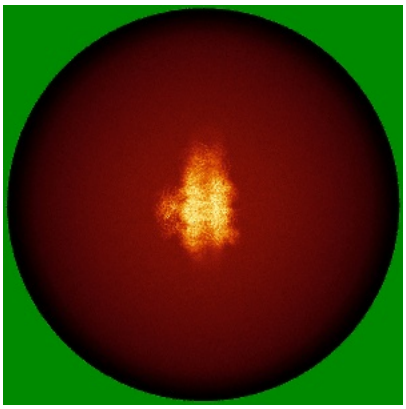
The images above show the largest variance slices of the map in three orthogonal directions.

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

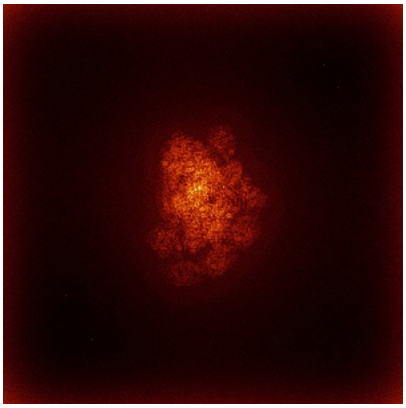
6.4.1 Primary map

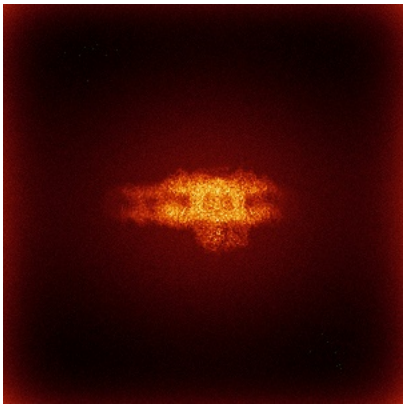

X

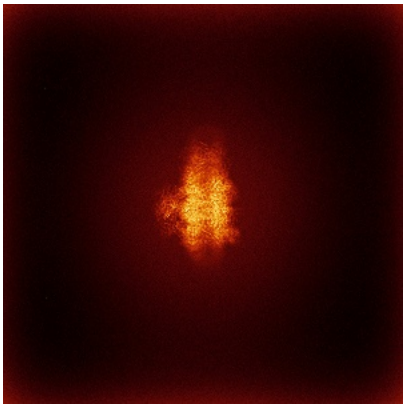

Y


Z

6.4.2 Raw map


X

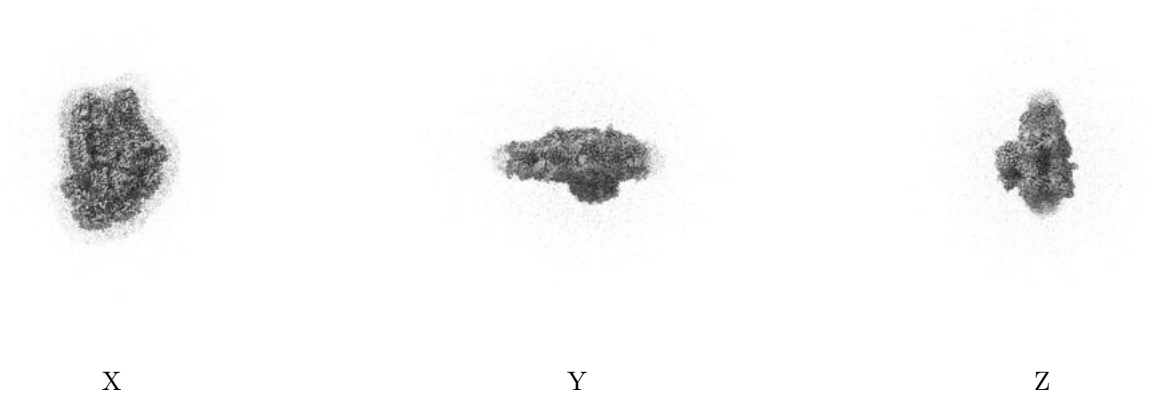

Y


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)

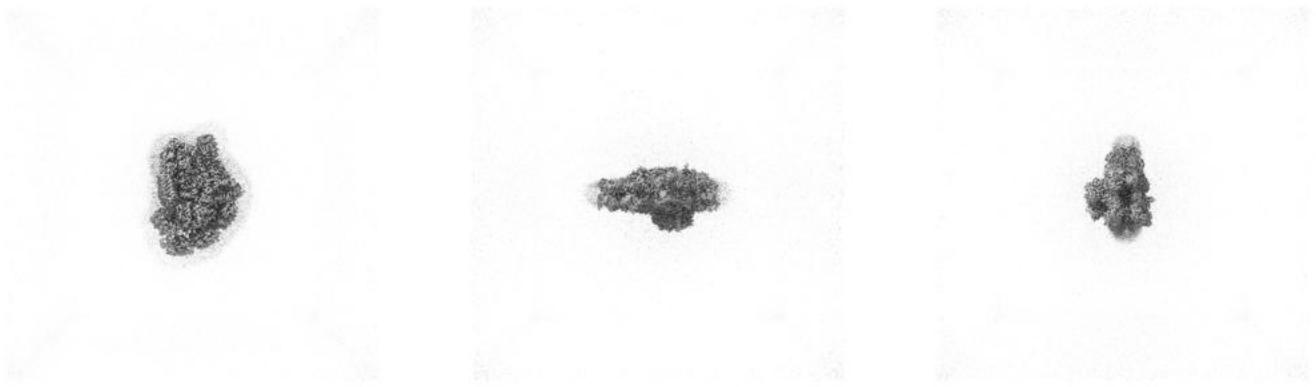
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

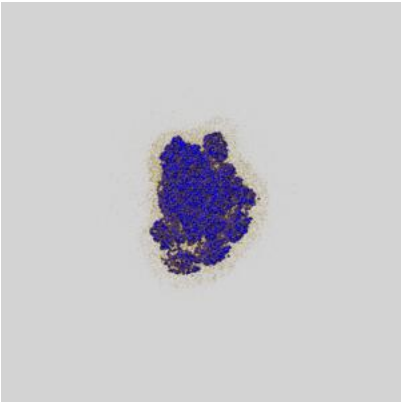
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

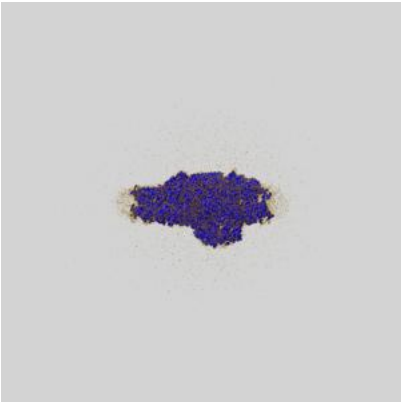
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

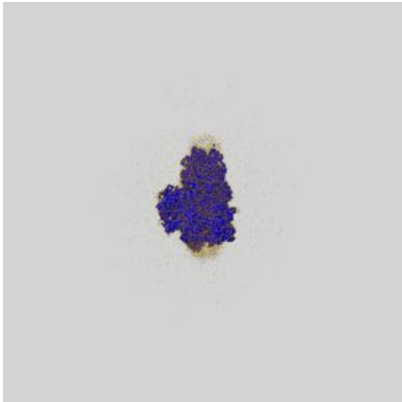
6.6.1 emd_64378_msk_1.map (i)



X



Y

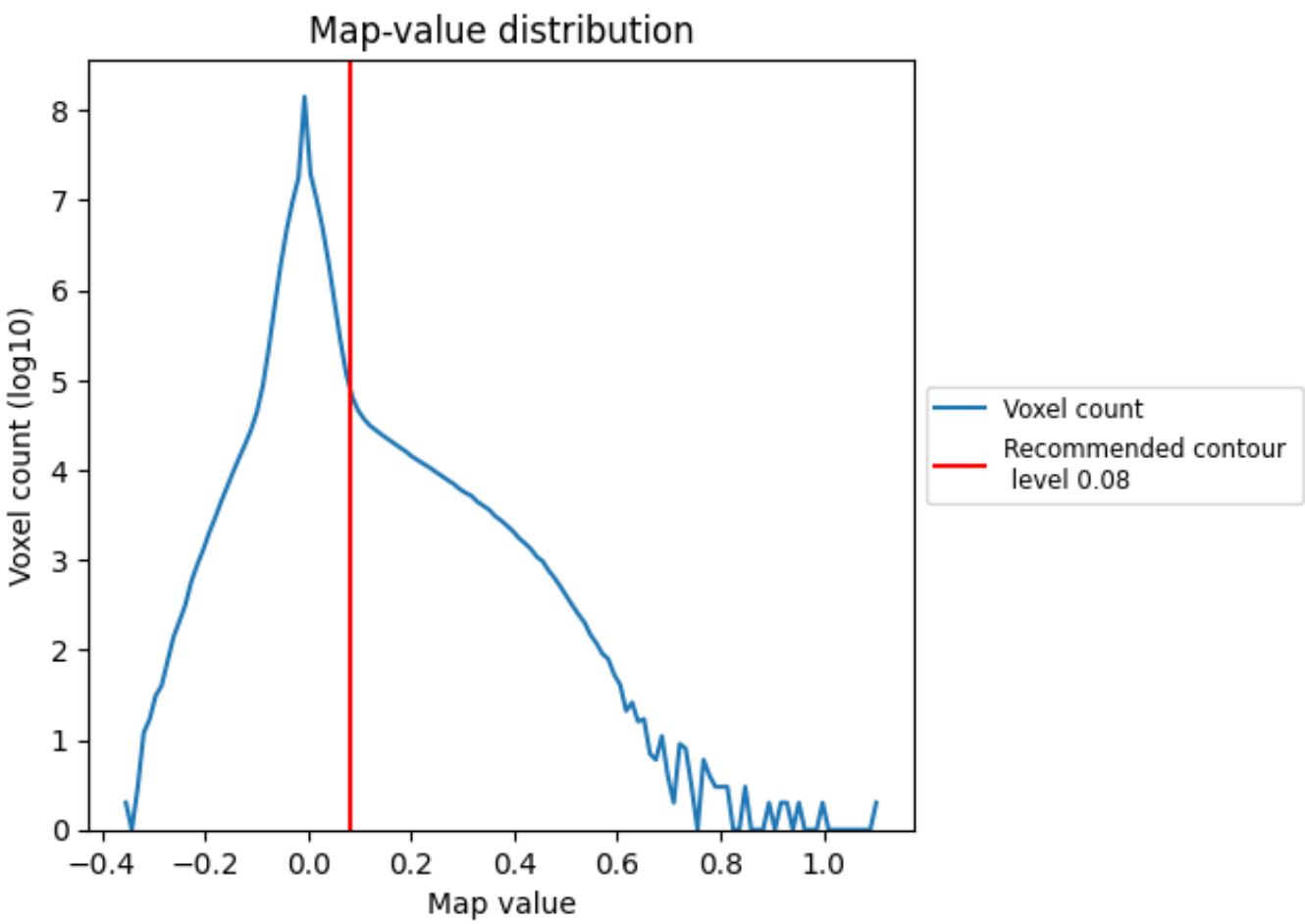


Z

7 Map analysis (i)

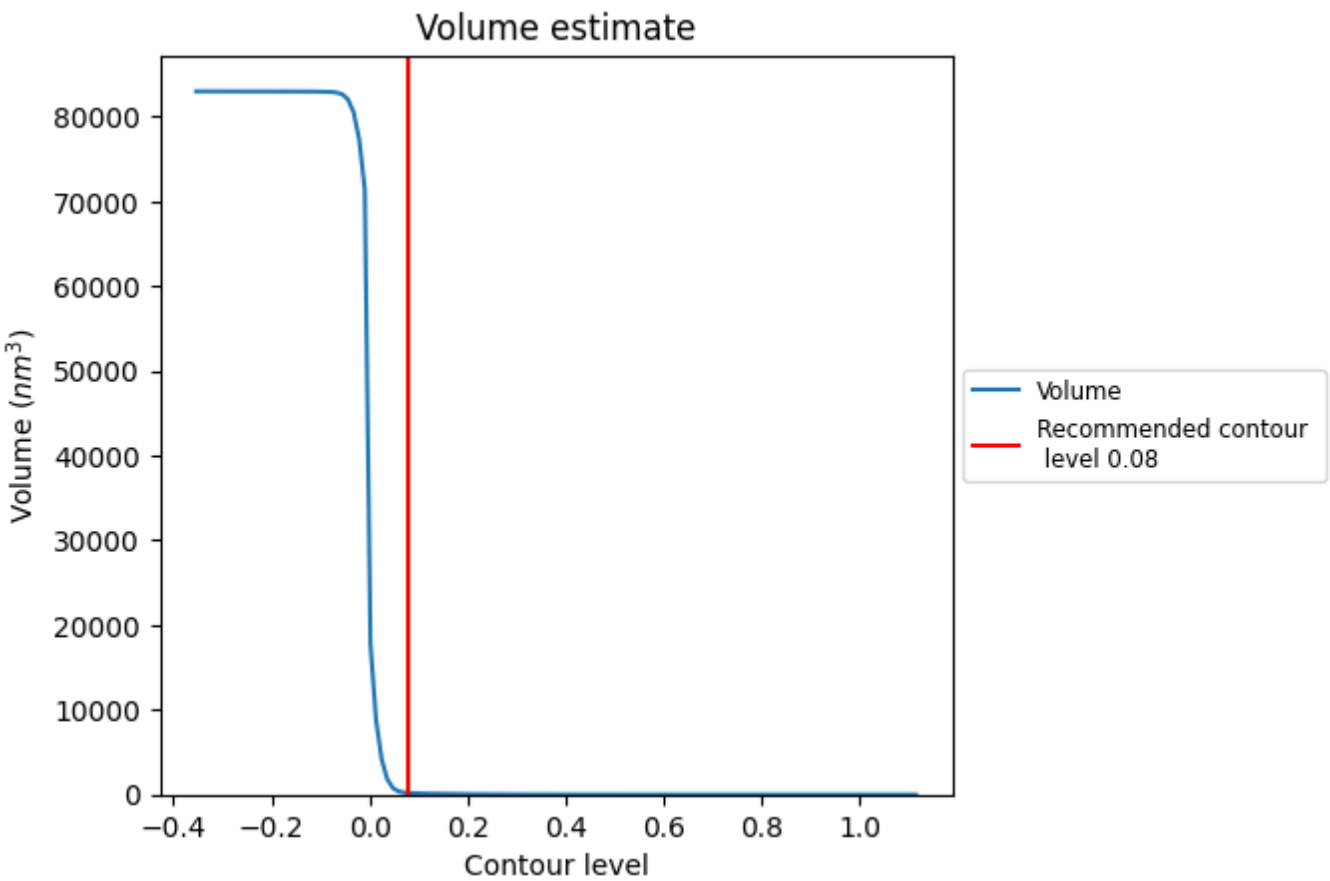
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

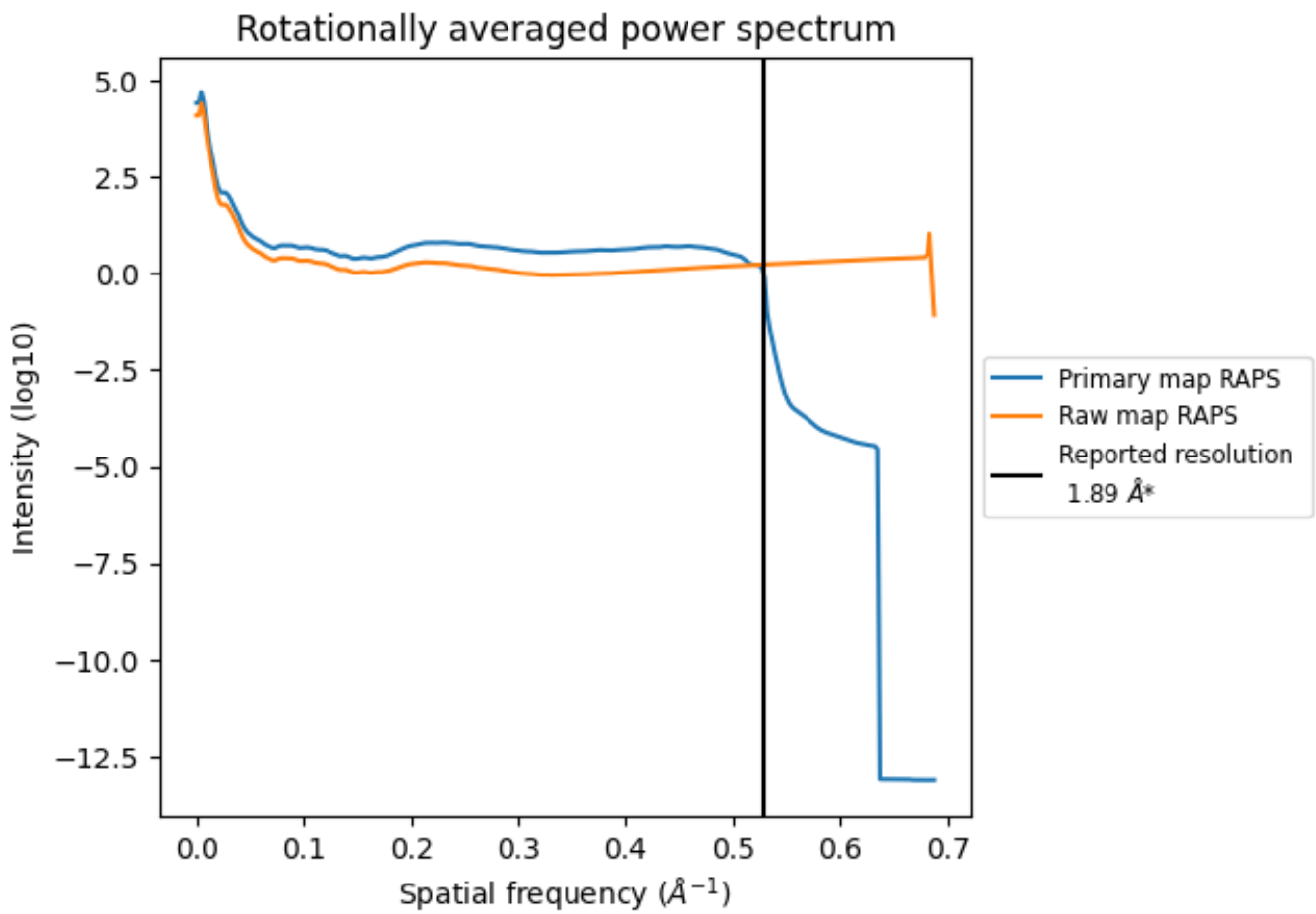
7.2 Volume estimate (i)



The volume at the recommended contour level is 189 nm^3; this corresponds to an approximate mass of 171 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)

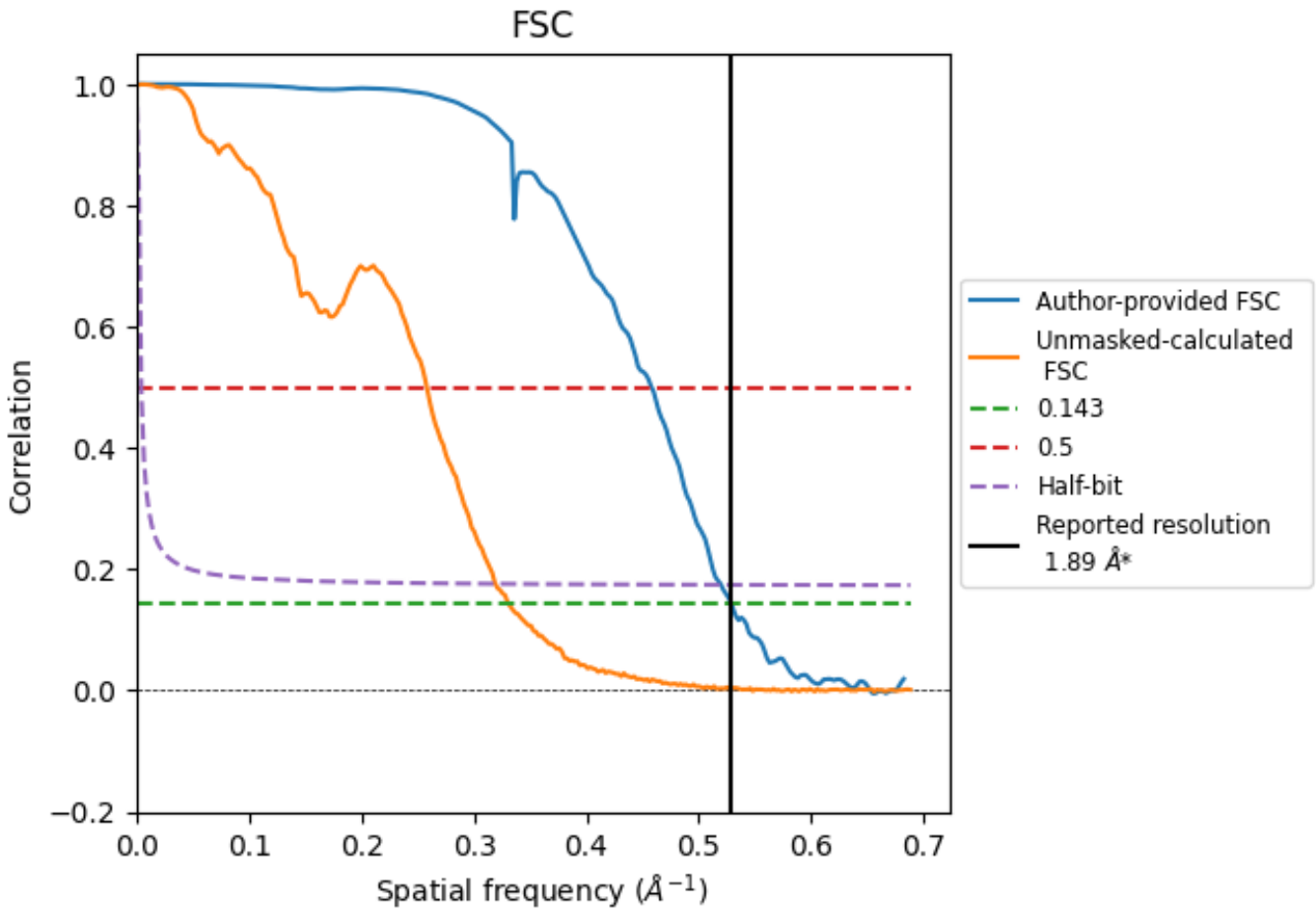


*Reported resolution corresponds to spatial frequency of 0.529 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.529 Å^{-1}

8.2 Resolution estimates (i)

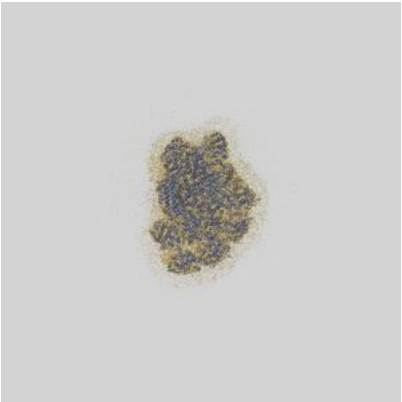
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.89	-	-
Author-provided FSC curve	1.89	2.18	1.92
Unmasked-calculated*	3.02	3.87	3.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 1.89 by more than 10 %

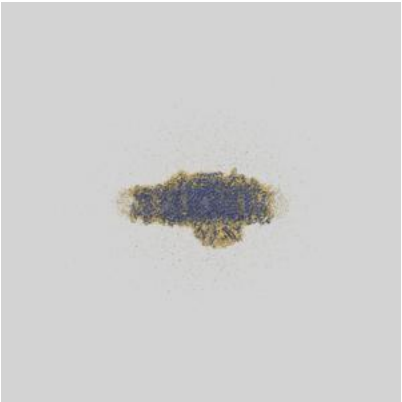
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-64378 and PDB model 9UOF. Per-residue inclusion information can be found in section 3 on page 24.

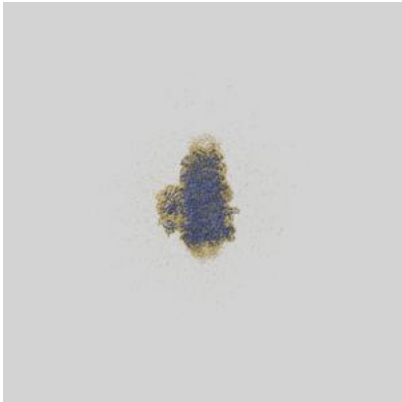
9.1 Map-model overlay (i)



X



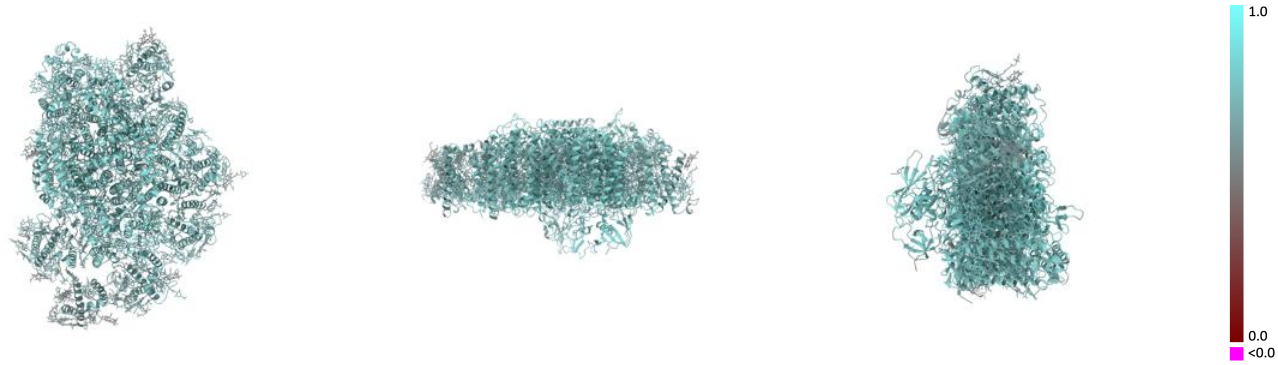
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

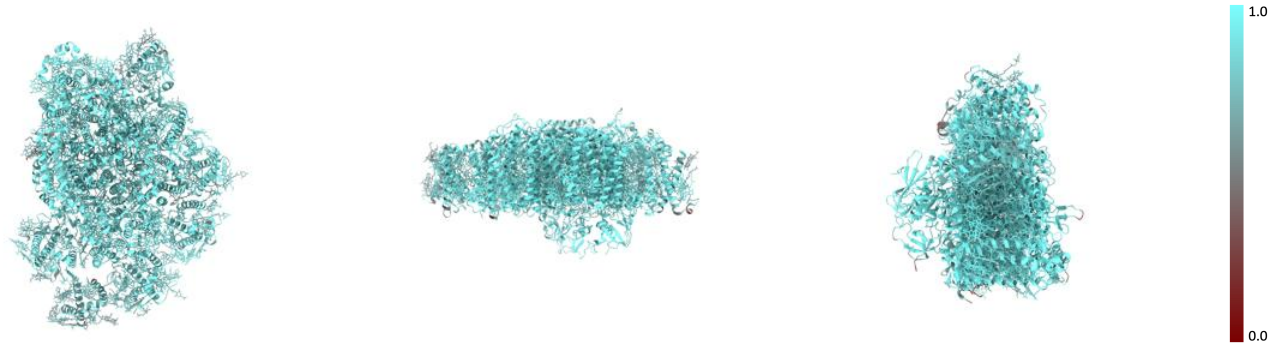
9.2 Q-score mapped to coordinate model (i)



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.

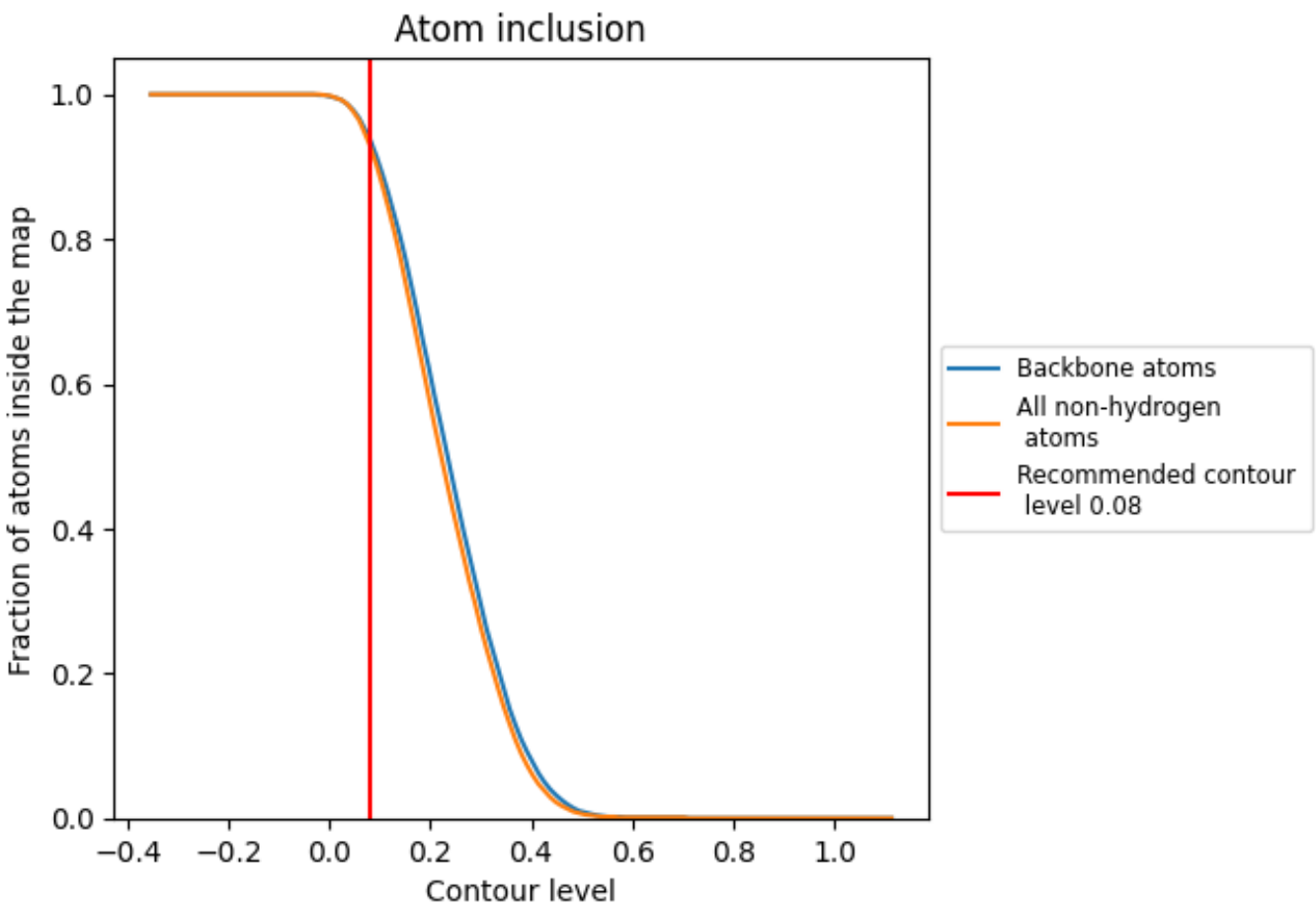
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9300	0.7370
A	0.9580	0.7640
B	0.9770	0.7850
C	0.9920	0.8000
D	0.9440	0.7530
E	0.9060	0.7410
F	0.9400	0.7380
I	0.9740	0.7650
J	0.8270	0.6700
L	0.9540	0.7540
M	0.9530	0.7490
O	0.9110	0.7000
P	0.8790	0.6780
Q	0.8560	0.6690
R	0.9380	0.7320
S	0.9110	0.7100
T	0.7480	0.6010
U	0.8360	0.6690