Full wwPDB EM Validation Report (i)

Sep 15, 2026 – 06:48 PM JST

PDB ID	:	9UH4 / pdb_00009uh4
EMDB ID	:	EMD-64154
Title	:	PSI-4 FCPI supercomplex from haptophyte Chrysotila roscoffensis
Authors	:	La Rocca, R.; Tsai, P.-C.; Kato, K.; Nakajima, Y.; Akita, F.; Shen, J.-R.
Deposited on	:	2025-04-14
Resolution	:	2.12 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:

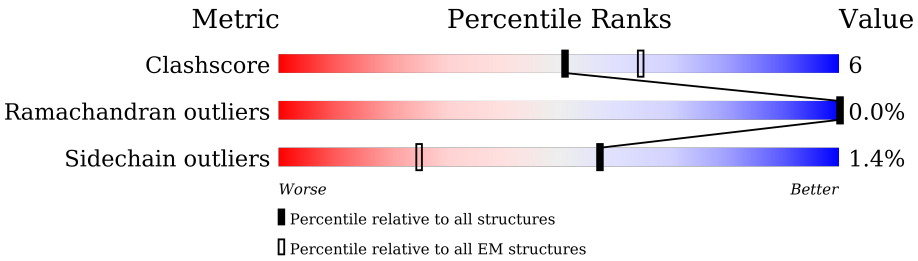
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

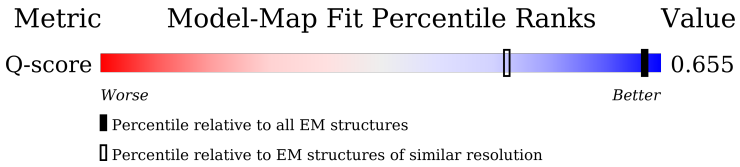
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.12 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	2398 (1.64 - 2.62)

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	90% 8% •
2	B	734	92% 7%
3	C	81	95% • •
4	D	142	88% 9% •

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Mol	Chain	Length	Quality of chain
5	E	67	90% 6%
6	F	184	81% 6% 12%
7	I	35	83% 14%
8	J	39	74% 26%
9	L	141	87% 12%
10	M	29	97%
11	U	191	68% 6% 26%
12	G	209	57% 17% 24%
13	H	169	7% 72% 15% 12%
14	K	200	14% 40% 7% 52%
15	k	89	53% 8% 39%

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 31069 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 I (FCPI-1).

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

- Molecule 12 is a protein called Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	158	1201	769	194	229	9	0	0

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	H	149	1128	725	185	206	12	0	0

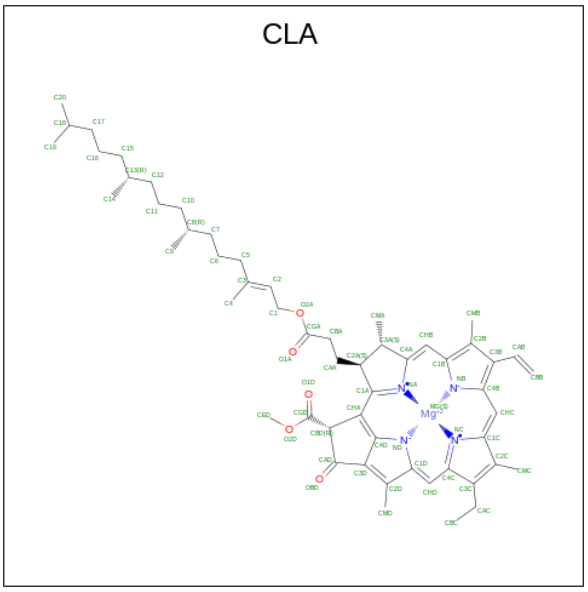
- Molecule 14 is a protein called Fucoxanthin chlorophyll a/c binding protein IX (FCPI-9).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	K	95	737	488	119	123	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	k	54	375	245	61	66	3	0	0

- Molecule 16 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
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
16	A	1	55	45	1	4	5	0
16	A	1	65	55	1	4	5	0
16	A	1	65	55	1	4	5	0
16	A	1	49	39	1	4	5	0
16	A	1	65	55	1	4	5	0
16	A	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	A	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
16	A	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	53	43	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	63	53	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	F	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	F	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
16	F	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
16	I	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	J	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
16	L	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
16	L	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	L	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
16	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
16	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
16	G	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	40	32	1	4	3	0

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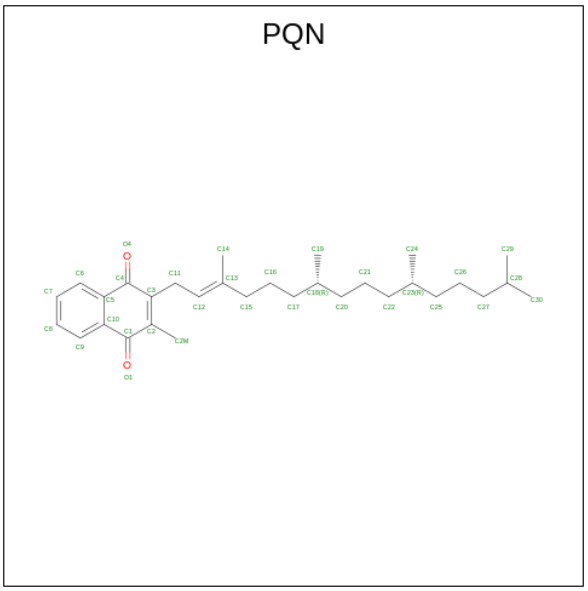
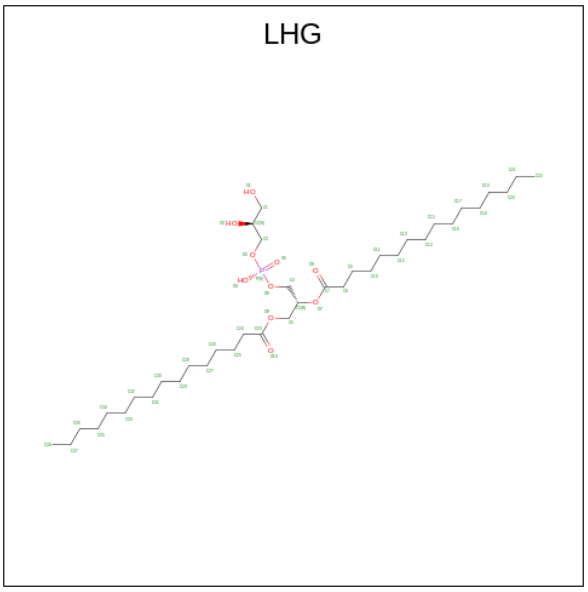
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	H	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
16	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
16	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	K	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
16	K	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
16	K	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	K	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
16	K	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
16	K	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
16	k	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
16	k	1	55	45	1	4	5	0

- Molecule 17 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	
17	A	1	33	31	2	0
17	B	1	33	31	2	0

- Molecule 18 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	
18	A	1	48	37	10	1	0

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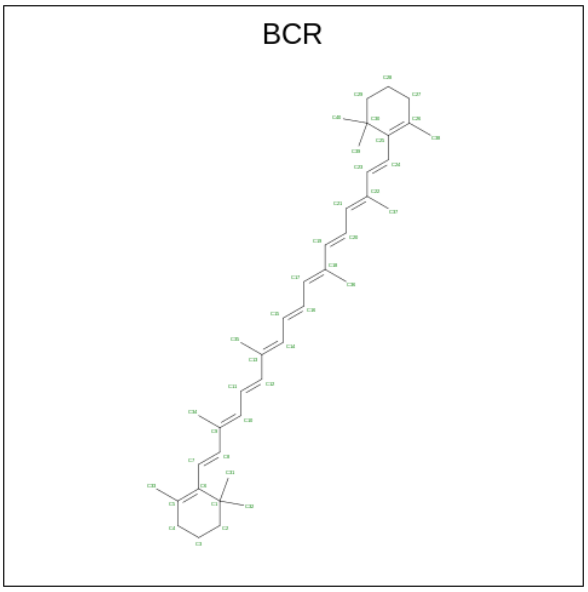
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	A	1	27	16	10	1	0
18	G	1	27	16	10	1	0

- Molecule 19 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	
19	A	1	40	40	0
19	A	1	40	40	0
19	A	1	40	40	0
19	A	1	40	40	0
19	B	1	40	40	0
19	B	1	40	40	0
19	B	1	40	40	0
19	B	1	40	40	0
19	B	1	40	40	0

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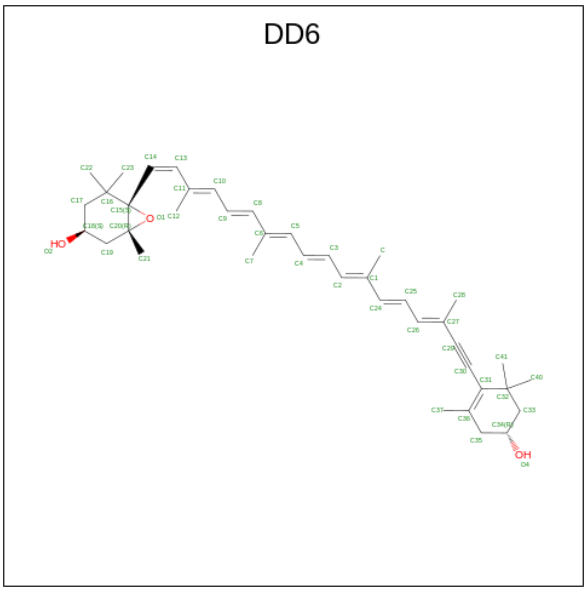
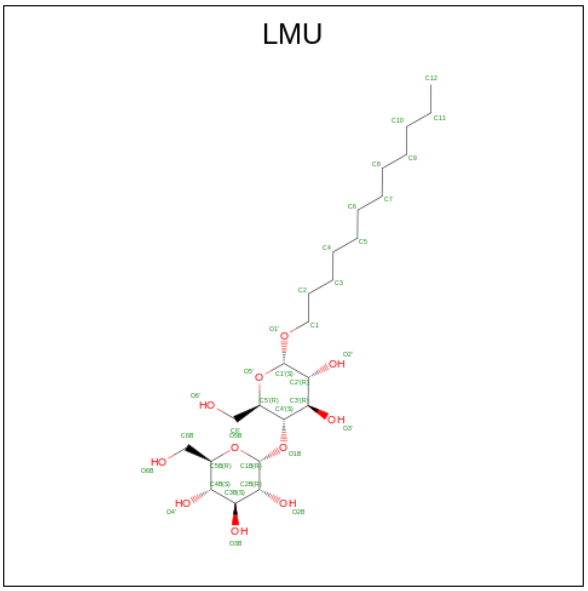
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
19	B	1	39	39	0
			Total	C	
19	F	1	40	40	0
			Total	C	
19	F	1	40	40	0
			Total	C	
19	I	1	40	40	0
			Total	C	
19	I	1	40	40	0
			Total	C	
19	J	1	40	40	0
			Total	C	
19	L	1	40	40	0
			Total	C	
19	L	1	40	40	0
			Total	C	
19	M	1	40	40	0
			Total	C	
19	k	1	40	40	0

- Molecule 20 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).



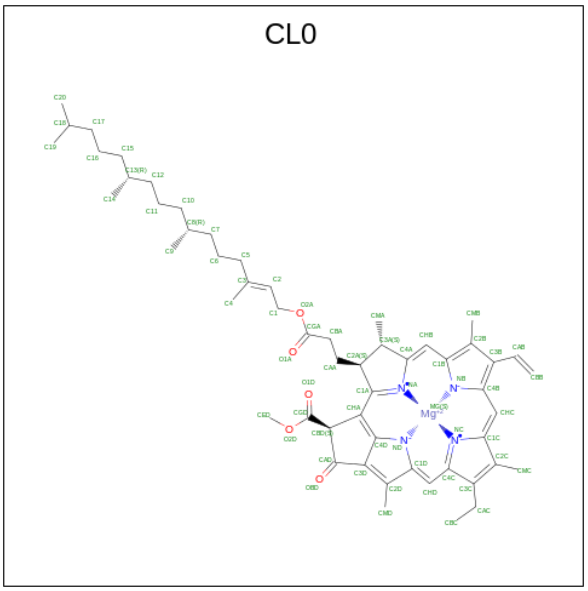
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	A	1	43	40	3	0
20	J	1	43	40	3	0
20	U	1	43	40	3	0
20	U	1	43	40	3	0
20	U	1	26	25	1	0
20	G	1	43	40	3	0
20	G	1	27	25	2	0
20	G	1	43	40	3	0
20	G	1	43	40	3	0
20	G	1	43	40	3	0
20	H	1	43	40	3	0
20	H	1	43	40	3	0
20	K	1	43	40	3	0

- Molecule 21 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



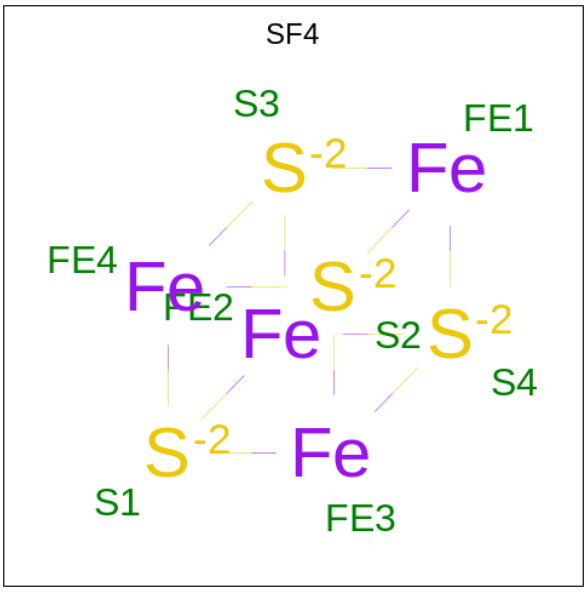
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	A	1	35	24	11	0
			Total	C	O	
21	A	1	35	24	11	0
			Total	C	O	
21	F	1	35	24	11	0
			Total	C	O	
21	J	1	35	24	11	0
			Total	C	O	
21	K	1	35	24	11	0

- 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

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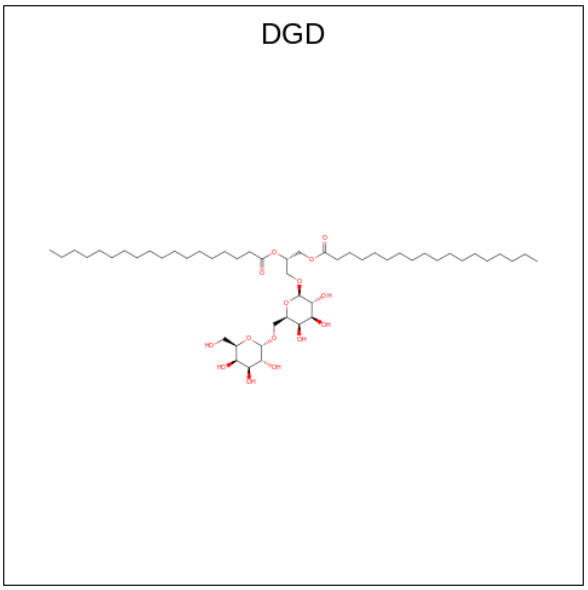
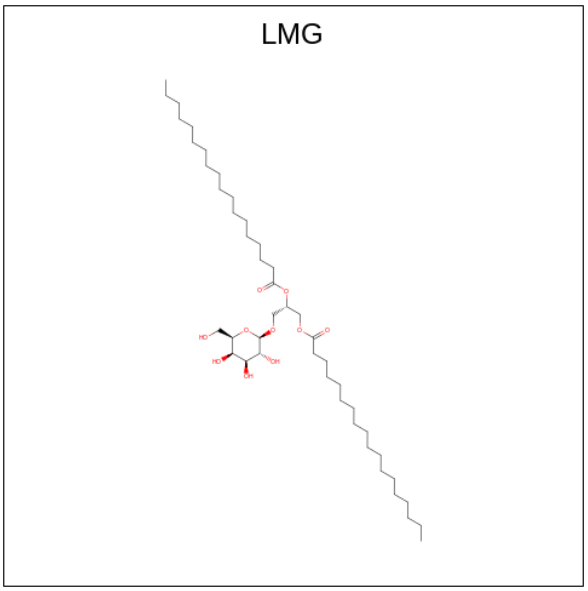
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
23	C	1	8	4	4	0

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



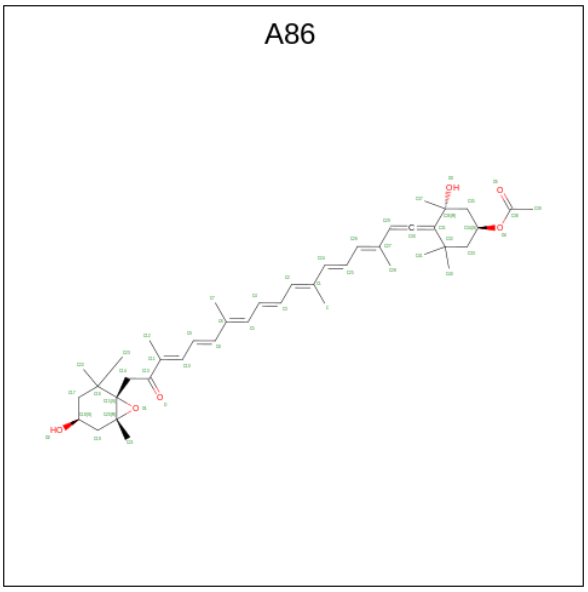
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	B	1	60	45	15	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



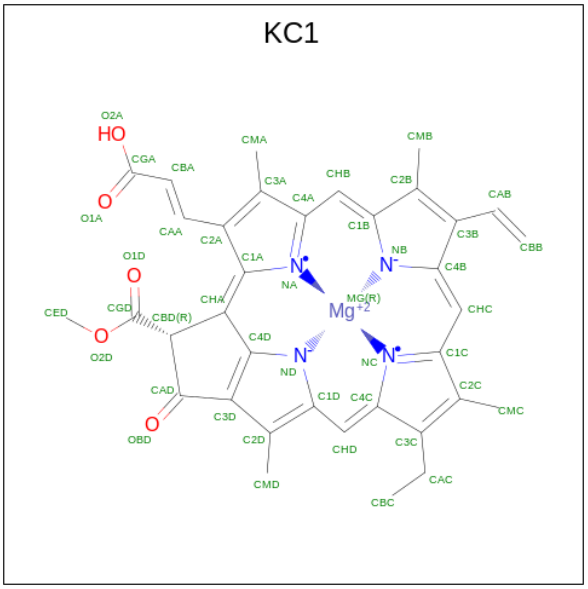
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	J	1	39	29	10	0
			Total	C	O	
25	U	1	32	22	10	0

- Molecule 26 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	
26	U	1	48	42	6	0

- Molecule 27 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	
27	U	1	45	35	1	4	5	0

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
28	A	132	132	132	0
28	B	146	146	146	0
28	C	32	32	32	0
28	D	19	19	19	0
28	E	8	8	8	0
28	F	24	24	24	0
28	J	1	1	1	0
28	L	14	14	14	0
28	M	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
28	U	3	3	3	0
			Total	O	
28	G	5	5	5	0
			Total	O	
28	H	1	1	1	0
			Total	O	
28	K	7	7	7	0
			Total	O	
28	k	2	2	2	0

3 Residue-property plots (i)

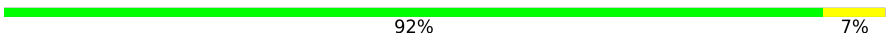
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

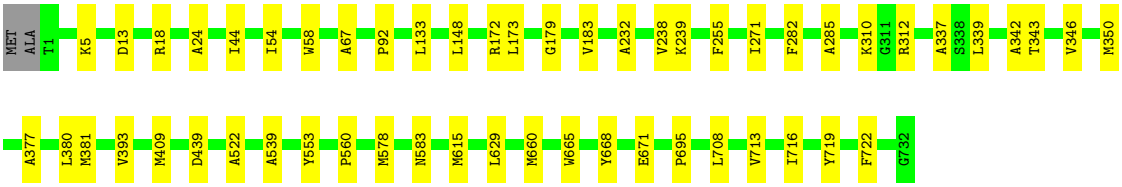
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 (psaA)

Chain A:

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

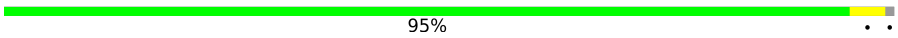
Chain B:





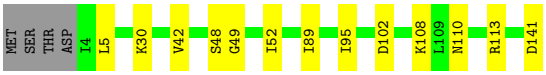
• Molecule 3: Photosystem I iron-sulfur center (psaC)

Chain C:



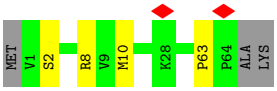
• Molecule 4: Photosystem I reaction center subunit II (psaD)

Chain D:



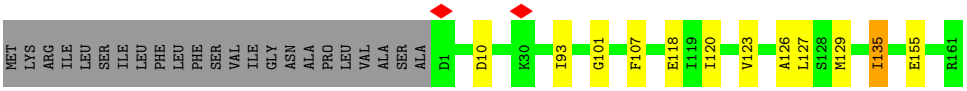
• Molecule 5: Photosystem I reaction center subunit IV (psaE)

Chain E: 90% 6%



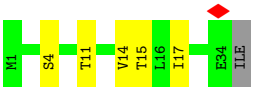
• Molecule 6: Photosystem I reaction center subunit III (psaF)

Chain F: 81% 6% 12%



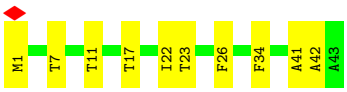
• Molecule 7: Photosystem I reaction center subunit VIII (psaI)

Chain I: 83% 14%



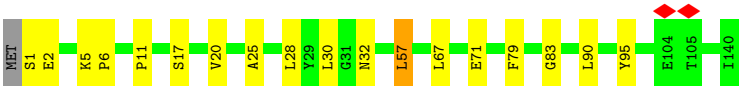
• Molecule 8: Photosystem I reaction center subunit IX (psaJ)

Chain J: 74% 26%



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

Chain L: 87% 12%

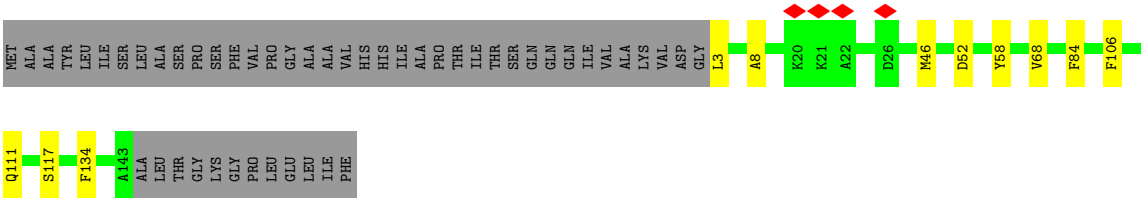


• Molecule 10: Photosystem I reaction center subunit XII (psaM)

Chain M: 97%

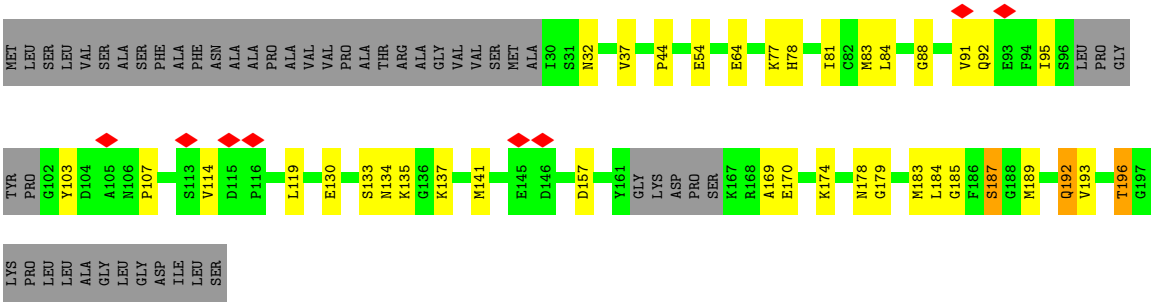
• Molecule 11: Fucoxanthin chlorophyll a/c binding protein I (FCPI-1)

Chain U: 68% 6% 26%



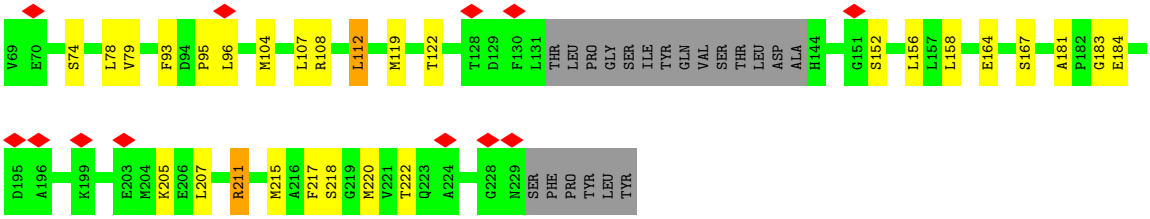
• Molecule 12: Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7)

Chain G:



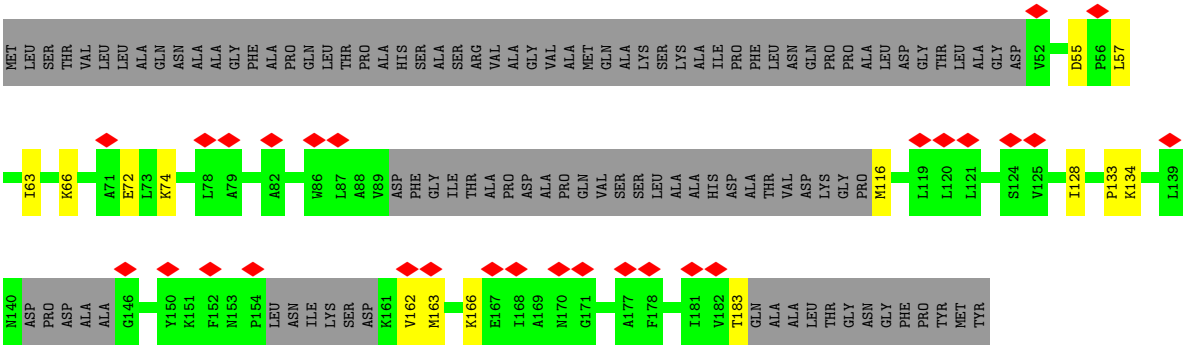
• Molecule 13: Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8)

Chain H:



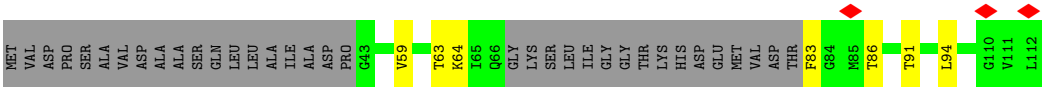
• Molecule 14: Fucoxanthin chlorophyll a/c binding protein IX (FCPI-9)

Chain K:



• Molecule 15: Photosystem I reaction center subunit psaK

Chain k:


MET
VAL
ASP
PRO
SER
ALA
VAL
ASP
ALA
ALA
SER
GLN
LEU
LEU
ALA
ILE
ALA
ASP
PRO
G43
V59
T63
K64
I65
Q66
GLY
LYS
SER
LEU
ILE
GLY
GLY
THR
LYS
HIS
ASP
GLU
MET
VAL
ASP
THR
F83
G84
M85
T86
T91
L94
G110
V111
L112

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22619	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	0.576	Depositor
Minimum map value	-0.256	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.065	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: LMU, DD6, LHG, A86, BCR, LMG, KC1, PQN, DGD, CLA, CL0, SF4

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	0.29	0/6007	0.48	1/8185 (0.0%)
2	B	0.30	0/6015	0.50	0/8205
3	C	0.18	0/609	0.41	0/826
4	D	0.30	0/1116	0.52	1/1503 (0.1%)
5	E	0.21	0/505	0.48	0/689
6	F	0.21	0/1275	0.44	0/1728
7	I	0.38	0/273	0.65	0/373
8	J	0.45	0/313	0.82	1/427 (0.2%)
9	L	0.21	0/1081	0.42	0/1470
10	M	0.24	0/218	0.52	0/295
11	U	0.28	0/1109	0.57	1/1499 (0.1%)
12	G	0.33	0/1226	0.70	1/1655 (0.1%)
13	H	0.32	0/1149	0.59	0/1546
14	K	0.33	0/752	0.63	0/1012
15	k	0.17	0/379	0.39	0/514
All	All	0.29	0/22027	0.52	5/29927 (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	H	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	42	ALA	N-CA-C	-6.01	106.56	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	169	ALA	N-CA-C	-5.56	108.28	114.62
1	A	398	HIS	CA-CB-CG	-5.33	108.47	113.80
4	D	49	GLY	CA-C-O	-5.18	118.85	122.22
11	U	68	VAL	N-CA-C	-5.13	107.83	112.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	H	211	ARG	Sidechain

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	5695	47	0
2	B	5805	0	5634	45	0
3	C	599	0	577	2	0
4	D	1092	0	1093	6	0
5	E	494	0	488	2	0
6	F	1246	0	1256	11	0
7	I	266	0	278	3	0
8	J	305	0	310	10	0
9	L	1056	0	1068	17	0
10	M	216	0	234	0	0
11	U	1082	0	1055	8	0
12	G	1201	0	1185	24	0
13	H	1128	0	1131	20	0
14	K	737	0	764	7	0
15	k	375	0	403	5	0
16	A	2540	0	2556	68	0
16	B	2439	0	2456	68	0
16	F	159	0	141	3	0
16	G	561	0	486	16	0
16	H	524	0	475	22	0
16	I	65	0	72	2	0
16	J	42	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	286	0	229	8	0
16	L	164	0	150	4	0
16	U	441	0	417	12	0
16	k	97	0	80	3	0
17	A	33	0	46	3	0
17	B	33	0	46	1	0
18	A	75	0	93	2	0
18	G	27	0	24	2	0
19	A	160	0	224	6	0
19	B	239	0	333	16	0
19	F	80	0	112	0	0
19	I	80	0	112	3	0
19	J	40	0	56	2	0
19	L	80	0	112	3	0
19	M	40	0	56	3	0
19	k	40	0	56	3	0
20	A	43	0	0	0	0
20	G	199	0	0	1	0
20	H	86	0	0	0	0
20	J	43	0	0	0	0
20	K	43	0	0	0	0
20	U	112	0	0	0	0
21	A	70	0	92	2	0
21	F	35	0	46	0	0
21	J	35	0	46	3	0
21	K	35	0	46	0	0
22	A	65	0	72	2	0
23	A	8	0	0	0	0
23	C	16	0	0	0	0
24	B	60	0	81	2	0
25	J	39	0	48	2	0
25	U	32	0	34	2	0
26	U	48	0	0	1	0
27	U	45	0	0	0	0
28	A	132	0	0	2	0
28	B	146	0	0	0	0
28	C	32	0	0	0	0
28	D	19	0	0	0	0
28	E	8	0	0	0	0
28	F	24	0	0	0	0
28	G	5	0	0	0	0
28	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	1	0	0	0	0
28	K	7	0	0	0	0
28	L	14	0	0	0	0
28	M	1	0	0	0	0
28	U	3	0	0	1	0
28	k	2	0	0	0	0
All	All	31069	0	29999	335	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 6.

All (335) 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)
13:H:122:THR:HA	13:H:220:MET:HE1	1.57	0.86
13:H:112:LEU:HD12	13:H:183:GLY:HA3	1.63	0.81
7:I:17:ILE:HD11	16:I:102:CLA:HAB	1.69	0.75
16:A:822:CLA:H91	19:A:844:BCR:H23C	1.70	0.74
16:A:803:CLA:H72	19:A:842:BCR:HC8	1.71	0.72
13:H:217:PHE:HA	13:H:220:MET:HE3	1.72	0.70
16:A:808:CLA:HBB2	16:A:811:CLA:HMA3	1.75	0.69
13:H:104:MET:HE1	16:H:306:CLA:HMA2	1.76	0.67
16:B:818:CLA:HMD2	19:B:838:BCR:HC7	1.77	0.67
12:G:91:VAL:HG13	12:G:95:ILE:HD13	1.76	0.66
16:H:305:CLA:HBB2	16:H:312:CLA:H151	1.81	0.63
1:A:322:PRO:HB3	9:L:1:SER:HB2	1.79	0.63
13:H:207:LEU:O	13:H:211:ARG:HB2	2.00	0.61
16:B:828:CLA:H111	6:F:93:ILE:HD11	1.83	0.60
8:J:1:MET:HG3	18:G:316:LHG:H241	1.84	0.60
16:A:816:CLA:HBB2	16:A:816:CLA:H151	1.82	0.59
11:U:8:ALA:O	28:U:301:HOH:O	2.17	0.59
1:A:207:GLN:HA	1:A:211:SER:HB2	1.84	0.59
12:G:114:VAL:HG11	12:G:119:LEU:HD11	1.83	0.59
11:U:58:TYR:HE2	16:U:207:CLA:HBA1	1.66	0.59
16:A:845:CLA:HBC2	2:B:583:ASN:HB2	1.85	0.58
2:B:13:ASP:HB3	2:B:18:ARG:HB2	1.86	0.58
16:B:819:CLA:H3A	16:B:836:CLA:HED3	1.85	0.58
13:H:217:PHE:HA	13:H:220:MET:CE	2.33	0.58
2:B:660:MET:HB2	16:B:803:CLA:C1C	2.34	0.57
12:G:91:VAL:HB	16:G:309:CLA:HBC3	1.87	0.57
16:A:836:CLA:H201	9:L:90:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:PHE:HA	16:A:833:CLA:HED1	1.86	0.56
16:B:819:CLA:HBB2	16:B:836:CLA:H52	1.87	0.56
1:A:491:ASN:HB2	16:A:831:CLA:HED2	1.87	0.56
2:B:393:VAL:HG13	2:B:539:ALA:HB1	1.88	0.56
16:A:831:CLA:HBA2	16:k:202:CLA:H11	1.88	0.55
16:B:849:CLA:H62	9:L:79:PHE:HB3	1.88	0.55
16:A:824:CLA:H91	16:A:826:CLA:H192	1.89	0.55
4:D:108:LYS:O	4:D:113:ARG:NH2	2.40	0.54
12:G:107:PRO:HD2	12:G:193:VAL:HG11	1.89	0.54
16:A:835:CLA:H71	16:A:853:CLA:H171	1.90	0.54
16:B:811:CLA:HBB2	16:B:847:CLA:H61	1.89	0.54
12:G:187:SER:HB2	16:G:308:CLA:HBC2	1.90	0.54
2:B:339:LEU:HB3	2:B:380:LEU:HD13	1.90	0.54
2:B:719:TYR:HB2	16:B:802:CLA:HED2	1.89	0.54
14:K:162:VAL:HG12	14:K:166:LYS:HE3	1.90	0.54
1:A:339:TRP:HB3	16:A:803:CLA:HAC1	1.89	0.53
1:A:416:LEU:HB3	16:A:849:CLA:HMC2	1.91	0.53
9:L:25:ALA:HB2	11:U:106:PHE:HB3	1.90	0.53
16:U:204:CLA:H42	16:U:211:CLA:HED2	1.90	0.53
16:A:845:CLA:HHB	16:B:802:CLA:H202	1.91	0.53
4:D:141:ASP:OD1	4:D:141:ASP:O	2.26	0.53
13:H:181:ALA:HB3	13:H:184:GLU:HB2	1.90	0.53
5:E:2:SER:HB2	5:E:63:PRO:HG3	1.91	0.53
16:B:831:CLA:H122	19:B:841:BCR:H311	1.89	0.53
25:U:201:LMG:H321	16:U:211:CLA:H42	1.91	0.53
16:H:305:CLA:HBB2	16:H:312:CLA:H171	1.91	0.52
16:B:825:CLA:H201	19:B:842:BCR:H11C	1.91	0.52
2:B:255:PHE:HZ	16:B:815:CLA:H71	1.73	0.52
8:J:41:ALA:HB2	21:J:101:LMU:H6'1	1.90	0.52
13:H:164:GLU:HA	13:H:167:SER:HB3	1.91	0.52
16:A:820:CLA:HHC	16:A:820:CLA:HBB1	1.92	0.52
16:k:201:CLA:HHC	16:k:201:CLA:HBB1	1.92	0.52
1:A:234:ILE:HD11	16:A:812:CLA:HAC1	1.91	0.52
16:B:808:CLA:HHC	16:B:808:CLA:HBB1	1.91	0.52
13:H:218:SER:HB3	16:H:312:CLA:H162	1.92	0.52
16:U:211:CLA:HBB1	16:U:211:CLA:HHC	1.91	0.51
13:H:205:LYS:HD2	16:H:302:CLA:HAA2	1.92	0.51
16:A:849:CLA:HHC	16:A:849:CLA:HBB1	1.92	0.51
2:B:346:VAL:O	2:B:350:MET:HB2	2.10	0.51
16:B:836:CLA:HED1	16:B:845:CLA:HHC	1.92	0.51
12:G:88:GLY:O	12:G:92:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:822:CLA:HBB1	16:B:822:CLA:HHC	1.92	0.51
16:B:834:CLA:HHC	16:B:834:CLA:HBB1	1.93	0.51
9:L:32:ASN:HB3	16:L:202:CLA:HAC1	1.93	0.51
16:H:308:CLA:HHC	16:H:308:CLA:HBB1	1.92	0.51
16:H:309:CLA:HHC	16:H:309:CLA:HBB1	1.93	0.51
1:A:279:LEU:HD13	16:A:815:CLA:HMA2	1.92	0.51
6:F:123:VAL:HB	25:J:103:LMG:HC72	1.92	0.51
16:A:847:CLA:H91	19:k:203:BCR:H291	1.91	0.51
16:B:807:CLA:H201	16:B:809:CLA:H192	1.93	0.51
16:A:854:CLA:H42	9:L:20:VAL:HG13	1.93	0.51
2:B:409:MET:HG3	19:B:846:BCR:H402	1.91	0.51
16:B:835:CLA:H193	19:I:101:BCR:H362	1.93	0.51
16:F:804:CLA:HHC	16:F:804:CLA:HBB1	1.92	0.51
16:K:203:CLA:HHC	16:K:203:CLA:HBB1	1.93	0.51
16:K:206:CLA:HHC	16:K:206:CLA:HBB1	1.92	0.50
16:K:205:CLA:HHC	16:K:205:CLA:HBB1	1.91	0.50
16:B:824:CLA:H11	19:B:839:BCR:H393	1.93	0.50
16:B:849:CLA:HHC	16:B:849:CLA:HBB1	1.93	0.50
16:F:802:CLA:HHC	16:F:802:CLA:HBB1	1.93	0.50
16:B:835:CLA:HHC	16:B:835:CLA:HBB1	1.93	0.50
16:G:303:CLA:HHC	16:G:303:CLA:HBB1	1.93	0.50
16:G:309:CLA:HHC	16:G:309:CLA:HBB1	1.92	0.50
16:A:831:CLA:HHC	16:A:831:CLA:HBB1	1.94	0.50
16:B:813:CLA:H143	19:B:839:BCR:HC32	1.93	0.50
8:J:34:PHE:HB3	21:J:101:LMU:H5B	1.94	0.50
2:B:342:ALA:HB2	16:B:820:CLA:H43	1.92	0.50
2:B:312:ARG:HH21	16:B:826:CLA:HBD	1.77	0.49
16:U:205:CLA:H92	16:U:206:CLA:HMA1	1.93	0.49
16:A:820:CLA:HBA2	25:U:201:LMG:H122	1.94	0.49
1:A:703:ALA:N	6:F:118:GLU:OE2	2.42	0.49
8:J:7:THR:OG1	25:J:103:LMG:O5	2.29	0.49
16:G:301:CLA:HHC	16:G:301:CLA:HBB1	1.94	0.49
16:H:302:CLA:HHC	16:H:302:CLA:HBB1	1.94	0.49
16:A:814:CLA:HHC	16:A:814:CLA:HBB1	1.94	0.49
12:G:103:TYR:HA	16:G:309:CLA:HED2	1.95	0.49
16:A:835:CLA:HHC	16:A:835:CLA:HBB1	1.94	0.49
1:A:570:ARG:NH1	28:A:906:HOH:O	2.46	0.49
13:H:152:SER:OG	16:H:308:CLA:OBD	2.31	0.49
16:U:208:CLA:HHC	16:U:208:CLA:HBB1	1.93	0.49
16:H:304:CLA:HBB1	16:H:304:CLA:HHC	1.93	0.49
16:B:807:CLA:HBB1	16:B:808:CLA:H202	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:825:CLA:H42	24:B:843:DGD:HB42	1.94	0.49
16:A:809:CLA:HBB2	21:A:848:LMU:H101	1.95	0.49
6:F:107:PHE:HB2	6:F:129:MET:HE1	1.95	0.49
16:A:817:CLA:HHC	16:A:817:CLA:HBB1	1.95	0.48
12:G:77:LYS:O	12:G:81:ILE:HD12	2.13	0.48
16:A:854:CLA:H12	9:L:30:LEU:HD11	1.95	0.48
16:B:807:CLA:H12	7:I:14:VAL:HG21	1.95	0.48
4:D:5:LEU:HD23	4:D:95:ILE:HD13	1.94	0.48
16:A:851:CLA:H172	6:F:101:GLY:HA2	1.95	0.48
16:B:819:CLA:HHB	16:B:836:CLA:O1D	2.12	0.48
1:A:230:PRO:HA	1:A:233:LEU:HD12	1.96	0.48
4:D:102:ASP:OD2	4:D:110:ASN:ND2	2.47	0.48
6:F:127:LEU:HB3	16:G:306:CLA:H41	1.94	0.48
12:G:174:LYS:HD3	16:G:303:CLA:HBD	1.94	0.48
16:A:815:CLA:HHC	16:A:815:CLA:HBB1	1.95	0.48
16:A:818:CLA:H52	16:A:849:CLA:H2	1.95	0.48
1:A:464:ASP:OD1	1:A:470:GLN:NE2	2.45	0.48
2:B:716:ILE:HG22	16:B:823:CLA:H52	1.96	0.48
2:B:522:ALA:HB2	16:B:832:CLA:HMA1	1.94	0.48
1:A:664:LEU:HD11	2:B:615:MET:HB2	1.96	0.48
9:L:5:LYS:NZ	11:U:111:GLN:O	2.46	0.48
14:K:163:MET:SD	16:K:202:CLA:HHB	2.54	0.48
16:A:819:CLA:HAA2	15:k:64:LYS:HE3	1.95	0.47
2:B:393:VAL:HG21	2:B:553:TYR:HB2	1.96	0.47
2:B:713:VAL:HG22	24:B:843:DGD:HBV1	1.96	0.47
16:G:310:CLA:HBA1	16:G:310:CLA:HBD	1.95	0.47
1:A:334:ILE:HG13	1:A:411:GLN:HE22	1.79	0.47
1:A:556:LYS:NZ	2:B:671:GLU:OE2	2.46	0.47
1:A:431:LEU:HD21	1:A:537:VAL:HG12	1.96	0.47
16:U:209:CLA:HHC	16:U:209:CLA:HBB1	1.96	0.47
13:H:107:LEU:HD13	16:H:306:CLA:HBA2	1.96	0.47
2:B:24:ALA:HA	16:B:825:CLA:H43	1.95	0.47
11:U:46:MET:HG2	16:U:207:CLA:HAC1	1.96	0.47
1:A:4:GLN:HG3	1:A:6:VAL:HG13	1.96	0.47
28:A:993:HOH:O	9:L:2:GLU:HB3	2.14	0.47
16:B:824:CLA:HBA2	16:B:824:CLA:H12	1.64	0.47
16:H:306:CLA:H62	16:H:306:CLA:H41	1.66	0.47
16:A:835:CLA:H101	8:J:17:THR:HG23	1.96	0.47
22:A:850:CL0:H35	16:B:801:CLA:O1D	2.15	0.47
16:B:822:CLA:H143	19:B:846:BCR:H20C	1.97	0.47
16:A:813:CLA:HHC	16:A:813:CLA:HBB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:845:CLA:H41	16:A:845:CLA:H61	1.76	0.46
22:A:850:CL0:O1D	16:B:802:CLA:HBB2	2.15	0.46
16:B:806:CLA:H102	16:B:806:CLA:H152	1.98	0.46
13:H:95:PRO:HB2	14:K:133:PRO:HG2	1.97	0.46
2:B:629:LEU:HD22	2:B:722:PHE:HA	1.97	0.46
2:B:339:LEU:HD11	16:B:805:CLA:H51	1.97	0.46
16:B:835:CLA:H41	16:B:835:CLA:H61	1.68	0.46
2:B:381:MET:HE1	19:B:841:BCR:H361	1.97	0.46
12:G:130:GLU:O	12:G:134:ASN:ND2	2.44	0.45
16:A:851:CLA:H12	16:B:848:CLA:HAA1	1.98	0.45
11:U:134:PHE:HE1	16:U:205:CLA:H202	1.80	0.45
2:B:668:TYR:OH	16:B:803:CLA:OBD	2.31	0.45
16:B:834:CLA:HBB2	17:B:837:PQN:H141	1.97	0.45
12:G:83:MET:HE3	12:G:178:ASN:HB2	1.98	0.45
17:A:837:PQN:H222	17:A:837:PQN:H18	1.69	0.45
7:I:11:THR:O	7:I:15:THR:OG1	2.33	0.45
16:H:303:CLA:H62	16:H:303:CLA:H41	1.78	0.45
16:A:816:CLA:H141	16:A:823:CLA:H193	1.99	0.45
2:B:282:PHE:HE1	16:B:817:CLA:HBB1	1.82	0.45
15:k:63:THR:HG21	15:k:91:THR:HG22	1.97	0.45
2:B:343:THR:HB	2:B:377:ALA:HB2	1.97	0.45
12:G:84:LEU:HD22	16:G:309:CLA:H93	1.99	0.45
1:A:351:GLY:HA2	1:A:388:GLY:HA2	1.97	0.45
2:B:285:ALA:HB2	16:B:817:CLA:HBC2	1.99	0.45
16:B:848:CLA:HHC	16:B:848:CLA:HBB1	1.99	0.45
15:k:83:PHE:HB3	15:k:86:THR:HG23	1.99	0.45
1:A:267:THR:OG1	1:A:283:ASP:OD1	2.30	0.45
19:B:839:BCR:H20C	19:B:839:BCR:H361	1.83	0.45
9:L:6:PRO:HB3	9:L:11:PRO:HA	1.99	0.44
12:G:179:GLY:O	12:G:183:MET:HG3	2.17	0.44
1:A:109:TRP:CD2	16:A:807:CLA:HED3	2.52	0.44
12:G:133:SER:O	12:G:135:LYS:NZ	2.45	0.44
16:G:310:CLA:HBD	16:G:310:CLA:HED2	1.87	0.44
9:L:5:LYS:HG3	9:L:17:SER:HB3	1.98	0.44
16:B:830:CLA:HHC	16:B:830:CLA:HBB1	1.98	0.44
5:E:8:ARG:NH2	6:F:155:GLU:OE1	2.50	0.44
6:F:129:MET:HG3	12:G:141:MET:HE1	2.00	0.44
13:H:156:LEU:HB3	16:H:309:CLA:HBC1	2.00	0.44
13:H:207:LEU:HD12	13:H:207:LEU:HA	1.65	0.44
1:A:111:ILE:HG13	1:A:112:VAL:HG13	1.99	0.44
2:B:578:MET:HG3	2:B:708:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:834:CLA:H191	9:L:57:LEU:HD11	2.00	0.44
8:J:1:MET:HG3	18:G:316:LHG:C24	2.47	0.44
16:L:202:CLA:H3A	16:L:202:CLA:HBA2	1.78	0.44
1:A:2:LYS:HD2	1:A:2:LYS:HA	1.82	0.44
1:A:7:VAL:HA	1:A:176:PRO:HA	1.99	0.44
16:A:824:CLA:H142	16:A:826:CLA:H18	2.00	0.44
2:B:92:PRO:HB2	16:B:849:CLA:HAA1	2.00	0.44
1:A:574:CYS:HB2	2:B:665:TRP:HB3	2.00	0.44
2:B:232:ALA:HB2	16:B:814:CLA:HMA2	1.99	0.44
12:G:32:ASN:HD22	12:G:32:ASN:HA	1.71	0.44
16:A:828:CLA:HBB1	16:A:829:CLA:HBA1	2.00	0.44
16:B:801:CLA:H122	19:B:842:BCR:H12C	1.99	0.43
16:A:828:CLA:H42	16:A:836:CLA:H2	2.00	0.43
2:B:173:LEU:HD23	2:B:173:LEU:HA	1.82	0.43
16:B:848:CLA:H202	16:B:848:CLA:H161	1.91	0.43
4:D:42:VAL:HG22	4:D:52:ILE:HG12	1.99	0.43
16:H:312:CLA:H12	16:H:312:CLA:HBA2	1.61	0.43
16:K:205:CLA:H12	16:K:205:CLA:H51	1.77	0.43
16:A:851:CLA:H191	6:F:126:ALA:HB1	2.00	0.43
16:B:818:CLA:HBB1	16:B:818:CLA:HHC	1.99	0.43
1:A:237:GLN:NE2	1:A:247:PHE:O	2.50	0.43
16:A:833:CLA:H51	16:A:833:CLA:H11	1.83	0.43
2:B:67:ALA:HB2	2:B:133:LEU:HB2	2.00	0.43
16:B:849:CLA:H12	9:L:67:LEU:HD12	2.00	0.43
16:U:207:CLA:H143	16:U:210:CLA:HBC1	2.00	0.43
14:K:55:ASP:OD1	14:K:55:ASP:O	2.37	0.43
1:A:364:MET:HE3	1:A:364:MET:HB2	1.83	0.43
16:A:833:CLA:H151	16:A:854:CLA:H202	2.00	0.43
19:B:838:BCR:H15C	19:B:838:BCR:H351	1.90	0.43
16:B:849:CLA:H143	9:L:83:GLY:HA2	2.00	0.43
19:L:205:BCR:H20C	19:L:205:BCR:H361	1.79	0.43
12:G:78:HIS:HB3	12:G:183:MET:SD	2.58	0.43
16:G:306:CLA:H152	16:G:306:CLA:H18	1.82	0.43
6:F:120:ILE:HG12	8:J:11:THR:HG22	2.00	0.43
12:G:184:LEU:HD11	16:G:307:CLA:HAC1	2.01	0.43
19:A:844:BCR:H15C	19:A:844:BCR:H351	1.86	0.43
16:H:305:CLA:H3A	16:H:306:CLA:H52	2.01	0.43
1:A:234:ILE:HD12	16:A:812:CLA:HHD	2.01	0.43
17:A:837:PQN:H141	16:F:802:CLA:HBB2	2.01	0.43
16:A:816:CLA:H91	16:A:825:CLA:H162	2.00	0.43
19:J:105:BCR:H15C	19:J:105:BCR:H351	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:LYS:HD3	2:B:310:LYS:HA	1.80	0.42
1:A:272:LEU:HD21	1:A:365:PRO:HD2	2.01	0.42
21:A:855:LMU:H22	21:A:855:LMU:H1'	1.58	0.42
19:L:205:BCR:H15C	19:L:205:BCR:H351	1.86	0.42
12:G:44:PRO:HG2	12:G:64:GLU:HG2	1.99	0.42
12:G:157:ASP:OD1	20:G:311:DD6:O4	2.36	0.42
19:A:843:BCR:H23C	16:A:849:CLA:HBC2	2.00	0.42
16:B:807:CLA:H122	16:B:807:CLA:H161	1.81	0.42
16:B:849:CLA:H41	16:B:849:CLA:H61	1.62	0.42
26:U:202:A86:C5	16:U:207:CLA:H2	2.49	0.42
16:H:302:CLA:H12	16:H:302:CLA:H52	1.87	0.42
14:K:128:ILE:HG12	16:K:203:CLA:HMB2	2.00	0.42
2:B:148:LEU:HD21	19:M:101:BCR:H342	2.02	0.42
2:B:172:ARG:HB2	16:B:844:CLA:HBC2	2.02	0.42
16:B:813:CLA:H92	16:B:813:CLA:H61	1.91	0.42
11:U:3:LEU:HD12	11:U:3:LEU:HA	1.95	0.42
16:G:308:CLA:CAD	16:H:308:CLA:H3A	2.50	0.42
13:H:207:LEU:HG	13:H:211:ARG:NH2	2.34	0.42
14:K:116:MET:HB3	16:K:206:CLA:HBC3	2.00	0.42
19:k:203:BCR:H20C	19:k:203:BCR:H361	1.84	0.42
19:B:846:BCR:H24C	19:B:846:BCR:H371	1.84	0.42
9:L:28:LEU:O	9:L:32:ASN:ND2	2.52	0.42
15:k:59:VAL:HG11	15:k:94:LEU:HB3	2.02	0.42
2:B:54:ILE:HD11	19:M:101:BCR:HC8	2.01	0.42
3:C:60:ASP:HA	3:C:61:PHE:HA	1.87	0.42
1:A:364:MET:HG3	1:A:497:SER:HB2	2.01	0.42
1:A:567:GLY:HA2	2:B:560:PRO:HD3	2.02	0.42
1:A:605:GLN:HB3	1:A:622:THR:HG23	2.02	0.42
16:A:824:CLA:H102	16:A:824:CLA:H61	1.88	0.42
16:A:828:CLA:H192	16:B:835:CLA:HBD	2.01	0.42
2:B:58:TRP:HA	16:B:807:CLA:HBB2	2.02	0.42
19:B:842:BCR:H20C	19:B:842:BCR:H361	1.88	0.42
1:A:564:PRO:HB3	1:A:711:ILE:HB	2.01	0.42
18:A:839:LHG:H282	18:A:839:LHG:H312	1.82	0.42
19:B:840:BCR:H20C	19:B:840:BCR:H361	1.88	0.42
19:I:103:BCR:H361	9:L:95:TYR:HB2	2.01	0.42
1:A:683:TYR:CE2	16:A:801:CLA:HMD1	2.55	0.42
2:B:238:VAL:HG23	2:B:239:LYS:HG2	2.02	0.42
8:J:22:ILE:HG23	16:J:104:CLA:HBB2	2.02	0.42
13:H:93:PHE:HD2	16:H:306:CLA:C1D	2.33	0.42
19:k:203:BCR:H11C	19:k:203:BCR:H341	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:ILE:HG23	16:B:816:CLA:HMA3	2.01	0.41
1:A:731:TRP:NE1	16:A:824:CLA:O1A	2.47	0.41
19:A:844:BCR:H20C	19:A:844:BCR:H361	1.85	0.41
12:G:54:GLU:H	12:G:54:GLU:HG3	1.60	0.41
1:A:229:LEU:HD22	16:A:814:CLA:HED1	2.02	0.41
16:B:806:CLA:H192	16:B:806:CLA:H71	2.02	0.41
19:J:105:BCR:H20C	19:J:105:BCR:H361	1.83	0.41
16:A:806:CLA:H12	16:A:806:CLA:HBA2	1.62	0.41
16:A:854:CLA:H72	16:L:203:CLA:H12	2.01	0.41
2:B:179:GLY:HA2	2:B:183:VAL:HB	2.02	0.41
1:A:555:ASP:OD1	1:A:555:ASP:N	2.53	0.41
18:A:839:LHG:H141	18:A:839:LHG:H112	1.85	0.41
16:A:853:CLA:H91	16:A:853:CLA:H112	1.80	0.41
2:B:5:LYS:HB2	2:B:5:LYS:HE2	1.81	0.41
8:J:23:THR:HA	8:J:26:PHE:CE2	2.55	0.41
13:H:78:LEU:HD11	14:K:133:PRO:HB2	2.02	0.41
16:L:204:CLA:HED2	16:L:204:CLA:HBD	1.89	0.41
16:k:202:CLA:H11	16:k:202:CLA:H51	1.88	0.41
16:I:102:CLA:H93	9:L:79:PHE:CE2	2.56	0.41
13:H:108:ARG:NH2	16:H:306:CLA:O1D	2.54	0.41
13:H:215:MET:HE2	16:H:306:CLA:HMC3	2.03	0.41
1:A:333:GLU:HB2	1:A:411:GLN:HE21	1.86	0.41
16:A:854:CLA:H91	16:A:854:CLA:H112	1.86	0.41
2:B:255:PHE:CG	16:B:815:CLA:HMB2	2.55	0.41
16:B:829:CLA:H62	16:B:829:CLA:H101	1.89	0.41
16:B:831:CLA:H51	16:B:831:CLA:H11	1.83	0.41
3:C:27:MET:HE3	3:C:27:MET:HB3	1.89	0.41
19:I:101:BCR:H15C	19:I:101:BCR:H351	1.89	0.41
19:M:101:BCR:H15C	19:M:101:BCR:H351	1.84	0.41
12:G:185:GLY:O	12:G:189:MET:HG3	2.21	0.41
1:A:87:ARG:HD2	1:A:150:TYR:OH	2.21	0.41
1:A:189:ASN:HB3	16:A:817:CLA:HMD1	2.03	0.41
1:A:460:ASP:HB3	16:A:829:CLA:HED3	2.02	0.41
16:A:808:CLA:HBA1	16:A:810:CLA:HMD2	2.03	0.41
16:A:828:CLA:CAD	19:L:201:BCR:H10C	2.51	0.41
2:B:695:PRO:HB3	16:B:834:CLA:C1C	2.51	0.41
4:D:30:LYS:HG2	4:D:89:ILE:HB	2.03	0.41
1:A:73:ILE:HD11	16:A:809:CLA:H121	2.03	0.40
1:A:669:ILE:HD13	1:A:669:ILE:HA	1.92	0.40
1:A:675:MET:HB2	16:A:801:CLA:C1C	2.51	0.40
1:A:691:ILE:HD13	16:A:851:CLA:HMD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:170:GLU:HG3	16:G:302:CLA:HED1	2.04	0.40
16:A:816:CLA:H72	16:A:816:CLA:H111	1.82	0.40
16:A:849:CLA:H152	16:A:849:CLA:H112	1.81	0.40
2:B:44:ILE:HG21	16:B:805:CLA:H192	2.03	0.40
6:F:135:ILE:H	6:F:135:ILE:HG13	1.67	0.40
15:k:59:VAL:O	15:k:63:THR:HG23	2.21	0.40
1:A:398:HIS:HA	1:A:401:ILE:HD12	2.03	0.40
1:A:709:LEU:HD21	17:A:837:PQN:H151	2.02	0.40
16:K:205:CLA:H41	16:K:205:CLA:H61	1.91	0.40
1:A:194:GLY:O	1:A:198:LEU:HB2	2.21	0.40
16:A:830:CLA:HHC	16:A:830:CLA:HAB	1.95	0.40
19:A:843:BCR:H362	16:A:849:CLA:HBA2	2.03	0.40
16:A:851:CLA:HAA2	16:B:827:CLA:HMB2	2.03	0.40
16:G:303:CLA:HAA1	16:G:304:CLA:HBB1	2.03	0.40
16:A:811:CLA:H102	16:A:811:CLA:H61	1.85	0.40
2:B:337:ALA:HB2	19:B:841:BCR:H372	2.04	0.40
19:B:839:BCR:H19C	16:B:844:CLA:H43	2.04	0.40
8:J:41:ALA:HB2	21:J:101:LMU:C6B	2.51	0.40
11:U:84:PHE:HZ	16:U:207:CLA:H162	1.86	0.40
12:G:192:GLN:O	12:G:196:THR:OG1	2.27	0.40
16:H:312:CLA:H93	16:H:312:CLA:H111	1.77	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%)	723 (98%)	16 (2%)	0	100	100
2	B	730/734 (100%)	713 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	136/142 (96%)	131 (96%)	4 (3%)	1 (1%)	18	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
6	F	159/184 (86%)	157 (99%)	2 (1%)	0	100	100
7	I	32/35 (91%)	30 (94%)	2 (6%)	0	100	100
8	J	37/39 (95%)	37 (100%)	0	0	100	100
9	L	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
10	M	27/29 (93%)	27 (100%)	0	0	100	100
11	U	139/191 (73%)	135 (97%)	4 (3%)	0	100	100
12	G	152/209 (73%)	142 (93%)	10 (7%)	0	100	100
13	H	145/169 (86%)	143 (99%)	2 (1%)	0	100	100
14	K	87/200 (44%)	85 (98%)	2 (2%)	0	100	100
15	k	50/89 (56%)	50 (100%)	0	0	100	100
All	All	2711/3062 (88%)	2646 (98%)	64 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	48	SER

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%)	601 (100%)	2 (0%)	86	91
2	B	590/591 (100%)	589 (100%)	1 (0%)	87	92
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%)	52 (98%)	1 (2%)	50	57
6	F	133/152 (88%)	131 (98%)	2 (2%)	57	65
7	I	31/32 (97%)	30 (97%)	1 (3%)	34	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	32/32 (100%)	32 (100%)	0	100	100
9	L	111/112 (99%)	109 (98%)	2 (2%)	51	59
10	M	21/21 (100%)	20 (95%)	1 (5%)	23	22
11	U	110/148 (74%)	108 (98%)	2 (2%)	51	59
12	G	130/167 (78%)	125 (96%)	5 (4%)	29	30
13	H	119/137 (87%)	112 (94%)	7 (6%)	18	15
14	K	77/153 (50%)	70 (91%)	7 (9%)	9	6
15	k	38/65 (58%)	38 (100%)	0	100	100
All	All	2234/2468 (90%)	2203 (99%)	31 (1%)	57	67

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	574	CYS
2	B	439	ASP
5	E	10	MET
6	F	10	ASP
6	F	135	ILE
7	I	4	SER
9	L	57	LEU
9	L	71	GLU
10	M	22	ILE
11	U	52	ASP
11	U	117	SER
12	G	37	VAL
12	G	137	LYS
12	G	187	SER
12	G	192	GLN
12	G	196	THR
13	H	74	SER
13	H	79	VAL
13	H	96	LEU
13	H	112	LEU
13	H	119	MET
13	H	158	LEU
13	H	222	THR
14	K	57	LEU
14	K	63	ILE

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Mol	Chain	Res	Type
14	K	66	LYS
14	K	72	GLU
14	K	74	LYS
14	K	134	LYS
14	K	183	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	A	377	GLN
1	A	432	ASN
2	B	39	ASN
2	B	112	ASN
2	B	169	ASN
2	B	227	ASN
2	B	264	GLN
2	B	641	GLN
3	C	3	ASN
4	D	99	HIS
4	D	118	ASN
6	F	15	ASN
6	F	122	ASN
9	L	32	ASN
11	U	122	GLN
12	G	32	ASN
12	G	178	ASN
13	H	172	GLN
13	H	229	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

180 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	$\#\|Z\| > 2$
16	CLA	A	851	1	69,73,73	1.21	7 (10%)	83,113,113	0.93	4 (4%)
16	CLA	A	801	-	69,73,73	1.17	8 (11%)	83,113,113	0.92	4 (4%)
16	CLA	B	816	2	64,68,73	1.25	7 (10%)	77,107,113	0.97	4 (5%)
16	CLA	A	812	1	49,53,73	1.44	7 (14%)	59,89,113	1.25	7 (11%)
16	CLA	A	827	1	54,58,73	1.41	7 (12%)	65,95,113	1.00	4 (6%)
16	CLA	G	306	12	69,73,73	1.26	7 (10%)	83,113,113	0.89	3 (3%)
16	CLA	A	854	1	69,73,73	1.18	7 (10%)	83,113,113	0.94	5 (6%)
16	CLA	I	102	-	69,73,73	1.17	7 (10%)	83,113,113	1.02	4 (4%)
16	CLA	L	203	9	69,73,73	1.15	7 (10%)	83,113,113	0.93	4 (4%)
16	CLA	H	308	13	45,49,73	1.42	6 (13%)	54,84,113	1.30	6 (11%)
16	CLA	B	808	2	69,73,73	1.25	7 (10%)	83,113,113	0.90	3 (3%)
16	CLA	A	803	1	69,73,73	1.16	7 (10%)	83,113,113	0.99	4 (4%)
16	CLA	B	845	2	69,73,73	1.23	7 (10%)	83,113,113	0.90	3 (3%)
20	DD6	H	311	-	39,45,45	1.59	7 (17%)	52,67,67	1.56	9 (17%)
16	CLA	K	202	14	46,50,73	1.42	8 (17%)	55,85,113	1.08	4 (7%)
16	CLA	H	309	13	49,53,73	1.42	7 (14%)	59,89,113	1.18	5 (8%)
16	CLA	A	806	1	69,73,73	1.17	7 (10%)	83,113,113	1.06	6 (7%)
16	CLA	B	804	2	49,53,73	1.46	8 (16%)	59,89,113	1.09	4 (6%)
20	DD6	G	313	-	39,45,45	1.62	8 (20%)	52,67,67	1.58	8 (15%)
16	CLA	H	304	13	48,52,73	1.39	8 (16%)	56,87,113	1.18	5 (8%)
16	CLA	B	817	28	69,73,73	1.20	7 (10%)	83,113,113	1.06	7 (8%)
16	CLA	B	803	-	69,73,73	1.18	7 (10%)	83,113,113	0.96	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	CLA	H	305	13	49,53,73	1.51	7 (14%)	59,89,113	0.98	3 (5%)
16	CLA	A	830	1	54,58,73	1.35	7 (12%)	65,95,113	1.01	3 (4%)
19	BCR	L	201	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
16	CLA	F	803	28	52,56,73	1.38	8 (15%)	62,92,113	1.18	5 (8%)
21	LMU	A	848	-	36,36,36	0.50	1 (2%)	47,47,47	0.98	2 (4%)
16	CLA	A	834	1	69,73,73	1.28	7 (10%)	83,113,113	0.95	4 (4%)
19	BCR	B	842	-	41,41,41	1.08	2 (4%)	56,56,56	1.16	4 (7%)
16	CLA	H	306	13	69,73,73	1.22	8 (11%)	83,113,113	1.15	7 (8%)
16	CLA	B	809	2	69,73,73	1.20	9 (13%)	83,113,113	0.94	4 (4%)
16	CLA	B	824	2	69,73,73	1.22	7 (10%)	83,113,113	1.01	5 (6%)
16	CLA	A	853	1	69,73,73	1.16	7 (10%)	83,113,113	0.95	4 (4%)
16	CLA	A	817	1	49,53,73	1.42	7 (14%)	59,89,113	1.21	6 (10%)
16	CLA	A	810	1	58,62,73	1.29	8 (13%)	69,99,113	1.07	5 (7%)
16	CLA	G	302	-	45,49,73	1.49	8 (17%)	54,84,113	1.05	4 (7%)
16	CLA	K	205	14	62,66,73	1.22	7 (11%)	74,104,113	1.30	7 (9%)
21	LMU	A	855	-	36,36,36	0.54	1 (2%)	47,47,47	0.96	1 (2%)
19	BCR	B	840	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	6 (10%)
16	CLA	B	830	28	49,53,73	1.43	8 (16%)	59,89,113	1.19	5 (8%)
16	CLA	A	818	28	69,73,73	1.18	7 (10%)	83,113,113	0.92	4 (4%)
19	BCR	A	842	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	4 (7%)
16	CLA	B	822	2	69,73,73	1.27	7 (10%)	83,113,113	0.98	5 (6%)
23	SF4	C	101	3	0,12,12	-	-	-		
16	CLA	B	814	2	59,63,73	1.35	7 (11%)	71,101,113	1.10	4 (5%)
16	CLA	G	305	12	65,69,73	1.19	6 (9%)	78,108,113	1.13	7 (8%)
16	CLA	K	206	28	43,48,73	1.52	8 (18%)	52,82,113	1.19	4 (7%)
19	BCR	L	205	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	6 (10%)
21	LMU	K	201	-	36,36,36	1.18	2 (5%)	47,47,47	1.37	6 (12%)
16	CLA	A	816	1	69,73,73	1.18	7 (10%)	83,113,113	0.99	4 (4%)
16	CLA	A	811	1	69,73,73	1.21	7 (10%)	83,113,113	0.93	3 (3%)
23	SF4	A	852	1,2	0,12,12	-	-	-		
25	LMG	J	103	-	39,39,55	0.87	1 (2%)	47,47,63	1.27	3 (6%)
16	CLA	A	845	28	69,73,73	1.17	7 (10%)	83,113,113	0.94	3 (3%)
16	CLA	G	304	12	47,51,73	1.39	6 (12%)	56,86,113	1.20	4 (7%)
19	BCR	J	105	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	4 (7%)
16	CLA	A	831	1	49,53,73	1.39	5 (10%)	59,89,113	1.21	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	BCR	F	801	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	3 (5%)
16	CLA	B	805	2	69,73,73	1.17	7 (10%)	83,113,113	0.95	4 (4%)
16	CLA	H	307	-	62,66,73	1.22	8 (12%)	74,104,113	1.00	4 (5%)
16	CLA	A	824	1	66,70,73	1.22	7 (10%)	79,109,113	1.06	5 (6%)
16	CLA	B	835	2	69,73,73	1.25	8 (11%)	83,113,113	1.02	4 (4%)
16	CLA	A	805	1	53,57,73	1.40	7 (13%)	62,93,113	1.05	4 (6%)
16	CLA	B	807	2	69,73,73	1.20	7 (10%)	83,113,113	0.95	3 (3%)
16	CLA	B	833	2	51,55,73	1.41	7 (13%)	61,91,113	1.06	5 (8%)
17	PQN	A	837	-	34,34,34	0.39	0	42,45,45	0.41	0
16	CLA	U	206	11	49,53,73	1.40	7 (14%)	59,89,113	1.07	4 (6%)
16	CLA	A	828	1	69,73,73	1.24	7 (10%)	83,113,113	0.93	3 (3%)
20	DD6	K	208	-	39,45,45	1.60	7 (17%)	52,67,67	1.63	9 (17%)
20	DD6	G	311	-	39,45,45	1.55	8 (20%)	52,67,67	1.51	7 (13%)
19	BCR	A	843	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	4 (7%)
16	CLA	H	303	13	65,69,73	1.22	5 (7%)	78,108,113	1.12	5 (6%)
20	DD6	U	212	-	39,45,45	1.61	6 (15%)	52,67,67	1.80	14 (26%)
16	CLA	G	301	12	49,53,73	1.40	6 (12%)	59,89,113	1.13	5 (8%)
20	DD6	G	312	-	24,28,45	1.78	6 (25%)	32,42,67	1.68	5 (15%)
18	LHG	A	840	16	26,26,48	0.83	0	29,32,54	1.33	3 (10%)
18	LHG	A	839	-	47,47,48	0.63	1 (2%)	50,53,54	1.25	6 (12%)
16	CLA	A	835	1	69,73,73	1.21	7 (10%)	83,113,113	0.98	4 (4%)
16	CLA	B	832	2	69,73,73	1.19	7 (10%)	83,113,113	0.94	3 (3%)
20	DD6	H	310	-	39,45,45	1.64	6 (15%)	52,67,67	1.67	10 (19%)
16	CLA	A	814	28	49,53,73	1.42	7 (14%)	59,89,113	1.14	5 (8%)
16	CLA	A	819	1	47,51,73	1.45	7 (14%)	56,86,113	1.11	4 (7%)
27	KC1	U	213	11	49,53,53	1.74	12 (24%)	63,89,89	1.02	4 (6%)
16	CLA	B	844	2	69,73,73	1.23	7 (10%)	83,113,113	0.92	3 (3%)
19	BCR	B	846	-	40,40,41	1.06	2 (5%)	54,54,56	1.31	8 (14%)
16	CLA	G	309	-	60,64,73	1.25	7 (11%)	72,102,113	1.09	6 (8%)
19	BCR	A	841	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	3 (5%)
19	BCR	B	841	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	5 (8%)
19	BCR	I	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	4 (7%)
16	CLA	B	819	2	57,61,73	1.27	8 (14%)	68,98,113	1.04	5 (7%)
16	CLA	K	207	-	50,54,73	1.36	7 (14%)	60,90,113	1.10	4 (6%)
19	BCR	B	838	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
16	CLA	A	820	1	55,59,73	1.38	8 (14%)	66,96,113	1.16	4 (6%)
24	DGD	B	843	-	61,61,67	0.92	2 (3%)	75,75,81	1.11	6 (8%)
16	CLA	L	202	9	53,57,73	1.37	8 (15%)	62,93,113	1.15	5 (8%)
16	CLA	B	823	2	69,73,73	1.24	8 (11%)	83,113,113	0.97	4 (4%)
16	CLA	U	210	11	69,73,73	1.16	5 (7%)	83,113,113	0.99	5 (6%)
16	CLA	K	203	14	59,63,73	1.26	7 (11%)	71,101,113	1.08	5 (7%)
16	CLA	B	820	28	67,71,73	1.22	8 (11%)	80,110,113	1.04	6 (7%)
16	CLA	B	801	28	69,73,73	1.19	7 (10%)	83,113,113	0.96	3 (3%)
20	DD6	U	214	-	24,26,45	1.84	5 (20%)	30,35,67	1.58	5 (16%)
26	A86	U	202	-	44,50,50	1.65	6 (13%)	51,76,76	1.52	8 (15%)
16	CLA	B	847	2	56,60,73	1.28	6 (10%)	67,97,113	1.07	4 (5%)
25	LMG	U	201	-	32,32,55	0.95	0	40,40,63	1.21	5 (12%)
16	CLA	U	205	11	69,73,73	1.20	7 (10%)	83,113,113	1.02	4 (4%)
16	CLA	A	826	1	69,73,73	1.30	8 (11%)	83,113,113	0.84	3 (3%)
16	CLA	F	804	6	50,54,73	1.39	7 (14%)	60,90,113	1.15	5 (8%)
16	CLA	A	802	1	59,63,73	1.26	7 (11%)	71,101,113	1.00	4 (5%)
16	CLA	B	825	2	69,73,73	1.26	7 (10%)	83,113,113	0.90	3 (3%)
21	LMU	F	806	-	36,36,36	1.20	2 (5%)	47,47,47	0.96	2 (4%)
16	CLA	H	301	-	43,48,73	1.48	6 (13%)	52,82,113	1.30	6 (11%)
19	BCR	F	805	-	41,41,41	1.03	2 (4%)	56,56,56	1.23	6 (10%)
16	CLA	A	823	1	69,73,73	1.27	8 (11%)	83,113,113	0.90	4 (4%)
16	CLA	U	207	-	69,73,73	1.14	6 (8%)	83,113,113	1.11	7 (8%)
16	CLA	L	204	28	54,58,73	1.36	8 (14%)	65,95,113	1.14	5 (7%)
16	CLA	U	209	-	46,50,73	1.40	6 (13%)	55,85,113	1.19	6 (10%)
16	CLA	H	302	13	64,68,73	1.26	8 (12%)	77,107,113	1.09	5 (6%)
16	CLA	F	802	28	69,73,73	1.20	7 (10%)	83,113,113	1.01	5 (6%)
16	CLA	B	811	2	59,63,73	1.27	6 (10%)	71,101,113	1.04	4 (5%)
20	DD6	A	846	-	39,45,45	1.55	8 (20%)	52,67,67	1.47	8 (15%)
16	CLA	A	809	1	66,70,73	1.25	7 (10%)	79,109,113	0.90	3 (3%)
16	CLA	B	848	2	69,73,73	1.28	8 (11%)	83,113,113	1.05	5 (6%)
20	DD6	U	203	-	39,45,45	1.63	6 (15%)	52,67,67	1.74	13 (25%)
16	CLA	A	836	28	69,73,73	1.17	7 (10%)	83,113,113	1.00	4 (4%)
16	CLA	A	815	1	69,73,73	1.22	7 (10%)	83,113,113	1.00	5 (6%)
16	CLA	k	202	28	59,63,73	1.32	8 (13%)	71,101,113	1.00	5 (7%)
16	CLA	A	813	1	54,58,73	1.39	7 (12%)	65,95,113	1.11	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	BCR	I	103	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	4 (7%)
16	CLA	G	315	12	49,53,73	1.35	6 (12%)	59,89,113	1.33	7 (11%)
16	CLA	A	832	1	55,59,73	1.36	8 (14%)	66,96,113	1.07	4 (6%)
16	CLA	B	834	28	69,73,73	1.20	7 (10%)	83,113,113	1.02	6 (7%)
16	CLA	A	833	1	69,73,73	1.22	7 (10%)	83,113,113	0.98	5 (6%)
16	CLA	A	804	1	69,73,73	1.18	8 (11%)	83,113,113	0.95	4 (4%)
16	CLA	B	849	2	69,73,73	1.19	7 (10%)	83,113,113	1.03	6 (7%)
16	CLA	J	104	8	46,50,73	1.43	7 (15%)	55,85,113	1.11	4 (7%)
16	CLA	U	211	11	56,60,73	1.37	8 (14%)	67,97,113	1.09	6 (8%)
19	BCR	A	844	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	5 (8%)
16	CLA	A	829	1	69,73,73	1.21	7 (10%)	83,113,113	0.93	3 (3%)
19	BCR	k	203	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	9 (16%)
20	DD6	J	102	-	39,45,45	1.59	8 (20%)	52,67,67	1.67	9 (17%)
16	CLA	U	208	11	50,54,73	1.36	7 (14%)	60,90,113	1.20	6 (10%)
16	CLA	B	821	28	59,63,73	1.23	6 (10%)	71,101,113	1.00	4 (5%)
16	CLA	A	838	18	56,60,73	1.30	8 (14%)	67,97,113	1.13	5 (7%)
20	DD6	G	314	-	39,45,45	1.56	8 (20%)	52,67,67	1.57	9 (17%)
16	CLA	B	806	2	69,73,73	1.21	7 (10%)	83,113,113	0.94	4 (4%)
19	BCR	B	839	-	41,41,41	1.06	2 (4%)	56,56,56	1.23	5 (8%)
19	BCR	M	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	5 (8%)
16	CLA	B	836	-	61,65,73	1.27	7 (11%)	73,103,113	1.09	6 (8%)
16	CLA	B	815	2	63,67,73	1.23	7 (11%)	75,105,113	0.99	4 (5%)
16	CLA	A	807	1	59,63,73	1.29	8 (13%)	71,101,113	1.11	6 (8%)
16	CLA	B	828	2	62,66,73	1.28	7 (11%)	74,104,113	1.04	6 (8%)
17	PQN	B	837	-	34,34,34	0.41	0	42,45,45	0.39	0
16	CLA	B	826	2	54,58,73	1.40	7 (12%)	65,95,113	1.01	4 (6%)
16	CLA	B	802	2	69,73,73	1.27	7 (10%)	83,113,113	0.82	4 (4%)
16	CLA	U	204	28	65,69,73	1.20	8 (12%)	78,108,113	1.01	5 (6%)
16	CLA	B	812	2	58,62,73	1.30	7 (12%)	69,99,113	1.03	4 (5%)
16	CLA	B	827	2	53,57,73	1.38	7 (13%)	62,93,113	1.02	3 (4%)
16	CLA	G	308	-	59,63,73	1.26	7 (11%)	71,101,113	1.11	6 (8%)
16	CLA	G	307	12	64,68,73	1.18	7 (10%)	77,107,113	1.03	4 (5%)
22	CL0	A	850	1	69,73,73	1.44	10 (14%)	83,113,113	1.05	5 (6%)
20	DD6	G	317	-	39,45,45	1.58	8 (20%)	52,67,67	1.54	10 (19%)
16	CLA	A	808	1	60,64,73	1.31	7 (11%)	72,102,113	0.97	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
16	CLA	A	847	1	64,68,73	1.32	8 (12%)	77,107,113	0.96	4 (5%)
23	SF4	C	102	3	0,12,12	-	-	-		
16	CLA	B	810	2	58,62,73	1.41	9 (15%)	73,100,113	1.01	4 (5%)
16	CLA	K	204	14	49,53,73	1.54	7 (14%)	59,89,113	1.01	3 (5%)
21	LMU	J	101	-	36,36,36	0.41	0	47,47,47	0.96	2 (4%)
16	CLA	H	312	-	69,73,73	1.11	5 (7%)	83,113,113	1.02	4 (4%)
16	CLA	A	825	1	69,73,73	1.24	7 (10%)	83,113,113	0.95	3 (3%)
16	CLA	G	303	-	49,53,73	1.43	8 (16%)	59,89,113	1.19	5 (8%)
16	CLA	B	818	2	50,54,73	1.40	7 (14%)	60,90,113	1.18	5 (8%)
16	CLA	B	813	2	63,67,73	1.27	8 (12%)	75,105,113	0.95	3 (4%)
18	LHG	G	316	-	26,26,48	0.35	0	29,32,54	0.43	0
16	CLA	A	849	1	69,73,73	1.20	6 (8%)	83,113,113	1.09	5 (6%)
16	CLA	G	310	12	49,53,73	1.44	7 (14%)	59,89,113	1.13	4 (6%)
16	CLA	B	829	28	69,73,73	1.17	7 (10%)	83,113,113	0.96	4 (4%)
16	CLA	A	821	28	69,73,73	1.21	9 (13%)	83,113,113	1.01	6 (7%)
16	CLA	k	201	15	46,50,73	1.45	5 (10%)	55,85,113	1.25	6 (10%)
16	CLA	A	822	28	69,73,73	1.14	7 (10%)	83,113,113	1.00	4 (4%)
16	CLA	B	831	2	62,66,73	1.33	8 (12%)	74,104,113	1.01	4 (5%)

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
16	CLA	A	851	1	-	6/39/115/115	-
16	CLA	A	801	-	-	1/39/115/115	-
16	CLA	B	816	2	-	0/33/109/115	-
16	CLA	A	812	1	-	2/15/91/115	-
16	CLA	A	827	1	-	3/21/97/115	-
16	CLA	G	306	12	-	10/39/115/115	-
16	CLA	A	854	1	-	6/39/115/115	-
16	CLA	I	102	-	-	4/39/115/115	-
16	CLA	L	203	9	-	1/39/115/115	-
16	CLA	H	308	13	-	2/10/86/115	-
16	CLA	B	808	2	-	5/39/115/115	-
16	CLA	A	803	1	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	845	2	-	3/39/115/115	-
20	DD6	H	311	-	-	11/26/80/80	0/3/3/3
16	CLA	K	202	14	-	0/12/88/115	-
16	CLA	H	309	13	-	4/15/91/115	-
16	CLA	A	806	1	-	8/39/115/115	-
16	CLA	B	804	2	-	4/15/91/115	-
20	DD6	G	313	-	-	6/26/80/80	0/3/3/3
16	CLA	H	304	13	-	1/13/90/115	-
16	CLA	B	817	28	-	5/39/115/115	-
16	CLA	B	803	-	-	3/39/115/115	-
16	CLA	H	305	13	-	2/15/91/115	-
16	CLA	A	830	1	-	0/21/97/115	-
19	BCR	L	201	-	-	10/29/63/63	0/2/2/2
16	CLA	F	803	28	-	3/19/95/115	-
21	LMU	A	848	-	-	10/21/61/61	0/2/2/2
16	CLA	A	834	1	-	9/39/115/115	-
19	BCR	B	842	-	-	7/29/63/63	0/2/2/2
16	CLA	H	306	13	-	6/39/115/115	-
16	CLA	B	809	2	-	6/39/115/115	-
16	CLA	B	824	2	-	3/39/115/115	-
16	CLA	A	853	1	-	11/39/115/115	-
16	CLA	A	817	1	-	3/15/91/115	-
16	CLA	A	810	1	-	4/26/102/115	-
16	CLA	G	302	-	-	1/10/86/115	-
16	CLA	K	205	14	-	5/31/107/115	-
21	LMU	A	855	-	-	8/21/61/61	0/2/2/2
19	BCR	B	840	-	-	6/29/63/63	0/2/2/2
16	CLA	B	830	28	-	0/15/91/115	-
16	CLA	A	818	28	-	3/39/115/115	-
19	BCR	A	842	-	-	10/29/63/63	0/2/2/2
16	CLA	B	822	2	-	2/39/115/115	-
23	SF4	C	101	3	-	-	0/6/5/5
16	CLA	B	814	2	-	8/27/103/115	-
16	CLA	G	305	12	-	13/35/111/115	-
16	CLA	K	206	28	-	1/10/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	L	205	-	-	8/29/63/63	0/2/2/2
21	LMU	K	201	-	-	12/21/61/61	0/2/2/2
16	CLA	A	816	1	-	2/39/115/115	-
16	CLA	A	811	1	-	3/39/115/115	-
23	SF4	A	852	1,2	-	-	0/6/5/5
25	LMG	J	103	-	-	22/34/54/70	0/1/1/1
16	CLA	A	845	28	-	7/39/115/115	-
16	CLA	G	304	12	-	3/13/89/115	-
19	BCR	J	105	-	-	10/29/63/63	0/2/2/2
16	CLA	A	831	1	-	4/15/91/115	-
19	BCR	F	801	-	-	10/29/63/63	0/2/2/2
16	CLA	B	805	2	-	7/39/115/115	-
16	CLA	H	307	-	-	7/31/107/115	-
16	CLA	A	824	1	-	5/36/112/115	-
16	CLA	B	835	2	-	8/39/115/115	-
16	CLA	A	805	1	-	3/20/96/115	-
16	CLA	B	807	2	-	5/39/115/115	-
16	CLA	B	833	2	-	2/18/94/115	-
17	PQN	A	837	-	-	3/23/43/43	0/2/2/2
16	CLA	U	206	11	-	2/15/91/115	-
16	CLA	A	828	1	-	3/39/115/115	-
20	DD6	K	208	-	-	11/26/80/80	0/3/3/3
20	DD6	G	311	-	-	7/26/80/80	0/3/3/3
19	BCR	A	843	-	-	4/29/63/63	0/2/2/2
16	CLA	H	303	13	-	4/35/111/115	-
20	DD6	U	212	-	-	14/26/80/80	0/3/3/3
16	CLA	G	301	12	-	3/15/91/115	-
20	DD6	G	312	-	-	6/19/50/80	0/2/2/3
18	LHG	A	840	16	-	6/31/31/53	-
18	LHG	A	839	-	-	19/52/52/53	-
16	CLA	A	835	1	-	1/39/115/115	-
16	CLA	B	832	2	-	3/39/115/115	-
20	DD6	H	310	-	-	15/26/80/80	0/3/3/3
16	CLA	A	814	28	-	3/15/91/115	-
16	CLA	A	819	1	-	1/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	KC1	U	213	11	-	0/15/71/71	-
16	CLA	B	844	2	-	5/39/115/115	-
19	BCR	B	846	-	-	17/27/61/63	0/2/2/2
16	CLA	G	309	-	-	8/29/105/115	-
19	BCR	A	841	-	-	7/29/63/63	0/2/2/2
19	BCR	B	841	-	-	6/29/63/63	0/2/2/2
19	BCR	I	101	-	-	9/29/63/63	0/2/2/2
16	CLA	B	819	2	-	5/25/101/115	-
16	CLA	K	207	-	-	4/17/93/115	-
19	BCR	B	838	-	-	9/29/63/63	0/2/2/2
16	CLA	A	820	1	-	3/23/99/115	-
24	DGD	B	843	-	-	25/49/89/95	0/2/2/2
16	CLA	L	202	9	-	6/20/96/115	-
16	CLA	B	823	2	-	5/39/115/115	-
16	CLA	U	210	11	-	3/39/115/115	-
16	CLA	K	203	14	-	3/27/103/115	-
16	CLA	B	820	28	-	5/37/113/115	-
16	CLA	B	801	28	-	2/39/115/115	-
20	DD6	U	214	-	-	3/14/37/80	0/1/1/3
26	A86	U	202	-	-	16/34/90/90	0/3/3/3
16	CLA	B	847	2	-	7/24/100/115	-
25	LMG	U	201	-	-	13/27/47/70	0/1/1/1
16	CLA	U	205	11	-	3/39/115/115	-
16	CLA	A	826	1	-	2/39/115/115	-
16	CLA	F	804	6	-	6/17/93/115	-
16	CLA	A	802	1	-	3/27/103/115	-
16	CLA	B	825	2	-	3/39/115/115	-
21	LMU	F	806	-	-	7/21/61/61	0/2/2/2
16	CLA	H	301	-	-	3/10/82/115	-
19	BCR	F	805	-	-	12/29/63/63	0/2/2/2
16	CLA	A	823	1	-	3/39/115/115	-
16	CLA	U	207	-	-	3/39/115/115	-
16	CLA	L	204	28	-	6/21/97/115	-
16	CLA	U	209	-	-	0/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	302	13	-	6/33/109/115	-
16	CLA	F	802	28	-	1/39/115/115	-
16	CLA	B	811	2	-	7/27/103/115	-
20	DD6	A	846	-	-	9/26/80/80	0/3/3/3
16	CLA	A	809	1	-	0/36/112/115	-
16	CLA	B	848	2	-	4/39/115/115	-
20	DD6	U	203	-	-	10/26/80/80	0/3/3/3
16	CLA	A	836	28	-	4/39/115/115	-
16	CLA	A	815	1	-	4/39/115/115	-
16	CLA	k	202	28	-	5/27/103/115	-
16	CLA	A	813	1	-	2/21/97/115	-
19	BCR	I	103	-	-	10/29/63/63	0/2/2/2
16	CLA	G	315	12	-	5/15/91/115	-
16	CLA	A	832	1	-	2/23/99/115	-
16	CLA	B	834	28	-	6/39/115/115	-
16	CLA	A	833	1	-	1/39/115/115	-
16	CLA	A	804	1	-	10/39/115/115	-
16	CLA	B	849	2	-	5/39/115/115	-
16	CLA	J	104	8	-	5/12/88/115	-
16	CLA	U	211	11	-	5/24/100/115	-
19	BCR	A	844	-	-	9/29/63/63	0/2/2/2
16	CLA	A	829	1	-	1/39/115/115	-
19	BCR	k	203	-	-	10/29/63/63	0/2/2/2
20	DD6	J	102	-	-	5/26/80/80	0/3/3/3
16	CLA	U	208	11	-	4/17/93/115	-
16	CLA	B	821	28	-	3/27/103/115	-
16	CLA	A	838	18	-	3/24/100/115	-
20	DD6	G	314	-	-	12/26/80/80	0/3/3/3
16	CLA	B	806	2	-	4/39/115/115	-
19	BCR	B	839	-	-	10/29/63/63	0/2/2/2
19	BCR	M	101	-	-	8/29/63/63	0/2/2/2
16	CLA	B	836	-	-	4/30/106/115	-
16	CLA	B	815	2	-	2/32/108/115	-
16	CLA	A	807	1	-	4/27/103/115	-
16	CLA	B	828	2	-	7/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PQN	B	837	-	-	1/23/43/43	0/2/2/2
16	CLA	B	826	2	-	1/21/97/115	-
16	CLA	B	802	2	-	3/39/115/115	-
16	CLA	U	204	28	-	12/35/111/115	-
16	CLA	B	812	2	-	2/26/102/115	-
16	CLA	B	827	2	-	3/20/96/115	-
16	CLA	G	308	-	-	4/27/103/115	-
16	CLA	G	307	12	-	7/33/109/115	-
22	CL0	A	850	1	-	9/39/115/115	-
20	DD6	G	317	-	-	12/26/80/80	0/3/3/3
16	CLA	A	808	1	-	0/29/105/115	-
16	CLA	A	847	1	-	6/33/109/115	-
23	SF4	C	102	3	-	-	0/6/5/5
16	CLA	B	810	2	-	0/25/101/115	-
16	CLA	K	204	14	-	5/15/91/115	-
21	LMU	J	101	-	-	9/21/61/61	0/2/2/2
16	CLA	H	312	-	-	21/39/115/115	-
16	CLA	A	825	1	-	6/39/115/115	-
16	CLA	G	303	-	-	5/15/91/115	-
16	CLA	B	818	2	-	1/17/93/115	-
16	CLA	B	813	2	-	1/32/108/115	-
18	LHG	G	316	-	-	22/31/31/53	-
16	CLA	A	849	1	-	9/39/115/115	-
16	CLA	G	310	12	-	7/15/91/115	-
16	CLA	B	829	28	-	1/39/115/115	-
16	CLA	A	821	28	-	7/39/115/115	-
16	CLA	k	201	15	-	1/12/88/115	-
16	CLA	A	822	28	-	2/39/115/115	-
16	CLA	B	831	2	-	3/31/107/115	-

All (1087) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	202	A86	C13-C11	-6.10	1.37	1.49
16	K	204	CLA	MG-NA	5.17	2.18	2.06
16	B	848	CLA	MG-NA	5.05	2.18	2.06
16	A	826	CLA	MG-NA	5.04	2.18	2.06
16	H	305	CLA	MG-NA	5.03	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	U	214	DD6	C26-C27	4.93	1.47	1.37
16	G	306	CLA	MG-NA	4.88	2.17	2.06
16	B	831	CLA	MG-NA	4.82	2.17	2.06
22	A	850	CL0	MG-NA	4.80	2.17	2.06
16	B	825	CLA	MG-NA	4.80	2.17	2.06
16	A	823	CLA	MG-NA	4.73	2.17	2.06
16	B	822	CLA	MG-NA	4.71	2.17	2.06
22	A	850	CL0	C4C-C3C	-4.69	1.37	1.45
16	A	834	CLA	MG-NA	4.68	2.17	2.06
16	A	823	CLA	C4C-C3C	-4.65	1.37	1.45
16	B	823	CLA	MG-NA	4.61	2.17	2.06
16	U	211	CLA	MG-NA	4.60	2.17	2.06
16	B	810	CLA	MG-NA	4.56	2.17	2.06
16	U	205	CLA	C4C-C3C	-4.54	1.37	1.45
16	A	825	CLA	MG-NA	4.54	2.17	2.06
16	B	802	CLA	C4C-C3C	-4.54	1.37	1.45
16	B	847	CLA	C4C-C3C	-4.51	1.37	1.45
16	A	828	CLA	MG-NA	4.51	2.17	2.06
16	B	822	CLA	C4C-C3C	-4.50	1.37	1.45
16	A	847	CLA	MG-NA	4.50	2.17	2.06
16	A	815	CLA	C4C-C3C	-4.50	1.37	1.45
16	B	844	CLA	MG-NA	4.49	2.16	2.06
16	G	307	CLA	C4C-C3C	-4.49	1.37	1.45
16	G	301	CLA	C4C-C3C	-4.48	1.37	1.45
16	B	814	CLA	MG-NA	4.48	2.16	2.06
20	H	310	DD6	C2-C1	4.48	1.41	1.35
16	A	832	CLA	C4C-C3C	-4.48	1.37	1.45
16	B	804	CLA	MG-NA	4.47	2.16	2.06
16	G	304	CLA	C4C-C3C	-4.47	1.37	1.45
16	B	808	CLA	C1C-C2C	-4.47	1.35	1.44
16	B	816	CLA	C4C-C3C	-4.46	1.37	1.45
16	U	206	CLA	C4C-C3C	-4.46	1.37	1.45
16	A	827	CLA	MG-NA	4.46	2.16	2.06
16	B	804	CLA	C4C-C3C	-4.46	1.37	1.45
16	G	308	CLA	C4C-C3C	-4.46	1.37	1.45
16	k	201	CLA	C1C-C2C	-4.46	1.35	1.44
16	B	808	CLA	C4C-C3C	-4.45	1.37	1.45
16	B	818	CLA	C4C-C3C	-4.45	1.37	1.45
16	A	838	CLA	C4C-C3C	-4.45	1.37	1.45
16	k	202	CLA	C4C-C3C	-4.45	1.37	1.45
16	H	304	CLA	C4C-C3C	-4.45	1.37	1.45
16	B	830	CLA	C4C-C3C	-4.44	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	849	CLA	C4C-C3C	-4.44	1.37	1.45
16	U	211	CLA	C4C-C3C	-4.44	1.37	1.45
16	A	849	CLA	C1C-C2C	-4.44	1.36	1.44
16	A	803	CLA	C1C-C2C	-4.44	1.36	1.44
16	U	210	CLA	C1C-C2C	-4.44	1.36	1.44
16	B	807	CLA	C4C-C3C	-4.44	1.37	1.45
16	B	803	CLA	C1C-C2C	-4.44	1.36	1.44
16	B	809	CLA	C1C-C2C	-4.44	1.36	1.44
20	U	212	DD6	C10-C11	4.44	1.41	1.35
16	B	813	CLA	C4C-C3C	-4.44	1.37	1.45
16	B	824	CLA	C4C-C3C	-4.44	1.37	1.45
26	U	202	A86	C5-C6	4.43	1.41	1.35
16	H	303	CLA	C4C-C3C	-4.43	1.37	1.45
16	A	812	CLA	MG-NA	4.43	2.16	2.06
16	A	823	CLA	C1C-C2C	-4.43	1.36	1.44
16	A	809	CLA	C4C-C3C	-4.43	1.37	1.45
16	A	818	CLA	C1C-C2C	-4.43	1.36	1.44
16	U	207	CLA	C4C-C3C	-4.42	1.37	1.45
16	U	209	CLA	C4C-C3C	-4.42	1.37	1.45
16	B	833	CLA	C4C-C3C	-4.42	1.37	1.45
16	A	825	CLA	C4C-C3C	-4.42	1.37	1.45
16	B	828	CLA	C4C-C3C	-4.42	1.37	1.45
16	B	832	CLA	C4C-C3C	-4.42	1.37	1.45
16	A	824	CLA	C4C-C3C	-4.42	1.37	1.45
16	A	801	CLA	C4C-C3C	-4.42	1.37	1.45
16	B	814	CLA	C4C-C3C	-4.42	1.37	1.45
16	B	835	CLA	C1C-C2C	-4.42	1.36	1.44
16	A	806	CLA	C4C-C3C	-4.41	1.37	1.45
16	A	812	CLA	C1C-C2C	-4.41	1.36	1.44
16	B	822	CLA	C1C-C2C	-4.41	1.36	1.44
16	A	802	CLA	C4C-C3C	-4.41	1.37	1.45
16	A	822	CLA	C4C-C3C	-4.41	1.37	1.45
16	A	808	CLA	C4C-C3C	-4.41	1.37	1.45
16	A	847	CLA	C4C-C3C	-4.41	1.37	1.45
16	A	818	CLA	C4C-C3C	-4.40	1.37	1.45
16	G	306	CLA	C4C-C3C	-4.40	1.37	1.45
24	B	843	DGD	O2G-C1B	4.40	1.46	1.34
16	B	827	CLA	MG-NA	4.40	2.16	2.06
16	A	829	CLA	C1C-C2C	-4.40	1.36	1.44
16	L	203	CLA	C4C-C3C	-4.40	1.37	1.45
16	A	813	CLA	C4C-C3C	-4.40	1.37	1.45
16	A	834	CLA	C4C-C3C	-4.40	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	812	CLA	C4C-C3C	-4.40	1.37	1.45
16	A	805	CLA	C4C-C3C	-4.40	1.37	1.45
16	H	305	CLA	C4C-C3C	-4.40	1.37	1.45
16	A	805	CLA	MG-NA	4.40	2.16	2.06
16	A	828	CLA	C4C-C3C	-4.40	1.37	1.45
16	A	815	CLA	MG-NA	4.39	2.16	2.06
16	A	810	CLA	C4C-C3C	-4.39	1.37	1.45
16	F	803	CLA	C1C-C2C	-4.39	1.36	1.44
16	B	806	CLA	C4C-C3C	-4.39	1.37	1.45
16	K	205	CLA	C4C-C3C	-4.39	1.37	1.45
16	B	825	CLA	C4C-C3C	-4.39	1.37	1.45
16	A	804	CLA	C4C-C3C	-4.39	1.37	1.45
16	A	820	CLA	C4C-C3C	-4.39	1.37	1.45
16	H	312	CLA	C4C-C3C	-4.39	1.37	1.45
16	A	814	CLA	C4C-C3C	-4.39	1.37	1.45
22	A	850	CL0	C1C-C2C	-4.39	1.36	1.44
16	A	821	CLA	MG-NA	4.38	2.16	2.06
16	G	302	CLA	C4C-C3C	-4.38	1.37	1.45
16	A	826	CLA	C1C-C2C	-4.38	1.36	1.44
16	B	811	CLA	C4C-C3C	-4.38	1.37	1.45
16	B	801	CLA	C4C-C3C	-4.38	1.37	1.45
16	B	845	CLA	C4C-C3C	-4.38	1.37	1.45
16	H	301	CLA	C1C-C2C	-4.38	1.36	1.44
16	J	104	CLA	C4C-C3C	-4.37	1.37	1.45
16	B	820	CLA	C1C-C2C	-4.37	1.36	1.44
16	B	834	CLA	C4C-C3C	-4.37	1.37	1.45
16	B	823	CLA	C4C-C3C	-4.37	1.37	1.45
16	B	805	CLA	C4C-C3C	-4.37	1.37	1.45
16	L	202	CLA	C4C-C3C	-4.37	1.37	1.45
16	A	827	CLA	C4C-C3C	-4.37	1.37	1.45
16	A	826	CLA	C4C-C3C	-4.36	1.37	1.45
16	F	804	CLA	C4C-C3C	-4.36	1.37	1.45
16	A	803	CLA	C4C-C3C	-4.36	1.37	1.45
16	H	302	CLA	C4C-C3C	-4.36	1.37	1.45
16	U	204	CLA	C4C-C3C	-4.36	1.37	1.45
16	K	204	CLA	C4C-C3C	-4.36	1.37	1.45
16	B	826	CLA	C4C-C3C	-4.36	1.37	1.45
16	I	102	CLA	C4C-C3C	-4.36	1.37	1.45
16	G	305	CLA	C4C-C3C	-4.36	1.37	1.45
16	H	306	CLA	C4C-C3C	-4.36	1.37	1.45
20	H	310	DD6	C5-C6	4.36	1.41	1.35
16	B	831	CLA	C4C-C3C	-4.36	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	835	CLA	C4C-C3C	-4.36	1.37	1.45
16	U	210	CLA	C4C-C3C	-4.35	1.37	1.45
16	B	821	CLA	C4C-C3C	-4.35	1.37	1.45
16	A	832	CLA	MG-NA	4.35	2.16	2.06
16	G	303	CLA	C4C-C3C	-4.35	1.37	1.45
16	B	845	CLA	MG-NA	4.35	2.16	2.06
16	B	809	CLA	C4C-C3C	-4.35	1.37	1.45
16	F	802	CLA	C4C-C3C	-4.35	1.37	1.45
16	A	833	CLA	C4C-C3C	-4.35	1.37	1.45
16	A	829	CLA	C4C-C3C	-4.35	1.37	1.45
16	A	851	CLA	C4C-C3C	-4.35	1.37	1.45
16	B	827	CLA	C4C-C3C	-4.35	1.37	1.45
16	U	208	CLA	C4C-C3C	-4.34	1.37	1.45
16	A	831	CLA	C4C-C3C	-4.34	1.37	1.45
16	A	836	CLA	C4C-C3C	-4.34	1.37	1.45
16	H	302	CLA	C1C-C2C	-4.34	1.36	1.44
16	B	810	CLA	C4C-C3C	-4.34	1.37	1.45
16	H	309	CLA	C1C-C2C	-4.34	1.36	1.44
16	B	803	CLA	C4C-C3C	-4.34	1.37	1.45
16	A	853	CLA	C4C-C3C	-4.34	1.37	1.45
16	K	206	CLA	C4C-C3C	-4.33	1.37	1.45
16	H	307	CLA	C4C-C3C	-4.33	1.37	1.45
16	A	854	CLA	C4C-C3C	-4.33	1.37	1.45
16	A	835	CLA	C4C-C3C	-4.33	1.37	1.45
16	A	817	CLA	C4C-C3C	-4.33	1.37	1.45
16	K	203	CLA	C4C-C3C	-4.33	1.37	1.45
16	A	853	CLA	C1C-C2C	-4.33	1.36	1.44
16	A	833	CLA	MG-NA	4.33	2.16	2.06
16	A	830	CLA	C1C-C2C	-4.33	1.36	1.44
16	G	301	CLA	C1C-C2C	-4.33	1.36	1.44
16	H	309	CLA	C4C-C3C	-4.33	1.37	1.45
16	A	851	CLA	C1C-C2C	-4.33	1.36	1.44
16	A	813	CLA	MG-NA	4.33	2.16	2.06
27	U	213	KC1	C4C-C3C	-4.33	1.37	1.45
16	A	807	CLA	C4C-C3C	-4.33	1.37	1.45
16	A	816	CLA	C4C-C3C	-4.33	1.37	1.45
16	G	310	CLA	C4C-C3C	-4.32	1.37	1.45
16	A	806	CLA	C1C-C2C	-4.32	1.36	1.44
16	A	825	CLA	C1C-C2C	-4.32	1.36	1.44
16	A	845	CLA	C4C-C3C	-4.32	1.37	1.45
16	L	204	CLA	C4C-C3C	-4.31	1.37	1.45
16	H	308	CLA	C4C-C3C	-4.31	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	811	CLA	C4C-C3C	-4.31	1.37	1.45
16	A	808	CLA	C1C-C2C	-4.31	1.36	1.44
16	B	816	CLA	C1C-C2C	-4.31	1.36	1.44
16	B	819	CLA	C4C-C3C	-4.30	1.37	1.45
16	A	832	CLA	C1C-C2C	-4.30	1.36	1.44
16	A	828	CLA	C1C-C2C	-4.30	1.36	1.44
16	B	802	CLA	C1C-C2C	-4.30	1.36	1.44
16	G	305	CLA	C1C-C2C	-4.30	1.36	1.44
16	A	809	CLA	C1C-C2C	-4.30	1.36	1.44
16	A	807	CLA	C1C-C2C	-4.30	1.36	1.44
16	B	826	CLA	C1C-C2C	-4.29	1.36	1.44
16	A	836	CLA	C1C-C2C	-4.29	1.36	1.44
16	B	829	CLA	C4C-C3C	-4.29	1.37	1.45
16	k	201	CLA	C4C-C3C	-4.29	1.37	1.45
16	A	811	CLA	C1C-C2C	-4.29	1.36	1.44
16	K	202	CLA	C4C-C3C	-4.28	1.37	1.45
16	A	811	CLA	MG-NA	4.28	2.16	2.06
16	A	804	CLA	C1C-C2C	-4.28	1.36	1.44
16	K	207	CLA	C4C-C3C	-4.28	1.37	1.45
16	B	828	CLA	C1C-C2C	-4.28	1.36	1.44
16	G	309	CLA	C4C-C3C	-4.28	1.37	1.45
16	B	815	CLA	C1C-C2C	-4.28	1.36	1.44
16	B	819	CLA	C1C-C2C	-4.28	1.36	1.44
26	U	202	A86	C2-C1	4.28	1.41	1.35
16	G	303	CLA	MG-NA	4.28	2.16	2.06
16	B	844	CLA	C1C-C2C	-4.28	1.36	1.44
16	U	211	CLA	C1C-C2C	-4.28	1.36	1.44
16	H	312	CLA	C1C-C2C	-4.28	1.36	1.44
16	B	811	CLA	C1C-C2C	-4.28	1.36	1.44
16	A	809	CLA	MG-NA	4.28	2.16	2.06
16	B	832	CLA	C1C-C2C	-4.28	1.36	1.44
16	A	822	CLA	C1C-C2C	-4.28	1.36	1.44
16	A	834	CLA	C1C-C2C	-4.27	1.36	1.44
16	A	847	CLA	C1C-C2C	-4.27	1.36	1.44
16	B	824	CLA	MG-NA	4.27	2.16	2.06
16	A	813	CLA	C1C-C2C	-4.27	1.36	1.44
16	A	827	CLA	C1C-C2C	-4.27	1.36	1.44
16	B	845	CLA	C1C-C2C	-4.27	1.36	1.44
16	B	836	CLA	C4C-C3C	-4.26	1.37	1.45
16	U	206	CLA	C1C-C2C	-4.26	1.36	1.44
16	A	817	CLA	C1C-C2C	-4.26	1.36	1.44
16	K	202	CLA	C1C-C2C	-4.26	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	817	CLA	C4C-C3C	-4.26	1.37	1.45
16	B	849	CLA	C1C-C2C	-4.26	1.36	1.44
16	U	207	CLA	C1C-C2C	-4.26	1.36	1.44
16	A	830	CLA	C4C-C3C	-4.25	1.37	1.45
16	B	815	CLA	C4C-C3C	-4.25	1.37	1.45
16	A	819	CLA	C1C-C2C	-4.25	1.36	1.44
16	B	805	CLA	C1C-C2C	-4.25	1.36	1.44
16	B	812	CLA	C1C-C2C	-4.25	1.36	1.44
24	B	843	DGD	O1G-C1A	4.25	1.45	1.33
16	B	817	CLA	C1C-C2C	-4.25	1.36	1.44
27	U	213	KC1	C1C-C2C	-4.25	1.36	1.44
16	L	202	CLA	C1C-C2C	-4.24	1.36	1.44
16	B	824	CLA	C1C-C2C	-4.24	1.36	1.44
16	B	827	CLA	C1C-C2C	-4.24	1.36	1.44
16	H	308	CLA	C1C-C2C	-4.24	1.36	1.44
16	A	820	CLA	C1C-C2C	-4.24	1.36	1.44
16	B	813	CLA	C1C-C2C	-4.24	1.36	1.44
16	K	204	CLA	C1C-C2C	-4.23	1.36	1.44
16	B	833	CLA	C1C-C2C	-4.23	1.36	1.44
16	F	803	CLA	MG-NA	4.23	2.16	2.06
16	H	304	CLA	C1C-C2C	-4.23	1.36	1.44
16	F	802	CLA	C1C-C2C	-4.23	1.36	1.44
16	K	203	CLA	C1C-C2C	-4.23	1.36	1.44
16	B	821	CLA	C1C-C2C	-4.23	1.36	1.44
16	B	829	CLA	C1C-C2C	-4.23	1.36	1.44
16	A	816	CLA	C1C-C2C	-4.23	1.36	1.44
16	B	806	CLA	C1C-C2C	-4.23	1.36	1.44
16	B	836	CLA	MG-NA	4.23	2.16	2.06
16	A	835	CLA	C1C-C2C	-4.22	1.36	1.44
16	L	203	CLA	C1C-C2C	-4.22	1.36	1.44
16	B	820	CLA	C4C-C3C	-4.22	1.37	1.45
16	K	206	CLA	C1C-C2C	-4.22	1.36	1.44
16	G	315	CLA	C1C-C2C	-4.22	1.36	1.44
16	B	808	CLA	MG-NA	4.22	2.16	2.06
16	A	831	CLA	C1C-C2C	-4.21	1.36	1.44
16	B	836	CLA	C1C-C2C	-4.21	1.36	1.44
16	A	814	CLA	C1C-C2C	-4.21	1.36	1.44
16	G	310	CLA	C1C-C2C	-4.21	1.36	1.44
16	H	307	CLA	C1C-C2C	-4.21	1.36	1.44
16	A	838	CLA	C1C-C2C	-4.21	1.36	1.44
20	U	212	DD6	C5-C6	4.21	1.41	1.35
16	G	306	CLA	C1C-C2C	-4.21	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	854	CLA	C1C-C2C	-4.21	1.36	1.44
16	A	808	CLA	MG-NA	4.21	2.16	2.06
16	A	801	CLA	C1C-C2C	-4.20	1.36	1.44
16	B	814	CLA	C1C-C2C	-4.20	1.36	1.44
16	B	823	CLA	C1C-C2C	-4.20	1.36	1.44
16	B	810	CLA	C1C-C2C	-4.20	1.36	1.44
16	k	202	CLA	MG-NA	4.20	2.16	2.06
16	A	833	CLA	C1C-C2C	-4.20	1.36	1.44
16	G	308	CLA	C1C-C2C	-4.20	1.36	1.44
16	A	821	CLA	C4C-C3C	-4.19	1.37	1.45
16	B	844	CLA	C4C-C3C	-4.19	1.37	1.45
16	B	806	CLA	MG-NA	4.19	2.16	2.06
16	B	804	CLA	C1C-C2C	-4.19	1.36	1.44
16	G	309	CLA	C1C-C2C	-4.19	1.36	1.44
16	k	202	CLA	C1C-C2C	-4.19	1.36	1.44
16	B	801	CLA	C1C-C2C	-4.19	1.36	1.44
16	A	849	CLA	C4C-C3C	-4.19	1.37	1.45
16	G	302	CLA	C1C-C2C	-4.18	1.36	1.44
16	A	812	CLA	C4C-C3C	-4.18	1.37	1.45
16	L	204	CLA	C1C-C2C	-4.18	1.36	1.44
16	B	833	CLA	MG-NA	4.18	2.16	2.06
16	A	845	CLA	C1C-C2C	-4.18	1.36	1.44
16	A	802	CLA	C1C-C2C	-4.18	1.36	1.44
16	B	834	CLA	C1C-C2C	-4.18	1.36	1.44
16	J	104	CLA	C1C-C2C	-4.18	1.36	1.44
16	A	805	CLA	C1C-C2C	-4.18	1.36	1.44
16	B	825	CLA	C1C-C2C	-4.18	1.36	1.44
16	A	807	CLA	MG-NA	4.18	2.16	2.06
16	G	315	CLA	C4C-C3C	-4.18	1.37	1.45
16	K	207	CLA	C1C-C2C	-4.18	1.36	1.44
20	U	214	DD6	C2-C1	4.18	1.41	1.35
16	A	819	CLA	C4C-C3C	-4.17	1.37	1.45
16	U	204	CLA	C1C-C2C	-4.17	1.36	1.44
16	A	810	CLA	C1C-C2C	-4.17	1.36	1.44
20	G	313	DD6	C5-C6	4.17	1.41	1.35
16	F	804	CLA	C1C-C2C	-4.17	1.36	1.44
16	B	848	CLA	C4C-C3C	-4.17	1.37	1.45
16	A	821	CLA	C1C-C2C	-4.17	1.36	1.44
16	B	848	CLA	C1C-C2C	-4.16	1.36	1.44
20	K	208	DD6	C10-C11	4.16	1.41	1.35
16	L	204	CLA	MG-NA	4.16	2.16	2.06
16	B	826	CLA	MG-NA	4.16	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	847	CLA	C1C-C2C	-4.15	1.36	1.44
16	B	830	CLA	C1C-C2C	-4.14	1.36	1.44
16	G	303	CLA	C1C-C2C	-4.14	1.36	1.44
16	F	803	CLA	C4C-C3C	-4.14	1.37	1.45
16	A	824	CLA	C1C-C2C	-4.14	1.36	1.44
16	B	807	CLA	C1C-C2C	-4.14	1.36	1.44
20	K	208	DD6	C5-C6	4.14	1.41	1.35
16	H	303	CLA	C1C-C2C	-4.13	1.36	1.44
16	B	820	CLA	MG-NA	4.13	2.16	2.06
16	U	208	CLA	C1C-C2C	-4.13	1.36	1.44
20	G	313	DD6	C10-C11	4.13	1.41	1.35
16	A	829	CLA	MG-NA	4.13	2.16	2.06
20	U	203	DD6	C5-C6	4.13	1.41	1.35
16	B	835	CLA	MG-NA	4.12	2.16	2.06
16	G	304	CLA	C1C-C2C	-4.12	1.36	1.44
16	H	302	CLA	MG-NA	4.12	2.16	2.06
20	U	203	DD6	C2-C1	4.12	1.41	1.35
16	A	817	CLA	MG-NA	4.12	2.16	2.06
27	U	213	KC1	C4D-ND	-4.12	1.32	1.37
16	B	818	CLA	C1C-C2C	-4.12	1.36	1.44
16	A	819	CLA	MG-NA	4.12	2.16	2.06
20	K	208	DD6	C2-C1	4.12	1.41	1.35
16	K	205	CLA	C1C-C2C	-4.11	1.36	1.44
16	H	301	CLA	C4C-C3C	-4.11	1.38	1.45
16	H	305	CLA	C1C-C2C	-4.10	1.36	1.44
16	I	102	CLA	C1C-C2C	-4.10	1.36	1.44
16	A	815	CLA	C1C-C2C	-4.10	1.36	1.44
16	F	802	CLA	MG-NA	4.09	2.16	2.06
16	B	831	CLA	C1C-C2C	-4.09	1.36	1.44
16	H	309	CLA	MG-NA	4.08	2.16	2.06
16	U	209	CLA	C1C-C2C	-4.08	1.36	1.44
16	B	807	CLA	MG-NA	4.08	2.16	2.06
20	H	311	DD6	C5-C6	4.08	1.41	1.35
16	K	206	CLA	MG-NA	4.07	2.15	2.06
16	U	205	CLA	C1C-C2C	-4.07	1.36	1.44
16	B	830	CLA	MG-NA	4.07	2.15	2.06
20	U	212	DD6	C2-C1	4.05	1.41	1.35
16	G	307	CLA	C1C-C2C	-4.05	1.36	1.44
20	G	317	DD6	C10-C11	4.05	1.41	1.35
16	B	801	CLA	MG-NA	4.05	2.15	2.06
20	G	312	DD6	C5-C6	4.05	1.41	1.35
16	B	834	CLA	MG-NA	4.03	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	830	CLA	MG-NA	4.03	2.15	2.06
16	B	816	CLA	MG-NA	4.02	2.15	2.06
16	L	202	CLA	MG-NA	4.02	2.15	2.06
20	G	313	DD6	C2-C1	4.02	1.41	1.35
20	G	317	DD6	C2-C1	4.01	1.41	1.35
20	G	317	DD6	C5-C6	4.01	1.41	1.35
20	J	102	DD6	C10-C11	4.00	1.41	1.35
16	B	802	CLA	MG-NA	4.00	2.15	2.06
22	A	850	CL0	MG-NC	4.00	2.15	2.06
16	A	814	CLA	MG-NA	3.99	2.15	2.06
16	A	810	CLA	MG-NA	3.99	2.15	2.06
16	A	835	CLA	MG-NA	3.98	2.15	2.06
20	J	102	DD6	C2-C1	3.97	1.41	1.35
27	U	213	KC1	C3B-C4B	-3.97	1.39	1.46
20	U	203	DD6	C10-C11	3.97	1.41	1.35
16	A	824	CLA	MG-NA	3.97	2.15	2.06
16	H	301	CLA	MG-NA	3.96	2.15	2.06
16	F	804	CLA	MG-NA	3.96	2.15	2.06
20	J	102	DD6	C5-C6	3.96	1.41	1.35
16	A	820	CLA	MG-NA	3.96	2.15	2.06
16	H	306	CLA	C1C-C2C	-3.95	1.36	1.44
16	B	828	CLA	MG-NA	3.95	2.15	2.06
16	U	205	CLA	MG-NA	3.94	2.15	2.06
16	I	102	CLA	MG-NA	3.94	2.15	2.06
16	A	851	CLA	MG-NA	3.93	2.15	2.06
16	B	809	CLA	MG-NA	3.93	2.15	2.06
16	B	802	CLA	MG-NC	3.92	2.15	2.06
20	G	312	DD6	C10-C11	3.92	1.41	1.35
20	H	311	DD6	C10-C11	3.92	1.41	1.35
20	H	311	DD6	C2-C1	3.91	1.41	1.35
16	B	812	CLA	MG-NA	3.91	2.15	2.06
16	B	832	CLA	MG-NA	3.90	2.15	2.06
16	J	104	CLA	MG-NA	3.90	2.15	2.06
16	G	310	CLA	MG-NA	3.90	2.15	2.06
16	G	309	CLA	MG-NA	3.90	2.15	2.06
20	G	311	DD6	C10-C11	3.90	1.40	1.35
16	B	813	CLA	MG-NA	3.87	2.15	2.06
16	H	306	CLA	MG-NA	3.87	2.15	2.06
16	k	201	CLA	MG-NA	3.86	2.15	2.06
16	G	304	CLA	MG-NA	3.86	2.15	2.06
16	B	818	CLA	MG-NA	3.86	2.15	2.06
16	A	849	CLA	MG-NA	3.84	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	311	DD6	C5-C6	3.84	1.40	1.35
16	B	803	CLA	MG-NA	3.83	2.15	2.06
20	H	310	DD6	C10-C11	3.82	1.40	1.35
16	B	815	CLA	MG-NA	3.82	2.15	2.06
16	A	854	CLA	MG-NA	3.81	2.15	2.06
16	A	816	CLA	MG-NA	3.80	2.15	2.06
16	B	817	CLA	MG-NA	3.79	2.15	2.06
16	K	207	CLA	MG-NA	3.78	2.15	2.06
16	U	206	CLA	MG-NA	3.77	2.15	2.06
27	U	213	KC1	MG-NA	3.77	2.15	2.06
16	A	845	CLA	MG-NA	3.77	2.15	2.06
16	A	804	CLA	MG-NA	3.77	2.15	2.06
16	G	302	CLA	MG-NA	3.76	2.15	2.06
20	G	314	DD6	C10-C11	3.75	1.40	1.35
16	A	834	CLA	MG-NC	3.75	2.15	2.06
16	G	308	CLA	MG-NA	3.74	2.15	2.06
16	B	829	CLA	MG-NA	3.74	2.15	2.06
16	U	204	CLA	MG-NA	3.73	2.15	2.06
16	B	811	CLA	MG-NA	3.70	2.15	2.06
16	H	303	CLA	MG-NA	3.68	2.15	2.06
20	G	314	DD6	C5-C6	3.68	1.40	1.35
27	U	213	KC1	C4A-C3A	-3.67	1.37	1.44
20	G	311	DD6	C2-C1	3.66	1.40	1.35
16	A	838	CLA	MG-NA	3.66	2.15	2.06
21	F	806	LMU	O5'-C1'	3.66	1.51	1.41
20	G	314	DD6	C2-C1	3.64	1.40	1.35
16	K	203	CLA	MG-NA	3.62	2.14	2.06
16	U	208	CLA	MG-NA	3.61	2.14	2.06
16	A	801	CLA	MG-NA	3.59	2.14	2.06
16	A	831	CLA	MG-NA	3.59	2.14	2.06
16	H	307	CLA	MG-NA	3.58	2.14	2.06
16	G	301	CLA	MG-NA	3.58	2.14	2.06
20	A	846	DD6	C10-C11	3.58	1.40	1.35
16	A	836	CLA	MG-NA	3.57	2.14	2.06
16	B	847	CLA	MG-NA	3.57	2.14	2.06
16	A	802	CLA	MG-NA	3.55	2.14	2.06
16	A	853	CLA	MG-NA	3.55	2.14	2.06
20	H	310	DD6	C26-C27	3.54	1.44	1.37
26	U	202	A86	C26-C27	3.53	1.40	1.35
16	A	806	CLA	MG-NA	3.53	2.14	2.06
16	B	849	CLA	MG-NA	3.51	2.14	2.06
16	K	204	CLA	MG-NC	3.51	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	202	CLA	MG-NA	3.49	2.14	2.06
16	B	805	CLA	MG-NA	3.49	2.14	2.06
16	G	315	CLA	MG-NA	3.49	2.14	2.06
20	A	846	DD6	C5-C6	3.48	1.40	1.35
16	U	209	CLA	MG-NA	3.47	2.14	2.06
16	H	305	CLA	MG-NC	3.47	2.14	2.06
20	A	846	DD6	C2-C1	3.43	1.40	1.35
16	H	304	CLA	MG-NA	3.42	2.14	2.06
16	B	819	CLA	MG-NA	3.42	2.14	2.06
21	K	201	LMU	O5'-C1'	3.38	1.50	1.41
16	U	210	CLA	MG-NA	3.38	2.14	2.06
20	A	846	DD6	C26-C27	3.36	1.44	1.37
16	A	847	CLA	MG-NC	3.35	2.14	2.06
20	U	214	DD6	C8-C6	-3.34	1.41	1.50
27	U	213	KC1	C1B-C2B	-3.34	1.38	1.45
20	G	313	DD6	C26-C27	3.34	1.44	1.37
16	A	818	CLA	MG-NA	3.34	2.14	2.06
19	A	844	BCR	C1-C6	-3.34	1.49	1.53
16	B	826	CLA	MG-NC	3.33	2.14	2.06
20	G	312	DD6	C24-C1	-3.33	1.41	1.50
19	A	843	BCR	C1-C6	-3.32	1.49	1.53
16	A	827	CLA	MG-NC	3.32	2.14	2.06
20	U	203	DD6	C26-C27	3.31	1.43	1.37
16	K	205	CLA	MG-NA	3.29	2.14	2.06
16	L	203	CLA	MG-NA	3.28	2.14	2.06
16	B	821	CLA	MG-NA	3.26	2.14	2.06
20	H	311	DD6	C26-C27	3.24	1.43	1.37
21	F	806	LMU	O5B-C1B	3.23	1.50	1.41
21	K	201	LMU	O5B-C1B	3.20	1.50	1.41
20	K	208	DD6	C26-C27	3.20	1.43	1.37
19	B	838	BCR	C1-C6	-3.20	1.49	1.53
16	B	814	CLA	MG-NC	3.19	2.13	2.06
16	B	831	CLA	MG-NC	3.19	2.13	2.06
16	A	803	CLA	MG-NA	3.19	2.13	2.06
16	B	810	CLA	MG-NC	3.19	2.13	2.06
16	G	306	CLA	MG-NC	3.18	2.13	2.06
16	H	308	CLA	MG-NA	3.17	2.13	2.06
16	A	828	CLA	MG-NC	3.15	2.13	2.06
19	k	203	BCR	C1-C6	-3.14	1.49	1.53
20	J	102	DD6	C26-C27	3.13	1.43	1.37
19	A	842	BCR	C1-C6	-3.13	1.49	1.53
16	U	207	CLA	MG-NA	3.11	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	823	CLA	MG-NC	3.08	2.13	2.06
16	G	310	CLA	MG-NC	3.07	2.13	2.06
16	A	822	CLA	MG-NA	3.06	2.13	2.06
16	A	826	CLA	MG-NC	3.06	2.13	2.06
16	G	307	CLA	MG-NA	3.05	2.13	2.06
20	U	212	DD6	C26-C27	3.05	1.43	1.37
16	B	825	CLA	MG-NC	3.03	2.13	2.06
19	L	201	BCR	C1-C6	-3.02	1.49	1.53
19	B	846	BCR	C1-C6	-3.00	1.49	1.53
19	J	105	BCR	C30-C25	-3.00	1.49	1.53
16	A	805	CLA	MG-NC	3.00	2.13	2.06
16	B	844	CLA	MG-NC	2.99	2.13	2.06
19	L	205	BCR	C30-C25	-2.98	1.49	1.53
16	A	851	CLA	MG-NC	2.97	2.13	2.06
19	B	839	BCR	C1-C6	-2.97	1.49	1.53
16	H	306	CLA	MG-NC	2.96	2.13	2.06
20	G	314	DD6	C26-C27	2.96	1.43	1.37
16	B	845	CLA	MG-NC	2.95	2.13	2.06
19	F	801	BCR	C1-C6	-2.95	1.49	1.53
22	A	850	CL0	C1D-C2D	-2.95	1.39	1.45
19	B	842	BCR	C30-C25	-2.94	1.49	1.53
16	B	835	CLA	MG-NC	2.91	2.13	2.06
19	L	201	BCR	C30-C25	-2.90	1.49	1.53
16	G	305	CLA	MG-NA	2.89	2.13	2.06
19	I	103	BCR	C1-C6	-2.88	1.49	1.53
20	G	311	DD6	C26-C27	2.88	1.43	1.37
16	B	817	CLA	C1B-C2B	-2.87	1.36	1.43
16	B	848	CLA	MG-NC	2.86	2.13	2.06
22	A	850	CL0	C3D-C4D	-2.84	1.37	1.44
19	B	841	BCR	C1-C6	-2.83	1.49	1.53
19	M	101	BCR	C30-C25	-2.82	1.49	1.53
16	B	833	CLA	MG-NC	2.82	2.13	2.06
19	I	103	BCR	C30-C25	-2.81	1.49	1.53
19	F	805	BCR	C1-C6	-2.81	1.49	1.53
16	A	808	CLA	MG-NC	2.81	2.12	2.06
16	A	819	CLA	MG-NC	2.79	2.12	2.06
16	A	825	CLA	MG-NC	2.79	2.12	2.06
16	A	820	CLA	MG-NC	2.77	2.12	2.06
20	A	846	DD6	C24-C1	-2.76	1.40	1.45
19	M	101	BCR	C1-C6	-2.75	1.50	1.53
19	I	101	BCR	C1-C6	-2.75	1.50	1.53
16	B	807	CLA	MG-NC	2.75	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	842	BCR	C30-C25	-2.74	1.50	1.53
16	A	809	CLA	MG-NC	2.73	2.12	2.06
19	B	840	BCR	C1-C6	-2.73	1.50	1.53
19	B	842	BCR	C1-C6	-2.72	1.50	1.53
16	A	821	CLA	MG-NC	2.70	2.12	2.06
20	G	317	DD6	C26-C27	2.70	1.42	1.37
16	k	202	CLA	C1D-C2D	-2.69	1.40	1.45
16	A	833	CLA	MG-NC	2.69	2.12	2.06
16	A	811	CLA	MG-NC	2.68	2.12	2.06
16	B	813	CLA	MG-NC	2.68	2.12	2.06
16	A	830	CLA	MG-NC	2.68	2.12	2.06
16	B	804	CLA	MG-NC	2.67	2.12	2.06
16	B	801	CLA	MG-NC	2.67	2.12	2.06
16	B	827	CLA	MG-NC	2.67	2.12	2.06
16	G	305	CLA	C1D-C2D	-2.67	1.40	1.45
27	U	213	KC1	C2A-C3A	2.66	1.42	1.37
16	B	806	CLA	MG-NC	2.66	2.12	2.06
16	A	835	CLA	MG-NC	2.66	2.12	2.06
16	B	836	CLA	MG-NC	2.66	2.12	2.06
16	U	211	CLA	MG-NC	2.66	2.12	2.06
16	K	206	CLA	MG-NC	2.66	2.12	2.06
16	G	302	CLA	C1D-C2D	-2.65	1.40	1.45
16	A	829	CLA	MG-NC	2.64	2.12	2.06
19	B	846	BCR	C30-C25	-2.64	1.50	1.53
27	U	213	KC1	MG-NC	2.64	2.12	2.06
16	B	845	CLA	C3D-C4D	-2.63	1.38	1.44
16	B	828	CLA	MG-NC	2.63	2.12	2.06
16	G	315	CLA	C3D-C4D	-2.62	1.38	1.44
16	B	832	CLA	MG-NC	2.62	2.12	2.06
22	A	850	CL0	MG-ND	-2.61	2.00	2.05
16	k	202	CLA	MG-NC	2.61	2.12	2.06
19	A	841	BCR	C1-C6	-2.60	1.50	1.53
22	A	850	CL0	MG-NB	-2.60	2.00	2.05
16	L	202	CLA	MG-NC	2.59	2.12	2.06
16	B	830	CLA	C1B-C2B	-2.59	1.37	1.43
16	B	808	CLA	MG-NC	2.58	2.12	2.06
16	A	812	CLA	MG-NC	2.58	2.12	2.06
16	A	820	CLA	C3D-C4D	-2.58	1.38	1.44
20	G	314	DD6	C8-C6	-2.57	1.40	1.45
16	k	201	CLA	C3D-C4D	-2.56	1.38	1.44
16	G	305	CLA	C3D-C4D	-2.56	1.38	1.44
16	A	823	CLA	C1D-C2D	-2.56	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	k	203	BCR	C30-C25	-2.55	1.50	1.53
16	B	849	CLA	C3D-C4D	-2.55	1.38	1.44
16	H	312	CLA	C3D-C4D	-2.55	1.38	1.44
19	B	841	BCR	C30-C25	-2.55	1.50	1.53
16	B	825	CLA	C3D-C4D	-2.54	1.38	1.44
20	G	314	DD6	C13-C11	-2.54	1.40	1.45
16	B	817	CLA	C3D-C4D	-2.53	1.38	1.44
20	U	214	DD6	C5-C6	2.53	1.41	1.35
16	F	803	CLA	MG-NC	2.53	2.12	2.06
16	A	818	CLA	C1B-NB	-2.52	1.34	1.37
16	B	819	CLA	C3D-C4D	-2.52	1.38	1.44
16	L	204	CLA	MG-NC	2.50	2.12	2.06
16	A	827	CLA	C3D-C4D	-2.50	1.38	1.44
16	A	803	CLA	C3D-C4D	-2.50	1.38	1.44
16	A	815	CLA	C1B-C2B	-2.50	1.37	1.43
20	A	846	DD6	C8-C6	-2.50	1.40	1.45
16	A	818	CLA	C1B-C2B	-2.50	1.37	1.43
16	B	802	CLA	C1D-C2D	-2.50	1.40	1.45
16	B	808	CLA	C1D-C2D	-2.49	1.40	1.45
16	K	203	CLA	C3D-C4D	-2.49	1.38	1.44
16	H	303	CLA	C1B-C2B	-2.49	1.37	1.43
19	B	838	BCR	C30-C25	-2.49	1.50	1.53
20	G	312	DD6	C2-C1	2.49	1.41	1.35
16	B	824	CLA	MG-NC	2.48	2.12	2.06
16	B	821	CLA	C3D-C4D	-2.48	1.38	1.44
16	U	208	CLA	C3D-C4D	-2.48	1.38	1.44
16	A	851	CLA	C3D-C4D	-2.48	1.38	1.44
19	J	105	BCR	C1-C6	-2.47	1.50	1.53
20	G	311	DD6	C24-C1	-2.47	1.40	1.45
16	B	831	CLA	C3D-C4D	-2.47	1.38	1.44
16	H	308	CLA	C3D-C4D	-2.47	1.38	1.44
16	A	801	CLA	C1B-C2B	-2.47	1.37	1.43
20	G	314	DD6	C24-C1	-2.47	1.40	1.45
16	A	835	CLA	C3D-C4D	-2.47	1.38	1.44
16	G	302	CLA	MG-NC	2.47	2.12	2.06
20	A	846	DD6	C13-C11	-2.47	1.40	1.45
19	F	801	BCR	C30-C25	-2.46	1.50	1.53
16	A	816	CLA	C1B-C2B	-2.46	1.37	1.43
16	U	204	CLA	C3D-C4D	-2.46	1.38	1.44
16	B	805	CLA	C3D-C4D	-2.46	1.38	1.44
16	U	207	CLA	C3D-C4D	-2.46	1.38	1.44
16	A	804	CLA	C3D-C4D	-2.46	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	807	CLA	MG-NC	2.46	2.12	2.06
16	A	845	CLA	MG-NC	2.46	2.12	2.06
16	B	825	CLA	C1D-C2D	-2.45	1.40	1.45
16	A	824	CLA	MG-NC	2.45	2.12	2.06
20	G	317	DD6	C24-C1	-2.45	1.40	1.45
16	A	853	CLA	C3D-C4D	-2.44	1.38	1.44
16	A	822	CLA	C3D-C4D	-2.44	1.38	1.44
16	A	801	CLA	C1D-C2D	-2.44	1.40	1.45
16	B	824	CLA	C3D-C4D	-2.44	1.38	1.44
16	B	812	CLA	C3D-C4D	-2.44	1.38	1.44
16	H	305	CLA	C3D-C4D	-2.44	1.38	1.44
16	B	822	CLA	C1D-C2D	-2.44	1.40	1.45
16	H	306	CLA	C3D-C4D	-2.44	1.38	1.44
16	H	309	CLA	C3D-C4D	-2.44	1.38	1.44
16	B	829	CLA	C3D-C4D	-2.44	1.38	1.44
16	B	847	CLA	C3D-C4D	-2.44	1.38	1.44
16	G	306	CLA	C3D-C4D	-2.44	1.38	1.44
16	A	832	CLA	MG-NC	2.43	2.12	2.06
16	B	815	CLA	C3D-C4D	-2.43	1.38	1.44
19	B	840	BCR	C30-C25	-2.43	1.50	1.53
16	B	816	CLA	MG-NC	2.43	2.12	2.06
16	U	204	CLA	C1D-C2D	-2.43	1.40	1.45
20	U	203	DD6	C13-C11	-2.43	1.40	1.45
16	L	203	CLA	C3D-C4D	-2.43	1.38	1.44
16	A	813	CLA	C3D-C4D	-2.43	1.38	1.44
16	A	813	CLA	C1B-C2B	-2.43	1.37	1.43
16	B	807	CLA	C3D-C4D	-2.42	1.38	1.44
19	F	805	BCR	C30-C25	-2.42	1.50	1.53
16	A	815	CLA	C3D-C4D	-2.42	1.38	1.44
16	B	835	CLA	C3D-C4D	-2.42	1.38	1.44
27	U	213	KC1	C1A-CHA	2.42	1.47	1.40
16	A	847	CLA	C3D-C4D	-2.42	1.38	1.44
16	H	304	CLA	C3D-C4D	-2.42	1.38	1.44
16	B	820	CLA	MG-NC	2.42	2.12	2.06
16	A	806	CLA	C3D-C4D	-2.42	1.38	1.44
16	G	303	CLA	MG-NC	2.42	2.12	2.06
16	B	818	CLA	C3D-C4D	-2.42	1.38	1.44
16	U	206	CLA	C3D-C4D	-2.41	1.38	1.44
16	B	806	CLA	C3D-C4D	-2.41	1.38	1.44
16	B	822	CLA	C3D-C4D	-2.41	1.38	1.44
16	B	832	CLA	C3D-C4D	-2.41	1.38	1.44
16	U	211	CLA	C1B-C2B	-2.41	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	816	CLA	C3D-C4D	-2.41	1.38	1.44
16	K	202	CLA	C3D-C4D	-2.41	1.38	1.44
16	U	205	CLA	C3D-C4D	-2.41	1.38	1.44
16	G	307	CLA	C3D-C4D	-2.41	1.38	1.44
16	A	831	CLA	C3D-C4D	-2.41	1.38	1.44
16	L	204	CLA	C3D-C4D	-2.41	1.38	1.44
20	G	312	DD6	C13-C11	-2.41	1.40	1.45
16	A	812	CLA	C3D-C4D	-2.41	1.38	1.44
16	U	205	CLA	MG-NC	2.41	2.12	2.06
16	A	827	CLA	C1D-C2D	-2.41	1.40	1.45
16	A	802	CLA	C3D-C4D	-2.41	1.38	1.44
16	A	854	CLA	C3D-C4D	-2.41	1.38	1.44
16	A	829	CLA	C3D-C4D	-2.40	1.38	1.44
16	B	814	CLA	C3D-C4D	-2.40	1.38	1.44
16	H	303	CLA	C3D-C4D	-2.40	1.38	1.44
16	B	826	CLA	C3D-C4D	-2.40	1.38	1.44
16	A	836	CLA	C3D-C4D	-2.40	1.38	1.44
16	B	833	CLA	C3D-C4D	-2.40	1.38	1.44
16	J	104	CLA	C3D-C4D	-2.40	1.38	1.44
16	B	827	CLA	C3D-C4D	-2.40	1.38	1.44
16	B	834	CLA	C3D-C4D	-2.40	1.38	1.44
16	H	301	CLA	C3D-C4D	-2.39	1.38	1.44
16	B	809	CLA	C3D-C4D	-2.39	1.38	1.44
16	A	818	CLA	C3D-C4D	-2.39	1.38	1.44
16	A	811	CLA	C3D-C4D	-2.39	1.38	1.44
16	B	810	CLA	C3D-C4D	-2.39	1.38	1.44
16	A	830	CLA	C3D-C4D	-2.39	1.38	1.44
16	B	812	CLA	MG-NC	2.39	2.11	2.06
16	B	848	CLA	C3D-C4D	-2.39	1.38	1.44
16	B	803	CLA	C1D-C2D	-2.39	1.40	1.45
16	B	813	CLA	C3D-C4D	-2.39	1.38	1.44
16	A	813	CLA	MG-NC	2.39	2.11	2.06
16	B	848	CLA	C1B-C2B	-2.39	1.37	1.43
16	G	308	CLA	C3D-C4D	-2.39	1.38	1.44
16	A	819	CLA	C3D-C4D	-2.39	1.38	1.44
16	B	820	CLA	C3D-C4D	-2.39	1.38	1.44
16	A	815	CLA	MG-NC	2.39	2.11	2.06
16	A	849	CLA	C3D-C4D	-2.38	1.38	1.44
16	A	823	CLA	C3D-C4D	-2.38	1.38	1.44
16	U	210	CLA	C3D-C4D	-2.38	1.38	1.44
16	K	206	CLA	C1D-C2D	-2.38	1.40	1.45
16	G	306	CLA	C1D-C2D	-2.38	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	205	CLA	CHB-C1B	2.38	1.44	1.39
16	U	211	CLA	C3D-C4D	-2.38	1.38	1.44
16	B	845	CLA	C1D-C2D	-2.38	1.40	1.45
16	A	809	CLA	C1D-C2D	-2.38	1.40	1.45
16	B	830	CLA	C3D-C4D	-2.38	1.38	1.44
22	A	850	CL0	C1B-C2B	-2.38	1.37	1.43
16	A	801	CLA	C3D-C4D	-2.37	1.38	1.44
16	H	306	CLA	C1D-C2D	-2.37	1.40	1.45
16	A	832	CLA	C3D-C4D	-2.37	1.38	1.44
16	B	815	CLA	MG-NC	2.37	2.11	2.06
16	B	808	CLA	C3D-C4D	-2.37	1.38	1.44
16	F	802	CLA	C3D-C4D	-2.37	1.38	1.44
16	A	818	CLA	C1D-C2D	-2.37	1.40	1.45
16	A	831	CLA	C1B-C2B	-2.37	1.37	1.43
16	A	833	CLA	C3D-C4D	-2.37	1.38	1.44
20	G	311	DD6	C8-C6	-2.37	1.40	1.45
16	B	828	CLA	C3D-C4D	-2.37	1.38	1.44
16	G	304	CLA	C1B-C2B	-2.36	1.37	1.43
16	A	828	CLA	C3D-C4D	-2.36	1.38	1.44
19	L	205	BCR	C1-C6	-2.36	1.50	1.53
16	A	824	CLA	C3D-C4D	-2.36	1.38	1.44
16	G	302	CLA	C3D-C4D	-2.36	1.38	1.44
16	F	802	CLA	MG-NC	2.36	2.11	2.06
16	K	204	CLA	C3D-C4D	-2.36	1.38	1.44
16	A	809	CLA	C3D-C4D	-2.36	1.38	1.44
16	A	838	CLA	C3D-C4D	-2.36	1.38	1.44
16	B	816	CLA	C3D-C4D	-2.36	1.38	1.44
16	A	849	CLA	MG-NC	2.36	2.11	2.06
19	B	839	BCR	C30-C25	-2.36	1.50	1.53
16	K	206	CLA	C1B-C2B	-2.36	1.37	1.43
16	A	805	CLA	C3D-C4D	-2.36	1.38	1.44
16	K	202	CLA	MG-NC	2.36	2.11	2.06
16	G	310	CLA	C3D-C4D	-2.36	1.38	1.44
16	G	305	CLA	C1B-C2B	-2.35	1.37	1.43
16	B	811	CLA	C3D-C4D	-2.35	1.38	1.44
16	H	312	CLA	C1D-C2D	-2.35	1.40	1.45
16	A	814	CLA	C1B-C2B	-2.35	1.37	1.43
16	G	301	CLA	C3D-C4D	-2.35	1.38	1.44
16	A	826	CLA	C3D-C4D	-2.34	1.38	1.44
16	B	848	CLA	MG-NB	2.34	2.10	2.05
19	A	843	BCR	C30-C25	-2.34	1.50	1.53
16	A	816	CLA	MG-NC	2.34	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	823	CLA	MG-NC	2.34	2.11	2.06
16	H	307	CLA	C3D-C4D	-2.34	1.38	1.44
16	B	822	CLA	MG-NC	2.34	2.11	2.06
16	A	825	CLA	C3D-C4D	-2.34	1.38	1.44
16	G	304	CLA	C3D-C4D	-2.34	1.38	1.44
16	A	810	CLA	MG-NC	2.34	2.11	2.06
16	B	828	CLA	C1D-C2D	-2.34	1.40	1.45
16	F	804	CLA	C3D-C4D	-2.34	1.38	1.44
16	B	823	CLA	C3D-C4D	-2.33	1.38	1.44
16	U	208	CLA	C1B-C2B	-2.33	1.37	1.43
16	G	309	CLA	C3D-C4D	-2.33	1.38	1.44
16	A	808	CLA	C3D-C4D	-2.33	1.38	1.44
16	L	202	CLA	C3D-C4D	-2.33	1.38	1.44
16	A	835	CLA	C1B-C2B	-2.33	1.37	1.43
16	B	806	CLA	C1D-C2D	-2.33	1.40	1.45
16	B	809	CLA	MG-NC	2.33	2.11	2.06
16	H	301	CLA	MG-NC	2.33	2.11	2.06
16	B	831	CLA	C1D-C2D	-2.33	1.40	1.45
16	K	205	CLA	C3D-C4D	-2.32	1.38	1.44
16	k	202	CLA	C3D-C4D	-2.32	1.38	1.44
20	G	311	DD6	C13-C11	-2.32	1.41	1.45
16	K	207	CLA	MG-NC	2.32	2.11	2.06
19	A	844	BCR	C30-C25	-2.32	1.50	1.53
16	A	820	CLA	C1D-C2D	-2.32	1.40	1.45
16	B	818	CLA	C1B-C2B	-2.32	1.37	1.43
16	H	305	CLA	C1D-C2D	-2.32	1.40	1.45
16	F	804	CLA	C1B-C2B	-2.31	1.37	1.43
16	K	207	CLA	C3D-C4D	-2.31	1.39	1.44
16	B	822	CLA	C1B-C2B	-2.31	1.37	1.43
16	I	102	CLA	C3D-C4D	-2.31	1.39	1.44
16	G	301	CLA	C1B-C2B	-2.31	1.37	1.43
16	A	807	CLA	C3D-C4D	-2.31	1.39	1.44
16	A	810	CLA	C3D-C4D	-2.31	1.39	1.44
20	G	312	DD6	C8-C6	-2.31	1.41	1.45
21	A	855	LMU	O1'-C1'	2.31	1.44	1.40
16	B	831	CLA	C1B-C2B	-2.31	1.37	1.43
16	A	814	CLA	C3D-C4D	-2.30	1.39	1.44
16	A	802	CLA	MG-NC	2.30	2.11	2.06
20	H	310	DD6	C8-C6	-2.30	1.41	1.45
16	B	808	CLA	C1B-C2B	-2.30	1.37	1.43
16	B	844	CLA	C3D-C4D	-2.30	1.39	1.44
16	B	823	CLA	C1D-C2D	-2.29	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	834	CLA	C3D-C4D	-2.29	1.39	1.44
16	A	826	CLA	C1D-C2D	-2.29	1.40	1.45
16	B	802	CLA	C3D-C4D	-2.29	1.39	1.44
16	F	803	CLA	C3D-C4D	-2.29	1.39	1.44
16	B	804	CLA	C3D-C4D	-2.29	1.39	1.44
16	A	817	CLA	C1B-C2B	-2.29	1.37	1.43
16	B	848	CLA	C1D-C2D	-2.29	1.40	1.45
16	B	807	CLA	C1D-C2D	-2.29	1.40	1.45
16	A	838	CLA	MG-NC	2.28	2.11	2.06
16	H	302	CLA	C1B-C2B	-2.28	1.37	1.43
16	B	834	CLA	MG-NC	2.28	2.11	2.06
16	B	829	CLA	MG-NC	2.28	2.11	2.06
16	B	803	CLA	C1B-C2B	-2.28	1.37	1.43
16	H	304	CLA	C1B-C2B	-2.28	1.37	1.43
20	G	317	DD6	C8-C6	-2.28	1.41	1.45
16	A	815	CLA	C1D-C2D	-2.28	1.40	1.45
16	B	819	CLA	C1D-C2D	-2.28	1.40	1.45
16	H	302	CLA	MG-NC	2.28	2.11	2.06
16	I	102	CLA	MG-NC	2.28	2.11	2.06
16	K	203	CLA	C1B-C2B	-2.28	1.37	1.43
16	G	309	CLA	C1B-C2B	-2.28	1.37	1.43
16	A	836	CLA	C1D-C2D	-2.28	1.40	1.45
16	U	209	CLA	C1B-C2B	-2.28	1.37	1.43
16	A	849	CLA	C1B-C2B	-2.27	1.37	1.43
16	U	205	CLA	C1B-C2B	-2.27	1.37	1.43
16	A	854	CLA	MG-NC	2.27	2.11	2.06
20	H	310	DD6	C13-C11	-2.27	1.41	1.45
16	B	849	CLA	C1B-C2B	-2.27	1.37	1.43
16	F	802	CLA	C1B-C2B	-2.27	1.37	1.43
16	J	104	CLA	MG-NC	2.27	2.11	2.06
16	B	811	CLA	C1D-C2D	-2.27	1.40	1.45
16	H	309	CLA	MG-NC	2.27	2.11	2.06
16	H	308	CLA	C1B-C2B	-2.26	1.37	1.43
16	G	303	CLA	C3D-C4D	-2.26	1.39	1.44
16	B	817	CLA	C1D-C2D	-2.26	1.40	1.45
16	A	817	CLA	C3D-C4D	-2.26	1.39	1.44
16	B	820	CLA	C1D-C2D	-2.26	1.40	1.45
16	A	817	CLA	MG-NC	2.26	2.11	2.06
16	B	849	CLA	C1D-C2D	-2.26	1.40	1.45
20	G	317	DD6	C13-C11	-2.25	1.41	1.45
16	B	836	CLA	C3D-C4D	-2.25	1.39	1.44
16	A	832	CLA	C1D-C2D	-2.25	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	811	CLA	MG-NC	2.25	2.11	2.06
16	A	821	CLA	C3D-C4D	-2.25	1.39	1.44
16	A	814	CLA	MG-NC	2.25	2.11	2.06
16	A	811	CLA	C1D-C2D	-2.25	1.40	1.45
20	G	313	DD6	C8-C6	-2.25	1.41	1.45
16	U	209	CLA	C3D-C4D	-2.25	1.39	1.44
16	A	847	CLA	C1D-C2D	-2.25	1.40	1.45
16	B	834	CLA	C1B-C2B	-2.25	1.38	1.43
20	J	102	DD6	C24-C1	-2.25	1.41	1.45
16	U	205	CLA	C1D-C2D	-2.25	1.40	1.45
16	H	302	CLA	C3D-C4D	-2.25	1.39	1.44
16	H	305	CLA	C1B-C2B	-2.24	1.38	1.43
16	A	819	CLA	C1D-C2D	-2.24	1.40	1.45
16	U	211	CLA	C1D-C2D	-2.24	1.40	1.45
16	B	801	CLA	C1B-C2B	-2.24	1.38	1.43
16	A	830	CLA	C1D-C2D	-2.24	1.40	1.45
16	B	844	CLA	C1D-C2D	-2.24	1.40	1.45
16	B	835	CLA	C1B-C2B	-2.24	1.38	1.43
20	J	102	DD6	C8-C6	-2.24	1.41	1.45
16	A	821	CLA	C1D-C2D	-2.24	1.40	1.45
16	H	309	CLA	C1B-C2B	-2.23	1.38	1.43
16	A	835	CLA	C1D-C2D	-2.23	1.40	1.45
16	A	836	CLA	MG-NC	2.23	2.11	2.06
20	H	311	DD6	C8-C6	-2.23	1.41	1.45
16	I	102	CLA	C1B-C2B	-2.23	1.38	1.43
19	I	101	BCR	C30-C25	-2.23	1.50	1.53
16	A	845	CLA	C3D-C4D	-2.23	1.39	1.44
16	H	312	CLA	C1B-C2B	-2.23	1.38	1.43
16	F	802	CLA	C1D-C2D	-2.23	1.40	1.45
16	A	820	CLA	C1B-C2B	-2.22	1.38	1.43
16	A	825	CLA	C1D-C2D	-2.22	1.40	1.45
16	A	845	CLA	C1D-C2D	-2.22	1.40	1.45
16	A	832	CLA	C1B-C2B	-2.22	1.38	1.43
16	B	813	CLA	C1D-C2D	-2.22	1.41	1.45
22	A	850	CL0	C1C-NC	-2.21	1.34	1.37
16	U	206	CLA	MG-NC	2.21	2.11	2.06
16	B	803	CLA	MG-NC	2.21	2.11	2.06
20	G	311	DD6	C25-C26	-2.21	1.36	1.43
16	B	826	CLA	C1D-C2D	-2.21	1.41	1.45
16	A	845	CLA	C1B-C2B	-2.21	1.38	1.43
16	B	830	CLA	MG-NC	2.21	2.11	2.06
16	B	835	CLA	C1D-C2D	-2.21	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	817	CLA	C1D-C2D	-2.21	1.41	1.45
16	J	104	CLA	C1D-C2D	-2.21	1.41	1.45
16	B	802	CLA	CHB-C1B	2.21	1.44	1.39
16	A	853	CLA	MG-NC	2.21	2.11	2.06
20	U	203	DD6	C8-C6	-2.21	1.41	1.45
16	K	204	CLA	C1D-C2D	-2.21	1.41	1.45
16	B	820	CLA	C1B-NB	-2.21	1.35	1.37
19	A	841	BCR	C30-C25	-2.21	1.50	1.53
16	B	809	CLA	C1D-C2D	-2.20	1.41	1.45
20	H	311	DD6	C24-C1	-2.20	1.41	1.45
16	L	203	CLA	C1D-C2D	-2.20	1.41	1.45
16	B	810	CLA	CAB-C3B	-2.20	1.46	1.50
16	G	309	CLA	MG-NC	2.20	2.11	2.06
16	A	810	CLA	C1D-C2D	-2.20	1.41	1.45
16	H	302	CLA	C1D-C2D	-2.20	1.41	1.45
16	B	804	CLA	C1D-C2D	-2.20	1.41	1.45
16	A	826	CLA	C1B-NB	-2.20	1.35	1.37
16	B	819	CLA	MG-NC	2.20	2.11	2.06
16	A	824	CLA	C1D-C2D	-2.20	1.41	1.45
16	G	301	CLA	C1D-C2D	-2.19	1.41	1.45
16	B	805	CLA	MG-NC	2.19	2.11	2.06
16	A	828	CLA	C1D-C2D	-2.19	1.41	1.45
16	B	809	CLA	C1B-C2B	-2.19	1.38	1.43
16	U	204	CLA	MG-NC	2.19	2.11	2.06
20	G	313	DD6	C13-C11	-2.19	1.41	1.45
16	A	824	CLA	C1B-C2B	-2.19	1.38	1.43
16	B	816	CLA	C1D-C2D	-2.19	1.41	1.45
16	B	849	CLA	MG-NC	2.18	2.11	2.06
16	G	303	CLA	C1B-C2B	-2.18	1.38	1.43
20	H	311	DD6	C13-C11	-2.18	1.41	1.45
16	A	814	CLA	C1D-C2D	-2.18	1.41	1.45
16	B	804	CLA	C1B-C2B	-2.18	1.38	1.43
20	K	208	DD6	C8-C6	-2.18	1.41	1.45
16	k	201	CLA	C1B-C2B	-2.18	1.38	1.43
16	A	854	CLA	C1D-C2D	-2.17	1.41	1.45
16	B	814	CLA	C1D-C2D	-2.17	1.41	1.45
25	J	103	LMG	C1-C2	2.17	1.58	1.52
16	A	804	CLA	MG-NC	2.17	2.11	2.06
16	K	206	CLA	C3D-C4D	-2.17	1.39	1.44
20	G	313	DD6	C24-C1	-2.17	1.41	1.45
16	A	807	CLA	C1D-C2D	-2.17	1.41	1.45
16	B	829	CLA	C1D-C2D	-2.17	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	F	803	CLA	C1D-C2D	-2.17	1.41	1.45
16	A	826	CLA	C1B-C2B	-2.17	1.38	1.43
16	B	803	CLA	C3D-C4D	-2.17	1.39	1.44
16	G	307	CLA	C1D-C2D	-2.17	1.41	1.45
16	A	819	CLA	C1B-C2B	-2.17	1.38	1.43
16	A	851	CLA	C1D-C2D	-2.17	1.41	1.45
16	B	827	CLA	C1B-C2B	-2.17	1.38	1.43
16	B	813	CLA	C1B-C2B	-2.17	1.38	1.43
20	K	208	DD6	C13-C11	-2.17	1.41	1.45
16	B	809	CLA	C1B-NB	-2.17	1.35	1.37
16	A	803	CLA	C1B-C2B	-2.16	1.38	1.43
20	G	314	DD6	C25-C26	-2.16	1.36	1.43
16	B	832	CLA	C1D-C2D	-2.16	1.41	1.45
16	F	804	CLA	MG-NC	2.16	2.11	2.06
16	B	805	CLA	C1B-C2B	-2.16	1.38	1.43
16	L	204	CLA	C1D-C2D	-2.16	1.41	1.45
16	A	808	CLA	C1D-C2D	-2.16	1.41	1.45
16	B	830	CLA	C1D-C2D	-2.15	1.41	1.45
16	A	832	CLA	C1B-NB	-2.15	1.35	1.37
16	L	202	CLA	C1D-C2D	-2.15	1.41	1.45
16	B	810	CLA	MG-NB	2.15	2.10	2.05
16	B	818	CLA	MG-NC	2.15	2.11	2.06
16	A	834	CLA	C1D-C2D	-2.15	1.41	1.45
20	J	102	DD6	C13-C11	-2.15	1.41	1.45
16	H	304	CLA	C1D-C2D	-2.15	1.41	1.45
16	B	834	CLA	C1D-C2D	-2.15	1.41	1.45
16	A	801	CLA	MG-NC	2.15	2.11	2.06
16	B	836	CLA	C1D-C2D	-2.15	1.41	1.45
16	A	822	CLA	C1B-C2B	-2.14	1.38	1.43
16	A	829	CLA	C1D-C2D	-2.14	1.41	1.45
27	U	213	KC1	C3B-C2B	2.14	1.41	1.37
16	A	802	CLA	C1B-C2B	-2.14	1.38	1.43
20	K	208	DD6	C24-C1	-2.14	1.41	1.45
16	K	205	CLA	C1B-C2B	-2.14	1.38	1.43
16	B	817	CLA	C1B-NB	-2.14	1.35	1.37
16	A	809	CLA	C1B-C2B	-2.13	1.38	1.43
16	A	853	CLA	C1D-C2D	-2.13	1.41	1.45
16	G	306	CLA	C1B-C2B	-2.13	1.38	1.43
16	B	824	CLA	C1B-C2B	-2.13	1.38	1.43
16	G	303	CLA	C1D-C2D	-2.13	1.41	1.45
16	B	816	CLA	C1B-C2B	-2.13	1.38	1.43
16	B	801	CLA	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	306	CLA	C1B-C2B	-2.13	1.38	1.43
16	B	833	CLA	C1D-C2D	-2.12	1.41	1.45
16	F	803	CLA	C1B-NB	-2.12	1.35	1.37
16	H	307	CLA	MG-NC	2.12	2.11	2.06
16	G	303	CLA	CHB-C1B	2.12	1.44	1.39
16	A	821	CLA	C1B-NB	-2.12	1.35	1.37
16	K	204	CLA	C1B-C2B	-2.12	1.38	1.43
16	B	821	CLA	C1B-C2B	-2.12	1.38	1.43
16	A	801	CLA	C1B-NB	-2.12	1.35	1.37
16	G	304	CLA	C1D-C2D	-2.12	1.41	1.45
16	B	813	CLA	MG-NB	2.12	2.10	2.05
16	A	806	CLA	C1D-C2D	-2.12	1.41	1.45
16	G	308	CLA	MG-NC	2.11	2.11	2.06
16	A	838	CLA	CHB-C1B	2.11	1.44	1.39
16	G	307	CLA	CHB-C1B	2.11	1.44	1.39
16	B	810	CLA	C1B-C2B	-2.11	1.38	1.43
27	U	213	KC1	C1B-NB	-2.11	1.35	1.37
16	G	310	CLA	C1D-C2D	-2.11	1.41	1.45
16	A	804	CLA	C1D-C2D	-2.11	1.41	1.45
16	B	827	CLA	C1D-C2D	-2.11	1.41	1.45
16	B	807	CLA	C1B-C2B	-2.11	1.38	1.43
16	G	308	CLA	C1D-C2D	-2.11	1.41	1.45
20	A	846	DD6	C25-C26	-2.10	1.36	1.43
16	K	203	CLA	C1D-C2D	-2.10	1.41	1.45
16	B	825	CLA	C1B-C2B	-2.10	1.38	1.43
16	A	823	CLA	C1B-NB	-2.10	1.35	1.37
16	F	803	CLA	C1B-C2B	-2.10	1.38	1.43
16	B	805	CLA	C1D-C2D	-2.10	1.41	1.45
16	A	816	CLA	C1B-NB	-2.10	1.35	1.37
16	H	302	CLA	C1B-NB	-2.10	1.35	1.37
16	B	828	CLA	CHB-C1B	2.10	1.44	1.39
16	B	845	CLA	C1B-C2B	-2.10	1.38	1.43
16	H	306	CLA	C1B-NB	-2.10	1.35	1.37
16	K	202	CLA	C1B-NB	-2.09	1.35	1.37
16	B	835	CLA	MG-NB	2.09	2.09	2.05
16	U	209	CLA	C1D-C2D	-2.09	1.41	1.45
16	G	310	CLA	C1B-C2B	-2.09	1.38	1.43
16	A	853	CLA	C1B-C2B	-2.09	1.38	1.43
20	G	317	DD6	C25-C26	-2.09	1.37	1.43
16	A	811	CLA	C1B-C2B	-2.09	1.38	1.43
16	G	308	CLA	C1B-C2B	-2.09	1.38	1.43
26	U	202	A86	C8-C6	-2.09	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	829	CLA	CHB-C1B	2.09	1.44	1.39
16	A	806	CLA	MG-NC	2.09	2.11	2.06
16	A	823	CLA	C1B-C2B	-2.09	1.38	1.43
16	A	822	CLA	C1D-C2D	-2.09	1.41	1.45
16	B	815	CLA	C1D-C2D	-2.09	1.41	1.45
16	B	847	CLA	C1D-C2D	-2.09	1.41	1.45
16	A	807	CLA	C1B-NB	-2.09	1.35	1.37
16	B	847	CLA	C1B-C2B	-2.08	1.38	1.43
26	U	202	A86	C24-C1	-2.08	1.41	1.45
16	A	808	CLA	C1B-C2B	-2.08	1.38	1.43
16	L	204	CLA	CHB-C1B	2.08	1.44	1.39
16	A	833	CLA	C1D-C2D	-2.08	1.41	1.45
16	B	824	CLA	C1D-C2D	-2.08	1.41	1.45
16	B	801	CLA	C1D-C2D	-2.08	1.41	1.45
16	A	803	CLA	C1D-C2D	-2.08	1.41	1.45
16	k	202	CLA	CHB-C1B	2.08	1.44	1.39
16	U	206	CLA	C1B-C2B	-2.08	1.38	1.43
20	J	102	DD6	C25-C26	-2.07	1.37	1.43
16	A	851	CLA	C1B-C2B	-2.07	1.38	1.43
18	A	839	LHG	O7-C5	-2.07	1.41	1.46
16	B	823	CLA	CHB-C1B	2.07	1.44	1.39
16	H	304	CLA	MG-NC	2.07	2.11	2.06
16	U	206	CLA	C1D-C2D	-2.07	1.41	1.45
20	G	313	DD6	C25-C26	-2.07	1.37	1.43
16	U	207	CLA	C1B-C2B	-2.07	1.38	1.43
16	A	804	CLA	C1B-NB	-2.07	1.35	1.37
16	B	821	CLA	C1D-C2D	-2.07	1.41	1.45
16	A	803	CLA	C1B-NB	-2.07	1.35	1.37
16	A	820	CLA	CHB-C1B	2.07	1.44	1.39
16	B	812	CLA	CHB-C1B	2.07	1.44	1.39
16	B	815	CLA	C1B-C2B	-2.06	1.38	1.43
16	A	810	CLA	C1B-C2B	-2.06	1.38	1.43
16	K	202	CLA	C1B-C2B	-2.06	1.38	1.43
16	B	812	CLA	C1D-C2D	-2.06	1.41	1.45
16	B	819	CLA	C1B-C2B	-2.06	1.38	1.43
16	K	205	CLA	C1D-C2D	-2.06	1.41	1.45
16	B	809	CLA	CHB-C1B	2.06	1.44	1.39
16	A	825	CLA	C1B-C2B	-2.06	1.38	1.43
16	A	805	CLA	C1D-C2D	-2.06	1.41	1.45
16	B	844	CLA	C1B-C2B	-2.06	1.38	1.43
16	B	832	CLA	C1B-C2B	-2.06	1.38	1.43
16	U	207	CLA	C1D-C2D	-2.06	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	207	CLA	CHB-C1B	2.06	1.44	1.39
16	A	836	CLA	CHB-C1B	2.05	1.44	1.39
16	B	818	CLA	C1D-C2D	-2.05	1.41	1.45
16	A	821	CLA	C1B-C2B	-2.05	1.38	1.43
16	A	804	CLA	C1B-C2B	-2.05	1.38	1.43
16	A	854	CLA	C1B-C2B	-2.05	1.38	1.43
16	U	208	CLA	C1D-C2D	-2.05	1.41	1.45
16	A	807	CLA	C1B-C2B	-2.05	1.38	1.43
16	I	102	CLA	C1D-C2D	-2.05	1.41	1.45
16	L	204	CLA	C1B-C2B	-2.05	1.38	1.43
16	A	829	CLA	C1B-C2B	-2.05	1.38	1.43
16	H	307	CLA	CHB-C1B	2.05	1.44	1.39
16	A	806	CLA	C1B-C2B	-2.05	1.38	1.43
16	K	203	CLA	MG-NC	2.05	2.11	2.06
16	B	831	CLA	C1B-NB	-2.05	1.35	1.37
16	A	838	CLA	C1D-C2D	-2.04	1.41	1.45
16	L	202	CLA	C1B-C2B	-2.04	1.38	1.43
16	G	302	CLA	C1B-C2B	-2.04	1.38	1.43
16	L	202	CLA	C1B-NB	-2.04	1.35	1.37
16	B	833	CLA	C1B-C2B	-2.04	1.38	1.43
16	A	810	CLA	C1B-NB	-2.04	1.35	1.37
16	H	304	CLA	CHB-C1B	2.04	1.44	1.39
20	U	212	DD6	C24-C1	-2.04	1.41	1.45
16	B	830	CLA	C1B-NB	-2.04	1.35	1.37
16	A	802	CLA	C1D-C2D	-2.04	1.41	1.45
16	F	804	CLA	C1D-C2D	-2.03	1.41	1.45
16	B	823	CLA	C1B-C2B	-2.03	1.38	1.43
16	B	806	CLA	CHB-C1B	2.03	1.44	1.39
16	A	834	CLA	C1B-C2B	-2.03	1.38	1.43
16	K	202	CLA	C1D-C2D	-2.03	1.41	1.45
16	k	202	CLA	C1B-NB	-2.03	1.35	1.37
21	A	848	LMU	O1'-C1'	2.03	1.43	1.40
16	G	309	CLA	C1D-C2D	-2.03	1.41	1.45
16	B	836	CLA	C1B-C2B	-2.03	1.38	1.43
16	A	813	CLA	C1D-C2D	-2.03	1.41	1.45
16	U	210	CLA	C1D-C2D	-2.03	1.41	1.45
16	B	826	CLA	C1B-C2B	-2.03	1.38	1.43
16	U	204	CLA	CHB-C1B	2.03	1.44	1.39
16	B	804	CLA	C1B-NB	-2.03	1.35	1.37
16	A	812	CLA	C1B-C2B	-2.03	1.38	1.43
16	U	208	CLA	MG-NC	2.03	2.11	2.06
16	A	827	CLA	C1B-C2B	-2.02	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	203	CLA	C1B-C2B	-2.02	1.38	1.43
16	U	204	CLA	C1B-C2B	-2.02	1.38	1.43
16	A	822	CLA	C1B-NB	-2.02	1.35	1.37
16	A	838	CLA	C1B-C2B	-2.02	1.38	1.43
16	K	207	CLA	C1B-C2B	-2.02	1.38	1.43
20	U	214	DD6	C25-C26	-2.02	1.37	1.43
16	B	814	CLA	C1B-C2B	-2.02	1.38	1.43
20	U	212	DD6	C8-C6	-2.02	1.41	1.45
16	H	309	CLA	C1D-C2D	-2.02	1.41	1.45
16	H	307	CLA	C1D-C2D	-2.02	1.41	1.45
16	G	307	CLA	C1B-C2B	-2.02	1.38	1.43
16	G	302	CLA	CHB-C1B	2.02	1.43	1.39
16	A	847	CLA	C1B-C2B	-2.02	1.38	1.43
16	B	820	CLA	C1B-C2B	-2.02	1.38	1.43
16	U	211	CLA	C1B-NB	-2.01	1.35	1.37
16	H	308	CLA	C1D-C2D	-2.01	1.41	1.45
16	H	307	CLA	C1B-C2B	-2.01	1.38	1.43
16	K	206	CLA	CHB-C1B	2.01	1.43	1.39
16	A	812	CLA	C1B-NB	-2.01	1.35	1.37
16	B	819	CLA	C1B-NB	-2.01	1.35	1.37
16	H	301	CLA	CHB-C1B	2.01	1.43	1.39
16	A	830	CLA	C1B-C2B	-2.01	1.38	1.43
16	G	315	CLA	C1B-C2B	-2.01	1.38	1.43
16	G	315	CLA	CHB-C1B	2.01	1.43	1.39
16	A	805	CLA	C1B-C2B	-2.00	1.38	1.43
16	A	828	CLA	CHB-C1B	2.00	1.43	1.39
16	A	847	CLA	MG-NB	2.00	2.09	2.05
16	L	203	CLA	MG-NC	2.00	2.11	2.06
16	A	833	CLA	C1B-C2B	-2.00	1.38	1.43
16	J	104	CLA	C1B-C2B	-2.00	1.38	1.43
16	B	810	CLA	C1D-C2D	-2.00	1.41	1.45
16	A	821	CLA	CHB-C1B	2.00	1.43	1.39

All (846) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	U	212	DD6	C3-C4-C5	5.24	134.21	123.47
16	G	315	CLA	CHD-C1D-ND	-4.92	119.93	124.45
16	H	306	CLA	O2A-C1-C2	4.51	120.47	108.64
20	J	102	DD6	C12-C11-C10	-4.46	116.67	122.92
16	K	205	CLA	O2A-C1-C2	4.40	120.21	108.64
20	U	203	DD6	C4-C3-C2	4.37	132.42	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	G	313	DD6	C4-C3-C2	4.31	132.31	123.47
20	H	310	DD6	C3-C4-C5	4.30	132.28	123.47
16	H	312	CLA	CHD-C1D-ND	-4.29	120.51	124.45
16	A	822	CLA	CHD-C1D-ND	-4.24	120.56	124.45
26	U	202	A86	C4-C3-C2	4.21	132.10	123.47
20	G	312	DD6	C4-C3-C2	4.19	132.06	123.47
16	A	803	CLA	CHD-C1D-ND	-4.16	120.63	124.45
18	A	839	LHG	O4-P-O5	4.15	132.77	112.24
20	G	317	DD6	C12-C11-C10	-4.15	117.11	122.92
16	A	849	CLA	CHD-C1D-ND	-4.15	120.64	124.45
20	H	311	DD6	C3-C4-C5	4.14	131.96	123.47
16	A	838	CLA	C4D-CHA-C1A	4.14	126.29	121.25
16	A	838	CLA	CHD-C1D-ND	-4.13	120.66	124.45
18	A	840	LHG	O4-P-O5	4.13	132.67	112.24
20	K	208	DD6	C12-C11-C10	-4.13	117.14	122.92
22	A	850	CL0	C5-C3-C2	4.10	129.42	121.12
20	A	846	DD6	C12-C11-C10	-4.10	117.18	122.92
20	G	317	DD6	C4-C3-C2	4.10	131.86	123.47
24	B	843	DGD	O2G-C1B-C2B	4.09	120.32	111.50
16	U	207	CLA	CHD-C1D-ND	-4.08	120.71	124.45
20	H	310	DD6	C12-C11-C10	-4.07	117.22	122.92
20	G	311	DD6	C4-C3-C2	4.06	131.79	123.47
20	G	314	DD6	C12-C11-C10	-4.04	117.26	122.92
20	G	311	DD6	C12-C11-C10	-4.02	117.29	122.92
20	G	313	DD6	C12-C11-C10	-4.02	117.29	122.92
20	U	203	DD6	C-C1-C2	-4.01	117.30	122.92
16	A	831	CLA	CHD-C1D-ND	-4.01	120.77	124.45
16	H	303	CLA	CHD-C1D-ND	-4.00	120.78	124.45
16	K	205	CLA	C4D-CHA-C1A	4.00	126.12	121.25
20	U	212	DD6	C12-C11-C10	-3.99	117.34	122.92
20	K	208	DD6	C3-C4-C5	3.95	131.57	123.47
16	B	818	CLA	CHD-C1D-ND	-3.94	120.83	124.45
16	G	308	CLA	CHD-C1D-ND	-3.93	120.84	124.45
16	U	210	CLA	CHD-C1D-ND	-3.92	120.85	124.45
16	A	812	CLA	CHD-C1D-ND	-3.92	120.85	124.45
20	H	311	DD6	C12-C11-C10	-3.92	117.44	122.92
16	G	303	CLA	C4D-CHA-C1A	3.91	126.01	121.25
16	A	802	CLA	CHD-C1D-ND	-3.91	120.86	124.45
20	U	203	DD6	C12-C11-C10	-3.91	117.45	122.92
16	L	203	CLA	CHD-C1D-ND	-3.89	120.88	124.45
16	G	307	CLA	CHD-C1D-ND	-3.89	120.88	124.45
20	J	102	DD6	C4-C3-C2	3.88	131.42	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	U	203	DD6	C24-C1-C2	3.86	124.87	118.94
16	B	807	CLA	C4D-CHA-C1A	3.85	125.94	121.25
16	K	206	CLA	C4D-CHA-C1A	3.84	125.92	121.25
16	H	301	CLA	CHD-C1D-ND	-3.83	120.93	124.45
16	A	806	CLA	CHD-C1D-ND	-3.83	120.93	124.45
20	H	310	DD6	C8-C6-C5	3.83	124.82	118.94
19	A	841	BCR	C2-C1-C6	3.83	116.37	110.48
20	J	102	DD6	C13-C11-C10	3.83	124.81	118.94
16	B	801	CLA	C4D-CHA-C1A	3.82	125.90	121.25
16	G	304	CLA	CHD-C1D-ND	-3.82	120.95	124.45
26	U	202	A86	C3-C4-C5	3.81	131.28	123.47
16	A	816	CLA	CHD-C1D-ND	-3.80	120.96	124.45
16	B	847	CLA	CHD-C1D-ND	-3.80	120.96	124.45
20	U	212	DD6	C7-C6-C5	-3.80	117.60	122.92
16	K	202	CLA	CHD-C1D-ND	-3.80	120.96	124.45
20	G	314	DD6	C8-C6-C5	3.78	124.75	118.94
16	B	816	CLA	C4D-CHA-C1A	3.78	125.85	121.25
16	H	301	CLA	C4D-CHA-C1A	3.78	125.85	121.25
16	G	305	CLA	CAA-C2A-C3A	-3.78	102.44	112.78
16	B	821	CLA	CHD-C1D-ND	-3.77	120.98	124.45
16	H	307	CLA	CHD-C1D-ND	-3.77	120.98	124.45
20	H	310	DD6	C4-C3-C2	3.77	131.20	123.47
20	K	208	DD6	C4-C3-C2	3.76	131.18	123.47
20	U	212	DD6	C8-C6-C5	3.76	124.71	118.94
16	B	810	CLA	CHD-C1D-ND	-3.75	121.01	124.45
16	G	305	CLA	CHD-C1D-ND	-3.75	121.01	124.45
16	B	818	CLA	C4D-CHA-C1A	3.75	125.81	121.25
16	F	804	CLA	C4D-CHA-C1A	3.75	125.81	121.25
19	M	101	BCR	C2-C1-C6	3.75	116.25	110.48
20	G	312	DD6	C12-C11-C10	-3.75	117.68	122.92
16	L	203	CLA	C4D-CHA-C1A	3.74	125.80	121.25
16	A	822	CLA	C4D-CHA-C1A	3.73	125.79	121.25
16	B	824	CLA	CHD-C1D-ND	-3.73	121.03	124.45
20	G	314	DD6	C-C1-C2	-3.72	117.71	122.92
16	H	308	CLA	CHD-C1D-ND	-3.72	121.03	124.45
16	U	206	CLA	CHD-C1D-ND	-3.72	121.03	124.45
16	B	816	CLA	CHD-C1D-ND	-3.71	121.05	124.45
16	A	819	CLA	C4D-CHA-C1A	3.70	125.75	121.25
16	A	831	CLA	C4D-CHA-C1A	3.68	125.73	121.25
16	A	833	CLA	CHD-C1D-ND	-3.68	121.08	124.45
16	B	812	CLA	CHD-C1D-ND	-3.67	121.08	124.45
20	G	314	DD6	C24-C1-C2	3.67	124.58	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	J	102	DD6	C3-C4-C5	3.67	131.00	123.47
16	A	824	CLA	CHD-C1D-ND	-3.67	121.08	124.45
16	I	102	CLA	CHD-C1D-ND	-3.66	121.09	124.45
16	B	830	CLA	CHD-C1D-ND	-3.66	121.09	124.45
16	k	201	CLA	CHD-C1D-ND	-3.66	121.09	124.45
16	G	304	CLA	C4D-CHA-C1A	3.66	125.70	121.25
16	G	309	CLA	C4D-CHA-C1A	3.66	125.70	121.25
16	F	804	CLA	CHD-C1D-ND	-3.65	121.10	124.45
16	B	836	CLA	C4D-CHA-C1A	3.65	125.69	121.25
20	U	214	DD6	C3-C4-C5	3.65	130.96	123.47
16	A	853	CLA	CHD-C1D-ND	-3.65	121.10	124.45
20	U	203	DD6	C3-C4-C5	3.65	130.94	123.47
16	G	309	CLA	CHD-C1D-ND	-3.65	121.10	124.45
20	U	214	DD6	C4-C3-C2	3.64	130.93	123.47
16	B	805	CLA	CHD-C1D-ND	-3.63	121.12	124.45
16	B	832	CLA	C4D-CHA-C1A	3.63	125.66	121.25
16	B	844	CLA	C4D-CHA-C1A	3.63	125.66	121.25
16	B	815	CLA	CHD-C1D-ND	-3.62	121.13	124.45
16	B	833	CLA	CHD-C1D-ND	-3.61	121.13	124.45
16	B	832	CLA	CHD-C1D-ND	-3.61	121.14	124.45
16	B	817	CLA	CHD-C1D-ND	-3.61	121.14	124.45
16	U	208	CLA	CHD-C1D-ND	-3.60	121.15	124.45
16	A	813	CLA	CHD-C1D-ND	-3.60	121.15	124.45
16	A	849	CLA	C4D-CHA-C1A	3.59	125.62	121.25
16	A	851	CLA	C4D-CHA-C1A	3.59	125.61	121.25
16	A	811	CLA	C4D-CHA-C1A	3.58	125.61	121.25
16	G	308	CLA	C4D-CHA-C1A	3.58	125.61	121.25
20	H	310	DD6	C-C1-C2	-3.58	117.91	122.92
16	G	307	CLA	C4D-CHA-C1A	3.58	125.60	121.25
16	U	205	CLA	CHD-C1D-ND	-3.58	121.17	124.45
20	U	214	DD6	C-C1-C2	-3.57	117.92	122.92
20	G	314	DD6	C7-C6-C5	-3.57	117.92	122.92
16	B	814	CLA	C4D-CHA-C1A	3.57	125.59	121.25
16	A	804	CLA	CHD-C1D-ND	-3.57	121.18	124.45
16	A	816	CLA	C4D-CHA-C1A	3.56	125.58	121.25
16	K	205	CLA	CHD-C1D-ND	-3.56	121.19	124.45
16	B	848	CLA	C4D-CHA-C1A	3.55	125.58	121.25
16	U	204	CLA	C4D-CHA-C1A	3.55	125.58	121.25
16	B	829	CLA	CHD-C1D-ND	-3.55	121.19	124.45
16	B	830	CLA	C4D-CHA-C1A	3.55	125.57	121.25
16	L	204	CLA	C4D-CHA-C1A	3.55	125.57	121.25
16	B	813	CLA	CHD-C1D-ND	-3.55	121.19	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	307	CLA	C4D-CHA-C1A	3.54	125.56	121.25
16	B	811	CLA	C4D-CHA-C1A	3.54	125.56	121.25
16	A	828	CLA	C4D-CHA-C1A	3.54	125.55	121.25
20	A	846	DD6	C-C1-C2	-3.54	117.97	122.92
16	H	309	CLA	CHD-C1D-ND	-3.54	121.20	124.45
16	A	833	CLA	C4D-CHA-C1A	3.53	125.55	121.25
16	B	807	CLA	CHD-C1D-ND	-3.53	121.21	124.45
16	B	831	CLA	C4D-CHA-C1A	3.53	125.54	121.25
19	F	801	BCR	C2-C1-C6	3.53	115.91	110.48
16	F	803	CLA	C4D-CHA-C1A	3.52	125.54	121.25
16	A	803	CLA	C4D-CHA-C1A	3.52	125.54	121.25
16	G	301	CLA	CHD-C1D-ND	-3.52	121.22	124.45
16	B	812	CLA	C4D-CHA-C1A	3.52	125.53	121.25
16	A	834	CLA	C4D-CHA-C1A	3.52	125.53	121.25
16	B	833	CLA	C4D-CHA-C1A	3.51	125.52	121.25
16	B	801	CLA	CHD-C1D-ND	-3.51	121.23	124.45
16	H	304	CLA	CHD-C1D-ND	-3.51	121.23	124.45
20	J	102	DD6	C7-C6-C5	-3.51	118.01	122.92
16	B	810	CLA	C4D-CHA-C1A	3.50	125.51	121.25
16	K	203	CLA	CHD-C1D-ND	-3.50	121.24	124.45
16	B	826	CLA	CHD-C1D-ND	-3.50	121.24	124.45
16	B	815	CLA	C4D-CHA-C1A	3.49	125.50	121.25
16	K	207	CLA	CHD-C1D-ND	-3.49	121.25	124.45
20	H	310	DD6	C7-C6-C5	-3.49	118.04	122.92
16	A	836	CLA	C4D-CHA-C1A	3.48	125.49	121.25
16	B	835	CLA	C4D-CHA-C1A	3.48	125.48	121.25
16	I	102	CLA	C4D-CHA-C1A	3.48	125.48	121.25
16	B	848	CLA	CHD-C1D-ND	-3.47	121.26	124.45
16	H	306	CLA	C4D-CHA-C1A	3.47	125.47	121.25
16	A	835	CLA	C4D-CHA-C1A	3.46	125.46	121.25
16	A	805	CLA	C4D-CHA-C1A	3.46	125.46	121.25
16	A	805	CLA	CHD-C1D-ND	-3.45	121.28	124.45
16	F	802	CLA	C4D-CHA-C1A	3.44	125.44	121.25
16	A	807	CLA	CHD-C1D-ND	-3.44	121.29	124.45
16	U	208	CLA	C4D-CHA-C1A	3.44	125.43	121.25
19	B	841	BCR	C15-C16-C17	-3.43	116.44	123.47
20	G	313	DD6	C-C1-C2	-3.43	118.12	122.92
20	K	208	DD6	C7-C6-C5	-3.43	118.12	122.92
16	A	813	CLA	C4D-CHA-C1A	3.42	125.41	121.25
16	A	819	CLA	CHD-C1D-ND	-3.42	121.31	124.45
16	B	827	CLA	CHD-C1D-ND	-3.42	121.31	124.45
16	A	814	CLA	CHD-C1D-ND	-3.42	121.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	315	CLA	C4D-CHA-C1A	3.42	125.41	121.25
16	L	204	CLA	CHD-C1D-ND	-3.40	121.33	124.45
18	A	840	LHG	O8-C23-C24	3.40	120.31	111.38
16	B	835	CLA	CHD-C1D-ND	-3.40	121.33	124.45
16	B	814	CLA	CAA-C2A-C3A	-3.40	103.47	112.78
20	G	311	DD6	C-C1-C2	-3.40	118.16	122.92
16	B	824	CLA	C4D-CHA-C1A	3.40	125.39	121.25
16	A	854	CLA	CHD-C1D-ND	-3.39	121.34	124.45
20	J	102	DD6	C-C1-C2	-3.39	118.18	122.92
16	A	853	CLA	C4D-CHA-C1A	3.39	125.37	121.25
16	A	820	CLA	C4D-CHA-C1A	3.39	125.37	121.25
16	A	829	CLA	CHD-C1D-ND	-3.39	121.34	124.45
16	A	854	CLA	C4D-CHA-C1A	3.38	125.36	121.25
16	B	814	CLA	CHD-C1D-ND	-3.38	121.35	124.45
16	A	810	CLA	C4D-CHA-C1A	3.38	125.36	121.25
16	A	834	CLA	CHD-C1D-ND	-3.38	121.35	124.45
26	U	202	A86	C7-C6-C5	-3.38	118.19	122.92
16	B	826	CLA	C4D-CHA-C1A	3.37	125.35	121.25
16	B	834	CLA	CHD-C1D-ND	-3.37	121.36	124.45
16	B	827	CLA	C4D-CHA-C1A	3.37	125.35	121.25
16	B	849	CLA	CHD-C1D-ND	-3.37	121.36	124.45
21	K	201	LMU	C2'-C3'-C4'	3.36	117.36	109.68
16	U	205	CLA	C4D-CHA-C1A	3.36	125.34	121.25
16	U	209	CLA	CHD-C1D-ND	-3.36	121.37	124.45
20	U	203	DD6	C7-C6-C5	-3.36	118.22	122.92
16	B	847	CLA	C4D-CHA-C1A	3.36	125.33	121.25
26	U	202	A86	C-C1-C2	-3.35	118.23	122.92
22	A	850	CL0	C4-C3-C2	-3.35	115.08	123.68
16	A	830	CLA	C4D-CHA-C1A	3.35	125.33	121.25
16	G	315	CLA	CMD-C2D-C1D	3.35	130.61	124.71
16	A	801	CLA	CHD-C1D-ND	-3.34	121.39	124.45
16	A	815	CLA	CHD-C1D-ND	-3.34	121.39	124.45
16	B	803	CLA	CHD-C1D-ND	-3.34	121.39	124.45
16	G	310	CLA	CHD-C1D-ND	-3.34	121.39	124.45
16	B	845	CLA	C4D-CHA-C1A	3.34	125.31	121.25
16	A	810	CLA	CHD-C1D-ND	-3.33	121.39	124.45
20	K	208	DD6	C-C1-C2	-3.33	118.26	122.92
20	G	317	DD6	C3-C4-C5	3.33	130.29	123.47
20	G	317	DD6	C7-C6-C5	-3.33	118.27	122.92
16	A	851	CLA	CHD-C1D-ND	-3.32	121.40	124.45
16	B	819	CLA	CHD-C1D-ND	-3.32	121.40	124.45
20	U	212	DD6	C-C1-C2	-3.32	118.27	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	812	CLA	C4D-CHA-C1A	3.32	125.29	121.25
16	B	834	CLA	C4D-CHA-C1A	3.32	125.29	121.25
16	U	206	CLA	C4D-CHA-C1A	3.32	125.29	121.25
16	A	808	CLA	CHD-C1D-ND	-3.32	121.41	124.45
16	K	207	CLA	C4D-CHA-C1A	3.31	125.28	121.25
20	J	102	DD6	C8-C6-C5	3.31	124.03	118.94
16	A	820	CLA	CHD-C1D-ND	-3.31	121.41	124.45
19	J	105	BCR	C2-C1-C6	3.31	115.58	110.48
16	A	847	CLA	C4D-CHA-C1A	3.30	125.27	121.25
16	B	829	CLA	C4D-CHA-C1A	3.30	125.27	121.25
16	H	309	CLA	C4D-CHA-C1A	3.30	125.27	121.25
16	A	807	CLA	C4A-NA-C1A	3.30	108.19	106.71
16	B	811	CLA	CHD-C1D-ND	-3.30	121.42	124.45
16	A	825	CLA	C4D-CHA-C1A	3.30	125.26	121.25
16	H	303	CLA	C4D-CHA-C1A	3.29	125.25	121.25
16	J	104	CLA	CHD-C1D-ND	-3.28	121.44	124.45
16	A	836	CLA	CHD-C1D-ND	-3.28	121.44	124.45
16	A	829	CLA	C4D-CHA-C1A	3.28	125.24	121.25
16	H	304	CLA	C4D-CHA-C1A	3.27	125.23	121.25
20	G	311	DD6	C7-C6-C5	-3.27	118.34	122.92
16	A	825	CLA	CHD-C1D-ND	-3.27	121.45	124.45
16	k	201	CLA	C4D-CHA-C1A	3.25	125.21	121.25
16	A	808	CLA	C4D-CHA-C1A	3.25	125.20	121.25
20	A	846	DD6	C24-C1-C2	3.25	123.92	118.94
20	H	310	DD6	C24-C1-C2	3.25	123.92	118.94
16	A	847	CLA	CHD-C1D-ND	-3.24	121.47	124.45
16	L	202	CLA	CHD-C1D-ND	-3.24	121.47	124.45
20	A	846	DD6	C7-C6-C5	-3.24	118.38	122.92
16	B	809	CLA	C4D-CHA-C1A	3.24	125.19	121.25
20	H	311	DD6	C7-C6-C5	-3.24	118.39	122.92
16	A	832	CLA	CHD-C1D-ND	-3.23	121.49	124.45
16	A	845	CLA	C4D-CHA-C1A	3.23	125.18	121.25
16	B	804	CLA	CHD-C1D-ND	-3.23	121.49	124.45
16	A	824	CLA	C4D-CHA-C1A	3.23	125.17	121.25
16	U	211	CLA	C4D-CHA-C1A	3.22	125.17	121.25
16	F	802	CLA	CHD-C1D-ND	-3.22	121.49	124.45
16	A	815	CLA	C4D-CHA-C1A	3.22	125.17	121.25
16	G	303	CLA	CHD-C1D-ND	-3.21	121.50	124.45
16	U	207	CLA	CAA-C2A-C3A	-3.21	103.98	112.78
16	A	817	CLA	C4D-CHA-C1A	3.21	125.15	121.25
16	G	310	CLA	C4D-CHA-C1A	3.20	125.15	121.25
16	L	202	CLA	C4D-CHA-C1A	3.20	125.14	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	835	CLA	CHD-C1D-ND	-3.20	121.51	124.45
24	B	843	DGD	C3G-O3G-C1D	-3.20	107.50	113.74
16	A	806	CLA	C4D-CHA-C1A	3.19	125.14	121.25
16	F	803	CLA	CHD-C1D-ND	-3.19	121.52	124.45
16	B	828	CLA	CHD-C1D-ND	-3.19	121.52	124.45
19	k	203	BCR	C2-C1-C6	3.19	115.39	110.48
16	A	807	CLA	C4D-CHA-C1A	3.19	125.13	121.25
16	k	202	CLA	C4D-CHA-C1A	3.19	125.13	121.25
16	A	827	CLA	C4D-CHA-C1A	3.18	125.12	121.25
20	H	311	DD6	C-C1-C2	-3.18	118.47	122.92
16	A	830	CLA	CHD-C1D-ND	-3.18	121.53	124.45
16	A	817	CLA	CHD-C1D-ND	-3.17	121.54	124.45
20	G	317	DD6	C-C1-C2	-3.17	118.48	122.92
16	B	809	CLA	CHD-C1D-ND	-3.17	121.54	124.45
16	B	828	CLA	C4D-CHA-C1A	3.17	125.11	121.25
16	A	802	CLA	C4D-CHA-C1A	3.16	125.10	121.25
16	B	805	CLA	C4D-CHA-C1A	3.16	125.10	121.25
16	U	210	CLA	C4D-CHA-C1A	3.16	125.09	121.25
16	K	203	CLA	C4D-CHA-C1A	3.16	125.09	121.25
16	B	820	CLA	CHA-C1A-NA	-3.15	119.17	126.40
16	G	301	CLA	C4D-CHA-C1A	3.15	125.08	121.25
16	H	302	CLA	C4D-CHA-C1A	3.14	125.07	121.25
16	U	207	CLA	C4D-CHA-C1A	3.14	125.07	121.25
16	G	305	CLA	C4D-CHA-C1A	3.14	125.07	121.25
16	k	202	CLA	C4A-NA-C1A	3.14	108.12	106.71
16	A	832	CLA	C4D-CHA-C1A	3.13	125.06	121.25
16	A	828	CLA	CHD-C1D-ND	-3.12	121.58	124.45
20	G	312	DD6	C7-C6-C5	-3.12	118.55	122.92
16	B	817	CLA	C4D-CHA-C1A	3.12	125.05	121.25
16	B	836	CLA	CHD-C1D-ND	-3.11	121.60	124.45
16	A	814	CLA	C4D-CHA-C1A	3.11	125.03	121.25
20	K	208	DD6	C8-C6-C5	3.10	123.70	118.94
16	G	302	CLA	C4D-CHA-C1A	3.10	125.02	121.25
16	J	104	CLA	C4D-CHA-C1A	3.09	125.01	121.25
16	A	809	CLA	C4D-CHA-C1A	3.09	125.01	121.25
16	B	823	CLA	C4D-CHA-C1A	3.08	125.00	121.25
20	U	214	DD6	C24-C1-C2	3.08	123.67	118.94
16	K	204	CLA	C4D-CHA-C1A	3.08	124.99	121.25
19	I	103	BCR	C15-C16-C17	-3.07	117.18	123.47
16	A	821	CLA	CHA-C1A-NA	-3.07	119.37	126.40
16	A	811	CLA	CHD-C1D-ND	-3.07	121.64	124.45
21	K	201	LMU	O5B-C5B-C4B	3.06	115.25	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	G	311	DD6	C24-C1-C2	3.06	123.63	118.94
16	B	806	CLA	C4D-CHA-C1A	3.06	124.97	121.25
16	B	822	CLA	C4D-CHA-C1A	3.05	124.96	121.25
20	G	312	DD6	C3-C4-C5	3.05	129.73	123.47
21	K	201	LMU	C1B-O1B-C4'	-3.05	110.42	117.96
16	H	302	CLA	CHD-C1D-ND	-3.05	121.65	124.45
16	A	804	CLA	C4D-CHA-C1A	3.04	124.95	121.25
16	H	305	CLA	C4D-CHA-C1A	3.04	124.94	121.25
16	B	849	CLA	C4D-CHA-C1A	3.03	124.94	121.25
19	B	841	BCR	C15-C14-C13	-3.03	122.99	127.31
16	A	809	CLA	CHD-C1D-ND	-3.03	121.67	124.45
20	J	102	DD6	C24-C1-C2	3.02	123.57	118.94
20	G	313	DD6	C7-C6-C5	-3.02	118.70	122.92
20	A	846	DD6	C4-C3-C2	3.01	129.65	123.47
26	U	202	A86	C8-C6-C5	3.01	123.56	118.94
16	B	813	CLA	C4D-CHA-C1A	3.01	124.91	121.25
25	J	103	LMG	O6-C1-O1	-3.00	102.86	109.97
16	H	302	CLA	CHA-C1A-NA	-3.00	119.53	126.40
16	A	845	CLA	CHD-C1D-ND	-3.00	121.70	124.45
16	B	806	CLA	CHD-C1D-ND	-2.99	121.70	124.45
20	G	311	DD6	C3-C4-C5	2.99	129.61	123.47
16	U	204	CLA	CHD-C1D-ND	-2.99	121.70	124.45
21	K	201	LMU	C4B-C3B-C2B	2.99	116.04	110.82
16	H	312	CLA	CHA-C1A-NA	-2.99	119.56	126.40
20	G	313	DD6	C24-C1-C2	2.99	123.53	118.94
26	U	202	A86	C24-C1-C2	2.98	123.52	118.94
16	H	308	CLA	C4D-CHA-C1A	2.98	124.88	121.25
20	U	203	DD6	C8-C6-C5	2.98	123.51	118.94
19	I	103	BCR	C27-C26-C25	2.96	127.03	122.73
20	K	208	DD6	C24-C1-C2	2.96	123.48	118.94
16	B	824	CLA	C1-O2A-CGA	2.93	124.14	116.44
16	A	818	CLA	CHD-C1D-ND	-2.93	121.76	124.45
26	U	202	A86	C28-C27-C26	-2.93	118.82	122.92
16	A	823	CLA	C4D-CHA-C1A	2.93	124.81	121.25
16	G	315	CLA	CHD-C1D-C2D	2.92	131.61	125.48
16	U	211	CLA	CHD-C1D-ND	-2.92	121.77	124.45
16	A	810	CLA	C4A-NA-C1A	2.92	108.02	106.71
20	G	317	DD6	C8-C6-C5	2.92	123.42	118.94
16	k	202	CLA	CHA-C1A-NA	-2.92	119.72	126.40
16	K	204	CLA	CHD-C1D-ND	-2.91	121.78	124.45
16	A	817	CLA	C4A-NA-C1A	2.91	108.01	106.71
20	U	212	DD6	C34-C35-C36	2.90	117.63	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	U	207	CLA	O2A-C1-C2	2.90	116.25	108.64
16	B	844	CLA	CHD-C1D-ND	-2.90	121.79	124.45
16	B	823	CLA	CHA-C1A-NA	-2.89	119.77	126.40
16	A	818	CLA	C4D-CHA-C1A	2.89	124.77	121.25
16	B	819	CLA	C4D-CHA-C1A	2.89	124.76	121.25
16	A	807	CLA	CHA-C1A-NA	-2.89	119.79	126.40
16	K	202	CLA	C4D-CHA-C1A	2.89	124.76	121.25
16	B	845	CLA	CHD-C1D-ND	-2.88	121.80	124.45
16	A	845	CLA	CHA-C1A-NA	-2.88	119.80	126.40
22	A	850	CL0	CHA-C1A-NA	-2.87	119.82	126.40
16	U	211	CLA	CHA-C1A-NA	-2.87	119.82	126.40
16	B	820	CLA	CHD-C1D-ND	-2.87	121.82	124.45
16	B	836	CLA	CHA-C1A-NA	-2.87	119.83	126.40
16	B	825	CLA	CHD-C1D-ND	-2.87	121.82	124.45
16	A	834	CLA	CHA-C1A-NA	-2.86	119.84	126.40
16	A	827	CLA	CHD-C1D-ND	-2.86	121.83	124.45
20	G	311	DD6	C8-C6-C5	2.86	123.33	118.94
16	G	306	CLA	C4D-CHA-C1A	2.86	124.73	121.25
16	A	812	CLA	CHA-C1A-NA	-2.85	119.86	126.40
16	B	823	CLA	CHD-C1D-ND	-2.85	121.83	124.45
16	B	802	CLA	CHA-C1A-NA	-2.85	119.87	126.40
16	B	804	CLA	C4D-CHA-C1A	2.85	124.72	121.25
16	K	206	CLA	CHD-C1D-ND	-2.84	121.84	124.45
16	B	803	CLA	CHA-C1A-NA	-2.84	119.89	126.40
20	A	846	DD6	C3-C4-C5	2.84	129.29	123.47
20	U	212	DD6	C24-C1-C2	2.84	123.30	118.94
16	F	803	CLA	CHA-C1A-NA	-2.84	119.90	126.40
16	A	815	CLA	CHA-C1A-NA	-2.83	119.91	126.40
16	A	817	CLA	CHA-C1A-NA	-2.83	119.92	126.40
16	B	848	CLA	CHA-C1A-NA	-2.83	119.92	126.40
16	A	825	CLA	CHA-C1A-NA	-2.83	119.92	126.40
19	k	203	BCR	C15-C16-C17	-2.83	117.69	123.47
16	B	809	CLA	CHA-C1A-NA	-2.83	119.93	126.40
16	A	801	CLA	CHA-C1A-NA	-2.82	119.94	126.40
19	M	101	BCR	C15-C16-C17	-2.82	117.70	123.47
20	H	311	DD6	C4-C3-C2	2.82	129.25	123.47
16	B	831	CLA	CHA-C1A-NA	-2.81	119.95	126.40
16	G	306	CLA	CHD-C1D-ND	-2.81	121.87	124.45
16	L	202	CLA	CHA-C1A-NA	-2.81	119.96	126.40
16	K	204	CLA	CHA-C1A-NA	-2.81	119.96	126.40
20	U	212	DD6	C4-C3-C2	2.81	129.23	123.47
26	U	202	A86	C17-C16-C15	2.81	112.03	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	303	CLA	CHA-C1A-NA	-2.81	119.97	126.40
16	H	306	CLA	C1-O2A-CGA	-2.81	109.08	116.44
16	B	822	CLA	CHA-C1A-NA	-2.81	119.97	126.40
16	B	806	CLA	CHA-C1A-NA	-2.80	119.98	126.40
19	L	205	BCR	C2-C1-C6	2.80	114.79	110.48
16	A	828	CLA	CHA-C1A-NA	-2.80	119.99	126.40
16	B	801	CLA	CHA-C1A-NA	-2.80	119.99	126.40
16	A	821	CLA	C4D-CHA-C1A	2.80	124.65	121.25
16	B	835	CLA	CHA-C1A-NA	-2.79	120.00	126.40
16	B	819	CLA	CHA-C1A-NA	-2.79	120.01	126.40
16	U	204	CLA	O2A-C1-C2	2.79	115.97	108.64
16	A	827	CLA	CHA-C1A-NA	-2.79	120.01	126.40
16	B	821	CLA	C4D-CHA-C1A	2.79	124.64	121.25
16	B	804	CLA	CHA-C1A-NA	-2.79	120.02	126.40
16	U	209	CLA	CHA-C1A-NA	-2.79	120.02	126.40
16	A	832	CLA	CHA-C1A-NA	-2.78	120.03	126.40
16	A	810	CLA	CHA-C1A-NA	-2.78	120.03	126.40
21	J	101	LMU	C3B-C4B-C5B	2.78	115.20	110.24
21	A	855	LMU	O1'-C1'-C2'	2.78	112.64	108.30
16	A	823	CLA	CHA-C1A-NA	-2.78	120.03	126.40
16	B	828	CLA	CHA-C1A-NA	-2.78	120.03	126.40
16	H	312	CLA	C4D-CHA-C1A	2.78	124.63	121.25
16	G	305	CLA	CHA-C1A-NA	-2.77	120.04	126.40
20	G	314	DD6	C3-C4-C5	2.77	129.15	123.47
19	I	103	BCR	C15-C14-C13	-2.77	123.36	127.31
19	B	840	BCR	C24-C23-C22	-2.77	122.05	126.23
20	H	311	DD6	C8-C6-C5	2.77	123.19	118.94
16	H	305	CLA	CHD-C1D-ND	-2.77	121.91	124.45
16	L	204	CLA	CHA-C1A-NA	-2.76	120.07	126.40
19	M	101	BCR	C15-C14-C13	-2.76	123.37	127.31
20	G	317	DD6	C24-C1-C2	2.76	123.18	118.94
16	H	305	CLA	CHA-C1A-NA	-2.76	120.08	126.40
20	A	846	DD6	C8-C6-C5	2.76	123.17	118.94
16	G	306	CLA	CHA-C1A-NA	-2.76	120.09	126.40
16	B	833	CLA	CHA-C1A-NA	-2.75	120.10	126.40
16	K	207	CLA	CHA-C1A-NA	-2.75	120.10	126.40
16	B	825	CLA	CHA-C1A-NA	-2.75	120.10	126.40
16	H	302	CLA	CHC-C4B-NB	-2.75	121.35	124.26
16	B	803	CLA	C4D-CHA-C1A	2.75	124.59	121.25
21	K	201	LMU	O5'-C5'-C4'	2.75	115.54	109.75
16	B	830	CLA	CHA-C1A-NA	-2.74	120.12	126.40
16	B	836	CLA	C4A-NA-C1A	2.74	107.94	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	814	CLA	CHA-C1A-NA	-2.74	120.12	126.40
16	U	209	CLA	C4D-CHA-C1A	2.74	124.58	121.25
16	F	802	CLA	CHA-C1A-NA	-2.74	120.13	126.40
16	B	834	CLA	CHA-C1A-NA	-2.73	120.14	126.40
16	A	814	CLA	CHA-C1A-NA	-2.73	120.14	126.40
16	A	835	CLA	CHA-C1A-NA	-2.73	120.14	126.40
16	G	310	CLA	CHA-C1A-NA	-2.73	120.15	126.40
20	H	311	DD6	C24-C1-C2	2.73	123.13	118.94
25	U	201	LMG	O6-C1-O1	-2.73	103.52	109.97
16	B	844	CLA	CHA-C1A-NA	-2.73	120.16	126.40
16	A	824	CLA	CHA-C1A-NA	-2.72	120.16	126.40
16	A	808	CLA	CHA-C1A-NA	-2.72	120.17	126.40
16	A	811	CLA	CHA-C1A-NA	-2.72	120.17	126.40
16	B	827	CLA	CHA-C1A-NA	-2.72	120.17	126.40
16	A	813	CLA	CHA-C1A-NA	-2.72	120.18	126.40
16	I	102	CLA	CHA-C1A-NA	-2.71	120.18	126.40
16	A	804	CLA	CHA-C1A-NA	-2.71	120.19	126.40
16	G	309	CLA	CHA-C1A-NA	-2.71	120.20	126.40
16	B	845	CLA	CHA-C1A-NA	-2.71	120.20	126.40
16	A	854	CLA	CHA-C1A-NA	-2.70	120.21	126.40
16	A	818	CLA	CHA-C1A-NA	-2.70	120.21	126.40
19	L	205	BCR	C11-C10-C9	-2.70	123.46	127.31
16	A	830	CLA	CHA-C1A-NA	-2.70	120.22	126.40
16	H	302	CLA	C4A-NA-C1A	2.70	107.92	106.71
16	A	847	CLA	CHA-C1A-NA	-2.70	120.22	126.40
16	A	819	CLA	CHA-C1A-NA	-2.70	120.22	126.40
16	A	805	CLA	CHA-C1A-NA	-2.70	120.22	126.40
16	A	806	CLA	O2A-C1-C2	2.69	115.71	108.64
21	A	848	LMU	O1'-C1'-C2'	2.69	112.51	108.30
16	U	210	CLA	CHA-C1A-NA	-2.69	120.23	126.40
16	F	803	CLA	C4A-NA-C1A	2.69	107.92	106.71
16	G	302	CLA	CHA-C1A-NA	-2.69	120.23	126.40
16	B	822	CLA	CHD-C1D-ND	-2.69	121.98	124.45
16	B	808	CLA	C4D-CHA-C1A	2.69	124.52	121.25
19	A	843	BCR	C28-C27-C26	-2.69	109.28	114.08
16	H	301	CLA	CHA-C1A-NA	-2.69	120.37	126.41
16	B	811	CLA	CHA-C1A-NA	-2.68	120.25	126.40
16	A	826	CLA	CHA-C1A-NA	-2.68	120.25	126.40
16	B	805	CLA	CHA-C1A-NA	-2.68	120.25	126.40
16	K	203	CLA	CHA-C1A-NA	-2.68	120.26	126.40
16	G	304	CLA	CHA-C1A-NA	-2.68	120.26	126.40
16	B	807	CLA	CHA-C1A-NA	-2.68	120.26	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	820	CLA	CHA-C1A-NA	-2.68	120.26	126.40
16	H	309	CLA	CHA-C1A-NA	-2.68	120.26	126.40
16	L	202	CLA	C4A-NA-C1A	2.68	107.91	106.71
16	G	308	CLA	CHA-C1A-NA	-2.68	120.27	126.40
16	A	836	CLA	CHA-C1A-NA	-2.68	120.27	126.40
16	F	803	CLA	C1-O2A-CGA	2.67	123.46	116.44
19	L	201	BCR	C15-C16-C17	-2.67	118.00	123.47
16	H	304	CLA	CHA-C1A-NA	-2.67	120.28	126.40
16	J	104	CLA	CHA-C1A-NA	-2.67	120.28	126.40
16	A	826	CLA	C4D-CHA-C1A	2.67	124.50	121.25
16	A	851	CLA	CHA-C1A-NA	-2.67	120.29	126.40
19	B	839	BCR	C11-C10-C9	-2.66	123.52	127.31
19	L	201	BCR	C27-C26-C25	2.66	126.59	122.73
16	B	847	CLA	CHA-C1A-NA	-2.66	120.31	126.40
16	F	804	CLA	CHA-C1A-NA	-2.66	120.31	126.40
16	B	812	CLA	CHA-C1A-NA	-2.66	120.32	126.40
16	A	826	CLA	CHD-C1D-ND	-2.65	122.02	124.45
16	B	829	CLA	CHA-C1A-NA	-2.65	120.32	126.40
16	U	205	CLA	CHA-C1A-NA	-2.65	120.33	126.40
16	A	809	CLA	CHA-C1A-NA	-2.65	120.33	126.40
16	K	202	CLA	CHA-C1A-NA	-2.65	120.33	126.40
16	G	301	CLA	CHA-C1A-NA	-2.65	120.34	126.40
16	A	849	CLA	CHA-C1A-NA	-2.64	120.34	126.40
16	A	821	CLA	CHD-C1D-ND	-2.64	122.02	124.45
16	B	817	CLA	CHA-C1A-NA	-2.64	120.35	126.40
16	B	813	CLA	CHA-C1A-NA	-2.64	120.35	126.40
16	k	201	CLA	CHA-C1A-NA	-2.64	120.35	126.40
16	U	208	CLA	CHA-C1A-NA	-2.64	120.36	126.40
16	A	832	CLA	C4A-NA-C1A	2.64	107.89	106.71
16	B	810	CLA	CHA-C1A-NA	-2.64	120.36	126.40
16	B	816	CLA	CHA-C1A-NA	-2.64	120.36	126.40
16	A	821	CLA	C4A-NA-C1A	2.64	107.89	106.71
16	A	801	CLA	C4D-CHA-C1A	2.63	124.45	121.25
20	J	102	DD6	C10-C9-C8	2.63	131.43	123.22
16	B	818	CLA	CHA-C1A-NA	-2.63	120.37	126.40
16	A	838	CLA	CHA-C1A-NA	-2.63	120.38	126.40
16	B	826	CLA	CHA-C1A-NA	-2.63	120.38	126.40
16	B	817	CLA	CHC-C4B-NB	-2.63	121.48	124.26
16	B	822	CLA	CHC-C4B-NB	-2.62	121.48	124.26
16	B	808	CLA	CHA-C1A-NA	-2.62	120.40	126.40
19	B	842	BCR	C27-C26-C25	2.62	126.54	122.73
19	J	105	BCR	C24-C23-C22	-2.62	122.28	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	823	CLA	CHD-C1D-ND	-2.62	122.05	124.45
16	B	831	CLA	CHD-C1D-ND	-2.62	122.05	124.45
16	U	206	CLA	CHA-C1A-NA	-2.62	120.40	126.40
16	B	849	CLA	CHA-C1A-NA	-2.61	120.41	126.40
16	U	204	CLA	CHA-C1A-NA	-2.61	120.42	126.40
16	K	206	CLA	CHA-C1A-NA	-2.61	120.54	126.41
19	B	839	BCR	C15-C16-C17	-2.61	118.13	123.47
16	H	306	CLA	CHA-C1A-NA	-2.60	120.44	126.40
19	L	205	BCR	C3-C4-C5	-2.60	109.43	114.08
20	H	310	DD6	C10-C9-C8	2.60	131.33	123.22
16	G	315	CLA	CHA-C1A-NA	-2.60	120.45	126.40
16	A	831	CLA	CHA-C1A-NA	-2.60	120.45	126.40
16	A	806	CLA	CHA-C1A-NA	-2.59	120.46	126.40
16	B	824	CLA	CHA-C1A-NA	-2.59	120.47	126.40
20	U	203	DD6	C26-C25-C24	2.59	131.30	123.22
16	K	205	CLA	CHA-C1A-NA	-2.59	120.47	126.40
16	G	303	CLA	C4A-NA-C1A	2.58	107.87	106.71
16	A	833	CLA	CHA-C1A-NA	-2.58	120.48	126.40
19	L	205	BCR	C27-C26-C25	2.58	126.48	122.73
16	A	816	CLA	CHA-C1A-NA	-2.58	120.49	126.40
19	A	842	BCR	C15-C16-C17	-2.58	118.20	123.47
16	B	825	CLA	C4D-CHA-C1A	2.57	124.38	121.25
16	B	832	CLA	CHA-C1A-NA	-2.57	120.51	126.40
16	H	301	CLA	C4A-NA-C1A	2.57	107.86	106.71
16	B	848	CLA	CHC-C4B-NB	-2.57	121.53	124.26
16	A	829	CLA	CHA-C1A-NA	-2.57	120.51	126.40
16	B	848	CLA	C4A-NA-C1A	2.57	107.86	106.71
16	H	303	CLA	CHA-C1A-NA	-2.57	120.52	126.40
24	B	843	DGD	C1D-O6D-C5D	-2.57	108.65	113.69
19	M	101	BCR	C27-C26-C25	2.56	126.45	122.73
16	L	202	CLA	C1-O2A-CGA	2.56	123.17	116.44
19	M	101	BCR	C3-C4-C5	-2.56	109.50	114.08
16	B	834	CLA	C4A-NA-C1A	2.56	107.86	106.71
24	B	843	DGD	O3G-C1D-C2D	2.55	112.29	108.30
16	L	203	CLA	CHA-C1A-NA	-2.55	120.57	126.40
18	A	840	LHG	C11-C10-C9	-2.54	101.50	114.42
19	F	801	BCR	C27-C26-C25	2.54	126.42	122.73
19	A	844	BCR	C33-C5-C6	-2.54	121.67	124.53
16	B	815	CLA	CHA-C1A-NA	-2.54	120.58	126.40
16	A	834	CLA	C4A-NA-C1A	2.54	107.85	106.71
16	A	831	CLA	CHC-C4B-NB	-2.54	121.57	124.26
16	H	308	CLA	CHA-C1A-NA	-2.54	120.58	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	U	201	LMG	O3-C3-C2	-2.54	104.48	110.35
16	H	307	CLA	CHA-C1A-NA	-2.54	120.59	126.40
19	B	841	BCR	C27-C26-C25	2.53	126.41	122.73
16	A	824	CLA	O2A-C1-C2	2.53	115.28	108.64
27	U	213	KC1	C4D-C3D-CAD	2.53	109.13	107.42
20	G	313	DD6	C3-C4-C5	2.53	128.65	123.47
16	K	205	CLA	C1-O2A-CGA	2.53	123.07	116.44
19	I	101	BCR	C15-C16-C17	-2.52	118.31	123.47
19	J	105	BCR	C27-C26-C25	2.52	126.39	122.73
19	k	203	BCR	C27-C26-C25	2.52	126.39	122.73
16	A	833	CLA	O2A-C1-C2	2.52	115.25	108.64
16	B	849	CLA	CHC-C4B-NB	-2.51	121.59	124.26
16	A	849	CLA	CHC-C4B-NB	-2.51	121.60	124.26
16	A	813	CLA	CHC-C4B-NB	-2.51	121.60	124.26
19	A	842	BCR	C15-C14-C13	-2.51	123.73	127.31
16	G	307	CLA	CHA-C1A-NA	-2.51	120.65	126.40
20	G	312	DD6	C8-C6-C5	2.51	122.79	118.94
19	B	846	BCR	C19-C18-C17	-2.50	119.24	124.81
16	A	814	CLA	C4A-NA-C1A	2.50	107.83	106.71
16	B	820	CLA	C4A-NA-C1A	2.49	107.83	106.71
19	F	805	BCR	C27-C26-C25	2.49	126.34	122.73
16	B	821	CLA	CHA-C1A-NA	-2.48	120.71	126.40
16	A	802	CLA	CHA-C1A-NA	-2.47	120.73	126.40
16	U	211	CLA	C4A-NA-C1A	2.47	107.82	106.71
20	K	208	DD6	C13-C11-C10	2.47	122.73	118.94
16	A	853	CLA	CHA-C1A-NA	-2.47	120.75	126.40
16	A	849	CLA	CHD-C1D-C2D	2.47	130.65	125.48
16	A	803	CLA	CHA-C1A-NA	-2.46	120.75	126.40
16	U	207	CLA	CHA-C1A-NA	-2.46	120.76	126.40
16	k	201	CLA	CHC-C4B-NB	-2.46	121.66	124.26
20	G	317	DD6	C37-C36-C31	-2.45	121.02	124.35
16	B	820	CLA	C4D-CHA-C1A	2.45	124.23	121.25
16	H	306	CLA	C4B-CHC-C1C	2.45	132.14	126.34
16	F	802	CLA	C4A-NA-C1A	2.44	107.81	106.71
20	U	203	DD6	C33-C32-C31	2.44	114.57	109.62
19	B	846	BCR	C24-C23-C22	-2.44	122.55	126.23
16	A	817	CLA	CHC-C4B-NB	-2.44	121.68	124.26
19	B	840	BCR	C27-C26-C25	2.43	126.26	122.73
16	H	303	CLA	CHC-C4B-NB	-2.42	121.69	124.26
18	A	839	LHG	C11-C10-C9	-2.42	102.12	114.42
20	G	313	DD6	C8-C6-C5	2.42	122.66	118.94
16	K	206	CLA	C4A-NA-C1A	2.42	107.79	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	848	LMU	C1'-C2'-C3'	2.42	115.03	110.00
19	A	842	BCR	C27-C26-C25	2.41	126.24	122.73
16	H	309	CLA	CHC-C4B-NB	-2.41	121.70	124.26
19	B	846	BCR	C19-C20-C21	-2.41	118.54	123.47
16	B	817	CLA	C3B-C4B-NB	-2.41	108.28	110.52
16	A	812	CLA	C4A-NA-C1A	2.41	107.79	106.71
16	U	210	CLA	C4A-NA-C1A	2.41	107.79	106.71
19	J	105	BCR	C15-C16-C17	-2.40	118.55	123.47
21	J	101	LMU	O1'-C1'-C2'	2.40	112.05	108.30
19	B	839	BCR	C33-C5-C6	-2.40	121.83	124.53
16	U	205	CLA	O2A-C1-C2	2.40	114.94	108.64
16	A	812	CLA	CHD-C1D-C2D	2.40	130.51	125.48
19	k	203	BCR	C15-C14-C13	-2.39	123.90	127.31
19	B	839	BCR	C15-C14-C13	-2.39	123.90	127.31
16	B	806	CLA	C4A-NA-C1A	2.39	107.78	106.71
16	A	822	CLA	CHA-C1A-NA	-2.39	120.93	126.40
16	L	204	CLA	C4A-NA-C1A	2.38	107.78	106.71
16	A	812	CLA	CMD-C2D-C1D	2.38	128.91	124.71
19	F	805	BCR	C11-C10-C9	-2.38	123.91	127.31
16	B	822	CLA	C4A-NA-C1A	2.38	107.78	106.71
16	B	835	CLA	C4A-NA-C1A	2.38	107.78	106.71
27	U	213	KC1	CBA-CAA-C2A	2.38	134.34	125.27
16	B	818	CLA	CHC-C4B-NB	-2.38	121.74	124.26
19	L	201	BCR	C15-C14-C13	-2.37	123.92	127.31
18	A	839	LHG	O8-C23-C24	2.37	119.35	111.91
19	L	205	BCR	C15-C14-C13	-2.37	123.93	127.31
19	B	838	BCR	C29-C30-C25	2.37	114.13	110.48
20	U	212	DD6	C9-C10-C11	2.36	130.69	127.31
16	H	312	CLA	CHD-C1D-C2D	2.36	130.44	125.48
16	F	804	CLA	CHC-C4B-NB	-2.36	121.75	124.26
16	B	834	CLA	CHC-C4B-NB	-2.36	121.76	124.26
20	H	310	DD6	C33-C32-C31	2.35	114.39	109.62
20	U	203	DD6	C13-C11-C10	2.35	122.54	118.94
20	U	212	DD6	C37-C36-C31	-2.34	121.16	124.35
16	A	854	CLA	C4A-NA-C1A	2.34	107.76	106.71
16	B	836	CLA	O2A-C1-C2	2.34	114.78	108.64
19	A	844	BCR	C15-C16-C17	-2.34	118.69	123.47
16	B	802	CLA	C4D-CHA-C1A	2.33	124.09	121.25
20	U	212	DD6	C14-C13-C11	2.33	129.15	125.53
19	L	205	BCR	C24-C23-C22	-2.33	122.71	126.23
16	A	815	CLA	C3B-C4B-NB	-2.33	108.35	110.52
19	B	838	BCR	C28-C27-C26	-2.33	109.92	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	843	BCR	C33-C5-C6	-2.33	121.91	124.53
20	U	214	DD6	C41-C32-C31	-2.33	106.77	110.47
19	L	201	BCR	C33-C5-C6	-2.33	121.92	124.53
16	H	301	CLA	CHD-C1D-C2D	2.32	130.35	125.48
16	B	830	CLA	CHC-C4B-NB	-2.32	121.80	124.26
25	U	201	LMG	O1-C7-C8	-2.32	105.30	110.90
19	I	101	BCR	C2-C1-C6	2.32	114.05	110.48
25	U	201	LMG	O1-C1-C2	-2.32	104.68	108.30
16	U	209	CLA	CHC-C4B-NB	-2.32	121.80	124.26
16	k	201	CLA	CMD-C2D-C1D	2.32	128.79	124.71
16	K	203	CLA	CHC-C4B-NB	-2.32	121.81	124.26
16	A	831	CLA	CHD-C1D-C2D	2.31	130.32	125.48
16	A	803	CLA	CHD-C1D-C2D	2.31	130.32	125.48
19	B	846	BCR	C17-C16-C15	-2.30	119.69	124.81
16	U	208	CLA	CHC-C4B-NB	-2.30	121.82	124.26
16	B	808	CLA	CHD-C1D-ND	-2.29	122.35	124.45
19	B	842	BCR	C10-C11-C12	-2.29	116.08	123.22
16	A	822	CLA	CHD-C1D-C2D	2.29	130.27	125.48
20	U	212	DD6	C33-C34-C35	2.29	113.43	110.30
16	B	809	CLA	C4A-NA-C1A	2.28	107.73	106.71
16	A	823	CLA	C4A-NA-C1A	2.28	107.73	106.71
19	k	203	BCR	C11-C10-C9	-2.28	124.06	127.31
19	A	841	BCR	C27-C26-C25	2.28	126.03	122.73
19	B	842	BCR	C16-C15-C14	-2.26	118.84	123.47
16	A	818	CLA	O2A-C1-C2	2.26	114.58	108.64
16	G	315	CLA	C2D-C1D-ND	-2.26	108.44	110.10
20	H	311	DD6	C33-C32-C31	2.25	114.18	109.62
19	B	838	BCR	C7-C8-C9	-2.25	122.83	126.23
16	B	811	CLA	C4A-NA-C1A	2.24	107.72	106.71
16	A	805	CLA	C4A-NA-C1A	2.24	107.71	106.71
20	G	314	DD6	C10-C9-C8	2.24	130.21	123.22
16	B	802	CLA	CHB-C1B-NB	-2.23	121.89	124.26
18	A	839	LHG	O8-C6-C5	-2.23	101.93	108.43
16	B	819	CLA	C2A-C1A-CHA	2.23	127.76	123.86
16	H	303	CLA	CHD-C1D-C2D	2.23	130.16	125.48
16	k	201	CLA	CHD-C1D-C2D	2.23	130.16	125.48
16	A	838	CLA	CHD-C1D-C2D	2.23	130.15	125.48
16	A	814	CLA	CHC-C4B-NB	-2.23	121.90	124.26
16	B	820	CLA	C2A-C1A-CHA	2.22	127.75	123.86
19	A	844	BCR	C15-C14-C13	-2.22	124.14	127.31
16	B	818	CLA	CHD-C1D-C2D	2.22	130.14	125.48
16	B	828	CLA	O2A-C1-C2	2.22	114.47	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	G	317	DD6	C13-C11-C10	2.22	122.35	118.94
16	G	305	CLA	C2A-C1A-CHA	2.22	127.74	123.86
16	U	207	CLA	CHD-C1D-C2D	2.22	130.13	125.48
19	A	844	BCR	C28-C27-C26	-2.22	110.12	114.08
16	B	821	CLA	CHD-C1D-C2D	2.21	130.12	125.48
20	G	314	DD6	C26-C25-C24	2.21	130.11	123.22
16	A	806	CLA	C1-O2A-CGA	2.20	122.22	116.44
16	A	821	CLA	C1D-ND-C4D	2.20	107.90	106.33
25	J	103	LMG	O3-C3-C2	-2.20	105.26	110.35
16	U	210	CLA	CHD-C1D-C2D	2.20	130.10	125.48
16	A	815	CLA	CHC-C4B-NB	-2.20	121.93	124.26
16	A	806	CLA	CHD-C1D-C2D	2.20	130.09	125.48
19	k	203	BCR	C2-C3-C4	2.19	116.28	111.38
16	G	304	CLA	CHD-C1D-C2D	2.19	130.08	125.48
21	F	806	LMU	C1B-O1B-C4'	-2.19	112.54	117.96
16	A	847	CLA	C4A-NA-C1A	2.19	107.69	106.71
24	B	843	DGD	O6E-C5E-C4E	2.19	113.67	109.69
16	A	836	CLA	O2A-C1-C2	2.19	114.38	108.64
16	G	301	CLA	CHC-C4B-NB	-2.18	121.94	124.26
16	A	835	CLA	CHC-C4B-NB	-2.18	121.94	124.26
27	U	213	KC1	C1A-NA-C4A	2.18	107.69	106.71
25	J	103	LMG	O5-C6-C5	-2.18	103.81	111.29
16	H	307	CLA	CHD-C1D-C2D	2.18	130.05	125.48
20	H	310	DD6	C13-C11-C10	2.18	122.28	118.94
16	G	303	CLA	CHC-C4B-NB	-2.18	121.95	124.26
19	A	841	BCR	C3-C4-C5	-2.18	110.19	114.08
22	A	850	CL0	C2A-C1A-CHA	2.18	127.66	123.86
16	G	309	CLA	CHC-C4B-NB	-2.17	121.95	124.26
20	U	203	DD6	C34-C35-C36	-2.17	107.52	111.85
16	B	817	CLA	CHD-C1D-C2D	2.17	130.04	125.48
19	F	805	BCR	C2-C1-C6	2.17	113.83	110.48
16	G	308	CLA	CHD-C1D-C2D	2.17	130.04	125.48
16	A	816	CLA	CHD-C1D-C2D	2.17	130.04	125.48
20	G	313	DD6	O1-C20-C19	-2.17	111.75	113.38
16	G	307	CLA	CHD-C1D-C2D	2.17	130.03	125.48
16	K	205	CLA	C1D-ND-C4D	2.17	107.88	106.33
16	B	847	CLA	CHD-C1D-C2D	2.17	130.03	125.48
16	F	802	CLA	CHC-C4B-NB	-2.16	121.97	124.26
16	H	308	CLA	CHC-C4B-NB	-2.16	121.97	124.26
16	I	102	CLA	CHD-C1D-C2D	2.16	130.01	125.48
19	B	846	BCR	C16-C15-C14	-2.16	119.05	123.47
16	G	309	CLA	CHD-C1D-C2D	2.16	130.00	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	308	CLA	CHD-C1D-C2D	2.16	130.00	125.48
16	K	205	CLA	CHD-C1D-C2D	2.15	130.00	125.48
16	G	308	CLA	C5-C3-C2	2.15	125.47	121.12
16	A	802	CLA	CHD-C1D-C2D	2.15	129.98	125.48
16	J	104	CLA	C4A-NA-C1A	2.14	107.67	106.71
16	G	309	CLA	C4A-NA-C1A	2.14	107.67	106.71
16	A	807	CLA	CAA-C2A-C1A	2.14	119.00	111.97
20	U	212	DD6	O1-C20-C19	-2.14	111.77	113.38
19	B	838	BCR	C33-C5-C6	-2.14	122.13	124.53
16	H	301	CLA	C2A-C1A-CHA	2.14	126.03	122.71
16	B	815	CLA	CHD-C1D-C2D	2.14	129.96	125.48
16	B	812	CLA	CHD-C1D-C2D	2.14	129.96	125.48
19	B	839	BCR	C28-C27-C26	-2.13	110.27	114.08
16	G	315	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
18	A	839	LHG	C27-C26-C25	-2.13	103.60	114.42
20	G	314	DD6	C4-C3-C2	2.13	127.84	123.47
19	F	805	BCR	C35-C13-C14	-2.13	119.94	122.92
16	A	801	CLA	C2A-C1A-CHA	2.13	127.58	123.86
19	I	101	BCR	C15-C14-C13	-2.13	124.27	127.31
16	G	308	CLA	C4A-NA-C1A	2.13	107.66	106.71
19	B	840	BCR	C2-C1-C6	2.13	113.76	110.48
20	H	311	DD6	C12-C11-C13	2.13	121.43	118.08
16	A	821	CLA	C2A-C1A-CHA	2.13	127.58	123.86
16	U	208	CLA	CHD-C1D-C2D	2.12	129.94	125.48
22	A	850	CL0	C4D-CHA-C1A	2.12	123.83	121.25
16	B	824	CLA	CHD-C1D-C2D	2.12	129.92	125.48
19	B	842	BCR	C15-C16-C17	-2.11	119.14	123.47
16	H	309	CLA	CHD-C1D-C2D	2.11	129.91	125.48
16	B	828	CLA	C2A-C1A-CHA	2.11	127.55	123.86
24	B	843	DGD	C3G-C2G-C1G	-2.11	106.81	111.79
19	A	843	BCR	C15-C16-C17	-2.10	119.16	123.47
16	B	817	CLA	CHB-C1B-NB	2.10	126.48	124.26
16	L	203	CLA	CHD-C1D-C2D	2.10	129.89	125.48
16	H	306	CLA	C2D-C1D-ND	-2.10	108.56	110.10
16	H	308	CLA	CAA-C2A-C3A	-2.10	111.20	116.10
16	U	211	CLA	CAA-C2A-C1A	2.10	118.85	111.97
20	A	846	DD6	C13-C11-C10	2.10	122.16	118.94
16	B	805	CLA	CHD-C1D-C2D	2.10	129.88	125.48
19	A	844	BCR	C29-C30-C25	2.09	113.71	110.48
16	U	211	CLA	CHC-C4B-NB	-2.09	122.04	124.26
16	B	829	CLA	CHD-C1D-C2D	2.09	129.87	125.48
16	B	802	CLA	C2A-C1A-CHA	2.09	127.52	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	F	804	CLA	CHD-C1D-C2D	2.09	129.87	125.48
19	B	840	BCR	C15-C16-C17	-2.09	119.19	123.47
16	U	209	CLA	C2A-C1A-CHA	2.09	127.52	123.86
21	F	806	LMU	O5'-C5'-C4'	2.09	114.16	109.75
16	A	819	CLA	C4A-NA-C1A	2.09	107.65	106.71
16	B	820	CLA	C1D-ND-C4D	2.09	107.82	106.33
16	U	206	CLA	CHD-C1D-C2D	2.09	129.86	125.48
19	F	805	BCR	C33-C5-C6	-2.09	122.18	124.53
19	B	840	BCR	C31-C1-C6	2.09	113.69	110.30
16	B	836	CLA	C1D-ND-C4D	2.09	107.82	106.33
16	B	831	CLA	C4A-NA-C1A	2.09	107.64	106.71
19	B	840	BCR	C1-C6-C5	-2.09	119.67	122.61
16	B	810	CLA	CHD-C1D-C2D	2.09	129.86	125.48
18	A	839	LHG	C18-C17-C16	-2.09	103.83	114.42
19	F	801	BCR	C16-C15-C14	-2.09	119.20	123.47
16	K	207	CLA	CHD-C1D-C2D	2.09	129.85	125.48
16	B	819	CLA	CHD-C1D-C2D	2.08	129.85	125.48
16	A	833	CLA	CHD-C1D-C2D	2.08	129.84	125.48
20	U	203	DD6	C15-C14-C13	2.08	130.39	125.99
16	H	304	CLA	CHC-C4B-NB	-2.08	122.06	124.26
16	A	813	CLA	CHD-C1D-C2D	2.08	129.84	125.48
19	B	841	BCR	C2-C1-C6	2.08	113.68	110.48
16	B	804	CLA	C4A-NA-C1A	2.08	107.64	106.71
16	L	204	CLA	CHD-C1D-C2D	2.07	129.83	125.48
19	B	841	BCR	C8-C7-C6	-2.07	121.38	127.20
16	k	202	CLA	CHD-C1D-ND	-2.07	122.55	124.45
16	A	804	CLA	CHD-C1D-C2D	2.07	129.83	125.48
19	F	805	BCR	C16-C15-C14	-2.07	119.23	123.47
19	B	846	BCR	C33-C5-C6	-2.07	122.20	124.53
19	B	846	BCR	C29-C30-C25	2.07	113.66	110.48
25	U	201	LMG	O2-C2-C1	-2.06	105.03	110.05
16	G	305	CLA	CHD-C1D-C2D	2.06	129.81	125.48
27	U	213	KC1	C1B-CHB-C4A	2.06	130.50	126.06
16	B	833	CLA	C4A-NA-C1A	2.06	107.63	106.71
16	A	812	CLA	C2D-C1D-ND	-2.06	108.59	110.10
16	G	305	CLA	C3B-C4B-NB	-2.06	108.61	110.52
16	B	816	CLA	CHD-C1D-C2D	2.06	129.80	125.48
16	G	302	CLA	CHD-C1D-ND	-2.06	122.56	124.45
16	B	830	CLA	CHD-C1D-C2D	2.06	129.79	125.48
16	B	828	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
16	U	204	CLA	CAA-CBA-CGA	2.05	119.26	113.25
16	G	302	CLA	CAA-C2A-C3A	-2.05	111.31	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	853	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	A	843	BCR	C29-C30-C25	2.05	113.64	110.48
16	A	807	CLA	CHD-C1D-C2D	2.05	129.78	125.48
16	B	803	CLA	C2A-C1A-CHA	2.05	127.44	123.86
19	I	101	BCR	C28-C27-C26	-2.05	110.42	114.08
16	U	208	CLA	O2D-CGD-CBD	2.05	114.91	111.27
16	A	817	CLA	C1D-ND-C4D	2.05	107.79	106.33
20	G	317	DD6	C28-C27-C29	2.05	120.89	116.84
16	B	849	CLA	CGD-CBD-CAD	-2.04	104.11	110.73
16	G	301	CLA	CHD-C1D-C2D	2.04	129.76	125.48
19	k	203	BCR	C7-C8-C9	-2.04	123.15	126.23
16	A	824	CLA	CHD-C1D-C2D	2.04	129.76	125.48
20	U	212	DD6	C12-C11-C13	2.04	121.29	118.08
19	k	203	BCR	C40-C30-C25	2.04	113.61	110.30
19	B	846	BCR	C27-C26-C25	2.04	125.69	122.73
20	K	208	DD6	C37-C36-C31	-2.04	121.58	124.35
16	A	820	CLA	CHD-C1D-C2D	2.04	129.75	125.48
16	B	826	CLA	CHD-C1D-C2D	2.04	129.75	125.48
16	B	834	CLA	CHD-C1D-C2D	2.04	129.75	125.48
16	K	202	CLA	CHD-C1D-C2D	2.04	129.75	125.48
16	H	306	CLA	CMC-C2C-C1C	2.03	128.14	125.04
16	k	202	CLA	O2A-C1-C2	2.03	113.98	108.64
16	U	209	CLA	C1D-ND-C4D	2.03	107.78	106.33
16	G	310	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
19	B	838	BCR	C24-C23-C22	-2.03	123.17	126.23
16	U	207	CLA	C3A-C2A-C1A	-2.03	98.30	101.34
19	k	203	BCR	C16-C15-C14	-2.02	119.33	123.47
21	K	201	LMU	C1B-C2B-C3B	2.02	114.21	110.00
20	U	203	DD6	C22-C16-C17	-2.02	105.47	108.98
19	B	838	BCR	C15-C16-C17	-2.02	119.33	123.47
16	A	827	CLA	C4A-NA-C1A	2.02	107.61	106.71
16	K	203	CLA	CHD-C1D-C2D	2.02	129.72	125.48
19	I	103	BCR	C38-C26-C25	-2.02	122.26	124.53
19	A	842	BCR	C11-C10-C9	-2.02	124.43	127.31
16	B	849	CLA	O2A-C1-C2	-2.01	103.35	108.64
16	B	833	CLA	CHD-C1D-C2D	2.01	129.70	125.48
16	H	304	CLA	CHD-C1D-C2D	2.01	129.70	125.48
16	B	823	CLA	CAA-C2A-C1A	2.01	118.56	111.97
16	A	854	CLA	CHD-C1D-C2D	2.00	129.68	125.48
16	A	838	CLA	O2D-CGD-CBD	2.00	114.83	111.27
16	A	810	CLA	CHD-C1D-C2D	2.00	129.68	125.48
16	A	851	CLA	C4A-NA-C1A	2.00	107.61	106.71

There are no chirality outliers.

All (1003) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	804	CLA	C1A-C2A-CAA-CBA
16	A	806	CLA	CBA-CGA-O2A-C1
16	A	806	CLA	O1A-CGA-O2A-C1
16	A	815	CLA	C3A-C2A-CAA-CBA
16	A	820	CLA	CBD-CGD-O2D-CED
16	A	820	CLA	O1D-CGD-O2D-CED
16	A	826	CLA	CHA-CBD-CGD-O1D
16	A	826	CLA	CHA-CBD-CGD-O2D
16	A	831	CLA	CHA-CBD-CGD-O1D
16	A	831	CLA	CHA-CBD-CGD-O2D
16	A	834	CLA	CHA-CBD-CGD-O1D
16	A	834	CLA	CHA-CBD-CGD-O2D
16	A	838	CLA	CBD-CGD-O2D-CED
16	A	838	CLA	O1D-CGD-O2D-CED
16	A	845	CLA	C2-C3-C5-C6
16	A	845	CLA	C4-C3-C5-C6
16	A	849	CLA	CHA-CBD-CGD-O1D
16	A	849	CLA	CHA-CBD-CGD-O2D
16	B	809	CLA	CHA-CBD-CGD-O1D
16	B	809	CLA	CHA-CBD-CGD-O2D
16	B	819	CLA	CHA-CBD-CGD-O1D
16	B	819	CLA	CHA-CBD-CGD-O2D
16	B	821	CLA	CHA-CBD-CGD-O2D
16	B	824	CLA	CBA-CGA-O2A-C1
16	B	824	CLA	O1A-CGA-O2A-C1
16	B	825	CLA	CHA-CBD-CGD-O2D
16	B	847	CLA	C1A-C2A-CAA-CBA
16	B	847	CLA	C3A-C2A-CAA-CBA
16	B	849	CLA	C1A-C2A-CAA-CBA
16	B	849	CLA	C2-C3-C5-C6
16	B	849	CLA	C4-C3-C5-C6
16	F	803	CLA	CBA-CGA-O2A-C1
16	F	803	CLA	O1A-CGA-O2A-C1
16	F	804	CLA	C1A-C2A-CAA-CBA
16	F	804	CLA	CHA-CBD-CGD-O1D
16	F	804	CLA	CHA-CBD-CGD-O2D
16	J	104	CLA	CHA-CBD-CGD-O1D
16	J	104	CLA	CHA-CBD-CGD-O2D
16	J	104	CLA	CAD-CBD-CGD-O1D
16	J	104	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	L	202	CLA	C1A-C2A-CAA-CBA
16	L	202	CLA	CBA-CGA-O2A-C1
16	L	202	CLA	O1A-CGA-O2A-C1
16	L	204	CLA	CBD-CGD-O2D-CED
16	L	204	CLA	O1D-CGD-O2D-CED
16	U	204	CLA	CHA-CBD-CGD-O1D
16	U	204	CLA	CHA-CBD-CGD-O2D
16	U	208	CLA	CBD-CGD-O2D-CED
16	U	208	CLA	O1D-CGD-O2D-CED
16	G	304	CLA	C1A-C2A-CAA-CBA
16	G	304	CLA	C3A-C2A-CAA-CBA
16	G	305	CLA	C2B-C3B-CAB-CBB
16	G	305	CLA	C4B-C3B-CAB-CBB
16	G	306	CLA	C1A-C2A-CAA-CBA
16	G	306	CLA	C3A-C2A-CAA-CBA
16	G	307	CLA	C4-C3-C5-C6
16	G	308	CLA	CHA-CBD-CGD-O1D
16	G	308	CLA	CHA-CBD-CGD-O2D
16	G	309	CLA	CHA-CBD-CGD-O1D
16	G	309	CLA	CHA-CBD-CGD-O2D
16	G	310	CLA	C1A-C2A-CAA-CBA
16	G	310	CLA	CBD-CGD-O2D-CED
16	G	310	CLA	O1D-CGD-O2D-CED
16	G	315	CLA	CHA-CBD-CGD-O1D
16	G	315	CLA	CHA-CBD-CGD-O2D
16	H	301	CLA	CHA-CBD-CGD-O1D
16	H	301	CLA	CHA-CBD-CGD-O2D
16	H	303	CLA	CBD-CGD-O2D-CED
16	H	303	CLA	O1D-CGD-O2D-CED
16	H	306	CLA	C1A-C2A-CAA-CBA
16	H	306	CLA	C3A-C2A-CAA-CBA
16	H	306	CLA	C2-C3-C5-C6
16	H	306	CLA	C4-C3-C5-C6
16	H	308	CLA	CBD-CGD-O2D-CED
16	H	308	CLA	O1D-CGD-O2D-CED
16	H	309	CLA	C1A-C2A-CAA-CBA
16	H	312	CLA	C2B-C3B-CAB-CBB
16	H	312	CLA	C4B-C3B-CAB-CBB
16	H	312	CLA	CBD-CGD-O2D-CED
16	H	312	CLA	O2A-C1-C2-C3
16	H	312	CLA	C1-C2-C3-C4
16	H	312	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
16	K	205	CLA	CHA-CBD-CGD-O1D
16	K	205	CLA	CHA-CBD-CGD-O2D
16	K	207	CLA	C1A-C2A-CAA-CBA
16	k	202	CLA	CHA-CBD-CGD-O1D
16	k	202	CLA	CHA-CBD-CGD-O2D
18	A	840	LHG	C3-O3-P-O5
18	G	316	LHG	C3-O3-P-O4
18	G	316	LHG	C3-O3-P-O5
18	G	316	LHG	C3-O3-P-O6
19	A	841	BCR	C20-C21-C22-C37
19	A	841	BCR	C21-C22-C23-C24
19	A	841	BCR	C23-C24-C25-C30
19	A	842	BCR	C1-C6-C7-C8
19	A	842	BCR	C7-C8-C9-C10
19	A	842	BCR	C21-C22-C23-C24
19	A	843	BCR	C7-C8-C9-C10
19	A	843	BCR	C7-C8-C9-C34
19	A	844	BCR	C1-C6-C7-C8
19	A	844	BCR	C7-C8-C9-C34
19	A	844	BCR	C20-C21-C22-C37
19	A	844	BCR	C21-C22-C23-C24
19	A	844	BCR	C37-C22-C23-C24
19	B	838	BCR	C1-C6-C7-C8
19	B	838	BCR	C37-C22-C23-C24
19	B	839	BCR	C6-C7-C8-C9
19	B	839	BCR	C37-C22-C23-C24
19	B	846	BCR	C1-C6-C7-C8
19	B	846	BCR	C16-C17-C18-C19
19	B	846	BCR	C20-C21-C22-C23
19	B	846	BCR	C20-C21-C22-C37
19	B	846	BCR	C23-C24-C25-C30
19	F	801	BCR	C7-C8-C9-C10
19	F	801	BCR	C7-C8-C9-C34
19	F	801	BCR	C37-C22-C23-C24
19	F	805	BCR	C1-C6-C7-C8
19	F	805	BCR	C7-C8-C9-C34
19	F	805	BCR	C37-C22-C23-C24
19	I	101	BCR	C11-C12-C13-C35
19	I	103	BCR	C1-C6-C7-C8
19	I	103	BCR	C7-C8-C9-C10
19	I	103	BCR	C7-C8-C9-C34
19	I	103	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
19	I	103	BCR	C37-C22-C23-C24
19	I	103	BCR	C23-C24-C25-C26
19	J	105	BCR	C7-C8-C9-C10
19	J	105	BCR	C7-C8-C9-C34
19	J	105	BCR	C11-C12-C13-C35
19	J	105	BCR	C21-C22-C23-C24
19	J	105	BCR	C37-C22-C23-C24
19	L	201	BCR	C21-C22-C23-C24
19	L	201	BCR	C37-C22-C23-C24
19	L	201	BCR	C23-C24-C25-C30
19	L	205	BCR	C22-C23-C24-C25
19	L	205	BCR	C23-C24-C25-C30
19	M	101	BCR	C1-C6-C7-C8
19	M	101	BCR	C7-C8-C9-C10
19	M	101	BCR	C7-C8-C9-C34
19	M	101	BCR	C23-C24-C25-C30
19	k	203	BCR	C1-C6-C7-C8
19	k	203	BCR	C6-C7-C8-C9
19	k	203	BCR	C7-C8-C9-C10
19	k	203	BCR	C7-C8-C9-C34
19	k	203	BCR	C10-C11-C12-C13
19	k	203	BCR	C37-C22-C23-C24
20	A	846	DD6	C9-C10-C11-C12
20	A	846	DD6	C9-C10-C11-C13
20	A	846	DD6	C10-C11-C13-C14
20	A	846	DD6	C12-C11-C13-C14
20	A	846	DD6	C5-C6-C8-C9
20	A	846	DD6	C7-C6-C8-C9
20	U	203	DD6	C1-C24-C25-C26
20	U	203	DD6	C2-C3-C4-C5
20	U	203	DD6	C3-C4-C5-C6
20	U	212	DD6	C11-C13-C14-C15
20	U	212	DD6	C5-C6-C8-C9
20	U	212	DD6	C7-C6-C8-C9
20	U	214	DD6	C2-C3-C4-C5
20	G	311	DD6	C9-C10-C11-C12
20	G	311	DD6	C9-C10-C11-C13
20	G	311	DD6	C11-C13-C14-C15
20	G	311	DD6	C2-C3-C4-C5
20	G	311	DD6	C4-C5-C6-C7
20	G	311	DD6	C4-C5-C6-C8
20	G	312	DD6	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
20	G	312	DD6	C4-C5-C6-C7
20	G	314	DD6	C-C1-C24-C25
20	G	314	DD6	C2-C1-C24-C25
20	G	314	DD6	C9-C10-C11-C12
20	G	314	DD6	C9-C10-C11-C13
20	G	314	DD6	C12-C11-C13-C14
20	G	317	DD6	C-C1-C24-C25
20	G	317	DD6	C2-C1-C24-C25
20	G	317	DD6	C10-C11-C13-C14
20	G	317	DD6	C12-C11-C13-C14
20	G	317	DD6	C24-C25-C26-C27
20	G	317	DD6	C2-C3-C4-C5
20	G	317	DD6	C4-C5-C6-C7
20	H	310	DD6	C9-C10-C11-C12
20	H	310	DD6	C9-C10-C11-C13
20	H	310	DD6	C10-C11-C13-C14
20	H	310	DD6	C12-C11-C13-C14
20	H	310	DD6	C11-C13-C14-C15
20	H	310	DD6	C4-C5-C6-C7
20	H	310	DD6	C4-C5-C6-C8
20	H	310	DD6	C5-C6-C8-C9
20	H	310	DD6	C7-C6-C8-C9
20	H	311	DD6	C10-C11-C13-C14
20	H	311	DD6	C12-C11-C13-C14
20	H	311	DD6	C13-C14-C15-O1
20	H	311	DD6	C4-C5-C6-C7
20	H	311	DD6	C4-C5-C6-C8
20	K	208	DD6	C2-C3-C4-C5
20	K	208	DD6	C4-C5-C6-C7
20	K	208	DD6	C4-C5-C6-C8
20	K	208	DD6	C5-C6-C8-C9
20	K	208	DD6	C7-C6-C8-C9
21	A	855	LMU	C2'-C1'-O1'-C1
21	A	855	LMU	O5'-C1'-O1'-C1
21	A	855	LMU	C2-C1-O1'-C1'
25	J	103	LMG	C2-C1-O1-C7
25	J	103	LMG	O6-C1-O1-C7
25	U	201	LMG	C2-C1-O1-C7
25	U	201	LMG	O6-C1-O1-C7
25	U	201	LMG	C11-C10-O7-C8
26	U	202	A86	C10-C11-C13-O
26	U	202	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
26	U	202	A86	C1-C24-C25-C26
26	U	202	A86	C2-C3-C4-C5
26	U	202	A86	C4-C5-C6-C7
26	U	202	A86	C4-C5-C6-C8
26	U	202	A86	C5-C6-C8-C9
26	U	202	A86	C7-C6-C8-C9
26	U	202	A86	C6-C8-C9-C10
16	H	312	CLA	O1D-CGD-O2D-CED
26	U	202	A86	C39-C38-O4-C34
16	H	312	CLA	O1A-CGA-O2A-C1
21	A	855	LMU	O5B-C1B-O1B-C4'
16	H	312	CLA	CBA-CGA-O2A-C1
25	U	201	LMG	C4-C5-C6-O5
22	A	850	CL0	CBD-CGD-O2D-CED
25	J	103	LMG	O9-C10-O7-C8
25	U	201	LMG	O9-C10-O7-C8
16	B	849	CLA	C3-C5-C6-C7
16	B	835	CLA	C4-C3-C5-C6
16	B	835	CLA	C2-C3-C5-C6
16	G	307	CLA	C2-C3-C5-C6
16	A	825	CLA	C2A-CAA-CBA-CGA
16	B	814	CLA	C2A-CAA-CBA-CGA
16	G	305	CLA	C2A-CAA-CBA-CGA
16	A	836	CLA	C3-C5-C6-C7
24	B	843	DGD	O6E-C5E-C6E-O5E
25	U	201	LMG	O6-C5-C6-O5
19	B	846	BCR	C17-C18-C19-C20
19	B	846	BCR	C19-C20-C21-C22
20	U	212	DD6	C24-C25-C26-C27
20	G	313	DD6	C24-C25-C26-C27
21	A	855	LMU	O5'-C5'-C6'-O6'
18	G	316	LHG	O2-C2-C3-O3
16	B	817	CLA	C3-C5-C6-C7
16	B	820	CLA	C3-C5-C6-C7
18	A	840	LHG	C8-C7-O7-C5
21	F	806	LMU	O5'-C5'-C6'-O6'
21	K	201	LMU	O5'-C5'-C6'-O6'
20	H	311	DD6	C2-C3-C4-C5
24	B	843	DGD	C4E-C5E-C6E-O5E
16	K	203	CLA	C3-C5-C6-C7
21	A	848	LMU	O5B-C5B-C6B-O6B
25	J	103	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
16	H	303	CLA	C4-C3-C5-C6
16	H	303	CLA	C2-C3-C5-C6
18	A	839	LHG	C23-C24-C25-C26
16	A	845	CLA	C2A-CAA-CBA-CGA
16	H	312	CLA	C2A-CAA-CBA-CGA
26	U	202	A86	O5-C38-O4-C34
18	G	316	LHG	C1-C2-C3-O3
25	J	103	LMG	C29-C28-O8-C9
21	F	806	LMU	C4'-C5'-C6'-O6'
20	U	203	DD6	C1-C2-C3-C4
20	U	203	DD6	C24-C25-C26-C27
20	H	310	DD6	C24-C25-C26-C27
16	A	824	CLA	C10-C11-C12-C13
21	A	848	LMU	C4B-C5B-C6B-O6B
16	H	312	CLA	C6-C7-C8-C9
16	B	834	CLA	C2A-CAA-CBA-CGA
19	A	842	BCR	C7-C8-C9-C34
19	A	842	BCR	C37-C22-C23-C24
19	B	838	BCR	C7-C8-C9-C34
19	B	839	BCR	C7-C8-C9-C34
19	B	846	BCR	C7-C8-C9-C34
20	J	102	DD6	C12-C11-C13-C14
20	U	212	DD6	C12-C11-C13-C14
20	G	313	DD6	C-C1-C24-C25
20	H	310	DD6	C-C1-C24-C25
20	H	311	DD6	C7-C6-C8-C9
20	K	208	DD6	C-C1-C24-C25
19	B	839	BCR	C21-C22-C23-C24
19	B	846	BCR	C7-C8-C9-C10
19	I	103	BCR	C21-C22-C23-C24
20	J	102	DD6	C10-C11-C13-C14
20	G	313	DD6	C2-C1-C24-C25
20	H	310	DD6	C2-C1-C24-C25
16	A	822	CLA	C13-C15-C16-C17
16	B	832	CLA	C13-C15-C16-C17
16	B	817	CLA	C8-C10-C11-C12
16	B	848	CLA	C13-C15-C16-C17
21	A	855	LMU	C4'-C5'-C6'-O6'
16	H	312	CLA	C15-C16-C17-C18
18	A	839	LHG	C28-C29-C30-C31
16	H	302	CLA	C11-C10-C8-C7
20	A	846	DD6	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
20	U	214	DD6	C1-C2-C3-C4
20	U	214	DD6	C3-C4-C5-C6
16	B	847	CLA	C2A-CAA-CBA-CGA
16	H	302	CLA	C2A-CAA-CBA-CGA
22	A	850	CL0	O1D-CGD-O2D-CED
16	A	801	CLA	C8-C10-C11-C12
16	A	811	CLA	C10-C11-C12-C13
16	H	312	CLA	C8-C10-C11-C12
16	B	831	CLA	C5-C6-C7-C8
19	B	838	BCR	C10-C11-C12-C13
19	F	805	BCR	C10-C11-C12-C13
20	J	102	DD6	C1-C24-C25-C26
20	U	212	DD6	C1-C24-C25-C26
20	G	314	DD6	C1-C24-C25-C26
21	K	201	LMU	O1'-C1-C2-C3
16	A	854	CLA	C15-C16-C17-C18
16	A	824	CLA	C5-C6-C7-C8
18	G	316	LHG	C4-O6-P-O3
16	B	844	CLA	C10-C11-C12-C13
16	A	849	CLA	C4-C3-C5-C6
16	A	847	CLA	C8-C10-C11-C12
16	L	204	CLA	C2A-CAA-CBA-CGA
21	F	806	LMU	O1'-C1-C2-C3
21	K	201	LMU	C4'-C5'-C6'-O6'
20	A	846	DD6	C1-C2-C3-C4
24	B	843	DGD	C1B-C2B-C3B-C4B
19	A	842	BCR	C20-C21-C22-C37
19	B	839	BCR	C20-C21-C22-C37
19	B	842	BCR	C11-C10-C9-C34
19	B	842	BCR	C20-C21-C22-C37
19	B	846	BCR	C35-C13-C14-C15
19	F	805	BCR	C20-C21-C22-C37
19	I	101	BCR	C20-C21-C22-C37
19	k	203	BCR	C16-C17-C18-C36
20	U	212	DD6	C4-C5-C6-C7
20	G	317	DD6	C9-C10-C11-C12
20	H	311	DD6	C9-C10-C11-C12
20	K	208	DD6	C9-C10-C11-C12
26	U	202	A86	C-C1-C2-C3
22	A	850	CL0	C3-C5-C6-C7
21	A	848	LMU	C4-C5-C6-C7
25	J	103	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
21	F	806	LMU	C5-C6-C7-C8
21	A	848	LMU	C7-C8-C9-C10
24	B	843	DGD	CEB-CFB-CGB-CHB
19	A	841	BCR	C20-C21-C22-C23
19	A	844	BCR	C20-C21-C22-C23
19	I	101	BCR	C20-C21-C22-C23
19	I	103	BCR	C20-C21-C22-C23
19	L	201	BCR	C20-C21-C22-C23
20	U	212	DD6	C4-C5-C6-C8
20	G	312	DD6	C4-C5-C6-C8
20	G	317	DD6	C9-C10-C11-C13
20	G	317	DD6	C4-C5-C6-C8
20	H	311	DD6	C9-C10-C11-C13
20	K	208	DD6	C9-C10-C11-C13
21	K	201	LMU	C2'-C1'-O1'-C1
26	U	202	A86	C24-C1-C2-C3
18	A	839	LHG	C24-C25-C26-C27
21	A	855	LMU	C2-C3-C4-C5
16	B	834	CLA	C16-C17-C18-C20
16	A	823	CLA	C4-C3-C5-C6
24	B	843	DGD	C7B-C8B-C9B-CAB
25	J	103	LMG	C4-C5-C6-O5
16	A	853	CLA	C14-C13-C15-C16
16	B	805	CLA	C11-C10-C8-C9
16	B	832	CLA	C14-C13-C15-C16
25	U	201	LMG	C29-C30-C31-C32
16	A	814	CLA	C2A-CAA-CBA-CGA
16	B	820	CLA	C2A-CAA-CBA-CGA
25	J	103	LMG	O10-C28-O8-C9
20	U	203	DD6	C-C1-C24-C25
18	A	839	LHG	C27-C28-C29-C30
24	B	843	DGD	C3B-C4B-C5B-C6B
19	B	838	BCR	C7-C8-C9-C10
19	B	839	BCR	C7-C8-C9-C10
20	U	203	DD6	C2-C1-C24-C25
20	G	314	DD6	C10-C11-C13-C14
25	J	103	LMG	C11-C10-O7-C8
25	J	103	LMG	C13-C14-C15-C16
22	A	850	CL0	C4B-C3B-CAB-CBB
18	A	839	LHG	C10-C11-C12-C13
21	J	101	LMU	C6-C7-C8-C9
24	B	843	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
16	B	848	CLA	C15-C16-C17-C18
18	A	839	LHG	C9-C10-C11-C12
21	A	848	LMU	C1-C2-C3-C4
21	A	848	LMU	C11-C10-C9-C8
24	B	843	DGD	C4A-C5A-C6A-C7A
16	A	804	CLA	C3A-C2A-CAA-CBA
16	F	804	CLA	C3A-C2A-CAA-CBA
16	G	303	CLA	C3A-C2A-CAA-CBA
16	K	204	CLA	C3A-C2A-CAA-CBA
21	F	806	LMU	C2-C1-O1'-C1'
24	B	843	DGD	C5A-C6A-C7A-C8A
25	J	103	LMG	C15-C16-C17-C18
16	B	834	CLA	C16-C17-C18-C19
18	A	840	LHG	O9-C7-O7-C5
20	J	102	DD6	C2-C3-C4-C5
20	U	212	DD6	C2-C3-C4-C5
20	G	313	DD6	C2-C3-C4-C5
16	A	807	CLA	C3-C5-C6-C7
16	A	806	CLA	C4-C3-C5-C6
16	A	821	CLA	C4-C3-C5-C6
16	A	853	CLA	C4-C3-C5-C6
16	A	823	CLA	C2-C3-C5-C6
22	A	850	CL0	C2B-C3B-CAB-CBB
21	J	101	LMU	C7-C8-C9-C10
16	K	205	CLA	C2-C1-O2A-CGA
16	B	828	CLA	C3-C5-C6-C7
19	A	841	BCR	C23-C24-C25-C26
19	A	842	BCR	C5-C6-C7-C8
19	A	843	BCR	C1-C6-C7-C8
19	A	843	BCR	C5-C6-C7-C8
19	A	844	BCR	C5-C6-C7-C8
19	A	844	BCR	C23-C24-C25-C26
19	A	844	BCR	C23-C24-C25-C30
19	B	838	BCR	C5-C6-C7-C8
19	B	839	BCR	C1-C6-C7-C8
19	B	839	BCR	C5-C6-C7-C8
19	B	841	BCR	C1-C6-C7-C8
19	B	841	BCR	C5-C6-C7-C8
19	B	841	BCR	C23-C24-C25-C26
19	B	841	BCR	C23-C24-C25-C30
19	B	842	BCR	C1-C6-C7-C8
19	B	842	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	B	846	BCR	C5-C6-C7-C8
19	B	846	BCR	C23-C24-C25-C26
19	F	801	BCR	C1-C6-C7-C8
19	F	805	BCR	C5-C6-C7-C8
19	I	103	BCR	C5-C6-C7-C8
19	I	103	BCR	C23-C24-C25-C30
19	L	201	BCR	C1-C6-C7-C8
19	L	201	BCR	C5-C6-C7-C8
19	L	201	BCR	C23-C24-C25-C26
19	L	205	BCR	C23-C24-C25-C26
19	M	101	BCR	C5-C6-C7-C8
19	k	203	BCR	C5-C6-C7-C8
18	A	839	LHG	C32-C33-C34-C35
21	F	806	LMU	C4-C5-C6-C7
16	A	804	CLA	C11-C12-C13-C15
16	A	821	CLA	C2-C3-C5-C6
16	A	853	CLA	C2-C3-C5-C6
16	B	805	CLA	C11-C10-C8-C7
16	B	844	CLA	C11-C10-C8-C7
16	G	305	CLA	C6-C7-C8-C10
24	B	843	DGD	CDB-CEB-CFB-CGB
20	H	310	DD6	C1-C2-C3-C4
16	G	306	CLA	C16-C17-C18-C20
18	G	316	LHG	C23-C24-C25-C26
19	B	846	BCR	C15-C16-C17-C18
21	K	201	LMU	O5'-C1'-O1'-C1
24	B	843	DGD	O6E-C1E-O5D-C6D
20	G	313	DD6	C1-C24-C25-C26
25	J	103	LMG	C19-C20-C21-C22
16	B	808	CLA	C3-C5-C6-C7
25	J	103	LMG	O7-C8-C9-O8
16	B	835	CLA	C15-C16-C17-C18
16	U	205	CLA	C4-C3-C5-C6
16	U	205	CLA	C2-C3-C5-C6
20	G	313	DD6	C27-C29-C30-C31
20	G	317	DD6	C27-C29-C30-C31
16	A	804	CLA	C11-C12-C13-C14
16	B	844	CLA	C11-C10-C8-C9
16	H	302	CLA	C11-C10-C8-C9
16	H	307	CLA	C11-C10-C8-C9
16	G	309	CLA	C3-C5-C6-C7
16	A	807	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	J	101	LMU	O5B-C5B-C6B-O6B
18	A	839	LHG	C30-C31-C32-C33
16	A	813	CLA	C1A-C2A-CAA-CBA
16	A	815	CLA	C1A-C2A-CAA-CBA
16	B	812	CLA	C1A-C2A-CAA-CBA
16	U	204	CLA	C1A-C2A-CAA-CBA
16	G	303	CLA	C1A-C2A-CAA-CBA
16	K	204	CLA	C1A-C2A-CAA-CBA
16	H	306	CLA	C13-C15-C16-C17
21	K	201	LMU	O5B-C1B-O1B-C4'
21	K	201	LMU	C2B-C1B-O1B-C4'
17	B	837	PQN	C23-C25-C26-C27
16	A	806	CLA	C2A-CAA-CBA-CGA
24	B	843	DGD	O1G-C1G-C2G-C3G
18	G	316	LHG	C7-C8-C9-C10
19	B	838	BCR	C20-C21-C22-C37
16	U	205	CLA	C8-C10-C11-C12
25	J	103	LMG	C7-C8-O7-C10
25	J	103	LMG	C18-C19-C20-C21
25	U	201	LMG	C31-C32-C33-C34
19	A	842	BCR	C20-C21-C22-C23
19	B	846	BCR	C12-C13-C14-C15
24	B	843	DGD	C2E-C1E-O5D-C6D
25	U	201	LMG	O1-C7-C8-O7
16	B	823	CLA	C6-C7-C8-C10
16	B	835	CLA	C11-C12-C13-C15
16	I	102	CLA	C11-C12-C13-C15
16	G	305	CLA	C11-C10-C8-C7
16	G	305	CLA	C11-C12-C13-C15
16	B	823	CLA	C6-C7-C8-C9
16	U	204	CLA	C11-C10-C8-C9
16	G	305	CLA	C6-C7-C8-C9
16	G	305	CLA	C11-C10-C8-C9
16	G	305	CLA	C11-C12-C13-C14
19	I	101	BCR	C14-C15-C16-C17
16	B	801	CLA	C2A-CAA-CBA-CGA
19	L	205	BCR	C7-C8-C9-C34
20	U	203	DD6	C12-C11-C13-C14
18	G	316	LHG	O1-C1-C2-C3
19	L	205	BCR	C7-C8-C9-C10
20	U	203	DD6	C10-C11-C13-C14
20	K	208	DD6	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
21	K	201	LMU	C2-C3-C4-C5
25	U	201	LMG	C12-C13-C14-C15
21	J	101	LMU	O1'-C1-C2-C3
20	G	314	DD6	C11-C13-C14-C15
20	G	317	DD6	C11-C13-C14-C15
16	B	813	CLA	C5-C6-C7-C8
16	A	834	CLA	C4-C3-C5-C6
16	A	854	CLA	C4-C3-C5-C6
25	U	201	LMG	C30-C31-C32-C33
18	G	316	LHG	C8-C7-O7-C5
16	L	202	CLA	C3A-C2A-CAA-CBA
16	U	204	CLA	C3A-C2A-CAA-CBA
21	F	806	LMU	C3-C4-C5-C6
25	J	103	LMG	C11-C12-C13-C14
21	K	201	LMU	C2-C1-O1'-C1'
16	B	844	CLA	C8-C10-C11-C12
18	G	316	LHG	C4-C5-C6-O8
25	U	201	LMG	O1-C7-C8-C9
16	B	811	CLA	O2A-C1-C2-C3
16	I	102	CLA	O2A-C1-C2-C3
16	B	814	CLA	C3-C5-C6-C7
16	B	835	CLA	C10-C11-C12-C13
16	A	849	CLA	C2-C3-C5-C6
25	J	103	LMG	C14-C15-C16-C17
16	A	834	CLA	C3-C5-C6-C7
16	B	811	CLA	C5-C6-C7-C8
18	G	316	LHG	O6-C4-C5-O7
24	B	843	DGD	C9A-CAA-CBA-CCA
25	J	103	LMG	C17-C18-C19-C20
18	G	316	LHG	O7-C5-C6-O8
26	U	202	A86	C10-C11-C13-C14
18	G	316	LHG	O9-C7-O7-C5
16	A	818	CLA	C4-C3-C5-C6
16	B	811	CLA	C4-C3-C5-C6
16	A	836	CLA	C2-C1-O2A-CGA
16	B	802	CLA	C2-C1-O2A-CGA
16	B	821	CLA	C2-C1-O2A-CGA
16	K	203	CLA	C2-C1-O2A-CGA
16	A	834	CLA	C2-C3-C5-C6
16	U	204	CLA	C6-C7-C8-C9
16	H	312	CLA	C11-C10-C8-C9
18	A	839	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
21	A	848	LMU	C2-C3-C4-C5
16	A	820	CLA	C4-C3-C5-C6
24	B	843	DGD	C3A-C4A-C5A-C6A
16	G	306	CLA	C16-C17-C18-C19
19	A	841	BCR	C1-C6-C7-C8
19	A	841	BCR	C5-C6-C7-C8
19	A	842	BCR	C23-C24-C25-C26
19	A	842	BCR	C23-C24-C25-C30
19	B	838	BCR	C23-C24-C25-C26
19	B	838	BCR	C23-C24-C25-C30
19	B	840	BCR	C5-C6-C7-C8
19	B	840	BCR	C23-C24-C25-C26
19	B	842	BCR	C23-C24-C25-C26
19	B	842	BCR	C23-C24-C25-C30
19	F	801	BCR	C5-C6-C7-C8
19	F	805	BCR	C23-C24-C25-C26
19	I	101	BCR	C5-C6-C7-C8
19	J	105	BCR	C23-C24-C25-C26
19	L	205	BCR	C5-C6-C7-C8
19	M	101	BCR	C23-C24-C25-C26
19	k	203	BCR	C23-C24-C25-C26
19	k	203	BCR	C23-C24-C25-C30
21	A	848	LMU	C9-C10-C11-C12
19	B	841	BCR	C17-C18-C19-C20
19	B	842	BCR	C21-C22-C23-C24
19	F	801	BCR	C21-C22-C23-C24
16	U	204	CLA	C10-C11-C12-C13
16	G	305	CLA	C8-C10-C11-C12
16	G	305	CLA	C14-C13-C15-C16
18	G	316	LHG	O6-C4-C5-C6
16	A	824	CLA	C12-C13-C15-C16
16	A	825	CLA	C12-C13-C15-C16
16	A	854	CLA	C2-C3-C5-C6
16	B	811	CLA	C2-C3-C5-C6
16	B	823	CLA	C2-C3-C5-C6
16	U	204	CLA	C6-C7-C8-C10
16	G	306	CLA	C11-C12-C13-C15
17	A	837	PQN	C17-C18-C20-C21
19	L	205	BCR	C9-C10-C11-C12
20	G	311	DD6	C24-C25-C26-C27
20	K	208	DD6	C24-C25-C26-C27
16	B	806	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	A	850	CL0	C8-C10-C11-C12
19	B	841	BCR	C20-C21-C22-C37
19	J	105	BCR	C20-C21-C22-C37
20	G	312	DD6	C9-C10-C11-C12
16	G	305	CLA	C12-C13-C15-C16
21	A	848	LMU	C3-C4-C5-C6
16	A	802	CLA	CAD-CBD-CGD-O2D
16	A	804	CLA	CAD-CBD-CGD-O2D
16	A	817	CLA	CAD-CBD-CGD-O2D
16	A	822	CLA	CAD-CBD-CGD-O2D
16	A	828	CLA	CAD-CBD-CGD-O2D
16	A	832	CLA	CAD-CBD-CGD-O2D
16	A	835	CLA	CAD-CBD-CGD-O2D
16	A	847	CLA	CAD-CBD-CGD-O2D
16	B	812	CLA	CAD-CBD-CGD-O2D
16	B	833	CLA	CAD-CBD-CGD-O2D
16	B	848	CLA	CAD-CBD-CGD-O2D
16	I	102	CLA	CAD-CBD-CGD-O2D
16	U	211	CLA	CAD-CBD-CGD-O2D
16	H	302	CLA	CAD-CBD-CGD-O2D
25	U	201	LMG	C29-C28-O8-C9
16	B	823	CLA	C4-C3-C5-C6
16	H	307	CLA	C4-C3-C5-C6
21	J	101	LMU	O5'-C1'-O1'-C1
21	K	201	LMU	C3-C4-C5-C6
24	B	843	DGD	C8B-C9B-CAB-CBB
16	A	803	CLA	CHA-CBD-CGD-O1D
16	A	803	CLA	CHA-CBD-CGD-O2D
16	A	806	CLA	CHA-CBD-CGD-O1D
16	A	806	CLA	CHA-CBD-CGD-O2D
16	A	851	CLA	CHA-CBD-CGD-O2D
16	A	853	CLA	CHA-CBD-CGD-O1D
16	A	853	CLA	CHA-CBD-CGD-O2D
16	B	808	CLA	CHA-CBD-CGD-O1D
16	B	808	CLA	CHA-CBD-CGD-O2D
16	B	820	CLA	CHA-CBD-CGD-O1D
16	B	820	CLA	CHA-CBD-CGD-O2D
16	B	821	CLA	CHA-CBD-CGD-O1D
16	B	825	CLA	CHA-CBD-CGD-O1D
16	U	207	CLA	CHA-CBD-CGD-O1D
16	G	307	CLA	CHA-CBD-CGD-O1D
16	G	307	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	H	302	CLA	CHA-CBD-CGD-O1D
16	H	307	CLA	CHA-CBD-CGD-O1D
16	H	307	CLA	CHA-CBD-CGD-O2D
19	B	839	BCR	C20-C21-C22-C23
24	B	843	DGD	C2B-C3B-C4B-C5B
24	B	843	DGD	O1G-C1G-C2G-O2G
26	U	202	A86	C13-C14-C15-O1
16	A	825	CLA	C4-C3-C5-C6
16	G	309	CLA	C4-C3-C5-C6
16	A	825	CLA	C2-C3-C5-C6
20	J	102	DD6	C27-C29-C30-C31
20	U	212	DD6	C27-C29-C30-C31
20	H	310	DD6	C27-C29-C30-C31
20	K	208	DD6	C27-C29-C30-C31
16	A	825	CLA	C14-C13-C15-C16
16	G	306	CLA	C11-C12-C13-C14
19	M	101	BCR	C37-C22-C23-C24
24	B	843	DGD	C6A-C7A-C8A-C9A
20	U	212	DD6	C10-C11-C13-C14
16	B	823	CLA	C1A-C2A-CAA-CBA
18	G	316	LHG	C24-C23-O8-C6
18	G	316	LHG	C5-C4-O6-P
18	A	839	LHG	C29-C30-C31-C32
18	G	316	LHG	C4-O6-P-O5
16	H	312	CLA	C16-C17-C18-C19
16	A	815	CLA	CAA-CBA-CGA-O2A
21	J	101	LMU	C5-C6-C7-C8
16	G	308	CLA	C6-C7-C8-C10
16	A	803	CLA	CAD-CBD-CGD-O1D
16	U	207	CLA	CAD-CBD-CGD-O1D
21	K	201	LMU	C4B-C5B-C6B-O6B
24	B	843	DGD	C2A-C1A-O1G-C1G
16	G	306	CLA	C6-C7-C8-C10
18	G	316	LHG	O10-C23-O8-C6
24	B	843	DGD	O1A-C1A-O1G-C1G
25	J	103	LMG	C7-C8-C9-O8
16	A	824	CLA	C14-C13-C15-C16
16	A	851	CLA	C11-C10-C8-C9
16	I	102	CLA	C11-C10-C8-C9
16	G	306	CLA	C6-C7-C8-C9
19	B	846	BCR	C22-C23-C24-C25
19	M	101	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
16	A	821	CLA	C8-C10-C11-C12
21	J	101	LMU	C2-C3-C4-C5
16	B	828	CLA	C5-C6-C7-C8
16	A	805	CLA	C1-C2-C3-C4
16	B	827	CLA	C1-C2-C3-C4
16	H	312	CLA	C3-C5-C6-C7
19	F	801	BCR	C14-C15-C16-C17
18	A	839	LHG	C24-C23-O8-C6
19	B	840	BCR	C23-C24-C25-C30
19	F	801	BCR	C23-C24-C25-C26
19	F	805	BCR	C23-C24-C25-C30
19	J	105	BCR	C5-C6-C7-C8
19	J	105	BCR	C23-C24-C25-C30
19	L	205	BCR	C1-C6-C7-C8
19	B	846	BCR	C11-C10-C9-C8
21	J	101	LMU	C2'-C1'-O1'-C1
18	A	839	LHG	C3-O3-P-O6
18	A	840	LHG	C3-O3-P-O6
18	A	840	LHG	C10-C11-C12-C13
21	A	855	LMU	C3-C4-C5-C6
16	A	818	CLA	C2-C3-C5-C6
16	A	834	CLA	C6-C7-C8-C10
16	G	309	CLA	C2-C3-C5-C6
16	H	307	CLA	C11-C10-C8-C7
16	H	312	CLA	C11-C10-C8-C7
16	A	804	CLA	C3-C5-C6-C7
16	B	835	CLA	C11-C12-C13-C14
17	A	837	PQN	C19-C18-C20-C21
20	H	310	DD6	C3-C4-C5-C6
20	H	311	DD6	C3-C4-C5-C6
16	G	307	CLA	C11-C12-C13-C15
18	G	316	LHG	C2-C3-O3-P
16	L	202	CLA	O2A-C1-C2-C3
16	A	806	CLA	C2-C3-C5-C6
16	A	828	CLA	C16-C17-C18-C20
16	H	312	CLA	C16-C17-C18-C20
24	B	843	DGD	O6D-C1D-O3G-C3G
16	A	807	CLA	C5-C6-C7-C8
16	G	307	CLA	C8-C10-C11-C12
16	U	204	CLA	C3-C5-C6-C7
16	B	814	CLA	C4-C3-C5-C6
16	A	827	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	B	843	DGD	C2D-C1D-O3G-C3G
16	A	815	CLA	C2A-CAA-CBA-CGA
16	G	309	CLA	C2A-CAA-CBA-CGA
16	K	207	CLA	C2A-CAA-CBA-CGA
16	B	848	CLA	C2C-C3C-CAC-CBC
16	A	853	CLA	C3A-C2A-CAA-CBA
16	B	805	CLA	C3A-C2A-CAA-CBA
16	B	814	CLA	C3A-C2A-CAA-CBA
16	B	849	CLA	C3A-C2A-CAA-CBA
16	G	310	CLA	C3A-C2A-CAA-CBA
16	K	207	CLA	C3A-C2A-CAA-CBA
20	G	314	DD6	C27-C29-C30-C31
16	A	849	CLA	C11-C10-C8-C9
16	B	817	CLA	C14-C13-C15-C16
16	H	307	CLA	C6-C7-C8-C9
16	B	805	CLA	C15-C16-C17-C18
19	B	840	BCR	C20-C21-C22-C37
19	F	801	BCR	C20-C21-C22-C37
19	F	805	BCR	C35-C13-C14-C15
19	L	201	BCR	C11-C10-C9-C34
20	G	314	DD6	C-C1-C2-C3
16	A	806	CLA	O2A-C1-C2-C3
20	G	312	DD6	C12-C11-C13-C14
16	G	315	CLA	CAA-CBA-CGA-O2A
16	A	851	CLA	C4-C3-C5-C6
16	A	853	CLA	C1A-C2A-CAA-CBA
16	B	805	CLA	C1A-C2A-CAA-CBA
16	H	309	CLA	CAA-CBA-CGA-O2A
16	G	303	CLA	CAA-CBA-CGA-O1A
16	B	803	CLA	C2A-CAA-CBA-CGA
18	A	839	LHG	C7-C8-C9-C10
18	A	839	LHG	O6-C4-C5-O7
18	A	840	LHG	O6-C4-C5-O7
16	H	309	CLA	CAA-CBA-CGA-O1A
16	A	834	CLA	C13-C15-C16-C17
16	G	301	CLA	CAA-CBA-CGA-O2A
24	B	843	DGD	CBB-CCB-CDB-CEB
16	A	804	CLA	C4-C3-C5-C6
16	B	808	CLA	C4-C3-C5-C6
16	B	814	CLA	C2-C3-C5-C6
16	G	315	CLA	CAA-CBA-CGA-O1A
19	B	840	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
19	F	805	BCR	C12-C13-C14-C15
19	L	201	BCR	C11-C10-C9-C8
20	G	314	DD6	C24-C1-C2-C3
24	B	843	DGD	O2G-C2G-C3G-O3G
16	B	829	CLA	C10-C11-C12-C13
26	U	202	A86	C1-C2-C3-C4
16	H	305	CLA	CAA-CBA-CGA-O2A
17	A	837	PQN	C18-C20-C21-C22
16	B	847	CLA	C4-C3-C5-C6
16	A	845	CLA	C2-C1-O2A-CGA
16	A	849	CLA	C2-C1-O2A-CGA
16	H	302	CLA	C2-C1-O2A-CGA
16	A	851	CLA	C2-C3-C5-C6
16	A	834	CLA	C14-C13-C15-C16
16	G	301	CLA	CAA-CBA-CGA-O1A
16	B	815	CLA	C10-C11-C12-C13
18	A	839	LHG	C16-C17-C18-C19
16	G	303	CLA	CAA-CBA-CGA-O2A
21	J	101	LMU	C4-C5-C6-C7
19	B	839	BCR	C23-C24-C25-C30
19	B	840	BCR	C1-C6-C7-C8
19	F	801	BCR	C23-C24-C25-C30
19	I	101	BCR	C1-C6-C7-C8
19	I	101	BCR	C23-C24-C25-C30
19	J	105	BCR	C1-C6-C7-C8
16	A	845	CLA	C10-C11-C12-C13
16	B	815	CLA	CAA-CBA-CGA-O2A
16	L	204	CLA	CAA-CBA-CGA-O2A
16	B	809	CLA	C4-C3-C5-C6
16	U	211	CLA	C4-C3-C5-C6
16	A	831	CLA	CAA-CBA-CGA-O2A
16	A	831	CLA	CAA-CBA-CGA-O1A
16	H	305	CLA	CAA-CBA-CGA-O1A
21	K	201	LMU	C5-C6-C7-C8
16	K	204	CLA	CAA-CBA-CGA-O2A
16	A	849	CLA	C10-C11-C12-C13
16	B	806	CLA	C4-C3-C5-C6
16	B	832	CLA	C12-C13-C15-C16
16	U	211	CLA	C2-C3-C5-C6
16	U	206	CLA	CAA-CBA-CGA-O2A
18	G	316	LHG	O1-C1-C2-O2
20	G	314	DD6	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
16	A	828	CLA	C16-C17-C18-C19
16	K	204	CLA	CAA-CBA-CGA-O1A
19	L	201	BCR	C16-C17-C18-C36
20	U	203	DD6	C4-C5-C6-C7
16	B	801	CLA	C4-C3-C5-C6
16	B	807	CLA	C4-C3-C5-C6
16	K	205	CLA	C4-C3-C5-C6
16	A	849	CLA	C8-C10-C11-C12
16	B	808	CLA	C2-C3-C5-C6
16	B	820	CLA	C14-C13-C15-C16
16	A	814	CLA	CAA-CBA-CGA-O2A
16	H	309	CLA	C3A-C2A-CAA-CBA
16	B	836	CLA	CAA-CBA-CGA-O2A
16	A	805	CLA	CAD-CBD-CGD-O2D
16	A	810	CLA	CAD-CBD-CGD-O2D
16	A	812	CLA	CAD-CBD-CGD-O2D
16	A	813	CLA	CAD-CBD-CGD-O2D
16	A	819	CLA	CAD-CBD-CGD-O2D
16	A	823	CLA	CAD-CBD-CGD-O2D
16	A	833	CLA	CAD-CBD-CGD-O2D
16	B	818	CLA	CAD-CBD-CGD-O2D
16	B	822	CLA	CAD-CBD-CGD-O2D
16	B	831	CLA	CAD-CBD-CGD-O2D
16	B	834	CLA	CAD-CBD-CGD-O2D
16	G	301	CLA	CAD-CBD-CGD-O2D
16	G	303	CLA	CAD-CBD-CGD-O2D
16	K	206	CLA	CAD-CBD-CGD-O2D
16	k	201	CLA	CAD-CBD-CGD-O2D
18	A	839	LHG	O9-C7-O7-C5
16	U	208	CLA	CAA-CBA-CGA-O2A
16	B	804	CLA	CAA-CBA-CGA-O2A
16	A	804	CLA	C2-C3-C5-C6
16	B	809	CLA	C2-C3-C5-C6
16	U	211	CLA	CAA-CBA-CGA-O2A
18	A	839	LHG	O8-C23-C24-C25
20	U	212	DD6	C2-C1-C24-C25
20	H	311	DD6	C5-C6-C8-C9
25	J	103	LMG	O1-C7-C8-C9
16	A	811	CLA	CAA-CBA-CGA-O2A
16	k	202	CLA	CAA-CBA-CGA-O2A
16	A	814	CLA	CAA-CBA-CGA-O1A
16	A	818	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
16	A	821	CLA	O2A-C1-C2-C3
16	A	824	CLA	O2A-C1-C2-C3
16	A	827	CLA	O2A-C1-C2-C3
16	B	814	CLA	O2A-C1-C2-C3
16	B	819	CLA	O2A-C1-C2-C3
16	B	834	CLA	O2A-C1-C2-C3
16	B	835	CLA	O2A-C1-C2-C3
16	L	204	CLA	O2A-C1-C2-C3
16	K	203	CLA	O2A-C1-C2-C3
22	A	850	CL0	O2A-C1-C2-C3
16	G	305	CLA	CBA-CGA-O2A-C1
16	B	804	CLA	CAA-CBA-CGA-O1A
16	U	206	CLA	CAA-CBA-CGA-O1A
16	A	816	CLA	CHA-CBD-CGD-O1D
16	A	816	CLA	CHA-CBD-CGD-O2D
16	A	821	CLA	CHA-CBD-CGD-O1D
16	A	827	CLA	CHA-CBD-CGD-O2D
16	A	829	CLA	CHA-CBD-CGD-O2D
16	A	851	CLA	CHA-CBD-CGD-O1D
16	B	802	CLA	CHA-CBD-CGD-O1D
16	B	802	CLA	CHA-CBD-CGD-O2D
16	B	804	CLA	CHA-CBD-CGD-O1D
16	B	804	CLA	CHA-CBD-CGD-O2D
16	B	807	CLA	CHA-CBD-CGD-O1D
16	B	807	CLA	CHA-CBD-CGD-O2D
16	B	822	CLA	CHA-CBD-CGD-O2D
16	B	826	CLA	CHA-CBD-CGD-O2D
16	B	828	CLA	CHA-CBD-CGD-O1D
16	B	828	CLA	CHA-CBD-CGD-O2D
16	U	210	CLA	CHA-CBD-CGD-O1D
16	U	210	CLA	CHA-CBD-CGD-O2D
16	G	304	CLA	CHA-CBD-CGD-O2D
22	A	850	CL0	CHA-CBD-CGD-O2D
16	B	847	CLA	C2-C3-C5-C6
16	B	809	CLA	CAA-CBA-CGA-O2A
16	G	306	CLA	CAA-CBA-CGA-O2A
16	A	817	CLA	CAA-CBA-CGA-O2A
16	A	821	CLA	CAA-CBA-CGA-O2A
16	B	803	CLA	CAA-CBA-CGA-O2A
16	B	806	CLA	CAA-CBA-CGA-O2A
16	B	845	CLA	CAA-CBA-CGA-O2A
16	G	309	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	H	312	CLA	CAA-CBA-CGA-O2A
16	A	849	CLA	C13-C15-C16-C17
20	A	846	DD6	C27-C29-C30-C31
16	F	804	CLA	CAA-CBA-CGA-O2A
16	A	854	CLA	C6-C7-C8-C9
20	U	212	DD6	C3-C4-C5-C6
16	A	805	CLA	C2B-C3B-CAB-CBB
16	A	807	CLA	C2B-C3B-CAB-CBB
16	A	810	CLA	C2B-C3B-CAB-CBB
16	A	812	CLA	C2B-C3B-CAB-CBB
16	A	825	CLA	C2B-C3B-CAB-CBB
16	A	832	CLA	C2B-C3B-CAB-CBB
16	A	834	CLA	C2B-C3B-CAB-CBB
16	A	838	CLA	C2B-C3B-CAB-CBB
16	A	845	CLA	C2B-C3B-CAB-CBB
16	A	847	CLA	C2B-C3B-CAB-CBB
16	A	851	CLA	C2B-C3B-CAB-CBB
16	A	853	CLA	C2B-C3B-CAB-CBB
16	A	854	CLA	C2B-C3B-CAB-CBB
16	B	805	CLA	C2B-C3B-CAB-CBB
16	B	811	CLA	C2B-C3B-CAB-CBB
16	B	819	CLA	C2B-C3B-CAB-CBB
16	B	824	CLA	C2B-C3B-CAB-CBB
16	B	825	CLA	C2B-C3B-CAB-CBB
16	B	827	CLA	C2B-C3B-CAB-CBB
16	B	833	CLA	C2B-C3B-CAB-CBB
16	B	836	CLA	C2B-C3B-CAB-CBB
16	B	845	CLA	C2B-C3B-CAB-CBB
16	B	847	CLA	C2B-C3B-CAB-CBB
16	F	803	CLA	C2B-C3B-CAB-CBB
16	J	104	CLA	C2B-C3B-CAB-CBB
16	L	202	CLA	C2B-C3B-CAB-CBB
16	L	204	CLA	C2B-C3B-CAB-CBB
16	U	204	CLA	C2B-C3B-CAB-CBB
16	U	210	CLA	C2B-C3B-CAB-CBB
16	G	302	CLA	C2B-C3B-CAB-CBB
16	G	310	CLA	C2B-C3B-CAB-CBB
16	G	315	CLA	C2B-C3B-CAB-CBB
16	H	301	CLA	C2B-C3B-CAB-CBB
16	H	306	CLA	C2B-C3B-CAB-CBB
16	K	204	CLA	C2B-C3B-CAB-CBB
16	K	207	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	k	202	CLA	C2B-C3B-CAB-CBB
16	A	810	CLA	CAA-CBA-CGA-O2A
16	k	202	CLA	CAA-CBA-CGA-O1A
16	U	204	CLA	CAA-CBA-CGA-O2A
16	B	828	CLA	C4-C3-C5-C6
16	B	807	CLA	C2-C3-C5-C6
16	B	811	CLA	C1A-C2A-CAA-CBA
16	B	844	CLA	C1A-C2A-CAA-CBA
16	F	802	CLA	C1A-C2A-CAA-CBA
16	H	304	CLA	C1A-C2A-CAA-CBA
16	U	208	CLA	CAA-CBA-CGA-O1A
16	B	834	CLA	C15-C16-C17-C18
16	B	809	CLA	CAA-CBA-CGA-O1A
16	B	836	CLA	CAA-CBA-CGA-O1A
16	U	211	CLA	CAA-CBA-CGA-O1A
25	J	103	LMG	O9-C10-C11-C12
16	G	310	CLA	CAA-CBA-CGA-O2A
16	A	836	CLA	C2A-CAA-CBA-CGA
16	A	847	CLA	C2A-CAA-CBA-CGA
16	G	307	CLA	C11-C12-C13-C14
16	A	802	CLA	CAA-CBA-CGA-O2A
16	B	803	CLA	CAA-CBA-CGA-O1A
16	B	835	CLA	C4B-C3B-CAB-CBB
18	A	839	LHG	C3-O3-P-O5
16	A	811	CLA	CAA-CBA-CGA-O1A
16	G	309	CLA	CAA-CBA-CGA-O1A
16	B	827	CLA	O2A-C1-C2-C3
19	I	101	BCR	C23-C24-C25-C26
16	B	811	CLA	CAA-CBA-CGA-O2A
16	B	847	CLA	CAA-CBA-CGA-O2A
16	G	308	CLA	C5-C6-C7-C8
16	A	803	CLA	C2A-CAA-CBA-CGA
16	A	804	CLA	C5-C6-C7-C8
16	A	821	CLA	CAA-CBA-CGA-O1A
16	B	817	CLA	C4-C3-C5-C6
16	H	307	CLA	C2-C3-C5-C6
16	B	817	CLA	C16-C17-C18-C19
16	A	845	CLA	CAD-CBD-CGD-O1D
16	B	805	CLA	CAD-CBD-CGD-O1D
16	B	831	CLA	CAD-CBD-CGD-O1D
16	L	203	CLA	CAD-CBD-CGD-O1D
22	A	850	CL0	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
16	B	845	CLA	CAA-CBA-CGA-O1A
16	H	312	CLA	CAA-CBA-CGA-O1A
16	A	804	CLA	CAA-CBA-CGA-O2A
25	J	103	LMG	O7-C10-C11-C12
16	A	817	CLA	CAA-CBA-CGA-O1A
16	U	204	CLA	CAA-CBA-CGA-O1A
16	B	814	CLA	CAA-CBA-CGA-O2A
16	B	828	CLA	CAA-CBA-CGA-O2A
21	A	848	LMU	C5-C6-C7-C8
16	B	807	CLA	C2A-CAA-CBA-CGA
16	A	803	CLA	CAA-CBA-CGA-O2A
16	A	847	CLA	CAA-CBA-CGA-O2A
16	A	836	CLA	C5-C6-C7-C8
16	A	853	CLA	C13-C15-C16-C17
18	G	316	LHG	C25-C26-C27-C28
16	A	810	CLA	CAA-CBA-CGA-O1A
16	F	804	CLA	CAA-CBA-CGA-O1A
19	B	846	BCR	C18-C19-C20-C21
16	B	836	CLA	C4-C3-C5-C6
20	U	212	DD6	C-C1-C24-C25
18	A	839	LHG	C34-C35-C36-C37
16	A	853	CLA	C11-C12-C13-C15
16	A	853	CLA	C12-C13-C15-C16
16	B	819	CLA	C3A-C2A-CAA-CBA
16	U	207	CLA	C3A-C2A-CAA-CBA
16	K	205	CLA	C2-C3-C5-C6
16	B	806	CLA	CAA-CBA-CGA-O1A
16	G	306	CLA	CAA-CBA-CGA-O1A
19	F	805	BCR	C7-C8-C9-C10
19	F	805	BCR	C11-C12-C13-C14
19	I	101	BCR	C21-C22-C23-C24
20	G	312	DD6	C10-C11-C13-C14
16	A	802	CLA	CAA-CBA-CGA-O1A
16	G	310	CLA	CAA-CBA-CGA-O1A
16	A	847	CLA	CAA-CBA-CGA-O1A
16	B	828	CLA	CAA-CBA-CGA-O1A
16	A	854	CLA	C5-C6-C7-C8
16	H	312	CLA	C5-C6-C7-C8
16	B	814	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

138 monomers are involved in 235 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	851	CLA	5	0
16	A	801	CLA	2	0
16	B	816	CLA	1	0
16	A	812	CLA	2	0
16	G	306	CLA	2	0
16	A	854	CLA	5	0
16	I	102	CLA	2	0
16	L	203	CLA	1	0
16	H	308	CLA	3	0
16	B	808	CLA	2	0
16	A	803	CLA	2	0
16	B	845	CLA	1	0
16	K	202	CLA	1	0
16	H	309	CLA	2	0
16	A	806	CLA	1	0
16	H	304	CLA	1	0
16	B	817	CLA	2	0
16	B	803	CLA	2	0
16	H	305	CLA	3	0
16	A	830	CLA	1	0
19	L	201	BCR	1	0
21	A	848	LMU	1	0
19	B	842	BCR	3	0
16	H	306	CLA	7	0
16	B	809	CLA	1	0
16	B	824	CLA	2	0
16	A	853	CLA	2	0
16	A	817	CLA	2	0
16	A	810	CLA	1	0
16	G	302	CLA	1	0
16	K	205	CLA	3	0
21	A	855	LMU	1	0
19	B	840	BCR	1	0
16	B	830	CLA	1	0
16	A	818	CLA	1	0
19	A	842	BCR	1	0
16	B	822	CLA	2	0
16	B	814	CLA	1	0
16	K	206	CLA	2	0
19	L	205	BCR	2	0
16	A	816	CLA	4	0
16	A	811	CLA	2	0
25	J	103	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	845	CLA	3	0
16	G	304	CLA	1	0
19	J	105	BCR	2	0
16	A	831	CLA	3	0
16	B	805	CLA	2	0
16	A	824	CLA	4	0
16	B	835	CLA	4	0
16	B	807	CLA	5	0
17	A	837	PQN	3	0
16	U	206	CLA	1	0
16	A	828	CLA	4	0
20	G	311	DD6	1	0
19	A	843	BCR	2	0
16	H	303	CLA	1	0
16	G	301	CLA	1	0
18	A	839	LHG	2	0
16	A	835	CLA	3	0
16	B	832	CLA	1	0
16	A	814	CLA	2	0
16	A	819	CLA	1	0
16	B	844	CLA	2	0
19	B	846	BCR	3	0
16	G	309	CLA	4	0
19	B	841	BCR	3	0
19	I	101	BCR	2	0
16	B	819	CLA	3	0
19	B	838	BCR	2	0
16	A	820	CLA	2	0
24	B	843	DGD	2	0
16	L	202	CLA	2	0
16	B	823	CLA	1	0
16	U	210	CLA	1	0
16	K	203	CLA	2	0
16	B	820	CLA	1	0
16	B	801	CLA	2	0
26	U	202	A86	1	0
16	B	847	CLA	1	0
25	U	201	LMG	2	0
16	U	205	CLA	2	0
16	A	826	CLA	2	0
16	F	804	CLA	1	0
16	B	825	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	823	CLA	1	0
16	U	207	CLA	5	0
16	L	204	CLA	1	0
16	U	209	CLA	1	0
16	H	302	CLA	3	0
16	F	802	CLA	2	0
16	B	811	CLA	1	0
16	A	809	CLA	2	0
16	B	848	CLA	3	0
16	A	836	CLA	2	0
16	A	815	CLA	2	0
16	k	202	CLA	2	0
16	A	813	CLA	1	0
19	I	103	BCR	1	0
16	B	834	CLA	4	0
16	A	833	CLA	3	0
16	B	849	CLA	6	0
16	J	104	CLA	1	0
16	U	211	CLA	3	0
19	A	844	BCR	3	0
16	A	829	CLA	2	0
19	k	203	BCR	3	0
16	U	208	CLA	1	0
16	B	806	CLA	2	0
19	B	839	BCR	4	0
19	M	101	BCR	3	0
16	B	836	CLA	4	0
16	B	815	CLA	2	0
16	A	807	CLA	1	0
16	B	828	CLA	1	0
17	B	837	PQN	1	0
16	B	826	CLA	1	0
16	B	802	CLA	3	0
16	U	204	CLA	1	0
16	B	827	CLA	1	0
16	G	308	CLA	2	0
16	G	307	CLA	1	0
22	A	850	CL0	2	0
16	A	808	CLA	2	0
16	A	847	CLA	1	0
21	J	101	LMU	3	0
16	H	312	CLA	5	0

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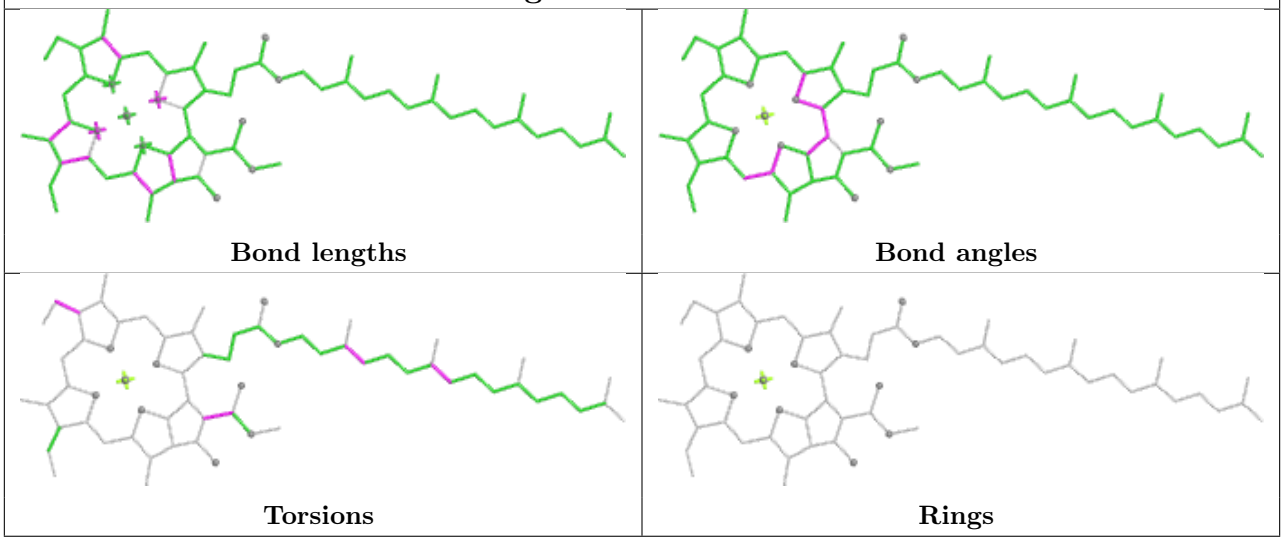
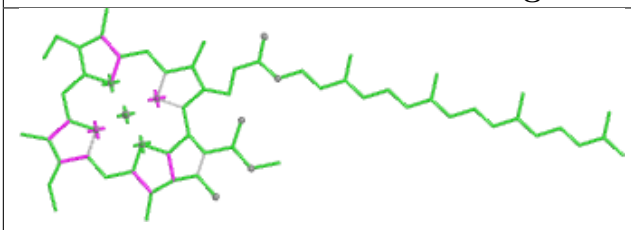
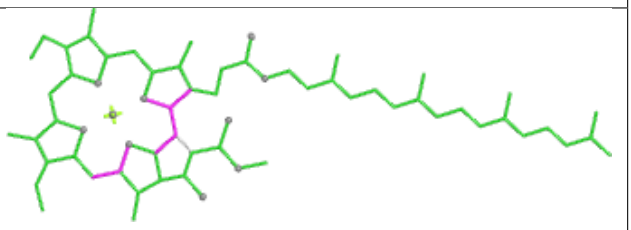
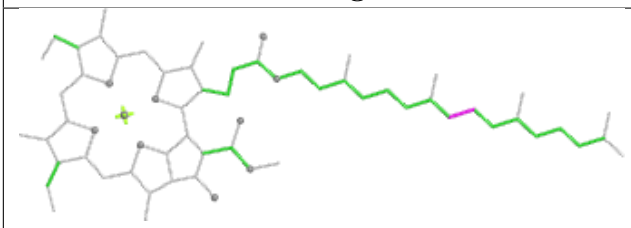
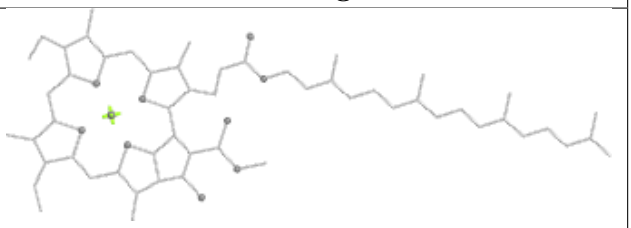
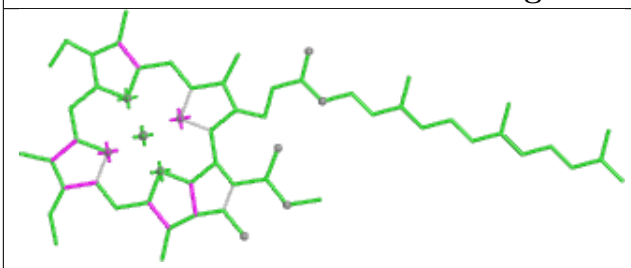
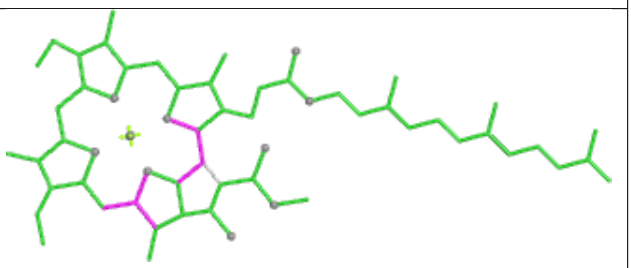
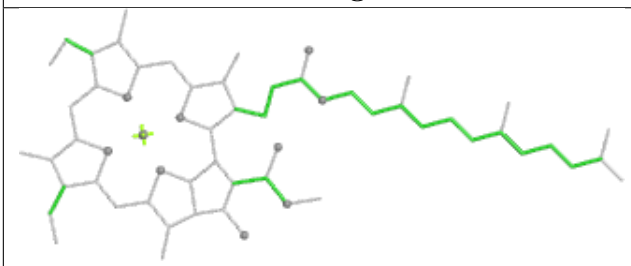
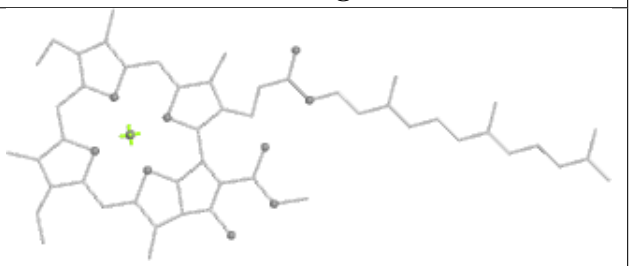
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	825	CLA	1	0
16	G	303	CLA	3	0
16	B	818	CLA	2	0
16	B	813	CLA	2	0
18	G	316	LHG	2	0
16	A	849	CLA	6	0
16	G	310	CLA	2	0
16	B	829	CLA	1	0
16	k	201	CLA	1	0
16	A	822	CLA	1	0
16	B	831	CLA	2	0

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.

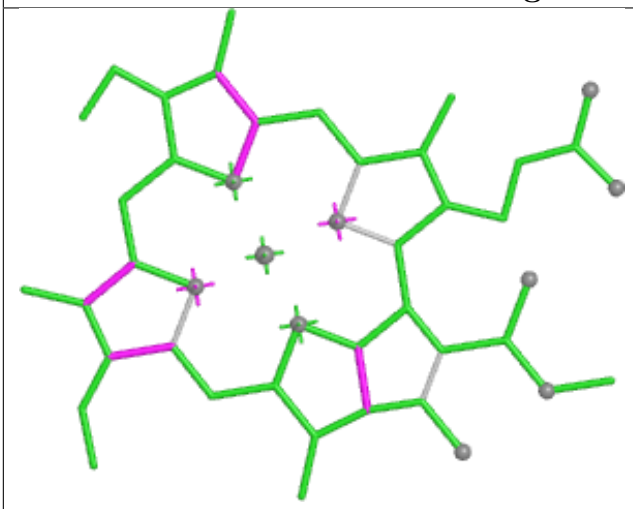
Ligand CLA A 851



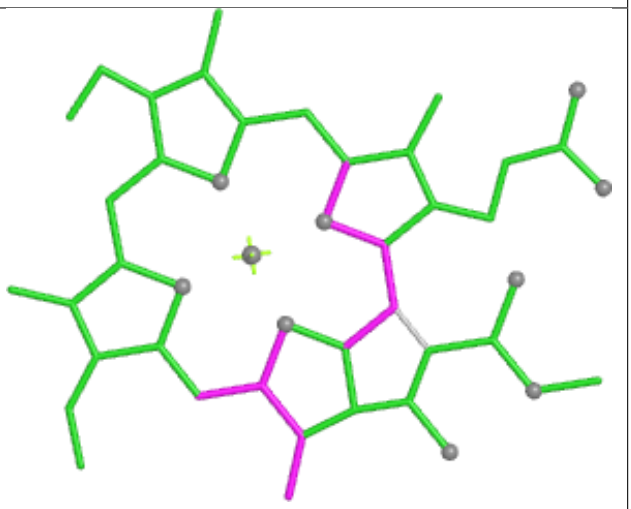
Ligand CLA A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

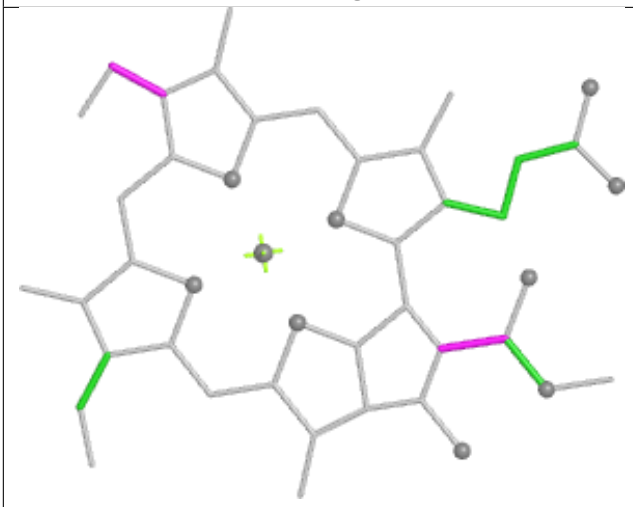
Ligand CLA A 812



Bond lengths

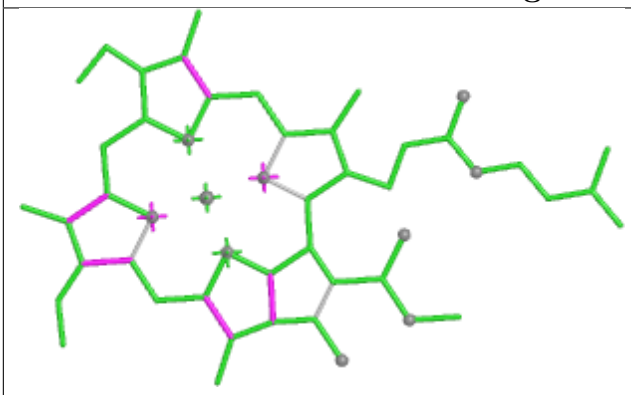
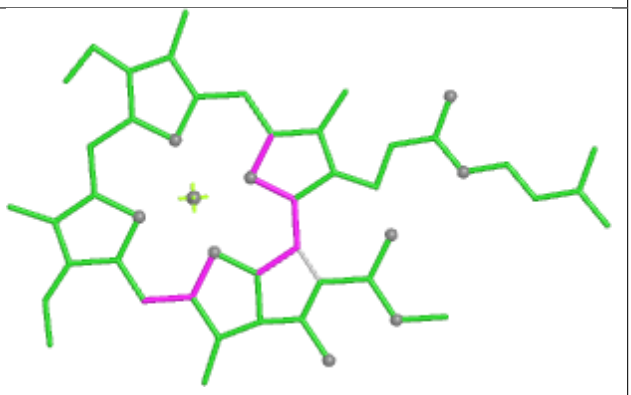
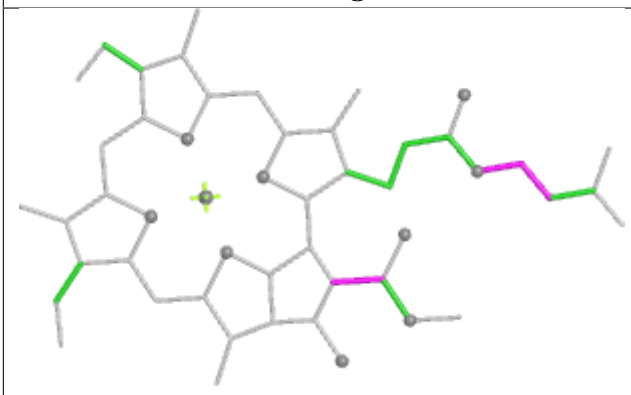
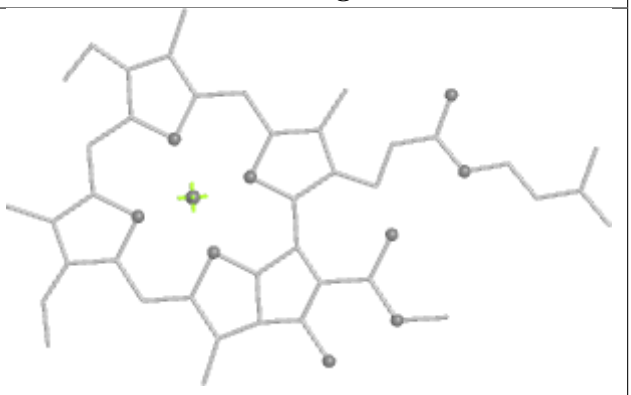


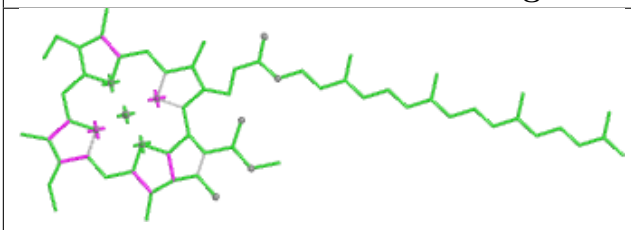
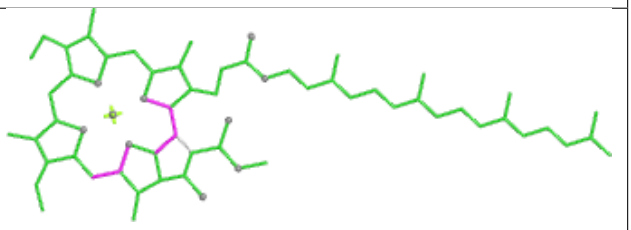
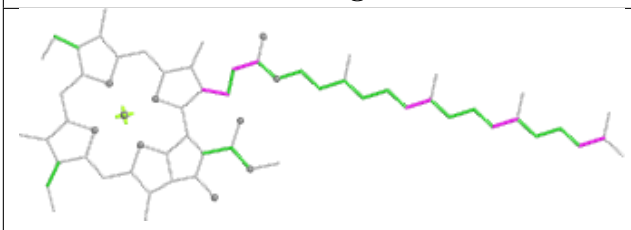
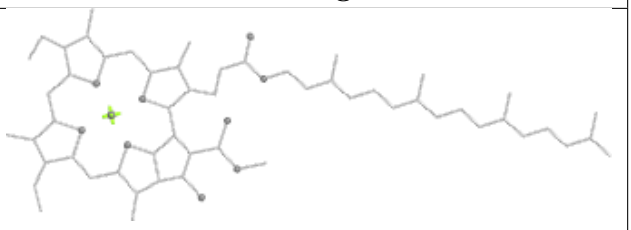
Bond angles



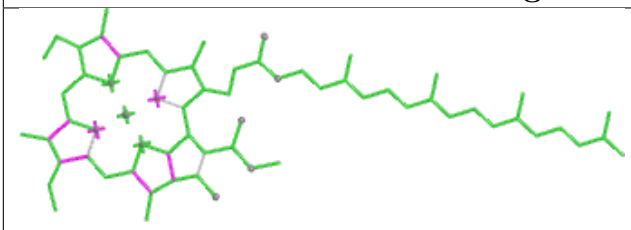
Torsions

Rings

Ligand CLA A 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 854



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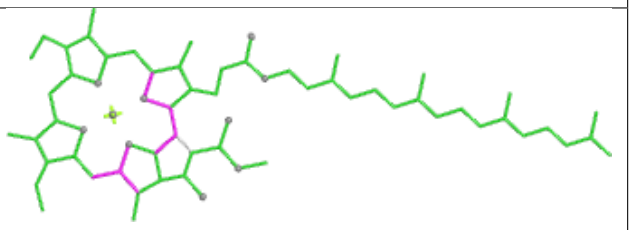

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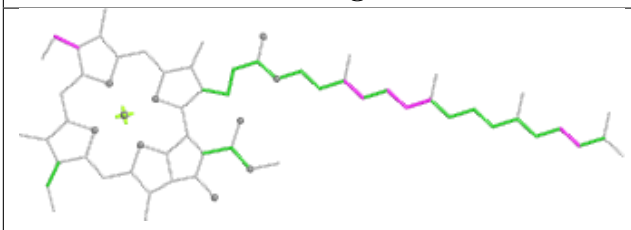

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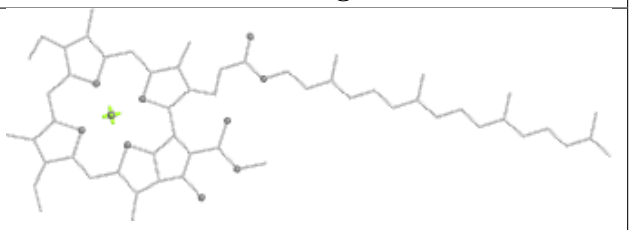
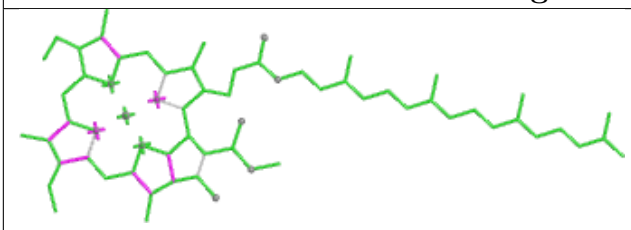


Rings

Ligand CLA I 102



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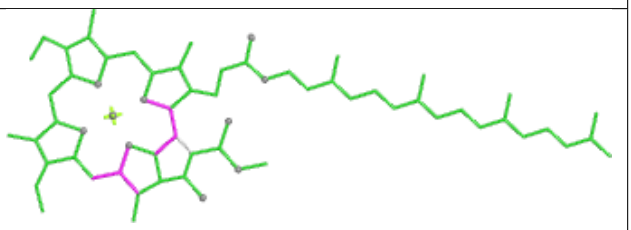
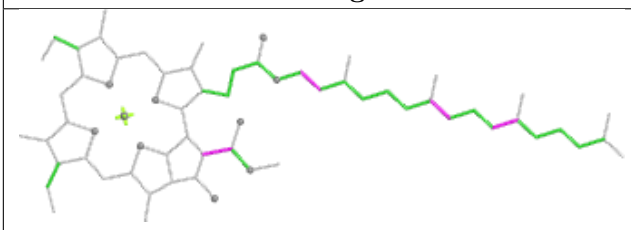


Bond angles



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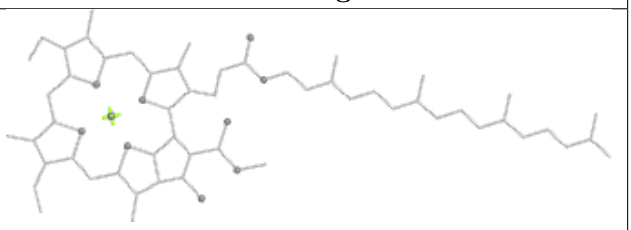
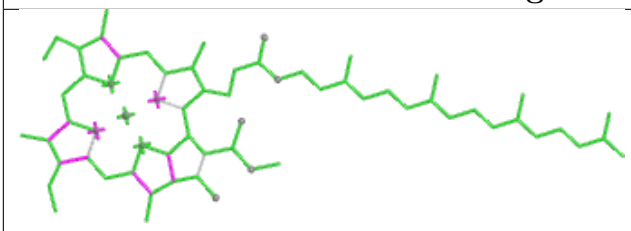


Rings

Ligand CLA L 203



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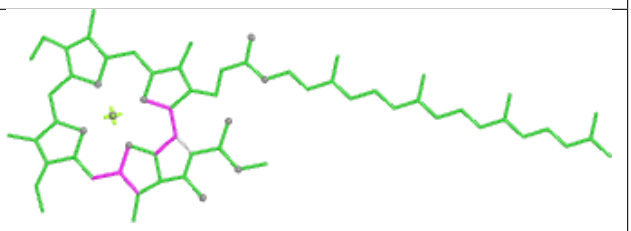

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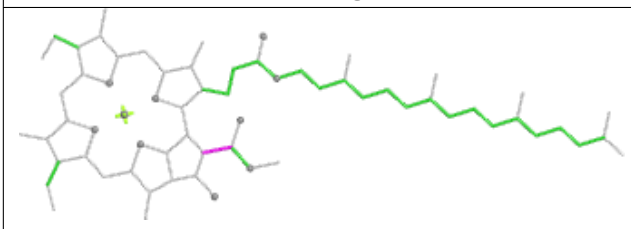

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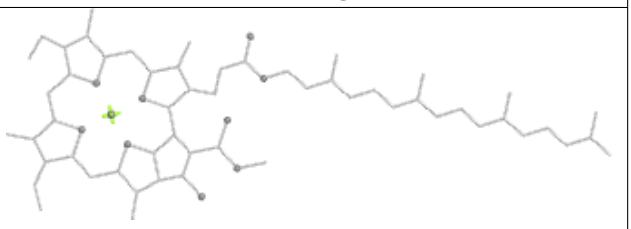
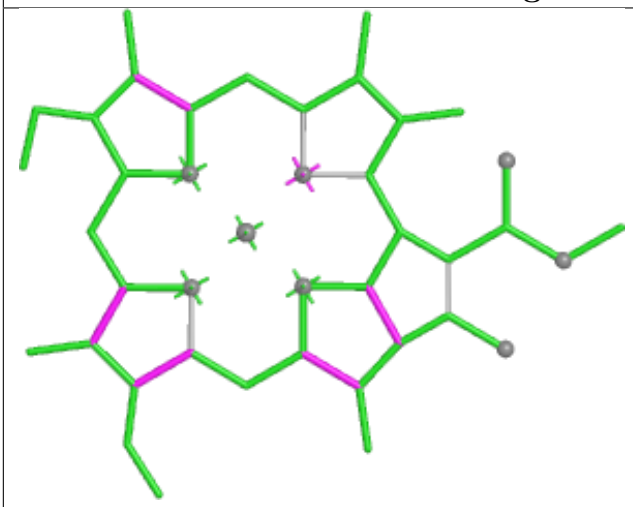


Rings

Ligand CLA H 308



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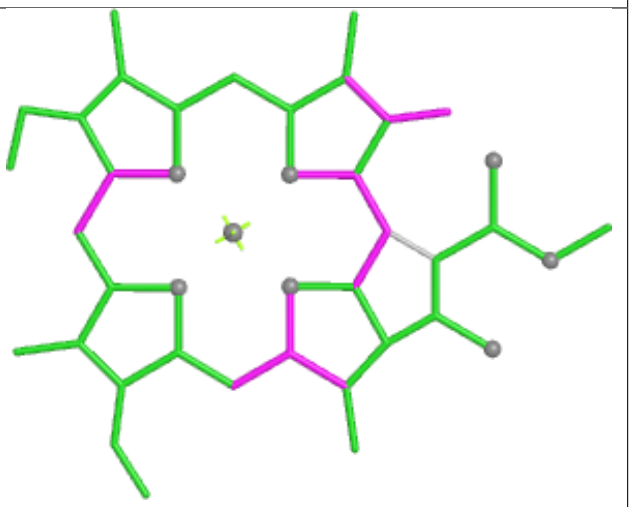

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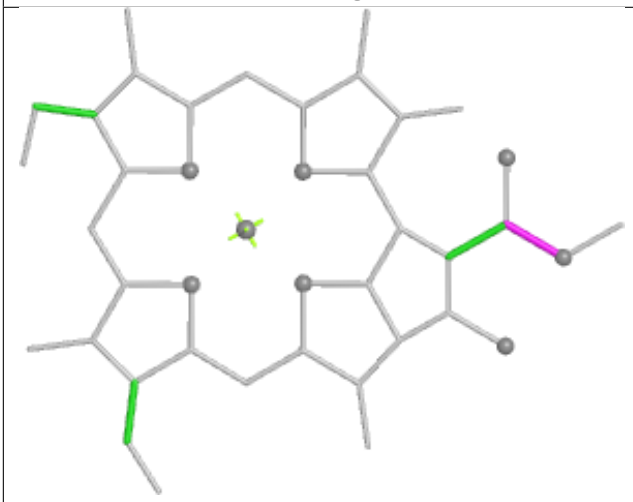

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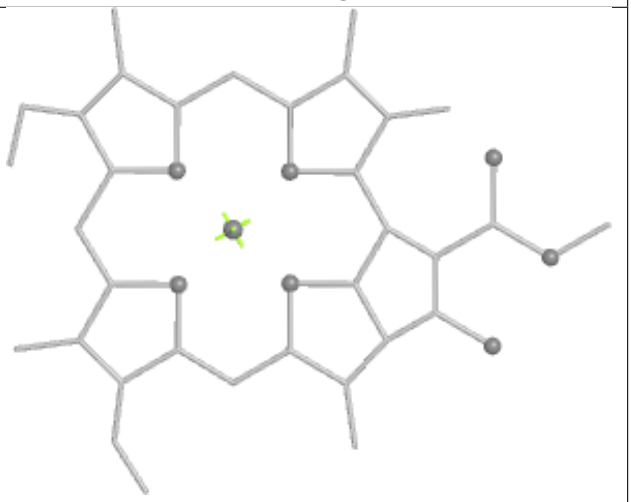
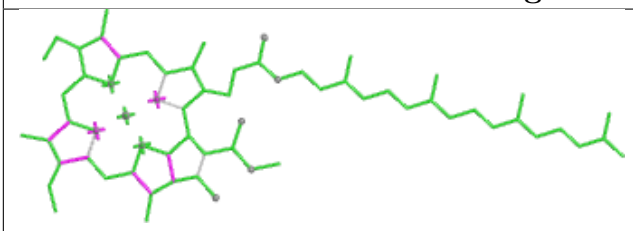


Rings

Ligand CLA B 808



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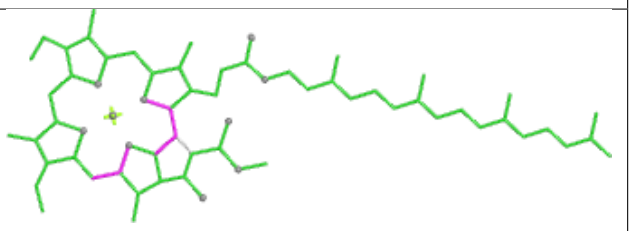

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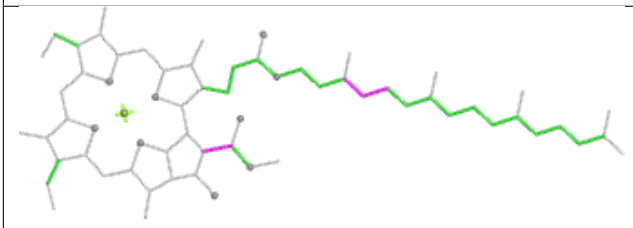

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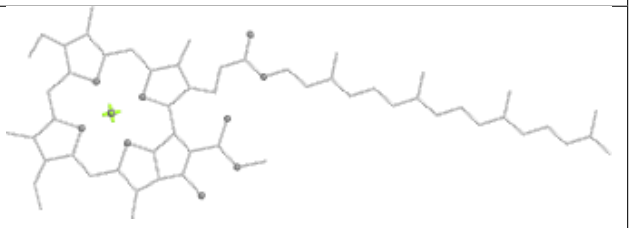
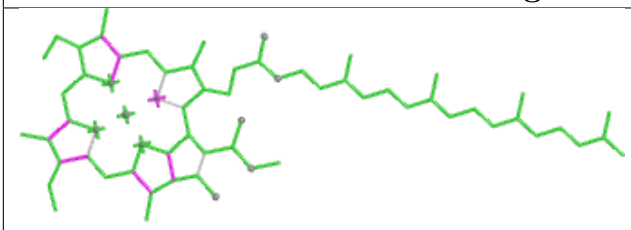


Rings

Ligand CLA A 803



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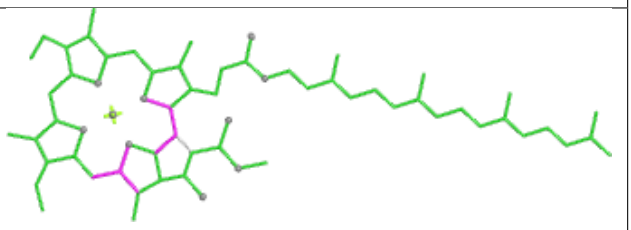

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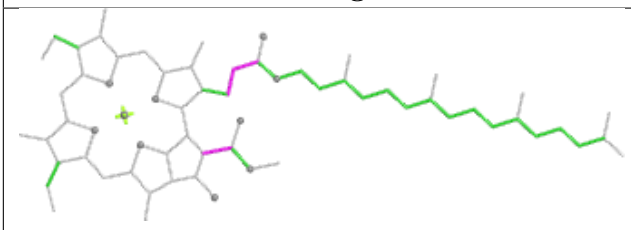

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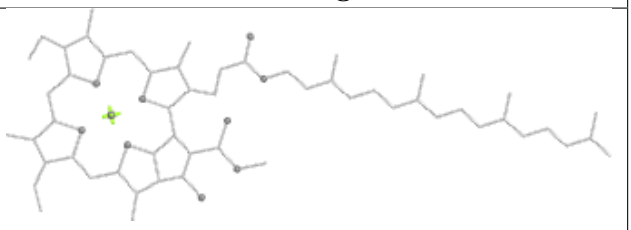
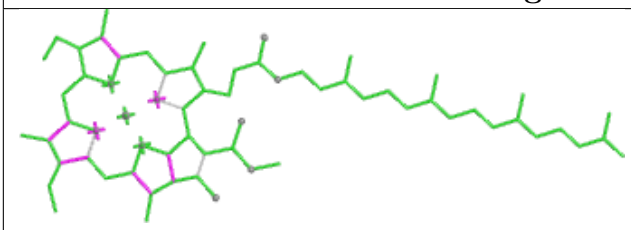


Rings

Ligand CLA B 845



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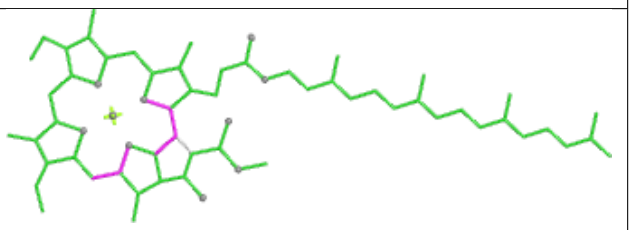

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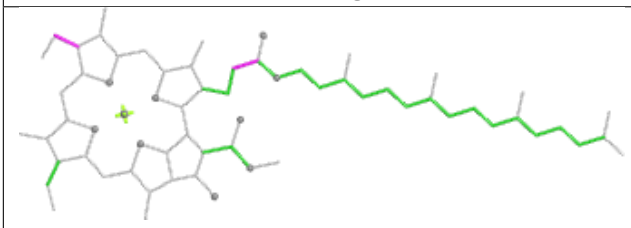

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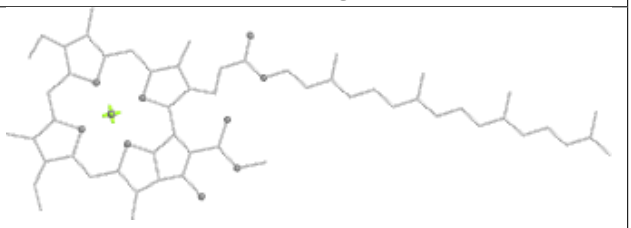
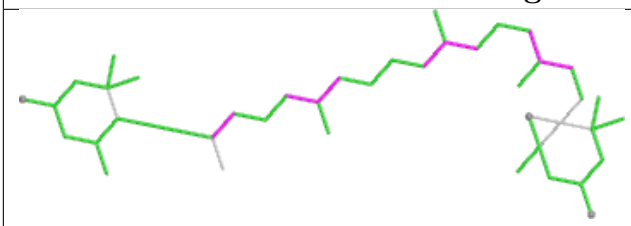


Rings

Ligand DD6 H 311



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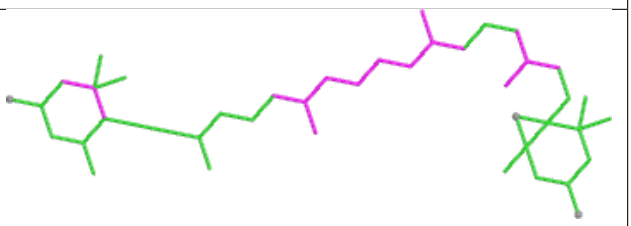
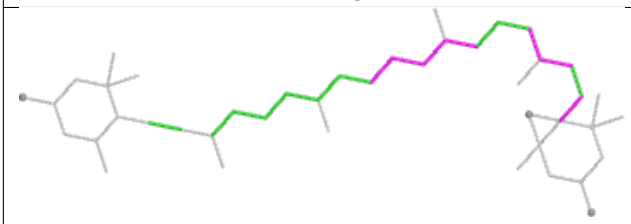


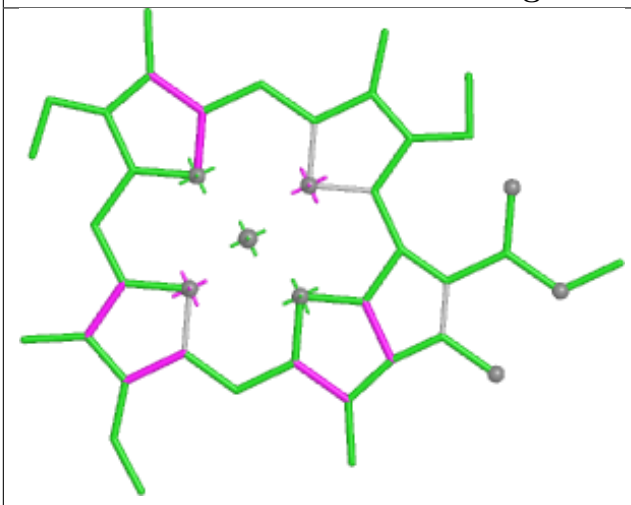
Bond angles



Torsions

Rings

Ligand CLA K 202



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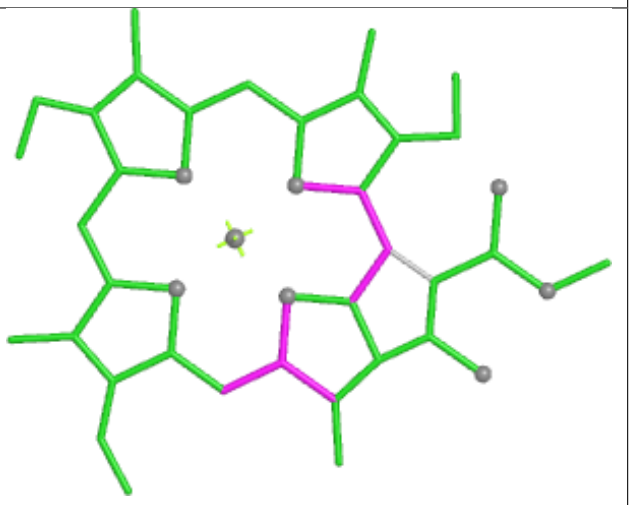

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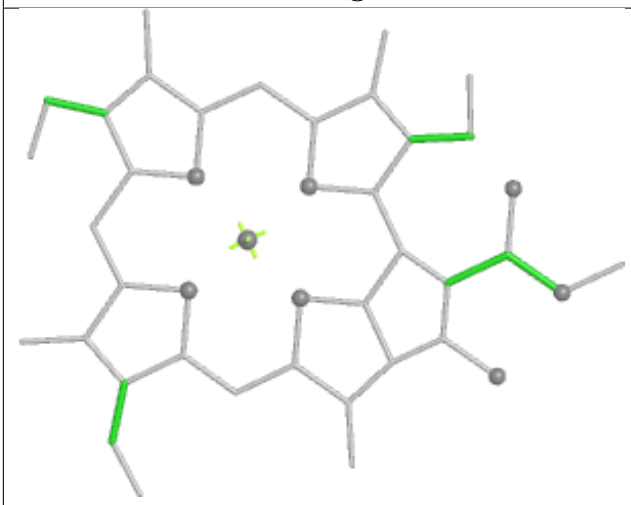
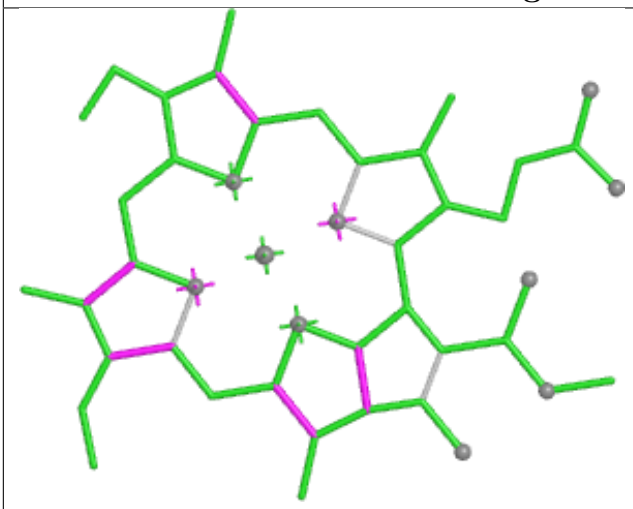


Torsions

Rings

Ligand CLA H 309



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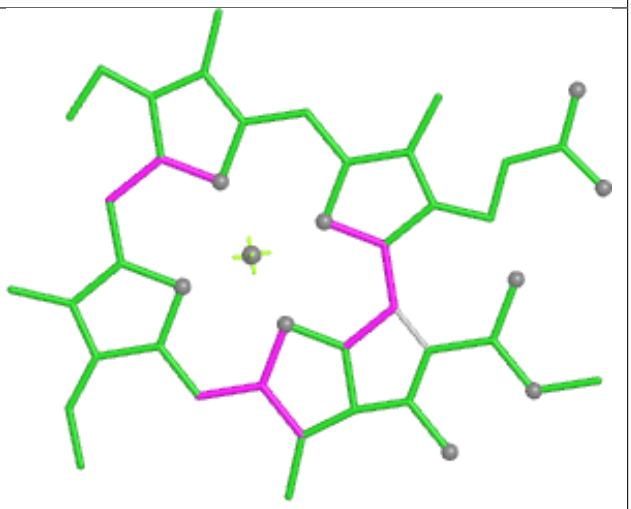

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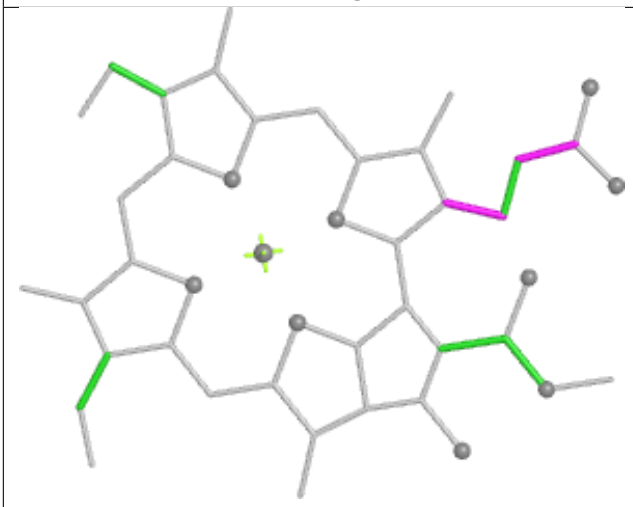
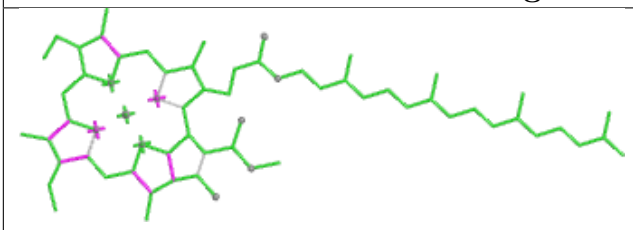


Torsions

Rings

Ligand CLA A 806



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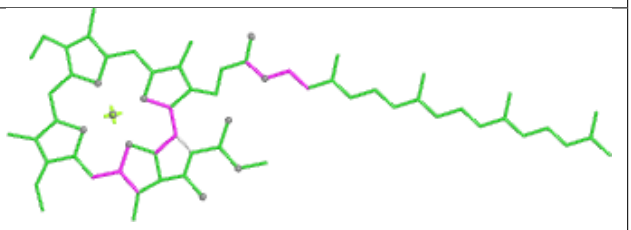

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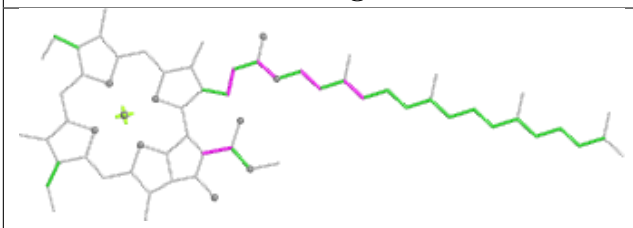
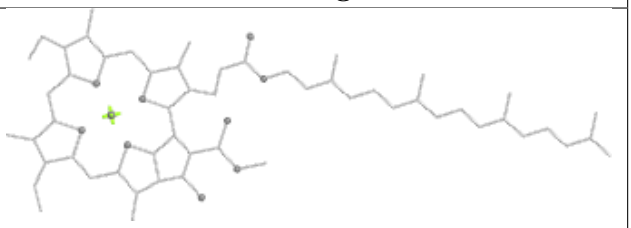
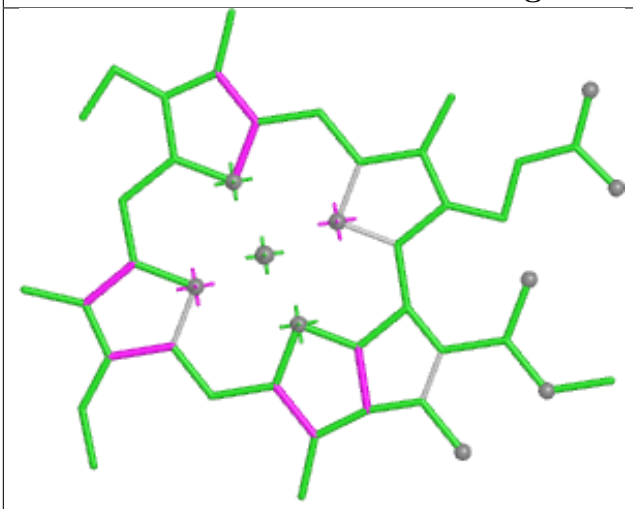


Torsions



Rings

Ligand CLA B 804



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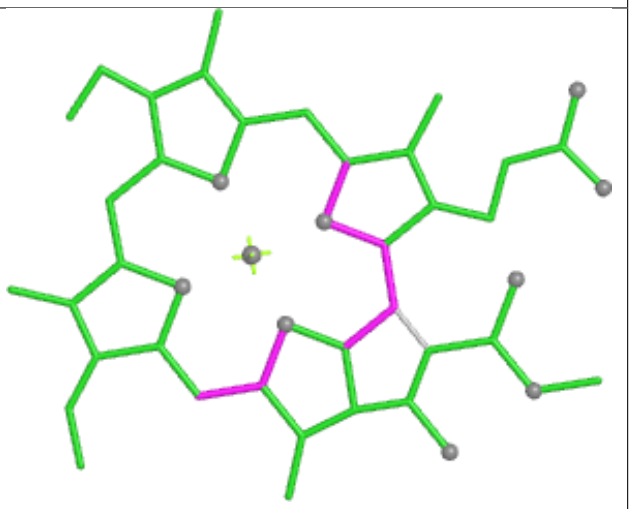

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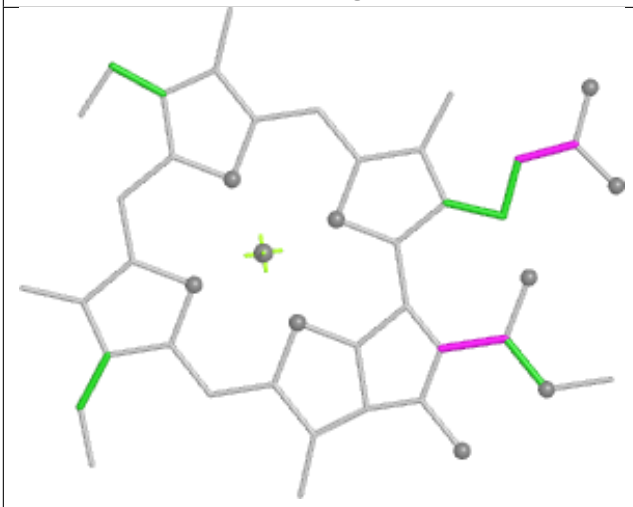
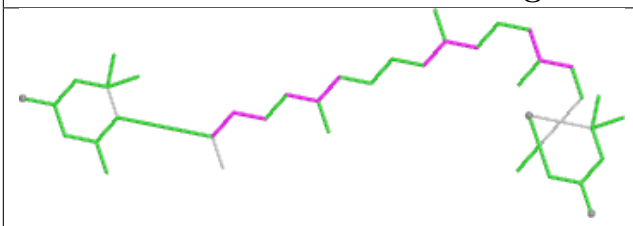


Torsions

Rings

Ligand DD6 G 313



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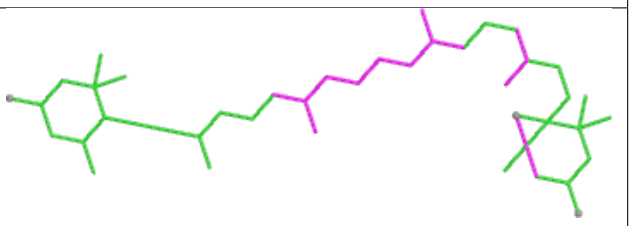
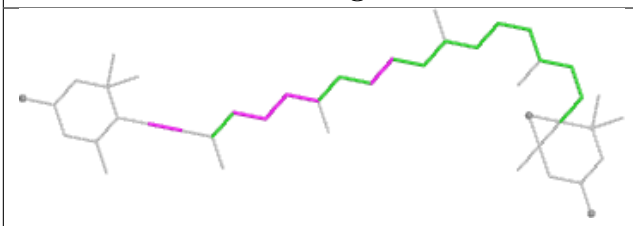
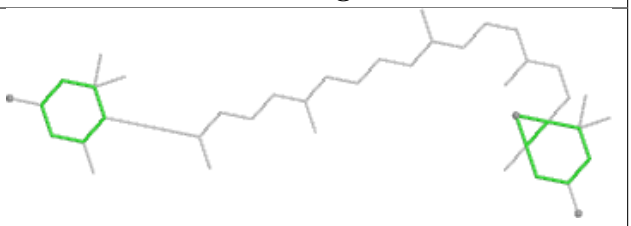


Bond angles

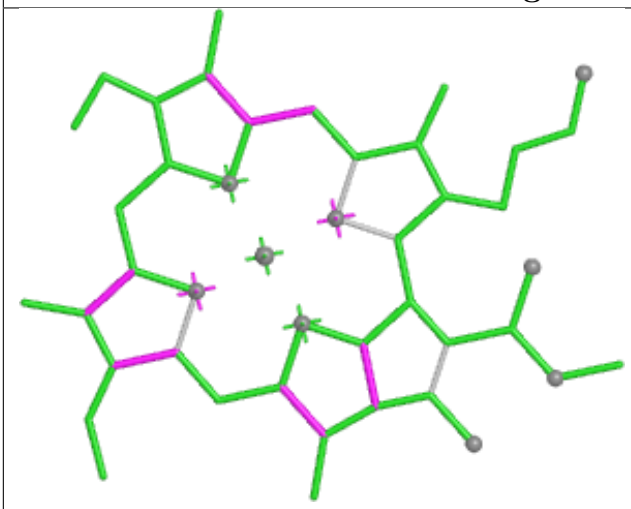


Torsions



Rings

Ligand CLA H 304



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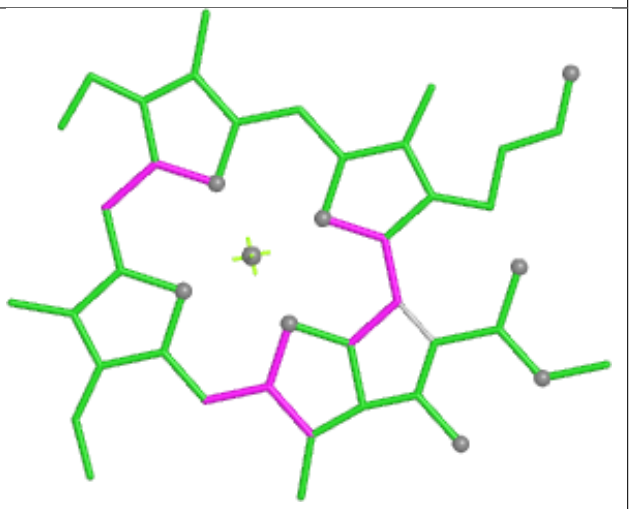
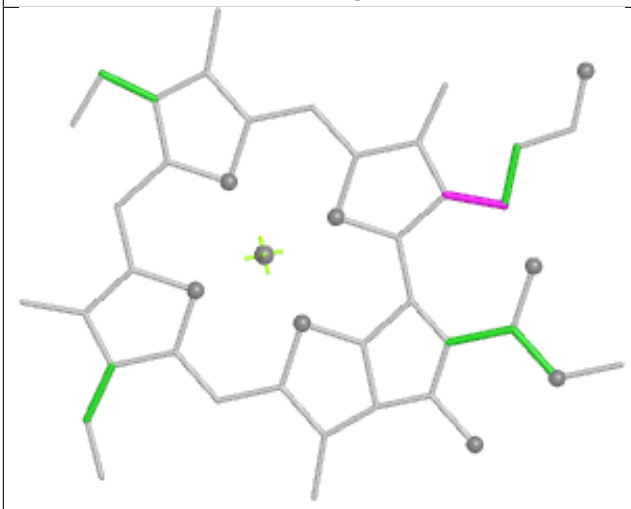
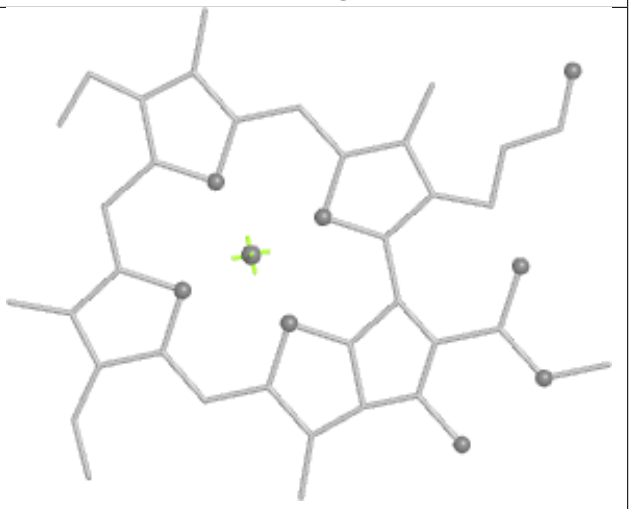


Bond angles

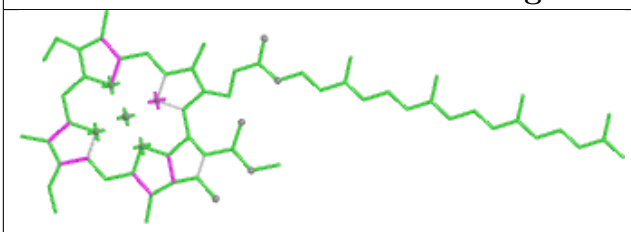


Torsions

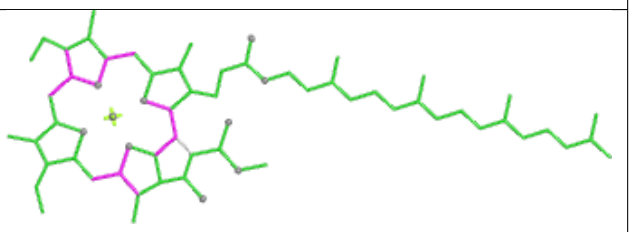


Rings

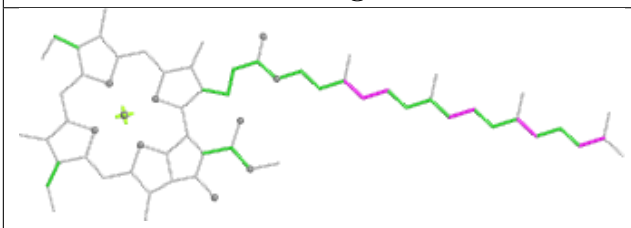
Ligand CLA B 817



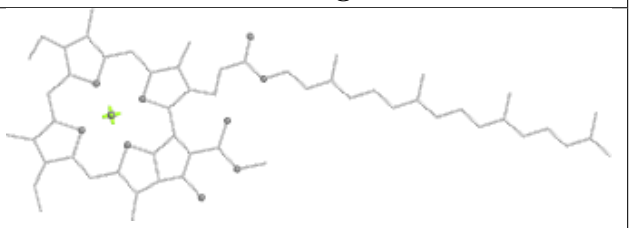
Bond lengths



Bond angles

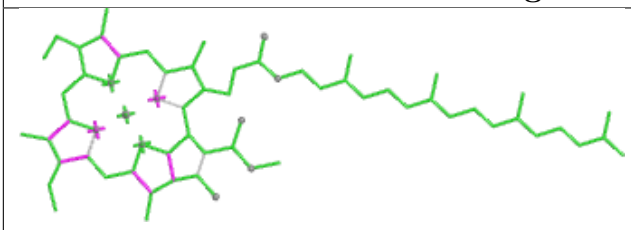


Torsions

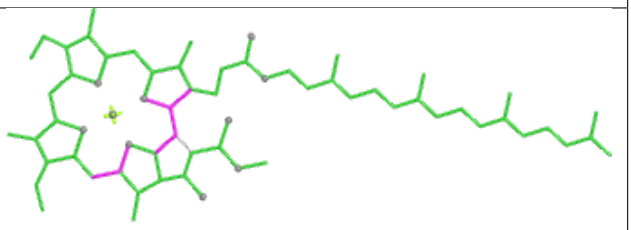


Rings

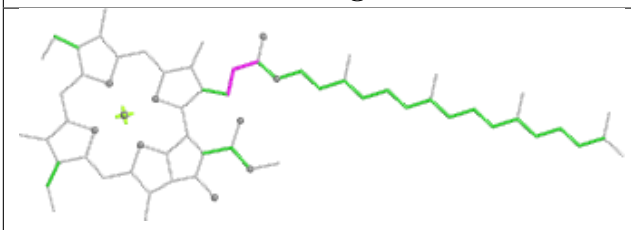
Ligand CLA B 803



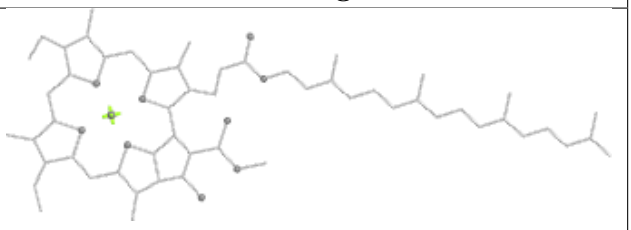
Bond lengths



Bond angles

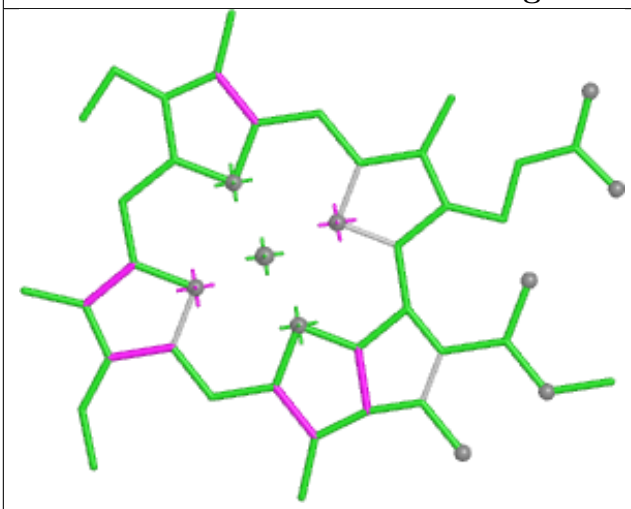


Torsions

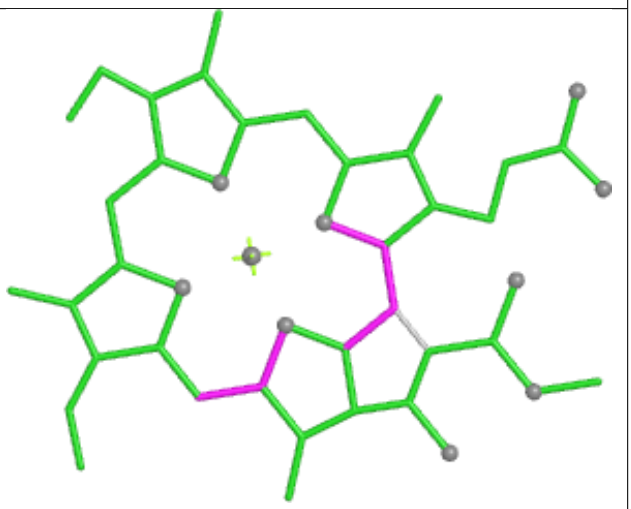


Rings

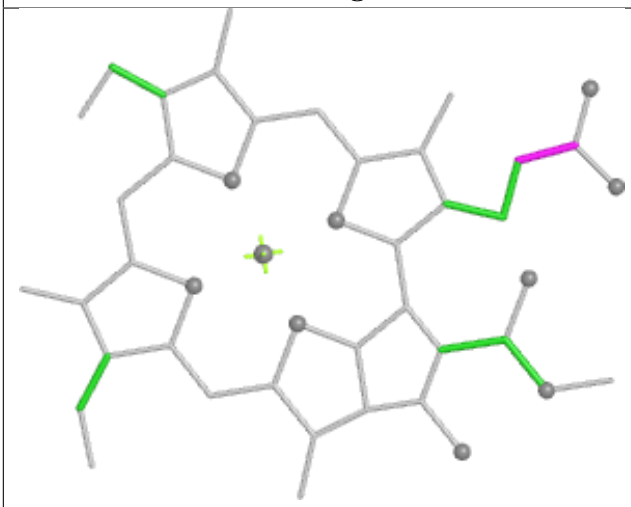
Ligand CLA H 305



Bond lengths



Bond angles



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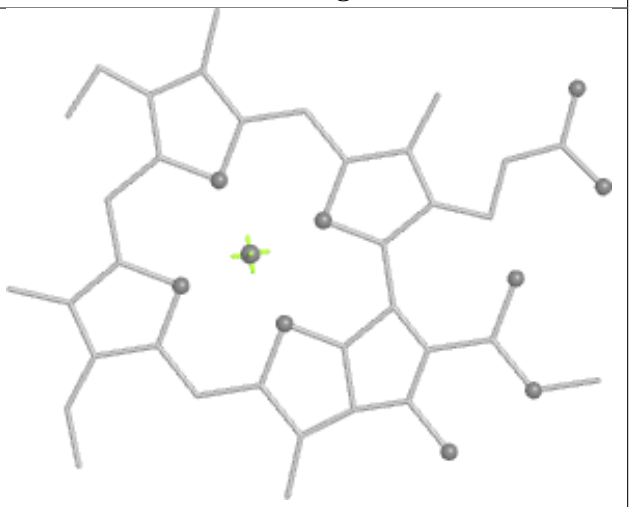
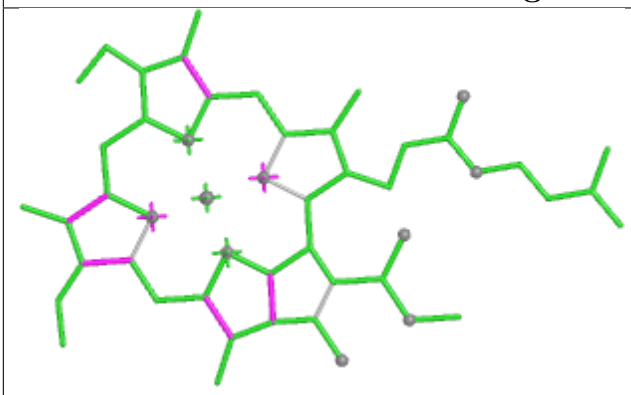
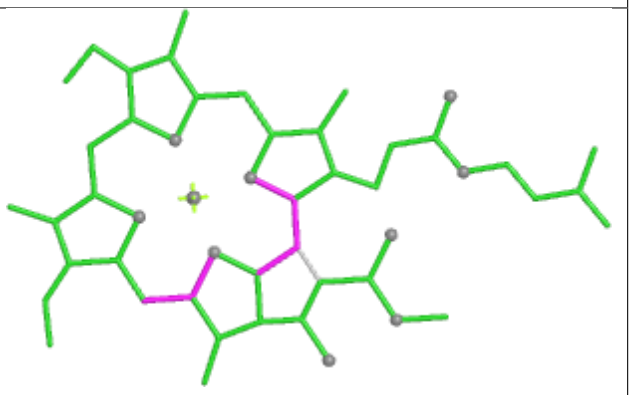
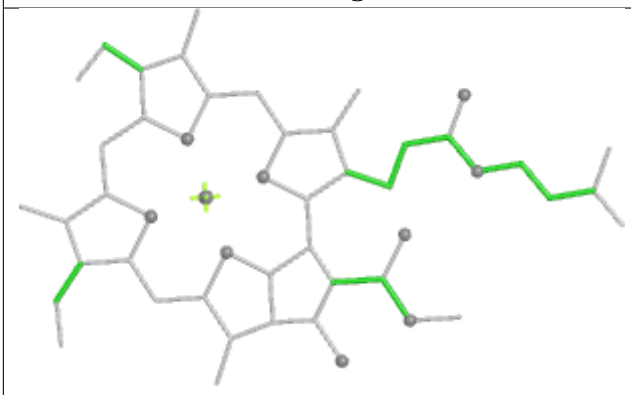
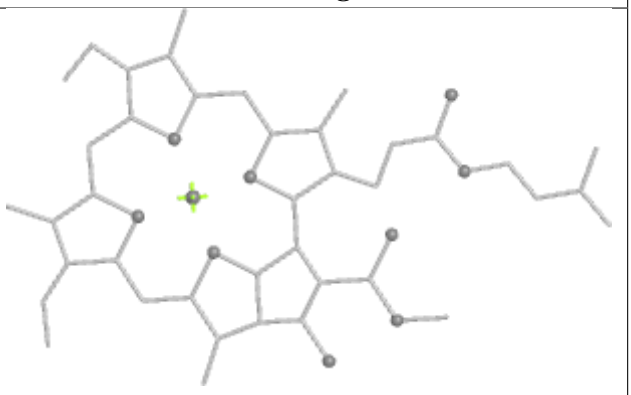
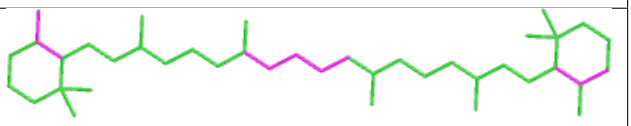
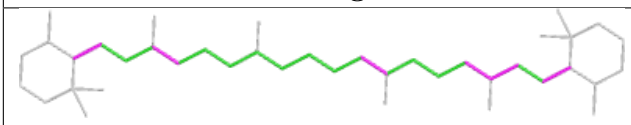
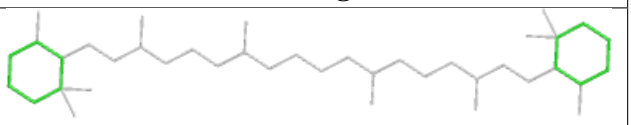
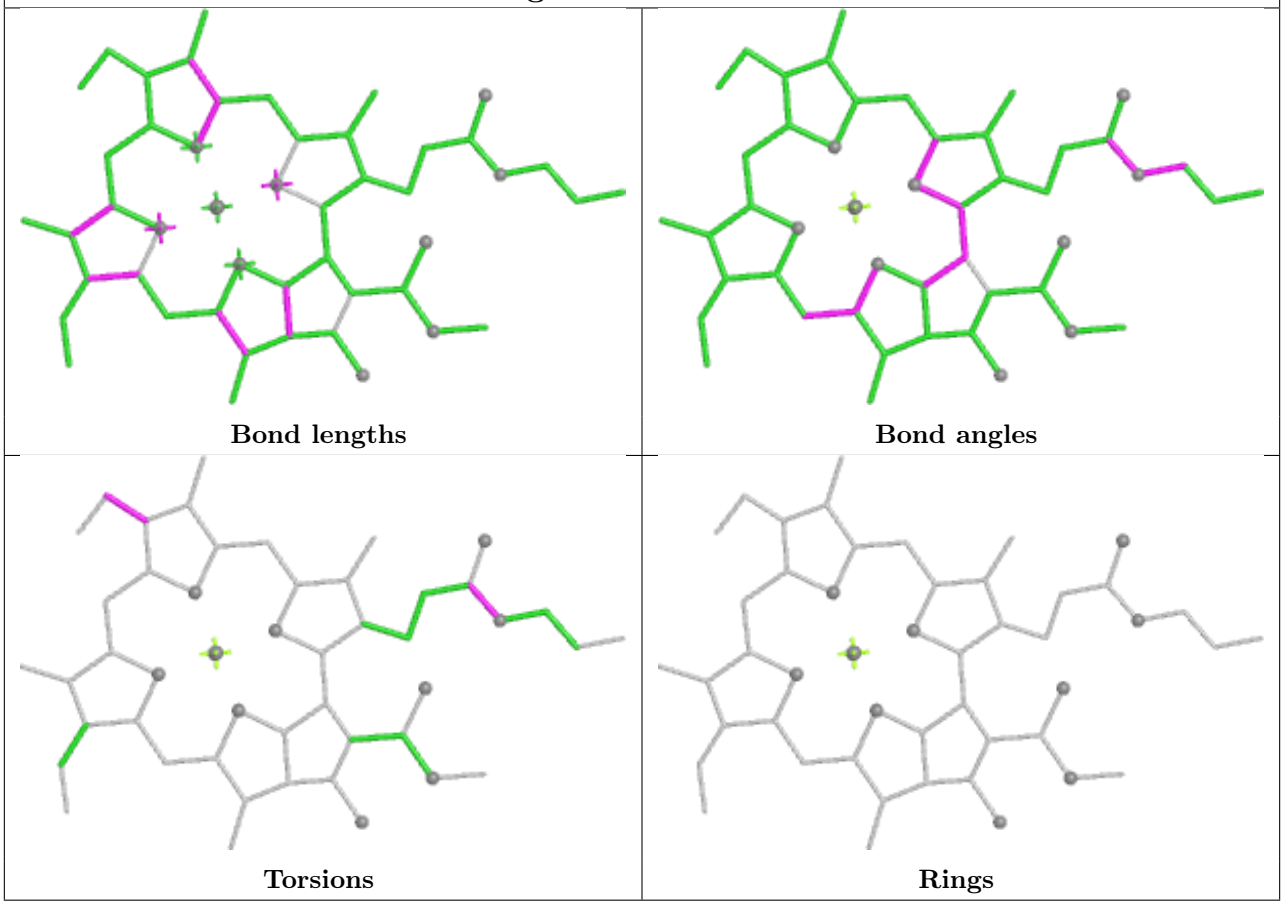


Rings

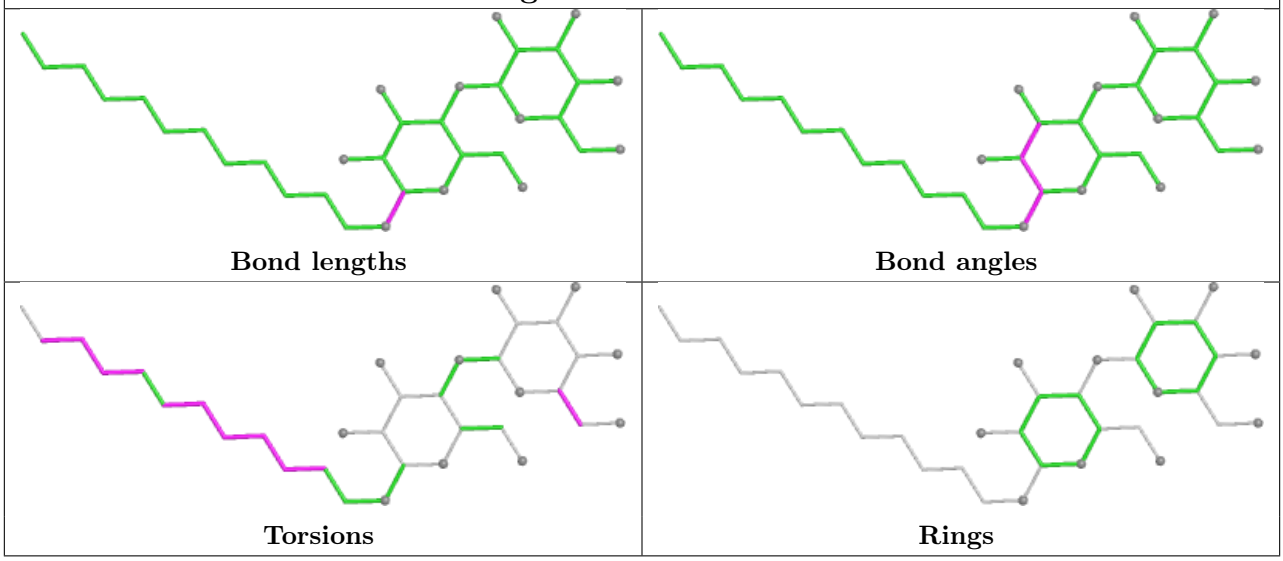
Ligand CLA A 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

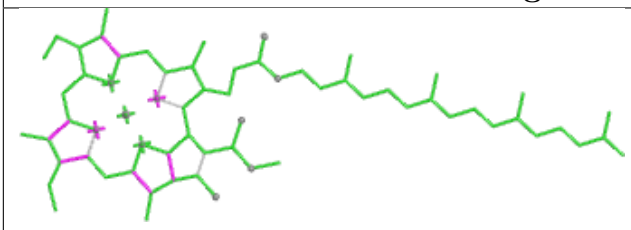
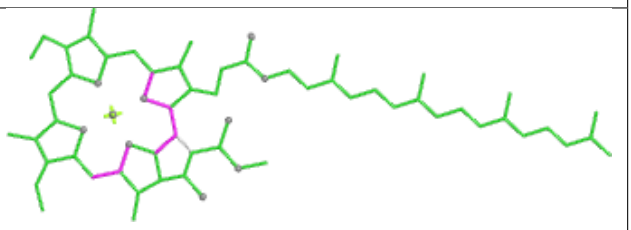
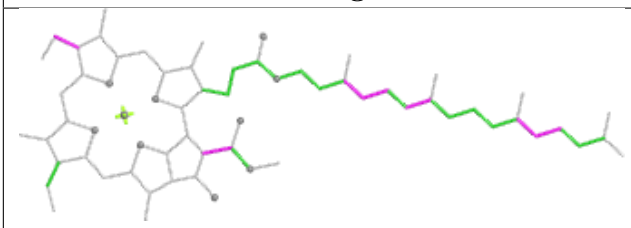
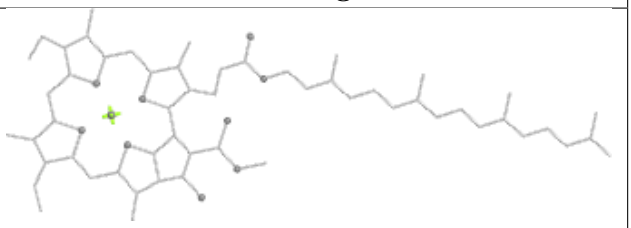
Ligand BCR L 201	
Bond lengths	 Bond angles
 Torsions	 Rings

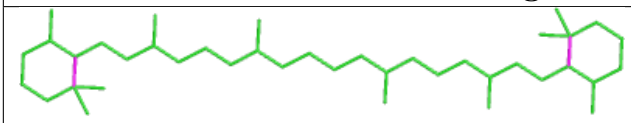
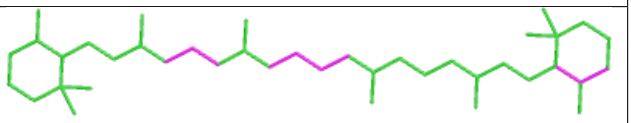
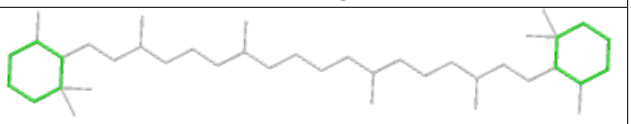
Ligand CLA F 803

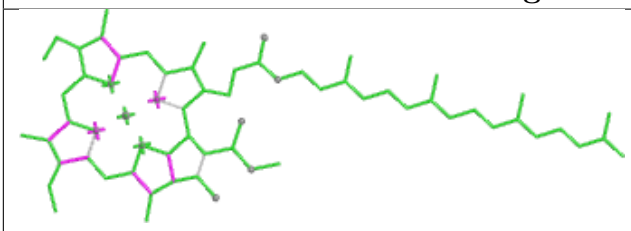
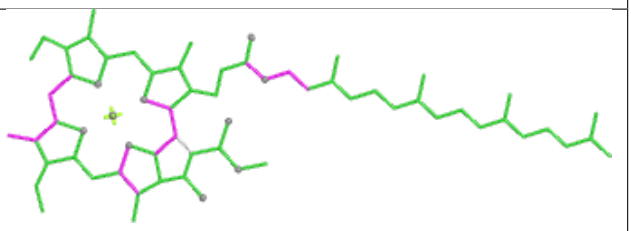
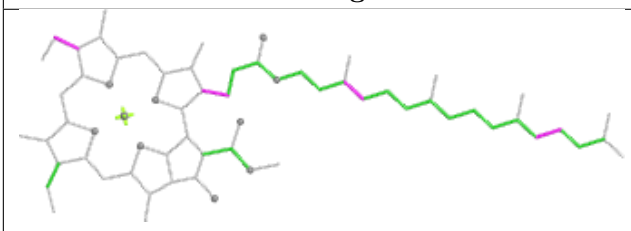
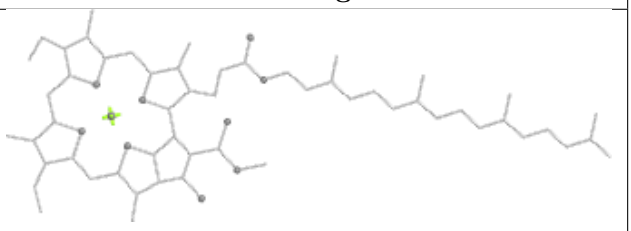


Ligand LMU A 848

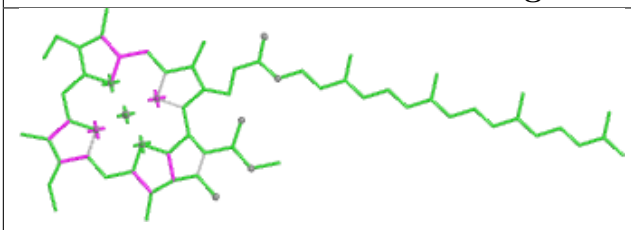


Ligand CLA A 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

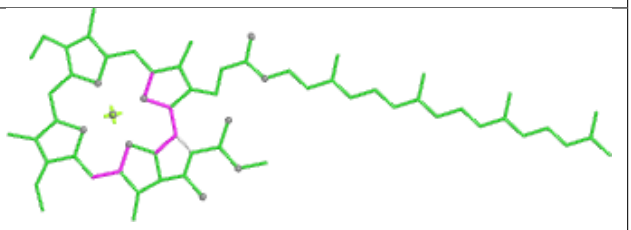
Ligand BCR B 842	
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand CLA H 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

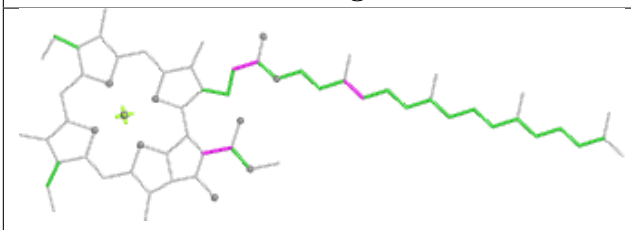
Ligand CLA B 809



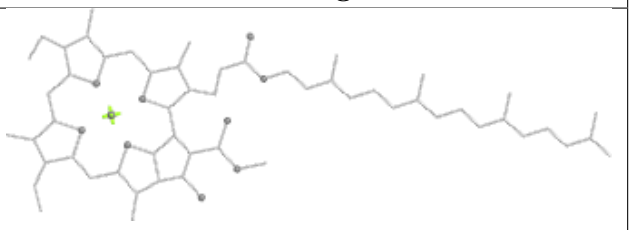
Bond lengths



Bond angles

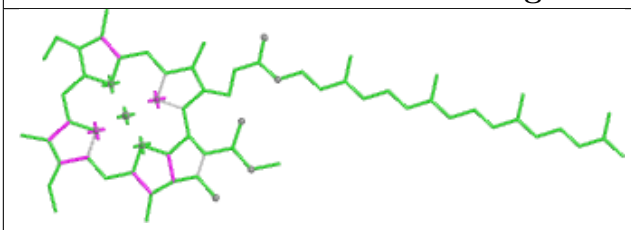


Torsions

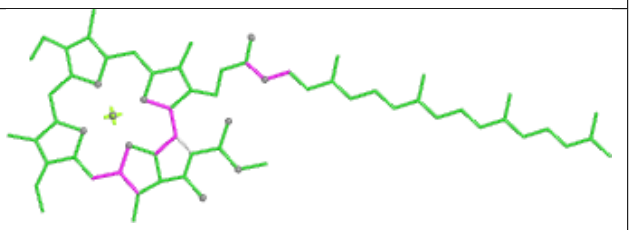


Rings

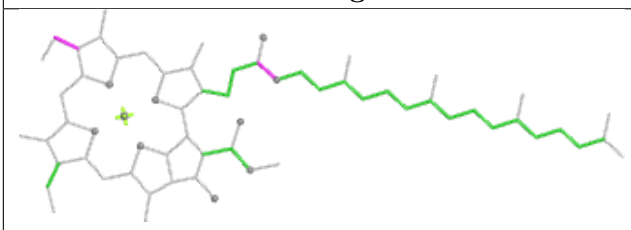
Ligand CLA B 824



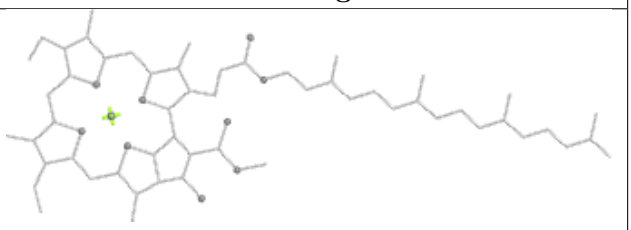
Bond lengths



Bond angles

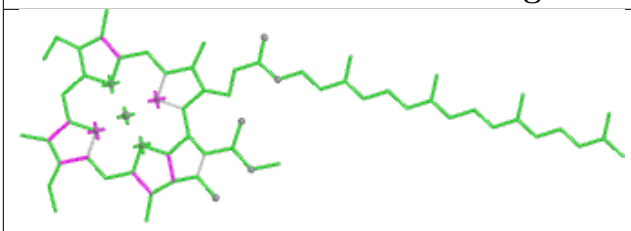


Torsions

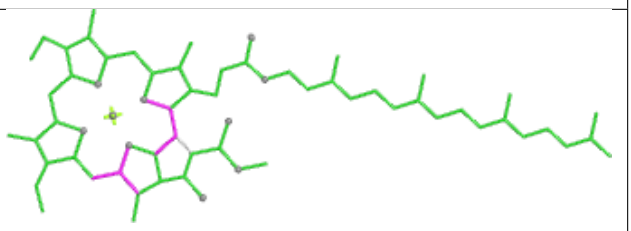


Rings

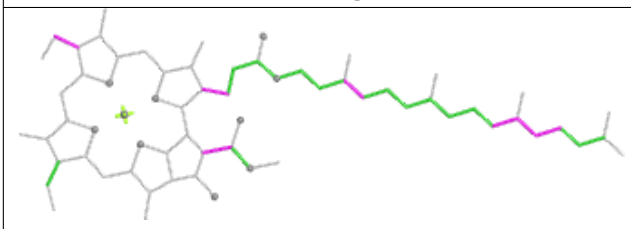
Ligand CLA A 853



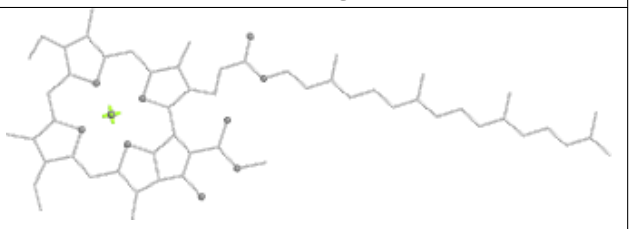
Bond lengths



Bond angles

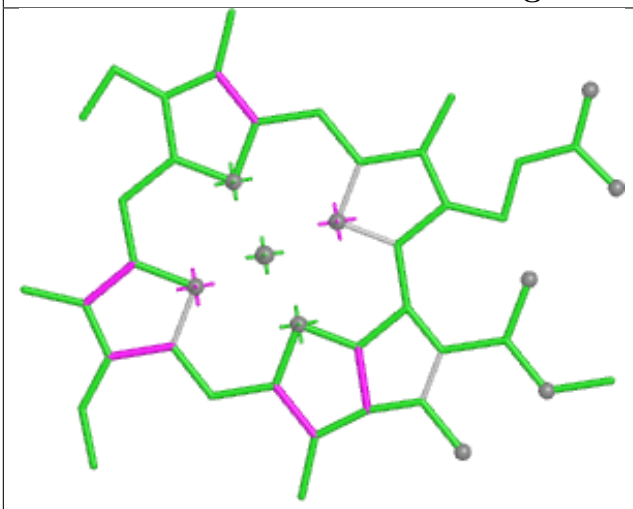


Torsions

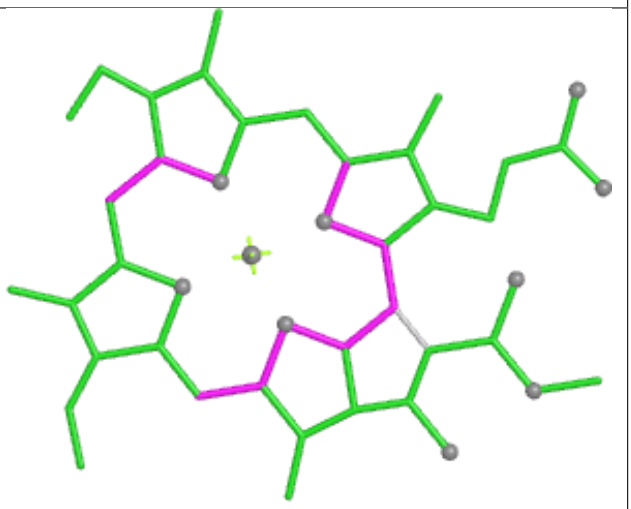


Rings

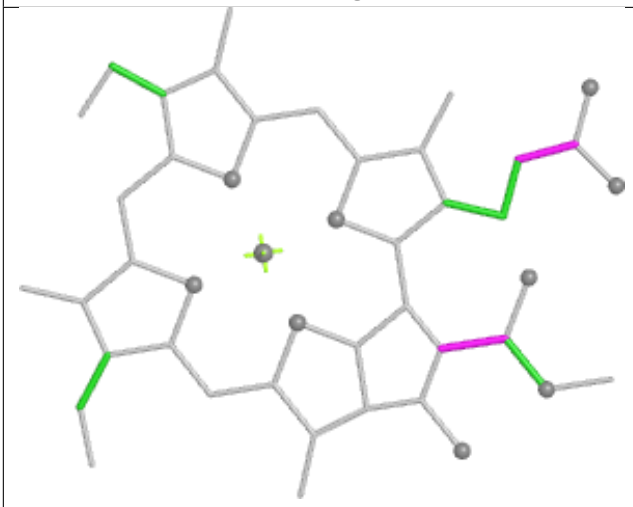
Ligand CLA A 817



Bond lengths

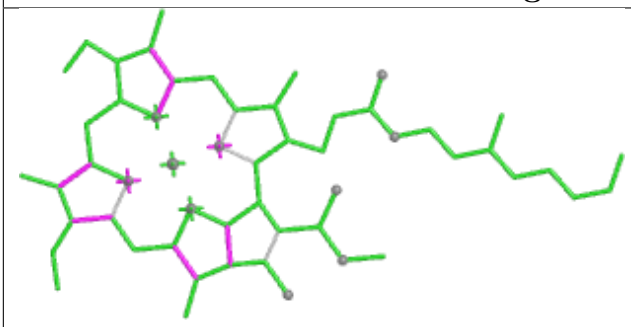
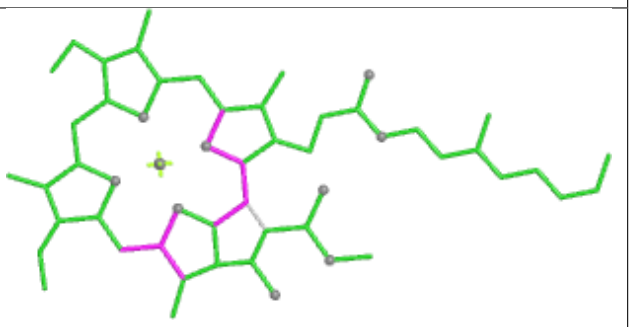
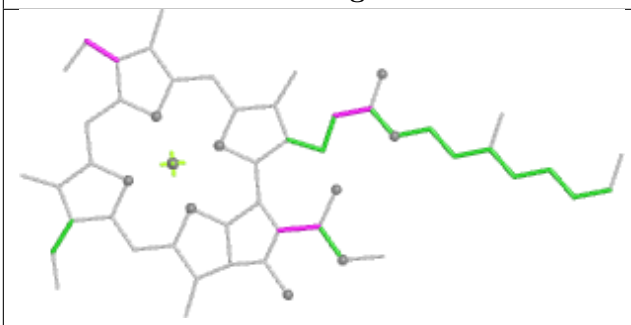
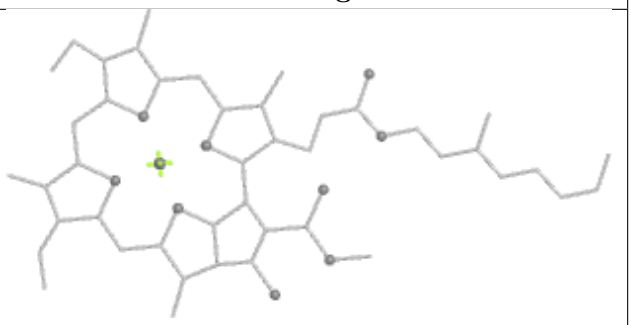


Bond angles

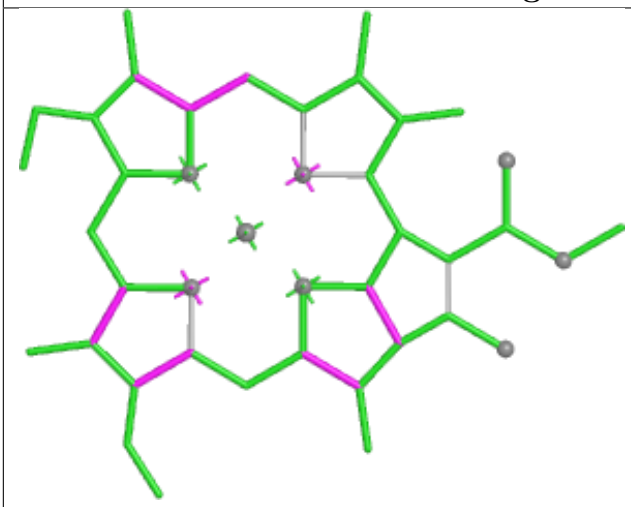


Torsions

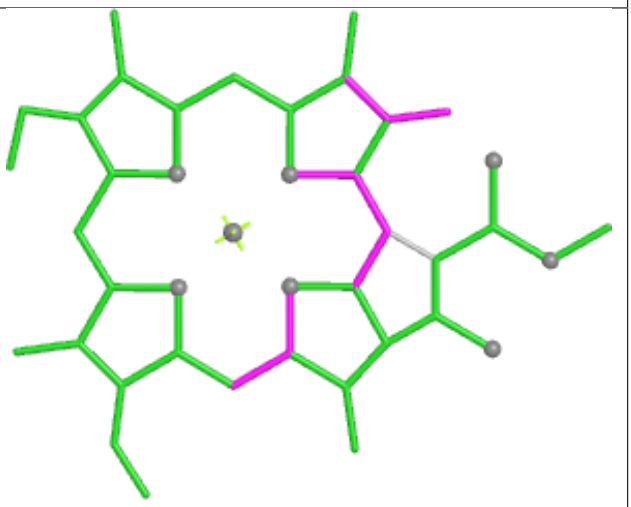
Rings

Ligand CLA A 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

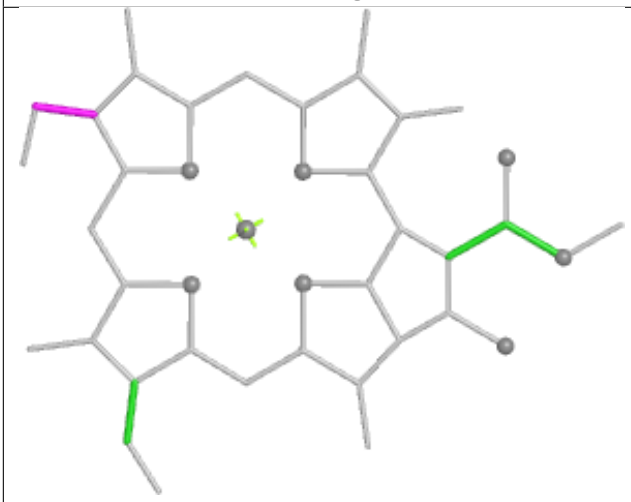
Ligand CLA G 302



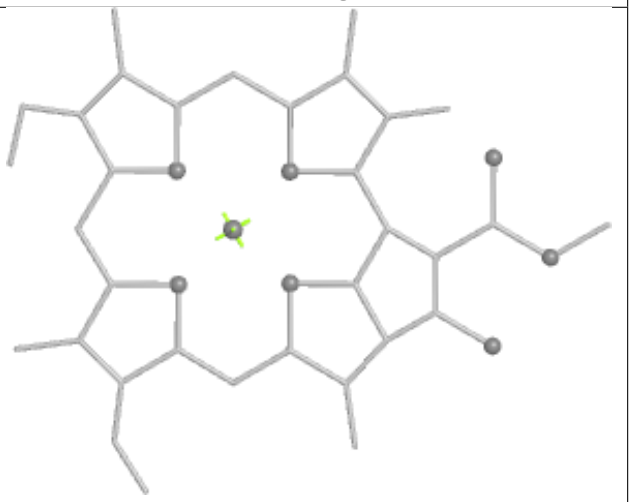
Bond lengths



Bond angles

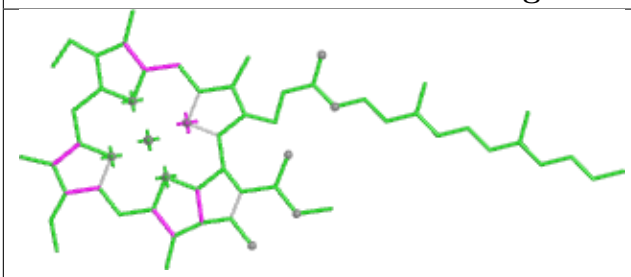


Torsions

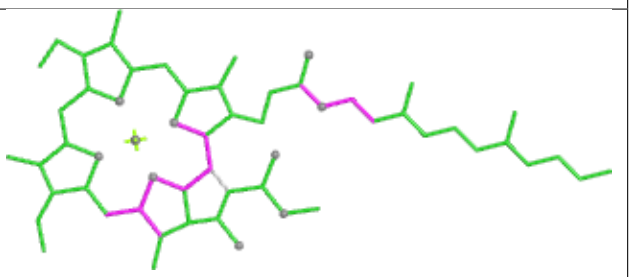


Rings

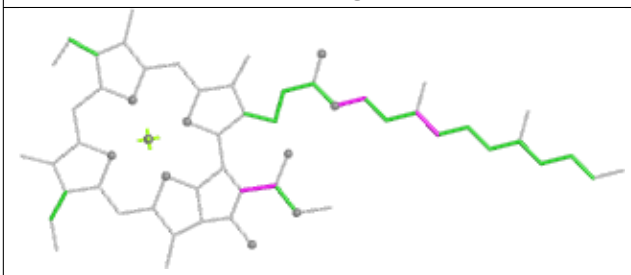
Ligand CLA K 205



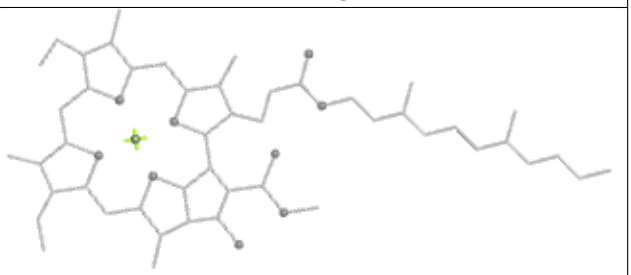
Bond lengths



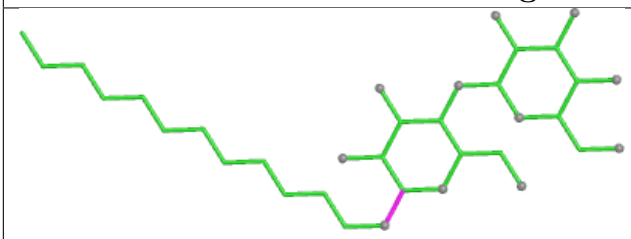
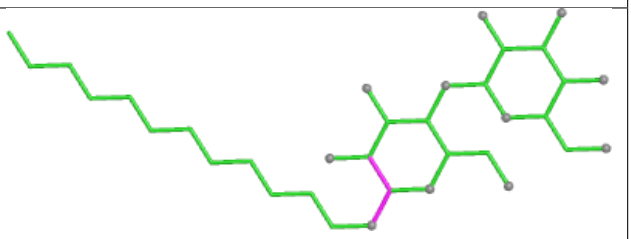
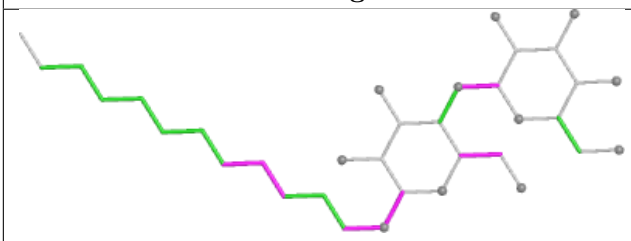
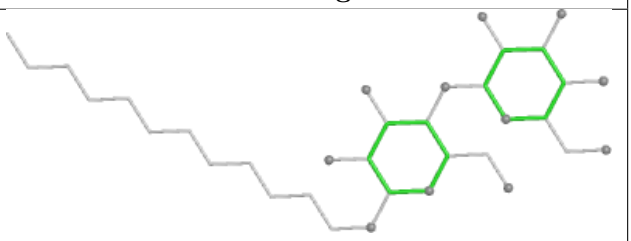
Bond angles

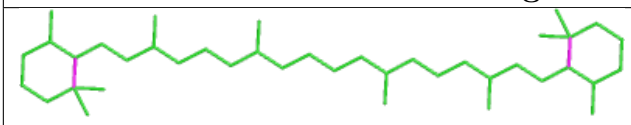
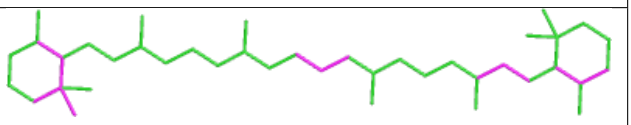
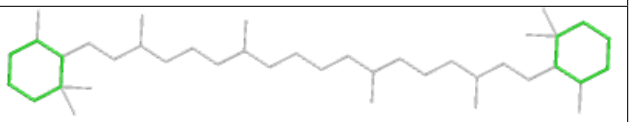


Torsions

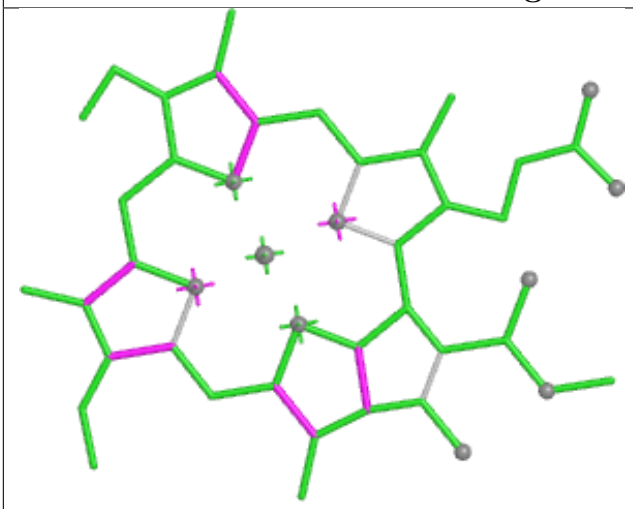


Rings

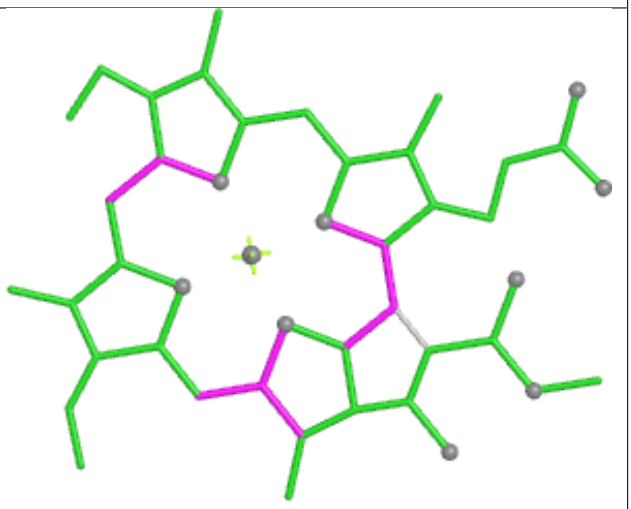
Ligand LMU A 855	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 840	
 Bond lengths	 Bond angles
Torsions	 Rings

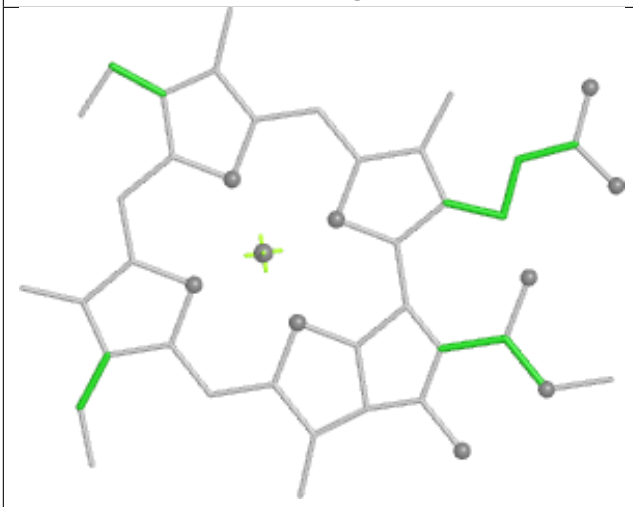
Ligand CLA B 830



Bond lengths



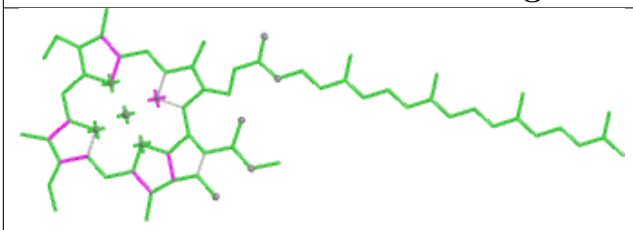
Bond angles



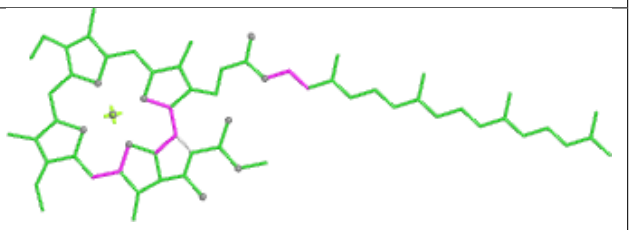
Torsions

Rings

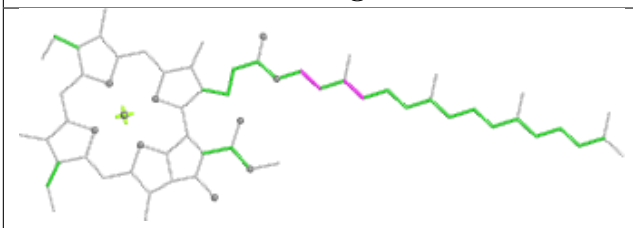
Ligand CLA A 818



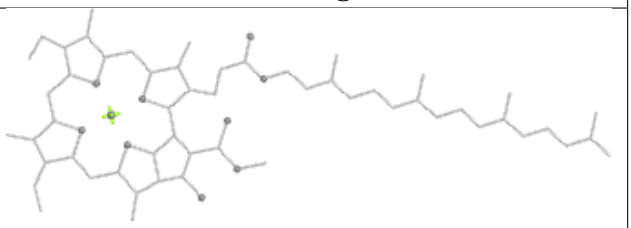
Bond lengths



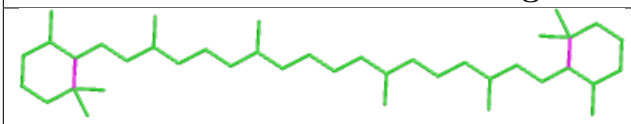
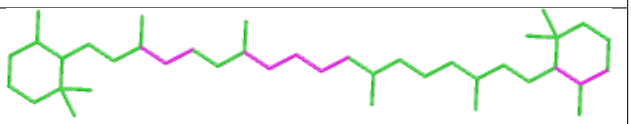
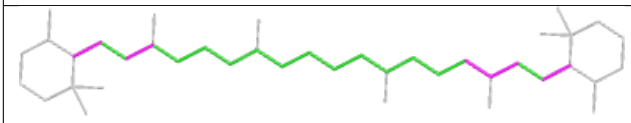
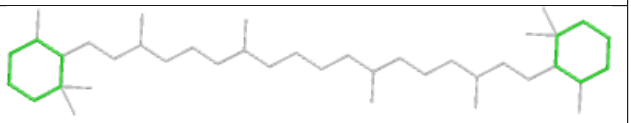
Bond angles

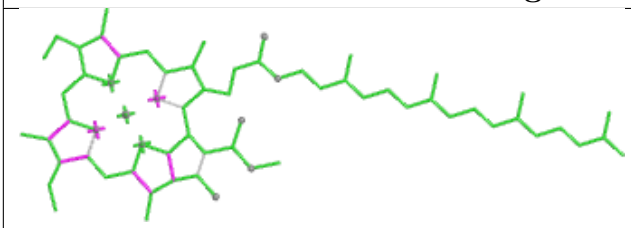
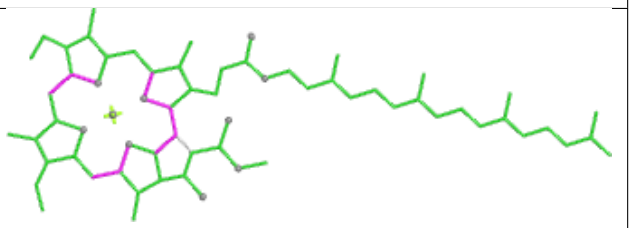
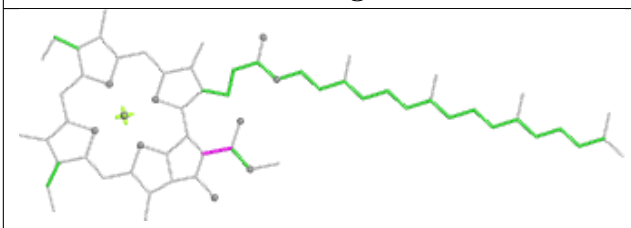
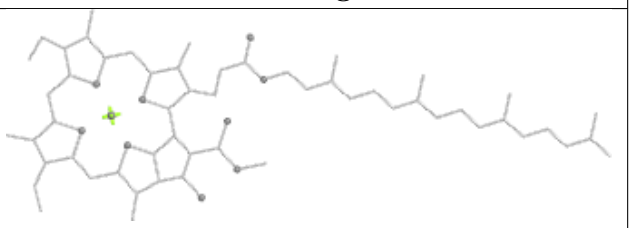


Torsions

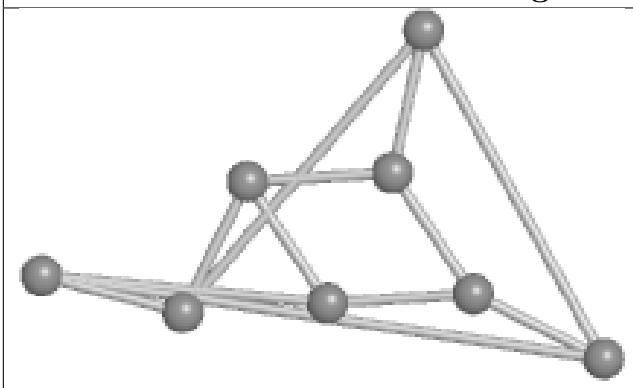


Rings

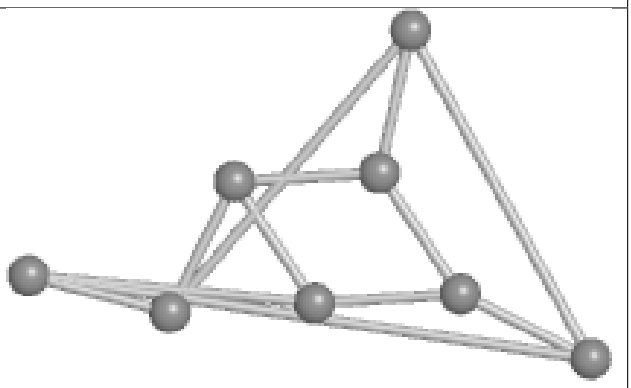
Ligand BCR A 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

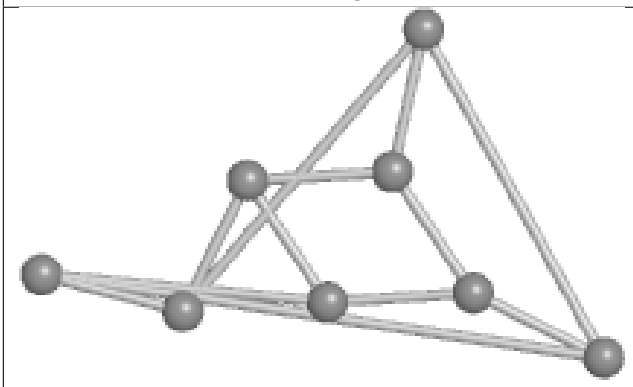
Ligand SF4 C 101



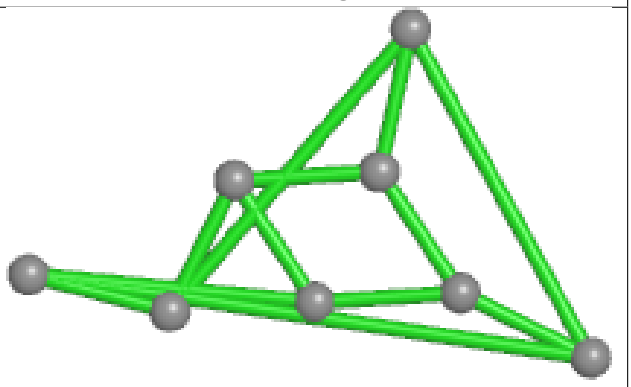
Bond lengths



Bond angles

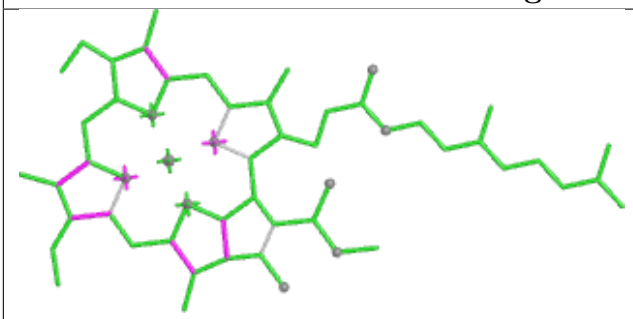


Torsions

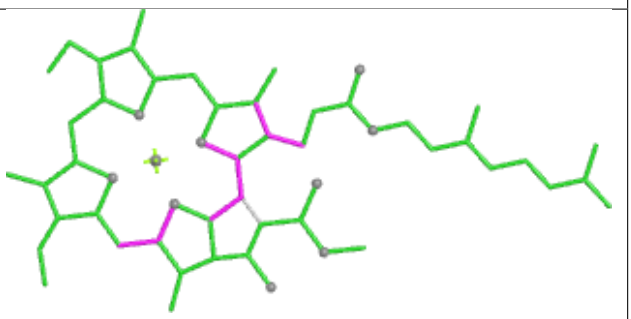


Rings

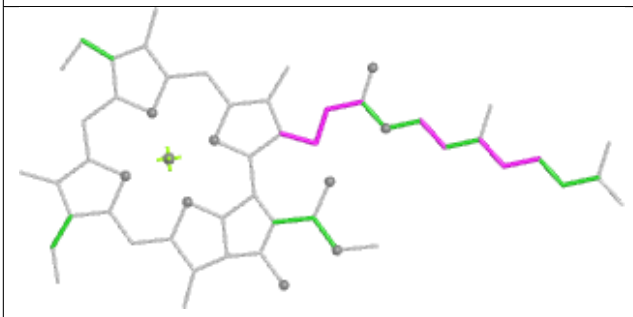
Ligand CLA B 814



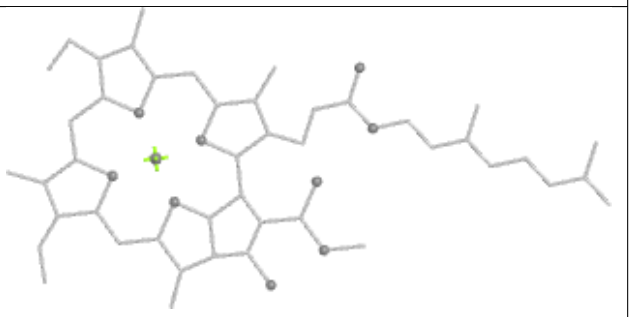
Bond lengths



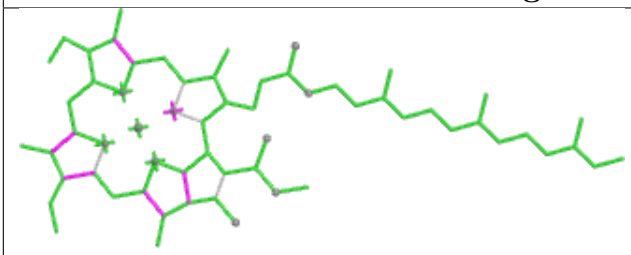
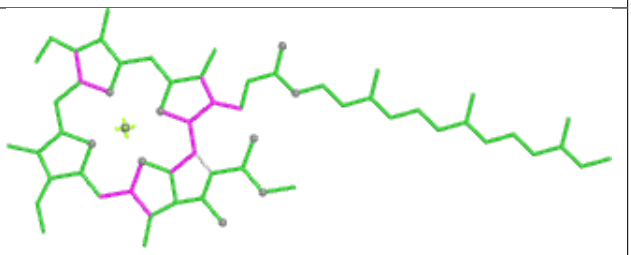
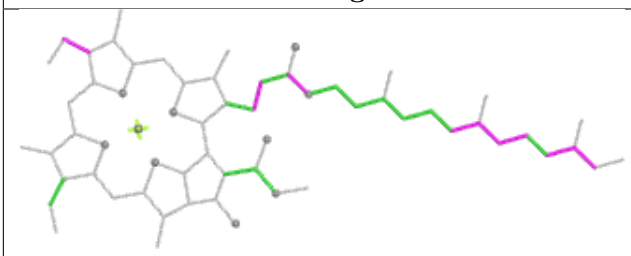
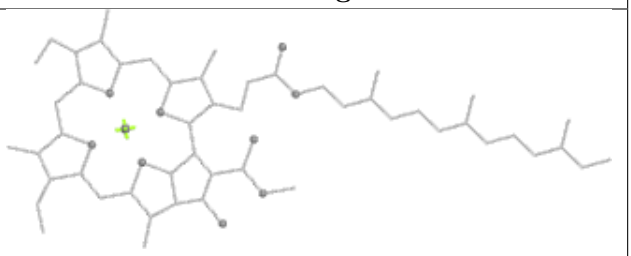
Bond angles

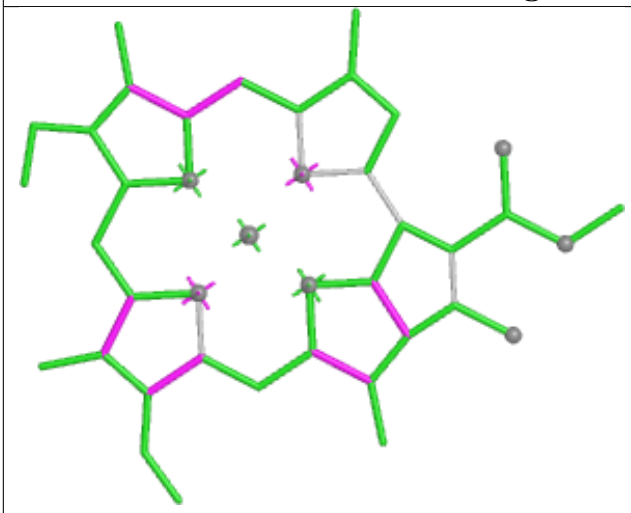
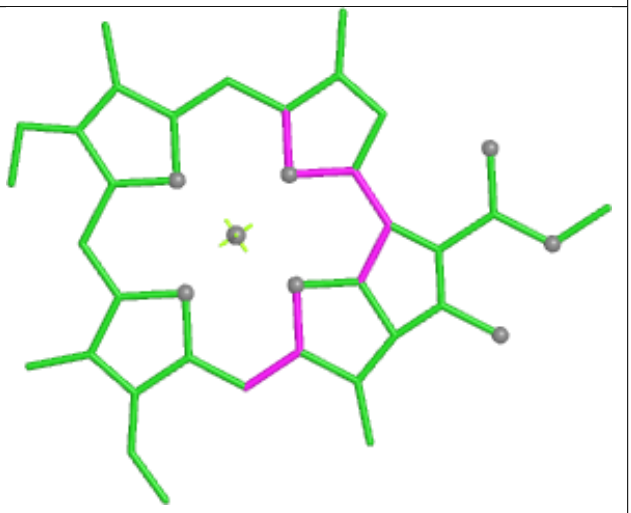
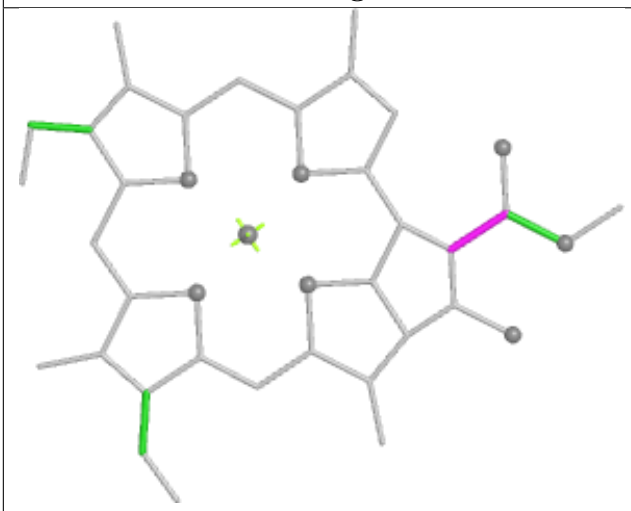
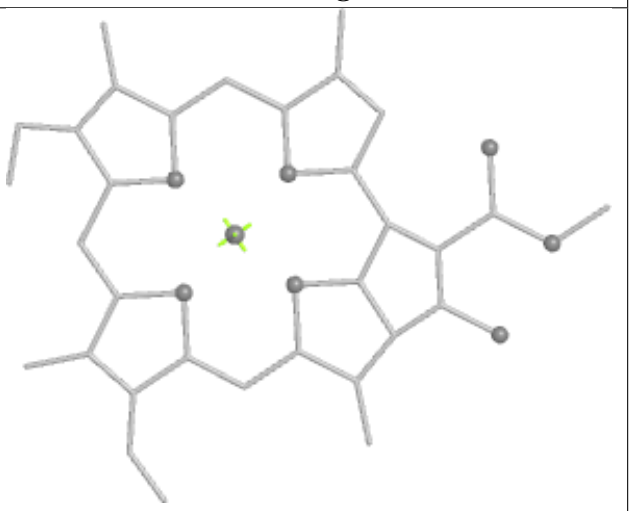


Torsions

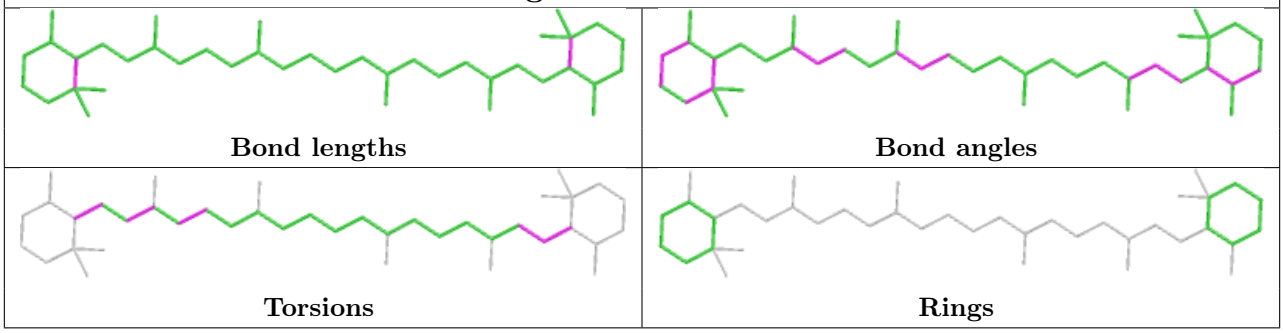


Rings

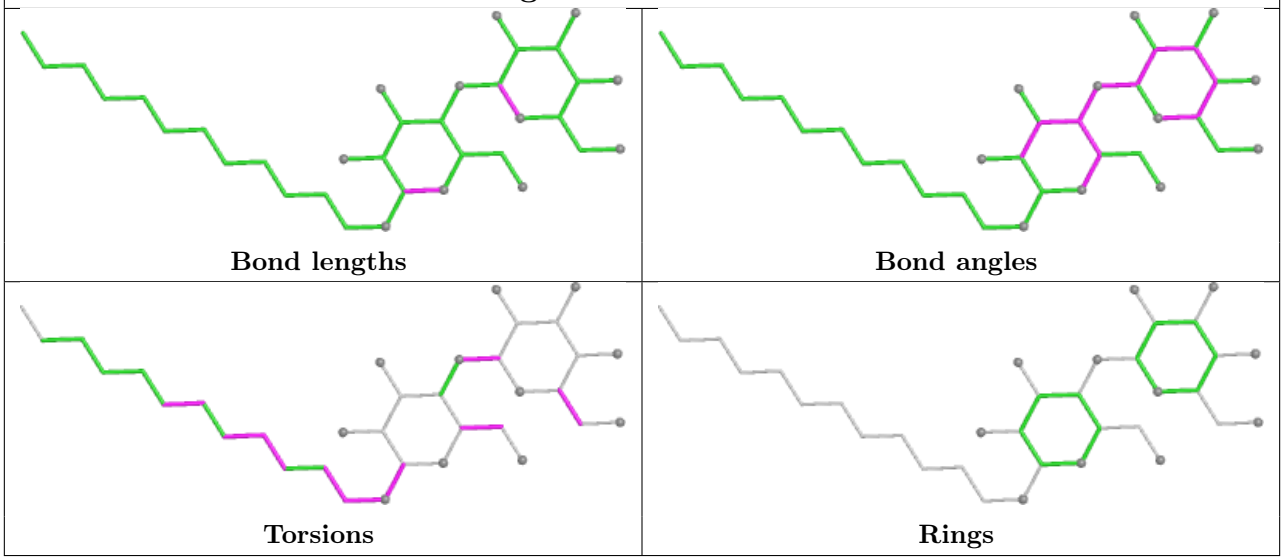
Ligand CLA G 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

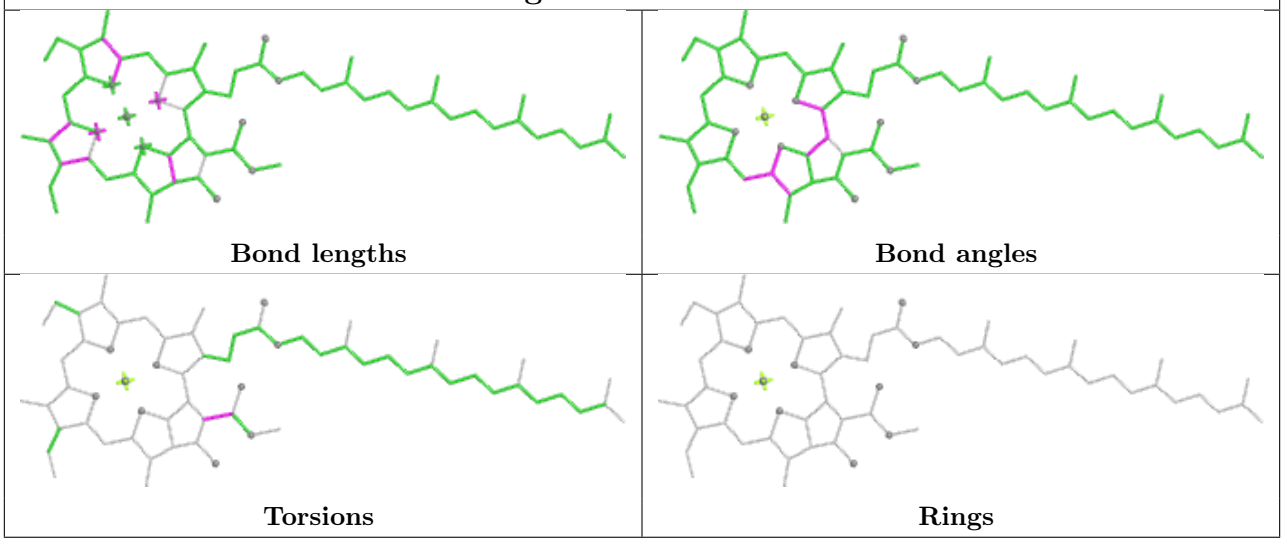
Ligand BCR L 205

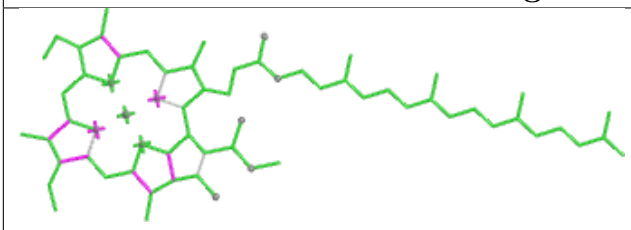
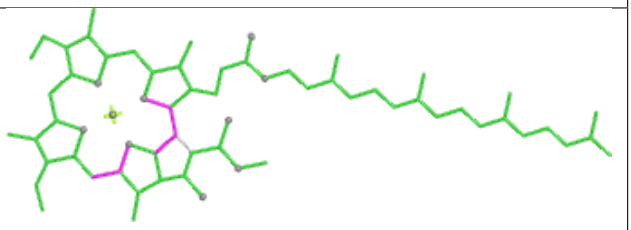
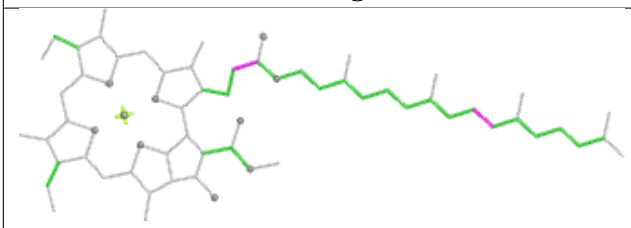
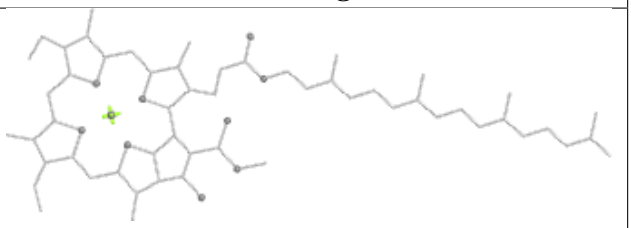


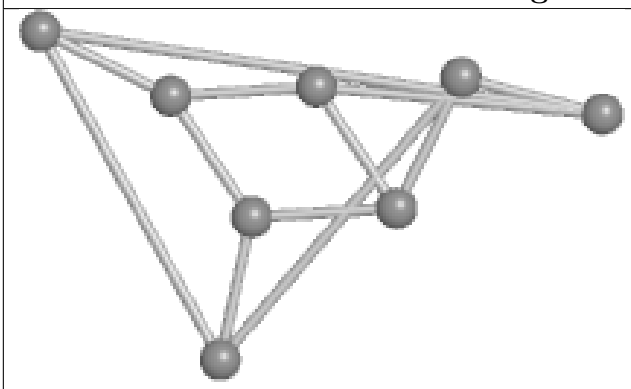
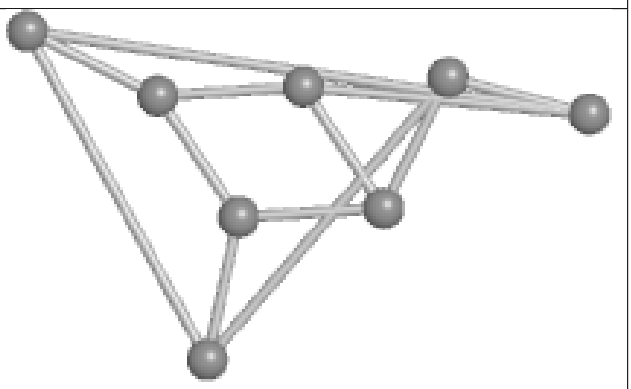
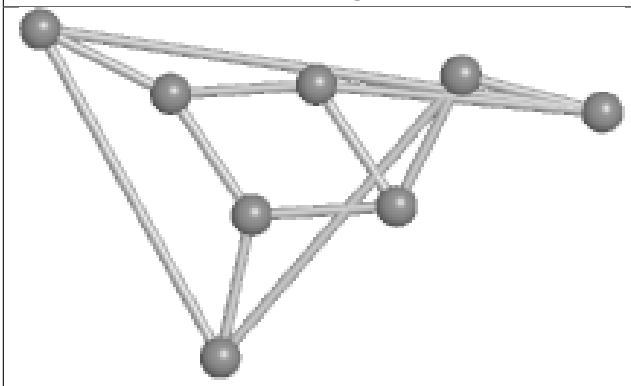
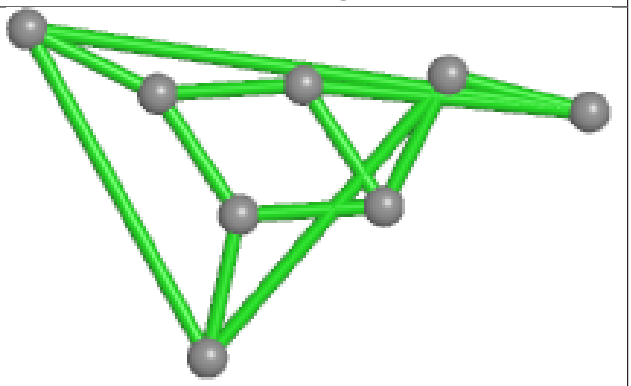
Ligand LMU K 201

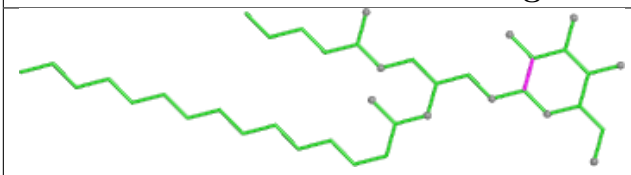
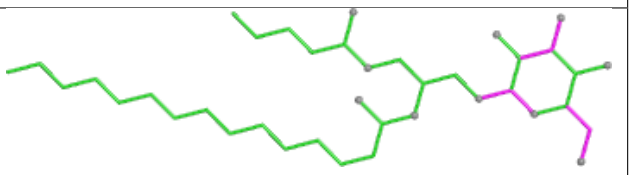
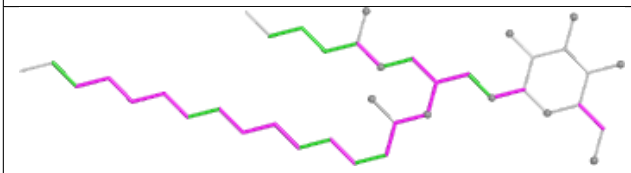
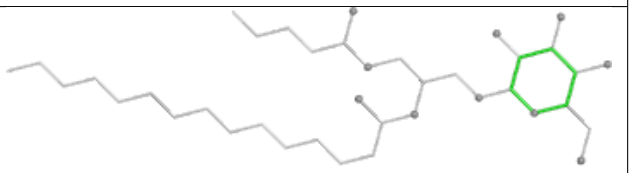


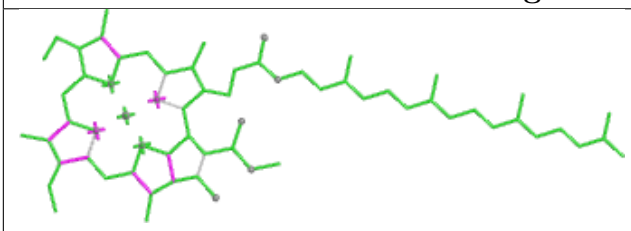
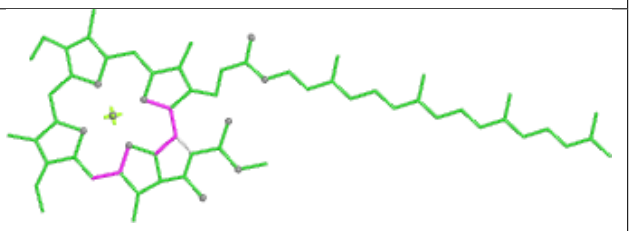
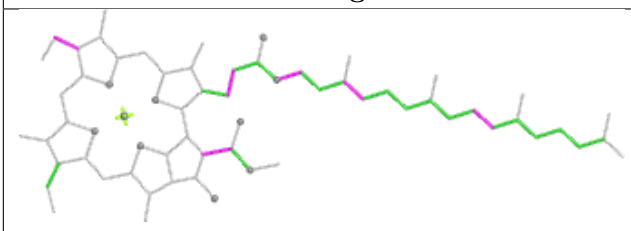
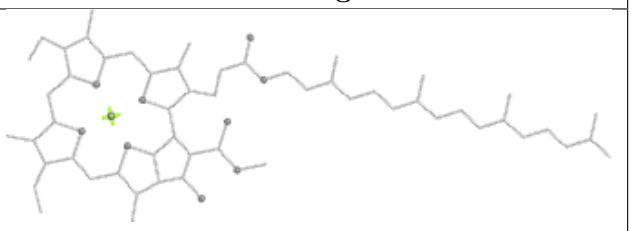
Ligand CLA A 816



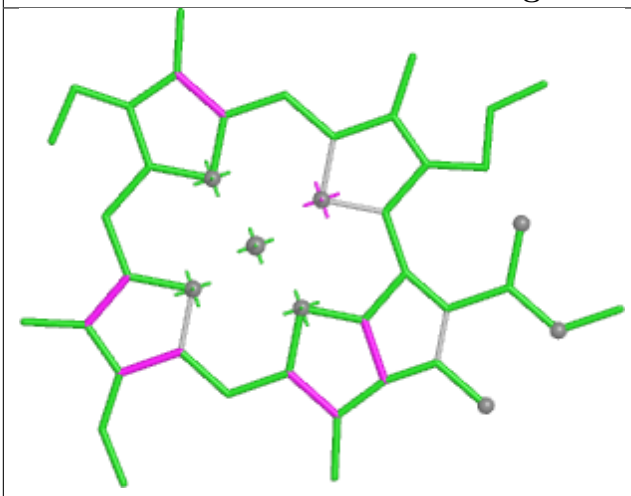
Ligand CLA A 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 A 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

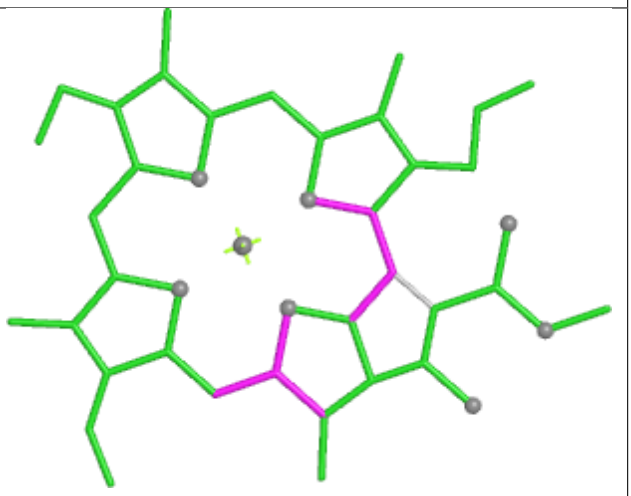
Ligand LMG J 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

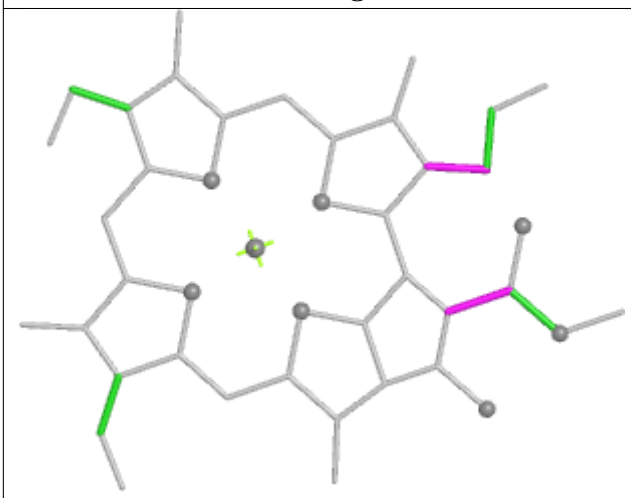
Ligand CLA G 304



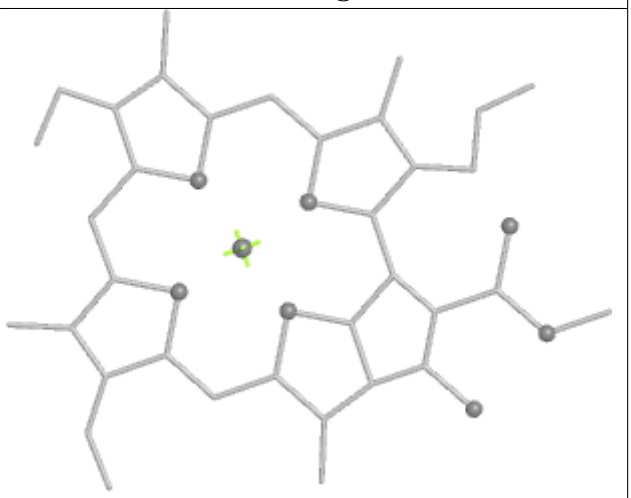
Bond lengths



Bond angles

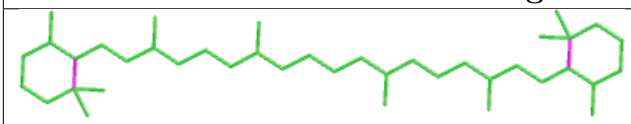


Torsions



Rings

Ligand BCR J 105



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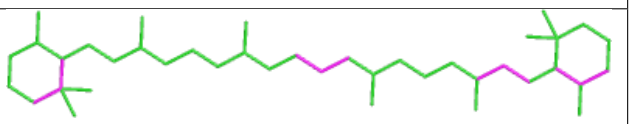
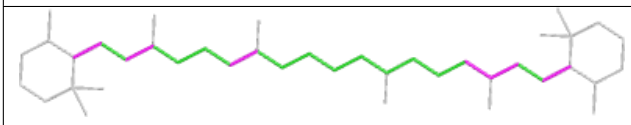


Bond angles



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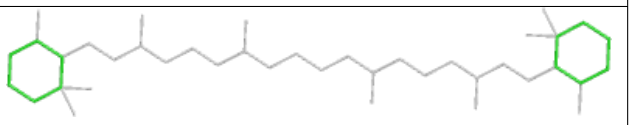
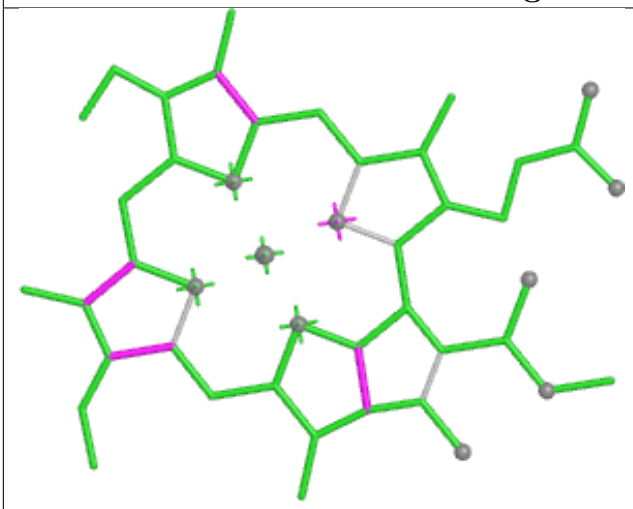
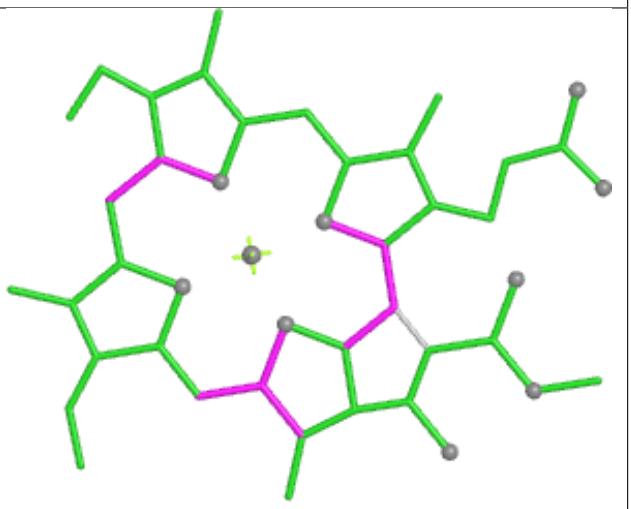


Rings

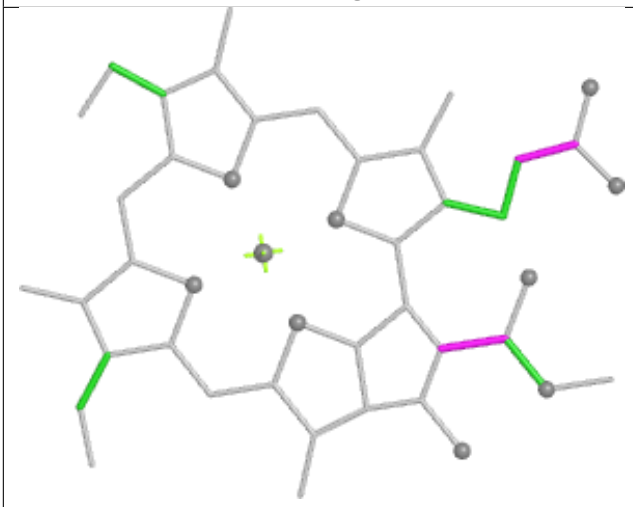
Ligand CLA A 831



Bond lengths



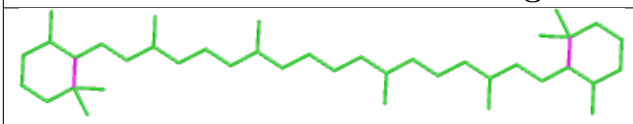
Bond angles



Torsions

Rings

Ligand BCR F 801



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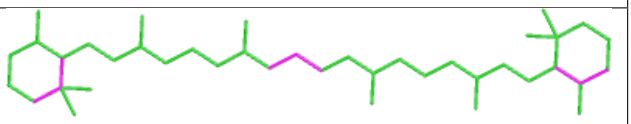
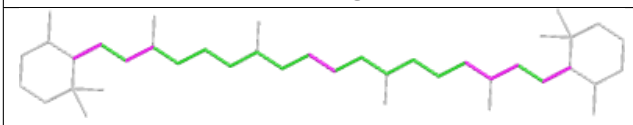


Bond angles



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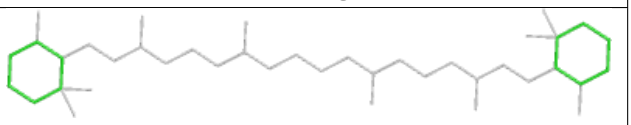
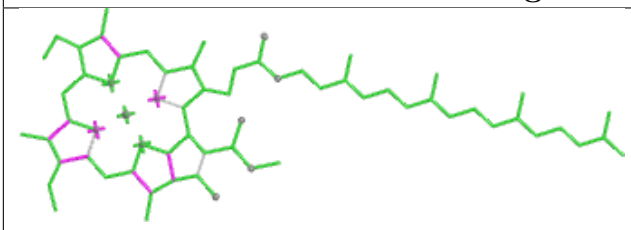
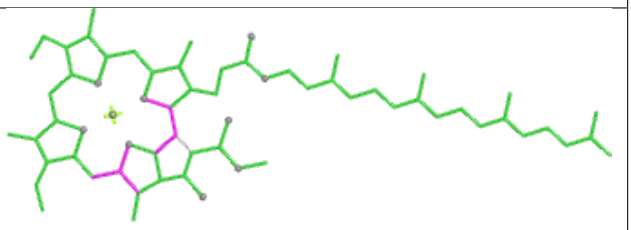
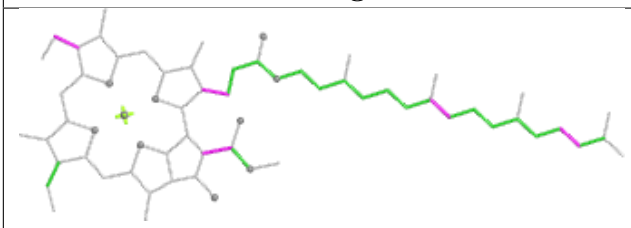
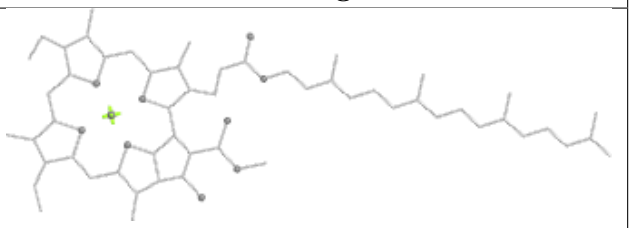
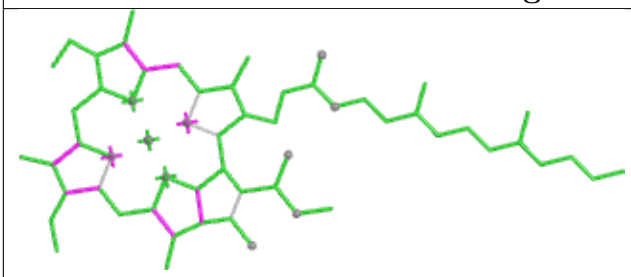
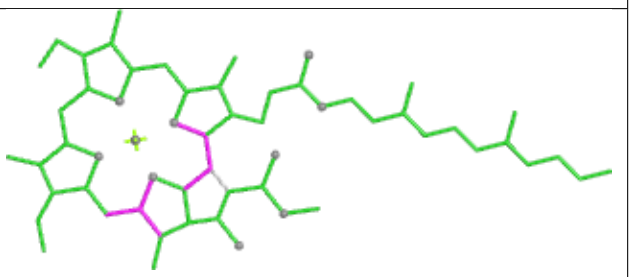
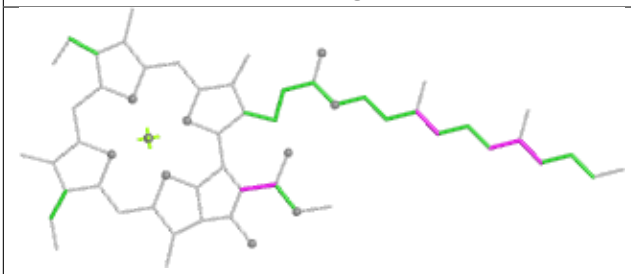
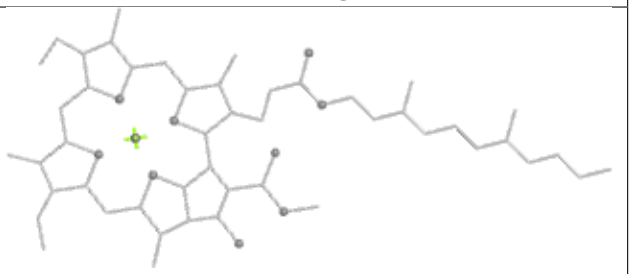
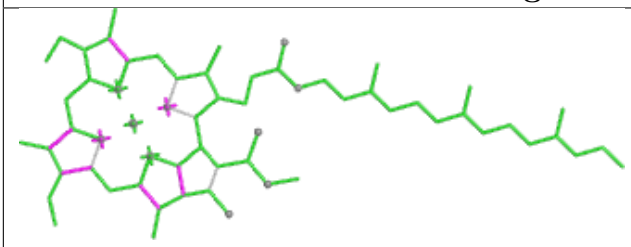
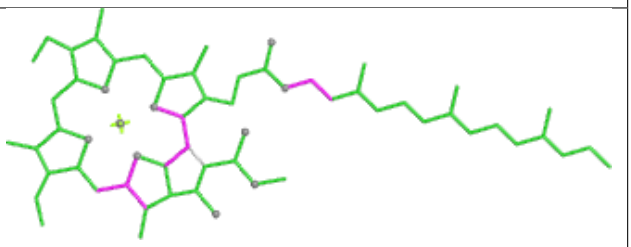
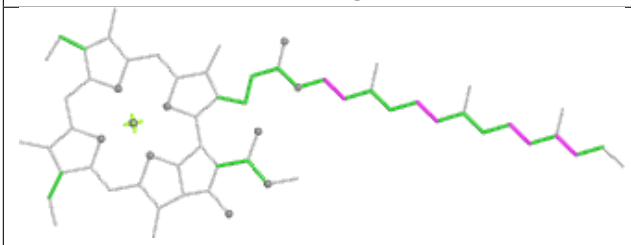
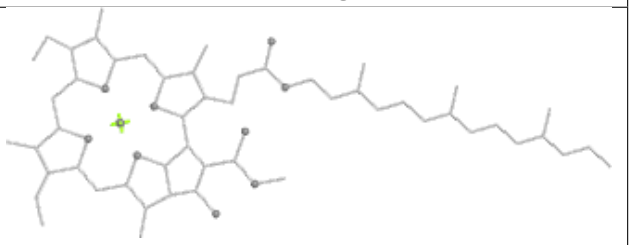
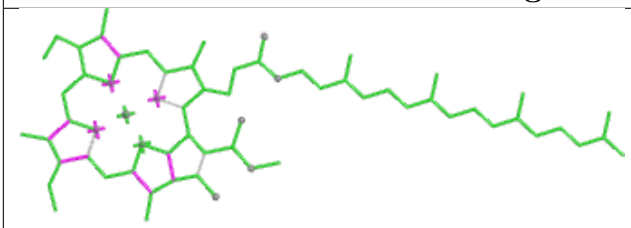
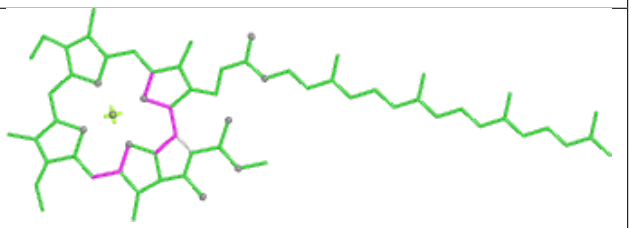
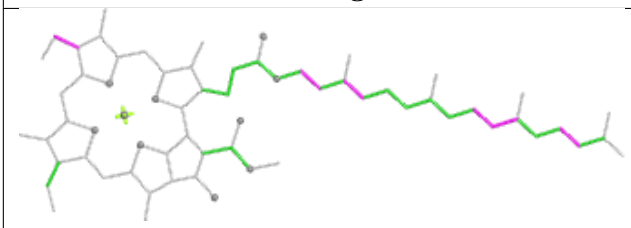
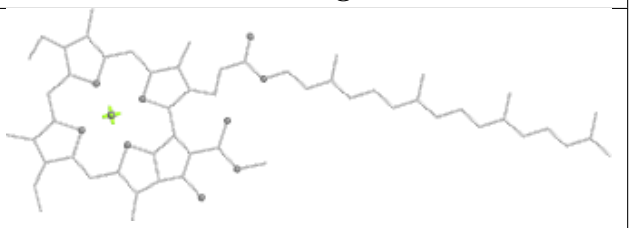


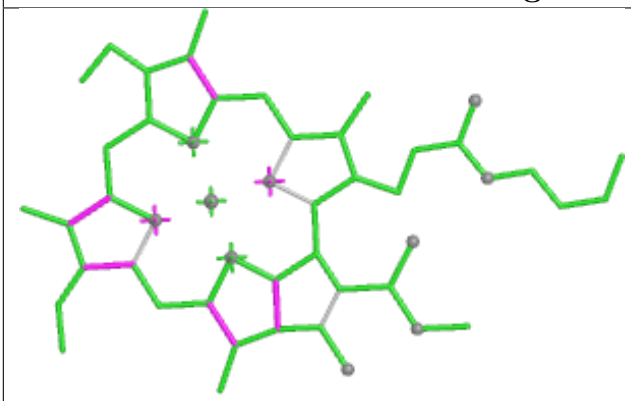
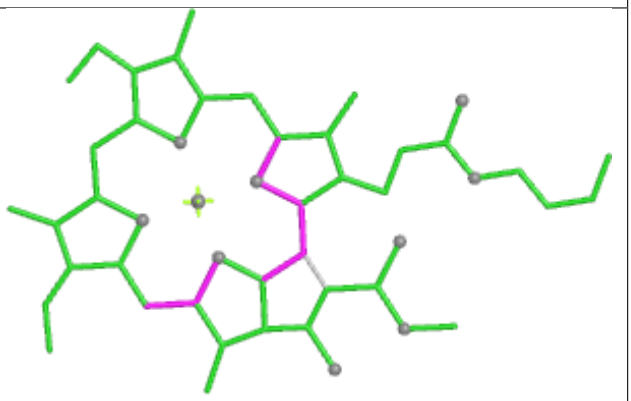
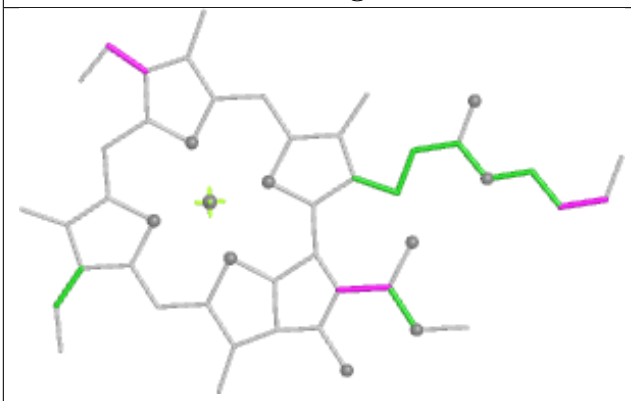
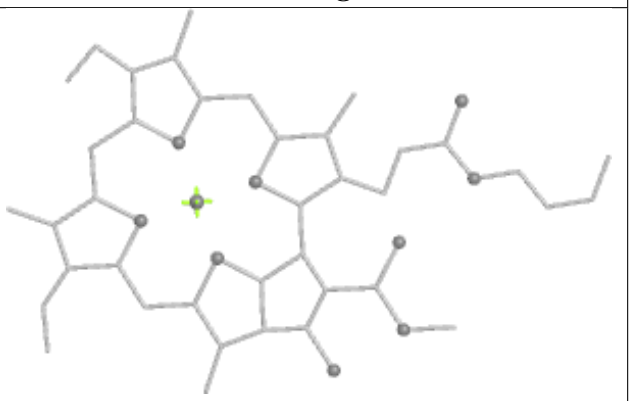
Rings

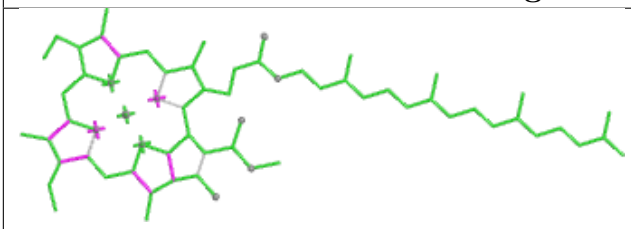
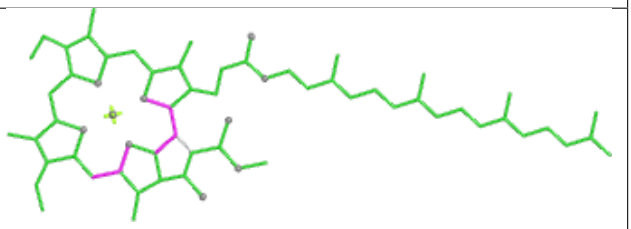
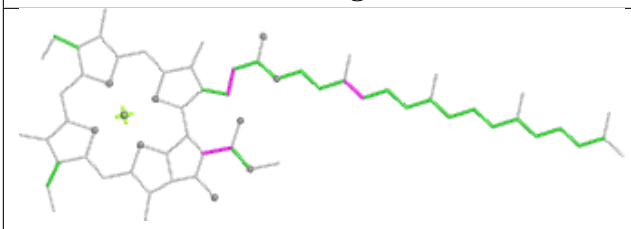
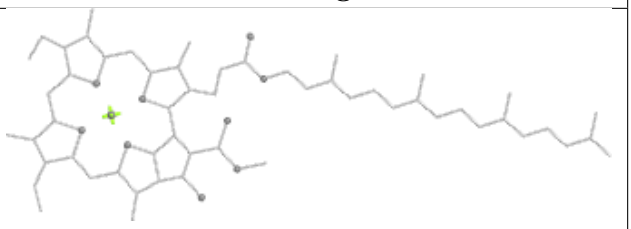
Ligand CLA B 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

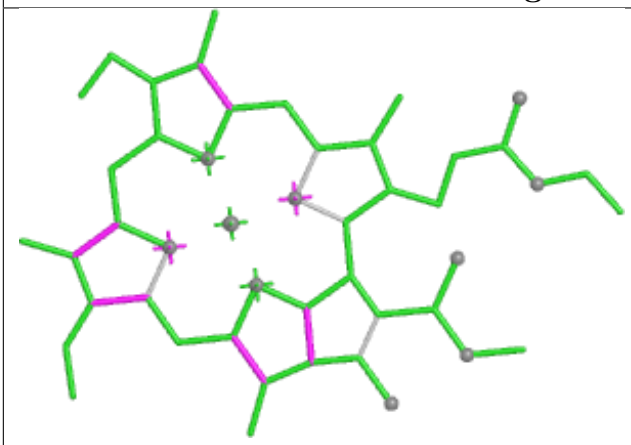
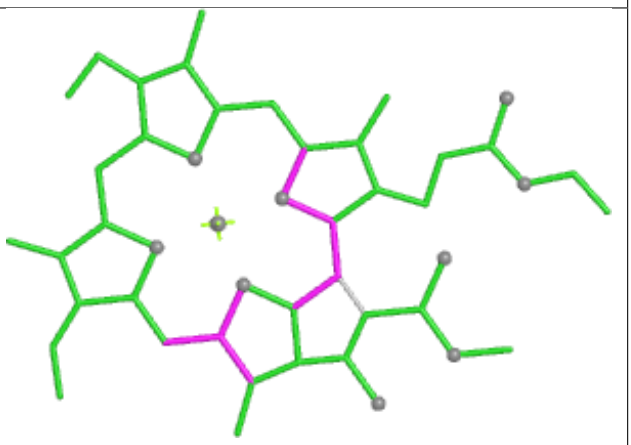
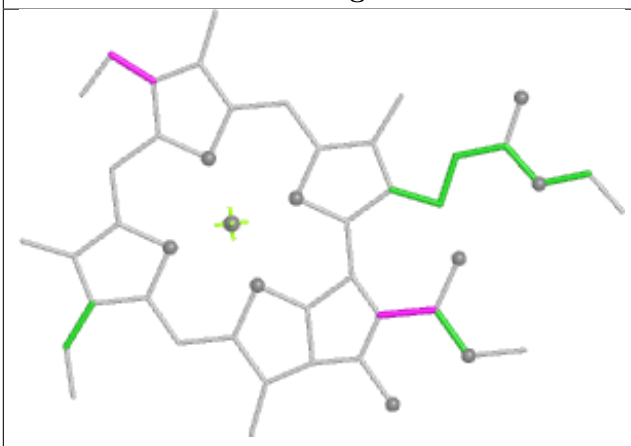
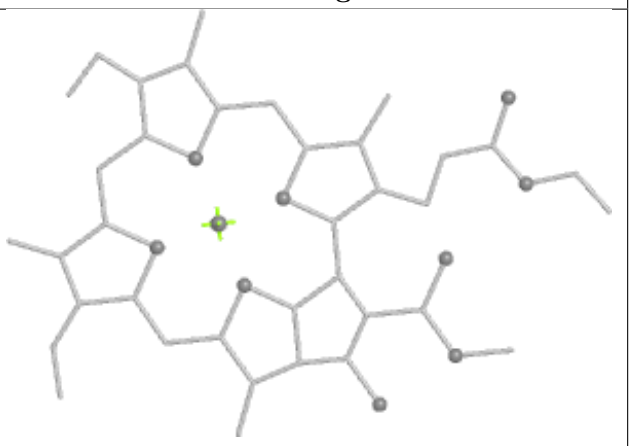
Ligand CLA H 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

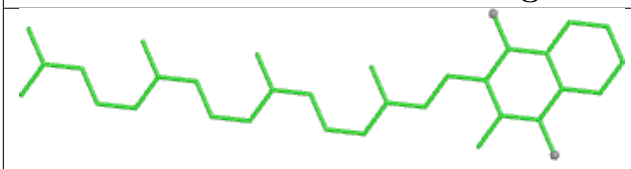
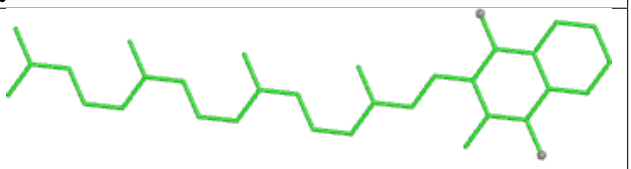
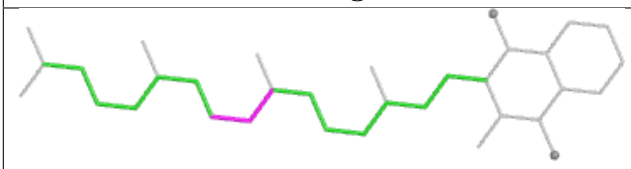
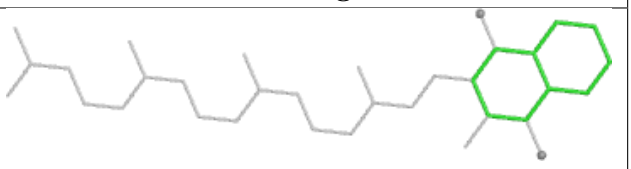
Ligand CLA A 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

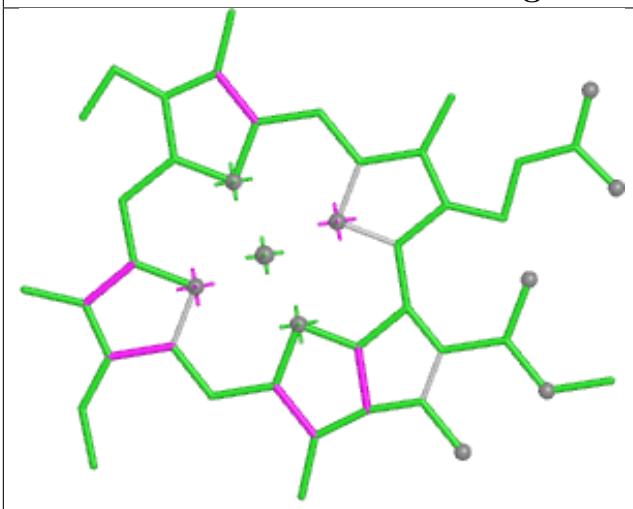
Ligand CLA A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

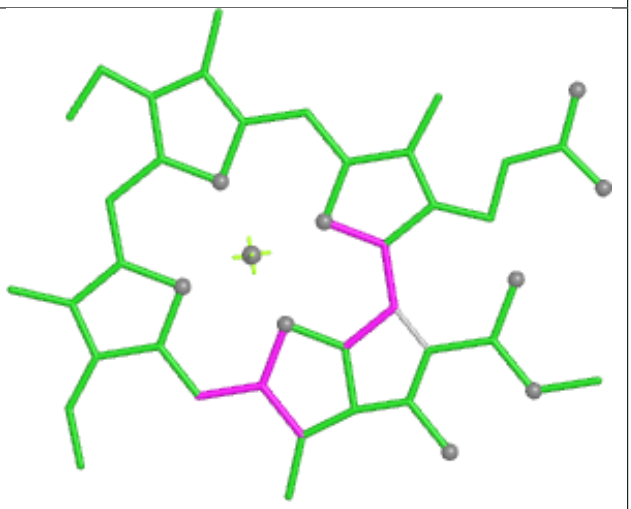
Ligand CLA B 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PQN A 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

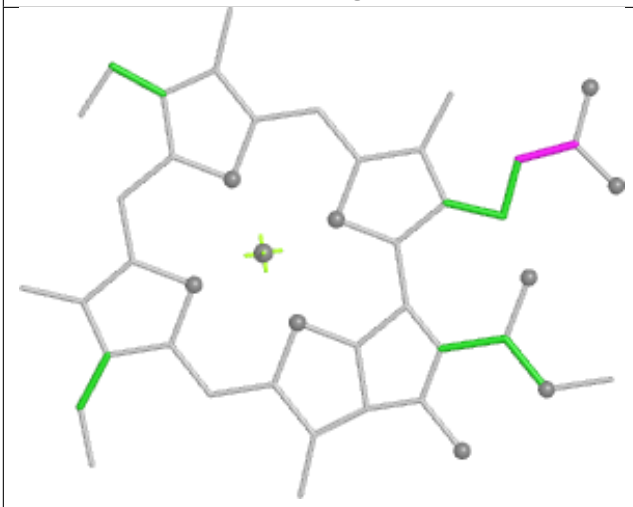
Ligand CLA U 206



Bond lengths



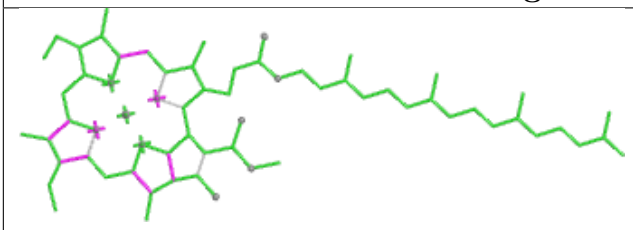
Bond angles



Torsions

Rings

Ligand CLA A 828



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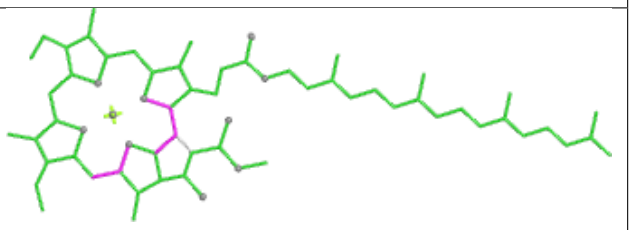
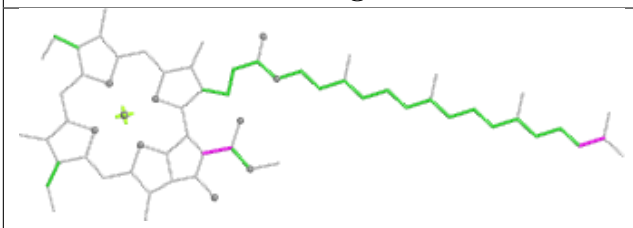


Bond angles



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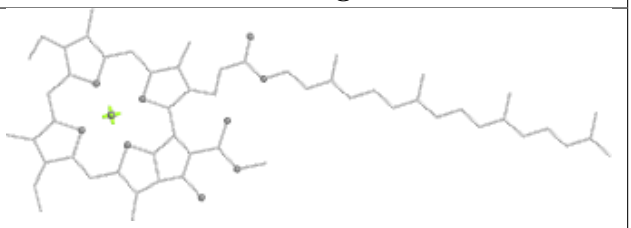
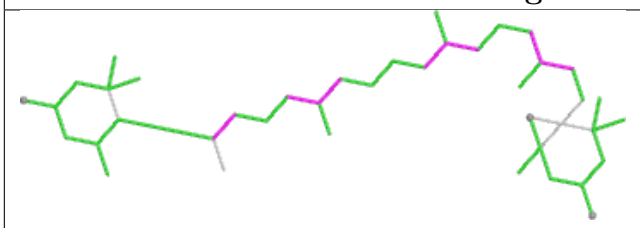
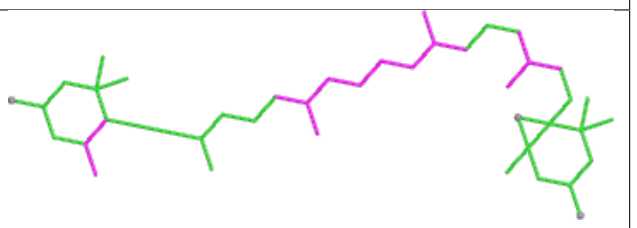
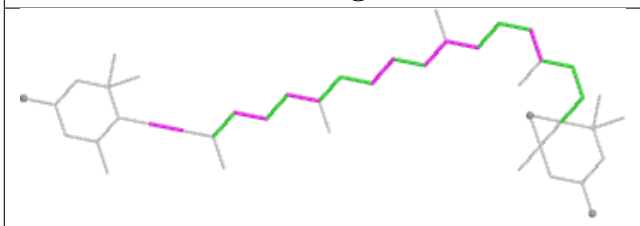
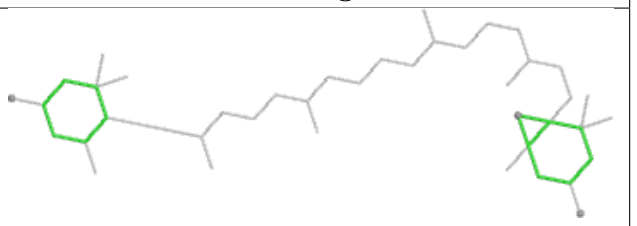
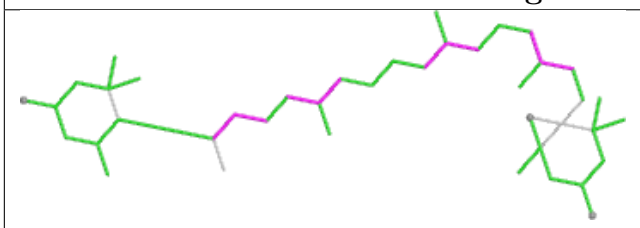
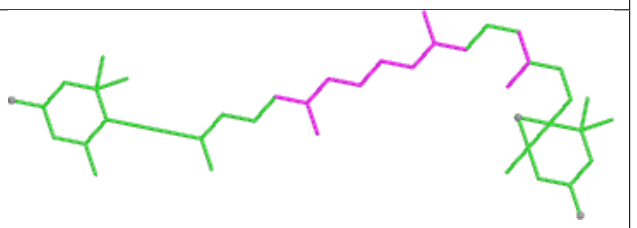
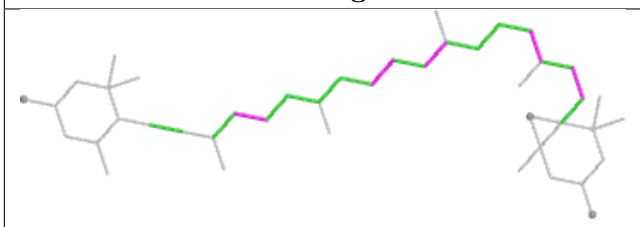
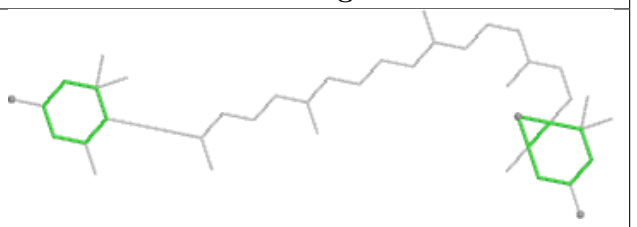
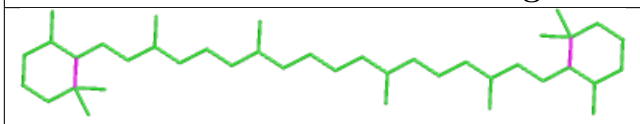
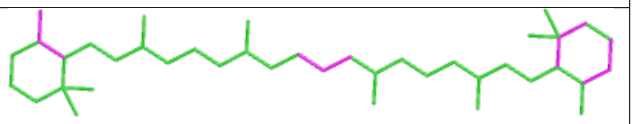
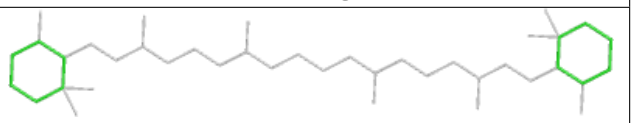
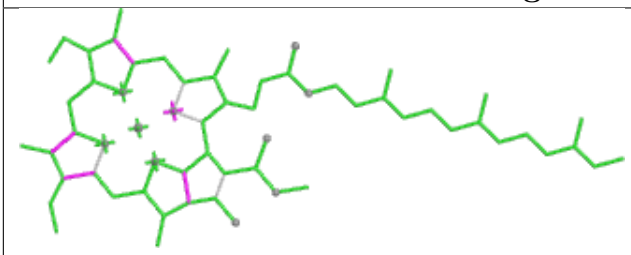
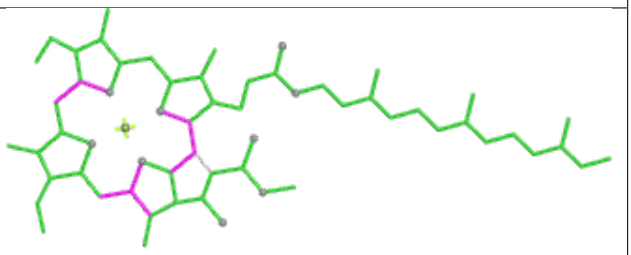
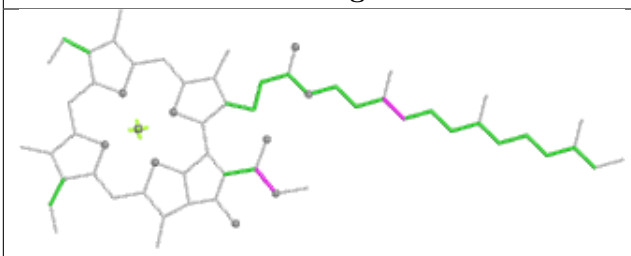
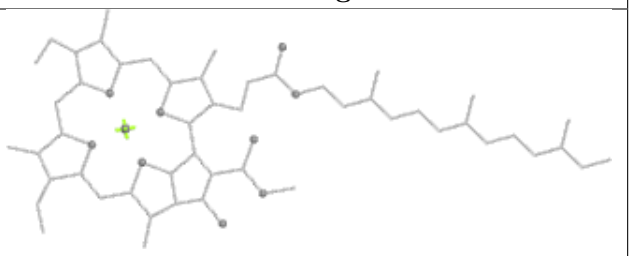


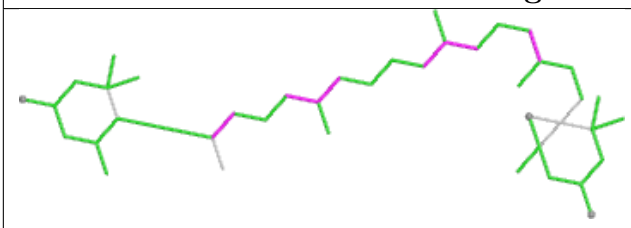
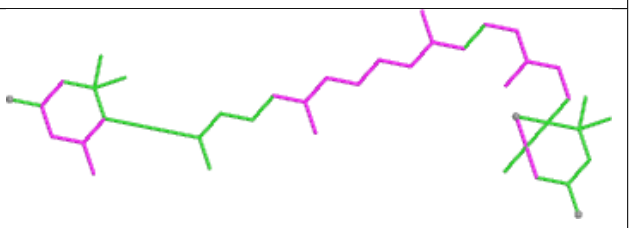
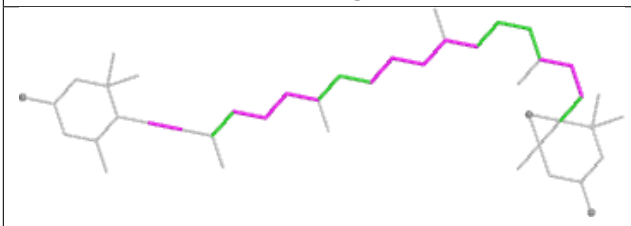
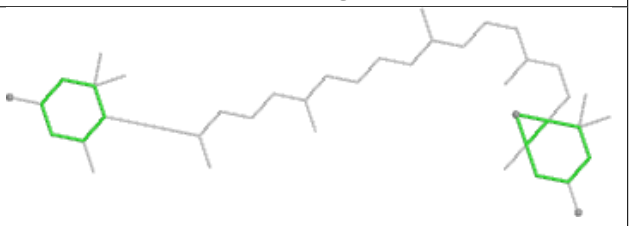
Rings

Ligand DD6 K 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

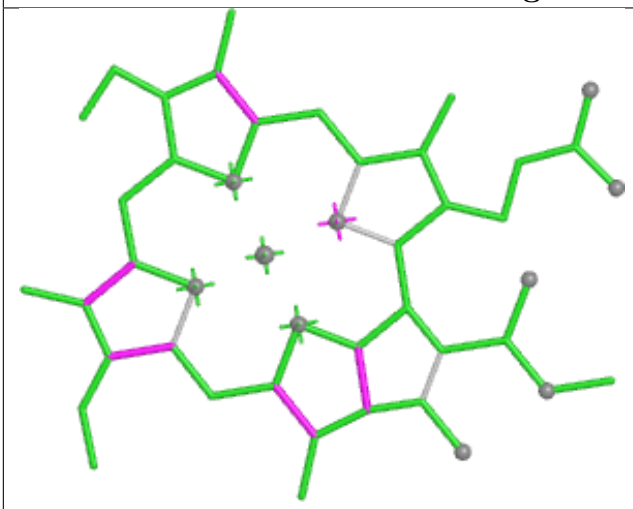
Ligand DD6 G 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 843	
 Bond lengths	 Bond angles
Torsions	 Rings

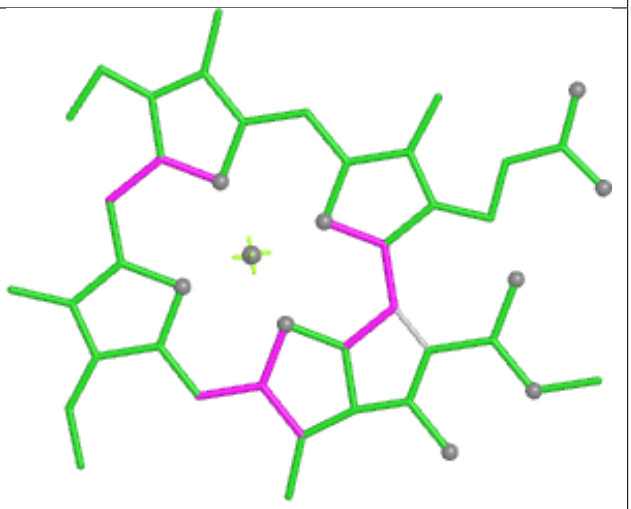
Ligand CLA H 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 U 212	
 Bond lengths	 Bond angles
 Torsions	 Rings

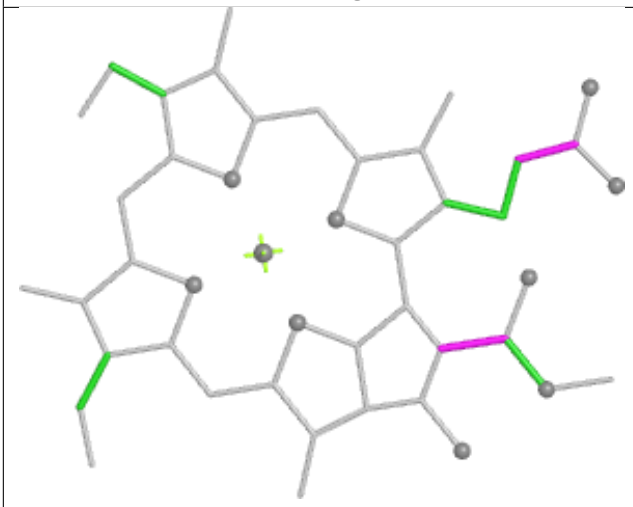
Ligand CLA G 301



Bond lengths



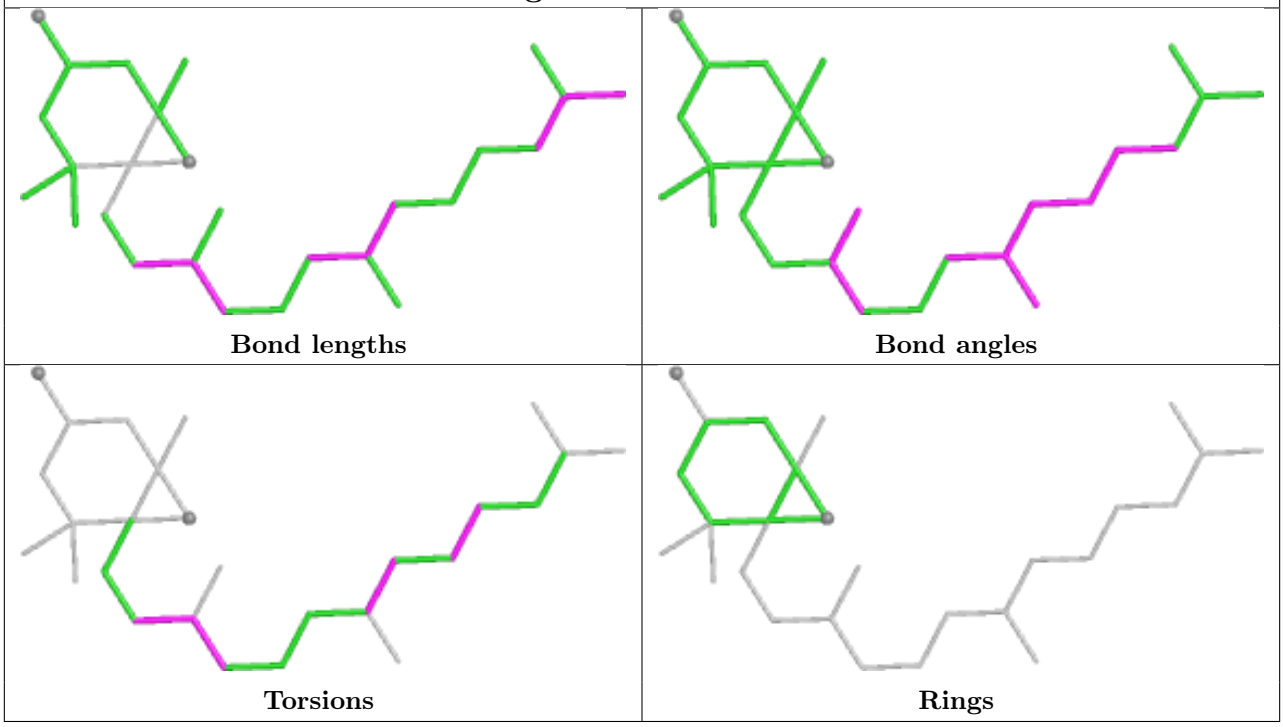
Bond angles



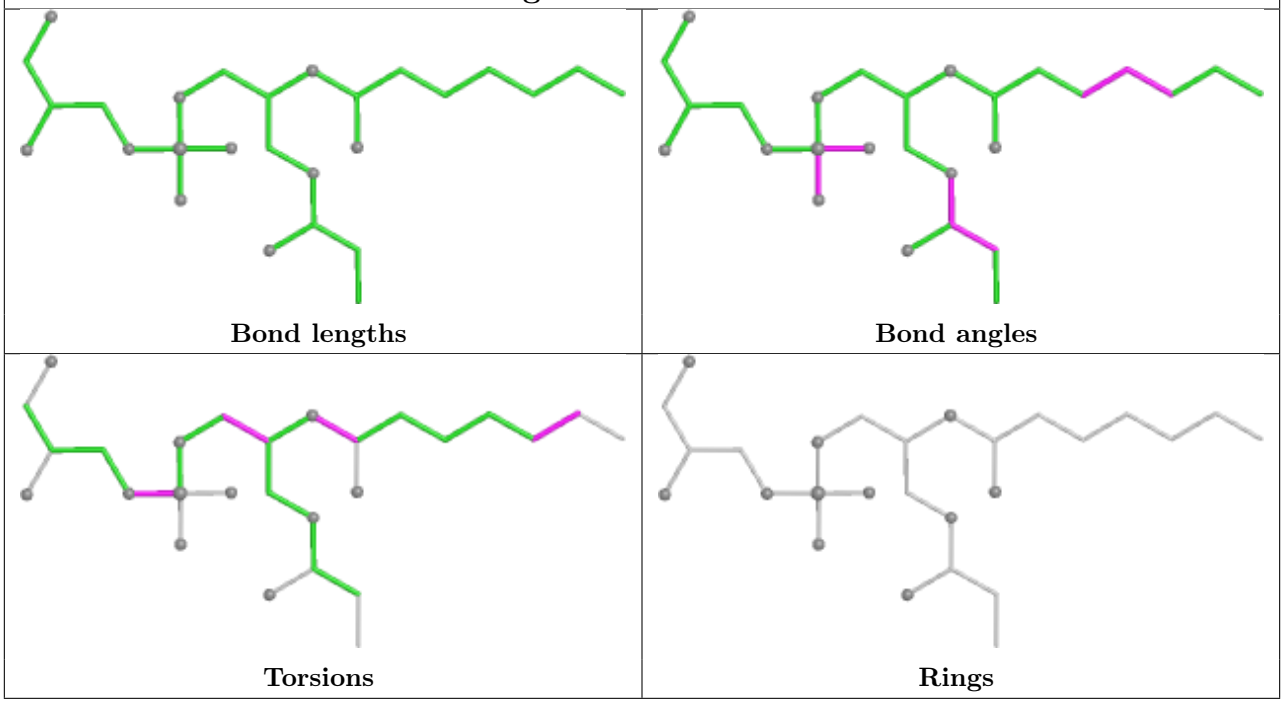
Torsions

Rings

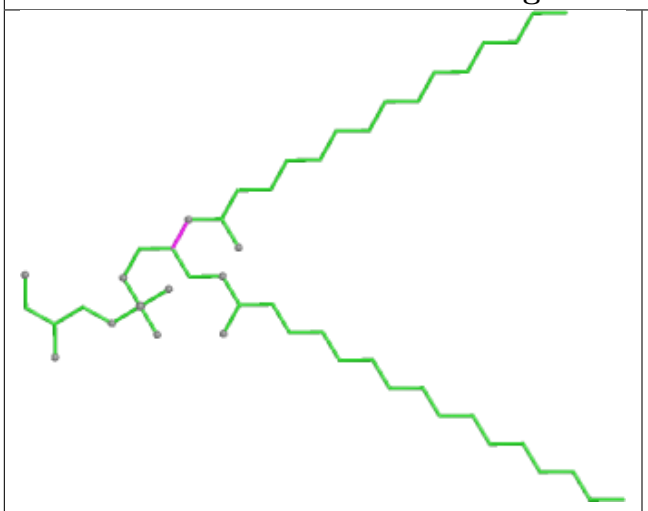
Ligand DD6 G 312



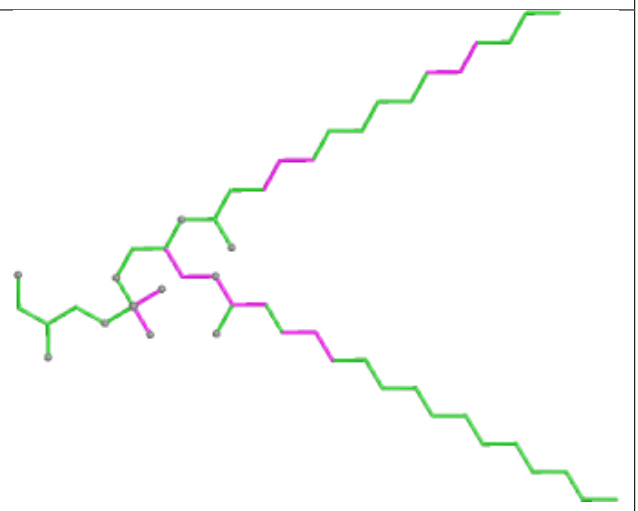
Ligand LHG A 840



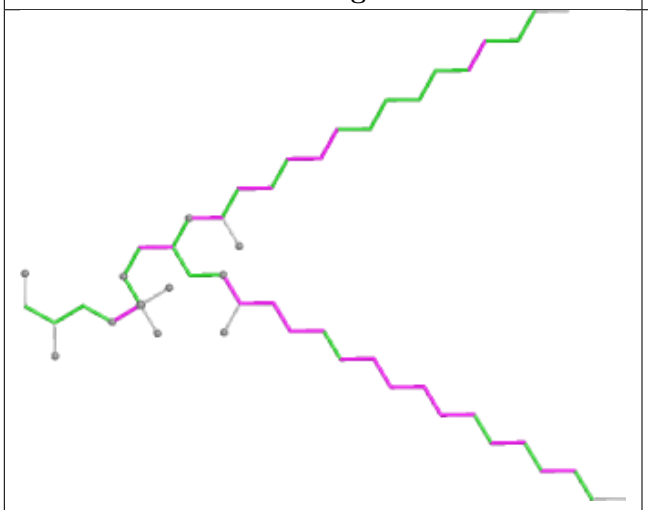
Ligand LHG A 839



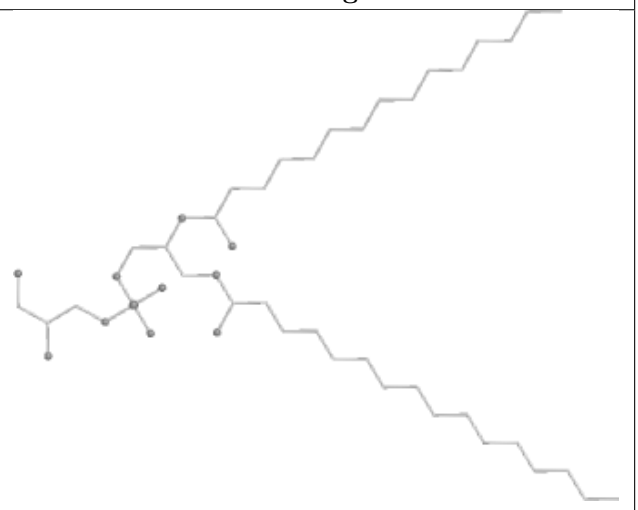
Bond lengths



Bond angles

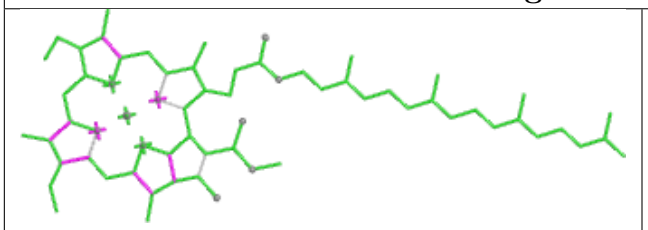


Torsions

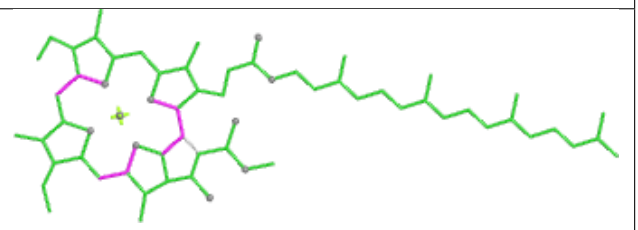


Rings

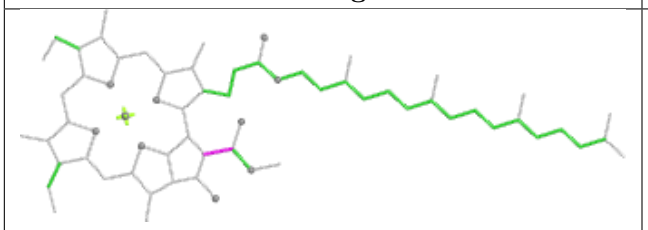
Ligand CLA A 835



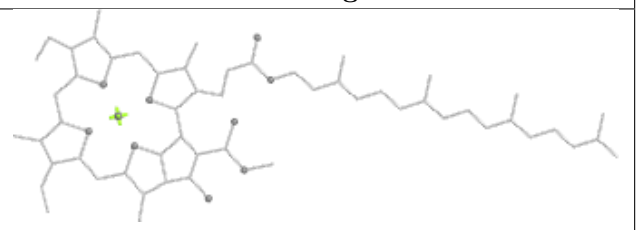
Bond lengths



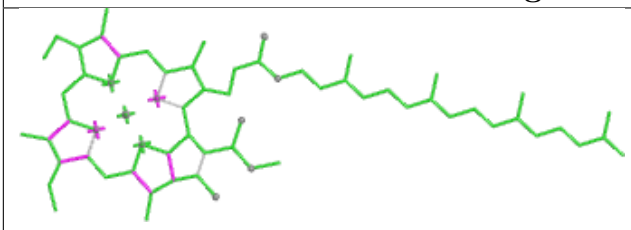
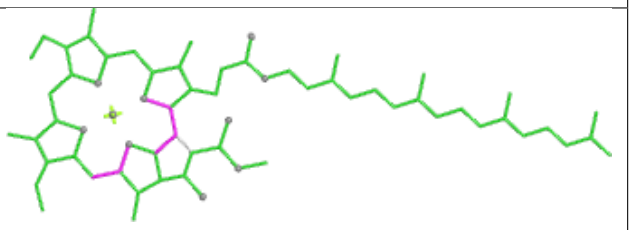
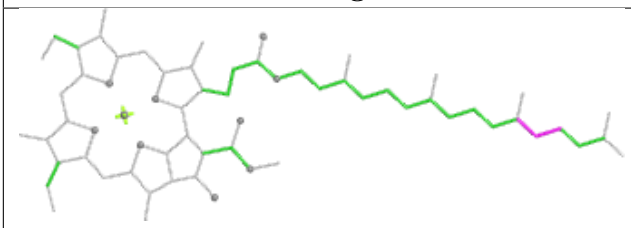
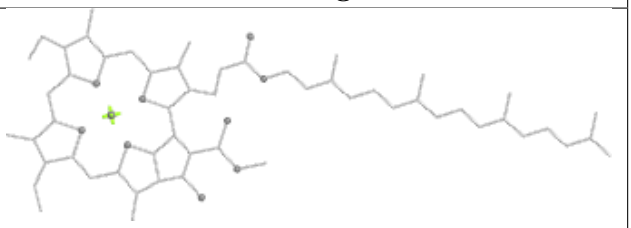
Bond angles

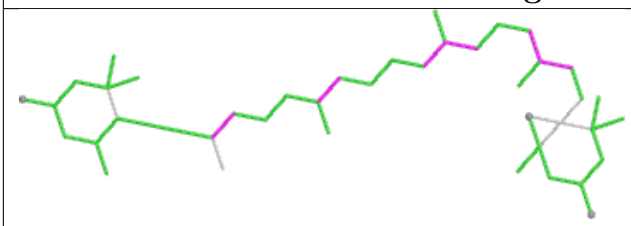
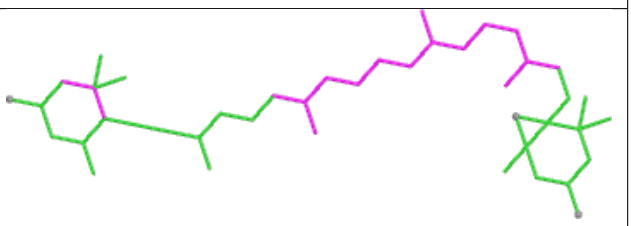
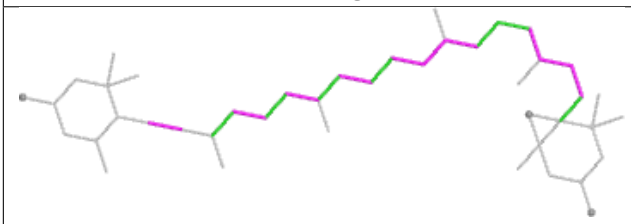


Torsions

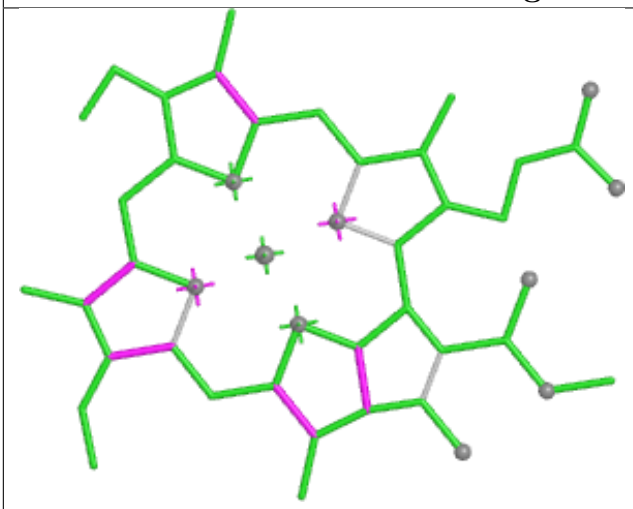


Rings

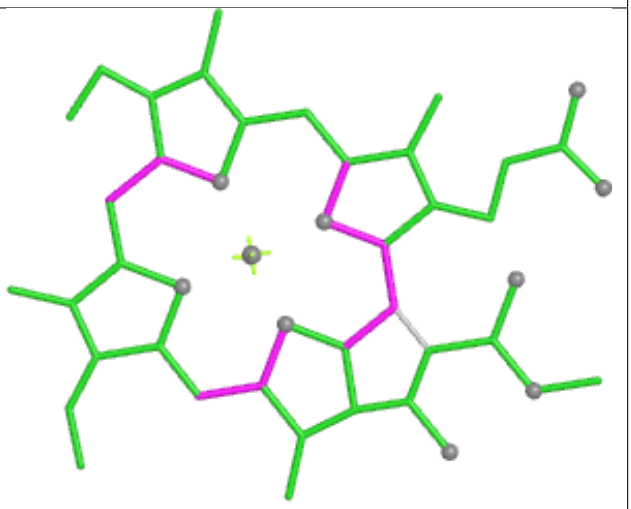
Ligand CLA B 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 H 310	
 Bond lengths	 Bond angles
 Torsions	Rings

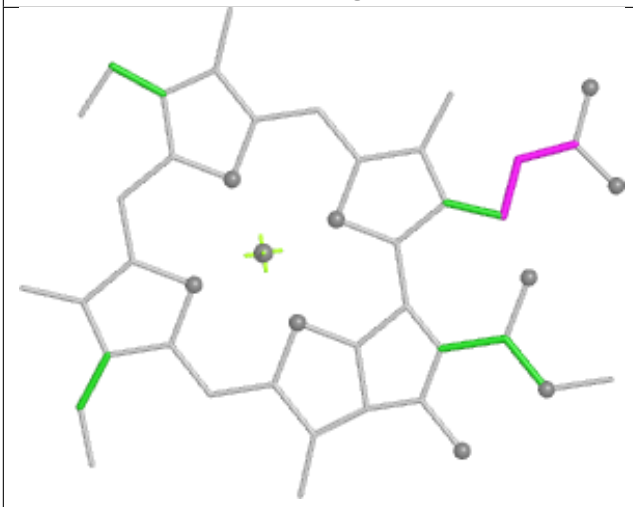
Ligand CLA A 814



Bond lengths



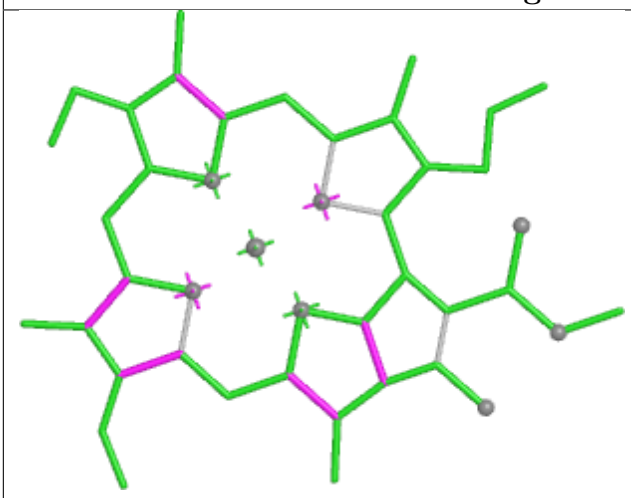
Bond angles



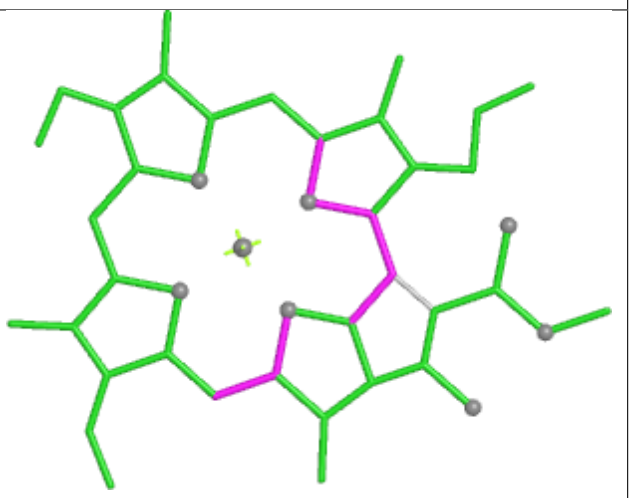
Torsions

Rings

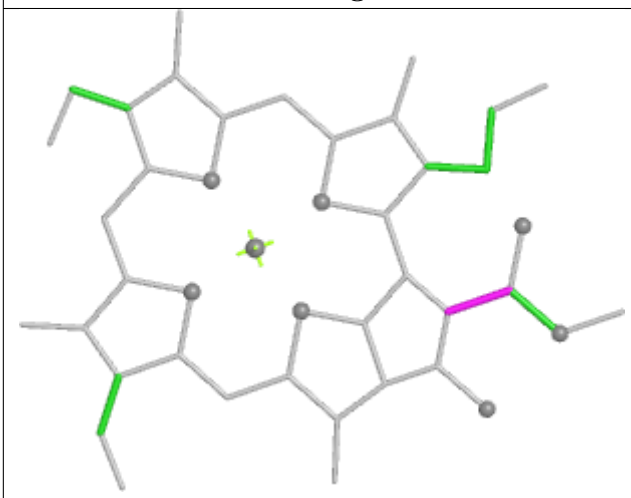
Ligand CLA A 819



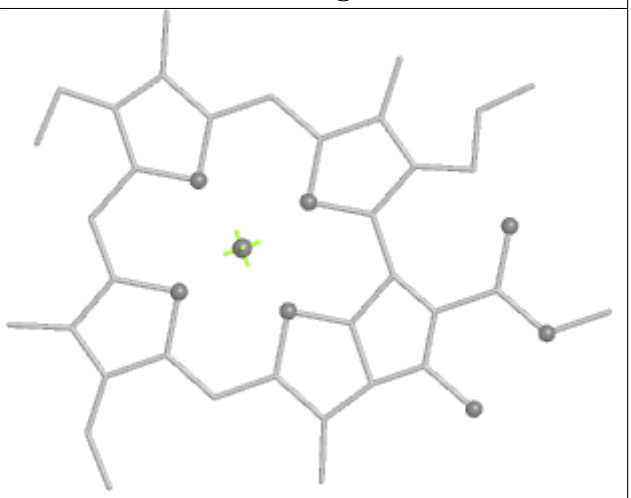
Bond lengths



Bond angles

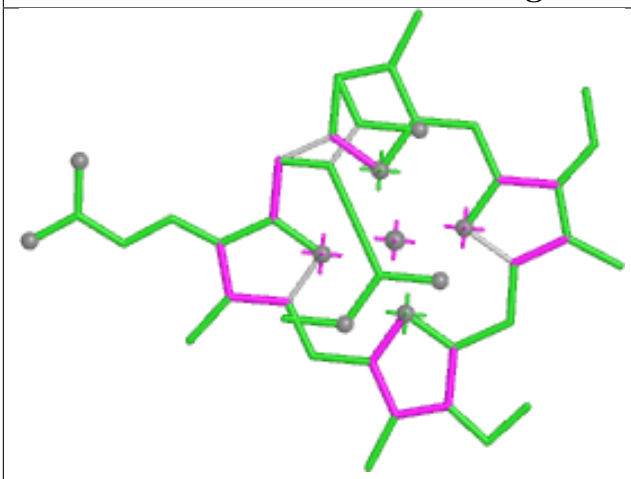


Torsions

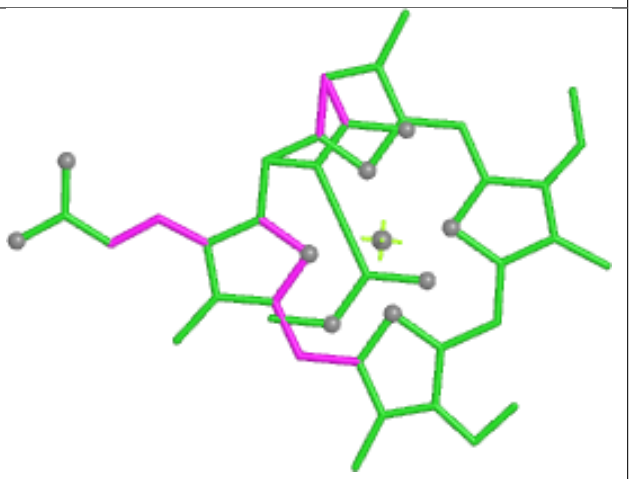


Rings

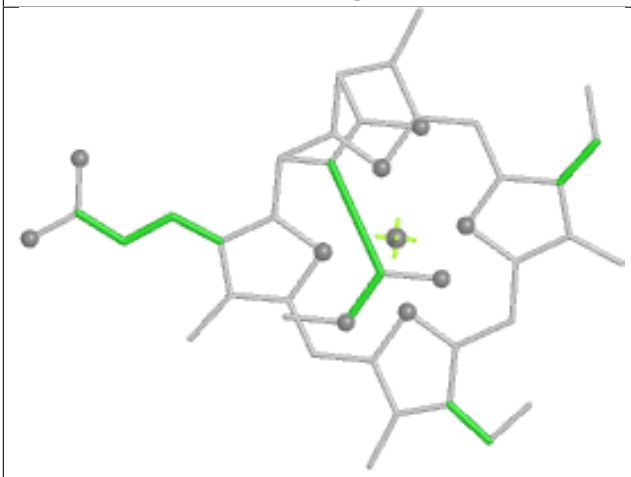
Ligand KC1 U 213



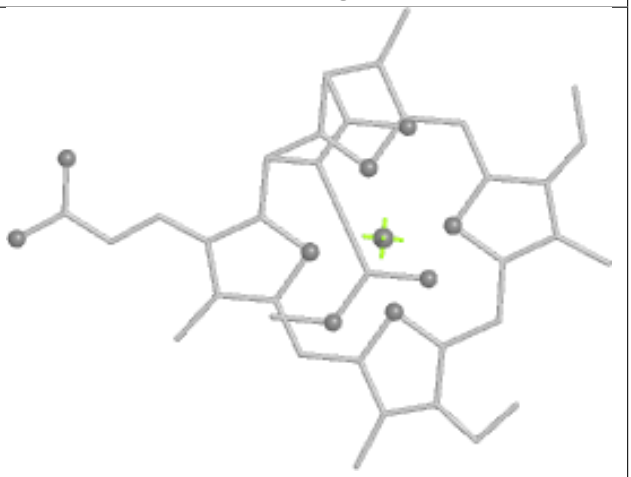
Bond lengths



Bond angles

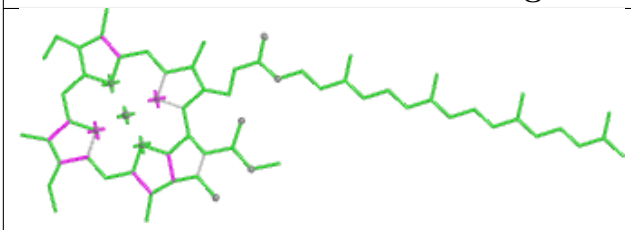


Torsions

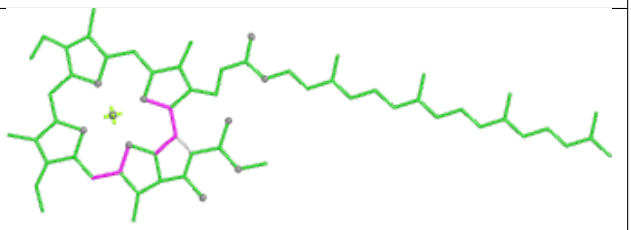


Rings

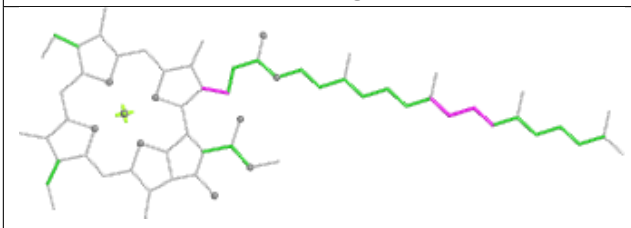
Ligand CLA B 844



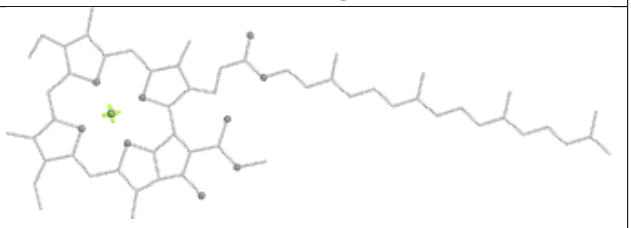
Bond lengths



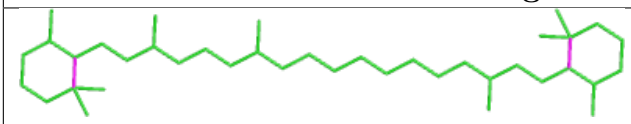
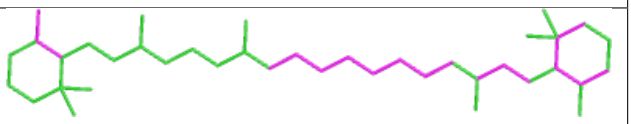
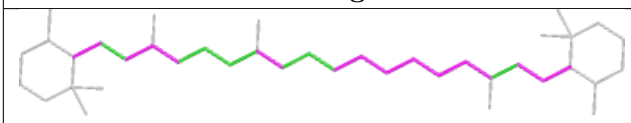
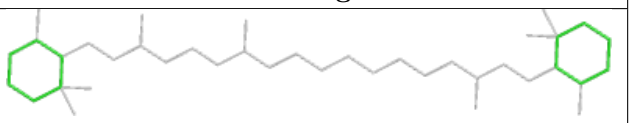
Bond angles

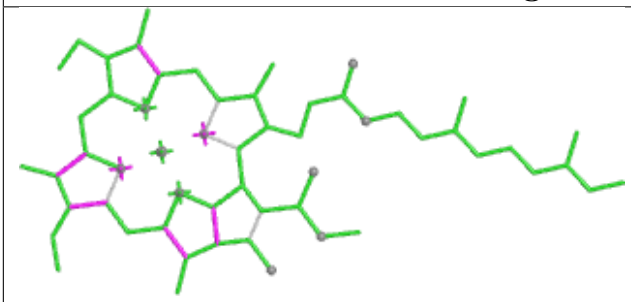
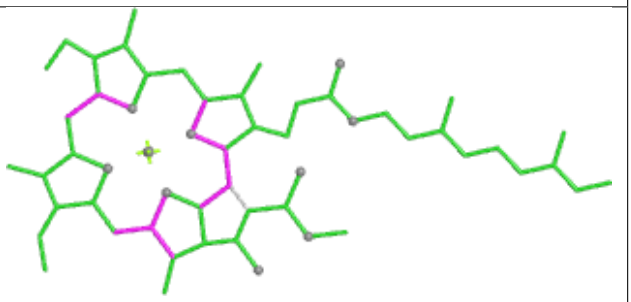
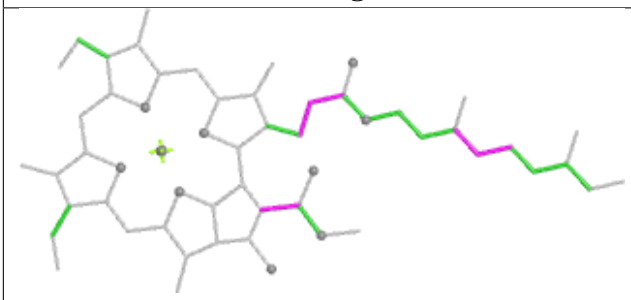
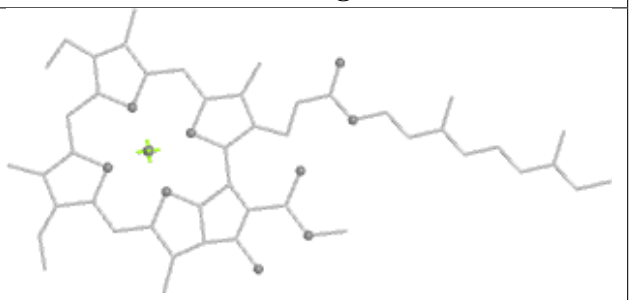


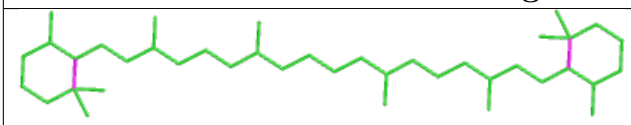
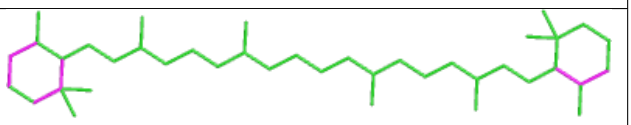
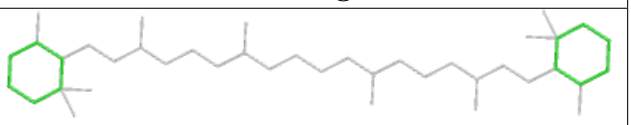
Torsions



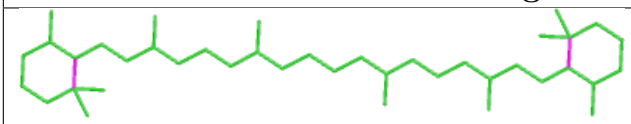
Rings

Ligand BCR B 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

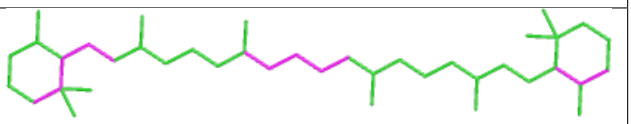
Ligand CLA G 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 841	
 Bond lengths	 Bond angles
Torsions	 Rings

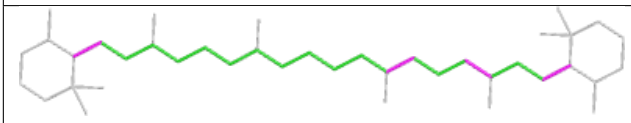
Ligand BCR B 841



Bond lengths



Bond angles



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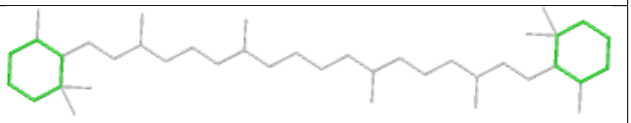
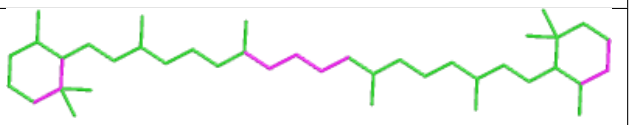


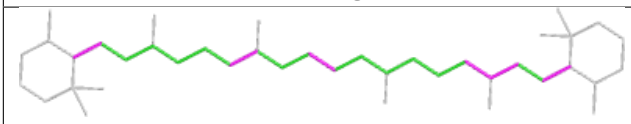
Rings

Ligand BCR I 101

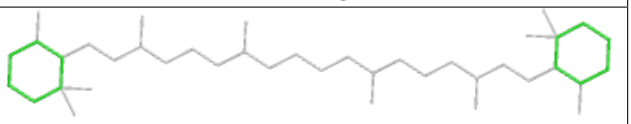
Bond lengths



Bond angles

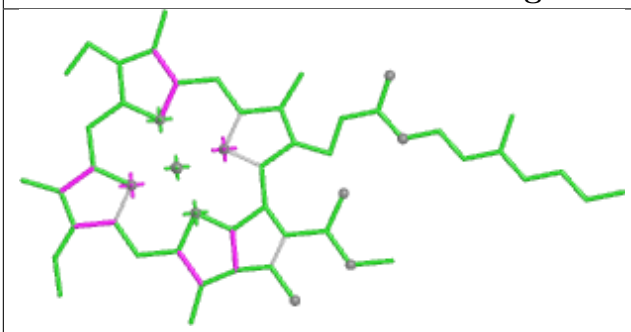


Torsions

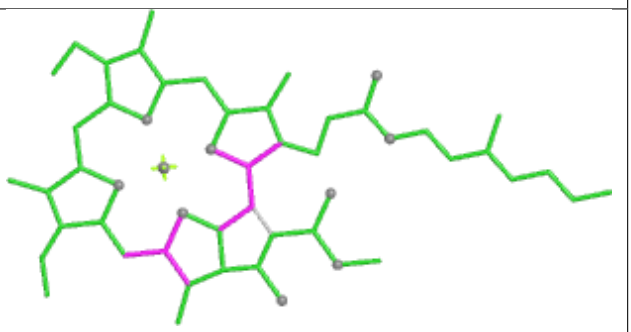


Rings

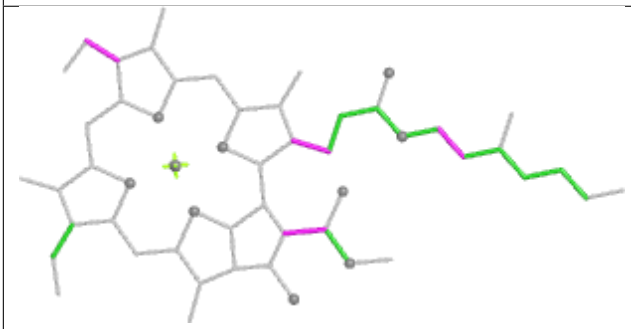
Ligand CLA B 819



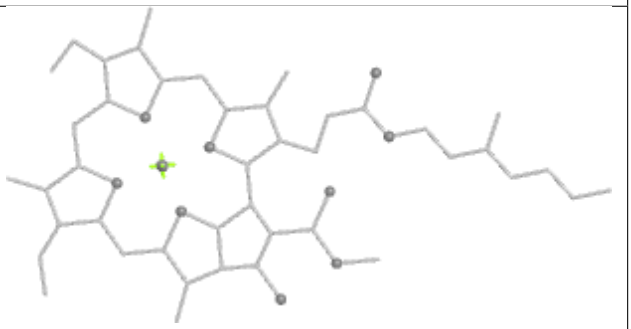
Bond lengths



Bond angles

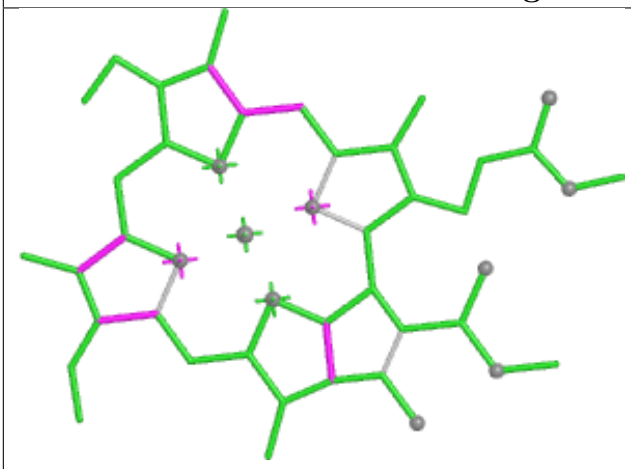


Torsions

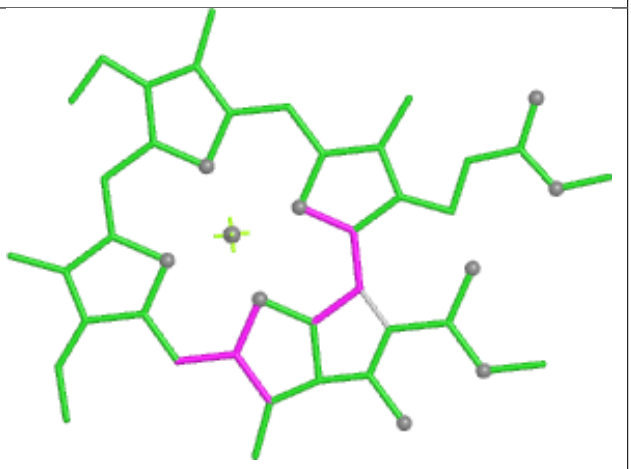


Rings

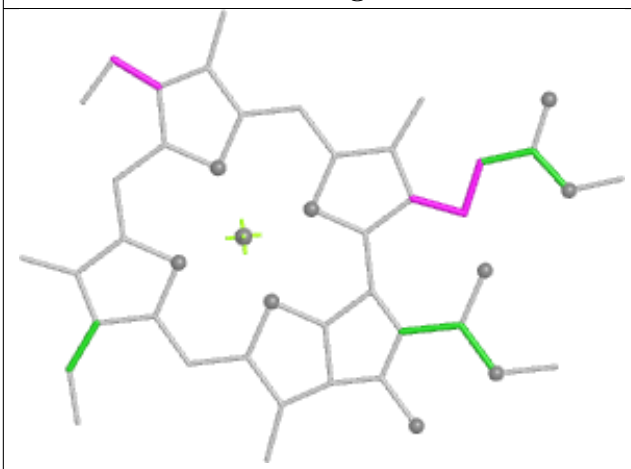
Ligand CLA K 207



Bond lengths



Bond angles



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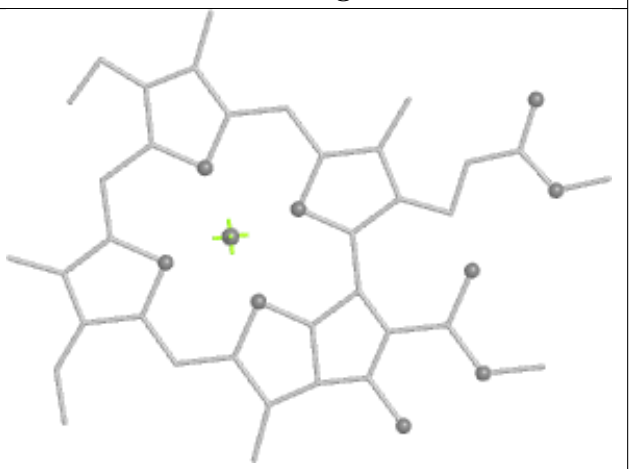
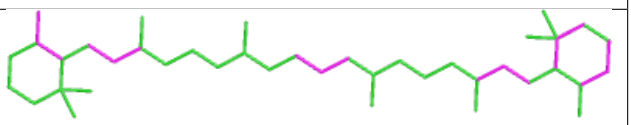


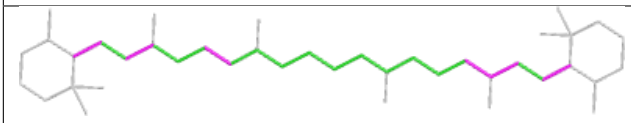
Rings

Ligand BCR B 838

Bond lengths



Bond angles



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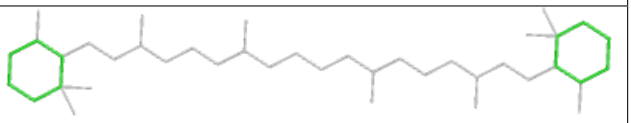
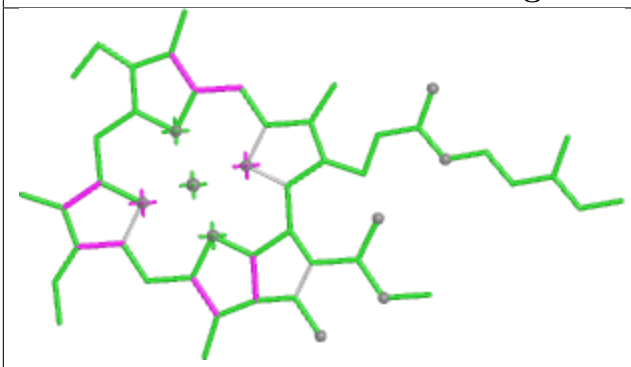
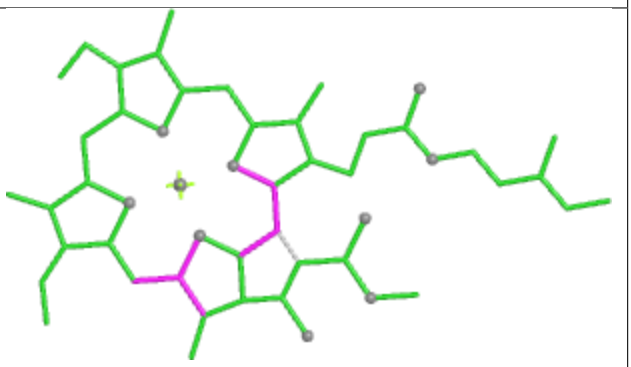


Rings

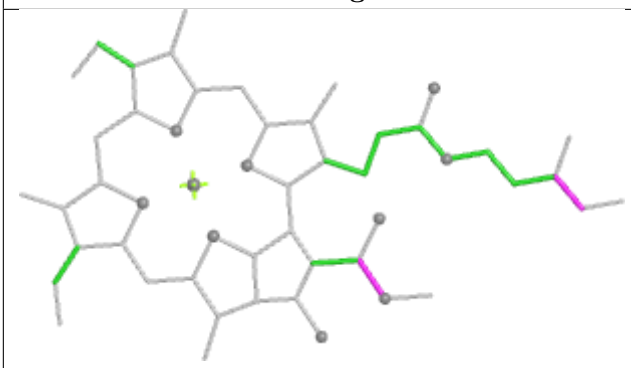
Ligand CLA A 820



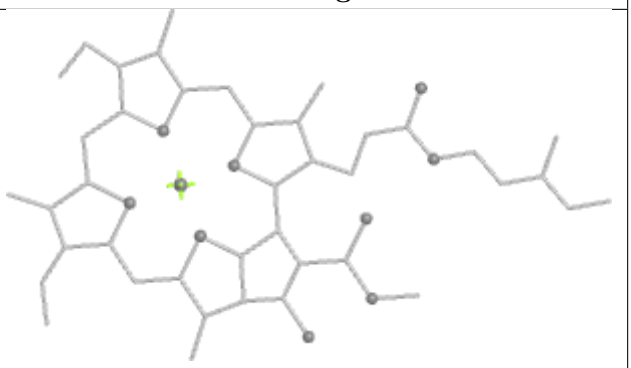
Bond lengths



Bond angles

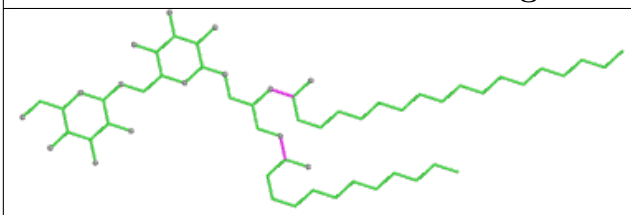


Torsions

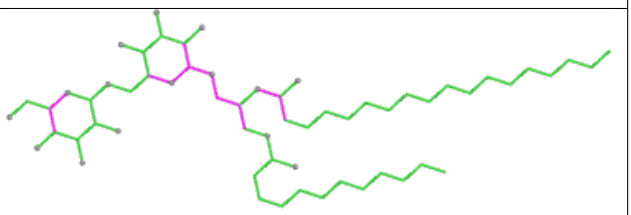


Rings

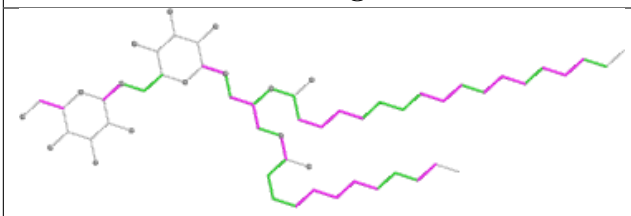
Ligand DGD B 843



Bond lengths



Bond angles



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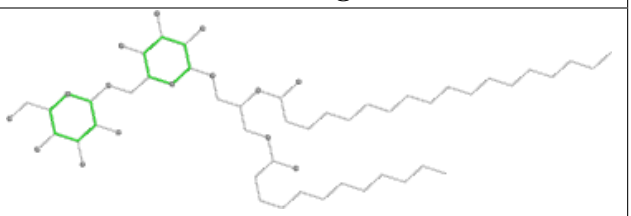
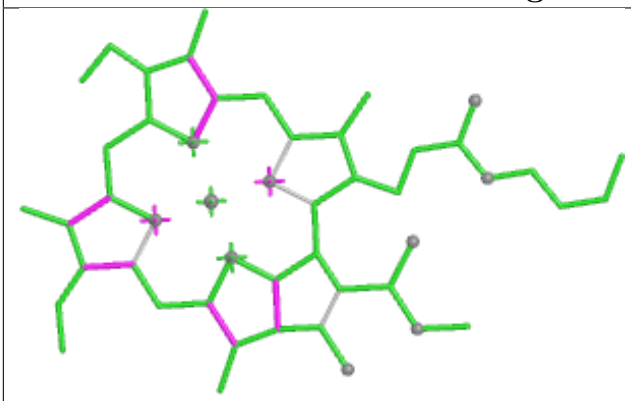
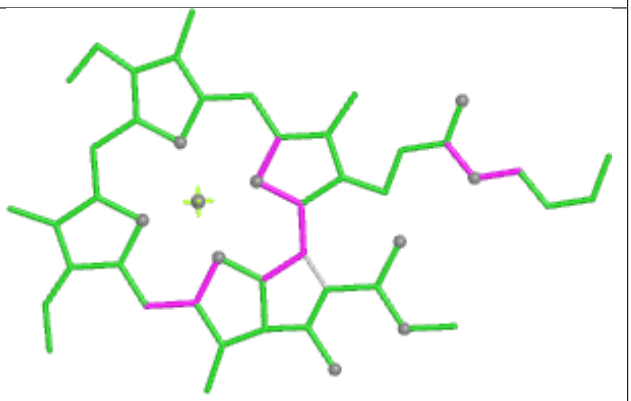
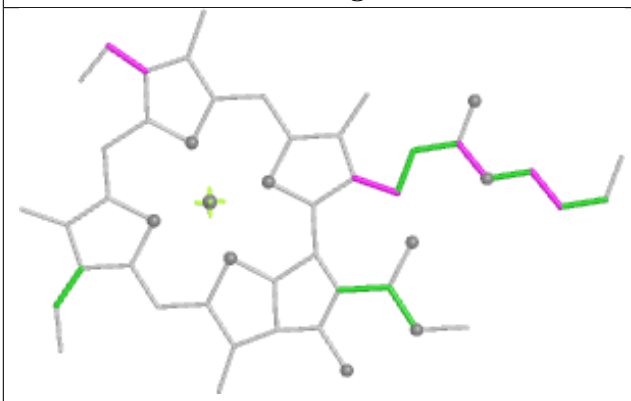
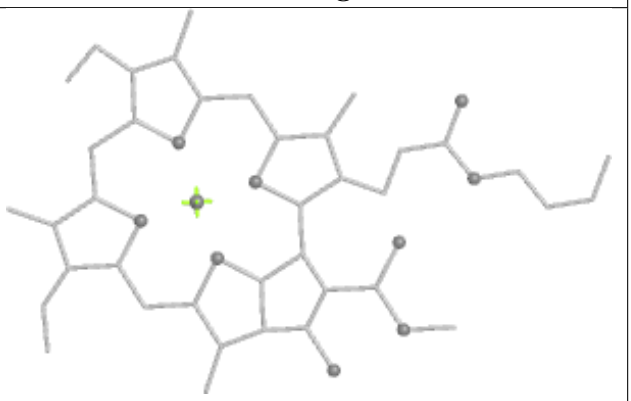
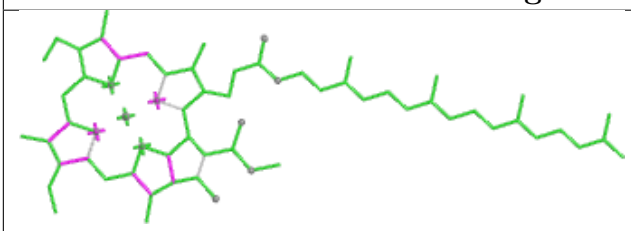
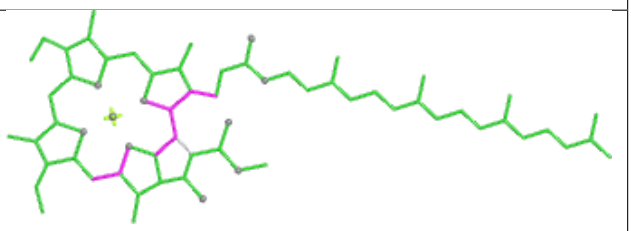
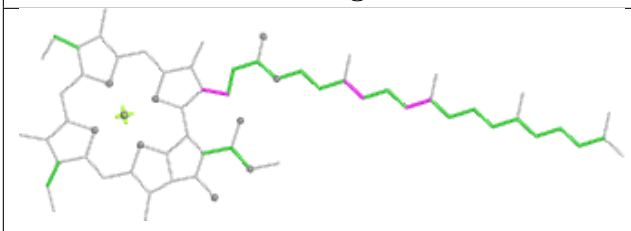
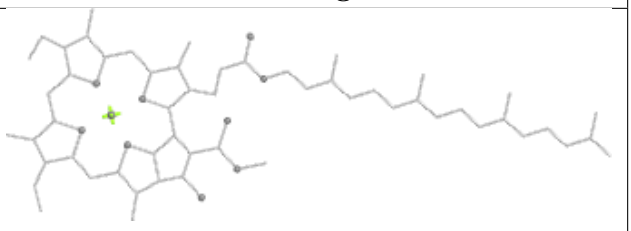
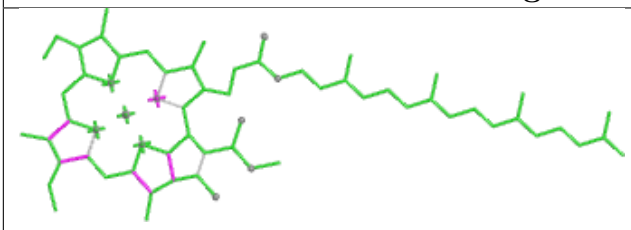
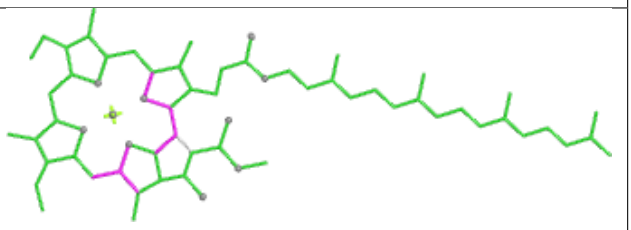
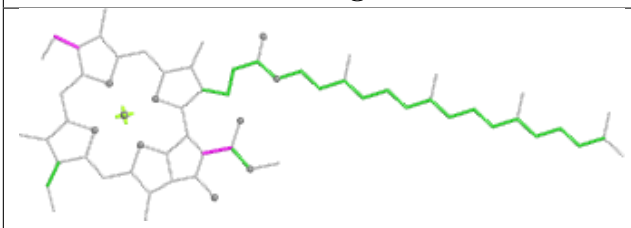
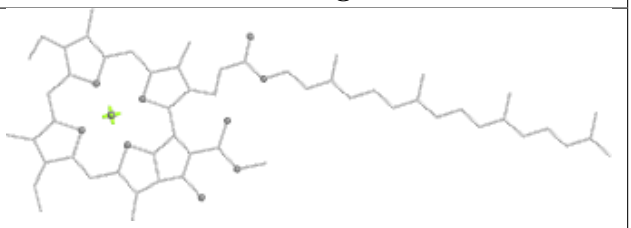


Rings

Ligand CLA L 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 210	
 Bond lengths	 Bond angles
 Torsions	 Rings

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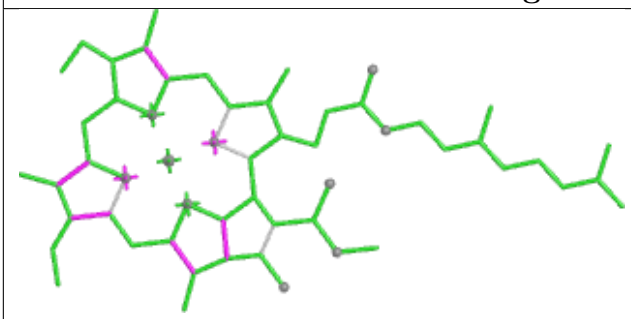
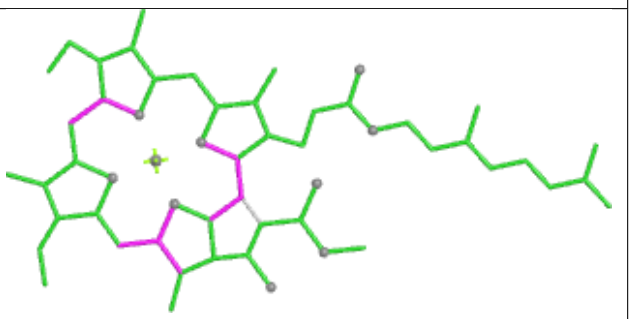
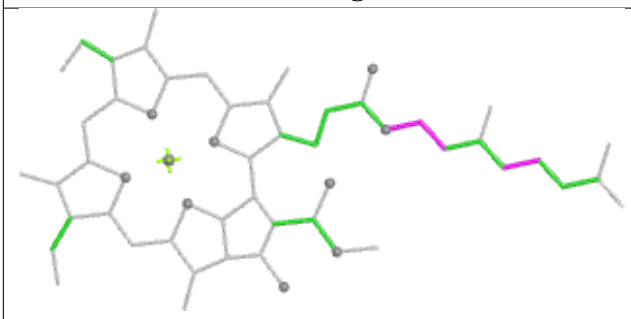
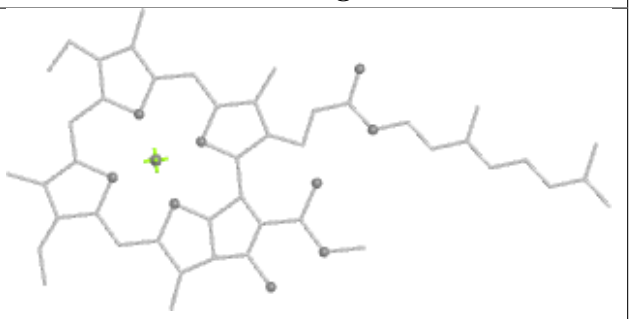
 Bond lengths	 Bond angles
 Torsions	 Rings

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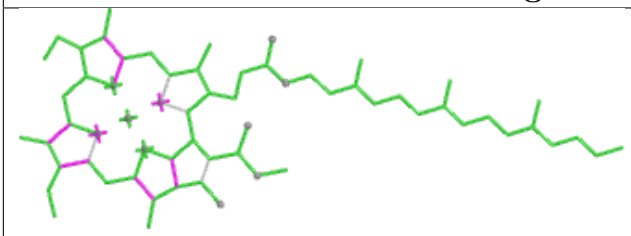
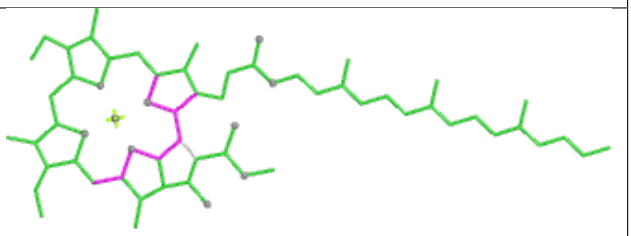
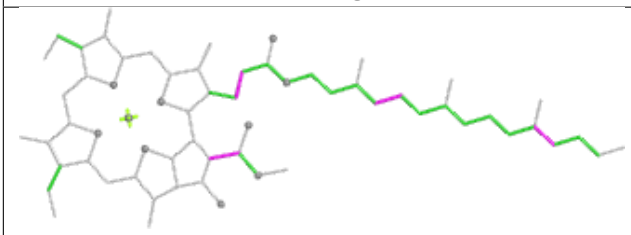
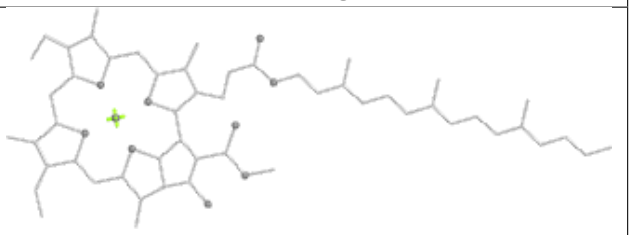
 Bond lengths	 Bond angles
 Torsions	 Rings

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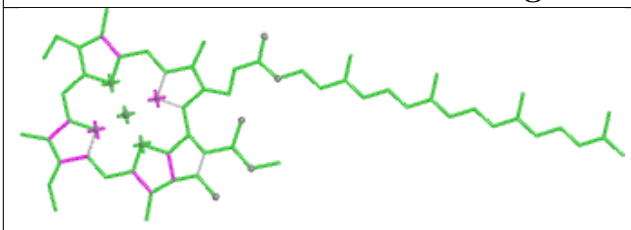
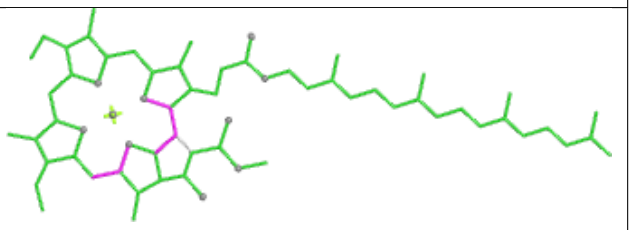
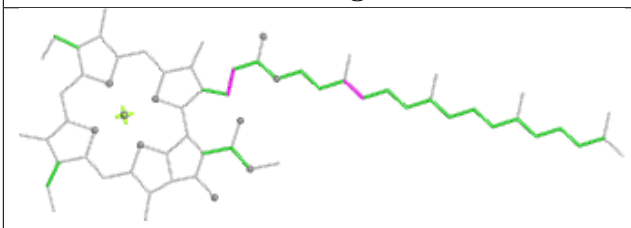
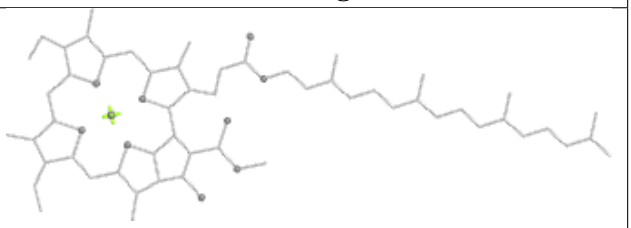
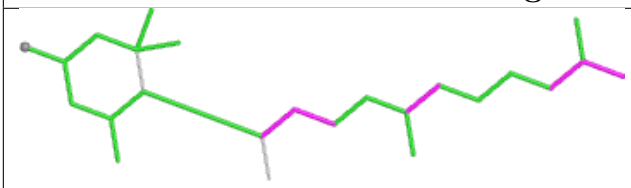
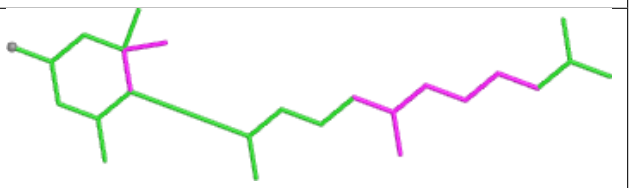
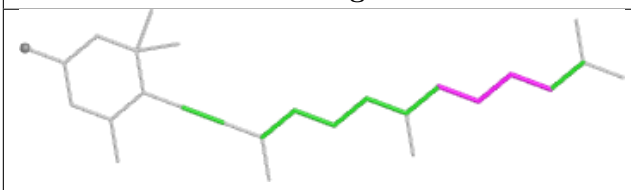
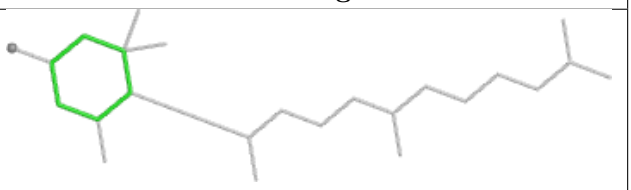
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 U 214	
 Bond lengths	 Bond angles
 Torsions	 Rings

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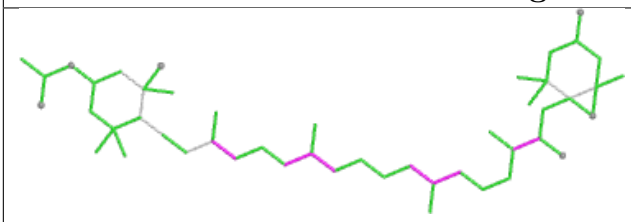
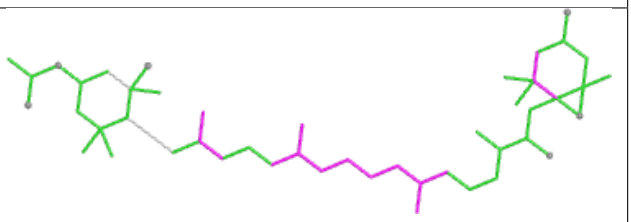
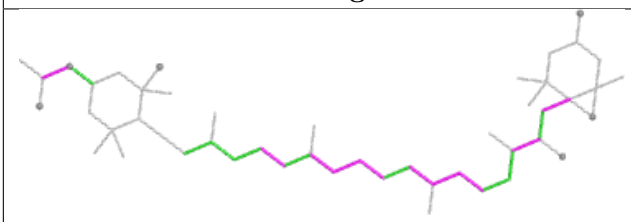
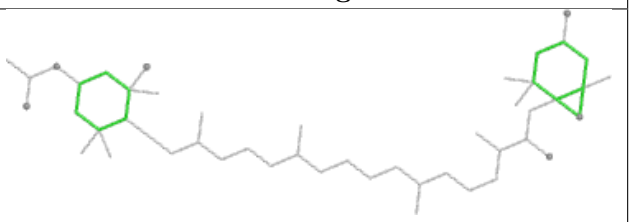
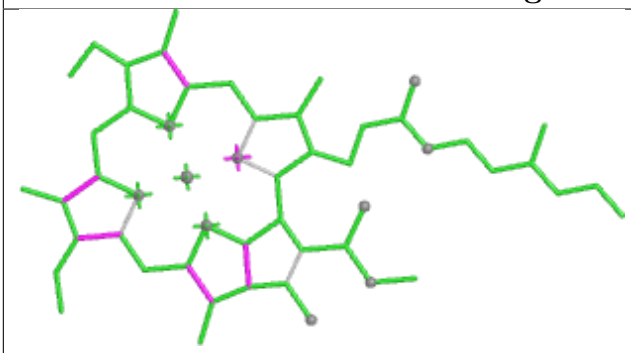
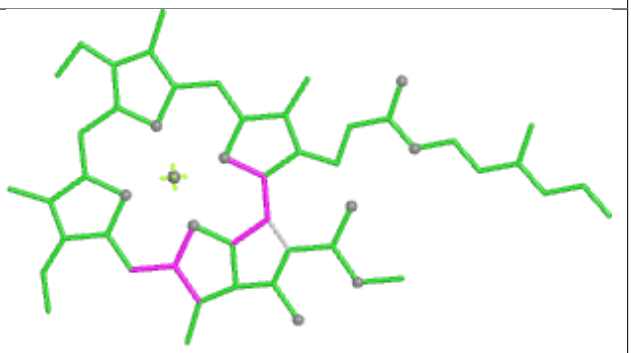
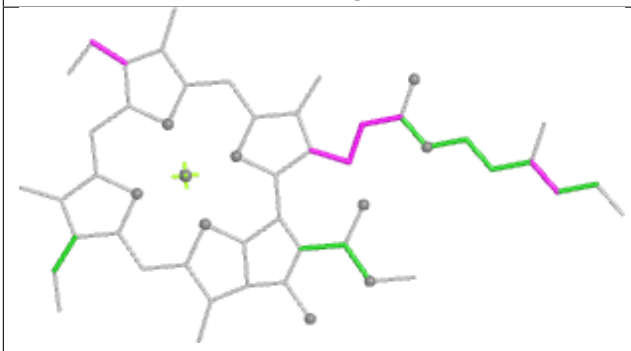
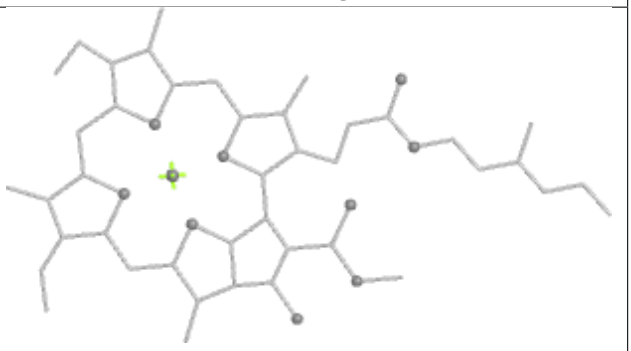
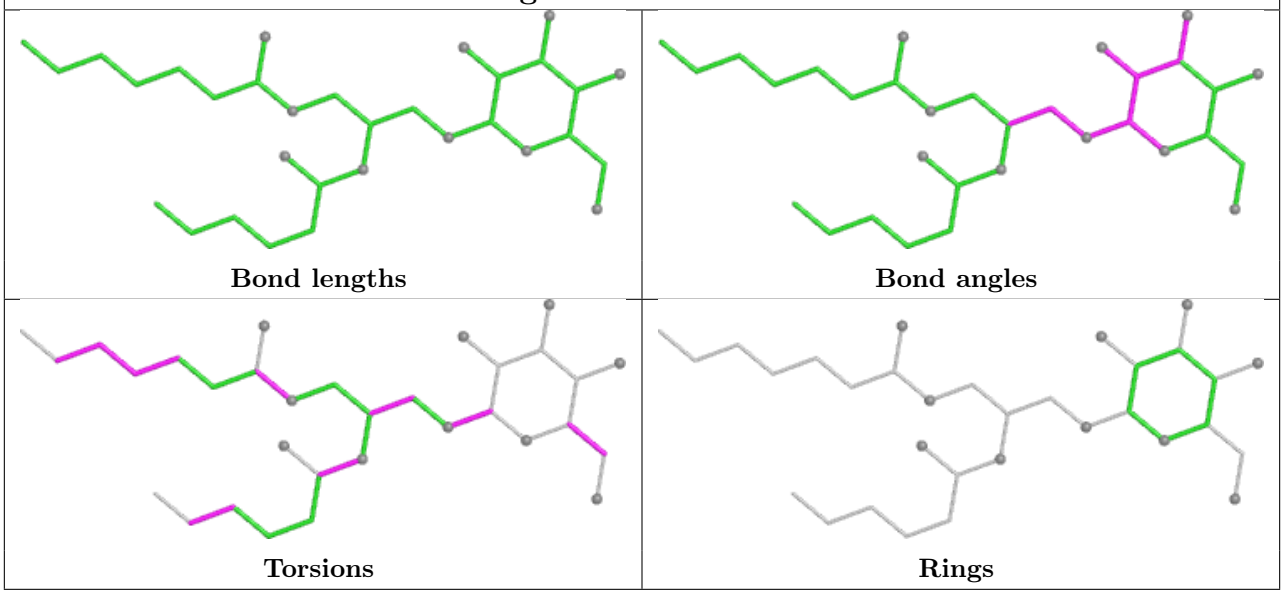
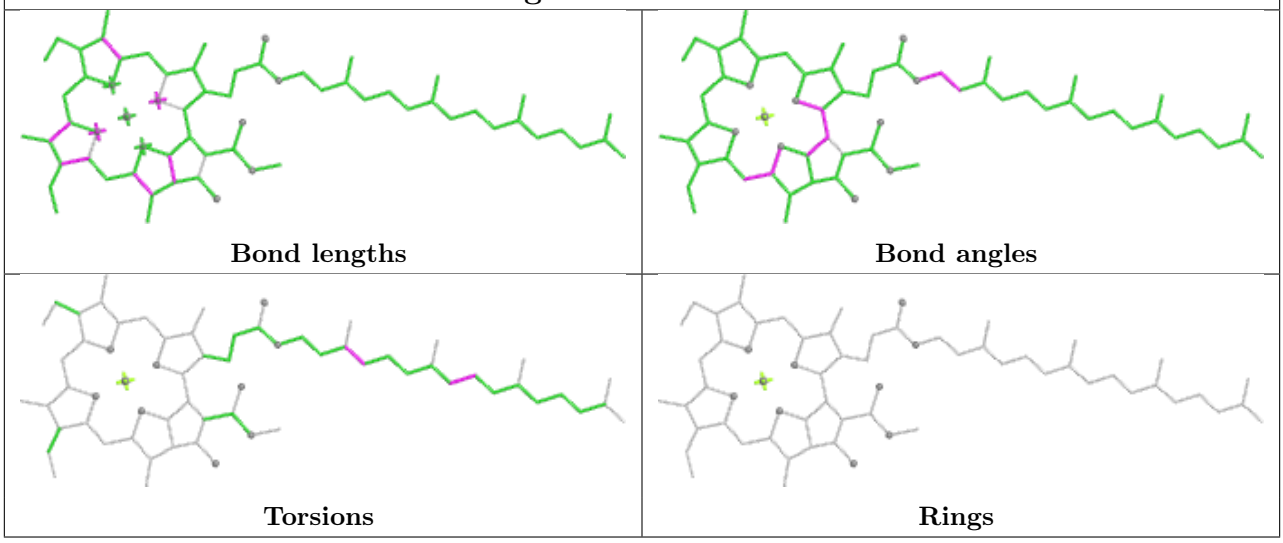
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

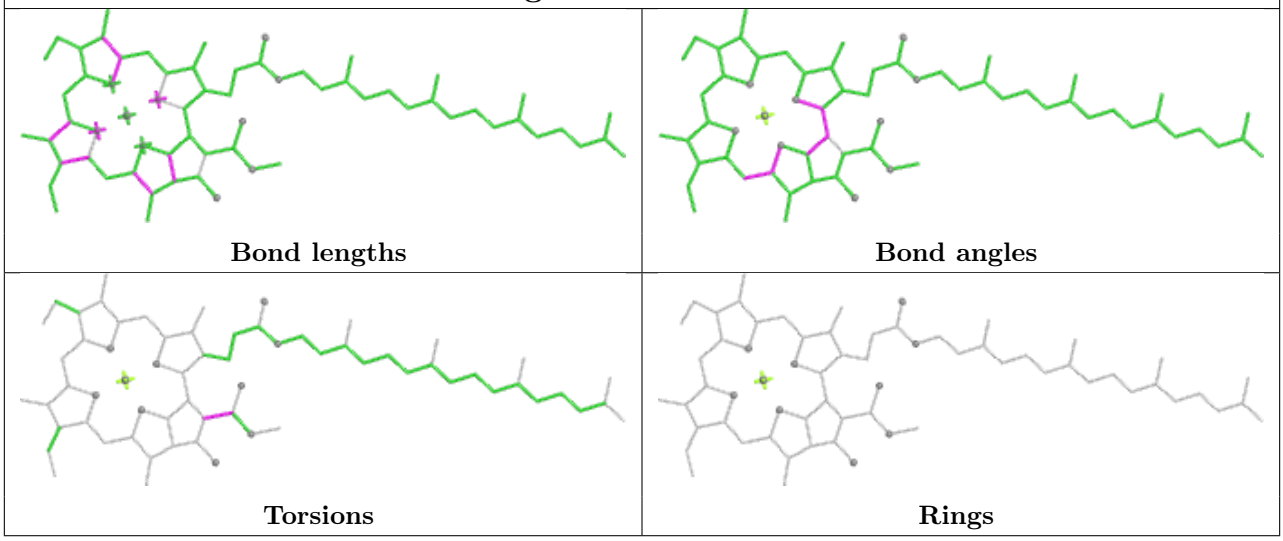
Ligand LMG U 201

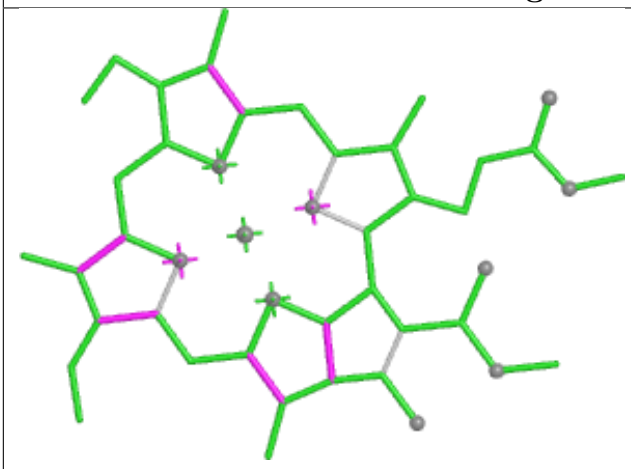
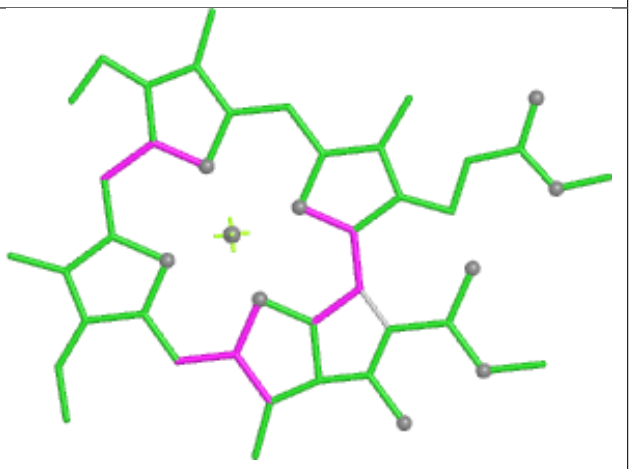
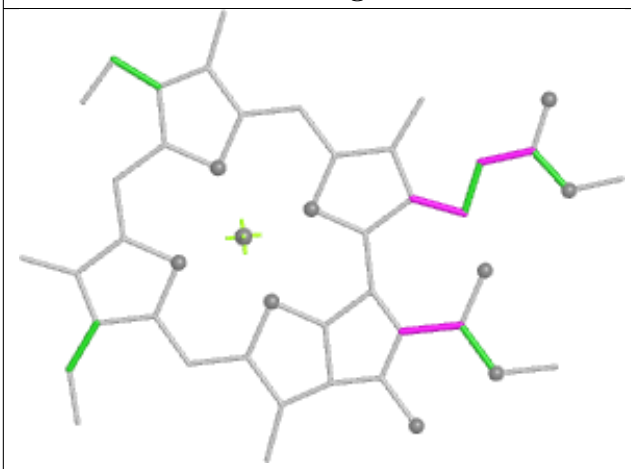
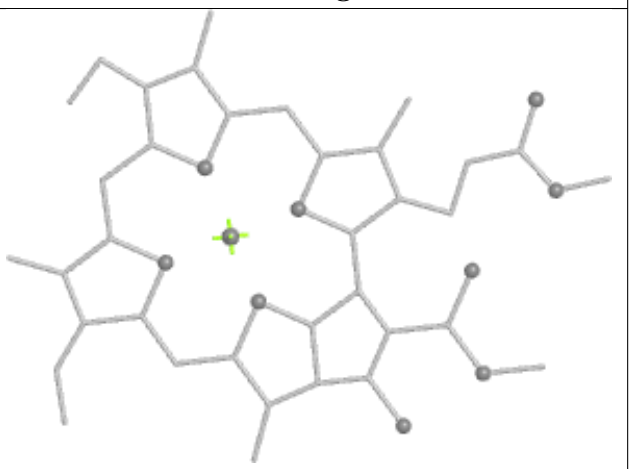


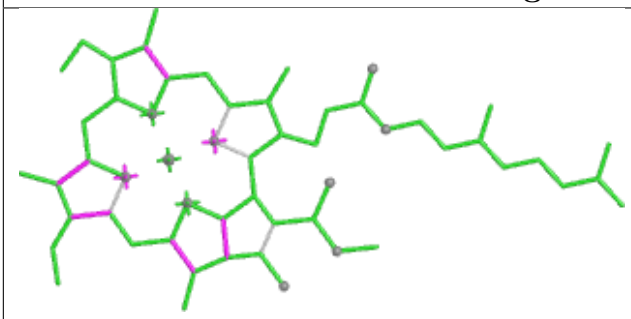
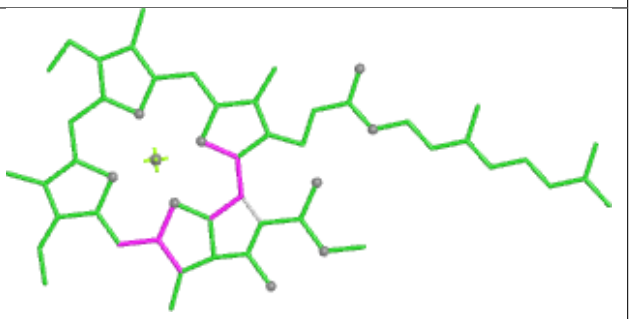
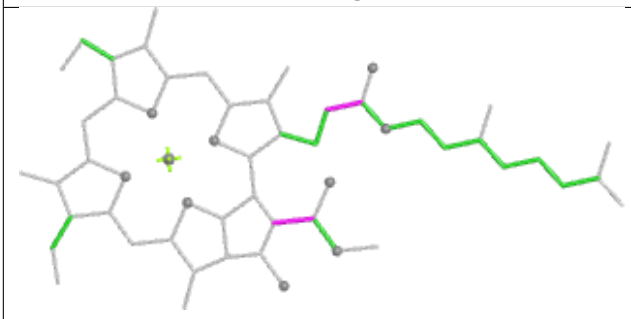
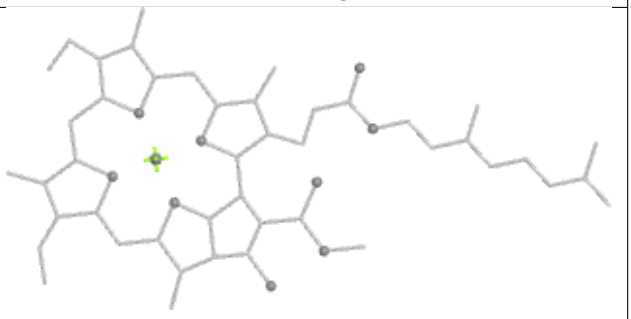
Ligand CLA U 205

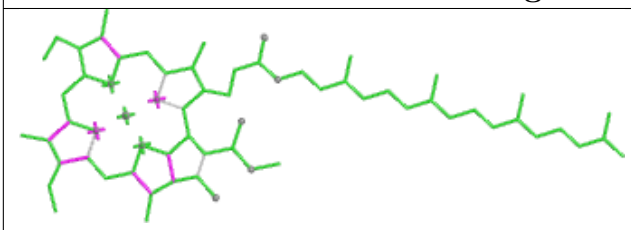
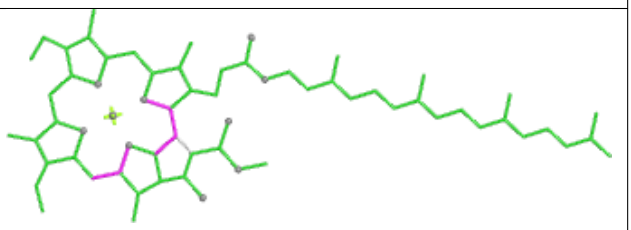
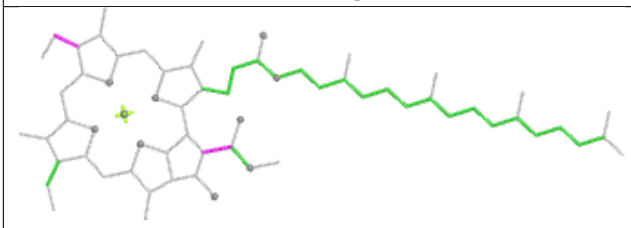
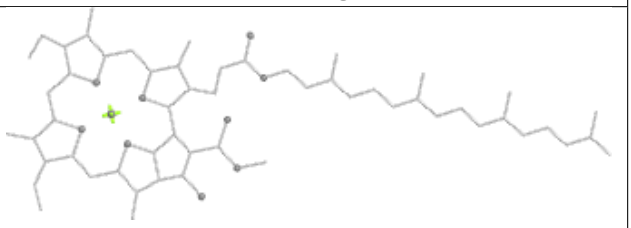


Ligand CLA A 826

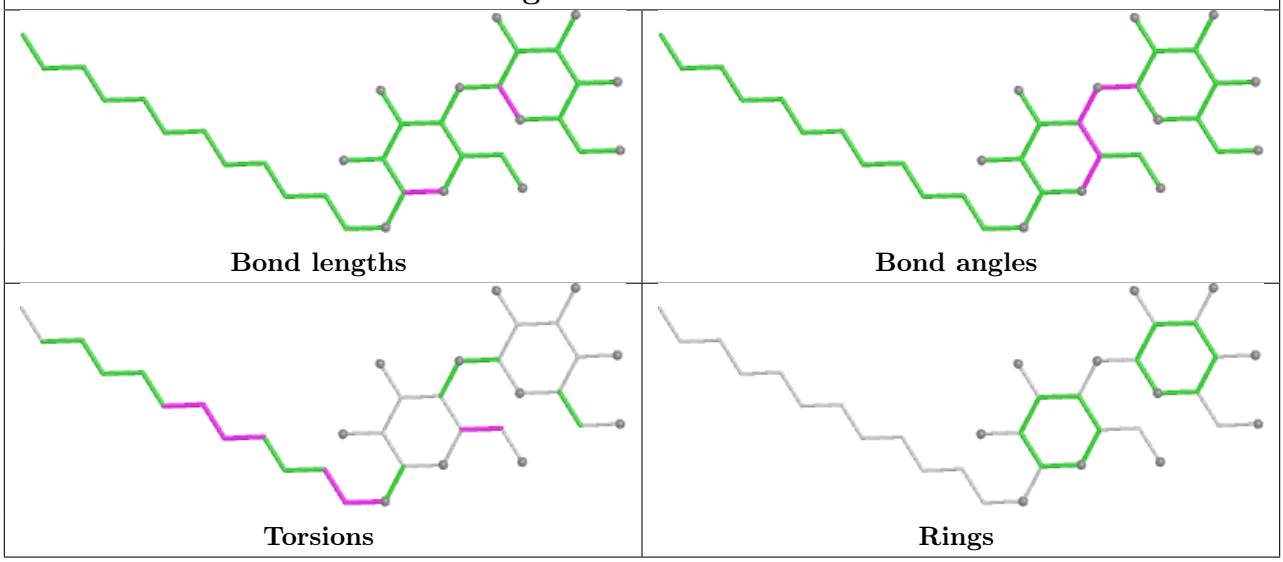


Ligand CLA F 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

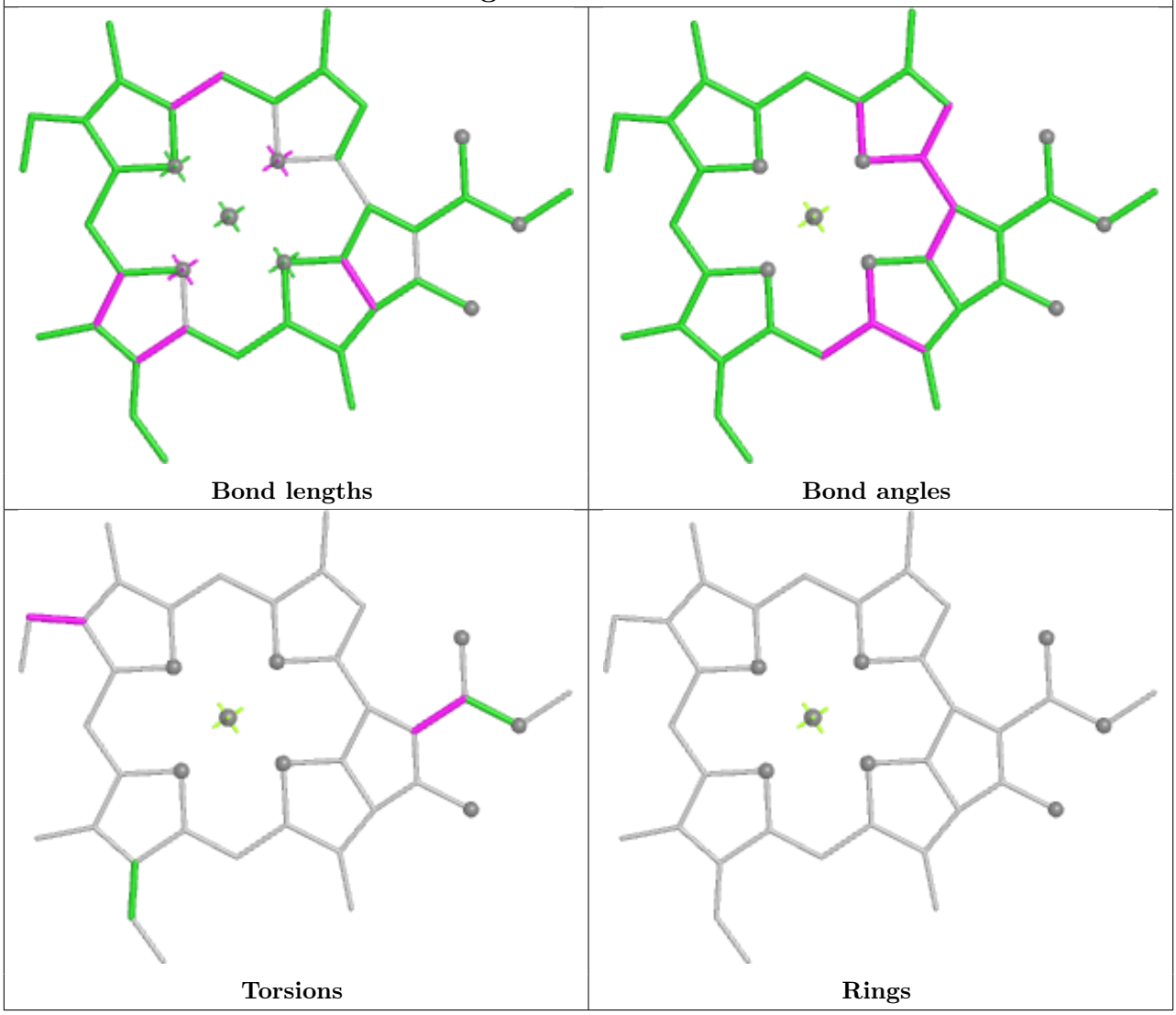
Ligand CLA A 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

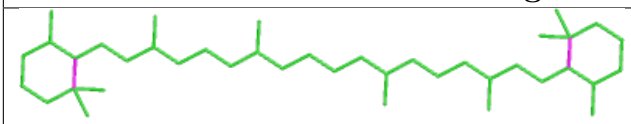
Ligand LMU F 806



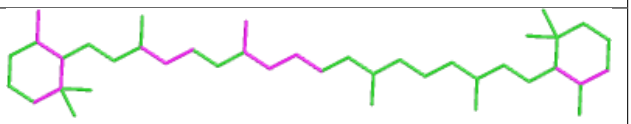
Ligand CLA H 301



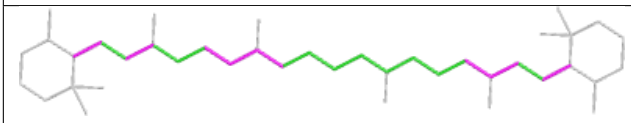
Ligand BCR F 805



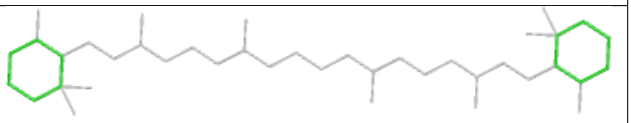
Bond lengths



Bond angles

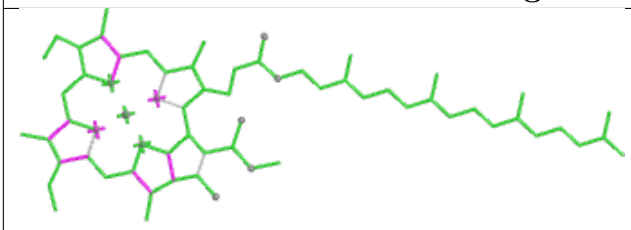


Torsions

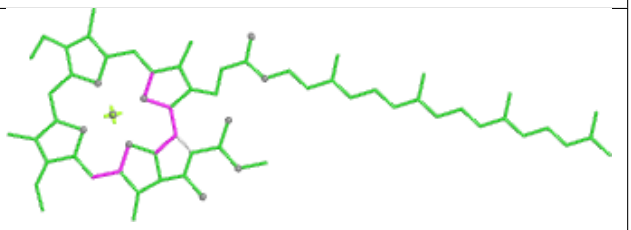


Rings

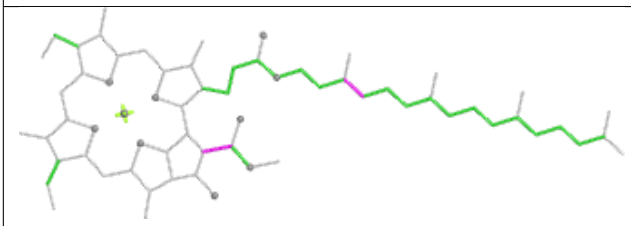
Ligand CLA A 823



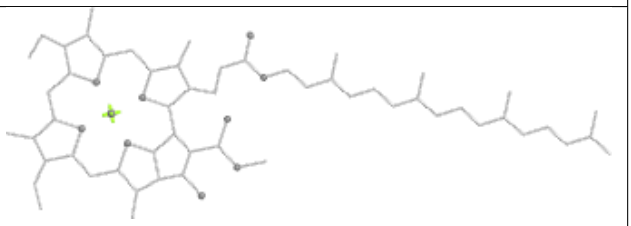
Bond lengths



Bond angles

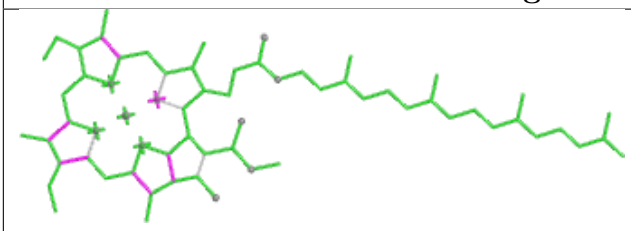


Torsions

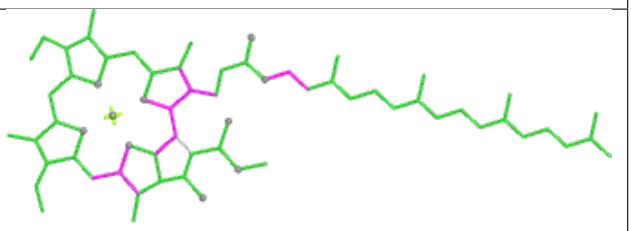


Rings

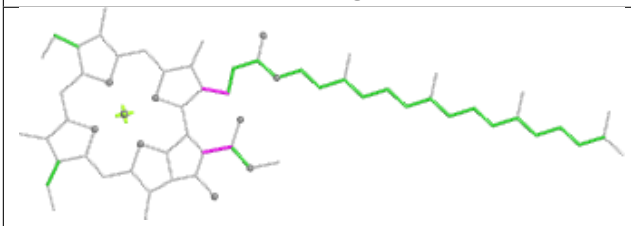
Ligand CLA U 207



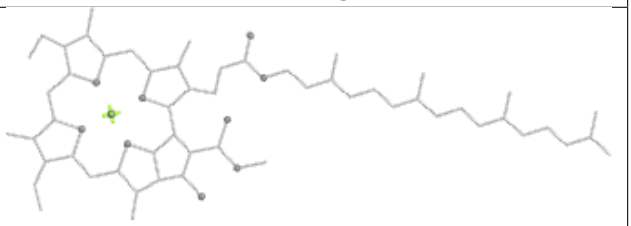
Bond lengths



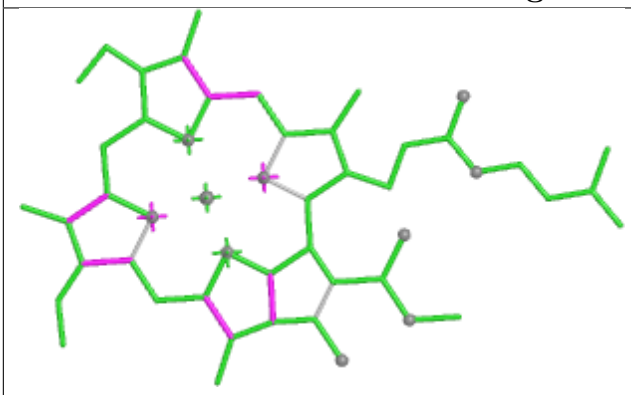
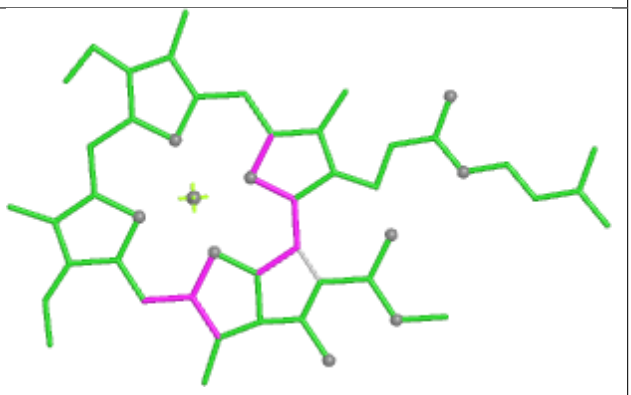
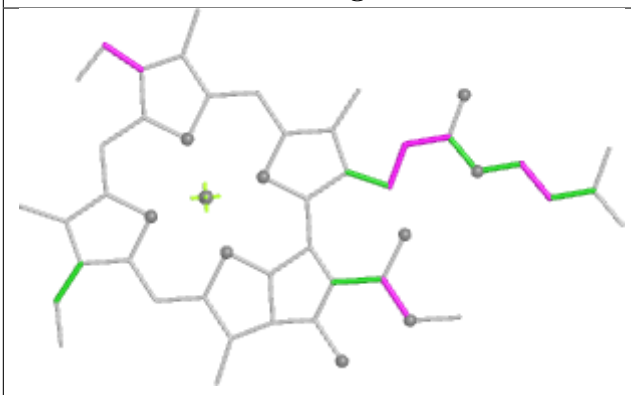
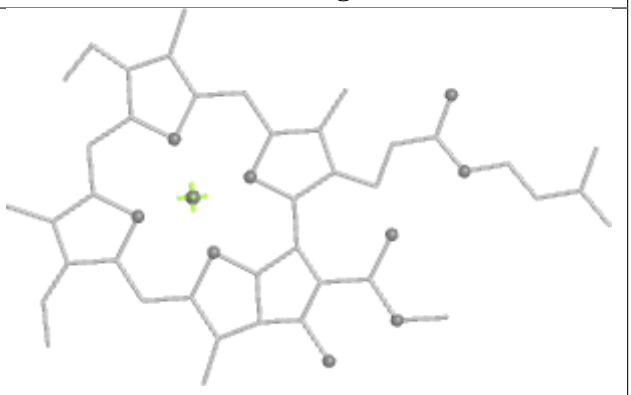
Bond angles



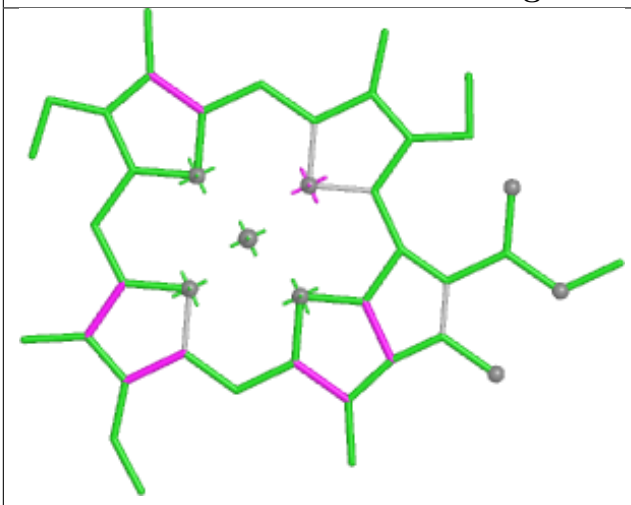
Torsions



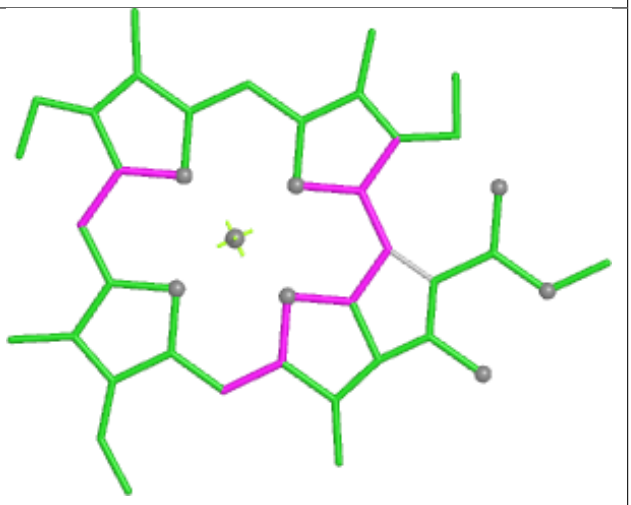
Rings

Ligand CLA L 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

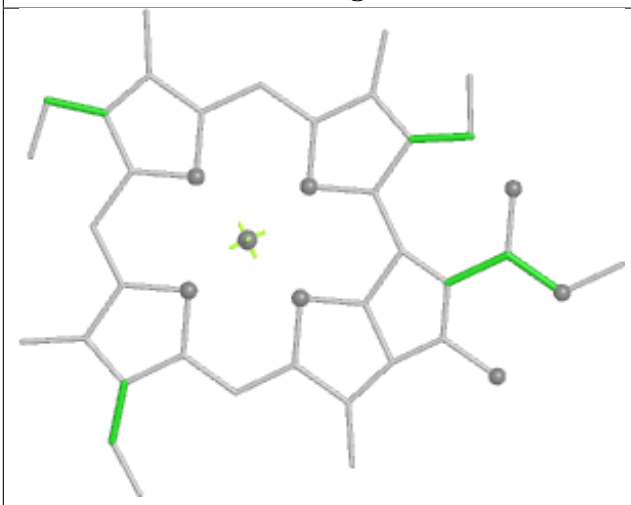
Ligand CLA U 209



Bond lengths



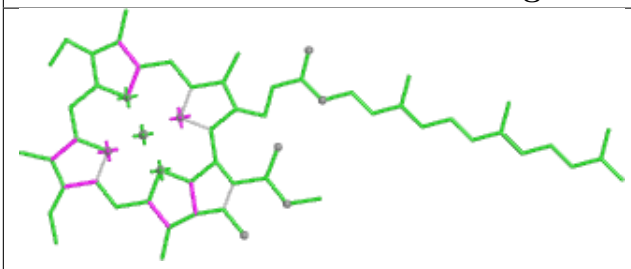
Bond angles



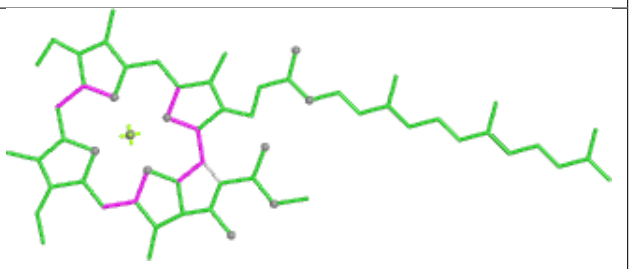
Torsions

Rings

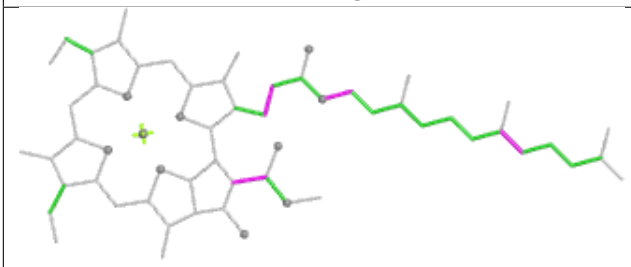
Ligand CLA H 302



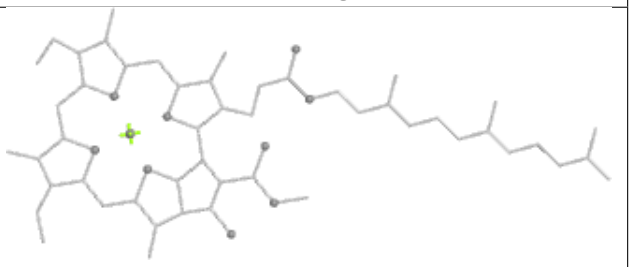
Bond lengths



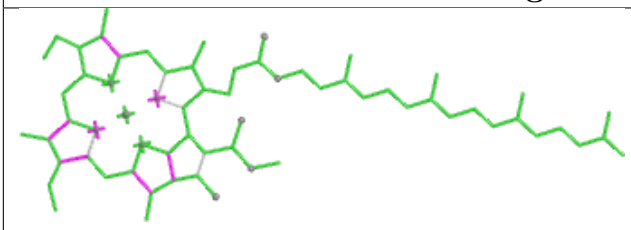
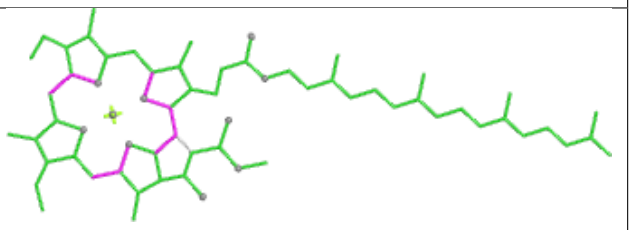
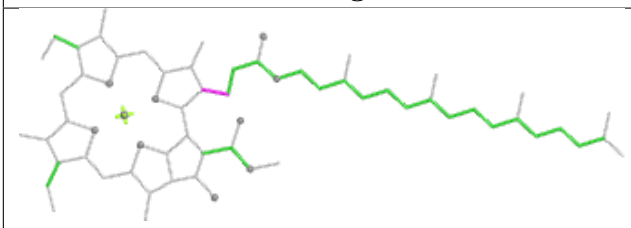
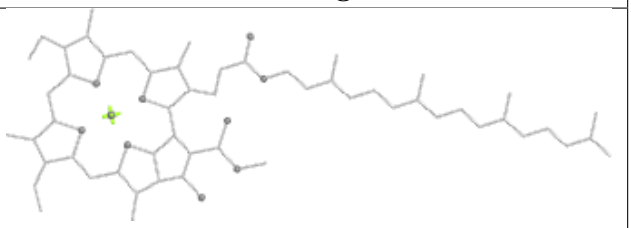
Bond angles

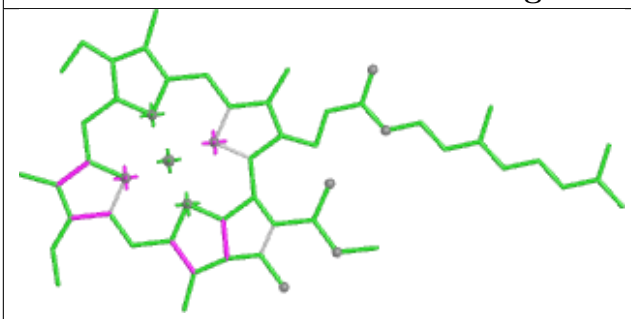
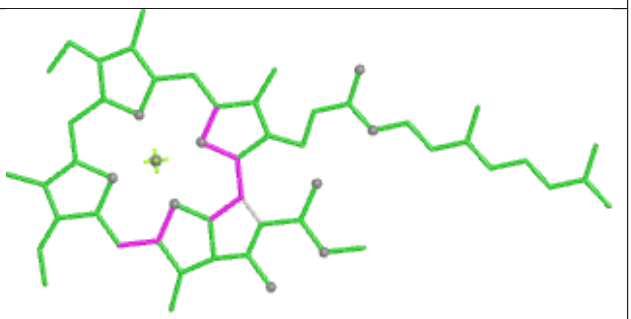
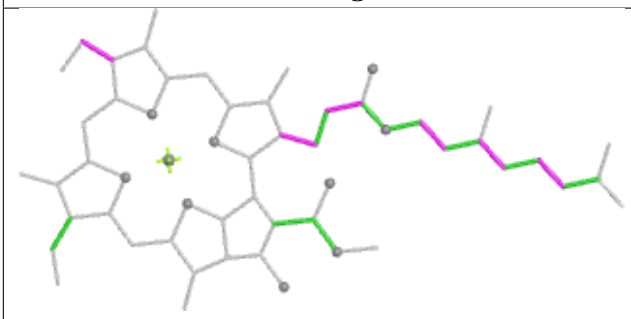
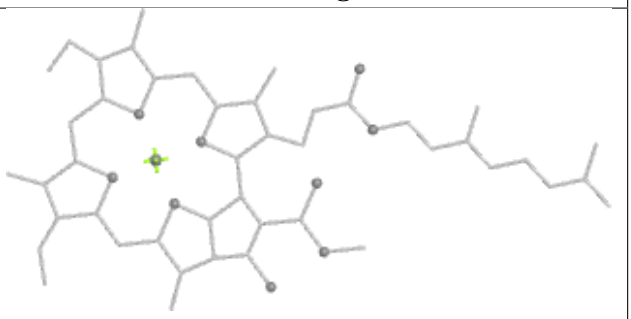


Torsions

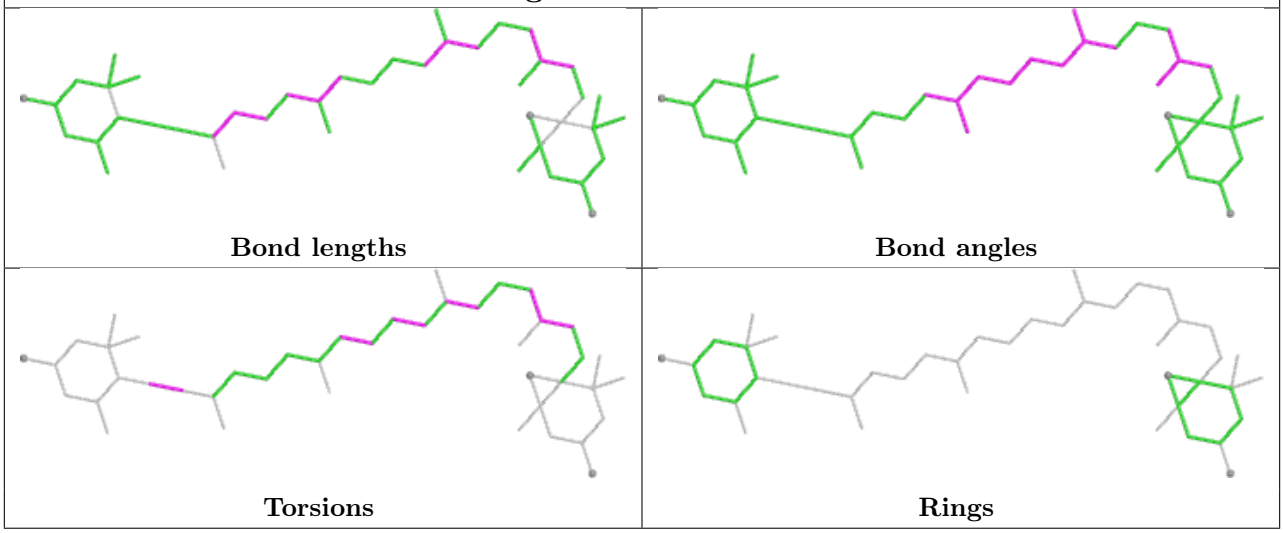


Rings

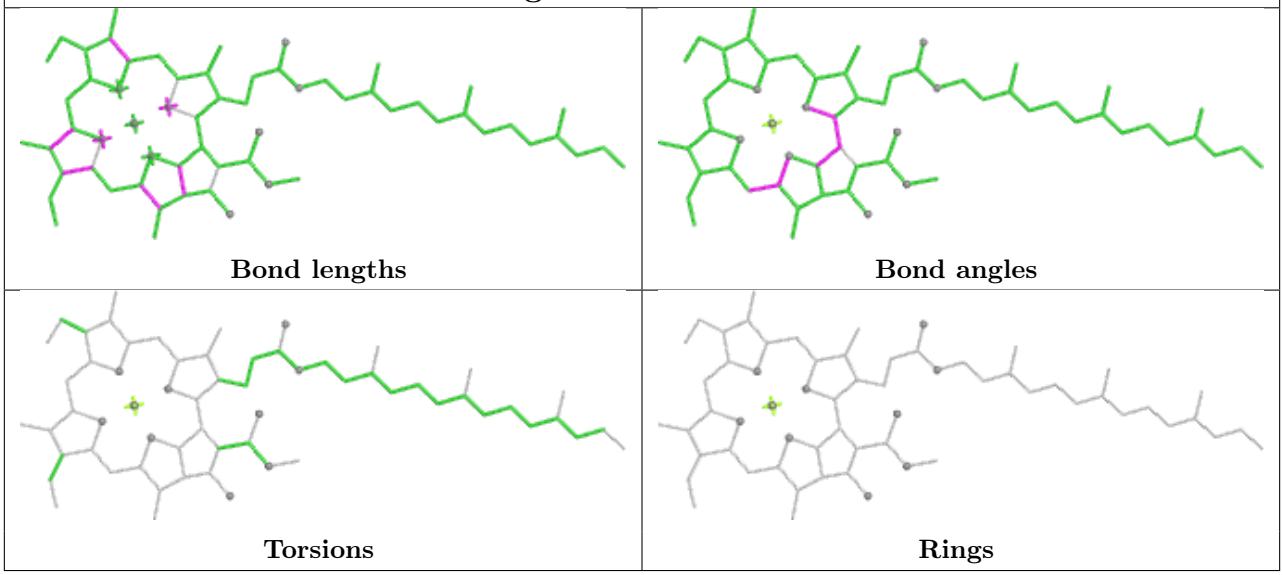
Ligand CLA F 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 A 846



Ligand CLA A 809



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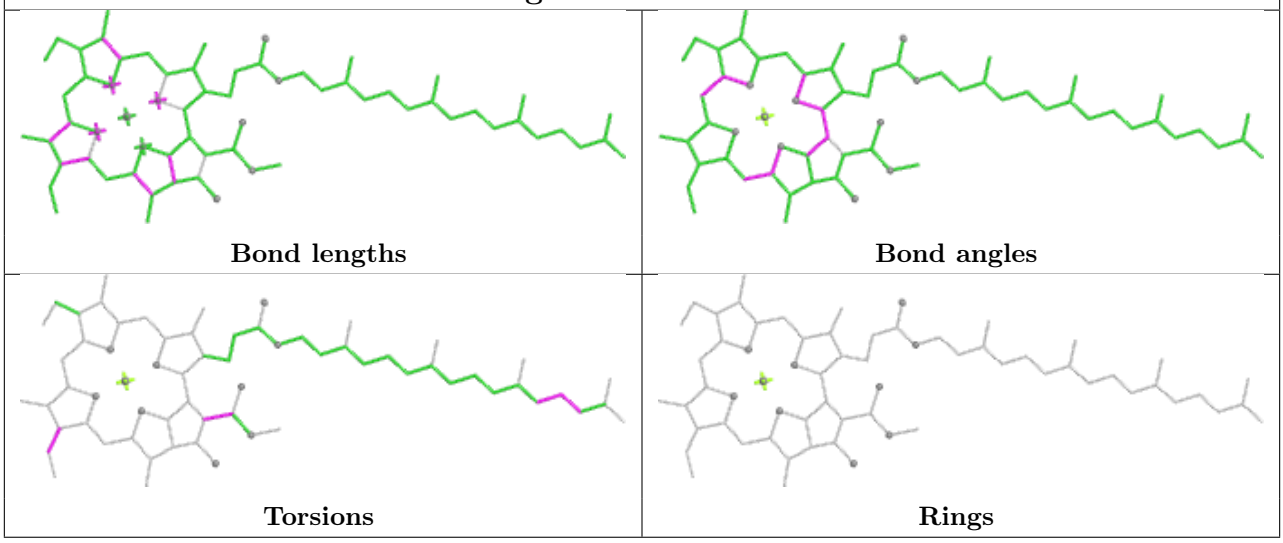
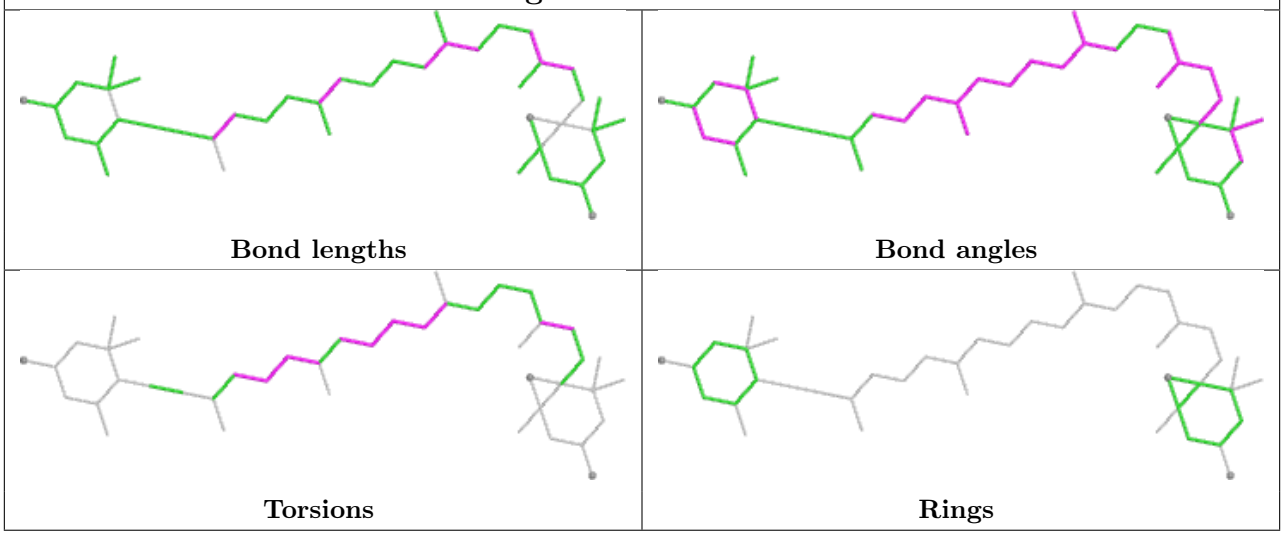


Ligand DD6 U 203



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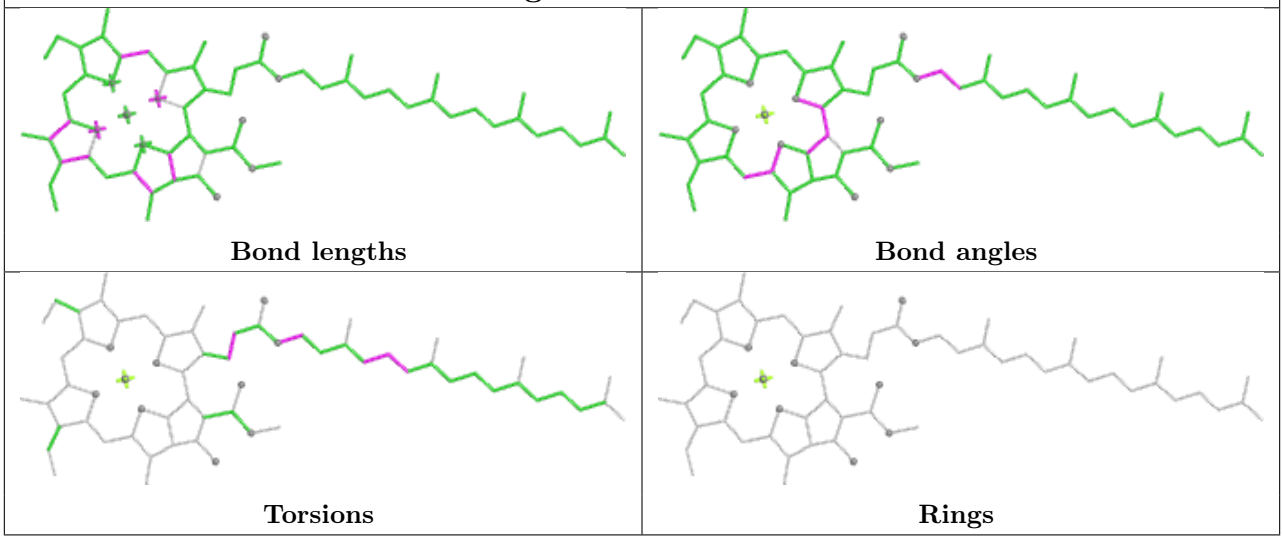
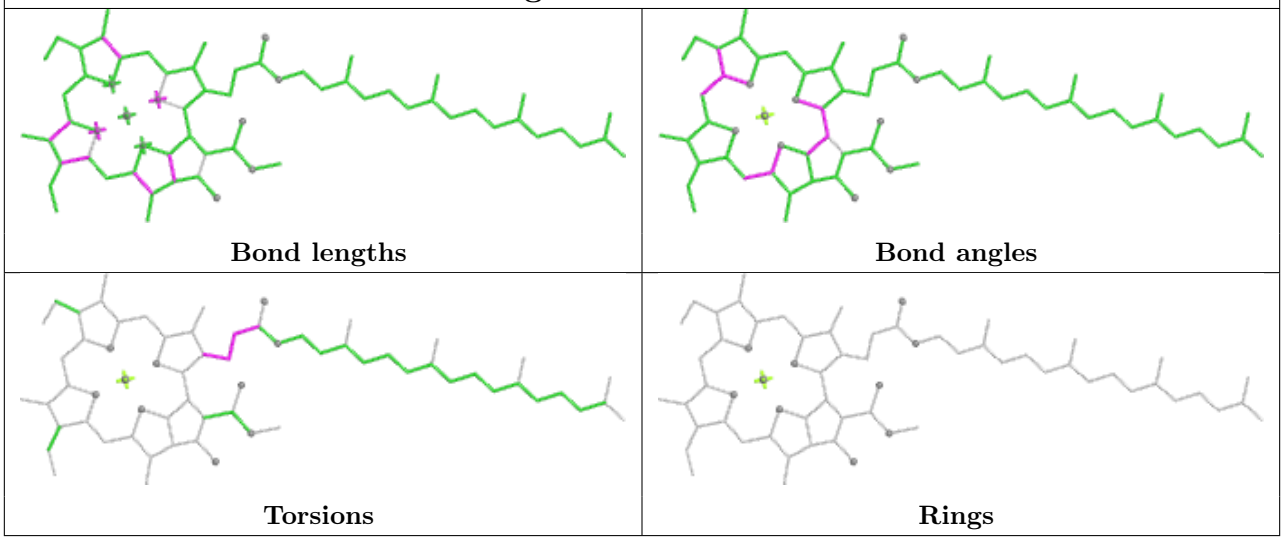
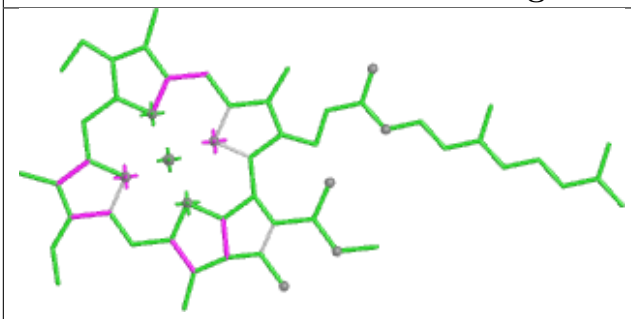
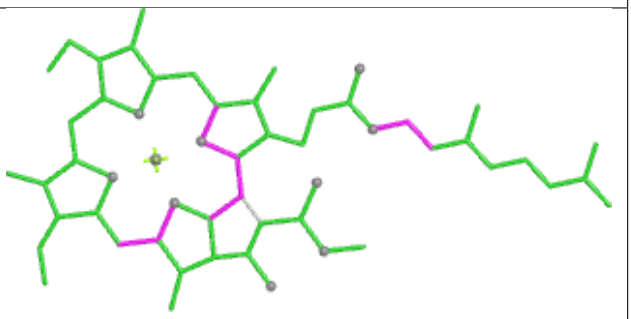
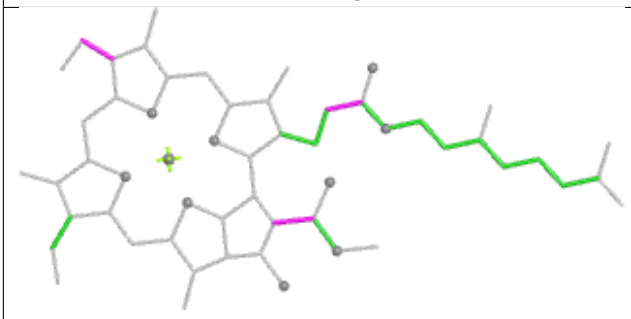
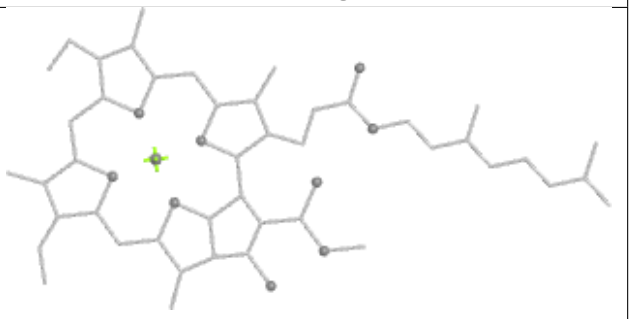


Ligand CLA A 815



Ligand CLA k 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

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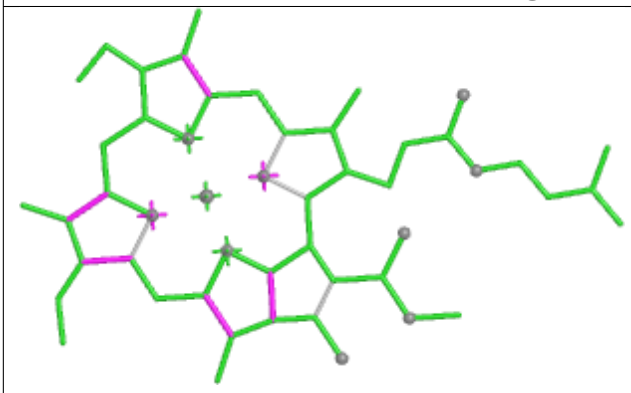
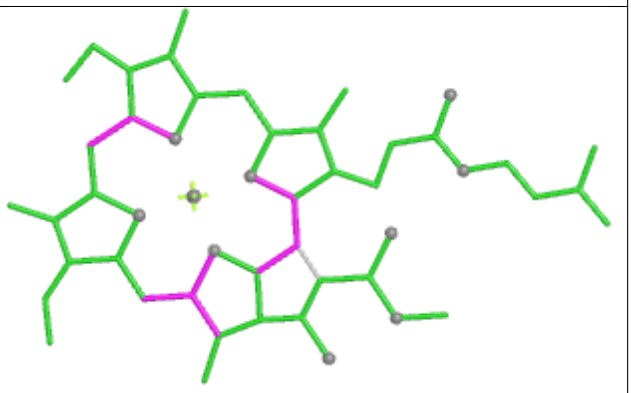
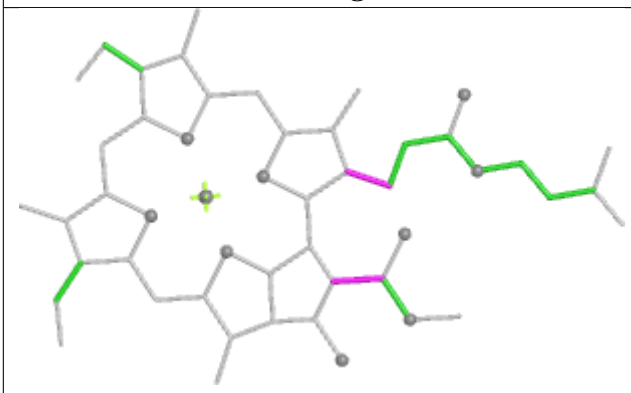
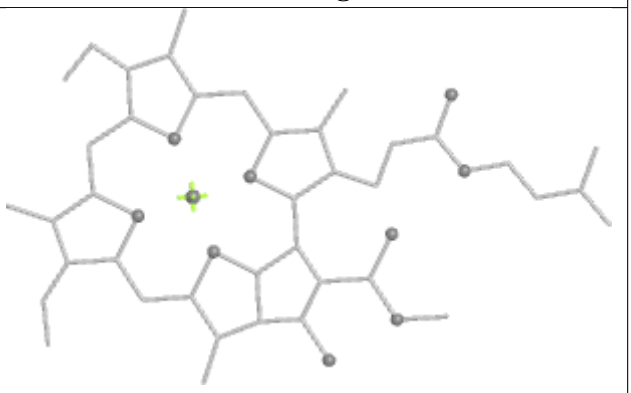
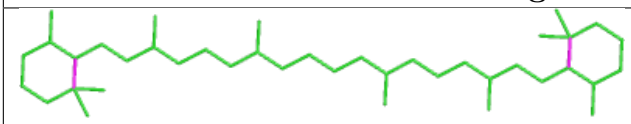
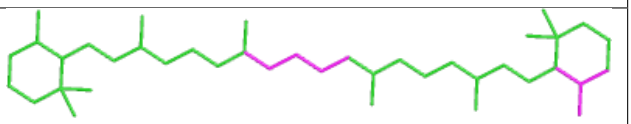
 Bond lengths	 Bond angles
 Torsions	 Rings

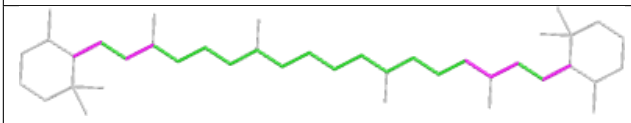
Ligand BCR I 103



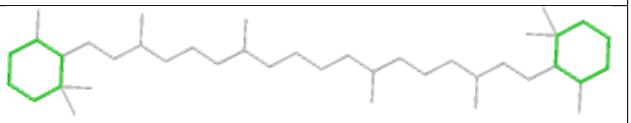
Bond lengths



Bond angles

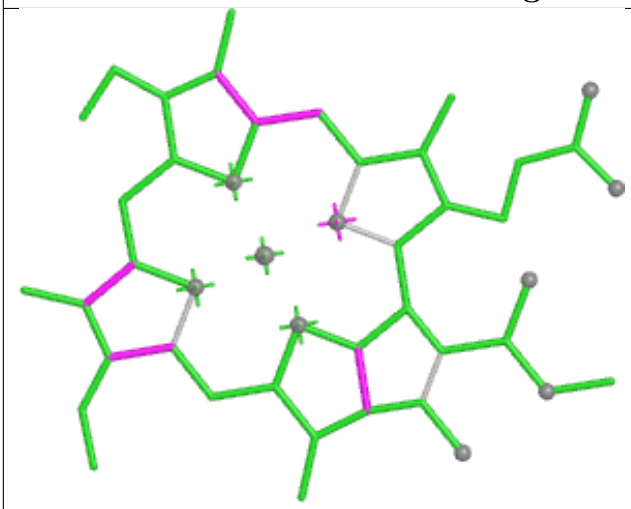


Torsions

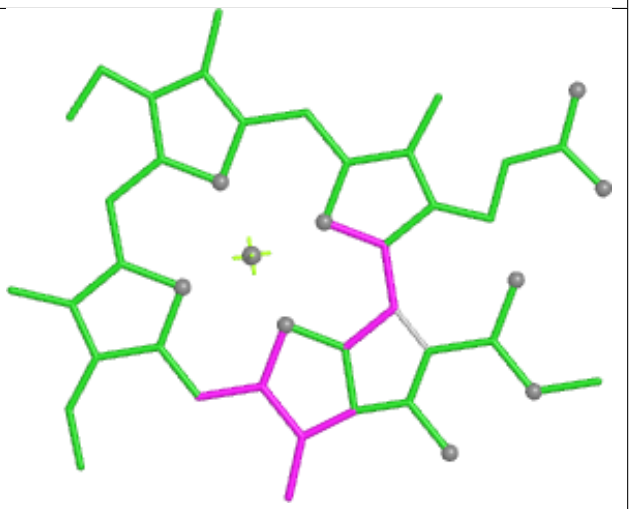


Rings

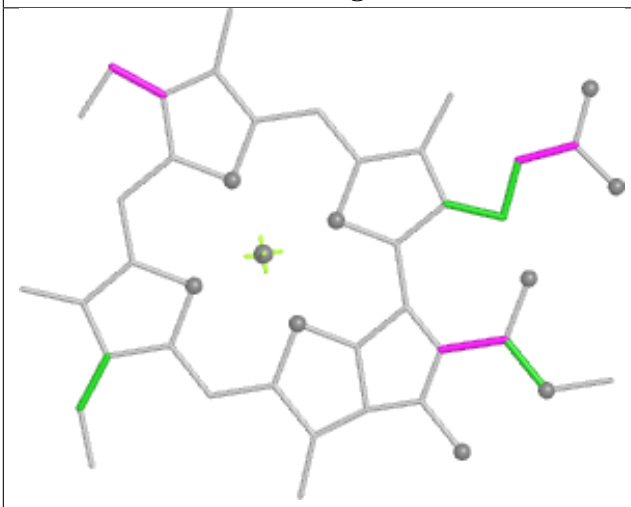
Ligand CLA G 315



Bond lengths



Bond angles



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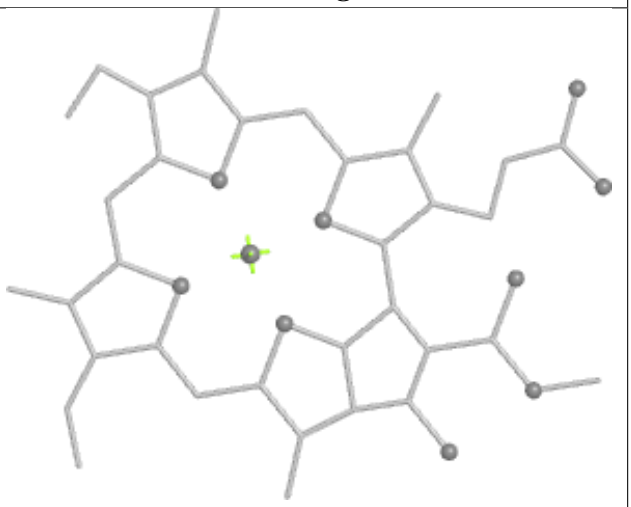
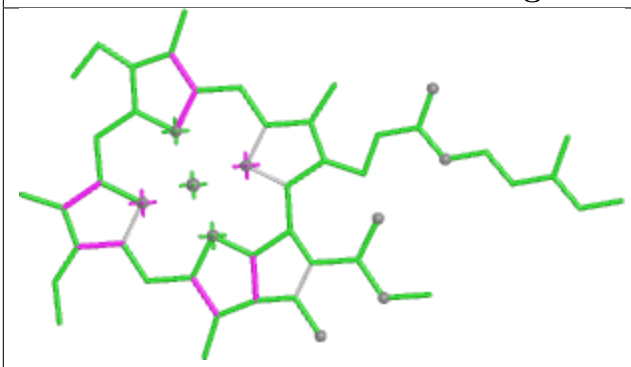
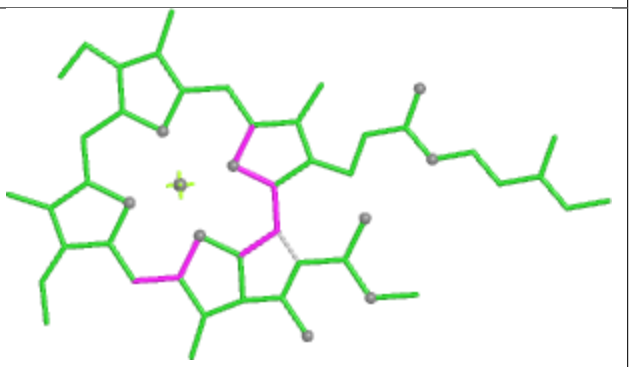
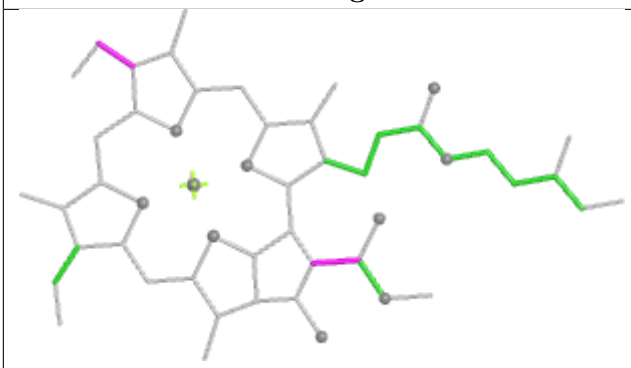
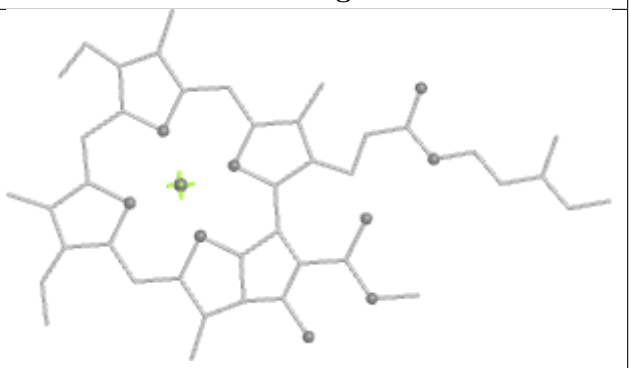
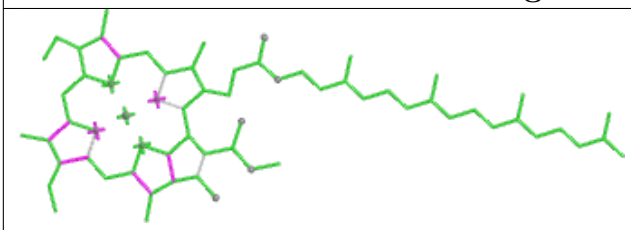
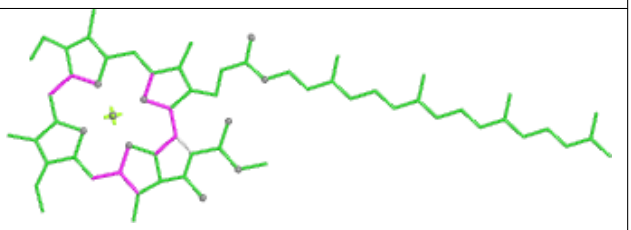
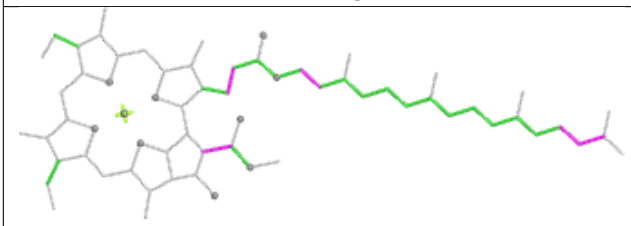
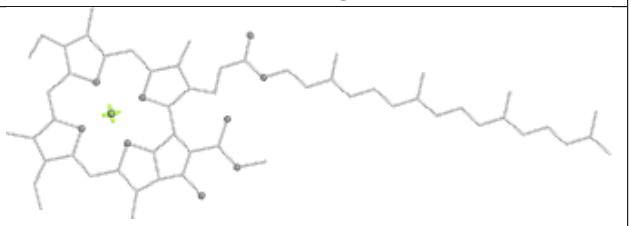
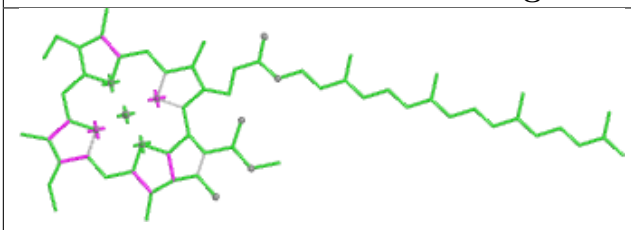
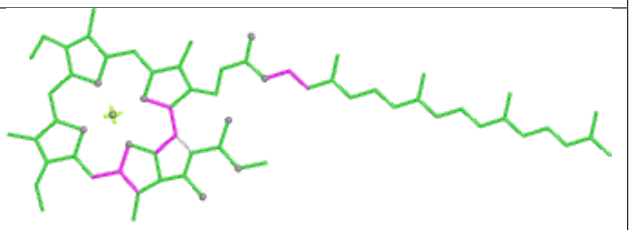
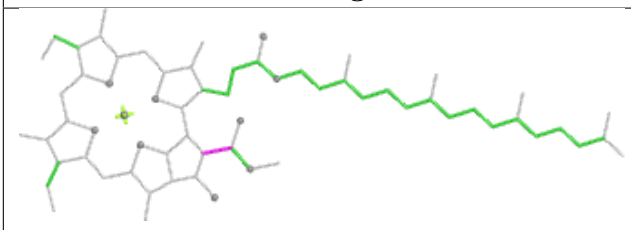
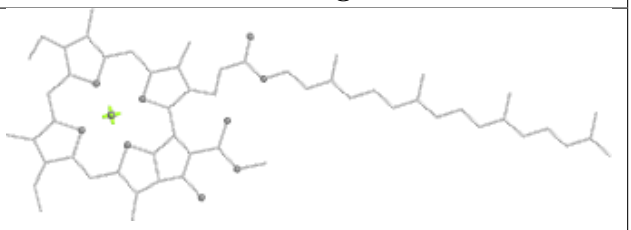


Rings

Ligand CLA A 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

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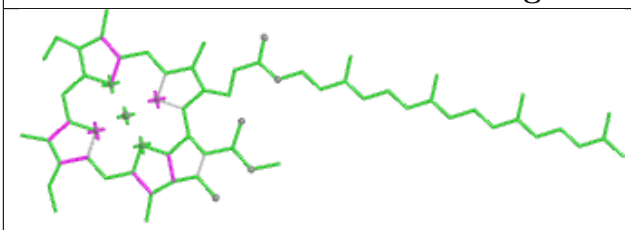
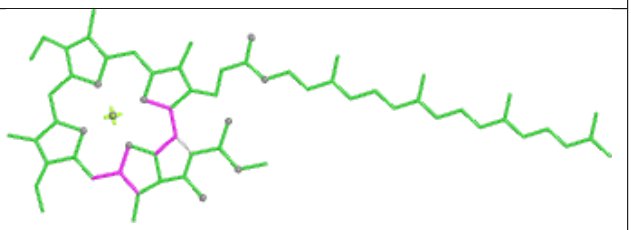
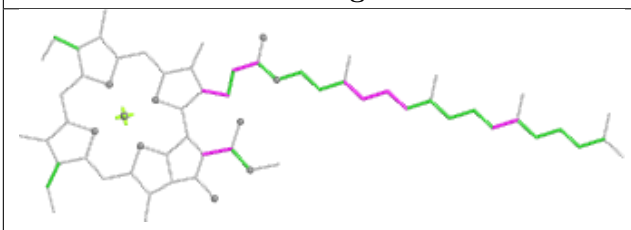
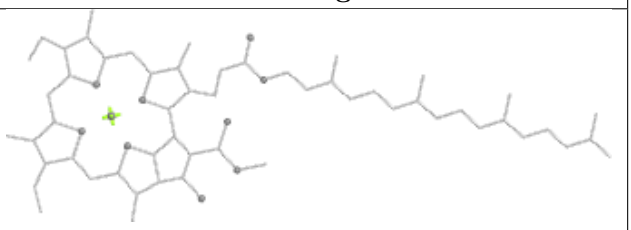
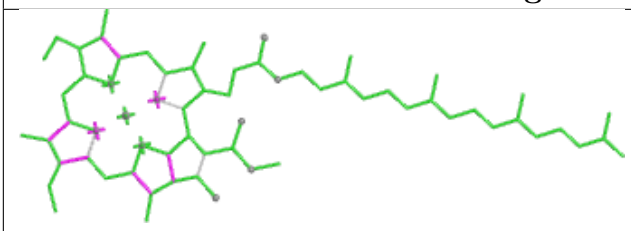
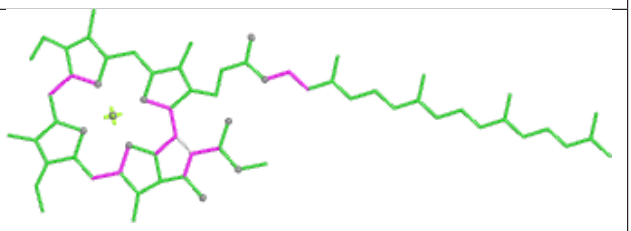
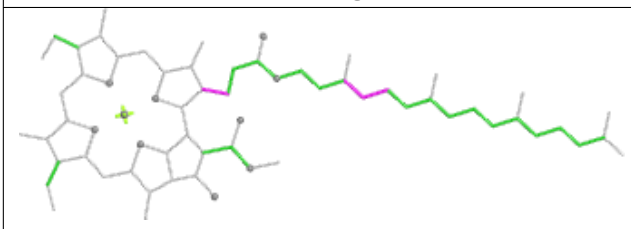
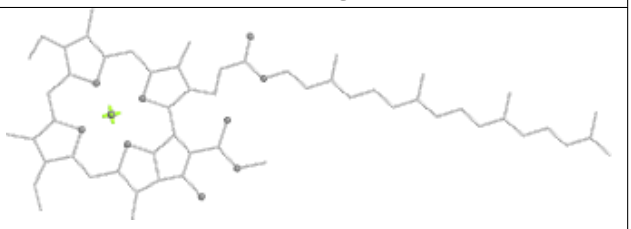
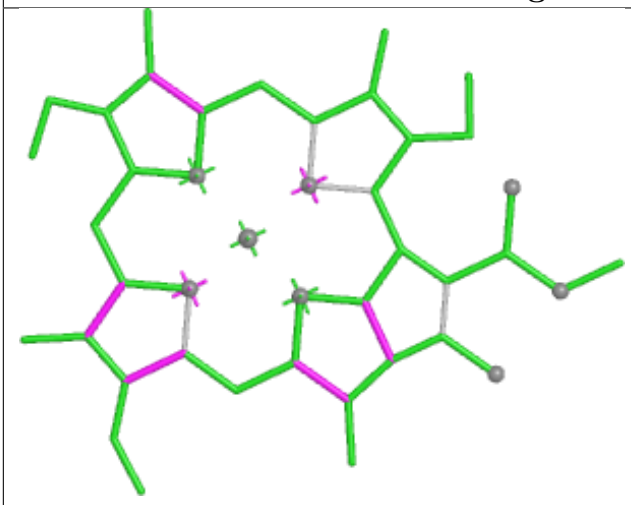
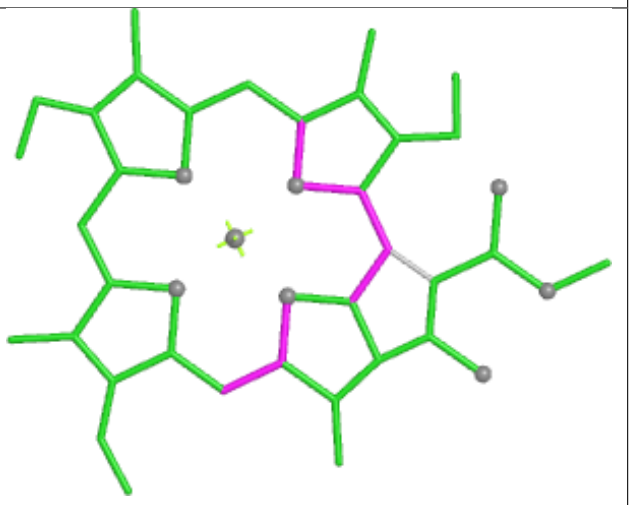
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

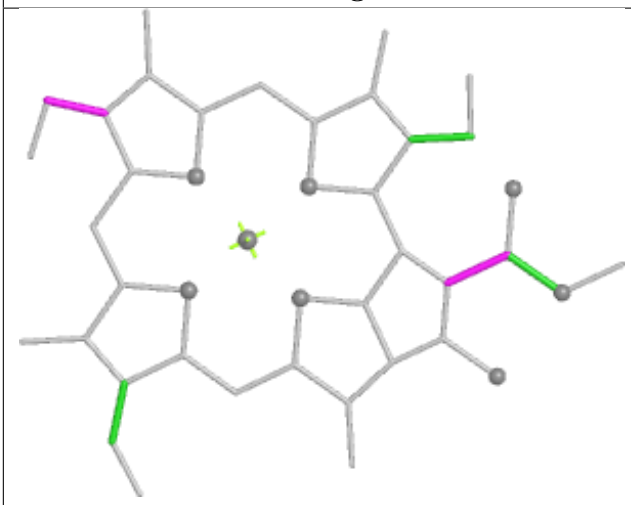
Ligand CLA J 104



Bond lengths



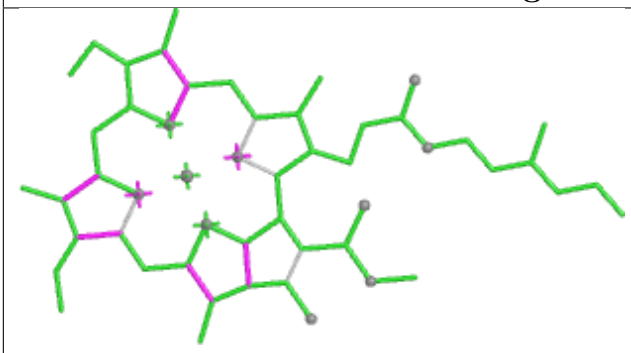
Bond angles



Torsions

Rings

Ligand CLA U 211



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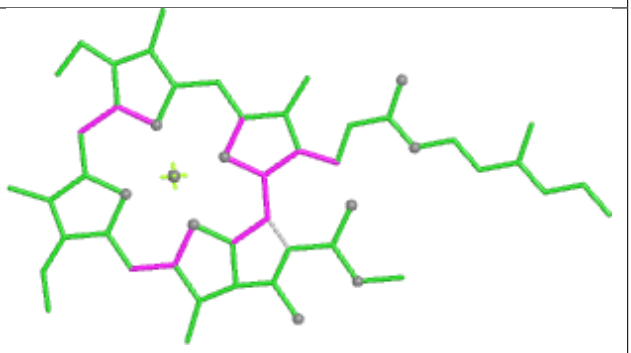
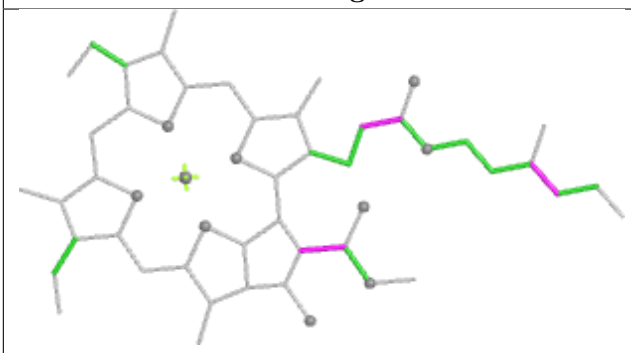


Bond angles



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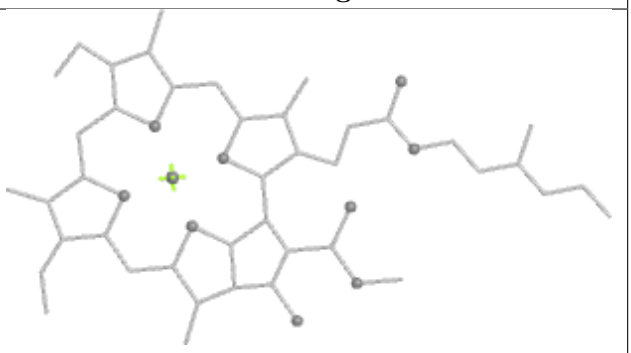
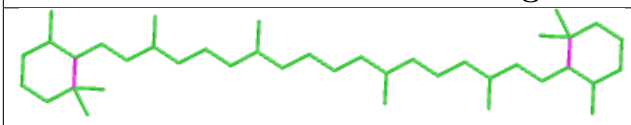


Rings

Ligand BCR A 844



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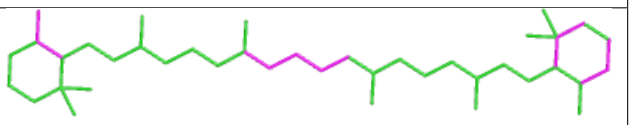
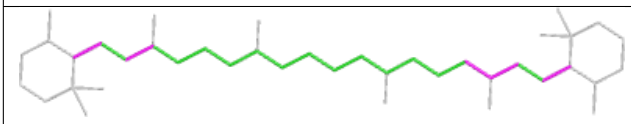


Bond angles



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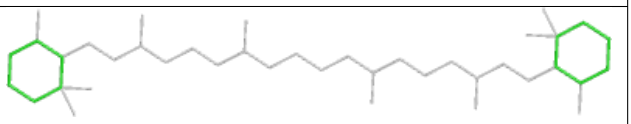
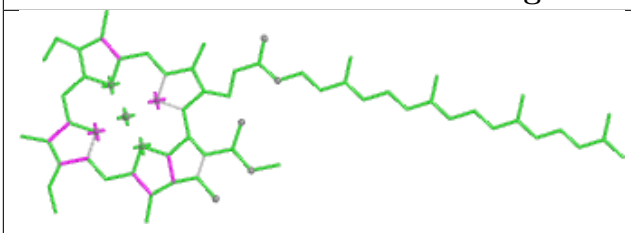
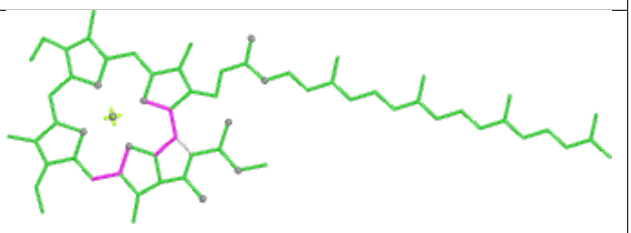


Rings

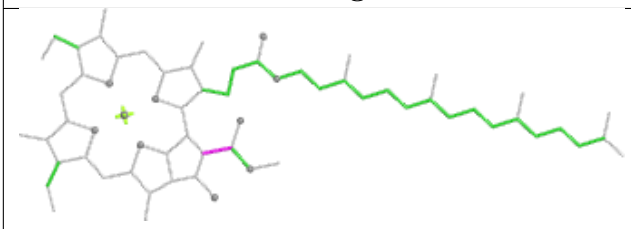
Ligand CLA A 829



Bond lengths



Bond angles



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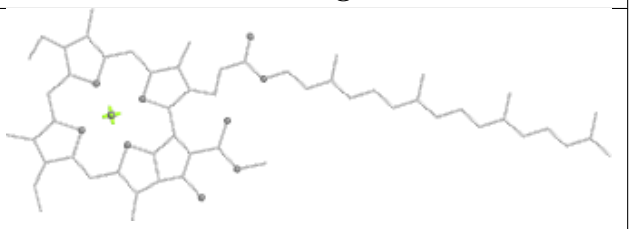
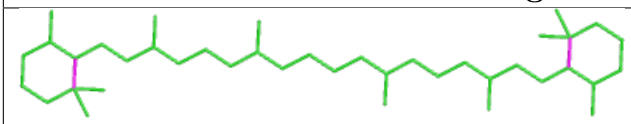
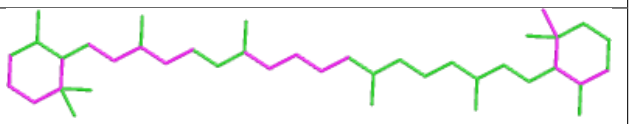
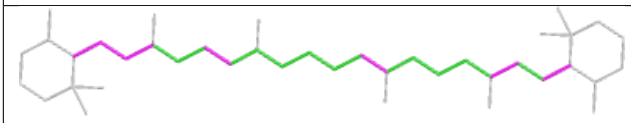
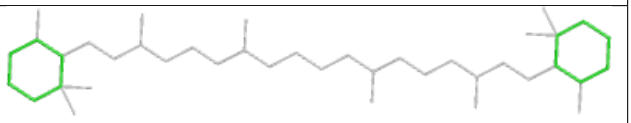
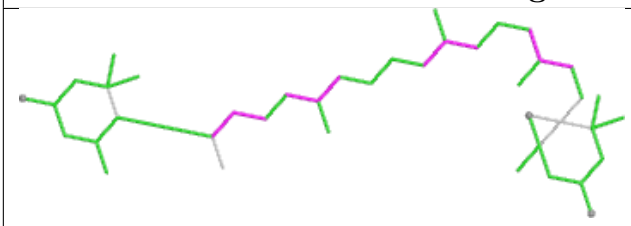
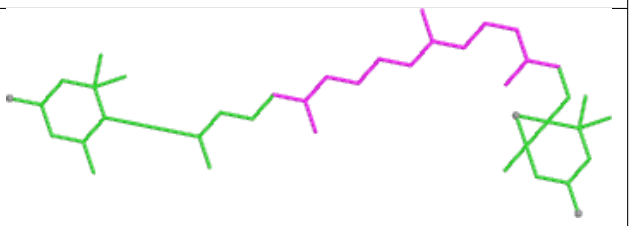
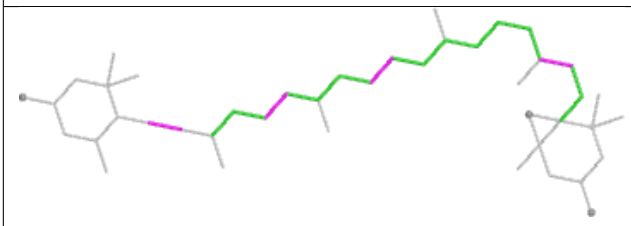
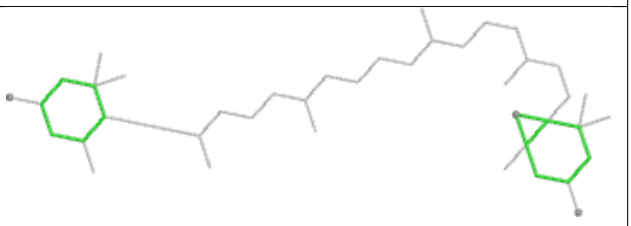
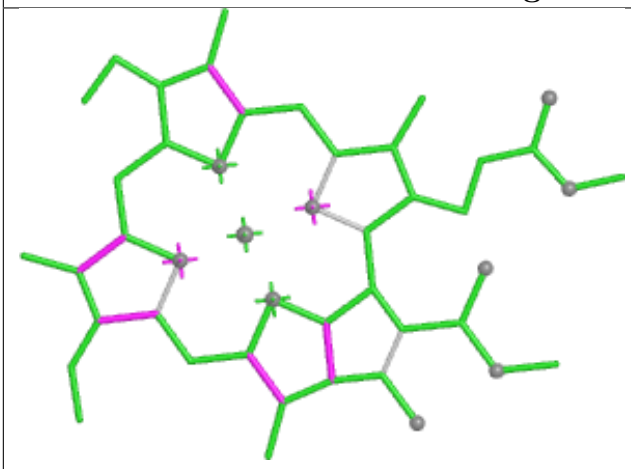
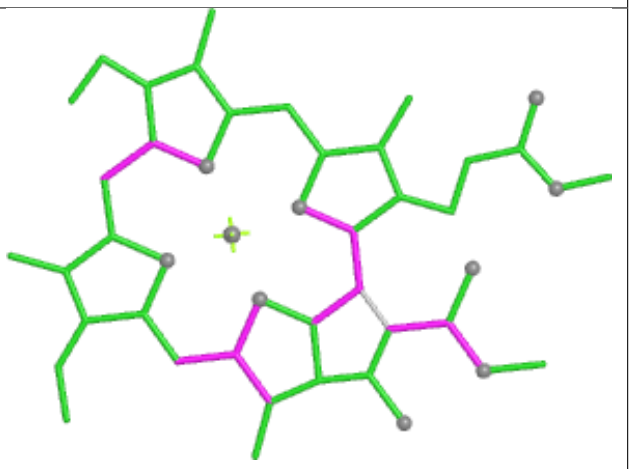
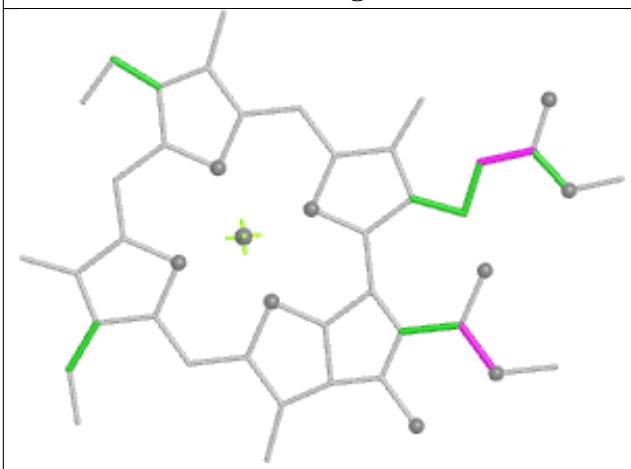
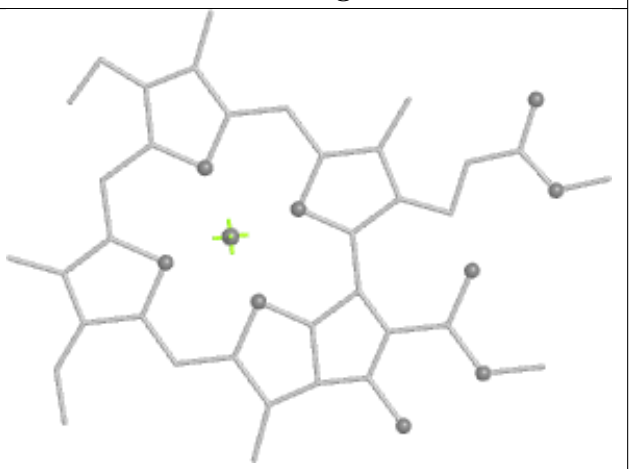
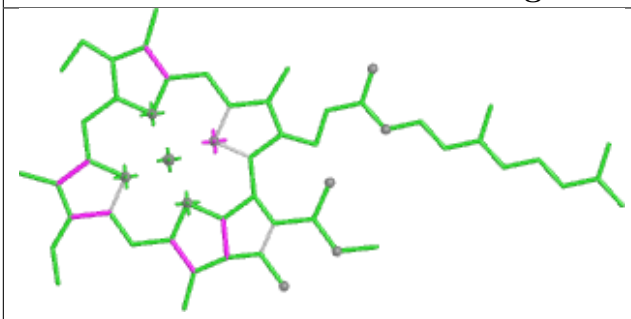
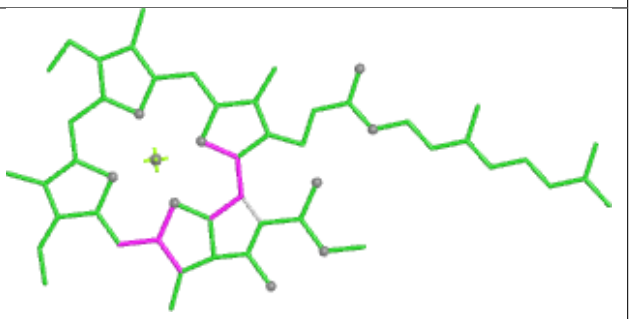
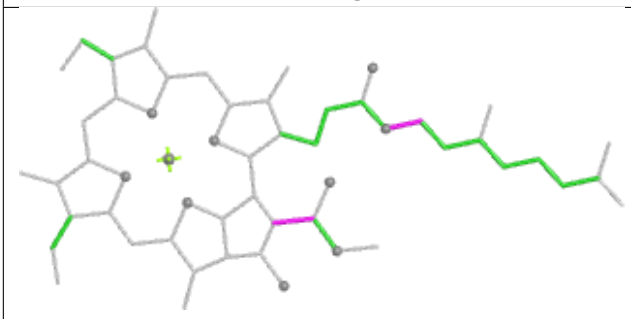
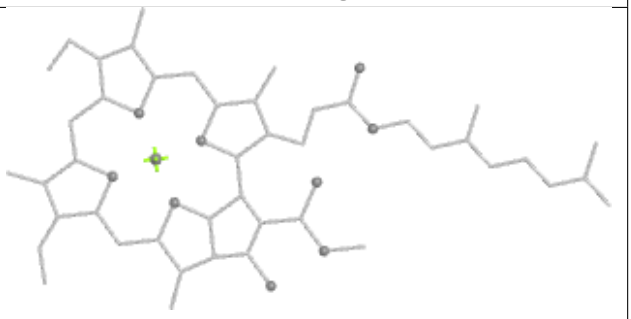


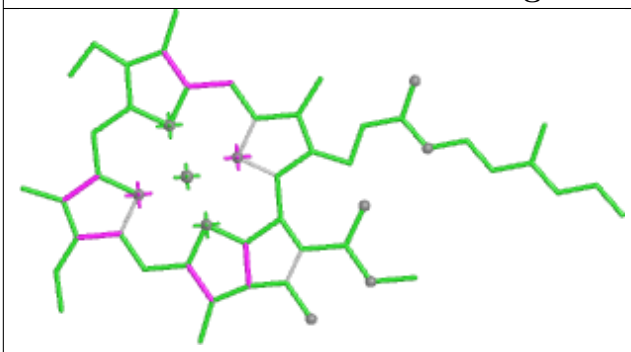
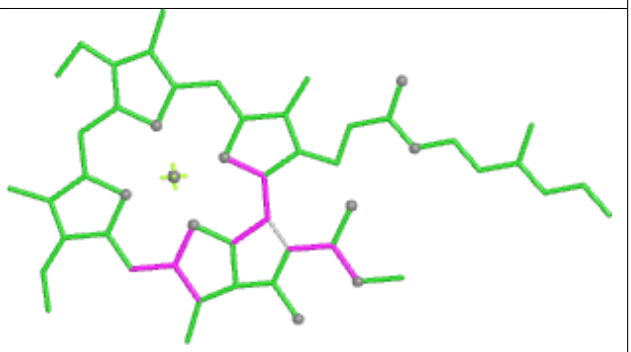
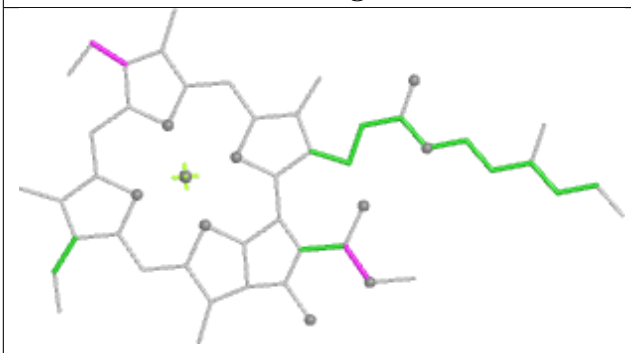
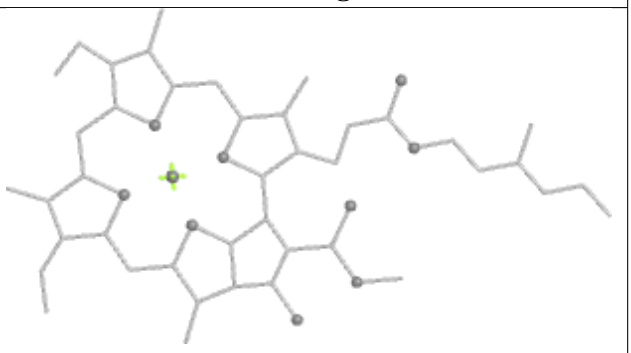
Rings

Ligand BCR k 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

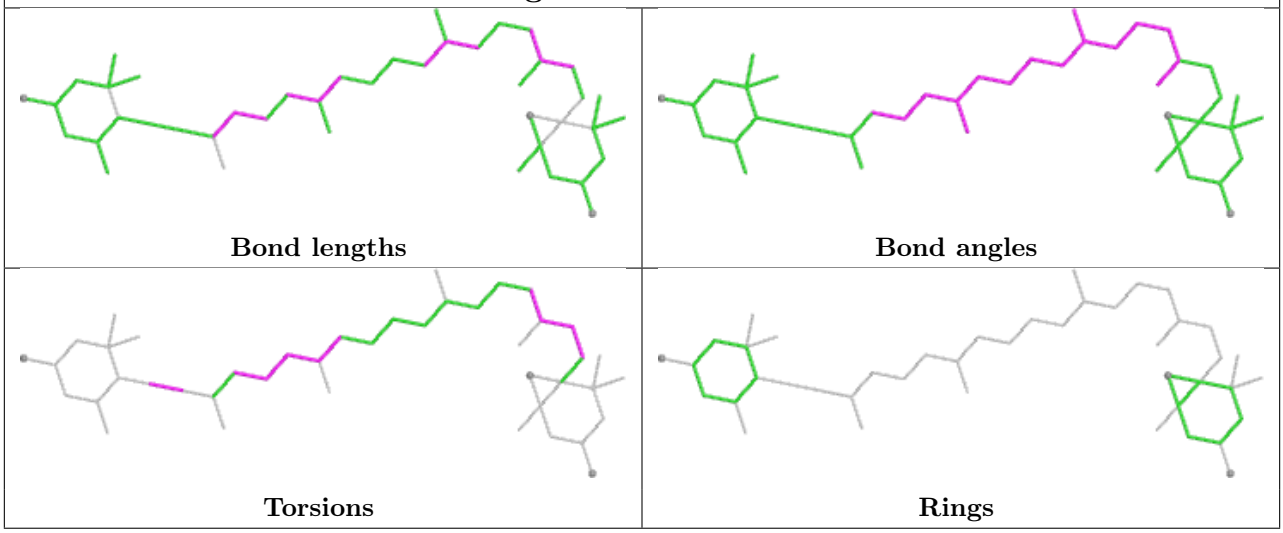
Ligand DD6 J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

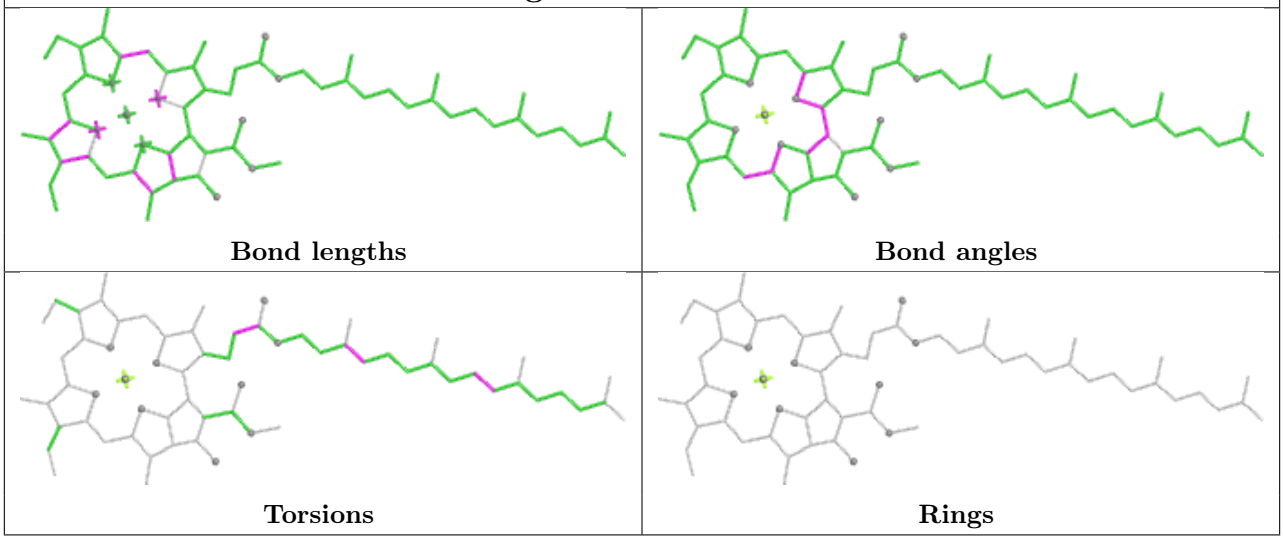
Ligand CLA B 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 G 314



Ligand CLA B 806



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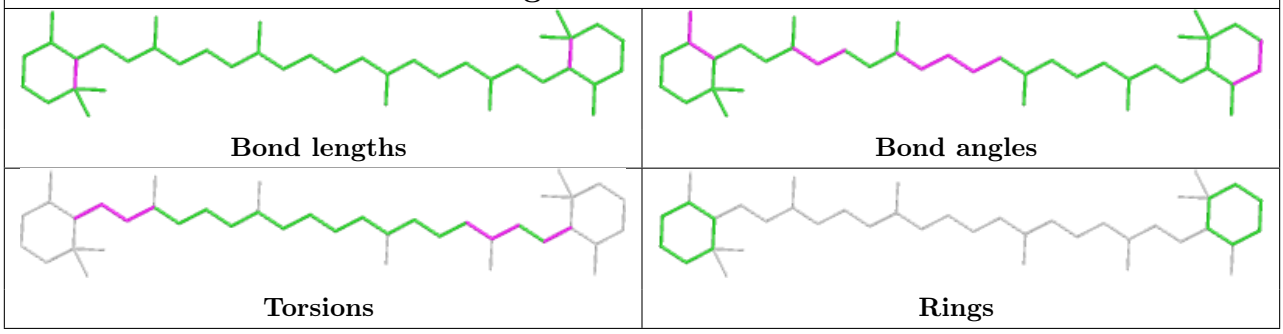
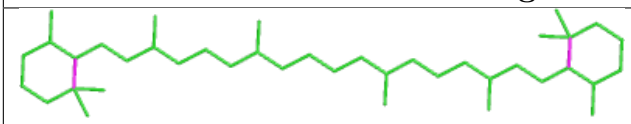
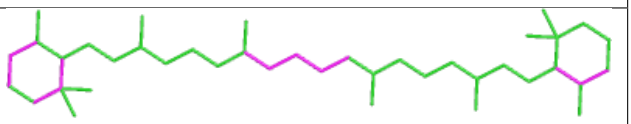


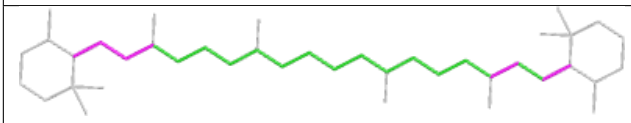
Ligand BCR M 101



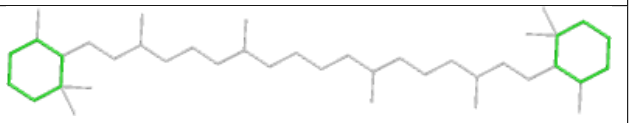
Bond lengths



Bond angles

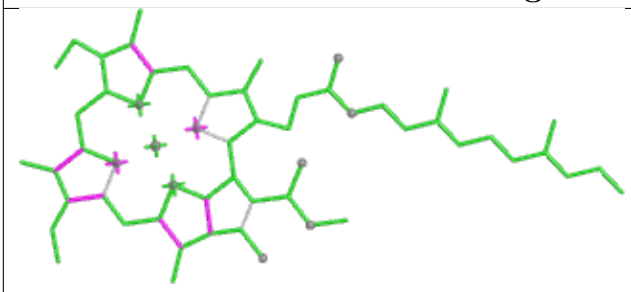


Torsions

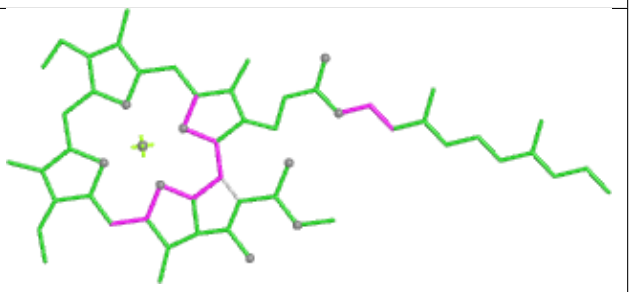


Rings

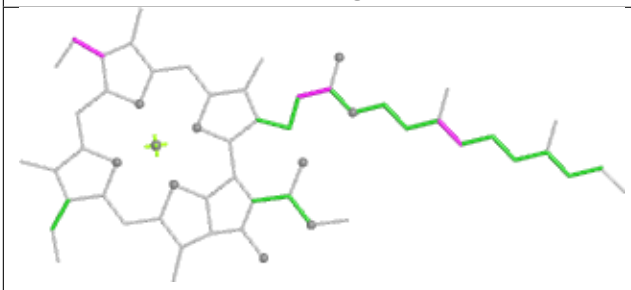
Ligand CLA B 836



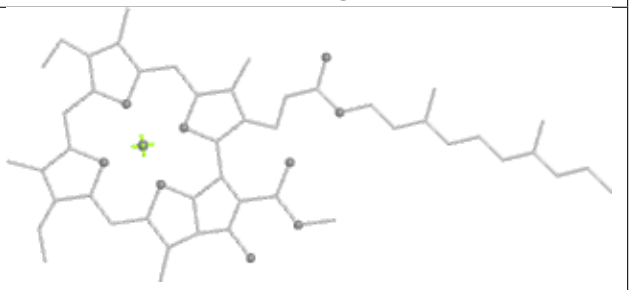
Bond lengths



Bond angles

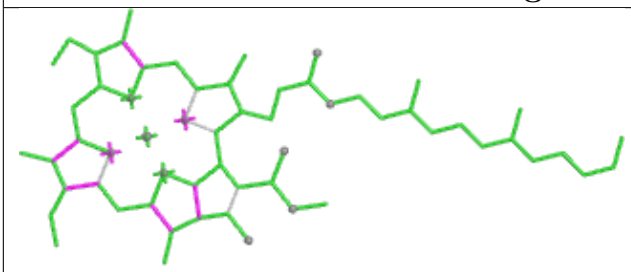


Torsions

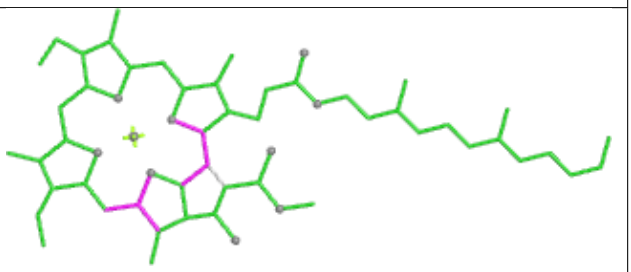


Rings

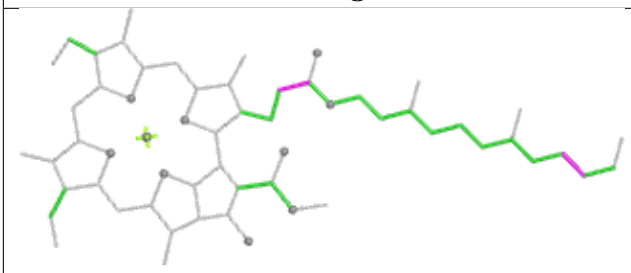
Ligand CLA B 815



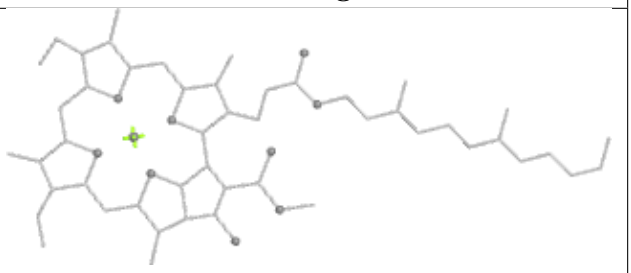
Bond lengths



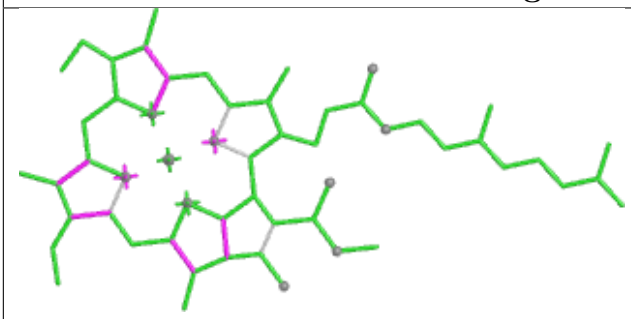
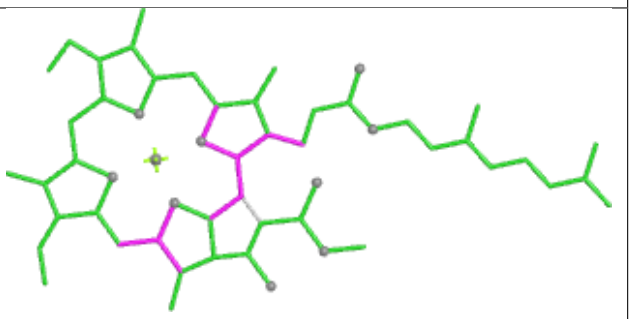
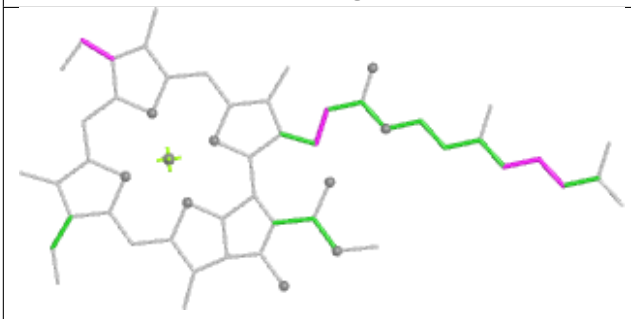
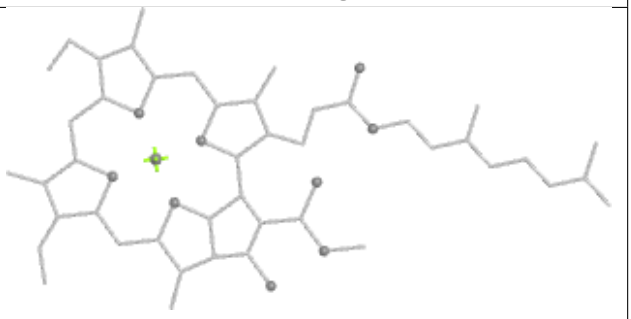
Bond angles

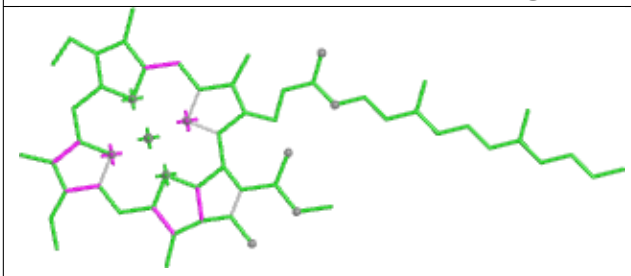
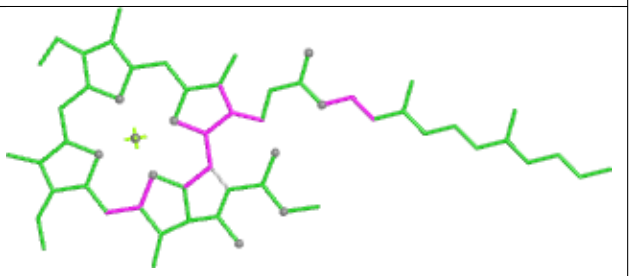
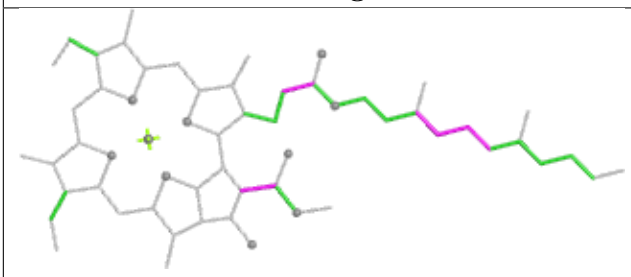
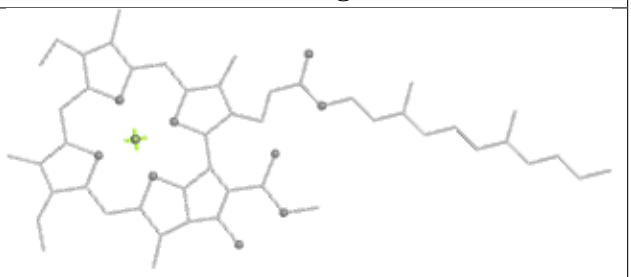


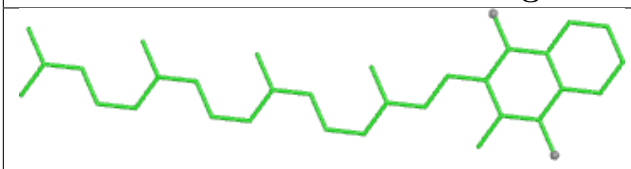
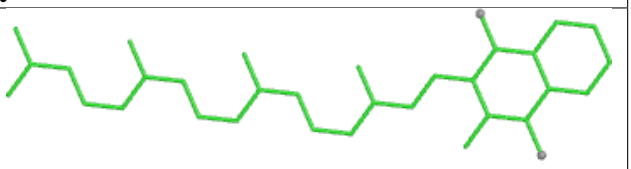
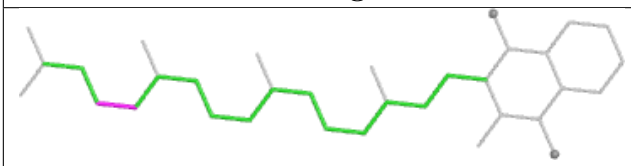
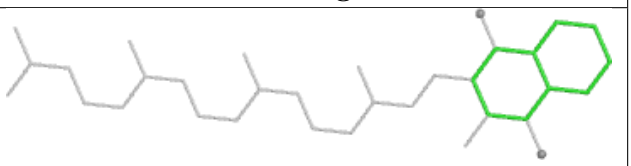
Torsions

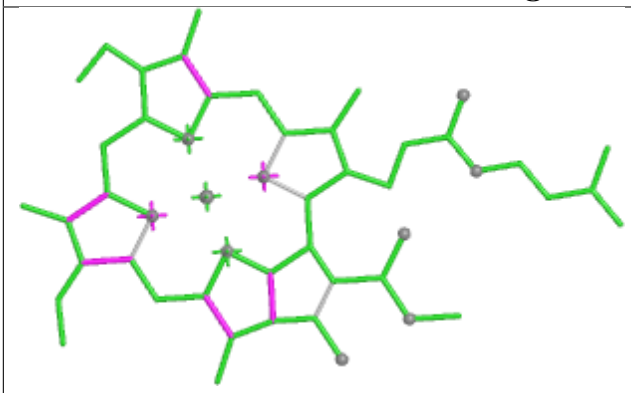
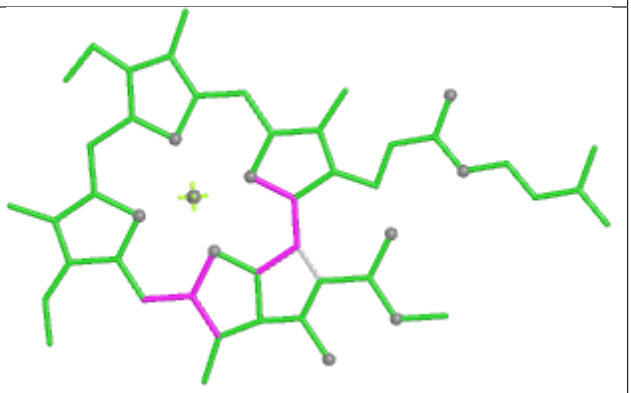
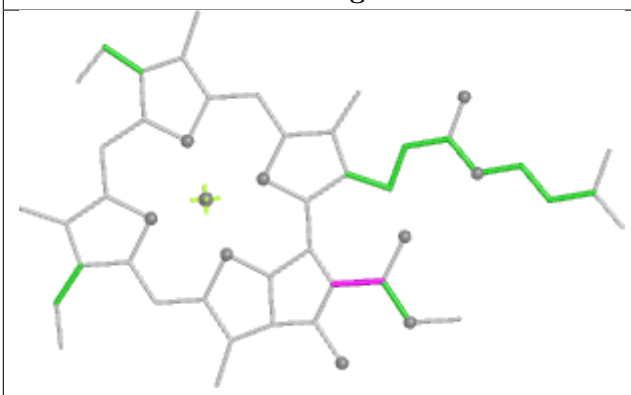
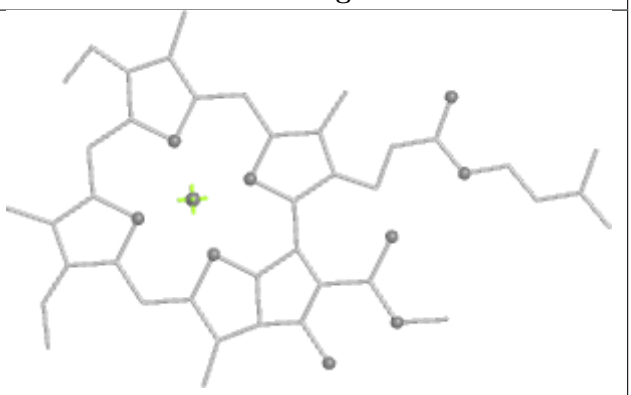


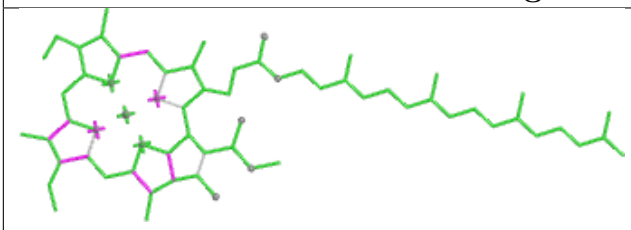
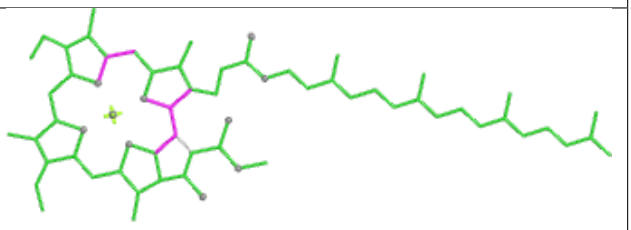
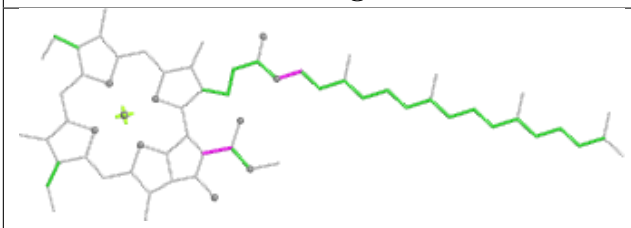
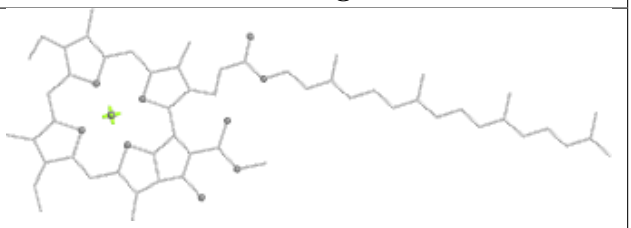
Rings

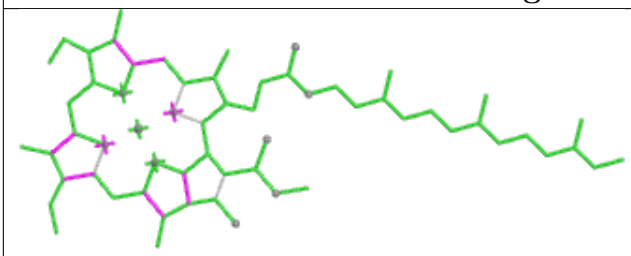
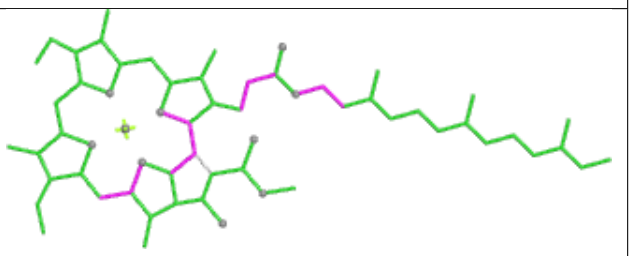
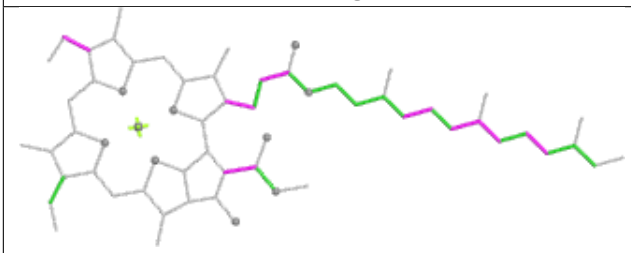
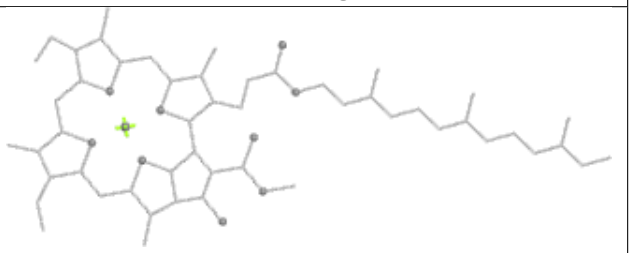
Ligand CLA A 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

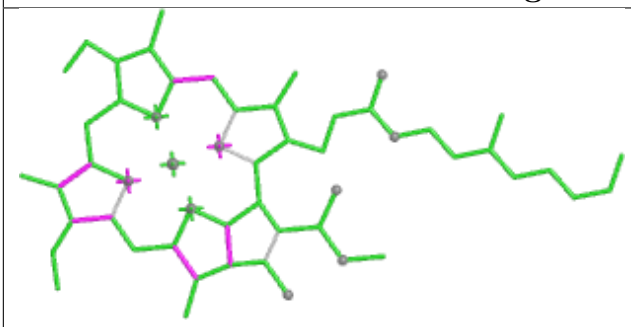
Ligand PQN B 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

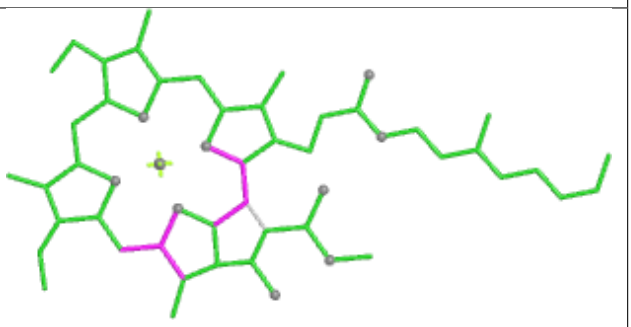
Ligand CLA B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

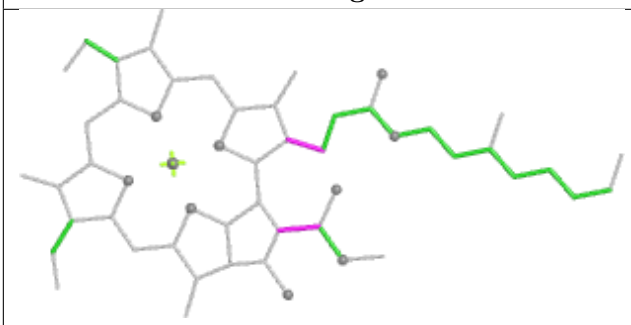
Ligand CLA B 812



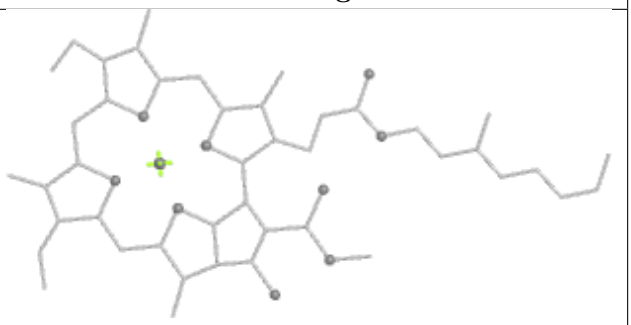
Bond lengths



Bond angles

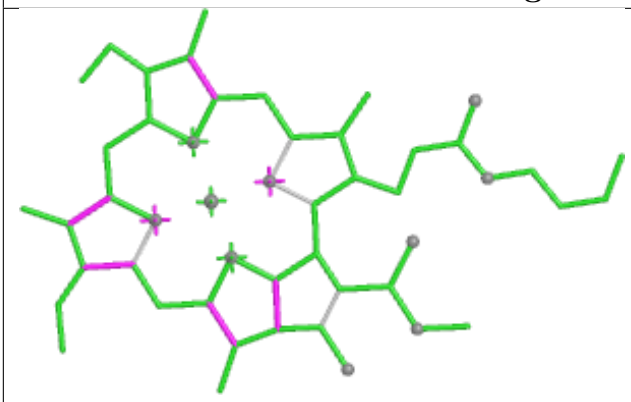


Torsions

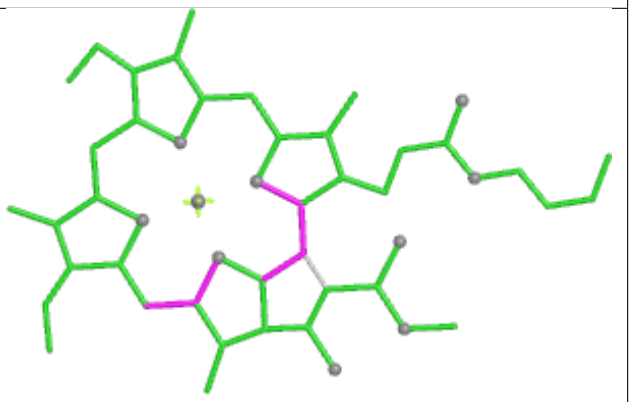


Rings

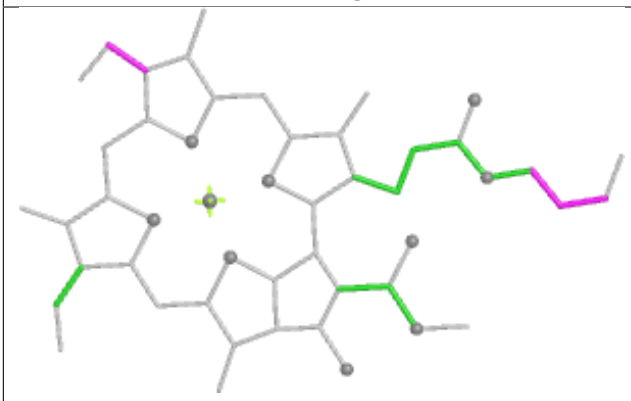
Ligand CLA B 827



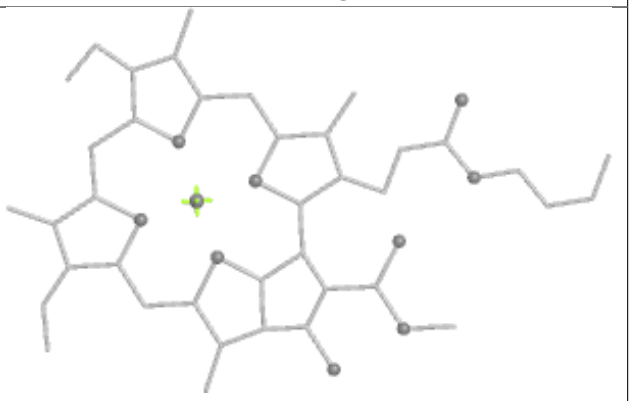
Bond lengths



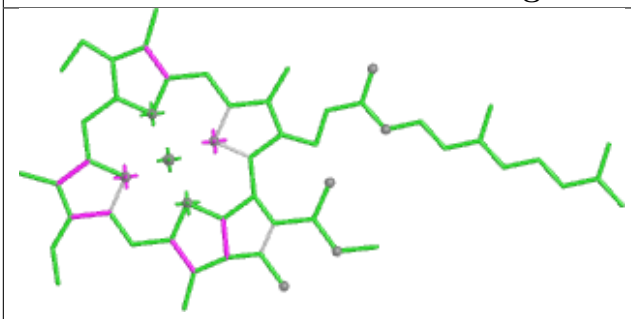
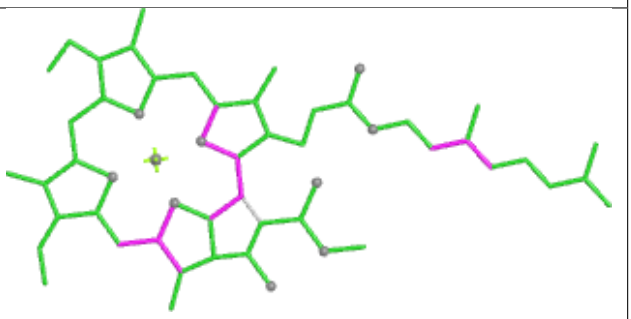
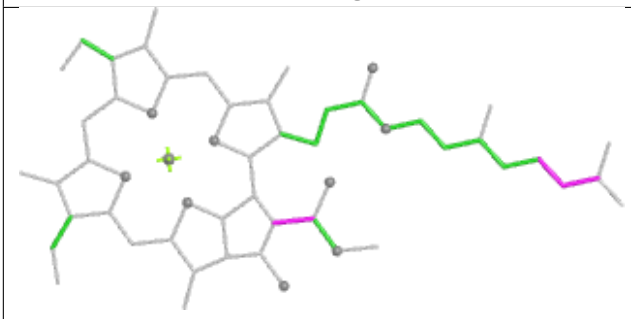
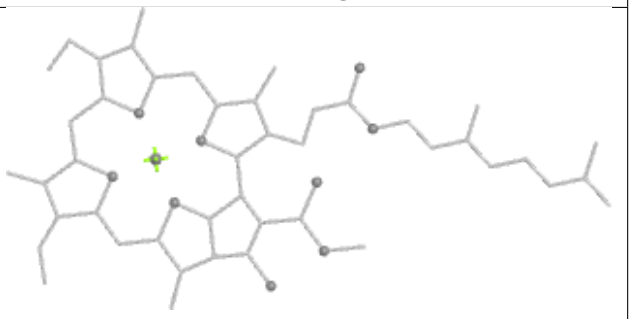
Bond angles

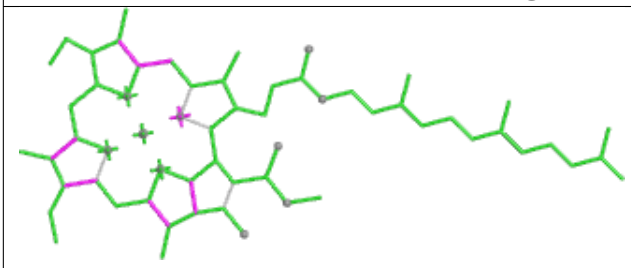
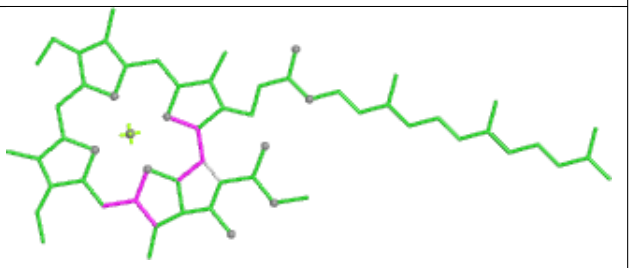
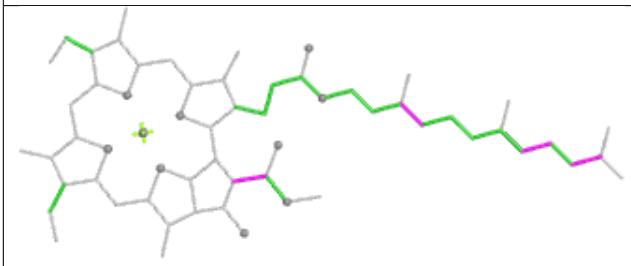
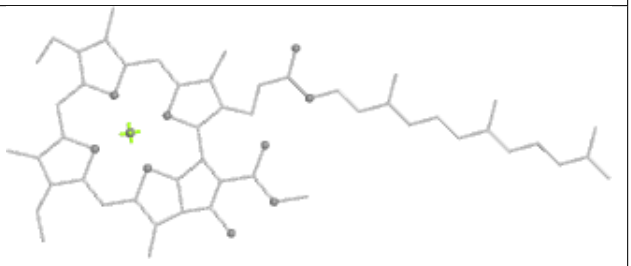


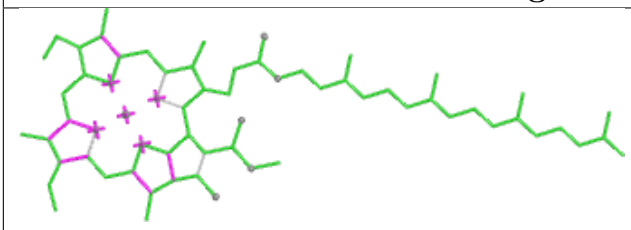
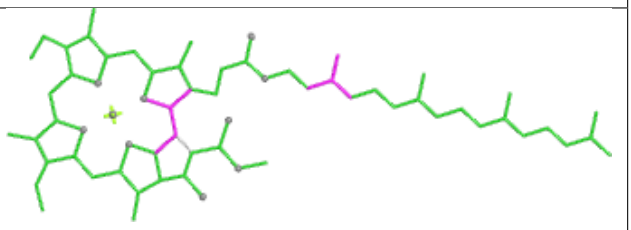
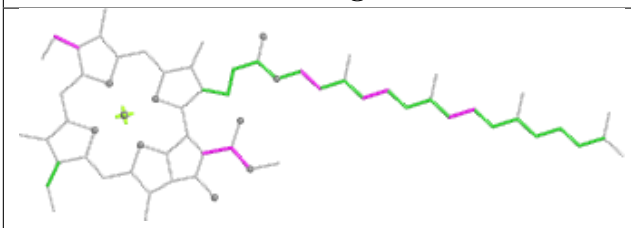
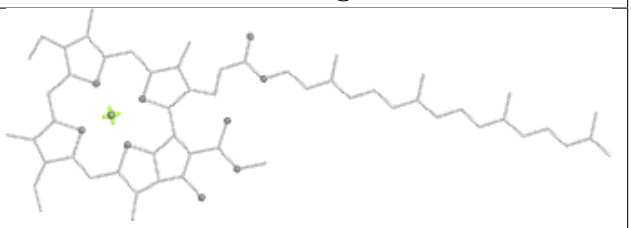
Torsions

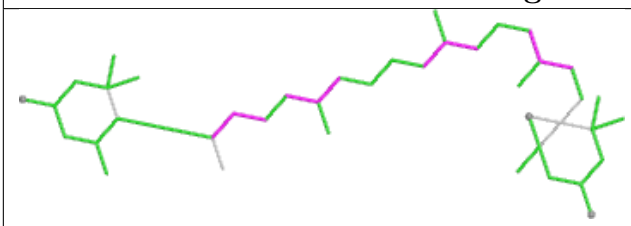
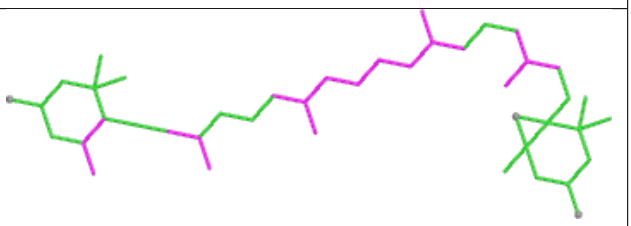
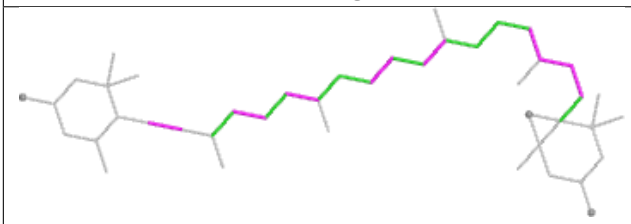


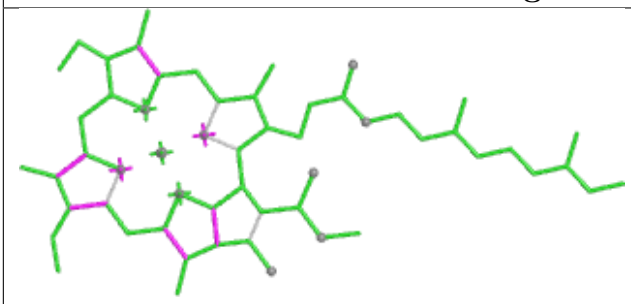
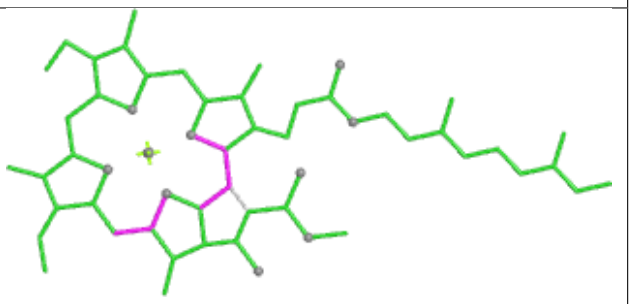
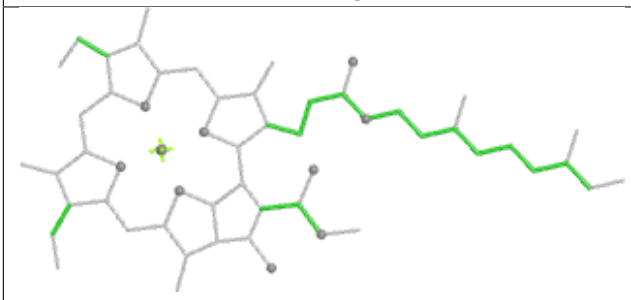
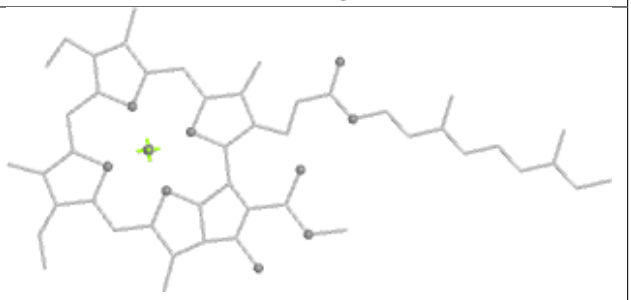
Rings

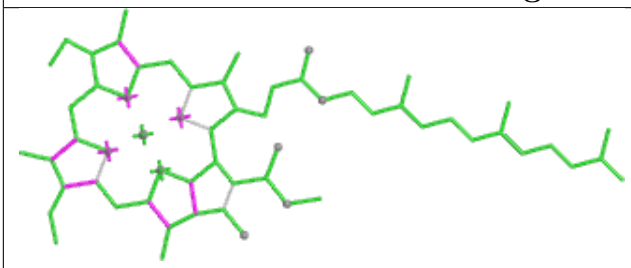
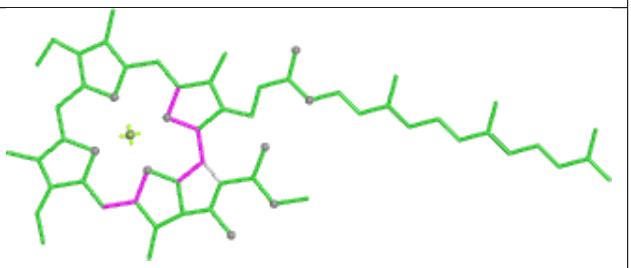
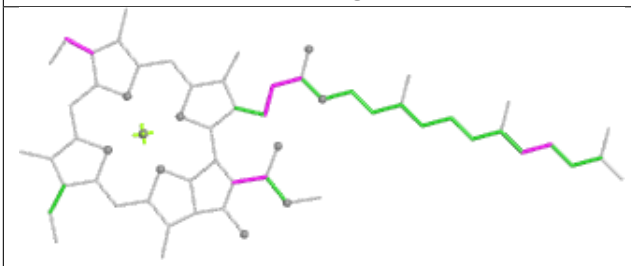
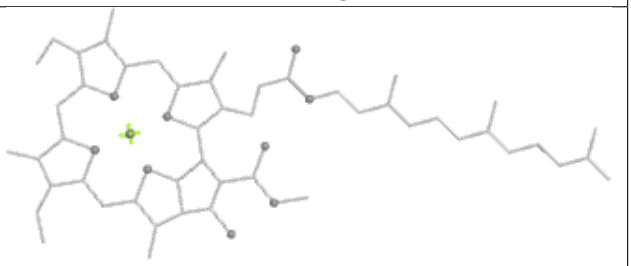
Ligand CLA G 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

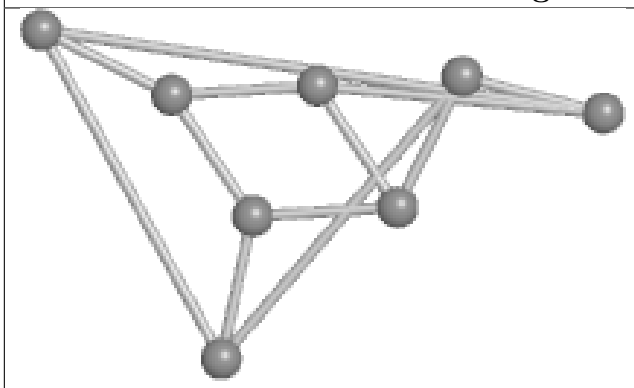
Ligand CL0 A 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 G 317	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 C 102



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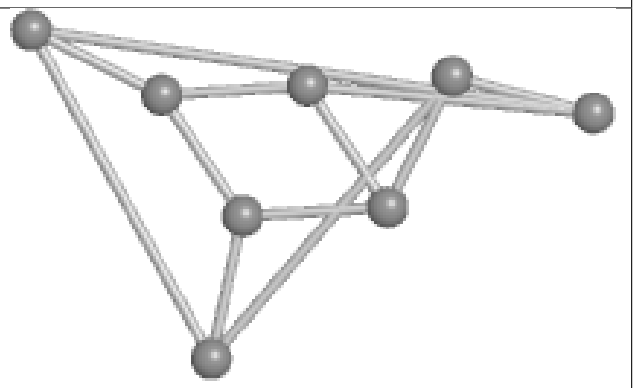

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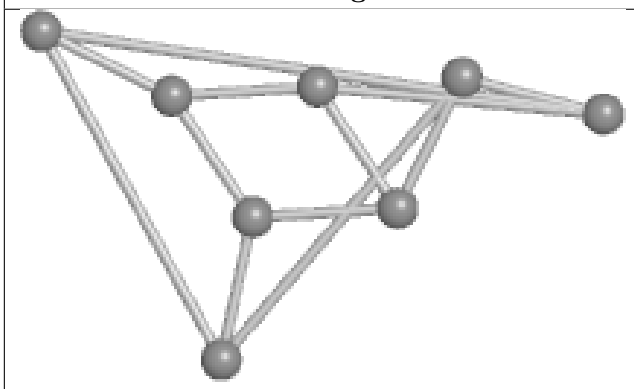

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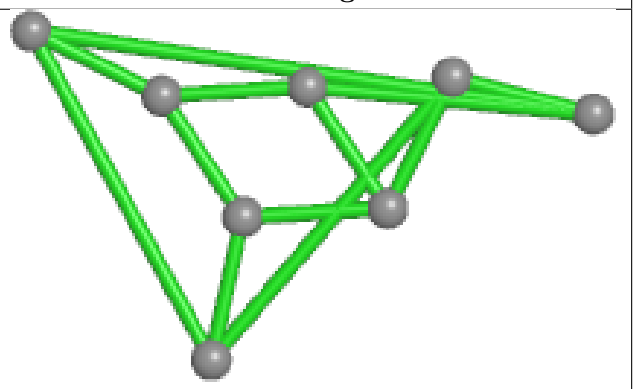
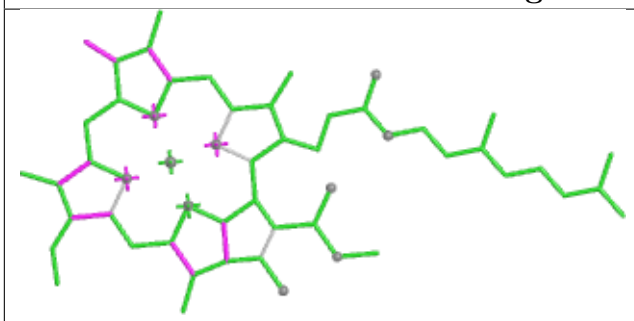


Rings

Ligand CLA B 810



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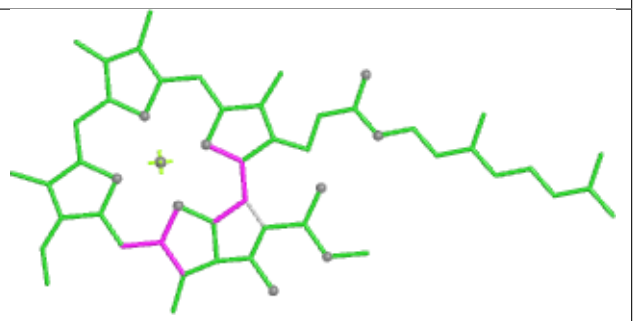

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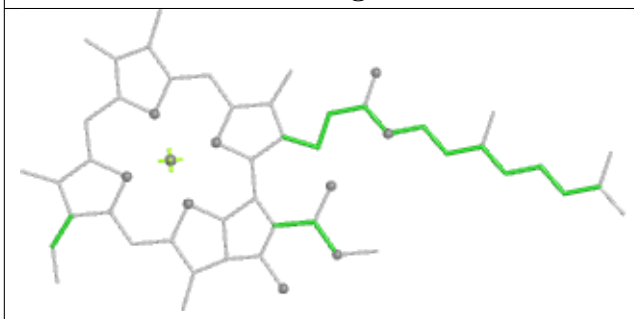

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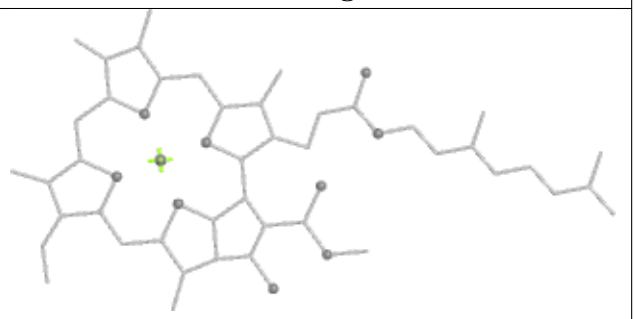
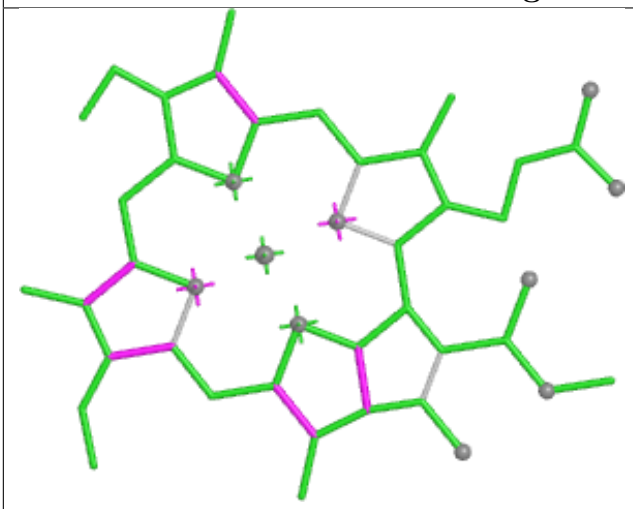


Rings

Ligand CLA K 204



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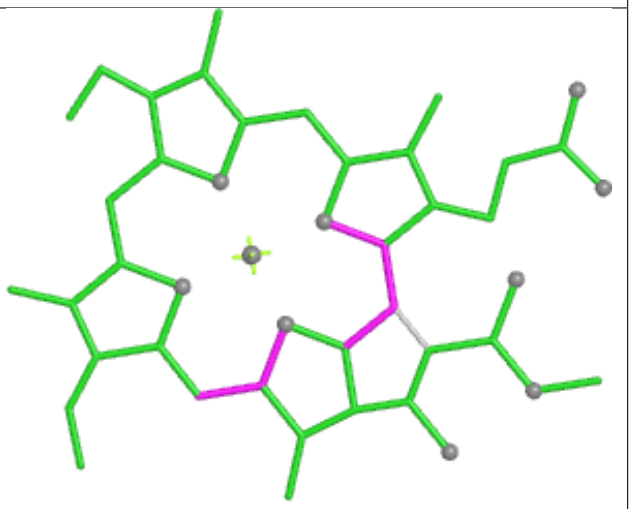

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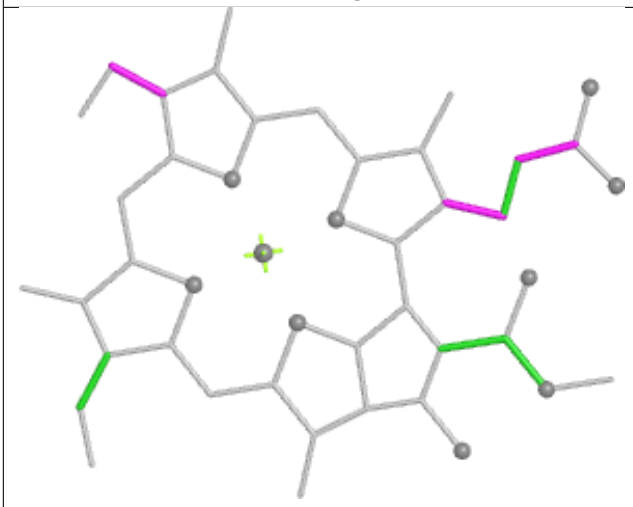
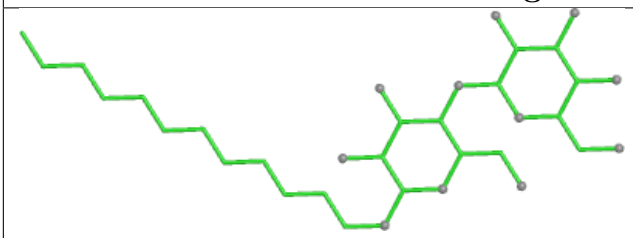


Torsions

Rings

Ligand LMU J 101



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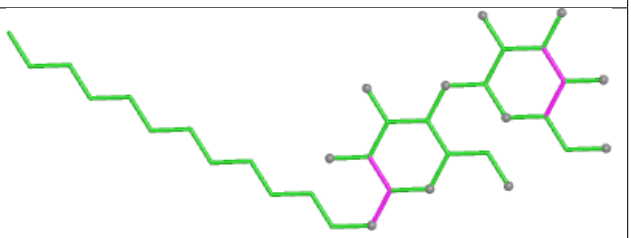

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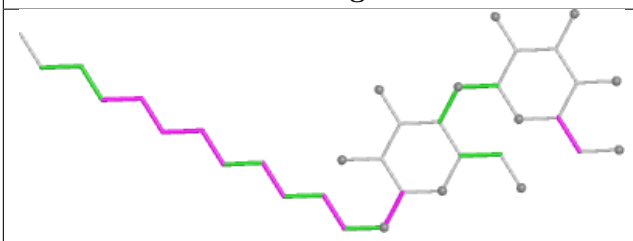

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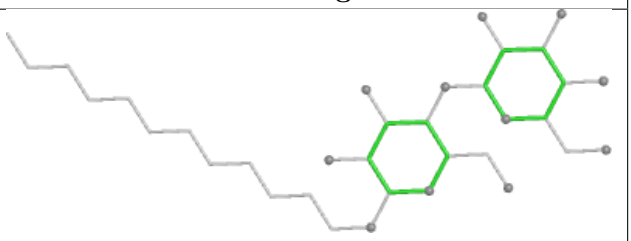
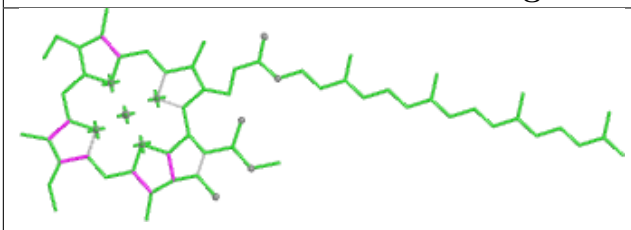
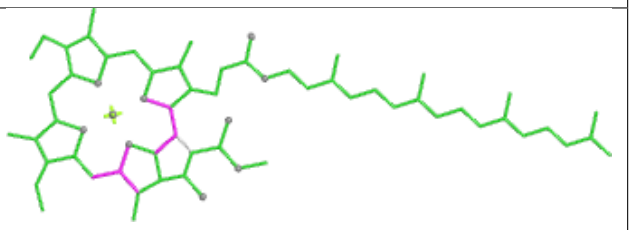
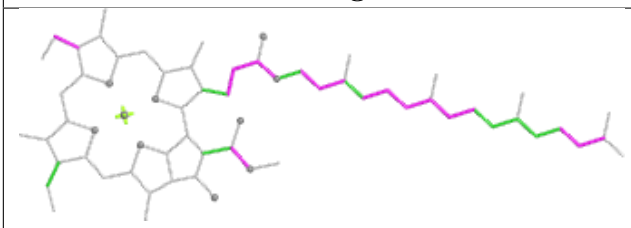
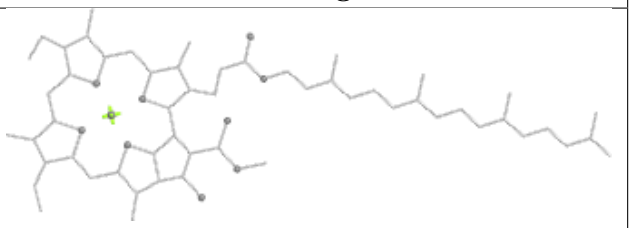
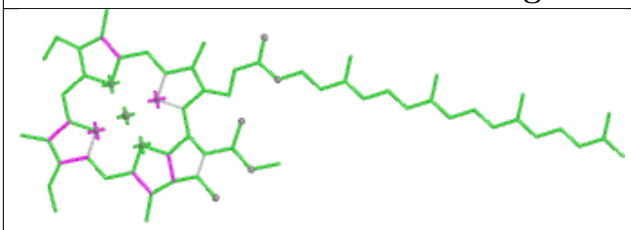
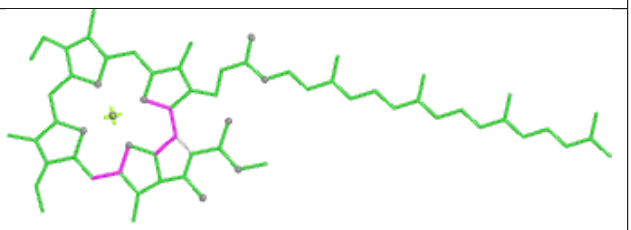
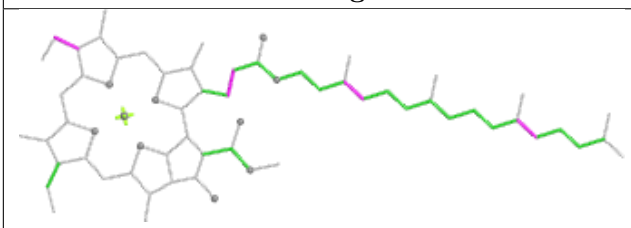
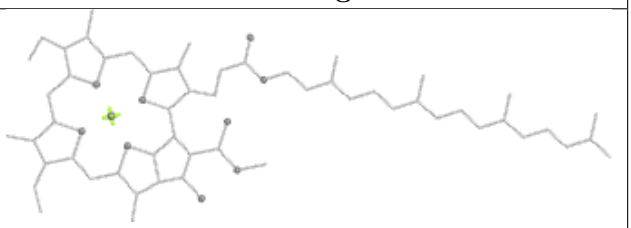
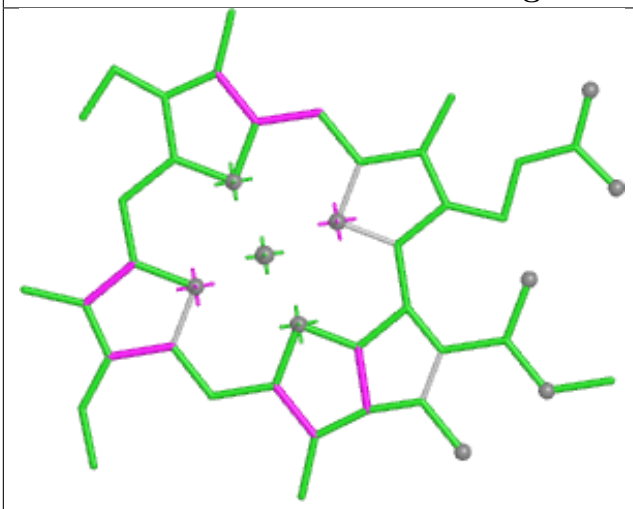


Rings

Ligand CLA H 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 303



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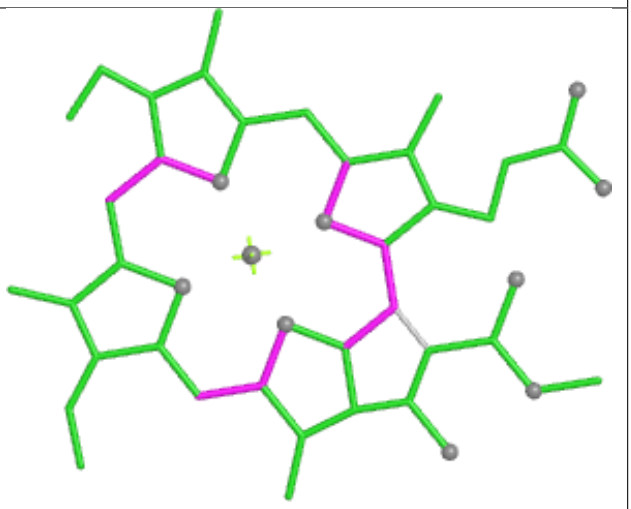
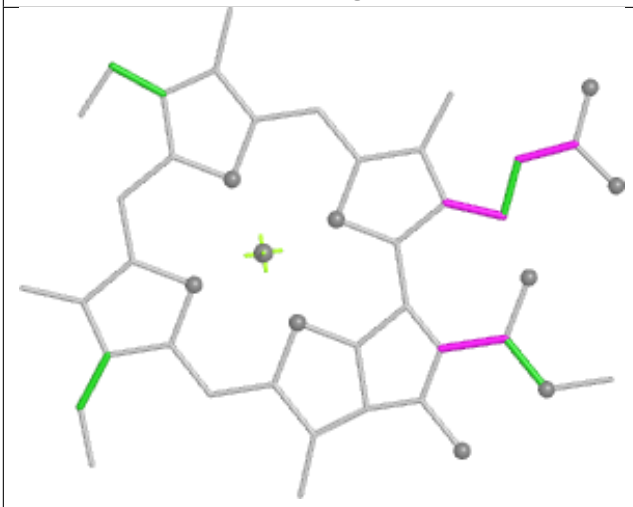


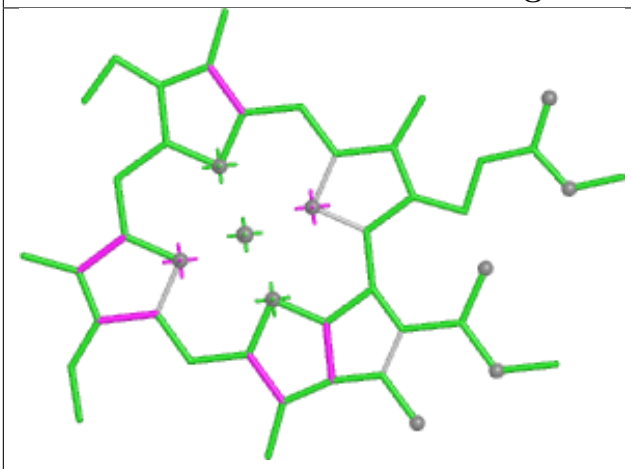
Bond angles



Torsions

Rings

Ligand CLA B 818



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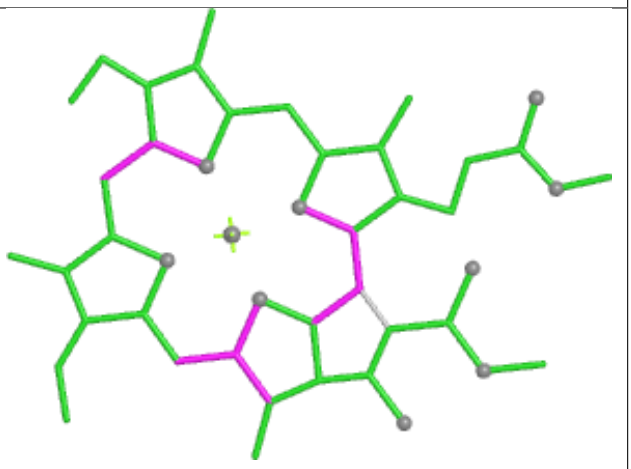

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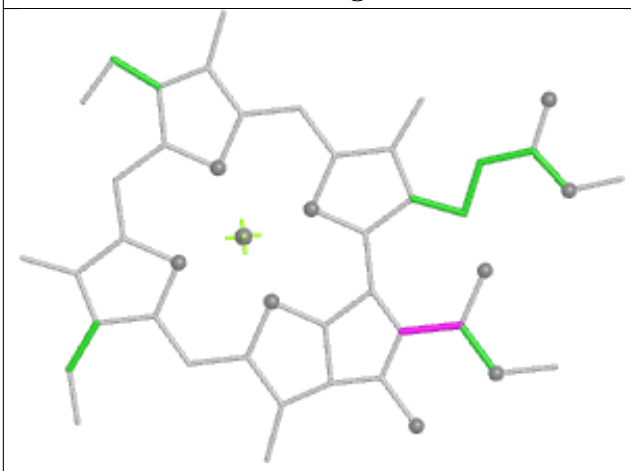
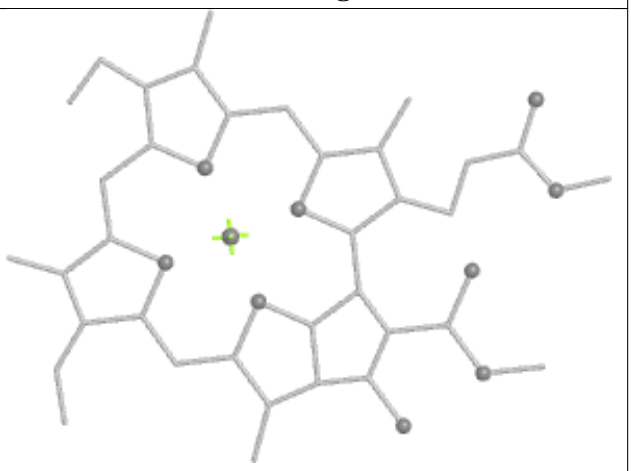
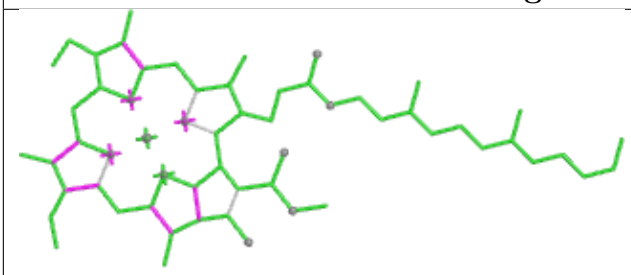


Torsions



Rings

Ligand CLA B 813



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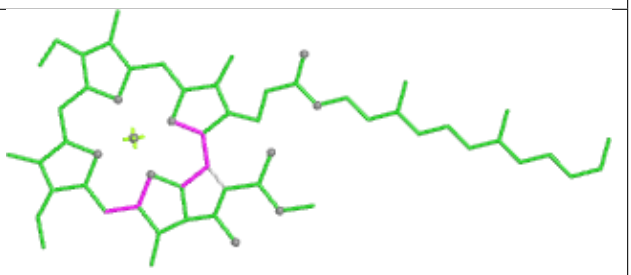
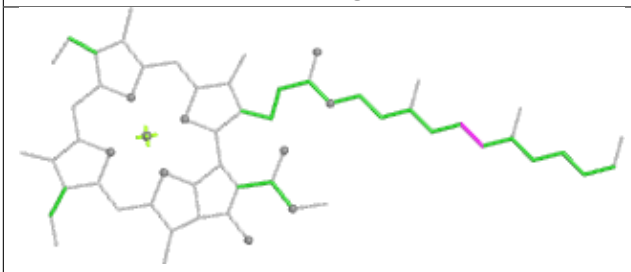


Bond angles



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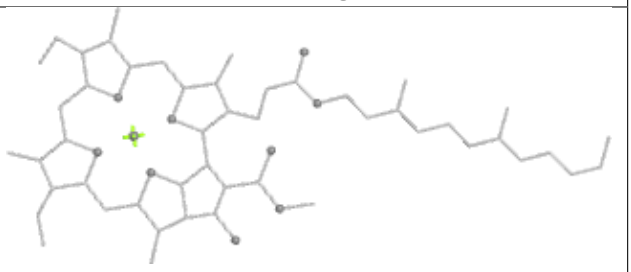
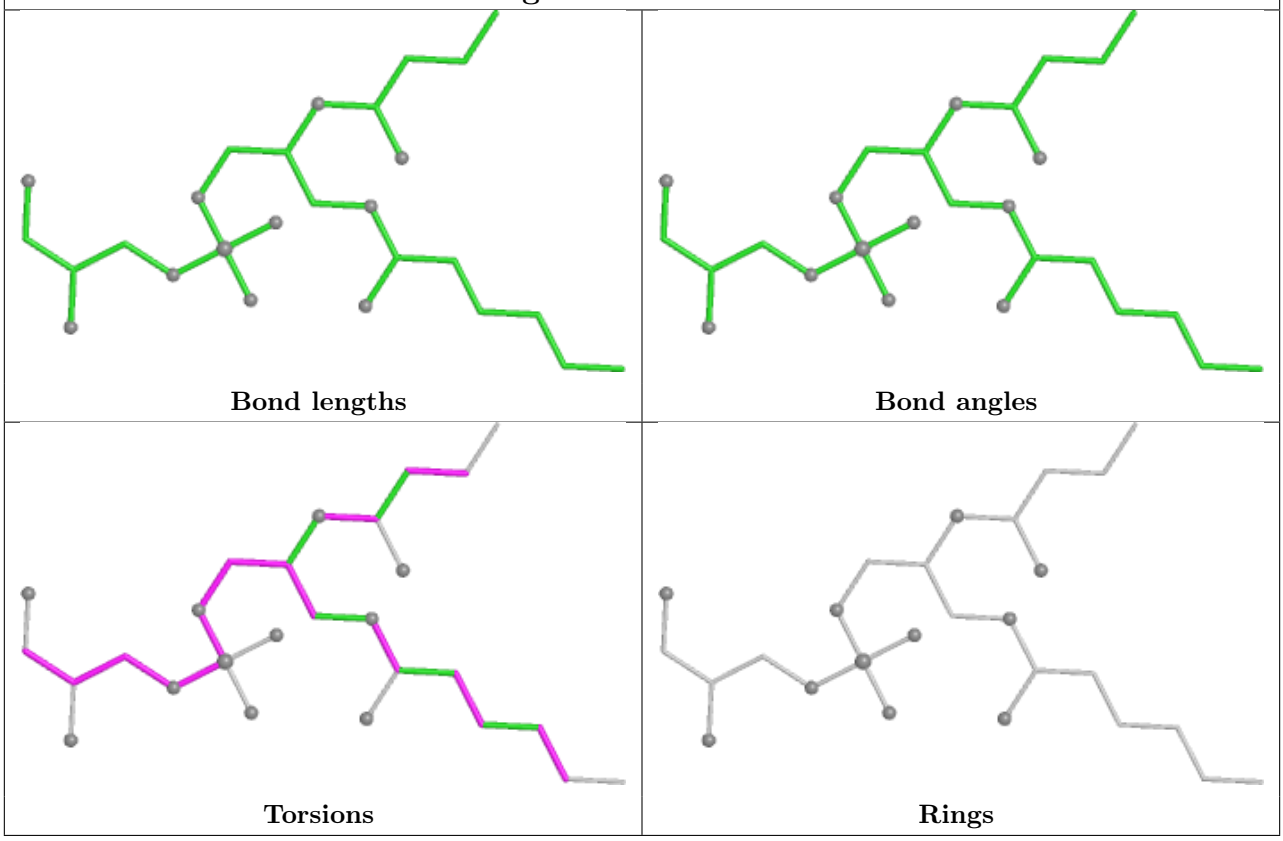
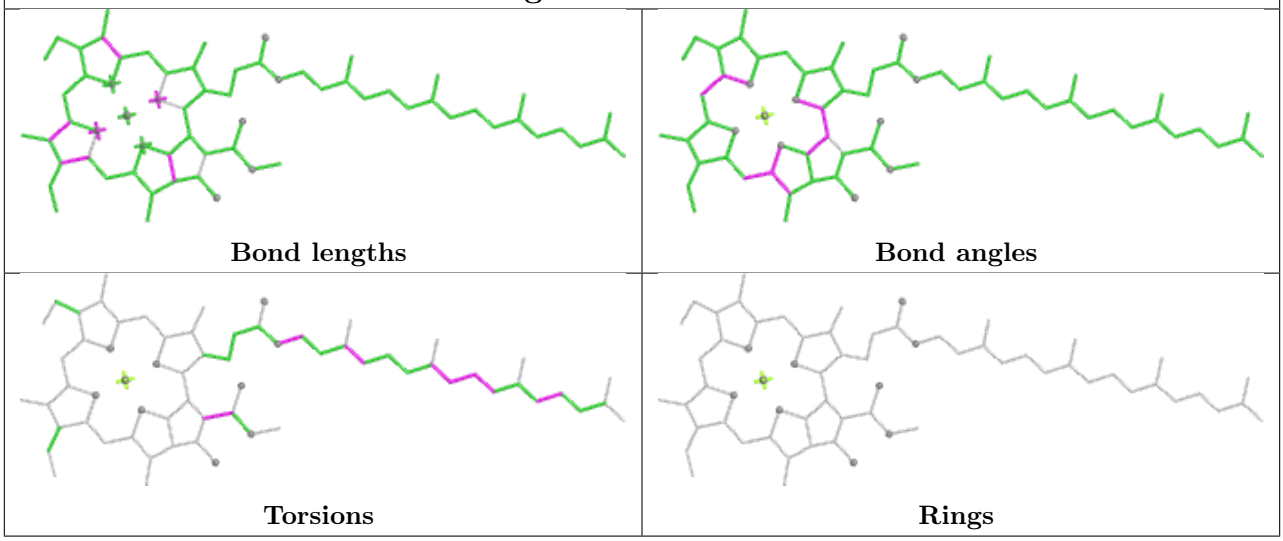


Rings

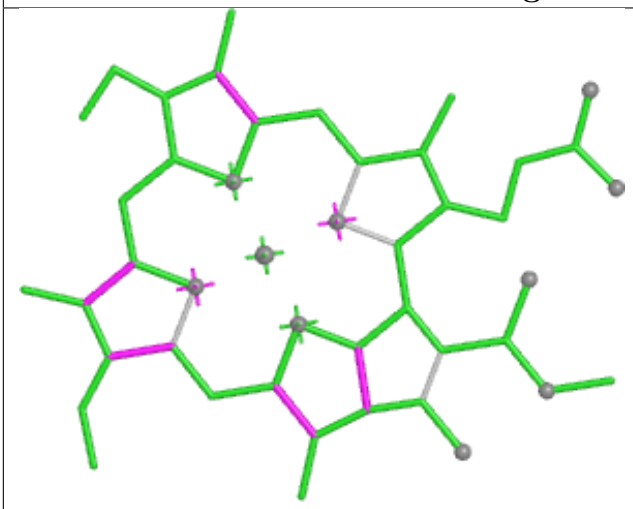
Ligand LHG G 316



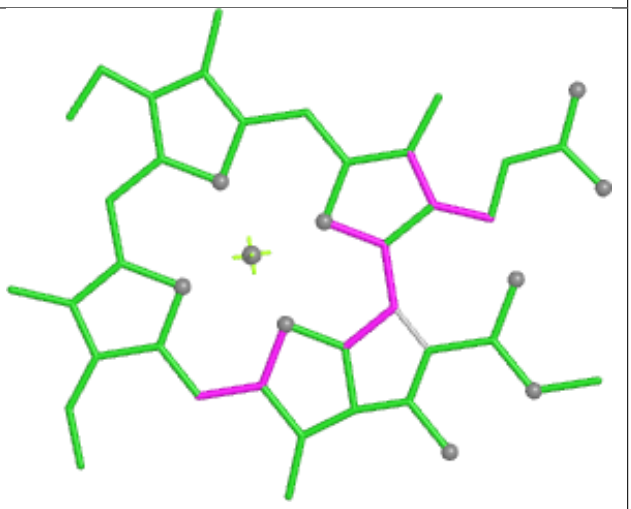
Ligand CLA A 849



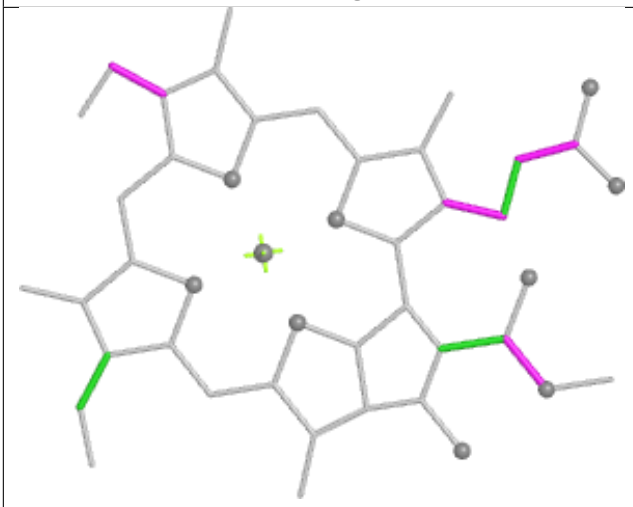
Ligand CLA G 310



Bond lengths



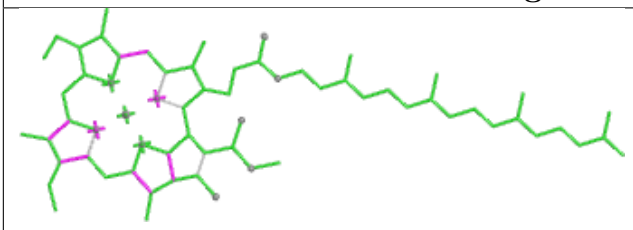
Bond angles



Torsions

Rings

Ligand CLA B 829



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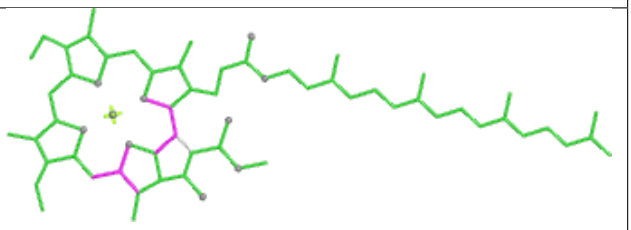
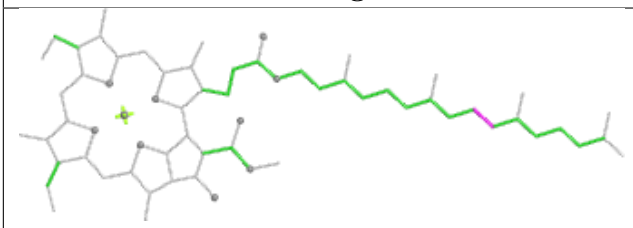
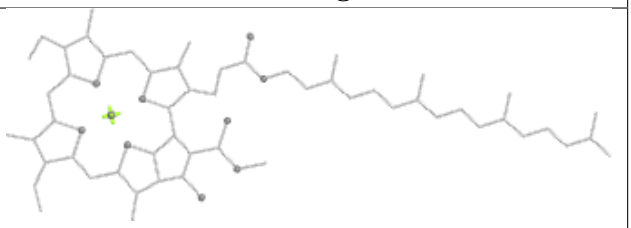


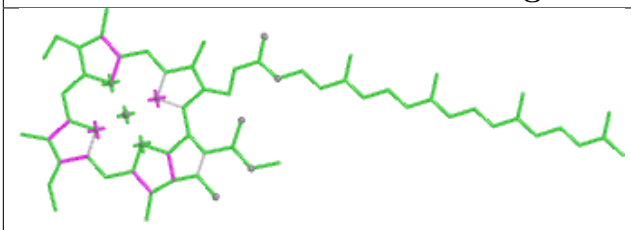
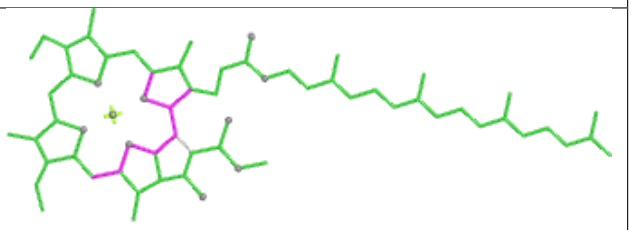
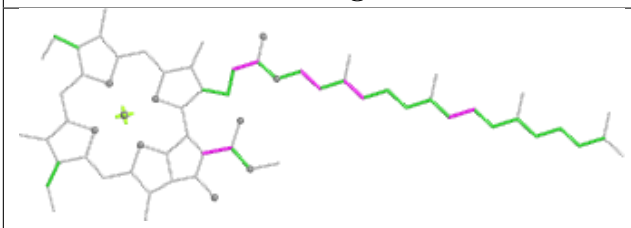
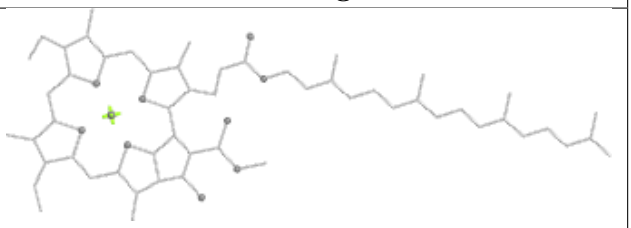
Bond angles

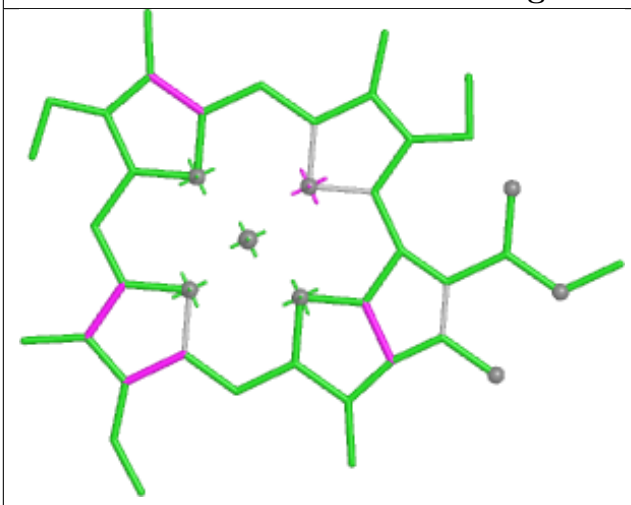
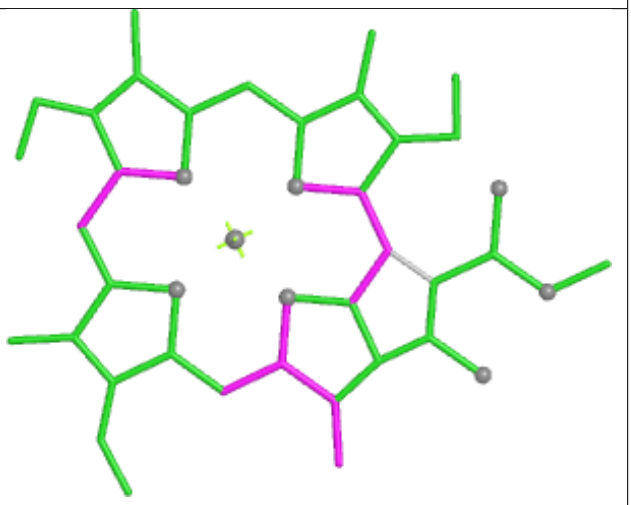
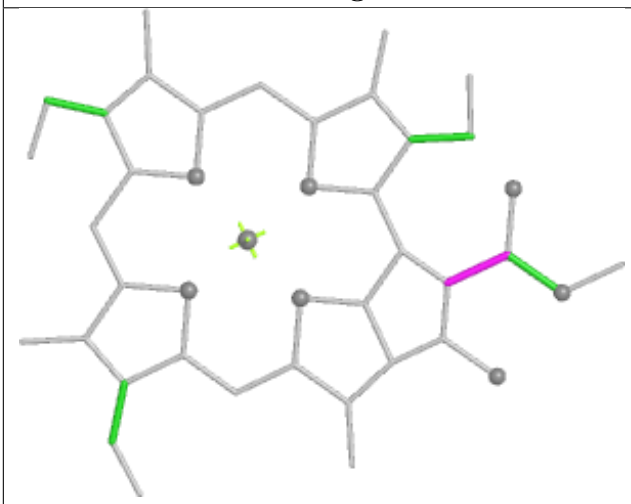
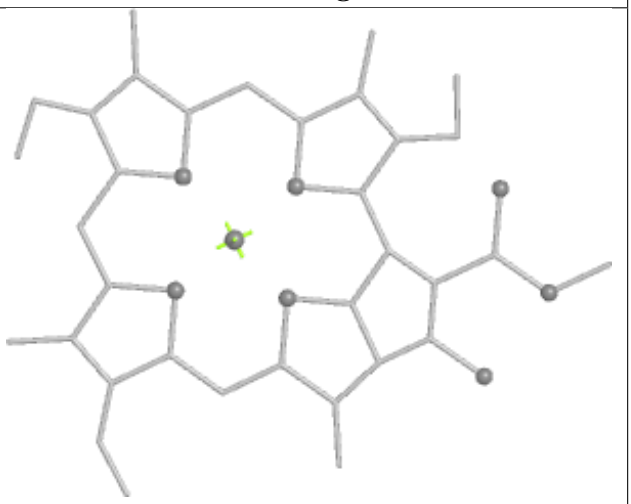


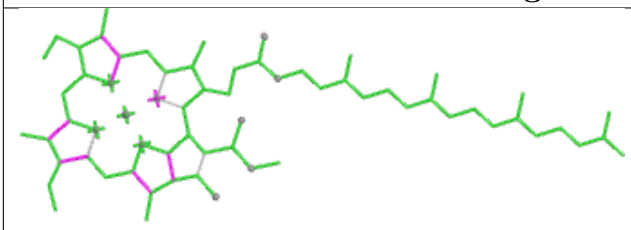
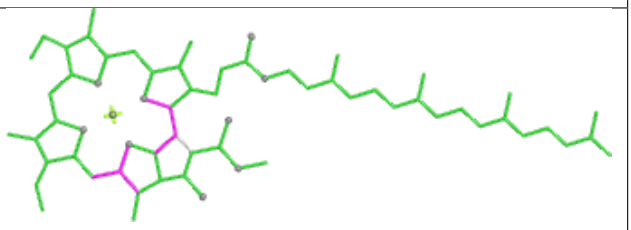
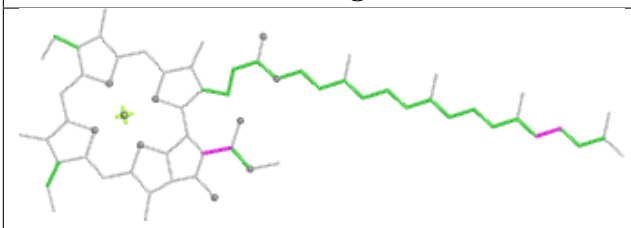
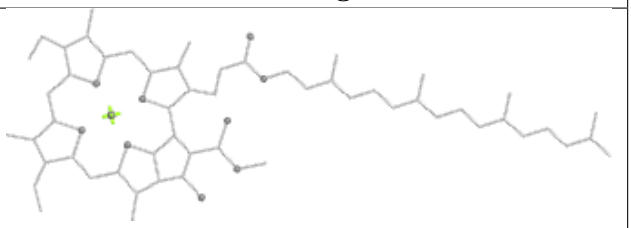
Torsions

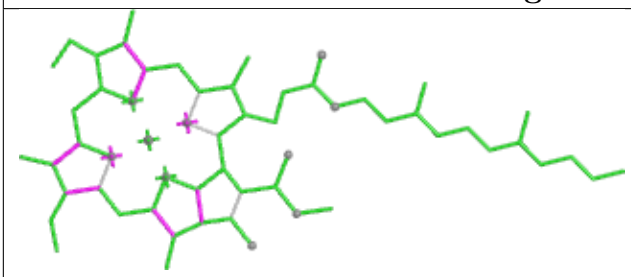
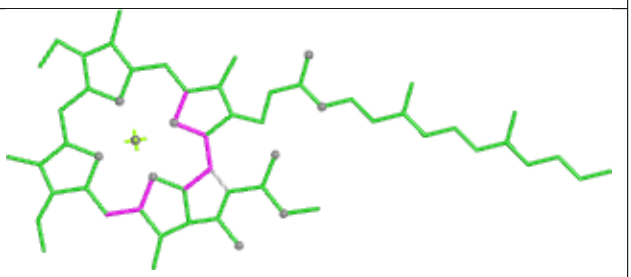
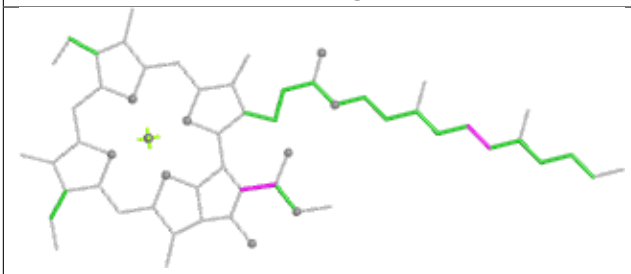
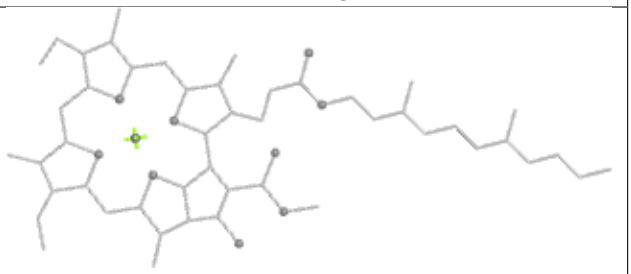


Rings

Ligand CLA A 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA k 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

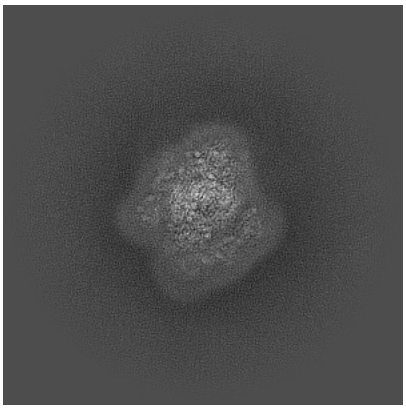
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-64154. These allow visual inspection of the internal detail of the map and identification of artifacts.

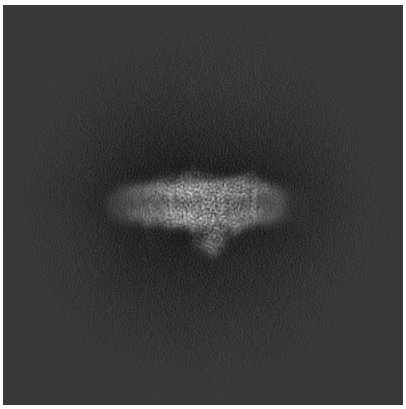
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

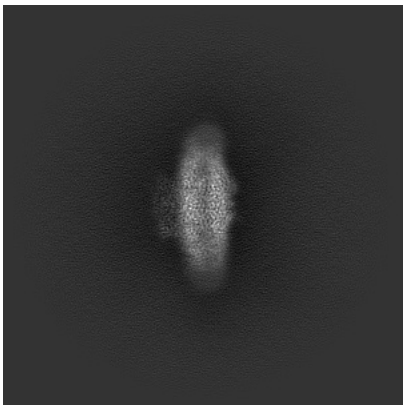
6.1.1 Primary map



X

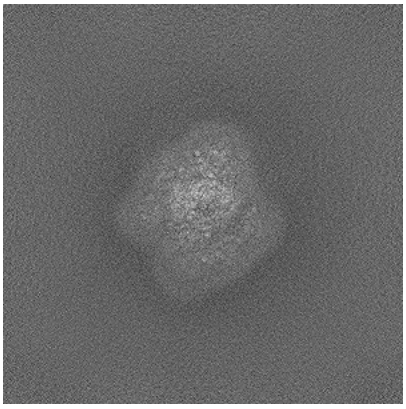


Y

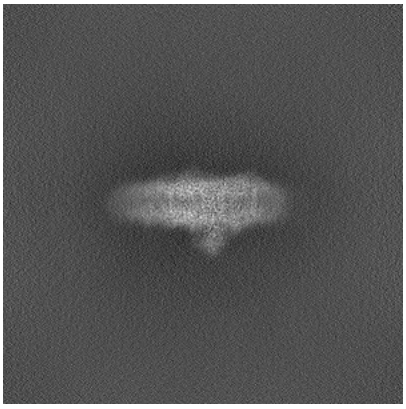


Z

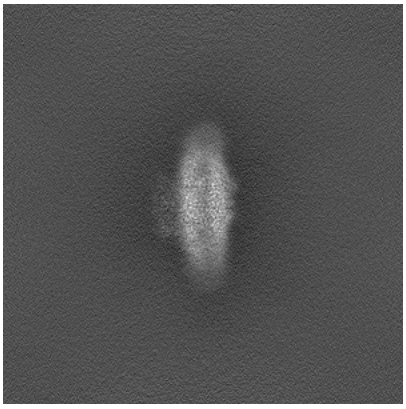
6.1.2 Raw map



X



Y

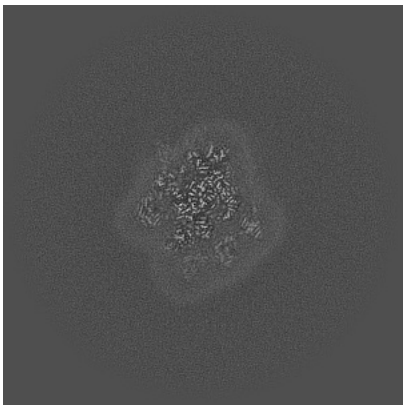


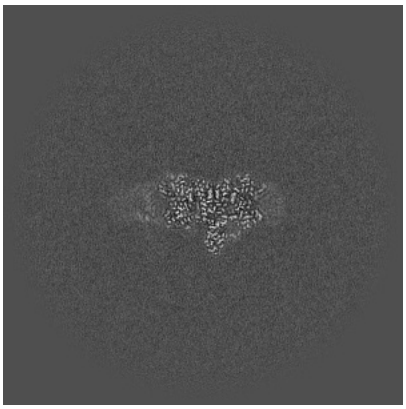
Z

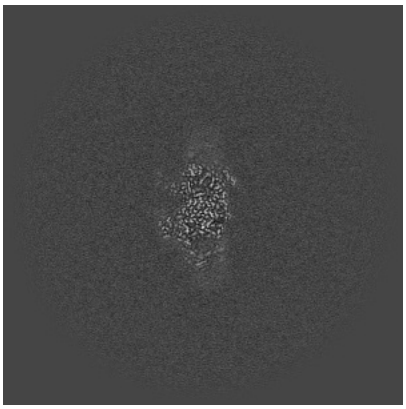
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

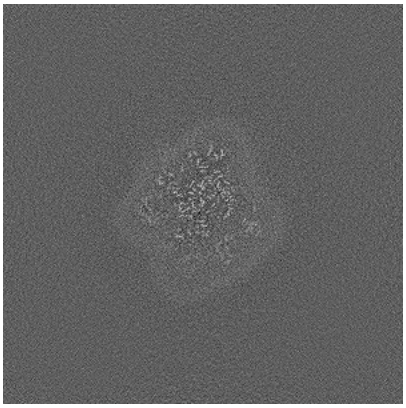
6.2.1 Primary map

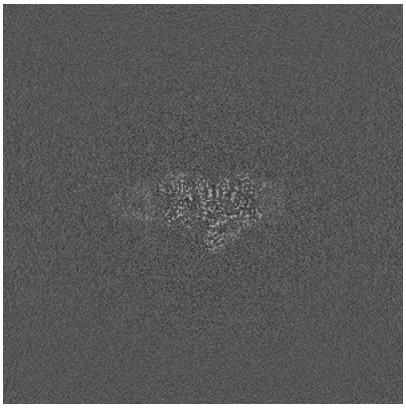

X Index: 300

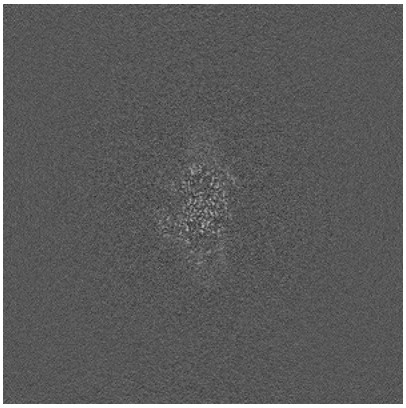

Y Index: 300


Z Index: 300

6.2.2 Raw map


X Index: 300

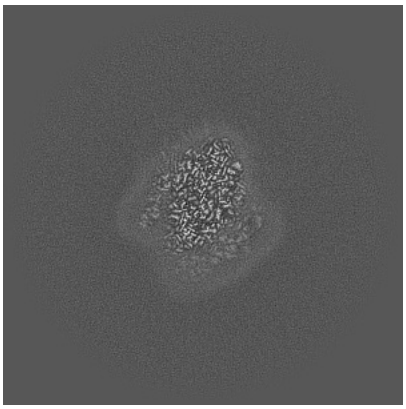

Y Index: 300


Z Index: 300

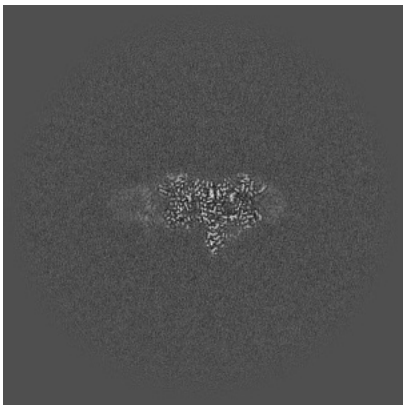
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

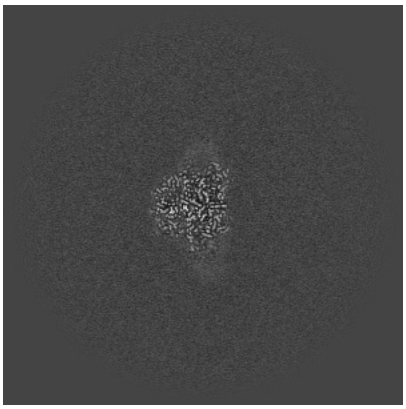
6.3.1 Primary map



X Index: 316

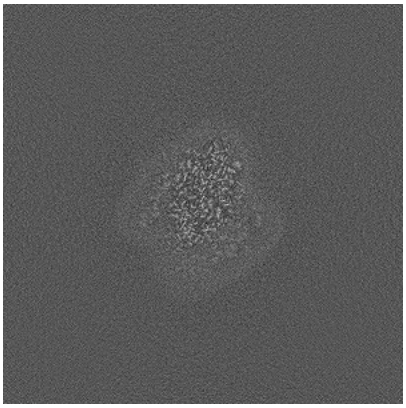


Y Index: 301

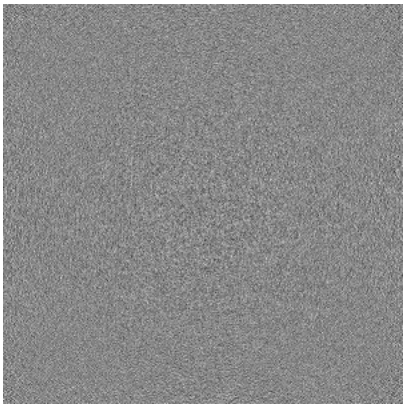


Z Index: 316

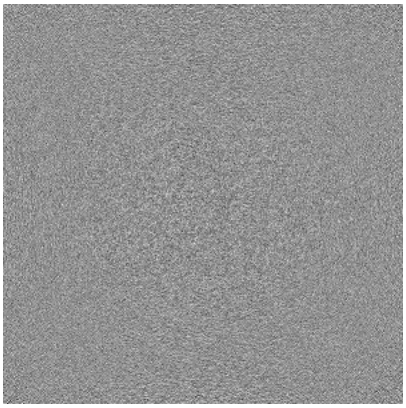
6.3.2 Raw map



X Index: 316



Y Index: 0

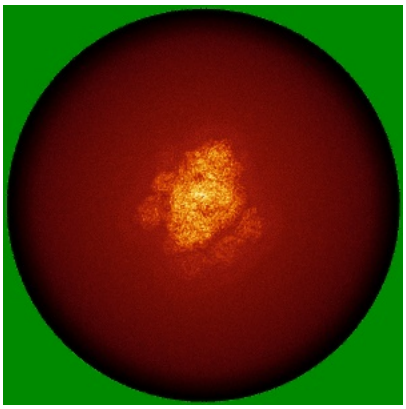


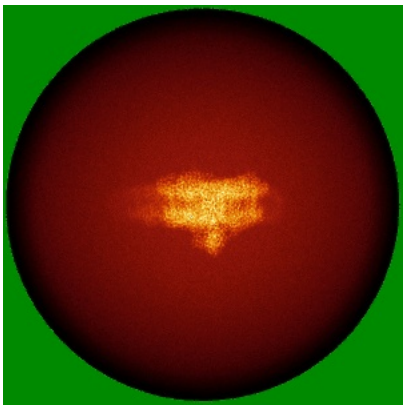
Z Index: 599

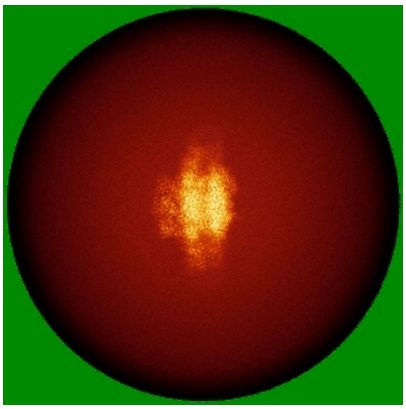
The images above show the largest variance slices of the map in three orthogonal directions.

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

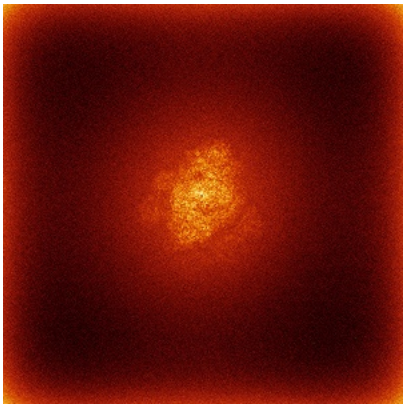
6.4.1 Primary map

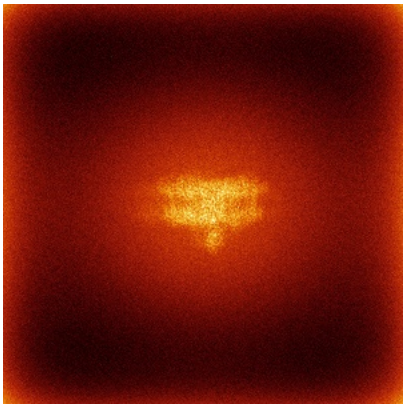

X

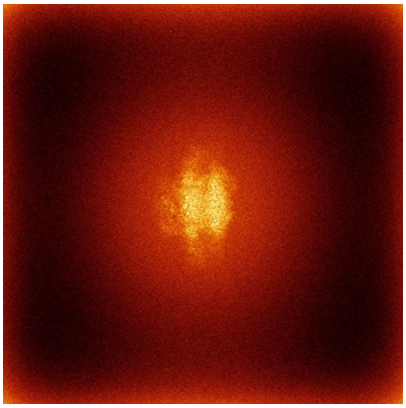

Y


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.

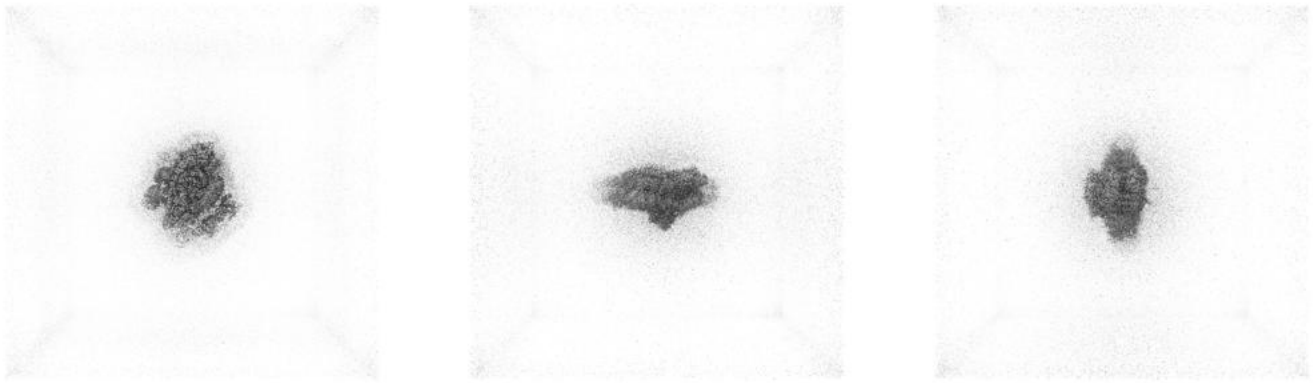
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. 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.

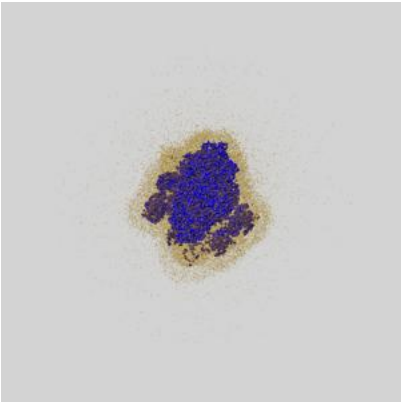
6.6 Mask visualisation (i)

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

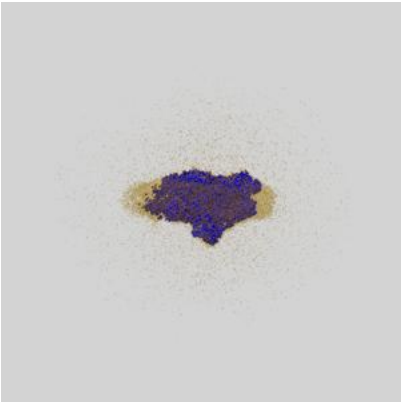
A mask typically either:

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

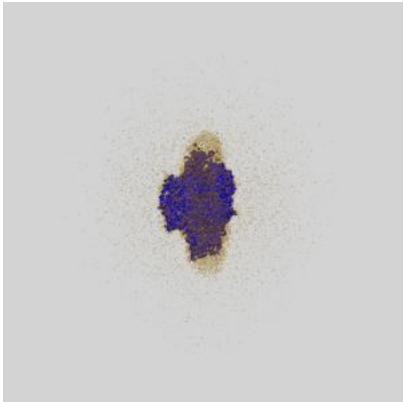
6.6.1 emd_64154_msk_1.map (i)



X



Y

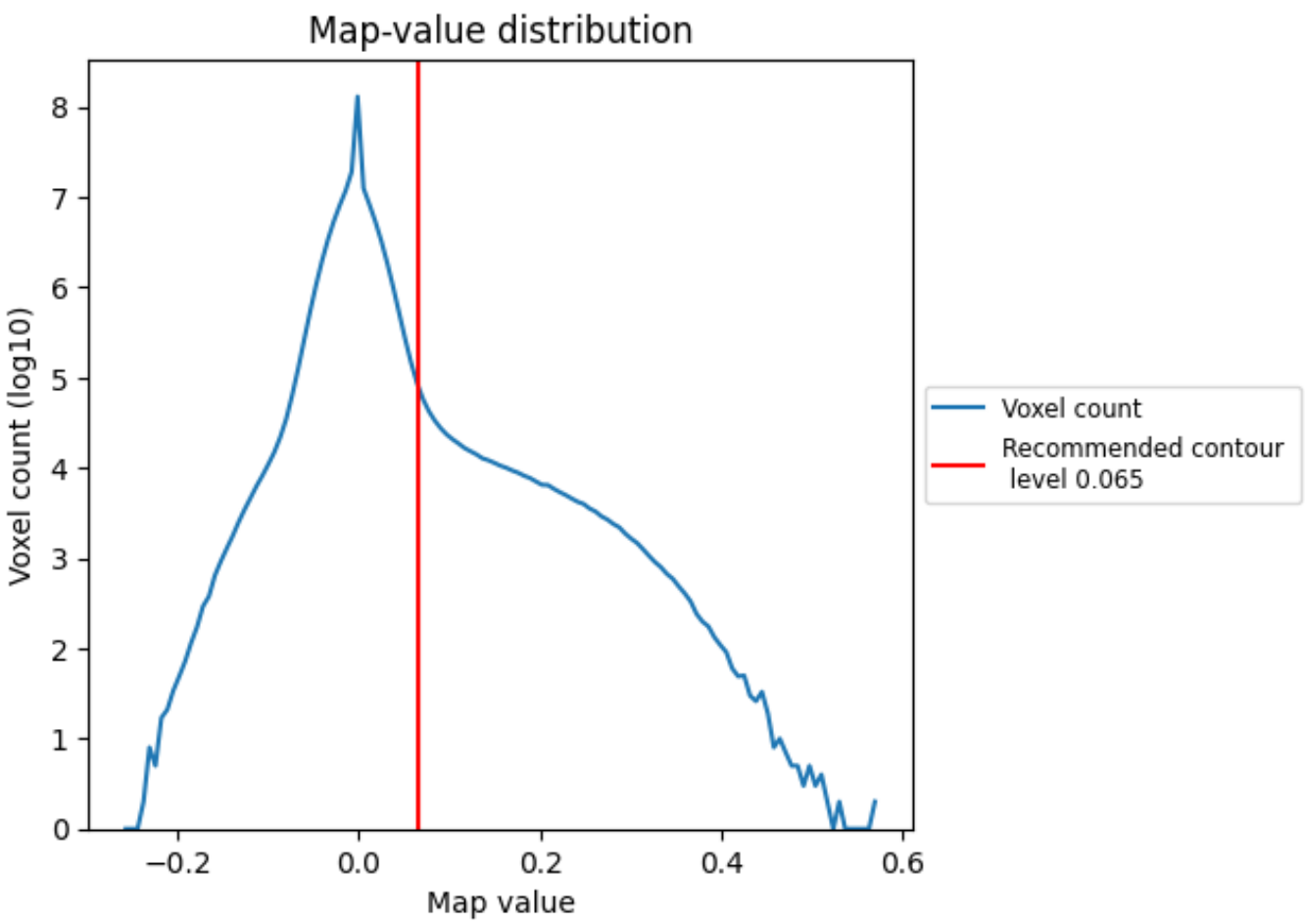


Z

7 Map analysis (i)

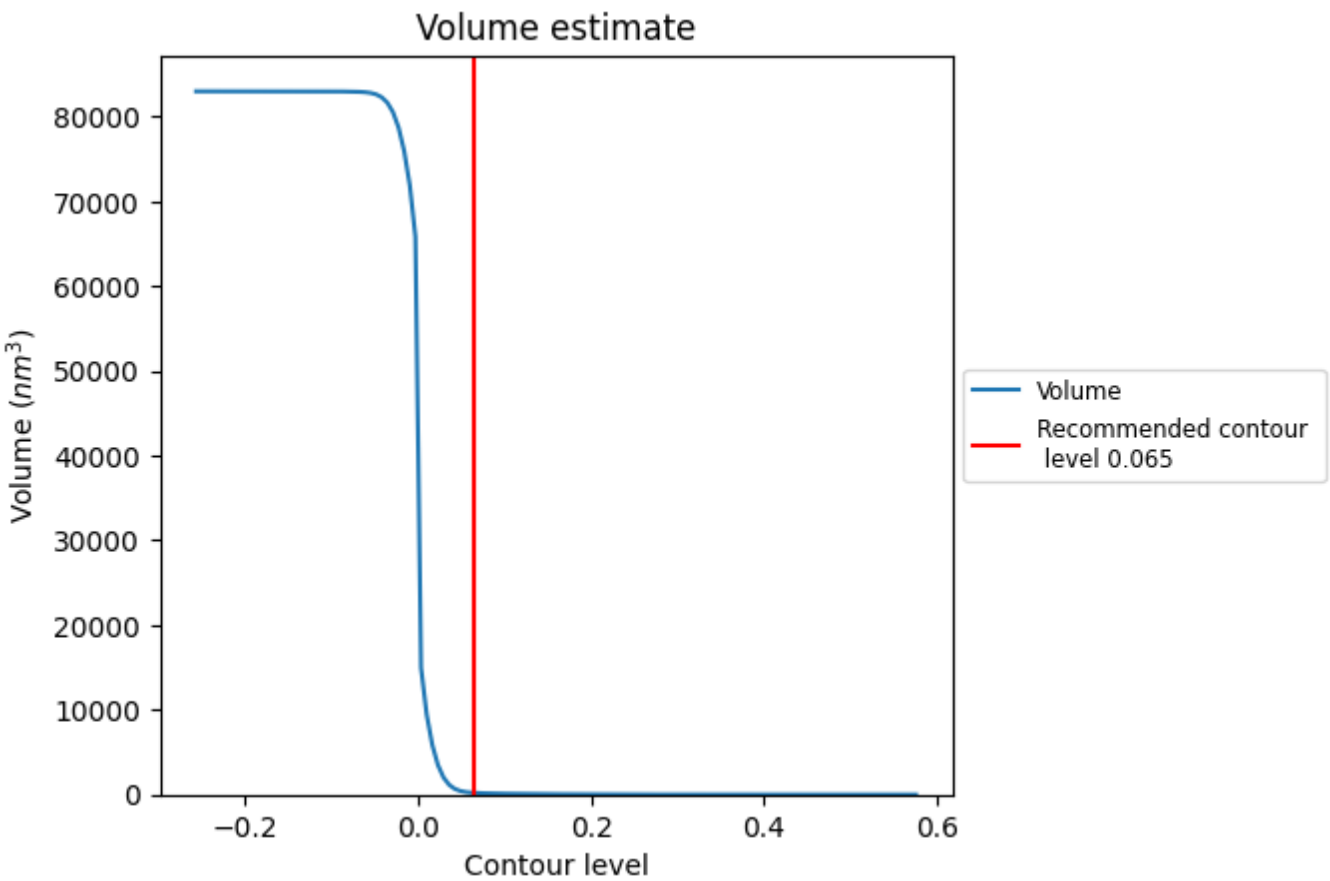
This section contains the results of statistical analysis of the map.

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.

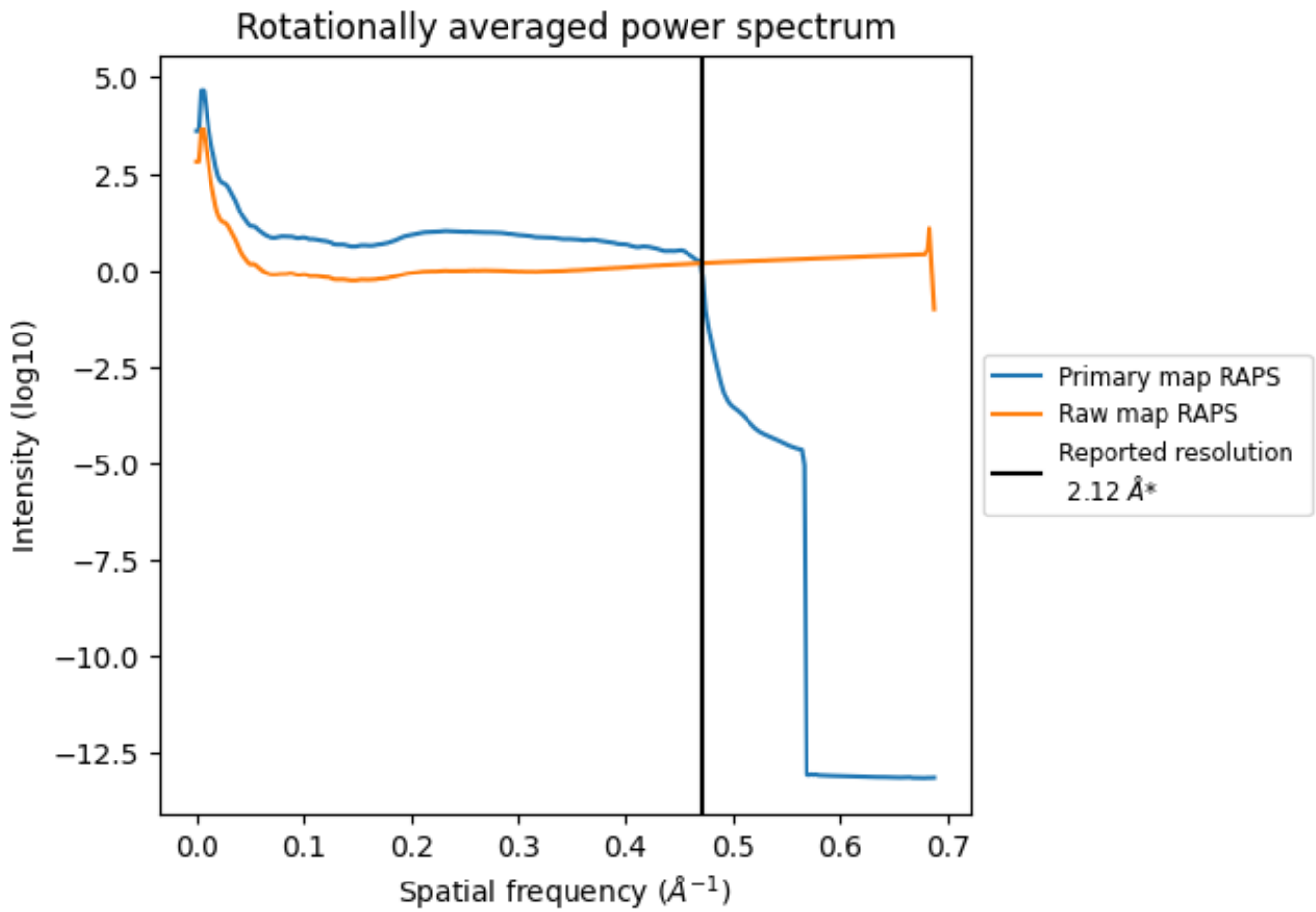
7.2 Volume estimate (i)



The volume at the recommended contour level is 203 nm^3; this corresponds to an approximate mass of 183 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)

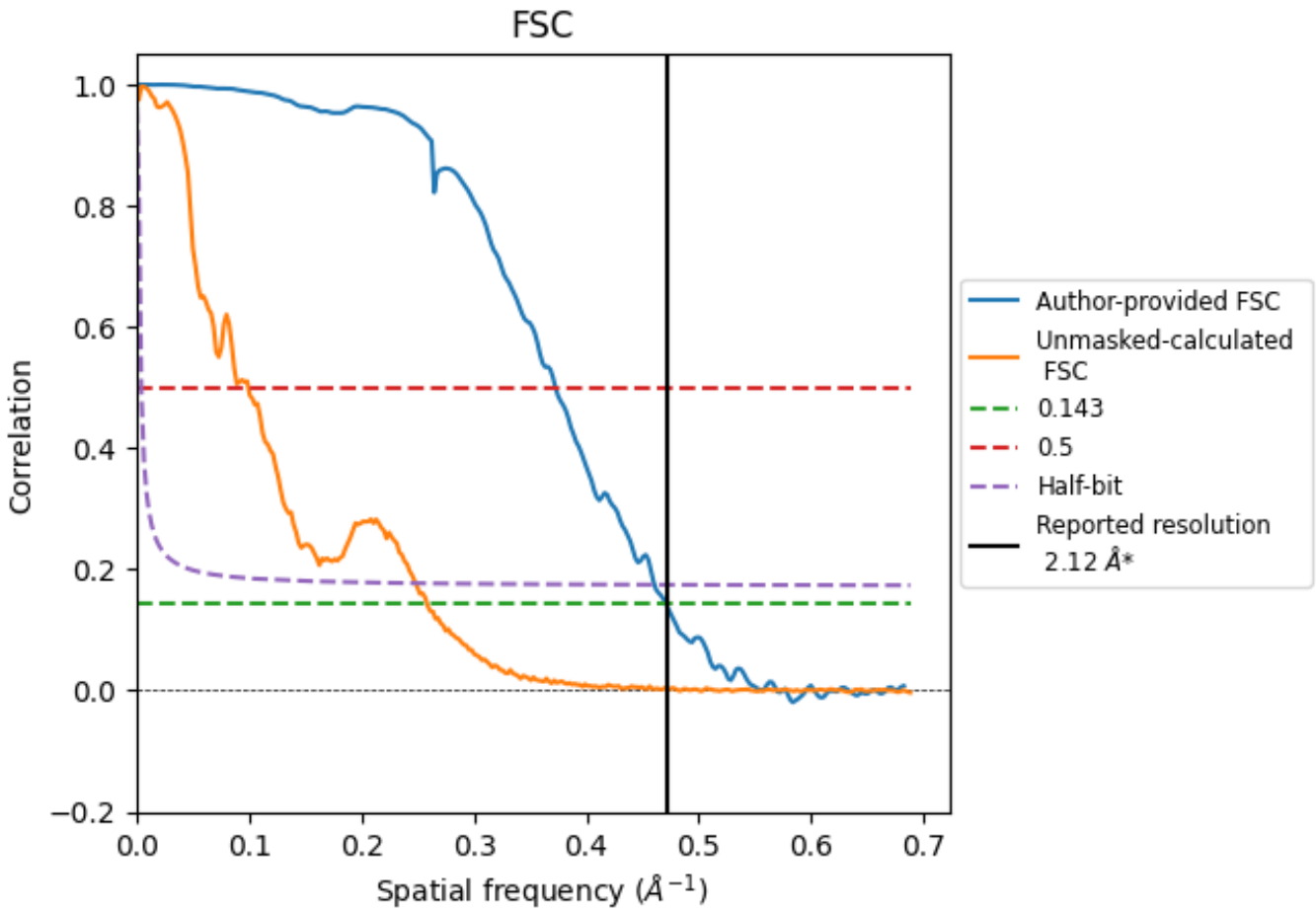


*Reported resolution corresponds to spatial frequency of 0.472 Å^{-1}

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 0.472 Å^{-1}

8.2 Resolution estimates (i)

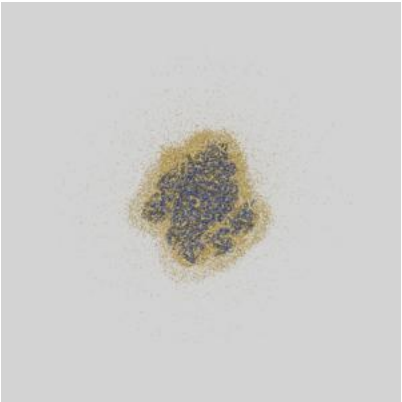
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.12	-	-
Author-provided FSC curve	2.12	2.68	2.17
Unmasked-calculated*	3.87	10.04	4.03

*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 3.87 differs from the reported value 2.12 by more than 10 %

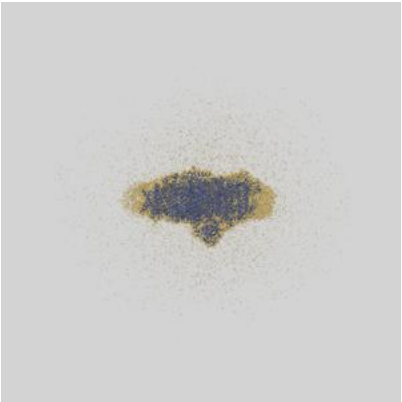
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-64154 and PDB model 9UH4. Per-residue inclusion information can be found in section 3 on page 23.

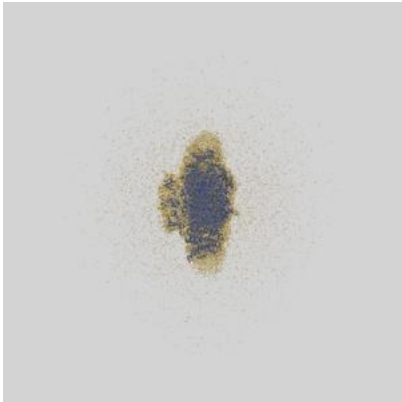
9.1 Map-model overlay (i)



X



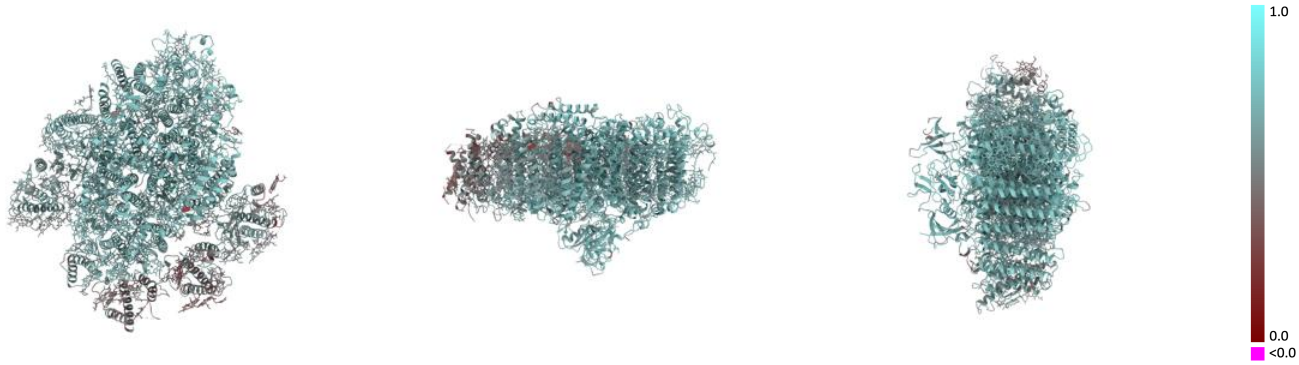
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065 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.

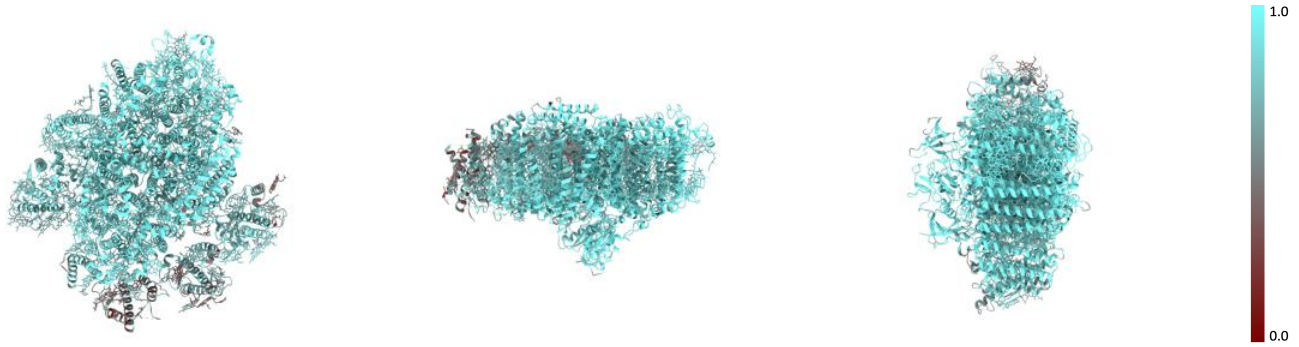
9.2 Q-score mapped to coordinate model (i)



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.

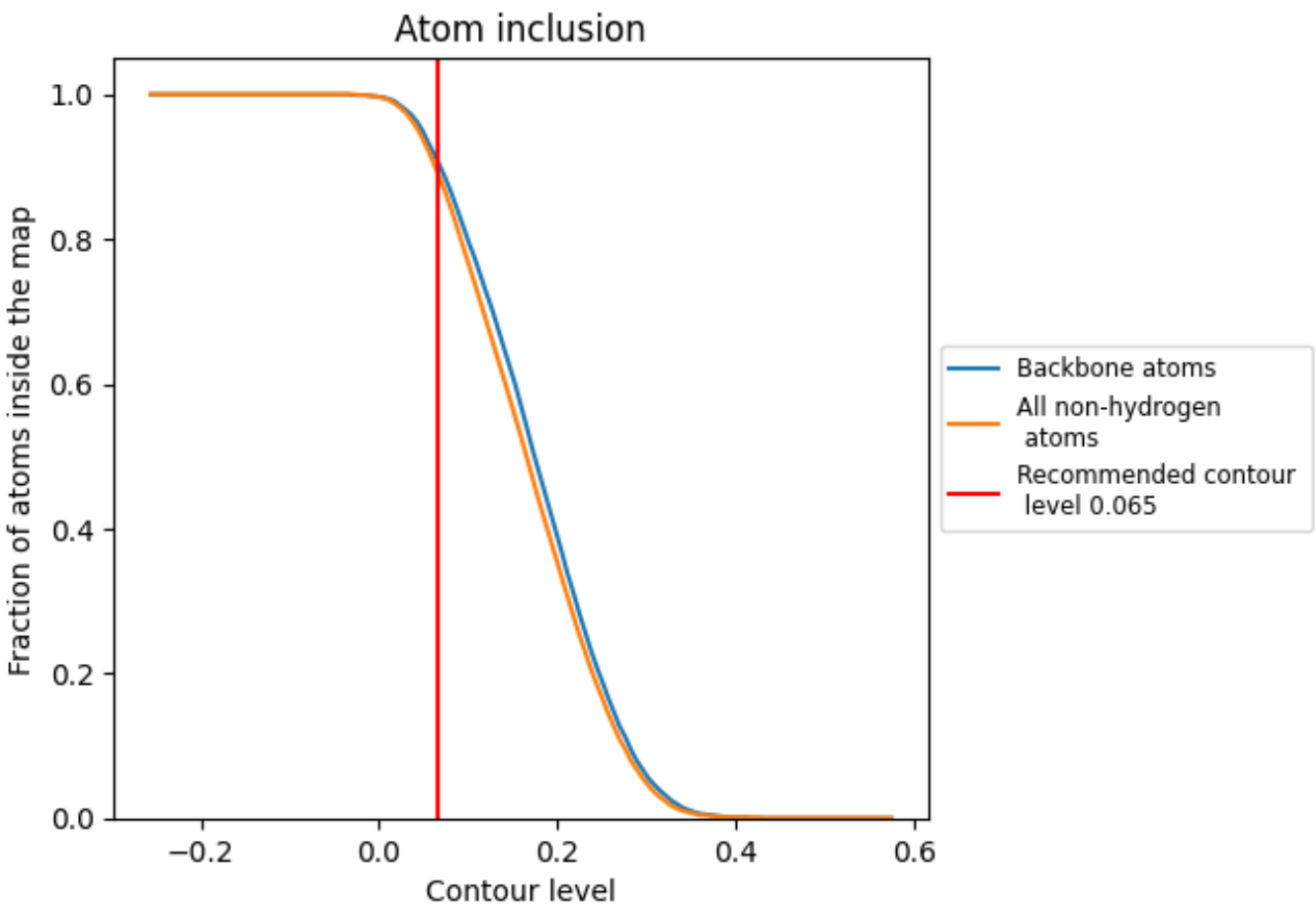
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.065).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.6550
A	0.9570	0.7000
B	0.9570	0.7010
C	0.9900	0.7210
D	0.9360	0.6750
E	0.9000	0.6590
F	0.9220	0.6710
G	0.7640	0.5610
H	0.6770	0.4970
I	0.8820	0.6410
J	0.9190	0.6580
K	0.4990	0.4400
L	0.9070	0.6540
M	0.9130	0.6530
U	0.7940	0.5820
k	0.7610	0.5750