Full wwPDB EM Validation Report (i)

Sep 15, 2026 – 12:41 AM JST

PDB ID	:	8J7B / pdb_00008j7b
EMDB ID	:	EMD-36037
Title	:	Coordinates of Cryo-EM structure of the Arabidopsis thaliana PSI in state 2 (PSI-ST2)
Authors	:	Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on	:	2023-04-27
Resolution	:	3.22 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:

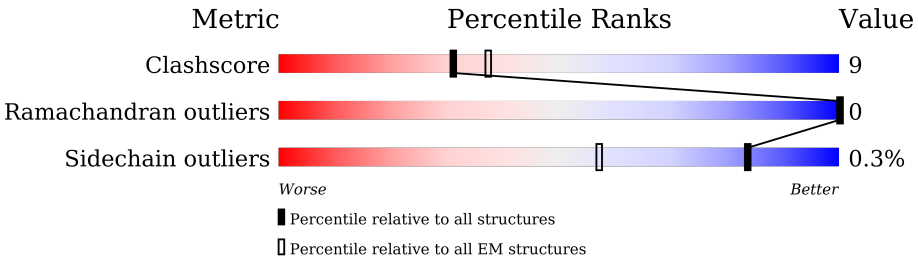
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

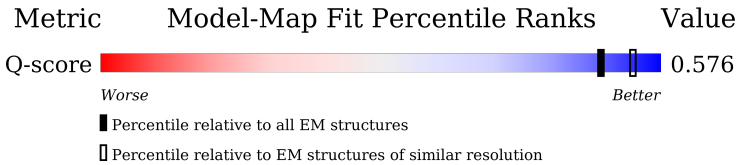
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.22 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	14612 (2.72 - 3.72)

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

Mol	Chain	Length	Quality of chain
1	1	241	65% 15% 20%
2	2	257	69% 9% 22%
3	3	273	70% 10% 20%
4	4	251	67% 11% 22%

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Mol	Chain	Length	Quality of chain
5	A	750	89% 10%
6	B	734	89% 11%
7	C	81	91% 7%
8	D	204	65% 5% 30%
9	E	143	43% 55%
10	F	221	63% 5% 31%
11	G	160	52% 5% 43%
12	H	145	56% 6% 38%
13	I	37	76% 8% 16%
14	J	44	77% 16% 7%
15	K	130	52% 13% 35%
16	L	219	66% 7% 27%

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 35077 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 Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	193	1496	975	248	268	5	0	0

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	201	1566	1024	256	282	4	0	0

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	218	1666	1088	270	303	5	0	0

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	196	1551	1013	253	282	3	0	0

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	737	5807	3807	986	996	18	0	0

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	732	5854	3842	997	1001	14	0	0

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	80	616	381	107	117	11	0	0

- Molecule 8 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	143	1128	723	195	206	4	0	0

- Molecule 9 is a protein called Photosystem I reaction center subunit IV A, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	E	64	517	331	92	94	0	0

- Molecule 10 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	152	1208	789	207	209	3	0	0

- Molecule 11 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	G	91	708	458	118	132	0	0

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	H	90	693	451	112	130	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	31	239	162	39	37	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	J	41	327	221	50	55	1	0	0

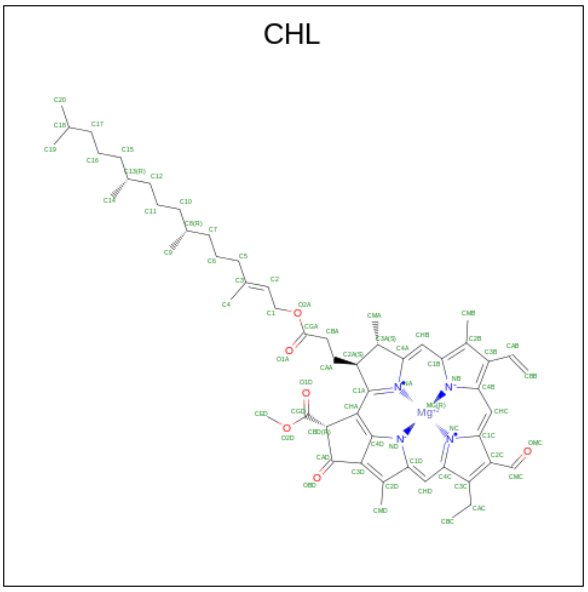
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K	84	593	373	104	113	3	0	0

- Molecule 16 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	L	160	1207	799	191	215	2	0	0

- Molecule 17 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	1	1	52	41	1	4	6	0
17	1	1	41	32	1	4	4	0
17	2	1	42	33	1	4	4	0
17	2	1	43	34	1	4	4	0

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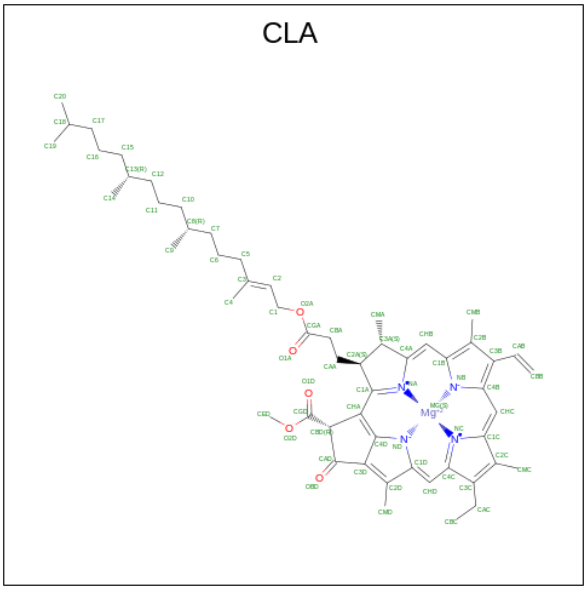
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	2	1	47	36	1	4	6	0
			Total	C	Mg	N	O	
17	2	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
17	2	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
17	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	4	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	4	1	41	32	1	4	4	0
			Total	C	Mg	N	O	
17	4	1	41	32	1	4	4	0
			Total	C	Mg	N	O	
17	4	1	46	35	1	4	6	0

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	1	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
18	1	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
18	1	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	1	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	1	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
18	1	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
18	1	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
18	1	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
18	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	1	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	1	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
18	2	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
18	2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	2	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
18	2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	2	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
18	2	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
18	2	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
18	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	2	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
18	3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	3	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
18	3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	3	1	54	44	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	3	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
18	3	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
18	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
18	4	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	4	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	4	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
18	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	4	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
18	4	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	4	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
18	4	1	43	33	1	4	5	0
			Total	C	Mg	N	O	
18	4	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	4	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	52	42	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
18	A	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	B	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
18	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	B	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	B	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
18	F	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	F	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
18	F	1	51	41	1	4	5	0

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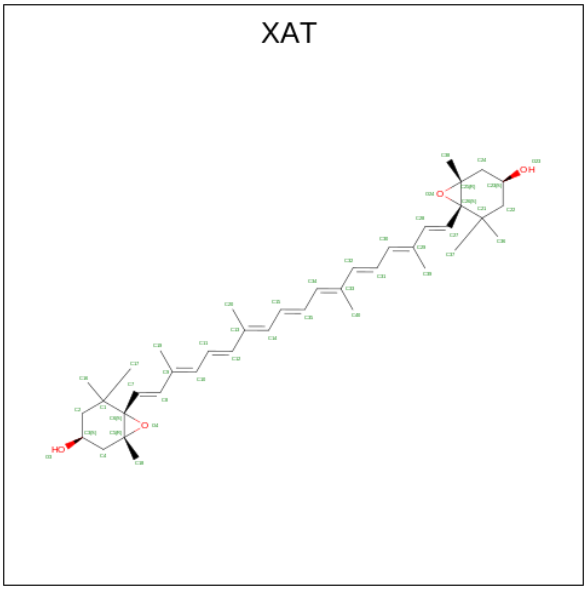
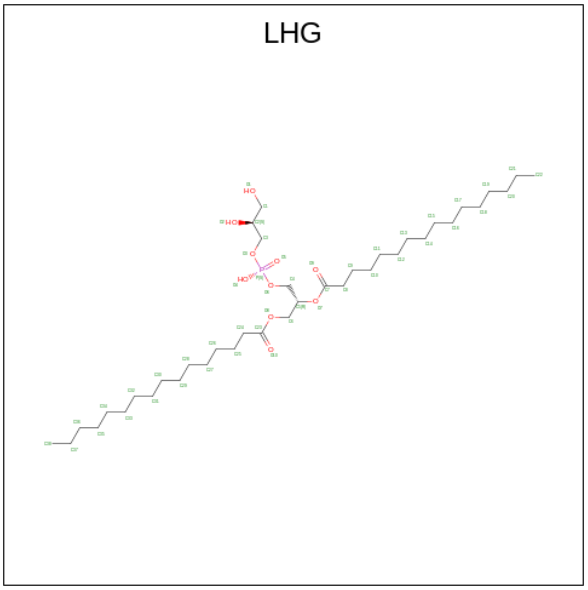
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	G	1	45	35	1	4	5	0
18	G	1	42	34	1	4	3	0
18	G	1	45	35	1	4	5	0
18	H	1	60	50	1	4	5	0
18	J	1	51	41	1	4	5	0
18	K	1	39	31	1	4	3	0
18	K	1	37	31	1	4	1	0
18	K	1	46	36	1	4	5	0
18	K	1	45	35	1	4	5	0
18	L	1	45	35	1	4	5	0
18	L	1	65	55	1	4	5	0
18	L	1	45	35	1	4	5	0

- Molecule 19 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



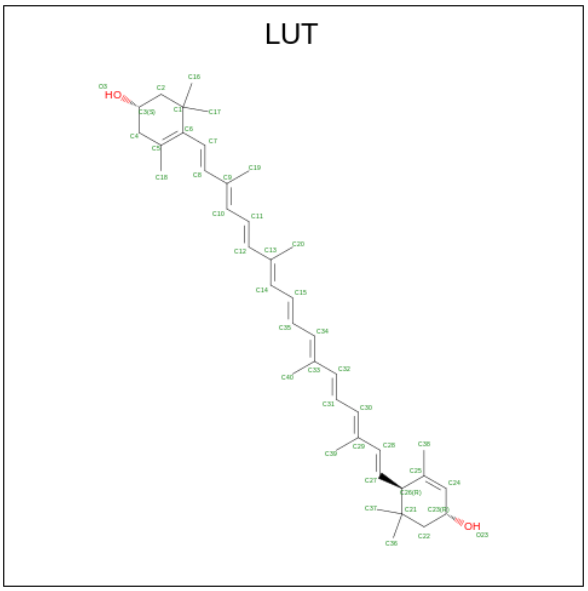
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
19	1	1	44	40	4	0
19	2	1	44	40	4	0
19	4	1	44	40	4	0

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



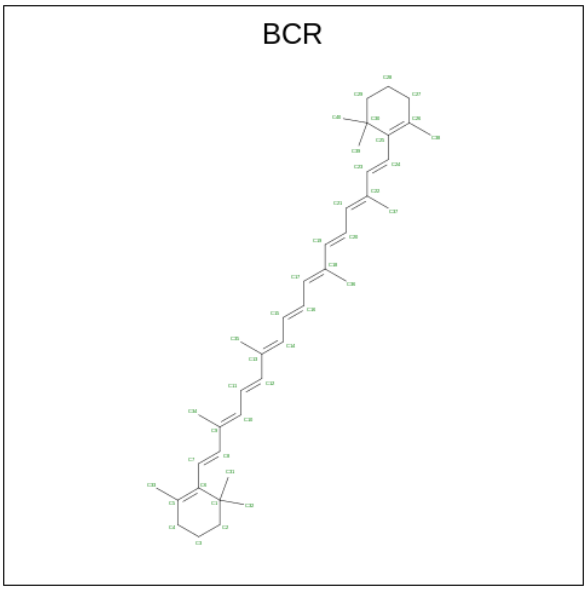
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	1	1	49	38	10	1	0
20	2	1	37	26	10	1	0
20	A	1	30	19	10	1	0
20	A	1	49	38	10	1	0
20	B	1	38	27	10	1	0
20	B	1	49	38	10	1	0

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	1	1	42	40	2	0
21	2	1	42	40	2	0
21	2	1	42	40	2	0
21	3	1	42	40	2	0
21	4	1	42	40	2	0

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
22	3	1	40	40	0
			Total	C	
22	4	1	40	40	0
			Total	C	
22	A	1	40	40	0
			Total	C	
22	A	1	40	40	0
			Total	C	
22	A	1	40	40	0
			Total	C	
22	A	1	40	40	0
			Total	C	
22	A	1	40	40	0
			Total	C	
22	A	1	40	40	0
			Total	C	
22	B	1	40	40	0
			Total	C	
22	B	1	40	40	0
			Total	C	
22	B	1	40	40	0
			Total	C	
22	B	1	40	40	0
			Total	C	
22	B	1	40	40	0
			Total	C	
22	B	1	40	40	0
			Total	C	
22	B	1	40	40	0
			Total	C	
22	B	1	40	40	0
			Total	C	
22	F	1	40	40	0
			Total	C	
22	G	1	40	40	0
			Total	C	
22	I	1	40	40	0
			Total	C	
22	J	1	40	40	0
			Total	C	
22	K	1	40	40	0
			Total	C	
22	K	1	40	40	0

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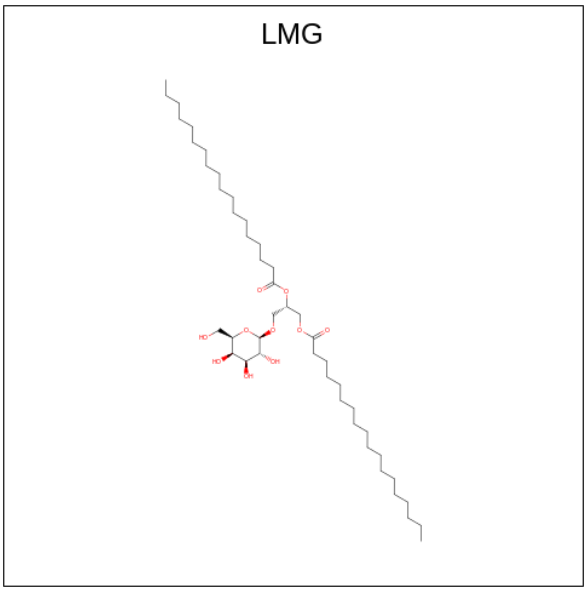
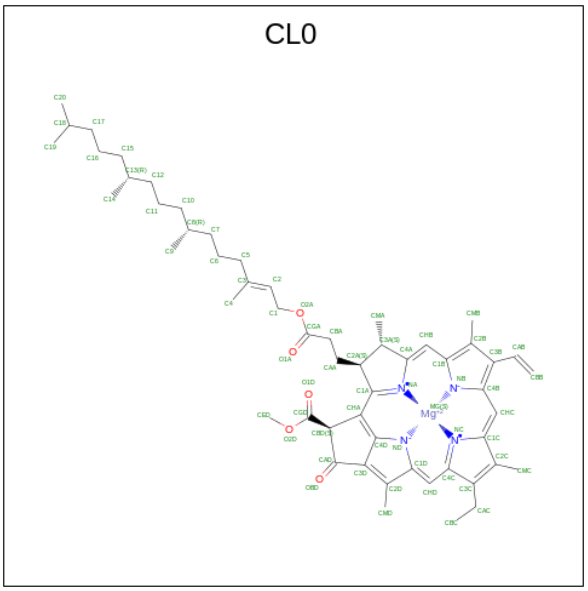
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
22	L	1	40	40	0
			Total	C	
22	L	1	40	40	0
			Total	C	
22	L	1	40	40	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



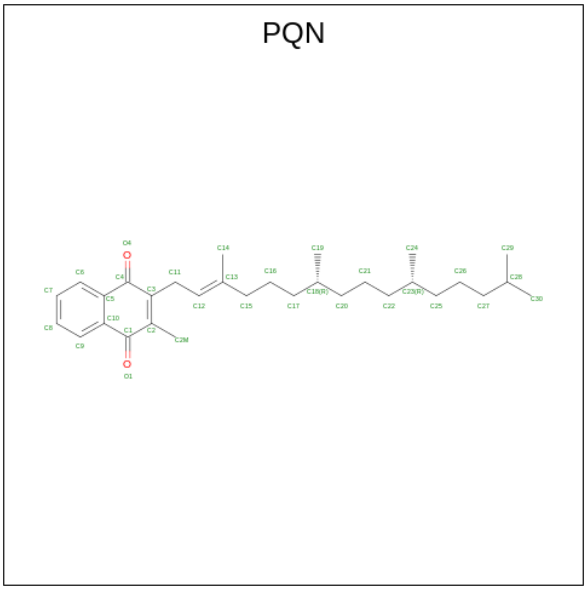
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	4	1	39	29	10	0
			Total	C	O	
23	4	1	33	23	10	0

- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



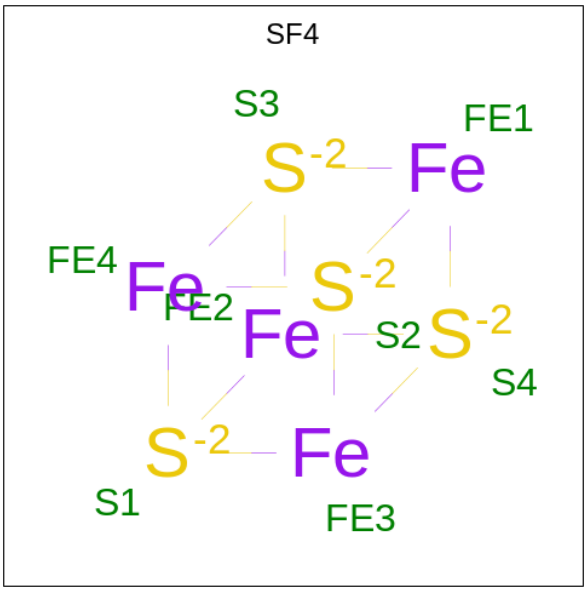
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	A	1	60	52	1	4	3	0

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



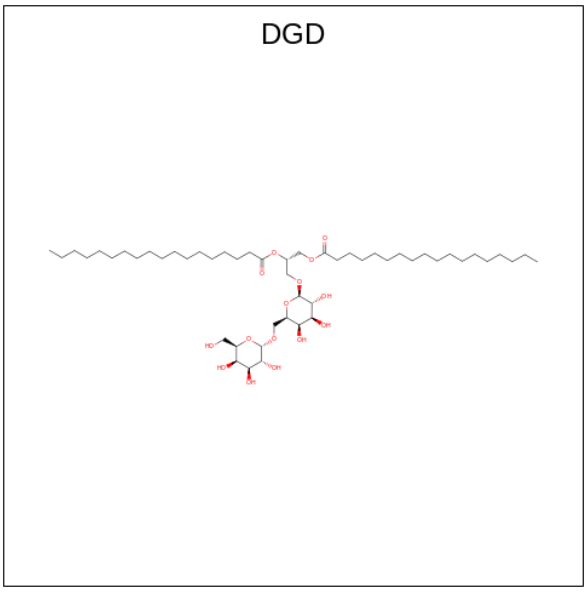
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	A	1	33	31	2	0
			Total	C	O	
25	B	1	33	31	2	0

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



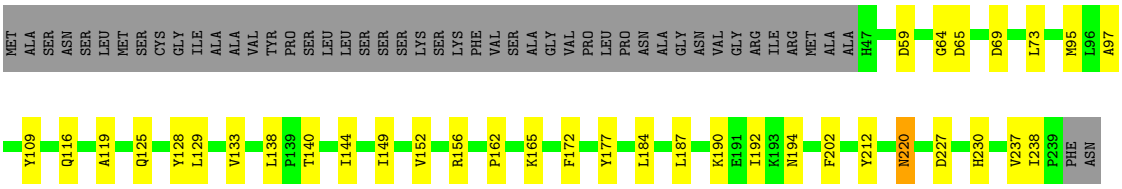
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	B	1	66	51	15	0

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.

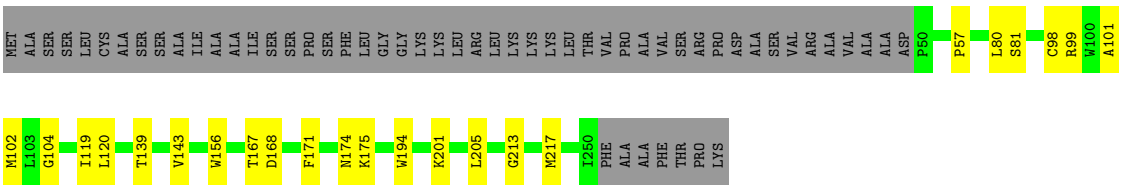
• Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic

Chain 1:



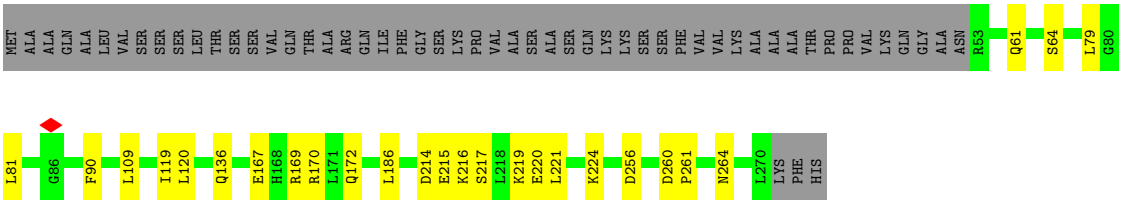
• Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

Chain 2:



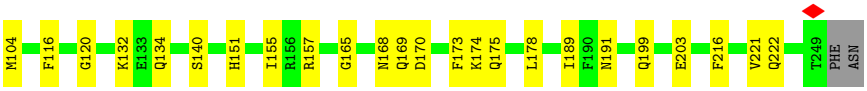
• Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

Chain 3:



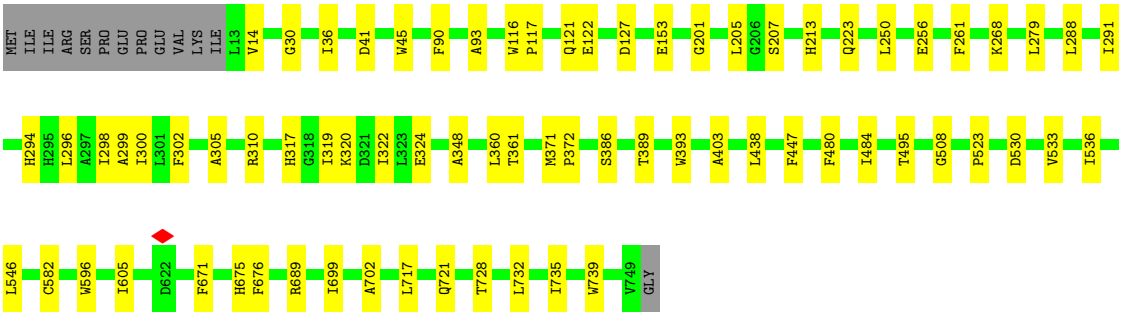
• Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic

Chain 4:



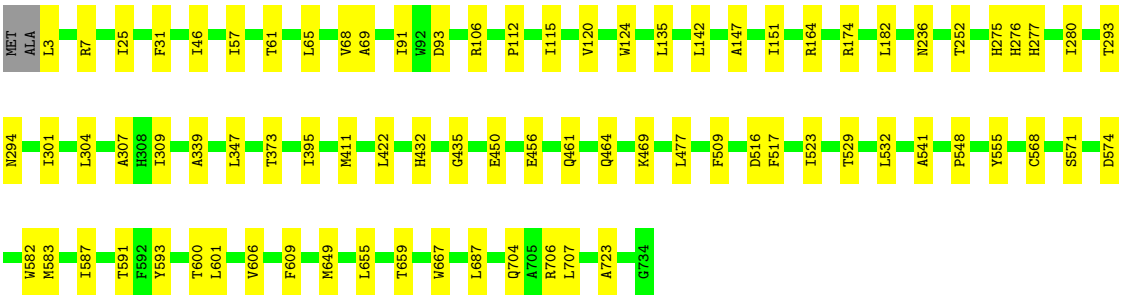
• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

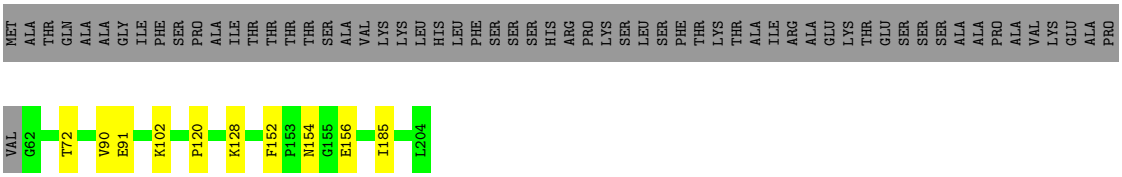


• Molecule 7: Photosystem I iron-sulfur center

Chain C:

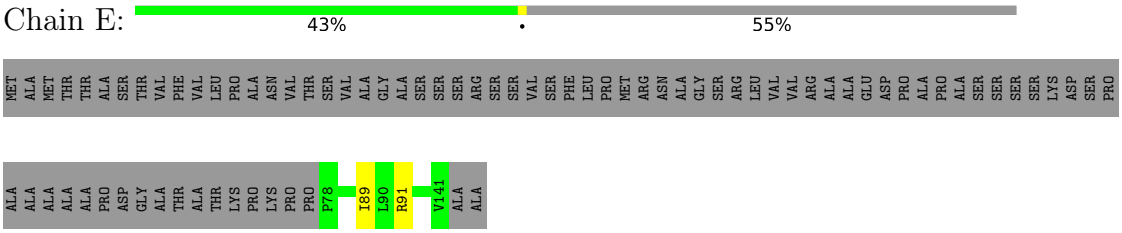
• Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic

Chain D:



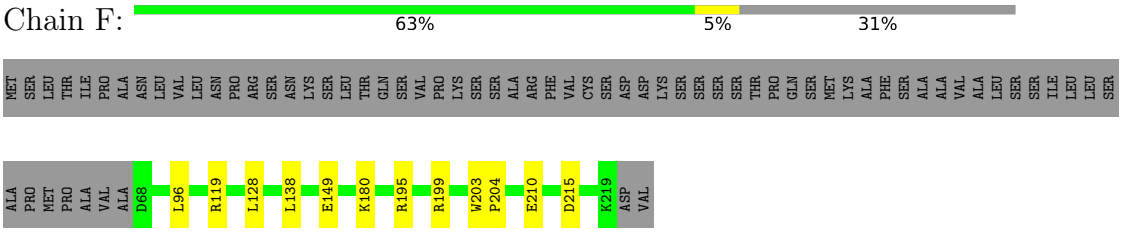
• Molecule 9: Photosystem I reaction center subunit IV A, chloroplastic

Chain E:



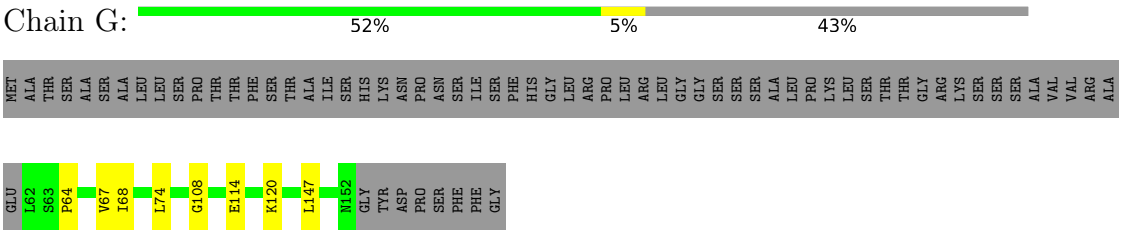
• Molecule 10: Photosystem I reaction center subunit III, chloroplastic

Chain F:



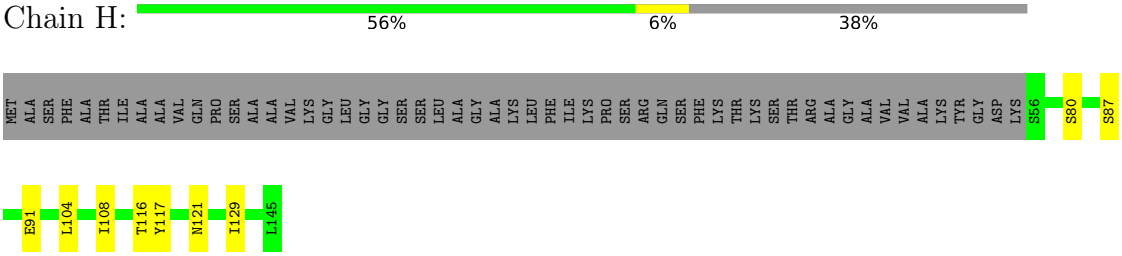
• Molecule 11: Photosystem I reaction center subunit V, chloroplastic

Chain G:



• Molecule 12: Photosystem I reaction center subunit VI-2, chloroplastic

Chain H:



• Molecule 13: Photosystem I reaction center subunit VIII

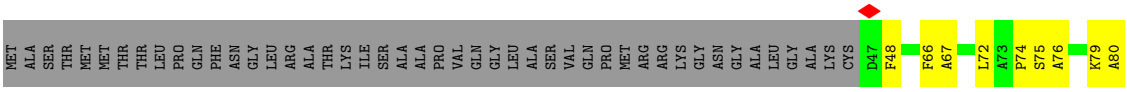
Chain I:

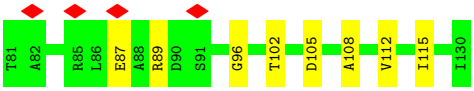
• Molecule 14: Photosystem I reaction center subunit IX

Chain J:

• Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic

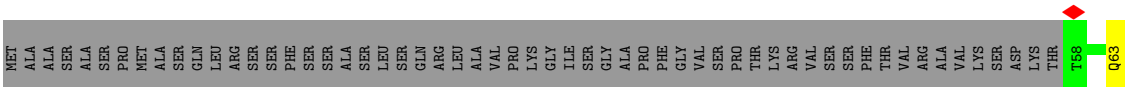
Chain K:

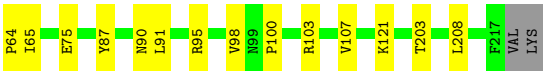




• Molecule 16: Photosystem I reaction center subunit XI, chloroplastic

Chain L:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137602	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	35.714	Depositor
Minimum map value	-22.642	Depositor
Average map value	0.012	Depositor
Map value standard deviation	1.070	Depositor
Recommended contour level	3.21	Depositor
Map size (Å)	365.232, 365.232, 365.232	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: CHL, DGD, PQN, LHG, CL0, CLA, XAT, LMG, LUT, BCR, 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	1	0.12	0/1546	0.32	0/2110
2	2	0.12	0/1622	0.28	0/2219
3	3	0.13	0/1717	0.30	0/2336
4	4	0.12	0/1599	0.29	0/2178
5	A	0.10	0/6005	0.25	0/8194
6	B	0.11	0/6065	0.28	1/8279 (0.0%)
7	C	0.12	0/629	0.38	0/852
8	D	0.10	0/1157	0.30	0/1563
9	E	0.08	0/528	0.23	0/715
10	F	0.11	0/1238	0.26	0/1670
11	G	0.08	0/724	0.25	0/981
12	H	0.10	0/713	0.27	0/968
13	I	0.12	0/245	0.29	0/333
14	J	0.10	0/336	0.25	0/458
15	K	0.16	0/599	0.50	3/809 (0.4%)
16	L	0.10	0/1244	0.27	0/1700
All	All	0.11	0/25967	0.28	4/35365 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	K	74	PRO	CA-N-CD	-7.69	101.24	112.00
15	K	74	PRO	N-CD-CG	-5.20	95.41	103.20
6	B	477	LEU	CB-CA-C	-5.12	110.26	117.23
15	K	74	PRO	CB-CG-CD	-5.12	89.72	106.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1496	0	1471	30	0
2	2	1566	0	1519	22	0
3	3	1666	0	1627	19	0
4	4	1551	0	1508	24	0
5	A	5807	0	5659	55	0
6	B	5854	0	5646	63	0
7	C	616	0	600	5	0
8	D	1128	0	1134	8	0
9	E	517	0	526	1	0
10	F	1208	0	1243	9	0
11	G	708	0	700	6	0
12	H	693	0	690	6	0
13	I	239	0	258	3	0
14	J	327	0	342	7	0
15	K	593	0	614	13	0
16	L	1207	0	1209	13	0
17	1	93	0	62	10	0
17	2	226	0	150	12	0
17	3	45	0	30	1	0
17	4	169	0	100	3	0
18	1	496	0	354	24	0
18	2	434	0	352	25	0
18	3	498	0	377	13	0
18	4	527	0	412	18	0
18	A	2533	0	2495	104	0
18	B	2284	0	2242	93	0
18	F	149	0	123	6	0
18	G	132	0	97	1	0
18	H	60	0	59	2	0
18	J	51	0	41	2	0
18	K	167	0	116	2	0
18	L	155	0	138	7	0
19	1	44	0	56	18	0
19	2	44	0	56	7	0
19	4	44	0	56	5	0
20	1	49	0	74	13	0
20	2	37	0	44	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	79	0	104	6	0
20	B	87	0	120	5	0
21	1	42	0	56	3	0
21	2	84	0	112	10	0
21	3	42	0	56	6	0
21	4	42	0	56	4	0
22	3	40	0	56	4	0
22	4	40	0	56	4	0
22	A	240	0	336	27	0
22	B	320	0	448	44	0
22	F	40	0	56	2	0
22	G	40	0	56	2	0
22	I	40	0	56	1	0
22	J	40	0	56	6	0
22	K	80	0	112	7	0
22	L	120	0	168	18	0
23	4	72	0	84	1	0
24	A	60	0	68	5	0
25	A	33	0	46	3	0
25	B	33	0	46	2	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	B	66	0	96	5	0
All	All	35077	0	34424	610	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 9.

All (610) 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)
18:B:814:CLA:H3A	22:B:845:BCR:H393	1.51	0.91
17:1:601:CHL:HBB1	20:1:615:LHG:H252	1.57	0.84
21:2:619:LUT:H8	21:2:619:LUT:H181	1.60	0.82
22:B:801:BCR:H12C	22:B:801:BCR:H341	1.63	0.81
3:3:79:LEU:HD13	18:A:813:CLA:H2	1.63	0.81
2:2:143:VAL:HG22	18:4:613:CLA:HBA2	1.61	0.80
4:4:104:MET:HE1	18:4:609:CLA:HAB	1.64	0.80
22:A:853:BCR:H12C	22:A:853:BCR:H341	1.68	0.76
1:1:202:PHE:CE1	19:1:614:XAT:H10	2.20	0.76
22:B:845:BCR:H16C	22:B:845:BCR:H20C	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:306:BCR:H321	22:L:306:BCR:HC8	1.68	0.75
18:3:612:CLA:HAB	18:3:607:CLA:HBA1	1.66	0.75
18:1:602:CLA:H51	19:1:614:XAT:H373	1.69	0.75
3:3:170:ARG:NH2	18:3:607:CLA:O1D	2.21	0.74
6:B:411:MET:HE2	22:B:846:BCR:H402	1.68	0.74
22:A:850:BCR:H16C	22:A:850:BCR:H351	1.69	0.74
18:A:814:CLA:HHC	18:A:814:CLA:HBB1	1.69	0.72
17:1:601:CHL:HBB1	17:1:601:CHL:HHC	1.72	0.72
18:B:812:CLA:HHC	18:B:812:CLA:HBB1	1.68	0.72
21:3:613:LUT:H401	21:3:613:LUT:H15	1.72	0.72
8:D:154:ASN:ND2	8:D:156:GLU:OE2	2.19	0.71
18:1:602:CLA:CBB	19:1:614:XAT:H32	2.21	0.71
17:4:605:CHL:HHC	17:4:605:CHL:HBB1	1.73	0.71
6:B:304:LEU:HA	18:B:822:CLA:HED1	1.72	0.70
21:4:616:LUT:H8	21:4:616:LUT:H171	1.73	0.70
18:1:602:CLA:HBB2	19:1:614:XAT:H32	1.73	0.69
17:1:601:CHL:HHC	20:1:615:LHG:H252	1.75	0.69
22:3:614:BCR:H403	22:3:614:BCR:H23C	1.74	0.69
3:3:256:ASP:O	3:3:264:ASN:ND2	2.26	0.69
18:A:805:CLA:H43	18:A:812:CLA:HBB1	1.73	0.68
3:3:215:GLU:N	3:3:215:GLU:OE2	2.23	0.68
1:1:97:ALA:HA	19:1:614:XAT:H181	1.76	0.68
3:3:81:LEU:HD13	18:3:601:CLA:H42	1.76	0.68
18:A:804:CLA:H191	18:A:844:CLA:H203	1.75	0.68
2:2:98:CYS:O	2:2:102:MET:HG3	1.93	0.67
1:1:172:PHE:HB2	18:1:609:CLA:HMD1	1.75	0.67
22:A:853:BCR:HC8	22:A:853:BCR:H311	1.75	0.67
16:L:107:VAL:HA	18:L:303:CLA:HED1	1.74	0.67
12:H:87:SER:O	12:H:91:GLU:HG3	1.95	0.67
18:A:829:CLA:H202	22:J:102:BCR:H19C	1.76	0.66
22:L:301:BCR:H21C	22:L:301:BCR:H361	1.77	0.66
1:1:187:LEU:HD13	18:1:609:CLA:HAA2	1.78	0.66
6:B:65:LEU:HD11	22:B:845:BCR:H282	1.75	0.66
18:B:805:CLA:H52	18:B:813:CLA:H61	1.78	0.66
13:I:24:MET:HE3	22:L:305:BCR:H352	1.78	0.65
18:A:804:CLA:HBD	18:A:804:CLA:HBA2	1.78	0.65
5:A:393:TRP:CD1	18:A:829:CLA:HAB	2.31	0.65
18:2:613:CLA:H2A	18:2:613:CLA:HED2	1.78	0.65
6:B:164:ARG:NH2	11:G:108:GLY:O	2.30	0.65
6:B:517:PHE:HA	18:B:837:CLA:HED1	1.79	0.65
18:B:828:CLA:H171	22:B:845:BCR:H362	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:J:102:BCR:HC8	22:J:102:BCR:H311	1.79	0.65
5:A:320:LYS:NZ	5:A:324:GLU:OE2	2.31	0.64
18:A:803:CLA:HBA2	6:B:655:LEU:HB2	1.79	0.64
25:A:855:PQN:H172	22:B:801:BCR:H382	1.78	0.64
18:A:802:CLA:H202	18:A:842:CLA:H2	1.80	0.64
16:L:65:ILE:HA	16:L:75:GLU:HG3	1.81	0.64
22:B:848:BCR:H403	22:B:848:BCR:H23C	1.80	0.63
22:B:847:BCR:HC8	22:B:847:BCR:H311	1.80	0.63
22:A:851:BCR:H16C	22:A:851:BCR:H351	1.80	0.63
22:K:205:BCR:H403	22:K:205:BCR:H23C	1.80	0.63
1:1:116:GLN:HG2	18:1:605:CLA:HBB2	1.80	0.63
22:B:801:BCR:HC8	22:B:801:BCR:H331	1.80	0.63
18:A:842:CLA:HBC2	25:A:855:PQN:H192	1.81	0.62
4:4:165:GLY:HA2	4:4:168:ASN:HD22	1.63	0.62
22:A:849:BCR:H383	22:A:849:BCR:H23C	1.80	0.62
6:B:574:ASP:OD1	6:B:706:ARG:NH1	2.31	0.62
6:B:307:ALA:HB3	18:B:822:CLA:HED3	1.80	0.62
18:B:841:CLA:HED1	18:B:822:CLA:HAB	1.80	0.62
2:2:119:ILE:HG22	2:2:120:LEU:HD12	1.81	0.61
18:3:607:CLA:HHC	18:3:607:CLA:HBB1	1.82	0.61
6:B:57:ILE:HA	18:B:806:CLA:HBC3	1.83	0.61
22:B:846:BCR:H343	18:B:822:CLA:HBB2	1.83	0.61
15:K:75:SER:OG	15:K:76:ALA:N	2.33	0.61
15:K:75:SER:O	15:K:89:ARG:NH2	2.34	0.61
1:1:73:LEU:HD12	19:1:614:XAT:H221	1.81	0.60
5:A:302:PHE:HE1	18:A:822:CLA:HAB	1.66	0.60
16:L:100:PRO:HA	16:L:103:ARG:HD3	1.83	0.60
22:A:851:BCR:H23C	22:A:851:BCR:H403	1.82	0.60
22:L:305:BCR:H321	22:L:305:BCR:HC8	1.82	0.60
22:G:204:BCR:HC8	22:G:204:BCR:H311	1.82	0.60
5:A:508:GLY:HA2	5:A:523:PRO:HB3	1.81	0.60
24:A:801:CL0:H15	24:A:801:CL0:H2	1.84	0.60
21:1:616:LUT:H391	21:1:616:LUT:H32	1.81	0.60
6:B:469:LYS:NZ	6:B:509:PHE:O	2.33	0.60
22:B:846:BCR:HC8	22:B:846:BCR:H311	1.84	0.60
4:4:100:GLY:O	4:4:104:MET:HG3	2.02	0.60
4:4:216:PHE:CD2	19:4:617:XAT:H14	2.37	0.60
18:1:609:CLA:HHC	18:1:609:CLA:HBB1	1.84	0.59
20:1:615:LHG:H151	18:4:614:CLA:HED3	1.83	0.59
22:K:205:BCR:H321	22:K:205:BCR:HC8	1.82	0.59
6:B:293:THR:HG22	6:B:294:ASN:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:732:LEU:HA	20:A:846:LHG:H383	1.83	0.59
18:A:821:CLA:HHC	18:A:821:CLA:HBB1	1.85	0.59
6:B:432:HIS:HB2	22:B:849:BCR:H402	1.84	0.59
12:H:117:TYR:O	12:H:121:ASN:ND2	2.30	0.59
18:4:613:CLA:HBD	18:4:613:CLA:HBA1	1.85	0.59
22:A:852:BCR:H403	22:A:852:BCR:H23C	1.85	0.59
6:B:68:VAL:HG11	6:B:124:TRP:HZ3	1.68	0.59
17:1:601:CHL:O1A	4:4:151:HIS:ND1	2.35	0.58
18:A:822:CLA:H2	18:A:826:CLA:HBB1	1.85	0.58
14:J:10:VAL:HG12	14:J:12:PRO:HD2	1.85	0.58
6:B:571:SER:OG	6:B:574:ASP:OD2	2.21	0.58
21:2:619:LUT:H172	18:4:610:CLA:HHC	1.84	0.58
6:B:600:THR:HG21	6:B:609:PHE:HB2	1.85	0.58
7:C:15:THR:HA	7:C:28:MET:HE3	1.86	0.58
22:4:618:BCR:HC8	22:4:618:BCR:H321	1.85	0.58
18:A:831:CLA:H172	20:A:846:LHG:H182	1.85	0.58
1:1:125:GLN:NE2	1:1:133:VAL:O	2.31	0.58
5:A:348:ALA:HB1	22:A:850:BCR:H393	1.86	0.58
17:1:601:CHL:HAA1	20:1:615:LHG:H141	1.85	0.58
5:A:288:LEU:HD23	5:A:291:ILE:HD12	1.86	0.58
6:B:147:ALA:O	6:B:151:ILE:HG13	2.04	0.58
4:4:178:LEU:HD21	4:4:189:ILE:HG22	1.86	0.57
18:A:820:CLA:H91	18:A:820:CLA:H151	1.86	0.57
5:A:36:ILE:O	5:A:45:TRP:NE1	2.29	0.57
5:A:438:LEU:HG	5:A:546:LEU:HB2	1.86	0.57
18:A:809:CLA:HAB	18:A:829:CLA:H122	1.86	0.57
18:A:809:CLA:H201	20:A:846:LHG:H211	1.86	0.57
2:2:104:GLY:HA2	19:2:617:XAT:H181	1.87	0.57
4:4:169:GLN:NE2	4:4:174:LYS:O	2.38	0.57
22:A:850:BCR:H311	22:A:850:BCR:HC8	1.86	0.57
3:3:186:LEU:HD11	22:3:614:BCR:H343	1.87	0.56
5:A:117:PRO:HB3	5:A:122:GLU:HB3	1.86	0.56
6:B:516:ASP:OD2	6:B:593:TYR:OH	2.21	0.56
22:B:843:BCR:H16C	22:B:843:BCR:H351	1.87	0.56
5:A:739:TRP:HH2	18:A:809:CLA:HBC2	1.70	0.56
15:K:102:THR:OG1	15:K:105:ASP:OD2	2.23	0.56
5:A:495:THR:OG1	18:A:836:CLA:OBD	2.21	0.56
4:4:82:LEU:HD13	18:4:602:CLA:H42	1.86	0.56
3:3:217:SER:O	3:3:221:LEU:HD12	2.06	0.56
5:A:294:HIS:HB2	18:A:819:CLA:C1B	2.36	0.56
6:B:707:LEU:HD11	27:B:850:DGD:HB81	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:395:ILE:HG13	6:B:541:ALA:HB1	1.89	0.55
18:A:825:CLA:H41	22:A:851:BCR:H15C	1.87	0.55
6:B:523:ILE:HG21	18:B:836:CLA:HAB	1.89	0.55
16:L:90:ASN:O	16:L:95:ARG:NH1	2.38	0.55
5:A:735:ILE:HD12	20:A:846:LHG:H382	1.87	0.55
18:H:201:CLA:HAA2	22:L:306:BCR:H342	1.89	0.55
5:A:279:LEU:HD21	5:A:372:PRO:HD2	1.89	0.55
18:A:808:CLA:H2	18:A:810:CLA:H42	1.87	0.55
17:2:615:CHL:HHC	17:2:615:CHL:HBB1	1.88	0.55
25:B:842:PQN:H272	18:B:840:CLA:H42	1.89	0.55
18:B:824:CLA:H141	18:B:824:CLA:H193	1.87	0.55
20:1:615:LHG:H171	20:1:615:LHG:H342	1.89	0.55
5:A:296:LEU:O	5:A:300:ILE:HG12	2.07	0.55
5:A:728:THR:HG23	20:A:846:LHG:H341	1.88	0.55
8:D:72:THR:HG23	8:D:120:PRO:HB2	1.88	0.55
6:B:704:GLN:HG3	27:B:850:DGD:HA22	1.89	0.54
18:B:831:CLA:HBC2	18:B:838:CLA:HMC3	1.89	0.54
6:B:373:THR:HG23	6:B:591:THR:HG21	1.90	0.54
13:I:27:LEU:HD22	22:L:305:BCR:H323	1.89	0.54
18:1:602:CLA:H2	19:1:614:XAT:H221	1.89	0.54
5:A:360:LEU:HD11	18:A:820:CLA:H8	1.90	0.54
22:A:853:BCR:H23C	22:A:853:BCR:H393	1.89	0.54
6:B:276:HIS:HB2	18:B:817:CLA:C1B	2.38	0.54
22:F:304:BCR:H14C	22:F:304:BCR:H10C	1.90	0.54
18:A:842:CLA:HBD	18:A:842:CLA:HBA1	1.90	0.53
1:1:95:MET:HE3	18:1:609:CLA:HAB	1.89	0.53
21:3:613:LUT:H161	21:3:613:LUT:H8	1.89	0.53
18:B:808:CLA:O1A	18:B:827:CLA:HBD	2.09	0.53
16:L:63:GLN:HG2	16:L:64:PRO:HD2	1.90	0.53
4:4:116:PHE:O	4:4:120:GLY:N	2.30	0.53
22:4:618:BCR:H383	22:4:618:BCR:H23C	1.91	0.53
18:B:805:CLA:H101	18:B:824:CLA:HBA1	1.89	0.53
1:1:237:VAL:HG13	1:1:238:ILE:HG23	1.90	0.53
18:A:830:CLA:CHA	18:A:830:CLA:HBA1	2.38	0.53
20:B:851:LHG:H261	20:B:851:LHG:H302	1.90	0.53
20:B:852:LHG:H121	18:B:822:CLA:H52	1.90	0.53
6:B:659:THR:HA	18:B:803:CLA:HAB	1.89	0.53
6:B:707:LEU:HD23	27:B:850:DGD:HA21	1.91	0.53
5:A:689:ARG:H	6:B:568:CYS:HB2	1.74	0.53
4:4:191:ASN:OD1	21:4:616:LUT:O23	2.27	0.53
1:1:64:GLY:HA3	1:1:192:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:25:ILE:HG21	27:B:850:DGD:HA72	1.91	0.52
18:B:828:CLA:H122	22:B:845:BCR:H372	1.91	0.52
22:B:849:BCR:H10C	14:J:38:THR:O	2.09	0.52
1:1:69:ASP:HA	19:1:614:XAT:O23	2.10	0.52
18:A:841:CLA:H143	18:F:302:CLA:HBC1	1.92	0.52
3:3:61:GLN:O	3:3:64:SER:OG	2.26	0.52
18:A:812:CLA:H141	18:A:812:CLA:H203	1.91	0.52
17:2:605:CHL:HHB	21:2:619:LUT:H392	1.91	0.52
18:A:844:CLA:HMB2	18:B:802:CLA:H203	1.90	0.52
5:A:389:THR:HG23	5:A:605:ILE:HG21	1.92	0.52
5:A:536:ILE:HG23	24:A:801:CL0:H70	1.92	0.52
4:4:170:ASP:OD1	4:4:173:PHE:N	2.42	0.52
5:A:403:ALA:HB2	22:A:851:BCR:H323	1.92	0.52
18:A:843:CLA:HMD3	22:B:848:BCR:H393	1.91	0.52
18:B:840:CLA:H122	22:L:305:BCR:H351	1.92	0.52
5:A:14:VAL:HG11	18:A:811:CLA:HED3	1.91	0.52
18:A:803:CLA:H2	6:B:655:LEU:HD22	1.92	0.52
25:B:842:PQN:H272	18:B:840:CLA:H11	1.91	0.52
16:L:90:ASN:HB3	18:L:302:CLA:HAC1	1.92	0.52
22:B:843:BCR:H311	22:B:843:BCR:HC8	1.92	0.51
5:A:699:ILE:HA	18:A:841:CLA:HED1	1.92	0.51
18:A:841:CLA:H72	18:B:832:CLA:H42	1.92	0.51
2:2:80:LEU:HD13	18:2:602:CLA:H71	1.92	0.51
3:3:214:ASP:OD1	3:3:216:LYS:N	2.44	0.51
5:A:256:GLU:OE2	5:A:268:LYS:NZ	2.44	0.51
18:A:806:CLA:H51	18:A:814:CLA:H12	1.93	0.51
7:C:47:ASP:OD2	8:D:128:LYS:NZ	2.41	0.51
6:B:236:ASN:HB3	6:B:252:THR:HG22	1.93	0.51
22:B:844:BCR:H382	22:B:844:BCR:H23C	1.93	0.51
2:2:167:THR:HG22	2:2:175:LYS:HD3	1.93	0.51
1:1:156:ARG:NH2	18:1:608:CLA:O1D	2.38	0.51
17:2:605:CHL:C2C	18:2:604:CLA:HBB2	2.41	0.51
18:B:832:CLA:HHC	18:B:832:CLA:HBB1	1.93	0.51
19:1:614:XAT:H242	19:1:614:XAT:H362	1.93	0.51
14:J:28:GLU:HG3	18:J:101:CLA:CHA	2.40	0.50
18:A:809:CLA:H202	18:A:809:CLA:H91	1.93	0.50
11:G:68:ILE:HG21	11:G:147:LEU:HG	1.93	0.50
15:K:108:ALA:O	15:K:112:VAL:HG23	2.10	0.50
12:H:80:SER:HB2	16:L:98:VAL:HG13	1.93	0.50
18:B:838:CLA:HHC	18:B:838:CLA:HBB1	1.93	0.50
18:1:602:CLA:ND	19:1:614:XAT:H382	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:104:MET:HE1	18:4:609:CLA:CAB	2.40	0.50
6:B:69:ALA:HB2	6:B:135:LEU:HB2	1.92	0.50
17:2:601:CHL:HHC	17:2:601:CHL:HBB1	1.94	0.49
18:A:811:CLA:H2A	18:A:811:CLA:HED2	1.93	0.49
6:B:450:GLU:OE2	10:F:119:ARG:NH1	2.44	0.49
6:B:120:VAL:HG21	18:B:808:CLA:HED1	1.94	0.49
18:4:614:CLA:CED	18:4:614:CLA:H2A	2.42	0.49
6:B:422:LEU:HD13	6:B:532:LEU:HA	1.94	0.49
2:2:104:GLY:HA3	19:2:617:XAT:H192	1.93	0.49
4:4:175:GLN:OE1	4:4:175:GLN:N	2.28	0.49
22:B:844:BCR:H352	18:B:828:CLA:H192	1.94	0.49
8:D:90:VAL:HG12	8:D:91:GLU:HG3	1.94	0.49
10:F:210:GLU:HG3	10:F:215:ASP:HB3	1.95	0.49
18:4:609:CLA:CGA	18:4:609:CLA:H3A	2.42	0.49
1:1:149:ILE:HA	1:1:152:VAL:HG22	1.94	0.49
5:A:447:PHE:O	18:A:835:CLA:HBB2	2.13	0.49
2:2:99:ARG:NH1	17:2:607:CHL:OBD	2.34	0.49
2:2:213:GLY:O	2:2:217:MET:HG3	2.12	0.49
18:A:844:CLA:H3A	18:A:844:CLA:O1A	2.13	0.49
18:B:819:CLA:HBB1	18:B:824:CLA:H93	1.95	0.49
5:A:261:PHE:HE1	18:A:818:CLA:HBB1	1.77	0.48
18:A:843:CLA:H152	22:L:301:BCR:H16C	1.95	0.48
6:B:395:ILE:HD13	6:B:555:TYR:HA	1.94	0.48
8:D:152:PHE:HB2	8:D:156:GLU:HG2	1.94	0.48
1:1:238:ILE:HD12	23:4:620:LMG:H132	1.94	0.48
21:2:616:LUT:H401	21:2:616:LUT:H15	1.95	0.48
15:K:79:LYS:O	15:K:87:GLU:N	2.45	0.48
17:2:605:CHL:C4C	18:2:604:CLA:HAB	2.44	0.48
6:B:91:ILE:HB	6:B:112:PRO:HB2	1.96	0.48
5:A:361:THR:HA	18:A:830:CLA:HBC2	1.96	0.48
5:A:739:TRP:CH2	18:A:809:CLA:HBC2	2.47	0.48
18:A:802:CLA:H202	18:A:802:CLA:H162	1.70	0.48
16:L:203:THR:HB	22:L:306:BCR:H333	1.94	0.48
17:1:601:CHL:NB	20:1:615:LHG:H131	2.29	0.48
10:F:199:ARG:HE	10:F:199:ARG:HB2	1.53	0.48
2:2:201:LYS:HE3	2:2:205:LEU:HD11	1.95	0.48
4:4:199:GLN:O	4:4:203:GLU:HG3	2.14	0.48
16:L:87:TYR:OH	18:L:303:CLA:O1A	2.30	0.48
1:1:177:TYR:HB2	18:1:609:CLA:HBA2	1.96	0.48
5:A:41:ASP:OD1	5:A:41:ASP:N	2.46	0.48
18:A:809:CLA:H151	18:A:804:CLA:H161	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:812:CLA:H92	18:A:812:CLA:H62	1.71	0.48
1:1:190:LYS:HD3	18:1:611:CLA:HAA2	1.95	0.48
17:1:601:CHL:H12	20:1:615:LHG:H181	1.96	0.48
19:2:617:XAT:H401	19:2:617:XAT:H15	1.95	0.48
5:A:717:LEU:HB3	5:A:721:GLN:HG2	1.95	0.48
18:A:806:CLA:H192	22:A:849:BCR:H363	1.96	0.48
25:A:855:PQN:H271	18:A:841:CLA:H91	1.96	0.48
3:3:220:GLU:O	3:3:224:LYS:HG3	2.14	0.47
4:4:151:HIS:HA	18:4:608:CLA:HAB	1.96	0.47
18:4:612:CLA:H91	18:4:612:CLA:H111	1.70	0.47
18:B:821:CLA:HBA1	18:B:821:CLA:HBD	1.95	0.47
4:4:157:ARG:NH2	18:4:608:CLA:O1D	2.33	0.47
18:B:830:CLA:HBC2	18:B:823:CLA:HBB1	1.96	0.47
15:K:48:PHE:HZ	18:K:204:CLA:HBC3	1.80	0.47
18:A:802:CLA:HBA1	18:A:802:CLA:H3A	1.43	0.47
18:B:814:CLA:H121	22:B:845:BCR:H363	1.97	0.47
6:B:106:ARG:HG3	6:B:115:ILE:HD11	1.95	0.47
18:B:805:CLA:H2	18:B:805:CLA:H61	1.58	0.47
11:G:64:PRO:HG2	11:G:67:VAL:HB	1.97	0.47
6:B:277:HIS:HA	6:B:280:ILE:HG12	1.95	0.47
18:B:818:CLA:H3A	18:B:818:CLA:HBA2	1.42	0.47
5:A:702:ALA:HB3	18:A:841:CLA:HED3	1.96	0.47
12:H:104:LEU:O	12:H:108:ILE:HG12	2.15	0.47
22:L:301:BCR:H361	22:L:301:BCR:C21	2.41	0.47
18:2:602:CLA:H192	18:2:602:CLA:H162	1.74	0.47
18:B:834:CLA:HBA1	18:B:834:CLA:H3A	1.57	0.47
18:F:302:CLA:H11	18:F:302:CLA:H52	1.72	0.47
18:1:602:CLA:CBB	19:1:614:XAT:H30	2.45	0.47
18:F:301:CLA:H62	18:F:301:CLA:H41	1.56	0.47
5:A:393:TRP:HD1	18:A:829:CLA:HAB	1.78	0.47
22:A:848:BCR:H403	22:A:848:BCR:H23C	1.96	0.47
2:2:102:MET:HE1	18:2:609:CLA:CBB	2.45	0.46
17:2:606:CHL:HHC	17:2:606:CHL:HBB1	1.97	0.46
3:3:90:PHE:HB2	18:3:602:CLA:H43	1.97	0.46
5:A:207:SER:HB3	5:A:299:ALA:HB2	1.97	0.46
6:B:31:PHE:HE1	18:B:804:CLA:HED1	1.80	0.46
10:F:128:LEU:HD21	14:J:38:THR:HG21	1.96	0.46
6:B:456:GLU:OE1	6:B:461:GLN:NE2	2.48	0.46
18:A:833:CLA:H61	18:A:833:CLA:H41	1.44	0.46
18:1:612:CLA:O2D	18:1:612:CLA:H2A	2.15	0.46
6:B:182:LEU:HD21	18:B:813:CLA:O1A	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:116:THR:HG23	13:I:10:ILE:HG23	1.97	0.46
21:1:616:LUT:H35	21:1:616:LUT:H401	1.79	0.46
18:A:805:CLA:H3A	18:A:805:CLA:HBA2	1.38	0.46
18:B:832:CLA:HBB2	22:B:801:BCR:H312	1.98	0.46
1:1:109:TYR:HE1	1:1:129:LEU:HA	1.80	0.46
21:2:616:LUT:H22	18:2:609:CLA:H12	1.98	0.46
18:A:820:CLA:HMB1	18:A:820:CLA:HBB1	1.98	0.46
6:B:46:ILE:HG21	18:B:805:CLA:H202	1.96	0.46
5:A:386:SER:HB3	18:A:829:CLA:HMA1	1.97	0.46
18:A:835:CLA:H161	18:A:835:CLA:H202	1.69	0.46
16:L:87:TYR:OH	18:L:302:CLA:HBB2	2.16	0.46
6:B:435:GLY:HA3	18:B:833:CLA:HAB	1.98	0.46
18:B:840:CLA:HBA1	18:B:840:CLA:H3A	1.66	0.46
18:1:603:CLA:H41	18:1:603:CLA:H62	1.67	0.46
22:K:202:BCR:H23C	22:K:202:BCR:H392	1.97	0.46
18:A:845:CLA:H3A	18:A:845:CLA:HBA1	1.46	0.46
6:B:548:PRO:HD2	7:C:62:PHE:CZ	2.51	0.46
10:F:138:LEU:HD22	10:F:149:GLU:HG2	1.98	0.46
1:1:238:ILE:O	1:1:238:ILE:HG13	2.15	0.45
18:B:837:CLA:H3A	18:B:837:CLA:HBA2	1.72	0.45
18:A:828:CLA:OBD	18:A:827:CLA:HAA2	2.16	0.45
18:A:833:CLA:HBA1	18:A:833:CLA:H3A	1.86	0.45
18:B:818:CLA:HBB1	18:B:818:CLA:HMB1	1.98	0.45
3:3:260:ASP:OD2	3:3:264:ASN:ND2	2.49	0.45
24:A:801:CL0:H51	24:A:801:CL0:H59	1.67	0.45
18:A:804:CLA:H143	22:A:853:BCR:H19C	1.98	0.45
18:H:201:CLA:H93	18:H:201:CLA:H62	1.78	0.45
1:1:212:TYR:HD1	1:1:220:ASN:HD21	1.62	0.45
20:1:615:LHG:H341	20:1:615:LHG:H371	1.50	0.45
2:2:194:TRP:HB2	18:2:609:CLA:O2A	2.16	0.45
3:3:119:ILE:HG13	3:3:120:LEU:HD23	1.98	0.45
22:A:853:BCR:H343	14:J:27:ILE:HG21	1.99	0.45
22:A:851:BCR:H351	22:A:851:BCR:C16	2.42	0.45
6:B:61:THR:HB	6:B:142:LEU:HD13	1.97	0.45
1:1:119:ALA:HB1	1:1:138:LEU:HD12	1.98	0.45
3:3:260:ASP:HA	3:3:261:PRO:HD3	1.86	0.45
21:3:613:LUT:H12	21:3:613:LUT:H191	1.98	0.45
6:B:301:ILE:HG21	18:B:824:CLA:HAC1	1.98	0.45
18:B:806:CLA:H72	18:B:806:CLA:H111	1.52	0.45
18:B:808:CLA:H141	18:B:808:CLA:H162	1.62	0.45
10:F:180:LYS:HB3	10:F:180:LYS:HE3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:805:CLA:H61	18:B:805:CLA:H93	1.66	0.45
18:B:827:CLA:H152	18:B:827:CLA:H111	1.39	0.45
7:C:62:PHE:HD2	8:D:185:ILE:HG21	1.82	0.45
21:2:619:LUT:H31	21:2:619:LUT:H391	1.82	0.45
6:B:339:ALA:HB2	22:B:847:BCR:H372	1.99	0.45
22:B:846:BCR:H332	20:B:852:LHG:H351	1.98	0.45
22:B:801:BCR:H383	22:B:801:BCR:H23C	1.99	0.45
1:1:190:LYS:O	1:1:194:ASN:ND2	2.42	0.45
5:A:201:GLY:O	5:A:205:LEU:HB2	2.16	0.45
18:A:806:CLA:HBA1	18:A:806:CLA:H3A	1.45	0.45
18:A:841:CLA:HBA2	18:A:841:CLA:H3A	1.41	0.44
18:B:805:CLA:HBA1	18:B:805:CLA:H3A	1.44	0.44
22:A:853:BCR:HC7	22:A:853:BCR:H331	1.82	0.44
6:B:687:LEU:HD11	16:L:91:LEU:HD13	1.99	0.44
2:2:81:SER:O	2:2:81:SER:OG	2.30	0.44
18:A:820:CLA:H62	18:A:820:CLA:H92	1.67	0.44
7:C:58:CYS:HB3	7:C:63:LEU:HD23	2.00	0.44
15:K:96:GLY:O	18:K:201:CLA:H3A	2.18	0.44
1:1:97:ALA:HA	19:1:614:XAT:C18	2.46	0.44
20:1:615:LHG:H342	20:1:615:LHG:H192	1.99	0.44
18:2:602:CLA:H41	18:2:602:CLA:H62	1.51	0.44
4:4:101:ARG:NH1	17:4:607:CHL:OBD	2.43	0.44
18:A:803:CLA:HBA1	18:A:803:CLA:H3A	1.63	0.44
18:A:842:CLA:H102	18:A:842:CLA:H62	1.78	0.44
18:2:612:CLA:H112	18:2:612:CLA:H71	1.68	0.44
18:2:602:CLA:H62	18:2:602:CLA:H102	1.83	0.44
18:4:602:CLA:H92	18:4:603:CLA:HHB	1.99	0.44
5:A:90:PHE:CG	18:A:808:CLA:HBC3	2.53	0.44
20:1:615:LHG:H261	20:1:615:LHG:H292	1.32	0.44
4:4:104:MET:HE1	18:4:609:CLA:HHC	1.99	0.44
9:E:89:ILE:HG22	9:E:91:ARG:H	1.82	0.44
11:G:120:LYS:HB3	11:G:120:LYS:HE3	1.71	0.44
18:G:201:CLA:CGA	18:G:201:CLA:H3A	2.48	0.44
22:K:202:BCR:H24C	22:K:202:BCR:H371	1.77	0.44
1:1:140:THR:O	1:1:144:ILE:HG13	2.17	0.44
18:1:609:CLA:HHC	18:1:609:CLA:CBB	2.47	0.44
22:B:847:BCR:H11C	22:B:847:BCR:H341	1.89	0.44
18:B:826:CLA:H102	18:B:826:CLA:H61	1.74	0.44
18:A:822:CLA:H141	18:A:822:CLA:H162	1.71	0.44
18:A:840:CLA:HMC2	18:A:833:CLA:HBC2	2.00	0.44
15:K:66:PHE:CD1	15:K:66:PHE:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:619:LUT:H35	21:2:619:LUT:H401	1.82	0.44
5:A:582:CYS:HB2	6:B:667:TRP:HB3	2.00	0.44
8:D:156:GLU:OE2	8:D:156:GLU:N	2.51	0.44
19:1:614:XAT:H35	19:1:614:XAT:H401	1.87	0.43
18:2:602:CLA:CGA	18:2:602:CLA:H3A	2.48	0.43
4:4:165:GLY:HA2	4:4:168:ASN:ND2	2.31	0.43
18:A:819:CLA:H3A	18:A:819:CLA:HBA2	1.63	0.43
22:A:853:BCR:H15C	22:A:853:BCR:H351	1.85	0.43
6:B:517:PHE:HE1	22:B:849:BCR:H271	1.83	0.43
22:B:846:BCR:H11C	22:B:846:BCR:H341	1.81	0.43
22:B:847:BCR:HC7	22:B:847:BCR:H331	1.85	0.43
18:B:825:CLA:H3A	18:B:825:CLA:HBA1	1.43	0.43
1:1:238:ILE:HD11	4:4:140:SER:HB3	1.99	0.43
2:2:57:PRO:O	3:3:172:GLN:HG2	2.19	0.43
18:3:601:CLA:H8	18:3:601:CLA:H51	1.74	0.43
6:B:395:ILE:HD12	6:B:555:TYR:HD1	1.82	0.43
18:3:603:CLA:HBA1	18:3:603:CLA:H3A	1.30	0.43
21:3:613:LUT:H181	21:3:613:LUT:H7	1.72	0.43
4:4:222:GLN:HE22	21:4:616:LUT:H41	1.83	0.43
5:A:371:MET:HE2	18:A:819:CLA:HAA2	2.00	0.43
15:K:67:ALA:HA	15:K:72:LEU:HD12	2.00	0.43
1:1:184:LEU:HD11	18:1:609:CLA:O2D	2.18	0.43
18:1:604:CLA:C1B	19:1:614:XAT:H42	2.48	0.43
4:4:134:GLN:OE1	4:4:134:GLN:C	2.61	0.43
5:A:317:HIS:HB3	5:A:322:ILE:HD11	1.99	0.43
5:A:676:PHE:CD2	22:A:852:BCR:H363	2.52	0.43
6:B:93:ASP:H	12:H:129:ILE:HD13	1.84	0.43
6:B:174:ARG:HB2	18:B:813:CLA:HBC2	2.00	0.43
18:B:822:CLA:H91	18:B:822:CLA:H111	1.82	0.43
18:3:609:CLA:HMB1	21:3:613:LUT:H26	2.01	0.43
5:A:480:PHE:O	5:A:484:ILE:HG12	2.18	0.43
18:A:825:CLA:H3A	18:A:825:CLA:HBA2	1.40	0.43
18:B:809:CLA:H92	18:B:809:CLA:H62	1.72	0.43
5:A:294:HIS:CE1	5:A:298:ILE:HG13	2.54	0.43
18:B:827:CLA:H193	27:B:850:DGD:HAN2	2.01	0.43
18:B:803:CLA:H61	18:B:803:CLA:H93	1.78	0.43
15:K:115:ILE:HG12	22:K:205:BCR:H313	2.01	0.43
20:2:618:LHG:O4	20:2:618:LHG:O2	2.33	0.43
5:A:93:ALA:HA	5:A:153:GLU:HG2	1.99	0.43
5:A:371:MET:HE2	18:A:819:CLA:HBD	2.00	0.43
1:1:128:TYR:HD1	18:1:604:CLA:HBA1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:602:CLA:H72	19:1:614:XAT:C37	2.49	0.43
2:2:171:PHE:HE2	17:2:615:CHL:HHB	1.84	0.43
19:4:617:XAT:H31	19:4:617:XAT:H391	1.92	0.43
5:A:530:ASP:HA	5:A:533:VAL:HG12	2.01	0.43
22:L:306:BCR:H373	18:L:303:CLA:HMA2	2.00	0.43
3:3:219:LYS:HA	3:3:219:LYS:HD2	1.83	0.43
5:A:223:GLN:HG2	5:A:250:LEU:HD21	2.01	0.43
22:B:846:BCR:H15C	22:B:846:BCR:H351	1.81	0.43
18:B:809:CLA:H41	18:B:809:CLA:H61	1.64	0.43
18:B:841:CLA:H121	18:B:841:CLA:H161	1.75	0.43
17:1:601:CHL:C2C	20:1:615:LHG:HC81	2.49	0.42
18:2:612:CLA:H142	18:2:612:CLA:H111	1.74	0.42
21:2:619:LUT:H181	21:2:619:LUT:C8	2.37	0.42
18:A:807:CLA:H93	18:A:807:CLA:H112	1.88	0.42
22:J:102:BCR:H11C	22:J:102:BCR:H341	1.83	0.42
18:L:303:CLA:H142	18:L:303:CLA:H111	1.72	0.42
2:2:168:ASP:HB3	2:2:171:PHE:O	2.19	0.42
20:2:618:LHG:HC81	20:2:618:LHG:HC41	2.01	0.42
17:4:615:CHL:HMC	17:4:607:CHL:OMC	2.18	0.42
18:A:835:CLA:H3A	18:A:835:CLA:HBA1	1.77	0.42
18:A:835:CLA:HHB	18:A:834:CLA:HAB	2.01	0.42
22:A:848:BCR:H11C	22:A:848:BCR:H341	1.90	0.42
6:B:583:MET:O	6:B:587:ILE:HG12	2.19	0.42
20:B:852:LHG:H121	18:B:822:CLA:H41	2.01	0.42
22:B:801:BCR:HC21	18:F:302:CLA:H51	2.00	0.42
22:B:845:BCR:H21C	22:B:845:BCR:H24C	1.78	0.42
10:F:203:TRP:CG	10:F:204:PRO:HD3	2.54	0.42
18:F:302:CLA:HAA2	14:J:22:LEU:HD11	2.02	0.42
18:1:604:CLA:C3B	19:1:614:XAT:H183	2.49	0.42
2:2:101:ALA:CB	2:2:217:MET:HG2	2.49	0.42
2:2:139:THR:O	2:2:143:VAL:HG23	2.19	0.42
21:3:613:LUT:H191	21:3:613:LUT:C12	2.48	0.42
4:4:221:VAL:HG11	18:4:612:CLA:HAC2	2.00	0.42
18:A:807:CLA:H193	18:A:807:CLA:H161	1.87	0.42
18:A:809:CLA:H71	22:J:102:BCR:H343	2.00	0.42
18:A:817:CLA:HBA1	18:A:817:CLA:H3A	1.65	0.42
22:A:851:BCR:H371	22:A:851:BCR:H24C	1.69	0.42
6:B:529:THR:HG21	6:B:582:TRP:CZ2	2.54	0.42
22:L:305:BCR:H24C	22:L:305:BCR:H371	1.81	0.42
18:A:807:CLA:HBA1	18:A:807:CLA:H3A	1.79	0.42
6:B:347:LEU:HD23	18:B:818:CLA:H72	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:614:XAT:H42	19:1:614:XAT:H162	2.01	0.42
21:2:616:LUT:H373	18:2:612:CLA:C2B	2.50	0.42
24:A:801:CL0:H51	24:A:801:CL0:H42	1.79	0.42
18:A:823:CLA:HAA2	15:K:80:ALA:HB3	2.02	0.42
18:A:834:CLA:HMA2	22:I:101:BCR:H272	2.02	0.42
6:B:649:MET:HE2	6:B:723:ALA:HB2	2.02	0.42
18:B:808:CLA:C1A	18:B:808:CLA:CGA	2.97	0.42
18:B:828:CLA:H3A	18:B:828:CLA:HBA2	1.30	0.42
22:B:801:BCR:H15C	22:B:801:BCR:H351	1.87	0.42
1:1:73:LEU:O	20:B:851:LHG:O1	2.28	0.42
18:A:804:CLA:O1D	18:A:804:CLA:H2A	2.19	0.42
6:B:373:THR:HB	18:B:827:CLA:HMB2	2.01	0.42
10:F:203:TRP:CD1	10:F:204:PRO:HD3	2.54	0.42
5:A:30:GLY:HA3	5:A:36:ILE:HG22	2.01	0.42
22:B:848:BCR:H403	22:B:848:BCR:C23	2.49	0.42
22:K:202:BCR:H351	22:K:202:BCR:H15C	1.80	0.42
18:3:605:CLA:O1D	18:3:605:CLA:H2A	2.20	0.42
22:B:846:BCR:H373	18:B:826:CLA:H121	2.01	0.42
22:B:801:BCR:H341	22:B:801:BCR:C12	2.37	0.42
22:L:305:BCR:H393	22:L:305:BCR:H23C	2.01	0.42
18:2:602:CLA:H122	19:2:617:XAT:H371	2.00	0.42
18:2:604:CLA:HBA1	18:2:604:CLA:H3A	1.92	0.42
6:B:294:ASN:HB2	11:G:114:GLU:HA	2.02	0.42
22:L:305:BCR:H20C	22:L:305:BCR:H361	1.88	0.42
1:1:65:ASP:OD2	1:1:65:ASP:C	2.62	0.42
18:B:840:CLA:H93	18:B:840:CLA:H61	1.91	0.42
1:1:227:ASP:OD2	1:1:230:HIS:HB2	2.20	0.41
2:2:102:MET:HE1	18:2:609:CLA:HBB2	2.01	0.41
18:A:844:CLA:H12	18:A:844:CLA:H52	1.84	0.41
18:A:839:CLA:H61	18:A:839:CLA:H41	1.77	0.41
22:A:851:BCR:H331	22:A:851:BCR:C8	2.49	0.41
6:B:275:HIS:HB3	18:B:817:CLA:HMB2	2.02	0.41
18:B:825:CLA:H93	18:B:825:CLA:H111	1.85	0.41
22:B:801:BCR:H24C	22:B:801:BCR:H371	1.87	0.41
8:D:102:LYS:HB2	8:D:102:LYS:HE2	1.91	0.41
17:1:601:CHL:C3B	20:1:615:LHG:H282	2.50	0.41
19:4:617:XAT:H32	18:4:602:CLA:HAB	2.00	0.41
5:A:310:ARG:HH22	15:K:79:LYS:HD3	1.85	0.41
18:A:804:CLA:HBA2	18:A:804:CLA:CBD	2.46	0.41
18:A:842:CLA:HBA2	20:A:846:LHG:H162	2.01	0.41
18:A:812:CLA:H111	18:A:812:CLA:H91	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:817:CLA:CGA	18:B:817:CLA:H3A	2.50	0.41
22:L:305:BCR:H23C	22:L:305:BCR:H402	2.02	0.41
21:1:616:LUT:H391	21:1:616:LUT:C32	2.49	0.41
18:2:609:CLA:HMD2	17:2:607:CHL:HBA2	2.01	0.41
19:2:617:XAT:H201	19:2:617:XAT:H35	2.02	0.41
18:2:608:CLA:H3A	18:2:608:CLA:HBA2	1.22	0.41
5:A:213:HIS:HB2	18:A:815:CLA:CHC	2.50	0.41
18:A:813:CLA:HBA2	18:A:813:CLA:H3A	1.75	0.41
18:A:830:CLA:H41	18:A:830:CLA:H62	1.68	0.41
18:B:824:CLA:H62	18:B:824:CLA:H41	1.55	0.41
18:A:821:CLA:HHC	18:A:821:CLA:CBB	2.50	0.41
18:A:809:CLA:H92	18:A:809:CLA:H62	1.77	0.41
18:A:830:CLA:H11	18:A:830:CLA:HBA2	1.55	0.41
22:B:848:BCR:H11C	22:B:848:BCR:H341	1.95	0.41
18:B:840:CLA:H111	18:B:840:CLA:H151	1.83	0.41
3:3:169:ARG:HB3	17:3:606:CHL:CMC	2.51	0.41
18:3:601:CLA:H2	18:3:601:CLA:H62	1.76	0.41
18:4:602:CLA:CGA	18:4:602:CLA:H3A	2.51	0.41
22:4:618:BCR:H11C	22:4:618:BCR:H341	1.92	0.41
22:A:851:BCR:H321	22:A:851:BCR:HC7	1.86	0.41
22:B:848:BCR:H20C	22:B:848:BCR:H361	1.92	0.41
18:B:818:CLA:H62	18:B:818:CLA:H41	1.77	0.41
18:B:823:CLA:HBA1	18:B:823:CLA:H3A	1.72	0.41
18:B:832:CLA:H143	18:B:832:CLA:H161	1.80	0.41
21:2:616:LUT:H11	21:2:616:LUT:H191	1.87	0.41
18:2:604:CLA:C2C	19:2:617:XAT:H183	2.50	0.41
18:3:602:CLA:H92	18:A:811:CLA:HMD1	2.02	0.41
19:4:617:XAT:H35	19:4:617:XAT:H401	1.89	0.41
21:4:616:LUT:H15	21:4:616:LUT:H201	1.96	0.41
18:A:825:CLA:HBB1	18:A:832:CLA:HBC2	2.02	0.41
18:B:809:CLA:H142	18:B:809:CLA:H111	1.91	0.41
18:B:802:CLA:HHC	18:B:802:CLA:HBB1	2.02	0.41
20:1:615:LHG:HC12	22:4:618:BCR:H291	2.03	0.41
18:A:805:CLA:HBA1	18:A:812:CLA:C1D	2.50	0.41
18:A:835:CLA:H93	18:A:835:CLA:H111	1.71	0.41
22:A:848:BCR:H23C	22:A:848:BCR:H392	2.02	0.41
22:A:850:BCR:H331	22:A:850:BCR:HC7	1.77	0.41
18:B:828:CLA:HBB1	18:B:806:CLA:HAB	2.03	0.41
18:B:828:CLA:H142	18:B:828:CLA:H112	1.90	0.41
22:B:845:BCR:H15C	22:B:845:BCR:H351	1.94	0.41
14:J:32:LEU:HD21	18:J:101:CLA:HBA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:156:TRP:CD2	18:2:608:CLA:HMA2	2.55	0.41
2:2:171:PHE:CE2	17:2:615:CHL:HHB	2.55	0.41
5:A:596:TRP:HE1	18:B:803:CLA:C1D	2.33	0.41
18:A:813:CLA:H2A	18:A:813:CLA:O2D	2.21	0.41
18:A:829:CLA:H72	18:A:829:CLA:H111	1.35	0.41
18:B:802:CLA:HBA1	18:B:802:CLA:H3A	1.29	0.41
18:B:820:CLA:C4B	22:B:843:BCR:H15C	2.50	0.41
22:G:204:BCR:HC7	22:G:204:BCR:H331	1.84	0.41
22:J:102:BCR:H15C	22:J:102:BCR:H351	1.82	0.41
22:L:301:BCR:H15C	22:L:301:BCR:H351	1.72	0.41
18:1:607:CLA:HBA2	18:1:607:CLA:H3A	1.23	0.41
18:2:602:CLA:HMC2	19:2:617:XAT:H391	2.03	0.41
5:A:116:TRP:O	5:A:121:GLN:NE2	2.38	0.41
5:A:305:ALA:HB2	18:A:822:CLA:HBC2	2.02	0.41
24:A:801:CL0:H12	18:B:802:CLA:CHB	2.51	0.41
18:A:813:CLA:H2A	18:A:813:CLA:CED	2.51	0.41
18:A:834:CLA:H162	18:A:834:CLA:H141	1.82	0.41
22:A:850:BCR:H11C	22:A:850:BCR:H341	1.84	0.41
18:A:812:CLA:H172	18:A:812:CLA:H13	1.73	0.41
6:B:464:GLN:NE2	18:B:836:CLA:OBD	2.44	0.41
6:B:601:LEU:HA	6:B:606:VAL:HG12	2.03	0.41
18:B:832:CLA:H62	18:B:832:CLA:H2	1.70	0.41
18:B:803:CLA:H202	18:B:803:CLA:H162	1.76	0.41
18:F:302:CLA:O1D	18:F:302:CLA:H2A	2.20	0.41
22:J:102:BCR:HC7	22:J:102:BCR:H331	1.90	0.41
16:L:121:LYS:HB3	16:L:121:LYS:HE3	1.84	0.41
16:L:208:LEU:HD23	16:L:208:LEU:HA	1.92	0.41
22:L:306:BCR:H15C	22:L:306:BCR:H351	1.84	0.41
2:2:174:ASN:HD22	17:2:615:CHL:C4D	2.33	0.41
4:4:155:ILE:HD13	4:4:155:ILE:HA	1.92	0.41
19:4:617:XAT:H11	19:4:617:XAT:H191	1.84	0.41
18:B:820:CLA:HBA2	18:B:820:CLA:H3A	1.32	0.41
22:L:305:BCR:H11C	22:L:305:BCR:H341	1.88	0.41
17:1:601:CHL:H61	17:1:601:CHL:H41	1.70	0.40
18:1:602:CLA:CGA	18:1:602:CLA:H3A	2.51	0.40
17:2:615:CHL:HBB1	17:2:615:CHL:CHC	2.50	0.40
18:2:612:CLA:H3A	18:2:612:CLA:HBA2	1.81	0.40
18:2:604:CLA:HED2	18:2:604:CLA:H2A	2.03	0.40
18:B:808:CLA:HAB	18:B:809:CLA:HAA2	2.03	0.40
18:B:814:CLA:H162	18:B:814:CLA:H141	1.81	0.40
18:B:824:CLA:H91	18:B:824:CLA:H112	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:75:SER:OG	15:K:105:ASP:OD1	2.27	0.40
22:3:614:BCR:H11C	22:3:614:BCR:H341	1.90	0.40
18:4:602:CLA:H91	18:4:602:CLA:H112	1.81	0.40
18:B:822:CLA:O1D	18:B:822:CLA:HBA1	2.21	0.40
18:3:601:CLA:H91	18:3:601:CLA:H112	1.87	0.40
5:A:319:ILE:HG21	18:A:826:CLA:HAC1	2.03	0.40
6:B:3:LEU:HD13	6:B:7:ARG:HH21	1.85	0.40
18:B:826:CLA:H111	18:B:826:CLA:H142	1.83	0.40
18:B:827:CLA:HBA2	18:B:827:CLA:H3A	1.39	0.40
22:B:843:BCR:H331	22:B:843:BCR:HC7	1.78	0.40
18:L:303:CLA:H112	18:L:303:CLA:H71	1.72	0.40
1:1:162:PRO:HA	1:1:165:LYS:HG3	2.03	0.40
19:1:614:XAT:H183	19:1:614:XAT:H7	1.85	0.40
18:2:602:CLA:H91	18:2:602:CLA:H111	1.82	0.40
20:2:618:LHG:HC91	22:3:614:BCR:HC41	2.04	0.40
5:A:671:PHE:O	5:A:675:HIS:ND1	2.54	0.40
18:A:809:CLA:H101	18:A:809:CLA:H13	1.92	0.40
18:B:813:CLA:O2D	18:B:813:CLA:H2A	2.22	0.40
18:B:832:CLA:CBB	22:B:801:BCR:H312	2.51	0.40
3:3:109:LEU:HD22	18:3:603:CLA:HBC1	2.04	0.40
3:3:167:GLU:OE1	3:3:170:ARG:NH1	2.54	0.40
6:B:432:HIS:CB	22:B:849:BCR:H402	2.49	0.40
10:F:195:ARG:HD2	10:F:195:ARG:HA	1.96	0.40
22:F:304:BCR:H361	22:F:304:BCR:H20C	1.80	0.40
11:G:74:LEU:HD12	11:G:74:LEU:HA	1.97	0.40
22:K:205:BCR:H24C	22:K:205:BCR:H371	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	191/241 (79%)	190 (100%)	1 (0%)	0	100	100
2	2	199/257 (77%)	198 (100%)	1 (0%)	0	100	100
3	3	216/273 (79%)	213 (99%)	3 (1%)	0	100	100
4	4	194/251 (77%)	191 (98%)	3 (2%)	0	100	100
5	A	735/750 (98%)	725 (99%)	10 (1%)	0	100	100
6	B	730/734 (100%)	716 (98%)	14 (2%)	0	100	100
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
8	D	141/204 (69%)	137 (97%)	4 (3%)	0	100	100
9	E	62/143 (43%)	61 (98%)	1 (2%)	0	100	100
10	F	150/221 (68%)	149 (99%)	1 (1%)	0	100	100
11	G	89/160 (56%)	88 (99%)	1 (1%)	0	100	100
12	H	88/145 (61%)	88 (100%)	0	0	100	100
13	I	29/37 (78%)	28 (97%)	1 (3%)	0	100	100
14	J	39/44 (89%)	38 (97%)	1 (3%)	0	100	100
15	K	82/130 (63%)	82 (100%)	0	0	100	100
16	L	158/219 (72%)	155 (98%)	3 (2%)	0	100	100
All	All	3181/3890 (82%)	3133 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	153/190 (80%)	151 (99%)	2 (1%)	61	75
2	2	163/205 (80%)	163 (100%)	0	100	100
3	3	167/211 (79%)	166 (99%)	1 (1%)	78	83
4	4	163/210 (78%)	162 (99%)	1 (1%)	78	83
5	A	598/610 (98%)	597 (100%)	1 (0%)	87	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B	599/600 (100%)	598 (100%)	1 (0%)	87	88
7	C	70/71 (99%)	70 (100%)	0	100	100
8	D	121/170 (71%)	121 (100%)	0	100	100
9	E	57/114 (50%)	57 (100%)	0	100	100
10	F	125/185 (68%)	124 (99%)	1 (1%)	73	80
11	G	77/133 (58%)	77 (100%)	0	100	100
12	H	75/113 (66%)	75 (100%)	0	100	100
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	36/39 (92%)	36 (100%)	0	100	100
15	K	61/95 (64%)	61 (100%)	0	100	100
16	L	126/174 (72%)	126 (100%)	0	100	100
All	All	2618/3153 (83%)	2611 (100%)	7 (0%)	84	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	59	ASP
1	1	220	ASN
3	3	136	GLN
4	4	132	LYS
5	A	127	ASP
6	B	309	ILE
10	F	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	131	ASN
1	1	220	ASN
3	3	242	GLN
3	3	263	ASN
3	3	265	ASN
4	4	168	ASN
4	4	194	ASN
4	4	222	GLN
4	4	224	ASN
4	4	236	GLN

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Mol	Chain	Res	Type
4	4	244	ASN
5	A	179	HIS
5	A	213	HIS
5	A	307	HIS
5	A	349	GLN
5	A	421	ASN
6	B	114	ASN
6	B	178	HIS
6	B	193	HIS
6	B	214	ASN
6	B	289	HIS
6	B	319	HIS
6	B	333	GLN
6	B	502	ASN
8	D	67	GLN
8	D	99	ASN
11	G	99	GLN
11	G	140	HIS
16	L	90	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)

201 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	$\#\|Z\| > 2$
18	CLA	A	843	-	69,73,73	1.26	6 (8%)	83,113,113	1.30	4 (4%)
18	CLA	A	825	-	59,63,73	1.37	6 (10%)	71,101,113	1.34	6 (8%)
18	CLA	B	833	6	49,53,73	1.49	6 (12%)	59,89,113	1.51	7 (11%)
19	XAT	2	617	-	39,47,47	1.78	7 (17%)	54,74,74	2.05	14 (25%)
18	CLA	A	810	5	54,58,73	1.42	9 (16%)	65,95,113	1.52	11 (16%)
18	CLA	3	601	-	64,68,73	1.31	8 (12%)	77,107,113	1.33	6 (7%)
18	CLA	G	203	11	49,53,73	1.48	7 (14%)	59,89,113	1.45	4 (6%)
18	CLA	2	602	2	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
17	CHL	4	615	4	44,49,74	2.29	16 (36%)	51,84,114	3.28	22 (43%)
21	LUT	3	613	-	42,43,43	1.71	8 (19%)	51,60,60	1.92	14 (27%)
18	CLA	A	835	5	69,73,73	1.25	7 (10%)	83,113,113	1.30	5 (6%)
23	LMG	4	620	-	33,33,55	0.24	0	41,41,63	0.33	0
18	CLA	2	612	2	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
18	CLA	A	806	5	69,73,73	1.25	8 (11%)	83,113,113	1.30	4 (4%)
18	CLA	A	812	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	5 (6%)
18	CLA	B	839	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
18	CLA	B	836	6	54,58,73	1.42	8 (14%)	65,95,113	3.43	11 (16%)
18	CLA	1	613	-	41,46,73	1.67	9 (21%)	52,81,113	1.61	8 (15%)
18	CLA	4	613	4	49,53,73	1.49	8 (16%)	59,89,113	1.58	6 (10%)
18	CLA	4	603	-	48,52,73	1.57	10 (20%)	61,88,113	1.50	6 (9%)
18	CLA	B	841	20	69,73,73	1.26	7 (10%)	83,113,113	1.30	5 (6%)
18	CLA	A	826	-	69,73,73	1.26	6 (8%)	83,113,113	1.29	4 (4%)
18	CLA	B	813	-	69,73,73	1.26	8 (11%)	83,113,113	1.36	8 (9%)
18	CLA	4	602	4	64,68,73	1.30	7 (10%)	77,107,113	1.33	7 (9%)
18	CLA	H	201	-	64,68,73	1.31	7 (10%)	77,107,113	1.32	4 (5%)
26	SF4	A	854	-	0,12,12	-	-	-		
17	CHL	1	601	1	55,60,74	2.21	17 (30%)	61,97,114	2.92	24 (39%)
18	CLA	A	820	5	69,73,73	1.26	7 (10%)	83,113,113	1.30	8 (9%)
18	CLA	2	609	-	51,55,73	1.44	8 (15%)	61,91,113	1.45	6 (9%)
22	BCR	B	845	-	41,41,41	1.80	8 (19%)	56,56,56	1.80	14 (25%)
18	CLA	A	819	5	63,67,73	1.32	7 (11%)	75,105,113	1.36	5 (6%)
18	CLA	A	830	-	69,73,73	1.26	7 (10%)	83,113,113	1.40	9 (10%)
18	CLA	B	821	6	51,55,73	1.44	7 (13%)	61,91,113	1.56	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
18	CLA	K	206	15	41,47,73	1.61	7 (17%)	49,81,113	1.52	6 (12%)
22	BCR	B	846	-	41,41,41	1.74	8 (19%)	56,56,56	1.70	10 (17%)
17	CHL	2	601	2	51,55,74	2.30	18 (35%)	57,91,114	3.00	22 (38%)
17	CHL	2	607	-	55,59,74	2.21	19 (34%)	62,96,114	2.91	24 (38%)
18	CLA	3	607	-	49,53,73	1.51	7 (14%)	59,89,113	1.45	6 (10%)
18	CLA	1	604	-	53,57,73	1.43	7 (13%)	62,93,113	1.48	6 (9%)
18	CLA	B	811	6	58,62,73	1.42	8 (13%)	73,100,113	1.45	7 (9%)
18	CLA	B	831	6	47,51,73	1.49	7 (14%)	56,86,113	1.47	5 (8%)
19	XAT	4	617	-	39,47,47	1.72	8 (20%)	54,74,74	1.72	12 (22%)
22	BCR	A	853	-	41,41,41	1.81	8 (19%)	56,56,56	1.75	14 (25%)
17	CHL	3	606	-	49,53,74	2.29	17 (34%)	59,89,114	2.92	20 (33%)
18	CLA	B	818	6	64,68,73	1.30	7 (10%)	77,107,113	1.34	6 (7%)
18	CLA	A	809	-	69,73,73	1.25	7 (10%)	83,113,113	1.30	5 (6%)
18	CLA	A	829	5	69,73,73	1.25	7 (10%)	83,113,113	1.29	5 (6%)
18	CLA	B	807	6	56,60,73	1.39	7 (12%)	67,97,113	1.40	5 (7%)
18	CLA	B	837	6	69,73,73	1.26	7 (10%)	83,113,113	1.32	7 (8%)
18	CLA	4	612	4	61,65,73	1.33	7 (11%)	73,103,113	1.36	6 (8%)
18	CLA	3	611	-	41,44,73	1.60	8 (19%)	49,77,113	1.50	4 (8%)
27	DGD	B	850	-	67,67,67	0.84	2 (2%)	81,81,81	0.94	4 (4%)
18	CLA	A	844	-	69,73,73	1.26	8 (11%)	83,113,113	1.31	7 (8%)
18	CLA	A	815	5	49,53,73	1.47	7 (14%)	59,89,113	1.45	4 (6%)
18	CLA	B	810	6	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
18	CLA	A	813	5	58,62,73	1.37	7 (12%)	69,99,113	1.41	6 (8%)
22	BCR	A	851	-	41,41,41	1.88	8 (19%)	56,56,56	2.48	19 (33%)
18	CLA	A	823	5	46,50,73	1.50	6 (13%)	55,85,113	1.48	4 (7%)
18	CLA	B	814	6	69,73,73	1.24	6 (8%)	83,113,113	1.30	7 (8%)
19	XAT	1	614	-	39,47,47	0.83	1 (2%)	54,74,74	3.20	18 (33%)
18	CLA	3	610	3	43,48,73	1.57	7 (16%)	51,83,113	1.50	5 (9%)
18	CLA	G	201	-	49,53,73	1.49	6 (12%)	59,89,113	1.44	4 (6%)
22	BCR	L	301	-	41,41,41	1.76	8 (19%)	56,56,56	2.17	12 (21%)
18	CLA	A	804	5	69,73,73	1.26	7 (10%)	83,113,113	1.38	7 (8%)
22	BCR	L	306	-	41,41,41	1.75	8 (19%)	56,56,56	1.91	16 (28%)
18	CLA	B	832	6	69,73,73	1.26	6 (8%)	83,113,113	1.26	6 (7%)
18	CLA	B	802	-	69,73,73	1.27	7 (10%)	83,113,113	1.27	5 (6%)
17	CHL	2	606	-	47,51,74	2.33	17 (36%)	52,86,114	3.11	21 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	1	605	-	50,54,73	1.47	7 (14%)	60,90,113	1.43	5 (8%)
18	CLA	1	609	-	46,50,73	1.51	8 (17%)	55,85,113	1.51	4 (7%)
22	BCR	B	847	-	41,41,41	1.73	8 (19%)	56,56,56	1.57	10 (17%)
18	CLA	1	610	20	41,46,73	1.67	8 (19%)	52,81,113	1.60	7 (13%)
20	LHG	B	852	-	48,48,48	0.27	0	51,54,54	0.33	0
17	CHL	4	607	-	50,54,74	2.27	17 (34%)	56,90,114	3.06	22 (39%)
18	CLA	B	812	6	47,51,73	1.51	6 (12%)	56,86,113	1.42	5 (8%)
20	LHG	2	618	18	36,36,48	0.31	0	39,42,54	0.53	1 (2%)
18	CLA	B	820	6	54,58,73	1.41	7 (12%)	65,95,113	1.44	6 (9%)
18	CLA	4	614	4	54,58,73	1.42	7 (12%)	65,95,113	1.45	6 (9%)
18	CLA	B	840	6	69,73,73	1.27	8 (11%)	83,113,113	1.28	5 (6%)
18	CLA	B	819	-	59,63,73	1.36	8 (13%)	71,101,113	1.38	6 (8%)
18	CLA	A	836	5	49,53,73	1.51	7 (14%)	59,89,113	1.45	5 (8%)
18	CLA	B	838	6	51,55,73	1.46	8 (15%)	61,91,113	1.41	7 (11%)
18	CLA	A	805	5	56,60,73	1.39	7 (12%)	67,97,113	1.41	4 (5%)
18	CLA	A	814	5	69,73,73	1.27	6 (8%)	83,113,113	1.28	6 (7%)
18	CLA	B	822	6	69,73,73	1.26	8 (11%)	83,113,113	1.38	9 (10%)
18	CLA	B	817	6	63,67,73	1.32	8 (12%)	75,105,113	1.34	6 (8%)
26	SF4	C	102	-	0,12,12	-	-	-		
25	PQN	A	855	-	34,34,34	0.41	0	42,45,45	0.42	0
18	CLA	G	202	11	46,50,73	1.51	8 (17%)	55,85,113	1.45	4 (7%)
18	CLA	K	201	15	42,45,73	1.57	8 (19%)	50,78,113	1.49	5 (10%)
18	CLA	A	842	5	69,73,73	1.26	9 (13%)	83,113,113	1.37	8 (9%)
18	CLA	B	803	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	5 (6%)
17	CHL	4	606	-	45,49,74	2.30	15 (33%)	57,84,114	3.07	20 (35%)
21	LUT	2	616	-	42,43,43	1.66	8 (19%)	51,60,60	2.02	12 (23%)
18	CLA	1	608	1	44,48,73	1.60	9 (20%)	56,83,113	1.58	7 (12%)
18	CLA	L	304	-	49,53,73	1.50	6 (12%)	59,89,113	1.47	5 (8%)
18	CLA	A	837	5	49,53,73	1.50	7 (14%)	59,89,113	1.44	5 (8%)
18	CLA	L	302	-	49,53,73	1.49	8 (16%)	59,89,113	1.48	6 (10%)
20	LHG	1	615	18	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
18	CLA	1	603	-	58,62,73	1.38	8 (13%)	69,99,113	1.39	6 (8%)
21	LUT	4	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.55	11 (21%)
18	CLA	A	845	20	54,58,73	1.42	7 (12%)	65,95,113	1.41	6 (9%)
18	CLA	3	612	-	43,48,73	1.54	8 (18%)	51,83,113	1.54	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	A	808	5	54,58,73	1.42	7 (12%)	65,95,113	1.43	8 (12%)
17	CHL	2	605	-	46,50,74	2.34	17 (36%)	52,85,114	3.09	21 (40%)
18	CLA	2	603	2	47,52,73	1.52	7 (14%)	56,88,113	1.44	4 (7%)
18	CLA	B	825	-	66,70,73	1.27	7 (10%)	79,109,113	1.35	10 (12%)
18	CLA	A	802	-	69,73,73	1.25	8 (11%)	83,113,113	1.34	7 (8%)
18	CLA	3	605	-	45,49,73	1.58	9 (20%)	57,84,113	1.57	6 (10%)
22	BCR	4	618	-	41,41,41	1.73	8 (19%)	56,56,56	1.69	10 (17%)
21	LUT	1	616	-	42,43,43	1.69	7 (16%)	51,60,60	2.00	12 (23%)
18	CLA	A	831	5	69,73,73	1.25	6 (8%)	83,113,113	1.30	6 (7%)
17	CHL	2	615	2	47,51,74	2.33	17 (36%)	52,86,114	3.15	23 (44%)
18	CLA	A	827	-	63,67,73	1.31	7 (11%)	75,105,113	1.36	6 (8%)
18	CLA	A	828	5	69,73,73	1.27	8 (11%)	83,113,113	1.31	6 (7%)
18	CLA	B	835	-	46,50,73	1.52	8 (17%)	55,85,113	1.46	6 (10%)
18	CLA	B	829	6	60,64,73	1.35	9 (15%)	72,102,113	1.35	6 (8%)
22	BCR	B	844	-	41,41,41	1.74	8 (19%)	56,56,56	1.79	12 (21%)
18	CLA	1	607	-	47,52,73	1.52	6 (12%)	56,88,113	1.44	5 (8%)
18	CLA	A	817	-	49,53,73	1.50	7 (14%)	59,89,113	1.44	5 (8%)
18	CLA	A	821	5	49,53,73	1.50	6 (12%)	59,89,113	1.44	5 (8%)
18	CLA	A	816	5	46,50,73	1.51	8 (17%)	55,85,113	1.46	5 (9%)
18	CLA	A	824	-	45,49,73	1.53	7 (15%)	54,84,113	1.51	7 (12%)
18	CLA	B	804	6	45,49,73	1.51	7 (15%)	54,84,113	1.56	5 (9%)
17	CHL	1	606	-	44,49,74	2.50	19 (43%)	48,84,114	3.08	21 (43%)
18	CLA	F	303	10	45,49,73	1.53	7 (15%)	54,84,113	1.52	6 (11%)
18	CLA	F	302	-	55,59,73	1.41	7 (12%)	66,96,113	1.43	6 (9%)
22	BCR	L	305	-	41,41,41	1.76	8 (19%)	56,56,56	1.75	14 (25%)
21	LUT	2	619	-	42,43,43	1.66	8 (19%)	51,60,60	1.88	12 (23%)
22	BCR	B	801	-	41,41,41	1.81	8 (19%)	56,56,56	1.77	13 (23%)
18	CLA	2	611	-	48,52,73	1.51	8 (16%)	58,88,113	1.50	5 (8%)
18	CLA	B	830	-	47,51,73	1.49	8 (17%)	56,86,113	1.46	5 (8%)
18	CLA	1	612	1	50,54,73	1.46	9 (18%)	60,90,113	1.49	5 (8%)
18	CLA	2	604	-	47,51,73	1.50	8 (17%)	55,86,113	1.48	4 (7%)
18	CLA	3	609	-	57,62,73	1.40	9 (15%)	68,100,113	1.34	7 (10%)
18	CLA	F	301	-	61,65,73	1.35	7 (11%)	73,103,113	1.32	6 (8%)
18	CLA	2	613	2	47,51,73	1.50	8 (17%)	56,86,113	1.45	5 (8%)
22	BCR	A	849	-	41,41,41	1.79	8 (19%)	56,56,56	1.95	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
22	BCR	J	102	-	41,41,41	1.75	8 (19%)	56,56,56	1.77	14 (25%)
18	CLA	4	609	-	58,62,73	1.36	8 (13%)	69,99,113	1.38	8 (11%)
18	CLA	A	818	5	64,68,73	1.29	7 (10%)	77,107,113	4.90	7 (9%)
18	CLA	4	611	-	44,49,73	1.56	8 (18%)	52,84,113	1.46	5 (9%)
20	LHG	A	847	18	29,29,48	0.33	0	32,35,54	0.43	0
22	BCR	3	614	-	41,41,41	1.73	8 (19%)	56,56,56	1.57	12 (21%)
18	CLA	B	808	-	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
18	CLA	J	101	-	55,59,73	1.42	6 (10%)	66,96,113	1.39	7 (10%)
18	CLA	A	807	5	69,73,73	1.27	7 (10%)	83,113,113	1.26	7 (8%)
20	LHG	A	846	-	48,48,48	0.27	0	51,54,54	0.33	0
18	CLA	B	815	6	47,51,73	1.48	7 (14%)	56,86,113	1.46	4 (7%)
18	CLA	B	823	6	49,53,73	1.49	8 (16%)	59,89,113	1.44	5 (8%)
18	CLA	B	827	6	69,73,73	1.26	7 (10%)	83,113,113	1.31	5 (6%)
22	BCR	F	304	-	41,41,41	1.84	7 (17%)	56,56,56	2.14	16 (28%)
18	CLA	A	834	5	69,73,73	1.26	7 (10%)	83,113,113	1.30	6 (7%)
18	CLA	2	610	20	41,45,73	2.58	9 (21%)	47,76,113	1.35	6 (12%)
25	PQN	B	842	-	34,34,34	0.42	0	42,45,45	0.40	0
18	CLA	B	828	-	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
22	BCR	K	202	-	41,41,41	1.74	8 (19%)	56,56,56	1.93	14 (25%)
18	CLA	3	608	-	45,49,73	1.50	7 (15%)	54,84,113	1.56	7 (12%)
18	CLA	1	602	1	58,62,73	1.36	7 (12%)	69,99,113	1.37	5 (7%)
18	CLA	2	608	-	49,53,73	1.48	6 (12%)	59,89,113	1.45	4 (6%)
18	CLA	B	826	6	66,70,73	1.29	8 (12%)	79,109,113	1.32	6 (7%)
18	CLA	B	816	6	59,63,73	1.35	7 (11%)	71,101,113	1.38	7 (9%)
18	CLA	L	303	16	69,73,73	1.25	6 (8%)	83,113,113	1.32	7 (8%)
18	CLA	B	824	-	69,73,73	1.25	7 (10%)	83,113,113	1.30	5 (6%)
18	CLA	B	809	6	69,73,73	1.25	7 (10%)	83,113,113	1.30	6 (7%)
18	CLA	A	832	5	54,58,73	1.41	7 (12%)	65,95,113	1.44	7 (10%)
23	LMG	4	619	-	39,39,55	0.22	0	47,47,63	0.24	0
18	CLA	A	833	5	60,64,73	1.34	7 (11%)	72,102,113	1.36	4 (5%)
18	CLA	A	841	5	69,73,73	1.26	7 (10%)	83,113,113	1.29	7 (8%)
18	CLA	4	601	4	50,54,73	1.45	6 (12%)	60,90,113	1.44	4 (6%)
17	CHL	4	605	-	44,49,74	2.35	16 (36%)	49,84,114	3.11	21 (42%)
18	CLA	A	840	5	56,60,73	1.40	7 (12%)	67,97,113	1.40	5 (7%)
18	CLA	3	602	-	59,63,73	1.37	7 (11%)	71,101,113	1.33	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
18	CLA	1	611	-	49,53,73	1.50	7 (14%)	59,89,113	1.44	4 (6%)
20	LHG	B	851	18	37,37,48	0.30	0	40,43,54	0.49	0
22	BCR	K	205	-	41,41,41	1.75	8 (19%)	56,56,56	1.97	16 (28%)
18	CLA	A	838	5	55,59,73	1.41	7 (12%)	66,96,113	1.40	8 (12%)
26	SF4	C	101	-	0,12,12	-	-	-		
18	CLA	K	203	-	49,53,73	1.49	7 (14%)	59,89,113	1.48	6 (10%)
18	CLA	A	839	-	59,63,73	1.35	7 (11%)	71,101,113	1.37	5 (7%)
22	BCR	B	849	-	41,41,41	1.75	8 (19%)	56,56,56	1.80	13 (23%)
22	BCR	I	101	-	41,41,41	1.72	8 (19%)	56,56,56	1.50	10 (17%)
18	CLA	K	204	15	50,54,73	1.48	9 (18%)	60,90,113	1.45	5 (8%)
22	BCR	B	843	-	41,41,41	1.78	8 (19%)	56,56,56	1.92	14 (25%)
18	CLA	A	822	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
18	CLA	4	608	4	49,53,73	1.48	8 (16%)	59,89,113	1.46	4 (6%)
18	CLA	3	603	-	49,53,73	1.49	7 (14%)	59,89,113	1.45	6 (10%)
22	BCR	A	850	-	41,41,41	1.82	8 (19%)	56,56,56	1.90	13 (23%)
18	CLA	4	610	-	46,50,73	1.51	7 (15%)	55,85,113	1.45	4 (7%)
18	CLA	A	803	-	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
18	CLA	B	806	6	69,73,73	1.25	7 (10%)	83,113,113	1.29	6 (7%)
18	CLA	A	811	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
24	CL0	A	801	5	64,67,73	2.08	20 (31%)	75,102,113	4.21	34 (45%)
18	CLA	B	834	6	64,68,73	1.31	7 (10%)	77,107,113	1.34	7 (9%)
18	CLA	3	604	-	44,49,73	1.55	8 (18%)	52,84,113	1.44	5 (9%)
18	CLA	B	805	6	69,73,73	1.27	7 (10%)	83,113,113	1.25	7 (8%)
22	BCR	A	848	-	41,41,41	1.73	8 (19%)	56,56,56	1.61	11 (19%)
22	BCR	B	848	-	41,41,41	1.72	8 (19%)	56,56,56	1.58	11 (19%)
22	BCR	A	852	-	41,41,41	1.74	8 (19%)	56,56,56	1.90	14 (25%)
22	BCR	G	204	-	41,41,41	1.73	8 (19%)	56,56,56	1.64	11 (19%)
18	CLA	4	604	-	47,51,73	1.59	9 (19%)	60,87,113	1.51	6 (10%)

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
18	CLA	A	843	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	825	-	-	9/27/103/115	-
18	CLA	B	833	6	-	4/15/91/115	-
19	XAT	2	617	-	-	16/31/93/93	0/4/4/4
18	CLA	A	810	5	-	5/21/97/115	-
18	CLA	3	601	-	-	13/33/109/115	-
18	CLA	G	203	11	-	3/15/91/115	-
18	CLA	2	602	2	-	17/39/115/115	-
17	CHL	4	615	4	-	0/10/86/117	-
21	LUT	3	613	-	-	6/29/67/67	0/2/2/2
18	CLA	A	835	5	-	18/39/115/115	-
23	LMG	4	620	-	-	7/28/48/70	0/1/1/1
18	CLA	2	612	2	-	17/39/115/115	-
18	CLA	A	806	5	-	20/39/115/115	-
18	CLA	A	812	-	-	19/39/115/115	-
18	CLA	B	839	-	-	10/39/115/115	-
18	CLA	B	836	6	-	7/21/97/115	-
18	CLA	1	613	-	-	0/4/80/115	-
18	CLA	4	613	4	-	4/15/91/115	-
18	CLA	4	603	-	-	6/13/89/115	-
18	CLA	B	841	20	-	22/39/115/115	-
18	CLA	A	826	-	-	9/39/115/115	-
18	CLA	B	813	-	-	15/39/115/115	-
18	CLA	4	602	4	-	6/33/109/115	-
18	CLA	H	201	-	-	17/33/109/115	-
26	SF4	A	854	-	-	-	0/6/5/5
17	CHL	1	601	1	-	10/24/100/117	-
18	CLA	A	820	5	-	14/39/115/115	-
18	CLA	2	609	-	-	9/18/94/115	-
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
18	CLA	A	819	5	-	16/32/108/115	-
18	CLA	A	830	-	-	13/39/115/115	-
18	CLA	B	821	6	-	3/18/94/115	-
18	CLA	K	206	15	-	0/8/80/115	-
22	BCR	B	846	-	-	8/29/63/63	0/2/2/2
17	CHL	2	601	2	-	7/19/95/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CHL	2	607	-	-	7/23/99/117	-
18	CLA	3	607	-	-	4/15/91/115	-
18	CLA	1	604	-	-	9/20/96/115	-
18	CLA	B	811	6	-	11/25/101/115	-
18	CLA	B	831	6	-	0/13/89/115	-
19	XAT	4	617	-	-	3/31/93/93	0/4/4/4
22	BCR	A	853	-	-	3/29/63/63	0/2/2/2
17	CHL	3	606	-	-	5/15/91/117	-
18	CLA	B	818	6	-	7/33/109/115	-
18	CLA	A	809	-	-	14/39/115/115	-
18	CLA	A	829	5	-	17/39/115/115	-
18	CLA	B	807	6	-	7/24/100/115	-
18	CLA	B	837	6	-	13/39/115/115	-
18	CLA	4	612	4	-	13/30/106/115	-
18	CLA	3	611	-	-	2/2/74/115	-
27	DGD	B	850	-	-	11/55/95/95	0/2/2/2
18	CLA	A	844	-	-	12/39/115/115	-
18	CLA	A	815	5	-	6/15/91/115	-
18	CLA	B	810	6	-	12/39/115/115	-
18	CLA	A	813	5	-	11/26/102/115	-
22	BCR	A	851	-	-	7/29/63/63	0/2/2/2
18	CLA	A	823	5	-	4/12/88/115	-
18	CLA	B	814	6	-	15/39/115/115	-
19	XAT	1	614	-	-	8/31/93/93	0/4/4/4
18	CLA	3	610	3	-	3/8/84/115	-
18	CLA	G	201	-	-	9/15/91/115	-
22	BCR	L	301	-	-	3/29/63/63	0/2/2/2
18	CLA	A	804	5	-	19/39/115/115	-
22	BCR	L	306	-	-	5/29/63/63	0/2/2/2
18	CLA	B	832	6	-	15/39/115/115	-
18	CLA	B	802	-	-	15/39/115/115	-
17	CHL	2	606	-	-	2/14/90/117	-
18	CLA	1	605	-	-	8/17/93/115	-
18	CLA	1	609	-	-	4/11/87/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	1	610	20	-	1/4/80/115	-
20	LHG	B	852	-	-	14/53/53/53	-
17	CHL	4	607	-	-	5/17/93/117	-
18	CLA	B	812	6	-	1/13/89/115	-
20	LHG	2	618	18	-	11/41/41/53	-
18	CLA	B	820	6	-	5/21/97/115	-
18	CLA	4	614	4	-	10/21/97/115	-
18	CLA	B	840	6	-	19/39/115/115	-
18	CLA	B	819	-	-	11/27/103/115	-
18	CLA	A	836	5	-	8/15/91/115	-
18	CLA	B	838	6	-	1/18/94/115	-
18	CLA	A	805	5	-	5/24/100/115	-
18	CLA	A	814	5	-	10/39/115/115	-
18	CLA	B	822	6	-	16/39/115/115	-
18	CLA	B	817	6	-	11/32/108/115	-
26	SF4	C	102	-	-	-	0/6/5/5
25	PQN	A	855	-	-	1/23/43/43	0/2/2/2
18	CLA	G	202	11	-	5/12/88/115	-
18	CLA	K	201	15	-	2/4/76/115	-
18	CLA	A	842	5	-	17/39/115/115	-
18	CLA	B	803	-	-	11/39/115/115	-
17	CHL	4	606	-	-	2/10/86/117	-
21	LUT	2	616	-	-	4/29/67/67	0/2/2/2
18	CLA	1	608	1	-	2/8/84/115	-
18	CLA	L	304	-	-	3/15/91/115	-
18	CLA	A	837	5	-	5/15/91/115	-
18	CLA	L	302	-	-	3/15/91/115	-
20	LHG	1	615	18	-	34/53/53/53	-
18	CLA	1	603	-	-	8/26/102/115	-
21	LUT	4	616	-	-	2/29/67/67	0/2/2/2
18	CLA	A	845	20	-	8/21/97/115	-
18	CLA	3	612	-	-	2/8/84/115	-
18	CLA	A	808	5	-	4/21/97/115	-
17	CHL	2	605	-	-	4/12/88/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	2	603	2	-	3/13/89/115	-
18	CLA	B	825	-	-	10/36/112/115	-
18	CLA	A	802	-	-	17/39/115/115	-
18	CLA	3	605	-	-	6/10/86/115	-
22	BCR	4	618	-	-	6/29/63/63	0/2/2/2
21	LUT	1	616	-	-	1/29/67/67	0/2/2/2
18	CLA	A	831	5	-	11/39/115/115	-
17	CHL	2	615	2	-	2/14/90/117	-
18	CLA	A	827	-	-	3/32/108/115	-
18	CLA	A	828	5	-	8/39/115/115	-
18	CLA	B	835	-	-	6/12/88/115	-
18	CLA	B	829	6	-	4/29/105/115	-
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2
18	CLA	1	607	-	-	8/13/89/115	-
18	CLA	A	817	-	-	5/15/91/115	-
18	CLA	A	821	5	-	1/15/91/115	-
18	CLA	A	816	5	-	4/12/88/115	-
18	CLA	A	824	-	-	4/10/86/115	-
18	CLA	B	804	6	-	2/10/86/115	-
17	CHL	1	606	-	-	0/10/86/117	-
18	CLA	F	303	10	-	2/10/86/115	-
18	CLA	F	302	-	-	5/23/99/115	-
22	BCR	L	305	-	-	2/29/63/63	0/2/2/2
21	LUT	2	619	-	-	5/29/67/67	0/2/2/2
22	BCR	B	801	-	-	3/29/63/63	0/2/2/2
18	CLA	2	611	-	-	5/13/89/115	-
18	CLA	B	830	-	-	2/13/89/115	-
18	CLA	1	612	1	-	6/17/93/115	-
18	CLA	2	604	-	-	8/11/88/115	-
18	CLA	3	609	-	-	9/25/101/115	-
18	CLA	F	301	-	-	16/30/106/115	-
18	CLA	2	613	2	-	6/13/89/115	-
22	BCR	A	849	-	-	6/29/63/63	0/2/2/2
22	BCR	J	102	-	-	2/29/63/63	0/2/2/2
18	CLA	4	609	-	-	8/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	818	5	-	13/33/109/115	-
18	CLA	4	611	-	-	6/10/86/115	-
20	LHG	A	847	18	-	2/34/34/53	-
22	BCR	3	614	-	-	3/29/63/63	0/2/2/2
18	CLA	B	808	-	-	18/39/115/115	-
18	CLA	J	101	-	-	9/23/99/115	-
18	CLA	A	807	5	-	13/39/115/115	-
20	LHG	A	846	-	-	5/53/53/53	-
18	CLA	B	815	6	-	2/13/89/115	-
18	CLA	B	823	6	-	8/15/91/115	-
18	CLA	B	827	6	-	22/39/115/115	-
22	BCR	F	304	-	-	12/29/63/63	0/2/2/2
18	CLA	A	834	5	-	9/39/115/115	-
18	CLA	2	610	20	-	5/10/70/115	-
25	PQN	B	842	-	-	6/23/43/43	0/2/2/2
18	CLA	B	828	-	-	19/39/115/115	-
22	BCR	K	202	-	-	2/29/63/63	0/2/2/2
18	CLA	3	608	-	-	3/10/86/115	-
18	CLA	1	602	1	-	6/26/102/115	-
18	CLA	2	608	-	-	7/15/91/115	-
18	CLA	B	826	6	-	6/36/112/115	-
18	CLA	B	816	6	-	6/27/103/115	-
18	CLA	L	303	16	-	11/39/115/115	-
18	CLA	B	824	-	-	14/39/115/115	-
18	CLA	B	809	6	-	18/39/115/115	-
18	CLA	A	832	5	-	6/21/97/115	-
23	LMG	4	619	-	-	5/34/54/70	0/1/1/1
18	CLA	A	833	5	-	7/29/105/115	-
18	CLA	A	841	5	-	14/39/115/115	-
18	CLA	4	601	4	-	7/17/93/115	-
17	CHL	4	605	-	-	2/10/86/117	-
18	CLA	A	840	5	-	8/24/100/115	-
18	CLA	3	602	-	-	11/27/103/115	-
18	CLA	1	611	-	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	B	851	18	-	5/42/42/53	-
22	BCR	K	205	-	-	9/29/63/63	0/2/2/2
18	CLA	A	838	5	-	6/23/99/115	-
26	SF4	C	101	-	-	-	0/6/5/5
18	CLA	K	203	-	-	6/15/91/115	-
18	CLA	A	839	-	-	11/27/103/115	-
22	BCR	B	849	-	-	7/29/63/63	0/2/2/2
22	BCR	I	101	-	-	0/29/63/63	0/2/2/2
18	CLA	K	204	15	-	12/17/93/115	-
22	BCR	B	843	-	-	1/29/63/63	0/2/2/2
18	CLA	A	822	-	-	13/39/115/115	-
18	CLA	4	608	4	-	6/15/91/115	-
18	CLA	3	603	-	-	8/15/91/115	-
22	BCR	A	850	-	-	4/29/63/63	0/2/2/2
18	CLA	4	610	-	-	4/12/88/115	-
18	CLA	A	803	-	-	21/39/115/115	-
18	CLA	B	806	6	-	12/39/115/115	-
18	CLA	A	811	-	-	10/39/115/115	-
24	CL0	A	801	5	-	8/35/95/115	-
18	CLA	B	834	6	-	9/33/109/115	-
18	CLA	3	604	-	-	2/10/86/115	-
18	CLA	B	805	6	-	16/39/115/115	-
22	BCR	A	848	-	-	0/29/63/63	0/2/2/2
22	BCR	B	848	-	-	0/29/63/63	0/2/2/2
22	BCR	A	852	-	-	13/29/63/63	0/2/2/2
22	BCR	G	204	-	-	2/29/63/63	0/2/2/2
18	CLA	4	604	-	-	6/11/87/115	-

All (1520) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	610	CLA	C1A-NA	12.67	1.40	1.29
24	A	801	CL0	C1D-ND	8.48	1.48	1.37
24	A	801	CL0	C3D-C4D	-6.44	1.34	1.46
17	2	606	CHL	O2D-CGD	5.18	1.45	1.33
17	4	606	CHL	O2D-CGD	5.17	1.45	1.33
17	2	605	CHL	O2D-CGD	5.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	607	CHL	O2D-CGD	5.15	1.45	1.33
17	2	615	CHL	O2D-CGD	5.14	1.45	1.33
17	2	607	CHL	O2D-CGD	5.11	1.45	1.33
22	A	853	BCR	C10-C9	5.10	1.42	1.35
17	2	601	CHL	O2D-CGD	5.08	1.45	1.33
17	3	606	CHL	O2D-CGD	5.06	1.45	1.33
22	B	801	BCR	C10-C9	5.05	1.42	1.35
22	F	304	BCR	C21-C22	5.02	1.42	1.35
22	F	304	BCR	C17-C18	5.00	1.42	1.35
22	B	845	BCR	C21-C22	4.99	1.42	1.35
17	1	606	CHL	CHD-C1D	4.92	1.47	1.38
17	1	606	CHL	CHC-C1C	4.92	1.48	1.38
17	1	606	CHL	C2C-C3C	4.91	1.47	1.36
22	A	850	BCR	C14-C13	4.89	1.42	1.35
21	3	613	LUT	C10-C9	4.87	1.42	1.35
22	A	851	BCR	C14-C13	4.84	1.42	1.35
22	A	851	BCR	C21-C22	4.81	1.42	1.35
21	1	616	LUT	C30-C29	4.79	1.42	1.35
22	A	849	BCR	C21-C22	4.73	1.42	1.35
17	1	601	CHL	C2C-C3C	4.73	1.46	1.36
17	2	615	CHL	C2C-C3C	4.73	1.46	1.36
17	2	606	CHL	C2C-C3C	4.72	1.46	1.36
19	2	617	XAT	C34-C33	4.71	1.42	1.35
22	A	850	BCR	C17-C18	4.71	1.42	1.35
17	1	606	CHL	C3D-C4D	-4.70	1.33	1.44
17	2	601	CHL	C2C-C3C	4.70	1.46	1.36
17	2	605	CHL	C2C-C3C	4.70	1.46	1.37
17	2	605	CHL	CHC-C1C	4.70	1.48	1.38
17	2	615	CHL	CHC-C1C	4.70	1.48	1.38
17	1	601	CHL	CHC-C1C	4.69	1.48	1.38
17	4	605	CHL	C3D-C4D	-4.69	1.33	1.44
17	2	607	CHL	CHC-C1C	4.69	1.48	1.38
19	2	617	XAT	C14-C13	4.69	1.42	1.35
22	A	851	BCR	C17-C18	4.68	1.42	1.35
17	2	601	CHL	C3D-C4D	-4.67	1.33	1.44
17	2	607	CHL	C3D-C4D	-4.67	1.33	1.44
17	1	601	CHL	C3D-C4D	-4.66	1.33	1.44
17	4	607	CHL	C3D-C4D	-4.66	1.33	1.44
17	4	605	CHL	C2C-C3C	4.66	1.46	1.37
17	4	615	CHL	O2D-CGD	4.66	1.45	1.30
17	4	606	CHL	C3C-C2C	4.66	1.46	1.36
17	2	601	CHL	CHC-C1C	4.66	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	606	CHL	CHC-C1C	4.66	1.48	1.38
17	1	606	CHL	O2D-CGD	4.65	1.45	1.30
17	4	605	CHL	O2D-CGD	4.65	1.45	1.30
17	2	615	CHL	CHD-C1D	4.65	1.47	1.38
17	3	606	CHL	C3D-C4D	-4.64	1.33	1.44
17	2	606	CHL	CHD-C1D	4.64	1.47	1.38
17	1	601	CHL	CHD-C1D	4.64	1.47	1.38
17	2	606	CHL	C3D-C4D	-4.63	1.33	1.44
17	1	601	CHL	O2D-CGD	4.62	1.45	1.30
17	4	615	CHL	C2C-C3C	4.62	1.46	1.36
17	2	605	CHL	C3D-C4D	-4.62	1.33	1.44
17	4	615	CHL	C3D-C4D	-4.61	1.33	1.44
17	2	607	CHL	C2C-C3C	4.60	1.46	1.36
22	A	849	BCR	C17-C18	4.60	1.41	1.35
17	2	615	CHL	C3D-C4D	-4.59	1.33	1.44
17	4	605	CHL	CHC-C1C	4.57	1.47	1.38
22	B	843	BCR	C14-C13	4.56	1.41	1.35
17	2	601	CHL	CHD-C1D	4.55	1.47	1.38
17	4	606	CHL	C3D-C4D	-4.54	1.33	1.44
17	4	606	CHL	CHC-C1C	4.54	1.47	1.38
21	3	613	LUT	C34-C33	4.53	1.41	1.35
17	3	606	CHL	O2A-CGA	4.53	1.46	1.30
17	4	605	CHL	CHD-C1D	4.52	1.47	1.38
17	4	607	CHL	CHC-C1C	4.52	1.47	1.38
17	4	615	CHL	CHC-C1C	4.50	1.47	1.38
21	2	616	LUT	C34-C33	4.49	1.41	1.35
17	2	607	CHL	CHD-C1D	4.49	1.47	1.38
17	2	605	CHL	CHD-C1D	4.49	1.47	1.38
17	4	607	CHL	C2C-C3C	4.48	1.46	1.36
17	4	607	CHL	O2A-CGA	4.48	1.45	1.30
17	4	615	CHL	CHD-C1D	4.44	1.47	1.38
22	A	851	BCR	C10-C9	4.44	1.41	1.35
17	3	606	CHL	C3C-C2C	4.44	1.46	1.36
17	4	606	CHL	CHD-C1D	4.43	1.47	1.38
17	3	606	CHL	CHD-C1D	4.41	1.47	1.38
17	1	606	CHL	CHD-C4C	4.38	1.49	1.39
22	B	845	BCR	C17-C18	4.36	1.41	1.35
17	3	606	CHL	CHC-C1C	4.36	1.47	1.38
17	4	607	CHL	CHD-C1D	4.33	1.46	1.38
22	B	844	BCR	C21-C22	4.32	1.41	1.35
17	2	607	CHL	O2A-CGA	4.32	1.46	1.33
22	F	304	BCR	C14-C13	4.29	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	843	BCR	C17-C18	4.27	1.41	1.35
22	F	304	BCR	C10-C9	4.26	1.41	1.35
22	K	205	BCR	C21-C22	4.26	1.41	1.35
22	L	301	BCR	C17-C18	4.26	1.41	1.35
17	1	601	CHL	O2A-CGA	4.24	1.45	1.33
22	L	301	BCR	C21-C22	4.24	1.41	1.35
19	4	617	XAT	C34-C33	4.23	1.41	1.35
22	L	306	BCR	C17-C18	4.23	1.41	1.35
22	B	849	BCR	C14-C13	4.22	1.41	1.35
20	1	615	LHG	O8-C23	4.22	1.45	1.33
22	B	843	BCR	C21-C22	4.22	1.41	1.35
22	J	102	BCR	C10-C9	4.22	1.41	1.35
22	A	849	BCR	C14-C13	4.21	1.41	1.35
21	1	616	LUT	C34-C33	4.21	1.41	1.35
24	A	801	CL0	C3D-C2D	4.21	1.45	1.37
22	L	306	BCR	C10-C9	4.21	1.41	1.35
27	B	850	DGD	O1G-C1A	4.20	1.45	1.33
22	L	306	BCR	C21-C22	4.20	1.41	1.35
19	4	617	XAT	C10-C9	4.20	1.41	1.35
22	K	202	BCR	C10-C9	4.20	1.41	1.35
22	B	843	BCR	C10-C9	4.19	1.41	1.35
21	2	616	LUT	C14-C13	4.19	1.41	1.35
19	2	617	XAT	C30-C29	4.19	1.41	1.35
22	L	301	BCR	C14-C13	4.19	1.41	1.35
24	A	801	CL0	O2A-CGA	4.19	1.45	1.33
21	1	616	LUT	C14-C13	4.18	1.41	1.35
19	2	617	XAT	C10-C9	4.18	1.41	1.35
19	4	617	XAT	C30-C29	4.18	1.41	1.35
22	K	205	BCR	C10-C9	4.18	1.41	1.35
22	J	102	BCR	C14-C13	4.18	1.41	1.35
17	2	606	CHL	CHD-C4C	4.18	1.48	1.39
22	B	801	BCR	C14-C13	4.17	1.41	1.35
22	B	846	BCR	C21-C22	4.17	1.41	1.35
22	A	850	BCR	C10-C9	4.16	1.41	1.35
17	2	615	CHL	CHD-C4C	4.16	1.48	1.39
19	4	617	XAT	C14-C13	4.16	1.41	1.35
22	J	102	BCR	C17-C18	4.15	1.41	1.35
22	B	849	BCR	C17-C18	4.15	1.41	1.35
22	B	801	BCR	C17-C18	4.15	1.41	1.35
22	L	306	BCR	C14-C13	4.15	1.41	1.35
22	B	844	BCR	C10-C9	4.15	1.41	1.35
22	J	102	BCR	C21-C22	4.15	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	305	BCR	C14-C13	4.15	1.41	1.35
22	L	305	BCR	C17-C18	4.14	1.41	1.35
22	A	853	BCR	C21-C22	4.13	1.41	1.35
20	1	615	LHG	O7-C7	4.13	1.46	1.34
22	G	204	BCR	C21-C22	4.13	1.41	1.35
17	4	605	CHL	CHD-C4C	4.13	1.48	1.39
17	2	601	CHL	CHD-C4C	4.13	1.48	1.39
22	L	301	BCR	C10-C9	4.12	1.41	1.35
22	A	853	BCR	C14-C13	4.12	1.41	1.35
17	2	605	CHL	CHD-C4C	4.12	1.48	1.39
22	4	618	BCR	C17-C18	4.12	1.41	1.35
22	B	846	BCR	C14-C13	4.12	1.41	1.35
22	L	305	BCR	C21-C22	4.12	1.41	1.35
22	B	846	BCR	C10-C9	4.11	1.41	1.35
22	L	305	BCR	C10-C9	4.11	1.41	1.35
21	1	616	LUT	C10-C9	4.11	1.41	1.35
24	A	801	CL0	C3C-C2C	4.11	1.45	1.36
22	B	801	BCR	C21-C22	4.10	1.41	1.35
22	A	849	BCR	C10-C9	4.10	1.41	1.35
22	B	847	BCR	C14-C13	4.10	1.41	1.35
22	K	202	BCR	C14-C13	4.10	1.41	1.35
22	A	853	BCR	C17-C18	4.10	1.41	1.35
22	A	852	BCR	C21-C22	4.10	1.41	1.35
27	B	850	DGD	O2G-C1B	4.09	1.45	1.34
22	B	849	BCR	C10-C9	4.09	1.41	1.35
17	1	601	CHL	CHD-C4C	4.09	1.48	1.39
22	A	852	BCR	C10-C9	4.09	1.41	1.35
22	A	852	BCR	C14-C13	4.09	1.41	1.35
22	4	618	BCR	C14-C13	4.09	1.41	1.35
22	B	846	BCR	C17-C18	4.09	1.41	1.35
17	2	607	CHL	CHD-C4C	4.08	1.48	1.39
22	K	202	BCR	C17-C18	4.08	1.41	1.35
22	K	205	BCR	C14-C13	4.08	1.41	1.35
22	A	852	BCR	C17-C18	4.08	1.41	1.35
22	K	202	BCR	C21-C22	4.08	1.41	1.35
22	A	848	BCR	C21-C22	4.07	1.41	1.35
22	B	844	BCR	C14-C13	4.07	1.41	1.35
21	2	619	LUT	C30-C29	4.07	1.41	1.35
22	3	614	BCR	C17-C18	4.07	1.41	1.35
21	2	619	LUT	C34-C33	4.06	1.41	1.35
22	4	618	BCR	C21-C22	4.06	1.41	1.35
17	3	606	CHL	CHD-C4C	4.06	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	614	BCR	C10-C9	4.05	1.41	1.35
21	2	619	LUT	C14-C13	4.05	1.41	1.35
22	B	847	BCR	C10-C9	4.05	1.41	1.35
22	B	845	BCR	C10-C9	4.05	1.41	1.35
22	G	204	BCR	C17-C18	4.04	1.41	1.35
21	2	619	LUT	C10-C9	4.04	1.41	1.35
22	B	849	BCR	C21-C22	4.04	1.41	1.35
22	B	844	BCR	C17-C18	4.04	1.41	1.35
22	4	618	BCR	C10-C9	4.04	1.41	1.35
22	K	205	BCR	C17-C18	4.03	1.41	1.35
22	B	847	BCR	C17-C18	4.03	1.41	1.35
22	3	614	BCR	C14-C13	4.03	1.41	1.35
17	4	615	CHL	CHD-C4C	4.02	1.48	1.39
21	4	616	LUT	C34-C33	4.01	1.41	1.35
17	2	601	CHL	O2A-CGA	4.01	1.45	1.33
22	A	848	BCR	C10-C9	4.01	1.41	1.35
18	L	304	CLA	C1D-ND	4.01	1.42	1.37
17	4	606	CHL	CHD-C4C	4.00	1.48	1.39
22	I	101	BCR	C17-C18	4.00	1.41	1.35
22	I	101	BCR	C10-C9	4.00	1.41	1.35
21	4	616	LUT	C30-C29	3.99	1.41	1.35
22	G	204	BCR	C10-C9	3.99	1.41	1.35
22	B	848	BCR	C10-C9	3.98	1.41	1.35
22	A	848	BCR	C17-C18	3.98	1.41	1.35
22	B	848	BCR	C17-C18	3.98	1.41	1.35
22	A	848	BCR	C14-C13	3.97	1.41	1.35
22	B	848	BCR	C14-C13	3.97	1.41	1.35
17	4	607	CHL	CHD-C4C	3.97	1.48	1.39
22	I	101	BCR	C14-C13	3.97	1.41	1.35
21	2	616	LUT	C10-C9	3.97	1.41	1.35
18	A	826	CLA	C1D-ND	3.95	1.42	1.37
22	G	204	BCR	C14-C13	3.95	1.41	1.35
21	4	616	LUT	C14-C13	3.95	1.41	1.35
21	3	613	LUT	C14-C13	3.95	1.41	1.35
18	F	303	CLA	C1D-ND	3.95	1.42	1.37
18	2	611	CLA	C1D-ND	3.94	1.42	1.37
18	3	609	CLA	C1D-ND	3.94	1.42	1.37
21	4	616	LUT	C10-C9	3.94	1.41	1.35
22	B	847	BCR	C21-C22	3.93	1.41	1.35
18	4	614	CLA	C1D-ND	3.93	1.42	1.37
18	A	836	CLA	C1D-ND	3.93	1.42	1.37
18	B	837	CLA	C1D-ND	3.93	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	834	CLA	C1D-ND	3.92	1.42	1.37
18	B	820	CLA	C1D-ND	3.91	1.42	1.37
18	A	816	CLA	C1D-ND	3.91	1.42	1.37
18	G	201	CLA	C1D-ND	3.91	1.42	1.37
18	A	820	CLA	C1D-ND	3.91	1.42	1.37
18	K	206	CLA	C1D-ND	3.91	1.42	1.37
18	1	611	CLA	C1D-ND	3.91	1.42	1.37
22	B	845	BCR	C14-C13	3.91	1.41	1.35
18	4	613	CLA	C1D-ND	3.91	1.42	1.37
18	4	611	CLA	C1D-ND	3.90	1.42	1.37
18	A	840	CLA	C1D-ND	3.90	1.42	1.37
18	A	817	CLA	C1D-ND	3.90	1.42	1.37
22	3	614	BCR	C21-C22	3.90	1.41	1.35
18	1	610	CLA	C1D-ND	3.90	1.42	1.37
18	1	613	CLA	C1D-ND	3.90	1.42	1.37
18	B	840	CLA	C1D-ND	3.90	1.42	1.37
18	K	201	CLA	C1D-ND	3.90	1.42	1.37
18	A	845	CLA	C1D-ND	3.90	1.42	1.37
18	3	611	CLA	C1D-ND	3.90	1.42	1.37
18	H	201	CLA	C1D-ND	3.90	1.42	1.37
18	3	604	CLA	C1D-ND	3.90	1.42	1.37
18	A	825	CLA	C1D-ND	3.90	1.42	1.37
18	A	813	CLA	C1D-ND	3.90	1.42	1.37
18	B	833	CLA	C1D-ND	3.90	1.42	1.37
18	A	804	CLA	C1D-ND	3.90	1.42	1.37
18	A	824	CLA	C1D-ND	3.90	1.42	1.37
18	3	603	CLA	C1D-ND	3.89	1.42	1.37
17	1	606	CHL	CHC-C4B	3.89	1.48	1.39
18	A	835	CLA	C1D-ND	3.89	1.42	1.37
18	1	607	CLA	C1D-ND	3.89	1.42	1.37
18	3	610	CLA	C1D-ND	3.89	1.42	1.37
18	2	602	CLA	C1D-ND	3.89	1.42	1.37
18	B	827	CLA	C1D-ND	3.89	1.42	1.37
18	G	202	CLA	C1D-ND	3.89	1.42	1.37
18	2	604	CLA	C1D-ND	3.88	1.42	1.37
18	3	601	CLA	C1D-ND	3.88	1.42	1.37
22	B	848	BCR	C21-C22	3.88	1.40	1.35
18	F	302	CLA	C1D-ND	3.88	1.42	1.37
18	A	832	CLA	C1D-ND	3.88	1.42	1.37
18	4	612	CLA	C1D-ND	3.88	1.42	1.37
18	2	612	CLA	C1D-ND	3.88	1.42	1.37
18	3	607	CLA	C1D-ND	3.88	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	613	CLA	C1D-ND	3.88	1.42	1.37
18	A	809	CLA	C1D-ND	3.88	1.42	1.37
18	2	603	CLA	C1D-ND	3.88	1.42	1.37
18	B	831	CLA	C1D-ND	3.87	1.42	1.37
18	A	821	CLA	C1D-ND	3.87	1.42	1.37
18	B	841	CLA	C1D-ND	3.87	1.42	1.37
18	A	806	CLA	C1D-ND	3.87	1.42	1.37
18	J	101	CLA	C1D-ND	3.87	1.42	1.37
22	A	850	BCR	C21-C22	3.87	1.40	1.35
18	A	823	CLA	C1D-ND	3.86	1.42	1.37
18	B	818	CLA	C1D-ND	3.86	1.42	1.37
18	1	612	CLA	C1D-ND	3.86	1.42	1.37
18	B	804	CLA	C1D-ND	3.86	1.42	1.37
18	3	602	CLA	C1D-ND	3.86	1.42	1.37
18	B	835	CLA	C1D-ND	3.86	1.42	1.37
18	A	808	CLA	C1D-ND	3.86	1.42	1.37
18	A	833	CLA	C1D-ND	3.86	1.42	1.37
18	B	830	CLA	C1D-ND	3.86	1.42	1.37
18	1	605	CLA	C1D-ND	3.86	1.42	1.37
18	A	837	CLA	C1D-ND	3.86	1.42	1.37
22	I	101	BCR	C21-C22	3.86	1.40	1.35
18	B	824	CLA	C1D-ND	3.86	1.42	1.37
18	B	810	CLA	C1D-ND	3.85	1.42	1.37
18	A	839	CLA	C1D-ND	3.85	1.42	1.37
18	B	812	CLA	C1D-ND	3.85	1.42	1.37
18	1	604	CLA	C1D-ND	3.85	1.42	1.37
18	A	841	CLA	C1D-ND	3.85	1.42	1.37
18	B	819	CLA	C1D-ND	3.85	1.42	1.37
18	G	203	CLA	C1D-ND	3.85	1.42	1.37
18	4	604	CLA	C1D-ND	3.85	1.42	1.37
18	A	838	CLA	C1D-ND	3.84	1.42	1.37
21	3	613	LUT	C30-C29	3.84	1.40	1.35
18	F	301	CLA	C1D-ND	3.84	1.42	1.37
18	A	807	CLA	C1D-ND	3.84	1.42	1.37
18	A	828	CLA	C1D-ND	3.84	1.42	1.37
18	B	822	CLA	C1D-ND	3.84	1.42	1.37
18	K	203	CLA	C1D-ND	3.84	1.42	1.37
18	B	839	CLA	C1D-ND	3.84	1.42	1.37
18	A	834	CLA	C1D-ND	3.83	1.42	1.37
18	3	605	CLA	C1D-ND	3.83	1.42	1.37
18	A	810	CLA	C1D-ND	3.83	1.42	1.37
18	B	815	CLA	C1D-ND	3.83	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	819	CLA	C1D-ND	3.83	1.42	1.37
18	3	612	CLA	C1D-ND	3.82	1.42	1.37
18	B	817	CLA	C1D-ND	3.82	1.42	1.37
18	A	822	CLA	C1D-ND	3.82	1.42	1.37
18	A	811	CLA	C1D-ND	3.82	1.42	1.37
18	2	608	CLA	C1D-ND	3.82	1.42	1.37
18	L	303	CLA	C1D-ND	3.82	1.42	1.37
18	A	818	CLA	C1D-ND	3.82	1.42	1.37
18	A	843	CLA	C1D-ND	3.82	1.42	1.37
18	B	813	CLA	C1D-ND	3.82	1.42	1.37
18	A	812	CLA	C1D-ND	3.81	1.42	1.37
18	A	805	CLA	C1D-ND	3.81	1.42	1.37
18	B	809	CLA	C1D-ND	3.81	1.42	1.37
18	B	821	CLA	C1D-ND	3.81	1.42	1.37
18	B	811	CLA	C1D-ND	3.81	1.42	1.37
18	B	807	CLA	C1D-ND	3.81	1.42	1.37
18	B	805	CLA	C1D-ND	3.81	1.42	1.37
18	B	814	CLA	C1D-ND	3.81	1.42	1.37
18	A	827	CLA	C1D-ND	3.81	1.42	1.37
18	4	603	CLA	C1D-ND	3.80	1.42	1.37
18	A	814	CLA	C1D-ND	3.80	1.42	1.37
18	A	844	CLA	C1D-ND	3.80	1.42	1.37
18	B	829	CLA	C1D-ND	3.80	1.42	1.37
18	2	610	CLA	C1D-ND	3.80	1.42	1.37
18	4	608	CLA	C1D-ND	3.80	1.42	1.37
18	4	610	CLA	C1D-ND	3.80	1.42	1.37
18	A	802	CLA	C1D-ND	3.79	1.42	1.37
21	2	616	LUT	C30-C29	3.79	1.40	1.35
18	A	831	CLA	C1D-ND	3.79	1.42	1.37
18	B	823	CLA	C1D-ND	3.79	1.42	1.37
18	A	815	CLA	C1D-ND	3.79	1.42	1.37
17	2	605	CHL	CHC-C4B	3.78	1.47	1.39
18	B	836	CLA	C1D-ND	3.78	1.42	1.37
18	B	816	CLA	C1D-ND	3.78	1.42	1.37
18	A	829	CLA	C1D-ND	3.78	1.42	1.37
18	B	838	CLA	C1D-ND	3.77	1.42	1.37
18	K	204	CLA	C1D-ND	3.77	1.42	1.37
18	1	602	CLA	C1D-ND	3.77	1.42	1.37
18	B	825	CLA	C1D-ND	3.77	1.42	1.37
18	4	602	CLA	C1D-ND	3.77	1.42	1.37
18	L	302	CLA	C1D-ND	3.77	1.42	1.37
18	1	603	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	826	CLA	C1D-ND	3.76	1.42	1.37
18	B	802	CLA	C1D-ND	3.76	1.42	1.37
18	3	608	CLA	C1D-ND	3.76	1.42	1.37
18	A	842	CLA	C1D-ND	3.76	1.42	1.37
18	2	609	CLA	C1D-ND	3.76	1.42	1.37
18	B	806	CLA	C1D-ND	3.76	1.42	1.37
18	4	601	CLA	C1D-ND	3.75	1.42	1.37
18	4	609	CLA	C1D-ND	3.75	1.42	1.37
18	1	608	CLA	C1D-ND	3.75	1.42	1.37
18	A	830	CLA	C1D-ND	3.75	1.42	1.37
18	B	803	CLA	C1D-ND	3.75	1.42	1.37
18	A	803	CLA	C1D-ND	3.74	1.42	1.37
17	4	605	CHL	OBD-CAD	3.74	1.28	1.22
17	2	606	CHL	OBD-CAD	3.74	1.28	1.22
17	1	601	CHL	CHC-C4B	3.73	1.47	1.39
17	4	606	CHL	OBD-CAD	3.73	1.28	1.22
17	2	615	CHL	OBD-CAD	3.72	1.28	1.22
17	2	601	CHL	OBD-CAD	3.72	1.28	1.22
17	3	606	CHL	OBD-CAD	3.72	1.28	1.22
18	B	832	CLA	C1D-ND	3.71	1.42	1.37
17	4	615	CHL	OBD-CAD	3.70	1.28	1.22
17	2	615	CHL	CHC-C4B	3.70	1.47	1.39
17	1	606	CHL	OBD-CAD	3.69	1.28	1.22
17	1	601	CHL	OBD-CAD	3.69	1.28	1.22
17	2	605	CHL	OBD-CAD	3.69	1.28	1.22
17	2	607	CHL	CHC-C4B	3.69	1.47	1.39
18	B	812	CLA	C4B-NB	3.68	1.42	1.37
17	1	606	CHL	CHB-C1B	3.68	1.47	1.39
17	2	606	CHL	CHC-C4B	3.68	1.47	1.39
17	4	607	CHL	OBD-CAD	3.66	1.28	1.22
17	2	601	CHL	CHC-C4B	3.66	1.47	1.39
18	B	828	CLA	C1D-ND	3.65	1.42	1.37
18	B	808	CLA	C1D-ND	3.64	1.42	1.37
17	2	607	CHL	OBD-CAD	3.64	1.28	1.22
17	4	605	CHL	CHC-C4B	3.61	1.47	1.39
18	B	805	CLA	C4B-NB	3.59	1.42	1.37
17	4	606	CHL	CHC-C4B	3.58	1.47	1.39
17	4	607	CHL	CHC-C4B	3.58	1.47	1.39
18	B	838	CLA	C4B-NB	3.55	1.42	1.37
18	A	821	CLA	C4B-NB	3.54	1.42	1.37
18	1	609	CLA	C1D-ND	3.52	1.42	1.37
17	3	606	CHL	CHC-C4B	3.51	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	615	CHL	CHC-C4B	3.51	1.47	1.39
18	A	814	CLA	C4B-NB	3.49	1.42	1.37
17	2	601	CHL	CHB-C1B	3.49	1.47	1.39
17	1	601	CHL	CHB-C1B	3.49	1.47	1.39
18	3	607	CLA	C4B-NB	3.49	1.42	1.37
18	3	611	CLA	C4B-NB	3.48	1.42	1.37
18	A	836	CLA	C4B-NB	3.48	1.42	1.37
17	2	606	CHL	CHB-C1B	3.48	1.47	1.39
18	B	828	CLA	C4B-NB	3.47	1.42	1.37
18	J	101	CLA	C4B-NB	3.46	1.42	1.37
17	2	605	CHL	CHB-C1B	3.46	1.47	1.39
17	4	605	CHL	CHB-C1B	3.45	1.47	1.39
18	B	802	CLA	C4B-NB	3.44	1.42	1.37
18	A	807	CLA	C4B-NB	3.44	1.42	1.37
18	B	832	CLA	C4B-NB	3.43	1.42	1.37
18	F	301	CLA	C4B-NB	3.43	1.42	1.37
18	A	817	CLA	C4B-NB	3.43	1.42	1.37
18	A	837	CLA	C4B-NB	3.43	1.42	1.37
18	4	611	CLA	C4B-NB	3.42	1.42	1.37
18	B	835	CLA	C4B-NB	3.42	1.42	1.37
18	A	819	CLA	C4B-NB	3.42	1.42	1.37
18	A	845	CLA	C4B-NB	3.42	1.42	1.37
18	1	607	CLA	C4B-NB	3.41	1.42	1.37
17	2	615	CHL	CHB-C1B	3.41	1.47	1.39
17	2	607	CHL	CHB-C1B	3.40	1.47	1.39
17	3	606	CHL	CHB-C1B	3.40	1.47	1.39
18	1	605	CLA	C4B-NB	3.40	1.42	1.37
18	L	302	CLA	C4B-NB	3.40	1.42	1.37
18	B	836	CLA	C4B-NB	3.40	1.42	1.37
18	F	303	CLA	C4B-NB	3.40	1.42	1.37
18	1	604	CLA	C4B-NB	3.39	1.42	1.37
18	3	610	CLA	C4B-NB	3.39	1.42	1.37
18	A	838	CLA	C4B-NB	3.39	1.42	1.37
18	A	814	CLA	C3B-C4B	3.38	1.50	1.42
17	4	606	CHL	CHB-C1B	3.38	1.47	1.39
18	3	605	CLA	C4B-NB	3.38	1.41	1.37
18	B	823	CLA	C4B-NB	3.38	1.41	1.37
18	K	201	CLA	C4B-NB	3.38	1.41	1.37
18	A	812	CLA	C4B-NB	3.37	1.41	1.37
18	4	610	CLA	C4B-NB	3.37	1.41	1.37
18	F	302	CLA	C4B-NB	3.37	1.41	1.37
18	G	201	CLA	C4B-NB	3.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	819	CLA	C4B-NB	3.37	1.41	1.37
18	3	602	CLA	C4B-NB	3.36	1.41	1.37
18	B	810	CLA	C4B-NB	3.36	1.41	1.37
18	3	604	CLA	C4B-NB	3.36	1.41	1.37
18	A	828	CLA	C4B-NB	3.36	1.41	1.37
18	2	613	CLA	C4B-NB	3.36	1.41	1.37
18	K	204	CLA	C4B-NB	3.36	1.41	1.37
18	4	601	CLA	C4B-NB	3.36	1.41	1.37
18	1	611	CLA	C4B-NB	3.36	1.41	1.37
18	A	841	CLA	C4B-NB	3.35	1.41	1.37
18	A	840	CLA	C4B-NB	3.35	1.41	1.37
18	3	609	CLA	C4B-NB	3.34	1.41	1.37
18	4	614	CLA	C4B-NB	3.34	1.41	1.37
18	A	834	CLA	C4B-NB	3.34	1.41	1.37
18	B	840	CLA	C4B-NB	3.34	1.41	1.37
18	A	808	CLA	C4B-NB	3.34	1.41	1.37
18	3	607	CLA	C3B-C4B	3.34	1.50	1.42
18	G	202	CLA	C4B-NB	3.34	1.41	1.37
18	B	834	CLA	C4B-NB	3.34	1.41	1.37
18	B	829	CLA	C4B-NB	3.33	1.41	1.37
18	2	611	CLA	C4B-NB	3.33	1.41	1.37
18	4	603	CLA	C4B-NB	3.33	1.41	1.37
18	B	811	CLA	C4B-NB	3.33	1.41	1.37
18	1	603	CLA	C4B-NB	3.33	1.41	1.37
18	B	826	CLA	C4B-NB	3.33	1.41	1.37
18	A	827	CLA	C4B-NB	3.33	1.41	1.37
18	B	827	CLA	C4B-NB	3.32	1.41	1.37
17	4	615	CHL	CHB-C1B	3.32	1.46	1.39
18	B	812	CLA	C3B-C4B	3.32	1.50	1.42
18	1	610	CLA	C4B-NB	3.32	1.41	1.37
18	K	206	CLA	C4B-NB	3.32	1.41	1.37
18	2	610	CLA	C4B-NB	3.31	1.41	1.37
17	4	607	CHL	CHB-C1B	3.31	1.46	1.39
18	B	815	CLA	C4B-NB	3.31	1.41	1.37
18	A	822	CLA	C4B-NB	3.31	1.41	1.37
18	1	612	CLA	C4B-NB	3.31	1.41	1.37
18	B	839	CLA	C4B-NB	3.31	1.41	1.37
18	A	816	CLA	C4B-NB	3.30	1.41	1.37
18	B	818	CLA	C4B-NB	3.30	1.41	1.37
18	B	817	CLA	C4B-NB	3.30	1.41	1.37
18	4	604	CLA	C4B-NB	3.30	1.41	1.37
18	A	825	CLA	C4B-NB	3.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	603	CLA	C4B-NB	3.30	1.41	1.37
18	A	813	CLA	C4B-NB	3.29	1.41	1.37
18	A	824	CLA	C4B-NB	3.29	1.41	1.37
18	A	820	CLA	C4B-NB	3.29	1.41	1.37
18	1	608	CLA	C4B-NB	3.29	1.41	1.37
18	1	613	CLA	C4B-NB	3.29	1.41	1.37
18	B	813	CLA	C4B-NB	3.28	1.41	1.37
18	L	303	CLA	C4B-NB	3.28	1.41	1.37
18	1	609	CLA	C4B-NB	3.28	1.41	1.37
18	A	810	CLA	C4B-NB	3.28	1.41	1.37
18	A	803	CLA	C4B-NB	3.28	1.41	1.37
18	B	830	CLA	C4B-NB	3.28	1.41	1.37
18	B	807	CLA	C4B-NB	3.27	1.41	1.37
18	A	843	CLA	C4B-NB	3.27	1.41	1.37
18	A	844	CLA	C4B-NB	3.27	1.41	1.37
18	L	304	CLA	C4B-NB	3.27	1.41	1.37
18	G	203	CLA	C4B-NB	3.27	1.41	1.37
18	K	203	CLA	C4B-NB	3.27	1.41	1.37
18	4	602	CLA	C4B-NB	3.26	1.41	1.37
18	A	831	CLA	C4B-NB	3.26	1.41	1.37
18	B	837	CLA	C4B-NB	3.26	1.41	1.37
18	4	608	CLA	C4B-NB	3.26	1.41	1.37
18	A	802	CLA	C4B-NB	3.26	1.41	1.37
18	A	805	CLA	C4B-NB	3.26	1.41	1.37
18	B	803	CLA	C4B-NB	3.25	1.41	1.37
18	1	602	CLA	C4B-NB	3.25	1.41	1.37
18	B	831	CLA	C4B-NB	3.25	1.41	1.37
18	B	825	CLA	C4B-NB	3.25	1.41	1.37
18	B	804	CLA	C4B-NB	3.25	1.41	1.37
18	B	820	CLA	C4B-NB	3.24	1.41	1.37
17	1	606	CHL	C3D-C2D	3.24	1.48	1.39
18	B	841	CLA	C4B-NB	3.24	1.41	1.37
18	2	603	CLA	C4B-NB	3.24	1.41	1.37
18	4	613	CLA	C4B-NB	3.23	1.41	1.37
18	A	826	CLA	C4B-NB	3.23	1.41	1.37
18	B	814	CLA	C4B-NB	3.23	1.41	1.37
18	B	822	CLA	C4B-NB	3.23	1.41	1.37
18	A	842	CLA	C4B-NB	3.23	1.41	1.37
18	H	201	CLA	C4B-NB	3.23	1.41	1.37
18	A	823	CLA	C4B-NB	3.23	1.41	1.37
18	3	601	CLA	C4B-NB	3.22	1.41	1.37
18	A	804	CLA	C4B-NB	3.22	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	833	CLA	C4B-NB	3.22	1.41	1.37
18	2	602	CLA	C4B-NB	3.21	1.41	1.37
18	A	832	CLA	C4B-NB	3.21	1.41	1.37
18	A	806	CLA	C4B-NB	3.21	1.41	1.37
17	1	606	CHL	C1D-C2D	3.21	1.51	1.45
18	B	805	CLA	C3B-C4B	3.21	1.50	1.42
18	A	830	CLA	C4B-NB	3.20	1.41	1.37
18	B	824	CLA	C4B-NB	3.20	1.41	1.37
18	B	832	CLA	C3B-C4B	3.20	1.50	1.42
18	B	806	CLA	C4B-NB	3.20	1.41	1.37
18	B	821	CLA	C4B-NB	3.20	1.41	1.37
18	B	828	CLA	C3B-C4B	3.20	1.50	1.42
18	B	808	CLA	C4B-NB	3.20	1.41	1.37
18	B	816	CLA	C4B-NB	3.19	1.41	1.37
18	B	802	CLA	C3B-C4B	3.19	1.50	1.42
18	A	839	CLA	C4B-NB	3.19	1.41	1.37
18	A	818	CLA	C4B-NB	3.18	1.41	1.37
18	A	821	CLA	C3B-C4B	3.18	1.50	1.42
18	4	612	CLA	C4B-NB	3.18	1.41	1.37
18	B	838	CLA	C3B-C4B	3.18	1.50	1.42
18	A	835	CLA	C4B-NB	3.18	1.41	1.37
18	B	833	CLA	C4B-NB	3.18	1.41	1.37
18	B	809	CLA	C4B-NB	3.17	1.41	1.37
18	2	604	CLA	C4B-NB	3.15	1.41	1.37
18	3	612	CLA	C4B-NB	3.15	1.41	1.37
24	A	801	CL0	CHB-C4A	-3.15	1.30	1.37
18	2	608	CLA	C4B-NB	3.15	1.41	1.37
18	4	609	CLA	C4B-NB	3.15	1.41	1.37
18	A	829	CLA	C4B-NB	3.14	1.41	1.37
18	2	612	CLA	C4B-NB	3.14	1.41	1.37
17	2	606	CHL	C1D-C2D	3.14	1.51	1.45
18	A	809	CLA	C4B-NB	3.13	1.41	1.37
18	A	815	CLA	C4B-NB	3.13	1.41	1.37
18	1	610	CLA	CAB-C3B	-3.11	1.44	1.50
18	A	807	CLA	C3B-C4B	3.11	1.50	1.42
18	3	608	CLA	C4B-NB	3.10	1.41	1.37
18	A	811	CLA	C4B-NB	3.10	1.41	1.37
17	2	606	CHL	C3D-C2D	3.10	1.47	1.39
18	2	610	CLA	CAB-C3B	-3.09	1.44	1.50
18	1	608	CLA	CAB-C3B	-3.09	1.44	1.50
18	K	204	CLA	C4D-ND	-3.09	1.33	1.37
17	1	601	CHL	C1D-C2D	3.08	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	609	CLA	C4B-NB	3.08	1.41	1.37
18	A	828	CLA	C3B-C4B	3.08	1.50	1.42
18	4	604	CLA	CAB-C3B	-3.07	1.44	1.50
18	4	603	CLA	CAB-C3B	-3.07	1.44	1.50
18	4	609	CLA	C3B-C4B	3.07	1.49	1.42
18	1	613	CLA	CAB-C3B	-3.06	1.44	1.50
18	1	609	CLA	C3B-C4B	3.06	1.49	1.42
17	3	606	CHL	C1D-C2D	3.06	1.51	1.45
18	B	810	CLA	C3B-C4B	3.05	1.49	1.42
18	B	811	CLA	CAB-C3B	-3.05	1.44	1.50
18	3	605	CLA	CAB-C3B	-3.05	1.44	1.50
17	2	601	CHL	C3D-C2D	3.04	1.47	1.39
17	2	605	CHL	C3D-C2D	3.04	1.47	1.39
17	4	605	CHL	C1D-C2D	3.04	1.51	1.45
17	2	615	CHL	C1D-C2D	3.04	1.51	1.45
17	2	615	CHL	C3D-C2D	3.04	1.47	1.39
17	4	615	CHL	C1D-C2D	3.03	1.51	1.45
18	F	301	CLA	C3B-C4B	3.03	1.49	1.42
18	4	611	CLA	C3B-C4B	3.03	1.49	1.42
17	2	607	CHL	C3D-C2D	3.03	1.47	1.39
18	A	808	CLA	C3B-C4B	3.02	1.49	1.42
17	2	601	CHL	C1D-C2D	3.02	1.51	1.45
17	4	606	CHL	C3D-C2D	3.02	1.47	1.39
18	3	604	CLA	C3B-C4B	3.01	1.49	1.42
18	A	810	CLA	C3B-C4B	3.01	1.49	1.42
18	A	828	CLA	C4D-ND	-3.00	1.33	1.37
17	1	601	CHL	C3D-C2D	3.00	1.47	1.39
18	B	841	CLA	C4D-ND	-3.00	1.33	1.37
18	G	202	CLA	C3B-C4B	2.99	1.49	1.42
18	A	837	CLA	C3B-C4B	2.99	1.49	1.42
18	J	101	CLA	C3B-C4B	2.99	1.49	1.42
18	1	611	CLA	C3B-C4B	2.98	1.49	1.42
18	B	826	CLA	C4D-ND	-2.98	1.33	1.37
18	A	824	CLA	C3B-C4B	2.98	1.49	1.42
18	A	836	CLA	C3B-C4B	2.98	1.49	1.42
18	3	609	CLA	C3B-C4B	2.97	1.49	1.42
18	F	303	CLA	C3B-C4B	2.97	1.49	1.42
18	A	829	CLA	C4D-ND	-2.97	1.33	1.37
18	B	834	CLA	C3B-C4B	2.97	1.49	1.42
18	B	829	CLA	C4D-ND	-2.97	1.33	1.37
18	B	840	CLA	C3B-C4B	2.97	1.49	1.42
18	1	609	CLA	C4D-ND	-2.97	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	201	CLA	C3B-C4B	2.97	1.49	1.42
18	A	840	CLA	C3B-C4B	2.97	1.49	1.42
22	B	845	BCR	C23-C22	-2.97	1.39	1.45
18	1	605	CLA	C4D-ND	-2.96	1.33	1.37
18	A	839	CLA	C4D-ND	-2.96	1.33	1.37
18	K	206	CLA	C4D-ND	-2.96	1.33	1.37
18	B	836	CLA	C3B-C4B	2.96	1.49	1.42
18	2	609	CLA	C4D-ND	-2.96	1.33	1.37
17	2	607	CHL	C1D-C2D	2.96	1.51	1.45
18	F	301	CLA	C4D-ND	-2.96	1.33	1.37
17	4	606	CHL	C1D-C2D	2.96	1.51	1.45
18	A	810	CLA	C4D-ND	-2.96	1.33	1.37
18	A	819	CLA	C3B-C4B	2.96	1.49	1.42
17	2	605	CHL	C1D-C2D	2.96	1.51	1.45
18	A	802	CLA	C3B-C4B	2.96	1.49	1.42
18	A	803	CLA	C4D-ND	-2.95	1.33	1.37
18	B	817	CLA	C4D-ND	-2.95	1.33	1.37
18	B	821	CLA	C4D-ND	-2.95	1.33	1.37
18	3	610	CLA	C3B-C4B	2.95	1.49	1.42
18	A	823	CLA	C3B-C4B	2.95	1.49	1.42
18	3	611	CLA	C3B-C4B	2.95	1.49	1.42
17	3	606	CHL	C3D-C2D	2.95	1.47	1.39
18	A	813	CLA	C3B-C4B	2.95	1.49	1.42
18	3	608	CLA	C4D-ND	-2.94	1.33	1.37
18	3	602	CLA	C4D-ND	-2.94	1.33	1.37
18	B	816	CLA	C4D-ND	-2.94	1.33	1.37
18	4	602	CLA	C3B-C4B	2.94	1.49	1.42
18	A	835	CLA	C3B-C4B	2.94	1.49	1.42
18	B	808	CLA	C4D-ND	-2.94	1.33	1.37
18	1	607	CLA	C3B-C4B	2.94	1.49	1.42
18	B	840	CLA	C4D-ND	-2.94	1.33	1.37
18	4	610	CLA	C3B-C4B	2.94	1.49	1.42
18	A	826	CLA	C4D-ND	-2.94	1.33	1.37
18	1	604	CLA	C3B-C4B	2.93	1.49	1.42
18	A	820	CLA	C3B-C4B	2.93	1.49	1.42
18	L	302	CLA	C3B-C4B	2.93	1.49	1.42
18	2	604	CLA	C4D-ND	-2.93	1.33	1.37
18	3	602	CLA	C3B-C4B	2.93	1.49	1.42
18	A	817	CLA	C3B-C4B	2.93	1.49	1.42
18	A	815	CLA	C3B-C4B	2.93	1.49	1.42
18	B	810	CLA	C4D-ND	-2.93	1.33	1.37
18	3	608	CLA	C3B-C4B	2.93	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	835	CLA	C3B-C4B	2.93	1.49	1.42
17	4	615	CHL	C3D-C2D	2.93	1.47	1.39
18	3	609	CLA	C4D-ND	-2.93	1.33	1.37
18	B	818	CLA	C3B-C4B	2.93	1.49	1.42
18	A	827	CLA	C3B-C4B	2.93	1.49	1.42
17	4	607	CHL	C3D-C2D	2.93	1.47	1.39
18	2	602	CLA	C4D-ND	-2.93	1.33	1.37
18	4	613	CLA	C4D-ND	-2.93	1.33	1.37
18	2	611	CLA	C3B-C4B	2.93	1.49	1.42
18	K	203	CLA	C4D-ND	-2.93	1.33	1.37
18	A	825	CLA	C3B-C4B	2.93	1.49	1.42
18	B	824	CLA	C4D-ND	-2.93	1.33	1.37
18	A	830	CLA	C4D-ND	-2.93	1.33	1.37
18	A	834	CLA	C4D-ND	-2.92	1.33	1.37
17	4	605	CHL	C3D-C2D	2.92	1.47	1.39
18	A	844	CLA	C3B-C4B	2.92	1.49	1.42
18	A	812	CLA	C4D-ND	-2.92	1.33	1.37
18	L	303	CLA	C3B-C4B	2.92	1.49	1.42
18	2	610	CLA	C4D-ND	-2.92	1.33	1.37
18	4	609	CLA	C4D-ND	-2.92	1.33	1.37
18	B	825	CLA	C3B-C4B	2.92	1.49	1.42
18	B	833	CLA	C4D-ND	-2.92	1.33	1.37
18	B	837	CLA	C4D-ND	-2.92	1.33	1.37
18	4	601	CLA	C3B-C4B	2.92	1.49	1.42
18	A	831	CLA	C4D-ND	-2.92	1.33	1.37
18	A	838	CLA	C3B-C4B	2.92	1.49	1.42
17	4	607	CHL	C1D-C2D	2.92	1.51	1.45
18	3	601	CLA	C4D-ND	-2.92	1.33	1.37
18	A	804	CLA	C4D-ND	-2.92	1.33	1.37
18	4	603	CLA	C4D-ND	-2.92	1.33	1.37
18	A	816	CLA	C3B-C4B	2.92	1.49	1.42
18	2	608	CLA	C4D-ND	-2.92	1.33	1.37
18	A	835	CLA	C4D-ND	-2.91	1.33	1.37
18	2	609	CLA	C3B-C4B	2.91	1.49	1.42
18	B	836	CLA	C4D-ND	-2.91	1.33	1.37
18	B	826	CLA	C3B-C4B	2.91	1.49	1.42
18	3	604	CLA	C4D-ND	-2.91	1.33	1.37
18	K	201	CLA	C4D-ND	-2.91	1.33	1.37
18	A	820	CLA	C4D-ND	-2.91	1.33	1.37
18	A	838	CLA	C4D-ND	-2.91	1.33	1.37
18	A	805	CLA	C3B-C4B	2.91	1.49	1.42
18	1	603	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	816	CLA	C4D-ND	-2.91	1.33	1.37
18	A	817	CLA	C4D-ND	-2.91	1.33	1.37
18	4	613	CLA	C3B-C4B	2.91	1.49	1.42
18	B	829	CLA	C3B-C4B	2.91	1.49	1.42
18	A	825	CLA	C4D-ND	-2.91	1.33	1.37
18	3	603	CLA	C3B-C4B	2.91	1.49	1.42
18	A	841	CLA	C3B-C4B	2.90	1.49	1.42
18	H	201	CLA	C3B-C4B	2.90	1.49	1.42
18	A	818	CLA	C4D-ND	-2.90	1.33	1.37
18	A	822	CLA	C3B-C4B	2.90	1.49	1.42
18	A	811	CLA	C3B-C4B	2.90	1.49	1.42
18	G	203	CLA	C3B-C4B	2.90	1.49	1.42
18	A	819	CLA	C4D-ND	-2.90	1.33	1.37
17	1	606	CHL	MG-NA	-2.90	1.99	2.06
18	1	603	CLA	C3B-C4B	2.90	1.49	1.42
18	4	612	CLA	C4D-ND	-2.90	1.33	1.37
18	A	831	CLA	C3B-C4B	2.90	1.49	1.42
18	B	832	CLA	C4D-ND	-2.90	1.33	1.37
18	2	602	CLA	C3B-C4B	2.90	1.49	1.42
18	A	812	CLA	C3B-C4B	2.90	1.49	1.42
22	A	850	BCR	C23-C22	-2.90	1.39	1.45
18	3	603	CLA	C4D-ND	-2.90	1.33	1.37
18	B	823	CLA	C4D-ND	-2.90	1.33	1.37
18	L	302	CLA	C4D-ND	-2.90	1.33	1.37
18	B	839	CLA	C3B-C4B	2.90	1.49	1.42
22	B	801	BCR	C8-C9	-2.90	1.39	1.45
18	A	842	CLA	C4D-ND	-2.90	1.33	1.37
18	A	811	CLA	C4D-ND	-2.89	1.33	1.37
18	B	811	CLA	C4D-ND	-2.89	1.33	1.37
18	B	828	CLA	C4D-ND	-2.89	1.33	1.37
24	A	801	CL0	CHC-C1C	2.89	1.44	1.38
18	A	803	CLA	C3B-C4B	2.89	1.49	1.42
18	A	839	CLA	C3B-C4B	2.89	1.49	1.42
18	K	206	CLA	C3B-C4B	2.89	1.49	1.42
18	A	843	CLA	C4D-ND	-2.89	1.33	1.37
18	2	603	CLA	C4D-ND	-2.89	1.33	1.37
18	4	602	CLA	C4D-ND	-2.89	1.33	1.37
18	A	841	CLA	C4D-ND	-2.89	1.33	1.37
18	B	837	CLA	C3B-C4B	2.89	1.49	1.42
18	4	610	CLA	C4D-ND	-2.89	1.33	1.37
18	B	830	CLA	C4D-ND	-2.89	1.33	1.37
18	4	608	CLA	C3B-C4B	2.89	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	822	CLA	C3B-C4B	2.89	1.49	1.42
18	B	833	CLA	C3B-C4B	2.89	1.49	1.42
18	B	813	CLA	C3B-C4B	2.89	1.49	1.42
18	3	601	CLA	C3B-C4B	2.88	1.49	1.42
18	2	613	CLA	C4D-ND	-2.88	1.33	1.37
18	B	804	CLA	C3B-C4B	2.88	1.49	1.42
18	B	807	CLA	C3B-C4B	2.88	1.49	1.42
18	4	614	CLA	C3B-C4B	2.88	1.49	1.42
18	B	827	CLA	C3B-C4B	2.88	1.49	1.42
18	B	814	CLA	C3B-C4B	2.88	1.49	1.42
18	4	612	CLA	C3B-C4B	2.88	1.49	1.42
22	I	101	BCR	C23-C22	-2.88	1.39	1.45
18	A	806	CLA	C3B-C4B	2.88	1.49	1.42
18	K	203	CLA	C3B-C4B	2.88	1.49	1.42
18	B	819	CLA	C4D-ND	-2.88	1.33	1.37
18	A	833	CLA	C4D-ND	-2.88	1.33	1.37
18	B	814	CLA	C4D-ND	-2.88	1.33	1.37
18	L	304	CLA	C4D-ND	-2.88	1.33	1.37
18	B	803	CLA	C3B-C4B	2.88	1.49	1.42
18	1	605	CLA	C3B-C4B	2.88	1.49	1.42
18	B	809	CLA	C3B-C4B	2.88	1.49	1.42
18	B	821	CLA	C3B-C4B	2.87	1.49	1.42
18	B	816	CLA	C3B-C4B	2.87	1.49	1.42
18	B	831	CLA	C3B-C4B	2.87	1.49	1.42
18	2	612	CLA	C4D-ND	-2.87	1.33	1.37
18	A	844	CLA	C4D-ND	-2.87	1.33	1.37
18	4	604	CLA	C4D-ND	-2.87	1.33	1.37
18	K	201	CLA	C3B-C4B	2.87	1.49	1.42
18	1	602	CLA	C3B-C4B	2.87	1.49	1.42
18	2	611	CLA	C4D-ND	-2.87	1.33	1.37
18	2	608	CLA	C3B-C4B	2.87	1.49	1.42
18	B	804	CLA	C4D-ND	-2.87	1.33	1.37
18	A	833	CLA	C3B-C4B	2.87	1.49	1.42
18	B	824	CLA	C3B-C4B	2.87	1.49	1.42
18	B	815	CLA	C3B-C4B	2.87	1.49	1.42
18	B	805	CLA	C4D-ND	-2.87	1.33	1.37
18	3	607	CLA	C4D-ND	-2.86	1.33	1.37
18	A	821	CLA	C4D-ND	-2.86	1.33	1.37
18	B	841	CLA	C3B-C4B	2.86	1.49	1.42
18	A	830	CLA	C3B-C4B	2.86	1.49	1.42
18	A	815	CLA	C4D-ND	-2.86	1.33	1.37
18	B	806	CLA	C4D-ND	-2.86	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	612	CLA	C3B-C4B	2.86	1.49	1.42
18	K	204	CLA	C3B-C4B	2.86	1.49	1.42
18	B	817	CLA	C3B-C4B	2.86	1.49	1.42
18	A	822	CLA	C4D-ND	-2.86	1.33	1.37
18	3	610	CLA	C4D-ND	-2.86	1.33	1.37
18	1	610	CLA	C4D-ND	-2.86	1.33	1.37
18	A	806	CLA	C4D-ND	-2.86	1.33	1.37
18	B	802	CLA	C4D-ND	-2.86	1.33	1.37
18	B	838	CLA	C4D-ND	-2.86	1.33	1.37
24	A	801	CL0	OBD-CAD	2.86	1.28	1.22
22	B	849	BCR	C23-C22	-2.86	1.39	1.45
18	A	807	CLA	C4D-ND	-2.86	1.33	1.37
18	A	840	CLA	C4D-ND	-2.86	1.33	1.37
18	B	822	CLA	C4D-ND	-2.86	1.33	1.37
18	A	805	CLA	C4D-ND	-2.85	1.33	1.37
18	H	201	CLA	C4D-ND	-2.85	1.33	1.37
18	B	815	CLA	C4D-ND	-2.85	1.33	1.37
22	B	847	BCR	C23-C22	-2.85	1.39	1.45
18	F	302	CLA	C3B-C4B	2.85	1.49	1.42
18	B	807	CLA	C4D-ND	-2.85	1.33	1.37
18	A	809	CLA	C3B-C4B	2.85	1.49	1.42
18	B	830	CLA	C3B-C4B	2.85	1.49	1.42
22	B	848	BCR	C23-C22	-2.85	1.39	1.45
18	B	827	CLA	C4D-ND	-2.85	1.33	1.37
18	B	823	CLA	C3B-C4B	2.84	1.49	1.42
18	A	814	CLA	C4D-ND	-2.84	1.33	1.37
18	A	832	CLA	C3B-C4B	2.84	1.49	1.42
18	4	611	CLA	C4D-ND	-2.84	1.33	1.37
18	B	809	CLA	C4D-ND	-2.84	1.33	1.37
18	3	611	CLA	C4D-ND	-2.84	1.33	1.37
18	A	827	CLA	C4D-ND	-2.84	1.33	1.37
18	A	832	CLA	C4D-ND	-2.84	1.33	1.37
18	A	834	CLA	C3B-C4B	2.84	1.49	1.42
18	B	834	CLA	C4D-ND	-2.84	1.33	1.37
18	B	839	CLA	C4D-ND	-2.84	1.33	1.37
18	B	803	CLA	C4D-ND	-2.84	1.33	1.37
18	A	826	CLA	C3B-C4B	2.84	1.49	1.42
18	B	820	CLA	C3B-C4B	2.84	1.49	1.42
18	4	601	CLA	C4D-ND	-2.84	1.33	1.37
18	L	304	CLA	C3B-C4B	2.83	1.49	1.42
17	2	615	CHL	C3B-C4B	2.83	1.49	1.42
18	4	614	CLA	C4D-ND	-2.83	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	303	CLA	C4D-ND	-2.83	1.33	1.37
18	B	808	CLA	C3B-C4B	2.83	1.49	1.42
18	G	203	CLA	C4D-ND	-2.83	1.33	1.37
18	A	845	CLA	C4D-ND	-2.83	1.33	1.37
18	B	831	CLA	C4D-ND	-2.83	1.33	1.37
18	A	842	CLA	C3B-C4B	2.83	1.49	1.42
18	B	820	CLA	C4D-ND	-2.83	1.33	1.37
18	1	608	CLA	C4D-ND	-2.83	1.33	1.37
18	G	202	CLA	C4D-ND	-2.83	1.33	1.37
18	1	613	CLA	C4D-ND	-2.82	1.33	1.37
18	B	818	CLA	C4D-ND	-2.82	1.33	1.37
17	1	601	CHL	C3B-C4B	2.82	1.49	1.42
18	A	824	CLA	C4D-ND	-2.82	1.33	1.37
18	2	613	CLA	C3B-C4B	2.82	1.49	1.42
18	A	843	CLA	C3B-C4B	2.82	1.49	1.42
18	1	604	CLA	C4D-ND	-2.82	1.33	1.37
18	A	845	CLA	C3B-C4B	2.82	1.49	1.42
18	1	602	CLA	C4D-ND	-2.81	1.33	1.37
22	3	614	BCR	C23-C22	-2.81	1.39	1.45
18	A	823	CLA	C4D-ND	-2.81	1.33	1.37
18	2	604	CLA	C3B-C4B	2.81	1.49	1.42
18	A	808	CLA	C4D-ND	-2.81	1.33	1.37
18	A	836	CLA	C4D-ND	-2.81	1.33	1.37
18	B	812	CLA	C4D-ND	-2.81	1.33	1.37
18	2	603	CLA	C3B-C4B	2.81	1.49	1.42
18	B	825	CLA	C4D-ND	-2.81	1.33	1.37
18	4	608	CLA	C4D-ND	-2.81	1.33	1.37
18	A	837	CLA	C4D-ND	-2.80	1.33	1.37
18	B	835	CLA	C4D-ND	-2.80	1.33	1.37
18	A	804	CLA	C3B-C4B	2.80	1.49	1.42
18	A	813	CLA	C4D-ND	-2.80	1.33	1.37
18	J	101	CLA	C4D-ND	-2.80	1.33	1.37
18	1	611	CLA	C4D-ND	-2.80	1.33	1.37
18	A	809	CLA	C4D-ND	-2.80	1.33	1.37
22	A	852	BCR	C8-C9	-2.80	1.39	1.45
18	A	818	CLA	C3B-C4B	2.79	1.49	1.42
18	F	302	CLA	C4D-ND	-2.79	1.33	1.37
18	3	605	CLA	C4D-ND	-2.79	1.33	1.37
18	3	612	CLA	C4D-ND	-2.79	1.33	1.37
18	1	612	CLA	C3B-C4B	2.79	1.49	1.42
22	B	846	BCR	C8-C9	-2.79	1.40	1.45
18	1	607	CLA	C4D-ND	-2.79	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	806	CLA	C3B-C4B	2.78	1.49	1.42
22	I	101	BCR	C8-C9	-2.78	1.40	1.45
22	A	852	BCR	C23-C22	-2.78	1.40	1.45
22	B	849	BCR	C8-C9	-2.78	1.40	1.45
22	G	204	BCR	C8-C9	-2.78	1.40	1.45
22	4	618	BCR	C8-C9	-2.78	1.40	1.45
22	B	845	BCR	C8-C9	-2.78	1.40	1.45
21	4	616	LUT	C8-C9	-2.77	1.40	1.45
18	B	813	CLA	C4D-ND	-2.77	1.33	1.37
18	3	612	CLA	C3B-C4B	2.77	1.49	1.42
18	F	303	CLA	C4D-ND	-2.77	1.33	1.37
22	A	849	BCR	C23-C22	-2.76	1.40	1.45
21	3	613	LUT	C8-C9	-2.76	1.40	1.45
18	2	613	CLA	C1B-C2B	2.76	1.49	1.43
18	B	819	CLA	C3B-C4B	2.76	1.49	1.42
18	G	201	CLA	C4D-ND	-2.76	1.33	1.37
22	A	848	BCR	C23-C22	-2.76	1.40	1.45
18	4	603	CLA	C1B-C2B	2.75	1.49	1.43
22	3	614	BCR	C8-C9	-2.75	1.40	1.45
22	G	204	BCR	C23-C22	-2.75	1.40	1.45
22	L	305	BCR	C8-C9	-2.74	1.40	1.45
18	1	612	CLA	C4D-ND	-2.73	1.33	1.37
18	B	818	CLA	C1B-C2B	2.73	1.49	1.43
17	1	606	CHL	C3B-C4B	2.73	1.49	1.42
18	1	612	CLA	C1B-C2B	2.73	1.49	1.43
18	A	829	CLA	C1B-C2B	2.73	1.49	1.43
18	B	814	CLA	C1B-C2B	2.73	1.49	1.43
22	B	847	BCR	C8-C9	-2.73	1.40	1.45
18	B	806	CLA	C1B-C2B	2.73	1.49	1.43
17	4	605	CHL	C3B-C4B	2.73	1.49	1.42
17	2	605	CHL	C3B-C4B	2.72	1.49	1.42
18	H	201	CLA	C1B-C2B	2.72	1.49	1.43
22	L	305	BCR	C23-C22	-2.72	1.40	1.45
18	A	802	CLA	C4D-ND	-2.72	1.33	1.37
18	1	608	CLA	C4B-C3B	2.72	1.49	1.43
18	A	843	CLA	C1B-C2B	2.72	1.49	1.43
18	A	829	CLA	C3B-C4B	2.72	1.49	1.42
22	A	853	BCR	C23-C22	-2.71	1.40	1.45
18	2	608	CLA	C1B-C2B	2.71	1.49	1.43
18	1	610	CLA	C1B-C2B	2.71	1.49	1.43
18	B	820	CLA	C1B-C2B	2.71	1.49	1.43
22	B	848	BCR	C8-C9	-2.71	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	613	CLA	C4B-C3B	2.71	1.49	1.43
18	A	804	CLA	C1B-C2B	2.71	1.49	1.43
18	A	824	CLA	C1B-C2B	2.71	1.49	1.43
18	3	601	CLA	C1B-C2B	2.71	1.49	1.43
18	4	614	CLA	C1B-C2B	2.71	1.49	1.43
17	1	606	CHL	C3A-C2A	-2.71	1.52	1.54
18	2	610	CLA	C1B-C2B	2.71	1.49	1.43
22	4	618	BCR	C23-C22	-2.71	1.40	1.45
18	A	826	CLA	C1B-C2B	2.71	1.49	1.43
22	L	301	BCR	C8-C9	-2.71	1.40	1.45
18	4	602	CLA	C1B-C2B	2.70	1.49	1.43
22	B	844	BCR	C23-C22	-2.70	1.40	1.45
22	K	205	BCR	C8-C9	-2.70	1.40	1.45
18	A	806	CLA	C1B-C2B	2.70	1.49	1.43
18	A	809	CLA	C1B-C2B	2.70	1.49	1.43
18	A	845	CLA	C1B-C2B	2.70	1.49	1.43
18	B	807	CLA	C1B-C2B	2.70	1.49	1.43
18	3	605	CLA	C1B-C2B	2.70	1.49	1.43
22	A	853	BCR	C8-C9	-2.70	1.40	1.45
18	3	610	CLA	C1B-C2B	2.70	1.49	1.43
18	1	605	CLA	C1B-C2B	2.70	1.49	1.43
21	2	619	LUT	C8-C9	-2.69	1.40	1.45
18	A	817	CLA	C1B-C2B	2.69	1.49	1.43
22	A	848	BCR	C8-C9	-2.69	1.40	1.45
18	1	603	CLA	C1B-C2B	2.69	1.49	1.43
18	B	841	CLA	C1B-C2B	2.69	1.49	1.43
18	A	827	CLA	C1B-C2B	2.69	1.49	1.43
18	B	826	CLA	C1B-C2B	2.69	1.49	1.43
18	1	602	CLA	C1B-C2B	2.69	1.49	1.43
18	2	611	CLA	C1B-C2B	2.69	1.49	1.43
18	A	818	CLA	C1B-C2B	2.69	1.49	1.43
18	3	602	CLA	C1B-C2B	2.69	1.49	1.43
18	A	830	CLA	C1B-C2B	2.68	1.49	1.43
22	J	102	BCR	C23-C22	-2.68	1.40	1.45
18	B	831	CLA	C1B-C2B	2.68	1.49	1.43
18	A	833	CLA	C1B-C2B	2.68	1.49	1.43
24	A	801	CL0	CHD-C1D	2.68	1.43	1.38
18	B	837	CLA	C1B-C2B	2.68	1.49	1.43
18	K	204	CLA	C1B-C2B	2.68	1.49	1.43
22	L	306	BCR	C23-C22	-2.68	1.40	1.45
18	A	823	CLA	C1B-C2B	2.68	1.49	1.43
18	B	823	CLA	C1B-C2B	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	205	BCR	C23-C22	-2.68	1.40	1.45
18	1	607	CLA	C1B-C2B	2.68	1.49	1.43
18	G	201	CLA	C1B-C2B	2.68	1.49	1.43
22	B	801	BCR	C23-C22	-2.67	1.40	1.45
18	B	833	CLA	C1B-C2B	2.67	1.49	1.43
18	B	819	CLA	C1B-C2B	2.67	1.49	1.43
18	J	101	CLA	C1B-C2B	2.67	1.49	1.43
18	L	304	CLA	C1B-C2B	2.67	1.49	1.43
21	1	616	LUT	C8-C9	-2.67	1.40	1.45
18	G	203	CLA	C1B-C2B	2.67	1.49	1.43
17	2	601	CHL	C3B-C4B	2.67	1.49	1.42
18	K	206	CLA	C1B-C2B	2.67	1.49	1.43
18	K	203	CLA	C1B-C2B	2.67	1.49	1.43
18	A	831	CLA	C1B-C2B	2.67	1.49	1.43
22	A	850	BCR	C8-C9	-2.67	1.40	1.45
22	J	102	BCR	C8-C9	-2.67	1.40	1.45
18	A	832	CLA	C1B-C2B	2.67	1.49	1.43
18	3	611	CLA	C1B-C2B	2.67	1.49	1.43
18	A	834	CLA	C1B-C2B	2.67	1.49	1.43
18	A	825	CLA	C1B-C2B	2.67	1.49	1.43
18	4	612	CLA	C1B-C2B	2.67	1.49	1.43
18	A	816	CLA	C1B-C2B	2.67	1.49	1.43
18	3	605	CLA	C4B-C3B	2.67	1.49	1.43
18	B	811	CLA	C4B-C3B	2.67	1.49	1.43
18	B	804	CLA	C1B-C2B	2.67	1.49	1.43
18	3	609	CLA	C1B-C2B	2.67	1.49	1.43
18	B	815	CLA	C1B-C2B	2.67	1.49	1.43
18	2	603	CLA	C1B-C2B	2.67	1.49	1.43
18	1	611	CLA	C1B-C2B	2.66	1.49	1.43
18	A	811	CLA	C1B-C2B	2.66	1.49	1.43
22	F	304	BCR	C8-C9	-2.66	1.40	1.45
18	B	811	CLA	C1B-C2B	2.66	1.49	1.43
18	B	827	CLA	C1B-C2B	2.66	1.49	1.43
22	B	844	BCR	C8-C9	-2.66	1.40	1.45
18	1	604	CLA	C1B-C2B	2.66	1.49	1.43
22	K	202	BCR	C23-C22	-2.66	1.40	1.45
18	3	612	CLA	C1B-C2B	2.66	1.49	1.43
24	A	801	CL0	C3B-C4B	2.66	1.49	1.42
18	3	608	CLA	C1B-C2B	2.66	1.49	1.43
18	A	840	CLA	C1B-C2B	2.66	1.49	1.43
18	B	821	CLA	C1B-C2B	2.66	1.49	1.43
22	B	846	BCR	C23-C22	-2.65	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	840	CLA	C1B-C2B	2.65	1.49	1.43
18	1	610	CLA	C4B-C3B	2.65	1.49	1.43
18	1	613	CLA	C1B-C2B	2.65	1.49	1.43
18	B	816	CLA	C1B-C2B	2.65	1.49	1.43
18	G	202	CLA	C1B-C2B	2.65	1.49	1.43
18	B	830	CLA	C1B-C2B	2.65	1.49	1.43
18	B	809	CLA	C1B-C2B	2.65	1.49	1.43
18	A	841	CLA	C1B-C2B	2.65	1.49	1.43
18	A	836	CLA	C1B-C2B	2.65	1.49	1.43
18	B	835	CLA	C1B-C2B	2.65	1.49	1.43
18	L	303	CLA	C1B-C2B	2.65	1.49	1.43
18	4	613	CLA	C1B-C2B	2.65	1.49	1.43
18	A	839	CLA	C1B-C2B	2.65	1.49	1.43
18	4	608	CLA	C1B-C2B	2.64	1.49	1.43
18	1	608	CLA	C1B-C2B	2.64	1.49	1.43
18	A	837	CLA	C1B-C2B	2.64	1.49	1.43
22	A	849	BCR	C8-C9	-2.64	1.40	1.45
18	A	819	CLA	C1B-C2B	2.64	1.49	1.43
18	A	813	CLA	C1B-C2B	2.64	1.49	1.43
18	A	805	CLA	C1B-C2B	2.64	1.49	1.43
18	K	201	CLA	C1B-C2B	2.64	1.49	1.43
18	B	829	CLA	C1B-C2B	2.64	1.49	1.43
18	A	820	CLA	C1B-C2B	2.64	1.49	1.43
18	F	301	CLA	C1B-C2B	2.64	1.49	1.43
18	F	303	CLA	C1B-C2B	2.64	1.49	1.43
18	1	609	CLA	C1B-C2B	2.63	1.49	1.43
17	2	606	CHL	C3B-C4B	2.63	1.48	1.42
22	K	202	BCR	C8-C9	-2.63	1.40	1.45
18	B	824	CLA	C1B-C2B	2.63	1.49	1.43
18	4	610	CLA	C1B-C2B	2.63	1.49	1.43
18	3	604	CLA	C1B-C2B	2.63	1.49	1.43
18	4	604	CLA	C1B-C2B	2.63	1.49	1.43
18	A	838	CLA	C1B-C2B	2.63	1.49	1.43
18	A	812	CLA	C1B-C2B	2.63	1.49	1.43
18	A	835	CLA	C1B-C2B	2.63	1.49	1.43
18	B	834	CLA	C1B-C2B	2.62	1.49	1.43
18	B	838	CLA	C1B-C2B	2.62	1.49	1.43
18	B	813	CLA	C1B-C2B	2.62	1.49	1.43
18	B	810	CLA	C1B-C2B	2.62	1.49	1.43
18	2	604	CLA	C1B-C2B	2.62	1.49	1.43
18	3	603	CLA	C1B-C2B	2.62	1.49	1.43
18	A	828	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	805	CLA	C1B-C2B	2.62	1.49	1.43
18	B	817	CLA	C1B-C2B	2.62	1.49	1.43
18	4	611	CLA	C1B-C2B	2.62	1.49	1.43
18	2	609	CLA	C1B-C2B	2.62	1.49	1.43
18	F	302	CLA	C1B-C2B	2.62	1.49	1.43
18	4	601	CLA	C1B-C2B	2.62	1.49	1.43
18	A	808	CLA	C1B-C2B	2.62	1.49	1.43
18	B	825	CLA	C1B-C2B	2.61	1.49	1.43
22	L	301	BCR	C23-C22	-2.61	1.40	1.45
18	4	603	CLA	C4B-C3B	2.61	1.49	1.43
18	A	815	CLA	C1B-C2B	2.61	1.49	1.43
22	L	306	BCR	C8-C9	-2.61	1.40	1.45
18	B	808	CLA	C1B-C2B	2.61	1.49	1.43
18	B	839	CLA	C1B-C2B	2.61	1.49	1.43
18	B	802	CLA	C1B-C2B	2.61	1.49	1.43
18	4	604	CLA	C4B-C3B	2.61	1.49	1.43
18	A	822	CLA	C1B-C2B	2.61	1.49	1.43
18	2	612	CLA	C1B-C2B	2.60	1.49	1.43
18	A	807	CLA	C1B-C2B	2.59	1.49	1.43
22	B	843	BCR	C8-C9	-2.59	1.40	1.45
18	B	836	CLA	C1B-C2B	2.59	1.49	1.43
18	A	821	CLA	C1B-C2B	2.58	1.49	1.43
18	2	602	CLA	C1B-C2B	2.58	1.49	1.43
18	2	610	CLA	C4B-C3B	2.58	1.49	1.43
17	1	606	CHL	C1B-C2B	2.57	1.49	1.43
18	B	803	CLA	C1B-C2B	2.57	1.49	1.43
18	L	302	CLA	C1B-C2B	2.57	1.49	1.43
18	A	803	CLA	C1B-C2B	2.56	1.49	1.43
17	2	606	CHL	C1B-C2B	2.56	1.49	1.43
22	B	843	BCR	C23-C22	-2.56	1.40	1.45
18	B	812	CLA	C1B-C2B	2.56	1.49	1.43
17	2	601	CHL	C1B-C2B	2.56	1.49	1.43
17	4	606	CHL	C1B-C2B	2.56	1.49	1.43
17	3	606	CHL	C3B-C4B	2.55	1.48	1.42
17	2	615	CHL	MG-NA	-2.54	2.00	2.06
18	A	810	CLA	C1B-C2B	2.54	1.49	1.43
24	A	801	CL0	CHD-C4C	2.54	1.45	1.39
18	B	828	CLA	C1B-C2B	2.53	1.49	1.43
17	4	607	CHL	C3B-C4B	2.53	1.48	1.42
17	3	606	CHL	C1B-C2B	2.53	1.49	1.43
17	4	605	CHL	C1B-C2B	2.53	1.49	1.43
17	4	615	CHL	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	832	CLA	C1B-C2B	2.51	1.49	1.43
18	A	842	CLA	C1B-C2B	2.51	1.49	1.43
22	A	851	BCR	C8-C9	-2.51	1.40	1.45
17	2	605	CHL	C1B-C2B	2.51	1.49	1.43
17	2	607	CHL	C3B-C4B	2.51	1.48	1.42
18	A	802	CLA	C1B-C2B	2.50	1.49	1.43
18	4	609	CLA	C1B-C2B	2.50	1.49	1.43
18	B	822	CLA	C1B-C2B	2.50	1.49	1.43
18	3	607	CLA	C1B-C2B	2.50	1.49	1.43
17	2	615	CHL	C1B-C2B	2.48	1.49	1.43
17	2	605	CHL	MG-NA	-2.45	2.00	2.06
17	1	601	CHL	C1B-C2B	2.45	1.49	1.43
18	A	844	CLA	C1B-C2B	2.45	1.49	1.43
17	1	606	CHL	C4C-C3C	2.44	1.49	1.45
17	4	607	CHL	C1B-C2B	2.44	1.49	1.43
18	A	814	CLA	C1B-C2B	2.43	1.49	1.43
17	1	601	CHL	MG-NA	-2.43	2.00	2.06
17	2	601	CHL	MG-NA	-2.43	2.00	2.06
22	A	851	BCR	C23-C22	-2.42	1.40	1.45
21	2	616	LUT	C8-C9	-2.42	1.40	1.45
17	2	606	CHL	C4C-C3C	2.41	1.49	1.45
18	A	828	CLA	CHC-C1C	2.41	1.43	1.38
17	2	606	CHL	MG-NA	-2.41	2.00	2.06
17	4	606	CHL	C4C-C3C	2.40	1.49	1.45
17	4	605	CHL	MG-NA	-2.39	2.00	2.06
24	A	801	CL0	C1D-C2D	2.39	1.50	1.45
17	4	605	CHL	C4C-C3C	2.38	1.49	1.44
17	2	607	CHL	C1B-C2B	2.38	1.48	1.43
17	2	601	CHL	C4C-C3C	2.37	1.49	1.45
18	4	609	CLA	CHC-C1C	2.37	1.43	1.38
24	A	801	CL0	C1B-C2B	2.36	1.48	1.43
17	2	605	CHL	C4C-C3C	2.35	1.49	1.44
21	2	616	LUT	C28-C29	-2.35	1.40	1.45
18	F	301	CLA	CHC-C1C	2.34	1.43	1.38
18	1	609	CLA	CMD-C2D	-2.34	1.45	1.50
22	I	101	BCR	C12-C13	-2.34	1.40	1.45
22	B	848	BCR	C19-C18	-2.34	1.40	1.45
18	A	844	CLA	CHC-C1C	2.34	1.43	1.38
18	B	825	CLA	CHC-C1C	2.33	1.43	1.38
21	2	616	LUT	C32-C33	-2.33	1.40	1.45
17	4	615	CHL	C4C-C3C	2.33	1.49	1.45
21	3	613	LUT	C28-C29	-2.33	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	845	BCR	C12-C13	-2.33	1.40	1.45
18	A	814	CLA	CHC-C1C	2.33	1.43	1.38
17	1	606	CHL	C4B-NB	-2.33	1.34	1.37
21	3	613	LUT	C32-C33	-2.33	1.40	1.45
22	A	850	BCR	C19-C18	-2.32	1.41	1.45
17	1	601	CHL	C4C-C3C	2.32	1.49	1.45
18	A	819	CLA	CHC-C1C	2.32	1.43	1.38
21	3	613	LUT	C12-C13	-2.32	1.41	1.45
22	3	614	BCR	C19-C18	-2.32	1.41	1.45
18	A	835	CLA	CHC-C1C	2.32	1.43	1.38
18	A	837	CLA	CHC-C1C	2.31	1.43	1.38
18	B	836	CLA	CHC-C1C	2.31	1.43	1.38
18	A	805	CLA	CHC-C1C	2.31	1.43	1.38
18	A	810	CLA	CHC-C1C	2.31	1.43	1.38
21	4	616	LUT	C32-C33	-2.31	1.41	1.45
17	2	607	CHL	MG-NA	-2.31	2.00	2.06
24	A	801	CL0	CHA-C1A	2.31	1.45	1.39
22	L	301	BCR	C12-C13	-2.30	1.41	1.45
17	2	615	CHL	C4C-C3C	2.30	1.49	1.45
22	F	304	BCR	C23-C22	-2.30	1.41	1.45
18	A	824	CLA	CHC-C1C	2.29	1.43	1.38
17	3	606	CHL	MG-NA	-2.29	2.00	2.06
17	4	606	CHL	MG-NA	-2.29	2.00	2.06
18	K	206	CLA	CHC-C1C	2.29	1.43	1.38
17	2	607	CHL	C4C-C3C	2.29	1.49	1.45
21	4	616	LUT	C12-C13	-2.29	1.41	1.45
18	B	804	CLA	CHC-C1C	2.29	1.43	1.38
22	I	101	BCR	C19-C18	-2.29	1.41	1.45
22	B	848	BCR	C12-C13	-2.29	1.41	1.45
18	A	803	CLA	CHC-C1C	2.29	1.43	1.38
18	2	602	CLA	CHC-C1C	2.28	1.43	1.38
18	B	828	CLA	CHC-C1C	2.28	1.43	1.38
18	1	608	CLA	CHC-C1C	2.28	1.43	1.38
22	G	204	BCR	C12-C13	-2.28	1.41	1.45
21	2	619	LUT	C32-C33	-2.28	1.41	1.45
18	B	822	CLA	CHC-C1C	2.28	1.43	1.38
22	A	848	BCR	C19-C18	-2.28	1.41	1.45
18	3	607	CLA	CHC-C1C	2.28	1.43	1.38
22	L	305	BCR	C12-C13	-2.28	1.41	1.45
18	B	837	CLA	CHC-C1C	2.28	1.43	1.38
18	A	827	CLA	CHC-C1C	2.28	1.43	1.38
18	1	605	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	815	CLA	CHC-C1C	2.27	1.43	1.38
21	2	619	LUT	C12-C13	-2.27	1.41	1.45
18	B	813	CLA	CHC-C1C	2.27	1.43	1.38
19	2	617	XAT	C28-C29	-2.27	1.41	1.45
18	J	101	CLA	CHC-C1C	2.27	1.43	1.38
24	A	801	CL0	MG-NC	2.27	2.11	2.06
24	A	801	CL0	CHC-C4B	2.27	1.44	1.39
17	4	606	CHL	C4B-C3B	2.27	1.48	1.43
18	B	829	CLA	CHC-C1C	2.27	1.43	1.38
18	A	811	CLA	CHC-C1C	2.26	1.43	1.38
18	B	811	CLA	CHC-C1C	2.26	1.43	1.38
18	1	604	CLA	CHC-C1C	2.26	1.43	1.38
18	4	610	CLA	CHC-C1C	2.26	1.43	1.38
18	B	824	CLA	CHC-C1C	2.26	1.43	1.38
18	2	609	CLA	CHC-C1C	2.26	1.43	1.38
18	B	805	CLA	CHC-C1C	2.26	1.43	1.38
18	A	808	CLA	CHC-C1C	2.26	1.43	1.38
18	A	833	CLA	CHC-C1C	2.26	1.43	1.38
18	A	836	CLA	CHC-C1C	2.26	1.43	1.38
22	B	847	BCR	C19-C18	-2.26	1.41	1.45
18	B	833	CLA	CHC-C1C	2.26	1.43	1.38
22	G	204	BCR	C19-C18	-2.25	1.41	1.45
18	4	602	CLA	CHC-C1C	2.25	1.43	1.38
17	4	607	CHL	C4C-C3C	2.25	1.48	1.45
18	4	611	CLA	CHC-C1C	2.25	1.43	1.38
18	A	809	CLA	CHC-C1C	2.25	1.43	1.38
18	2	612	CLA	CHC-C1C	2.25	1.43	1.38
18	B	818	CLA	CHC-C1C	2.25	1.43	1.38
22	3	614	BCR	C12-C13	-2.25	1.41	1.45
18	3	608	CLA	CHC-C1C	2.25	1.43	1.38
18	A	841	CLA	CHC-C1C	2.25	1.43	1.38
18	1	613	CLA	CHC-C1C	2.25	1.43	1.38
18	2	608	CLA	CHC-C1C	2.25	1.43	1.38
22	4	618	BCR	C12-C13	-2.25	1.41	1.45
22	B	847	BCR	C12-C13	-2.25	1.41	1.45
18	B	814	CLA	CHC-C1C	2.24	1.43	1.38
17	4	615	CHL	C4B-C3B	2.24	1.48	1.43
18	A	802	CLA	CHC-C1C	2.24	1.43	1.38
18	B	816	CLA	CHC-C1C	2.24	1.43	1.38
18	B	810	CLA	CHC-C1C	2.24	1.43	1.38
18	B	809	CLA	CHC-C1C	2.24	1.43	1.38
18	K	203	CLA	CHC-C1C	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	601	CLA	CHC-C1C	2.24	1.43	1.38
24	A	801	CL0	MG-NB	2.24	2.10	2.05
18	B	831	CLA	CHC-C1C	2.24	1.43	1.38
18	4	613	CLA	CHC-C1C	2.24	1.43	1.38
18	A	812	CLA	CHC-C1C	2.24	1.43	1.38
18	A	816	CLA	CHC-C1C	2.24	1.43	1.38
18	A	838	CLA	CHC-C1C	2.24	1.43	1.38
18	B	815	CLA	CHC-C1C	2.24	1.43	1.38
22	L	301	BCR	C20-C19	2.23	1.40	1.34
18	3	611	CLA	CHC-C1C	2.23	1.43	1.38
18	A	823	CLA	CHC-C1C	2.23	1.43	1.38
18	B	835	CLA	CHC-C1C	2.23	1.43	1.38
22	A	848	BCR	C12-C13	-2.23	1.41	1.45
18	B	821	CLA	CHC-C1C	2.23	1.43	1.38
18	3	610	CLA	CHC-C1C	2.23	1.43	1.38
22	B	849	BCR	C12-C13	-2.23	1.41	1.45
18	F	302	CLA	CHC-C1C	2.23	1.43	1.38
18	A	822	CLA	CHC-C1C	2.23	1.43	1.38
18	B	803	CLA	CHC-C1C	2.23	1.43	1.38
21	4	616	LUT	C28-C29	-2.23	1.41	1.45
22	B	801	BCR	C12-C13	-2.23	1.41	1.45
18	A	845	CLA	CHC-C1C	2.23	1.43	1.38
18	A	831	CLA	CHC-C1C	2.23	1.43	1.38
18	B	807	CLA	CHC-C1C	2.23	1.43	1.38
18	1	610	CLA	CHC-C1C	2.22	1.43	1.38
18	B	827	CLA	CHC-C1C	2.22	1.43	1.38
18	G	203	CLA	CHC-C1C	2.22	1.43	1.38
18	1	603	CLA	CHC-C1C	2.22	1.43	1.38
18	L	304	CLA	CHC-C1C	2.22	1.43	1.38
18	A	832	CLA	CHC-C1C	2.22	1.43	1.38
18	B	812	CLA	CHC-C1C	2.22	1.43	1.38
18	A	807	CLA	CHC-C1C	2.22	1.43	1.38
18	A	840	CLA	CHC-C1C	2.22	1.43	1.38
18	2	613	CLA	CHC-C1C	2.22	1.43	1.38
18	4	601	CLA	CHC-C1C	2.22	1.43	1.38
18	G	201	CLA	CHC-C1C	2.22	1.43	1.38
17	3	606	CHL	C4C-C3C	2.22	1.48	1.45
18	A	839	CLA	CHC-C1C	2.22	1.43	1.38
17	2	607	CHL	C1B-NB	-2.22	1.35	1.37
18	3	605	CLA	CHC-C1C	2.22	1.43	1.38
18	4	604	CLA	CHC-C1C	2.22	1.43	1.38
18	B	834	CLA	CHC-C1C	2.22	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	303	CLA	CHC-C1C	2.21	1.43	1.38
18	3	609	CLA	CHC-C1C	2.21	1.43	1.38
18	A	806	CLA	CHC-C1C	2.21	1.43	1.38
18	B	841	CLA	CHC-C1C	2.21	1.43	1.38
18	1	611	CLA	CHC-C1C	2.21	1.43	1.38
18	1	602	CLA	CHC-C1C	2.21	1.43	1.38
18	B	840	CLA	CHC-C1C	2.21	1.43	1.38
18	A	825	CLA	CHC-C1C	2.21	1.43	1.38
22	B	849	BCR	C19-C18	-2.21	1.41	1.45
17	1	606	CHL	C1B-NB	-2.21	1.35	1.37
18	A	813	CLA	CHC-C1C	2.21	1.43	1.38
22	A	853	BCR	C19-C18	-2.21	1.41	1.45
22	B	844	BCR	C12-C13	-2.21	1.41	1.45
17	2	615	CHL	C1B-NB	-2.21	1.35	1.37
22	A	849	BCR	C19-C18	-2.20	1.41	1.45
22	B	846	BCR	C19-C18	-2.20	1.41	1.45
18	K	201	CLA	CHC-C1C	2.20	1.43	1.38
18	4	603	CLA	CHC-C1C	2.20	1.43	1.38
18	3	602	CLA	CHC-C1C	2.20	1.43	1.38
22	A	852	BCR	C19-C18	-2.20	1.41	1.45
18	B	817	CLA	CHC-C1C	2.20	1.43	1.38
18	F	303	CLA	CHC-C1C	2.20	1.43	1.38
21	2	619	LUT	C28-C29	-2.20	1.41	1.45
18	A	829	CLA	CHC-C1C	2.20	1.43	1.38
18	A	817	CLA	CHC-C1C	2.20	1.43	1.38
24	A	801	CL0	CHB-C1B	2.20	1.44	1.39
18	4	614	CLA	CHC-C1C	2.20	1.43	1.38
18	A	804	CLA	CHC-C1C	2.20	1.43	1.38
18	B	832	CLA	CHC-C1C	2.20	1.43	1.38
22	B	801	BCR	C19-C18	-2.20	1.41	1.45
18	B	830	CLA	CHC-C1C	2.20	1.43	1.38
18	A	830	CLA	CHC-C1C	2.20	1.43	1.38
18	A	820	CLA	CHC-C1C	2.19	1.43	1.38
18	B	823	CLA	CHC-C1C	2.19	1.43	1.38
18	L	302	CLA	CHC-C1C	2.19	1.43	1.38
18	4	608	CLA	CHC-C1C	2.19	1.43	1.38
18	A	826	CLA	CHC-C1C	2.19	1.43	1.38
18	2	603	CLA	CHC-C1C	2.19	1.43	1.38
22	K	205	BCR	C19-C18	-2.19	1.41	1.45
22	J	102	BCR	C19-C18	-2.19	1.41	1.45
18	2	610	CLA	CHC-C1C	2.19	1.43	1.38
18	1	607	CLA	CHC-C1C	2.19	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	604	CLA	CHC-C1C	2.19	1.43	1.38
22	4	618	BCR	C19-C18	-2.19	1.41	1.45
18	A	842	CLA	CMB-C2B	-2.19	1.46	1.50
18	B	826	CLA	CHC-C1C	2.18	1.43	1.38
22	A	853	BCR	C12-C13	-2.18	1.41	1.45
18	A	842	CLA	MG-NB	-2.18	2.01	2.05
18	B	808	CLA	CHC-C1C	2.18	1.43	1.38
18	4	612	CLA	CHC-C1C	2.18	1.43	1.38
21	2	616	LUT	C12-C13	-2.18	1.41	1.45
18	G	202	CLA	CHC-C1C	2.18	1.42	1.38
22	L	305	BCR	C19-C18	-2.17	1.41	1.45
18	K	204	CLA	CHC-C1C	2.17	1.42	1.38
18	B	838	CLA	CHC-C1C	2.17	1.42	1.38
24	A	801	CL0	C1C-C2C	2.17	1.48	1.44
18	B	819	CLA	CHC-C1C	2.17	1.42	1.38
18	A	821	CLA	CHC-C1C	2.17	1.42	1.38
24	A	801	CL0	CHA-C4D	2.17	1.42	1.38
22	B	846	BCR	C12-C13	-2.16	1.41	1.45
18	2	611	CLA	CHC-C1C	2.16	1.42	1.38
18	A	834	CLA	CHC-C1C	2.16	1.42	1.38
19	4	617	XAT	C32-C33	-2.16	1.41	1.45
18	B	820	CLA	CHC-C1C	2.16	1.42	1.38
22	K	202	BCR	C19-C18	-2.16	1.41	1.45
18	A	843	CLA	CHC-C1C	2.16	1.42	1.38
22	A	850	BCR	C12-C13	-2.16	1.41	1.45
18	3	603	CLA	CHC-C1C	2.16	1.42	1.38
19	4	617	XAT	C8-C9	-2.15	1.41	1.45
18	B	839	CLA	CHC-C1C	2.15	1.42	1.38
18	A	844	CLA	MG-NB	-2.15	2.01	2.05
19	4	617	XAT	C28-C29	-2.15	1.41	1.45
22	A	849	BCR	C12-C13	-2.15	1.41	1.45
18	A	803	CLA	MG-NB	-2.15	2.01	2.05
18	B	802	CLA	CHC-C1C	2.15	1.42	1.38
18	2	604	CLA	CHC-C1C	2.14	1.42	1.38
21	1	616	LUT	C12-C13	-2.14	1.41	1.45
18	B	808	CLA	CMD-C2D	-2.14	1.46	1.50
18	B	806	CLA	CHC-C1C	2.14	1.42	1.38
18	H	201	CLA	CHC-C1C	2.14	1.42	1.38
17	1	601	CHL	C1B-NB	-2.14	1.35	1.37
17	4	607	CHL	MG-NA	-2.14	2.01	2.06
18	A	842	CLA	CMD-C2D	-2.14	1.46	1.50
22	J	102	BCR	C12-C13	-2.14	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	818	CLA	CHC-C1C	2.13	1.42	1.38
18	B	802	CLA	CMD-C2D	-2.12	1.46	1.50
22	K	202	BCR	C12-C13	-2.12	1.41	1.45
18	2	604	CLA	MG-NB	-2.12	2.01	2.05
17	2	605	CHL	C1B-NB	-2.12	1.35	1.37
18	B	808	CLA	MG-NB	-2.11	2.01	2.05
17	2	601	CHL	C4B-NB	-2.11	1.35	1.37
17	4	615	CHL	MG-NA	-2.11	2.01	2.06
18	K	201	CLA	CBD-CAD	2.11	1.56	1.51
22	B	843	BCR	C19-C18	-2.11	1.41	1.45
22	B	845	BCR	C19-C18	-2.11	1.41	1.45
18	3	612	CLA	MG-NB	-2.11	2.01	2.05
17	2	615	CHL	C4B-NB	-2.11	1.35	1.37
18	B	826	CLA	MG-NB	-2.11	2.01	2.05
18	4	604	CLA	MG-NB	-2.11	2.01	2.05
17	2	601	CHL	C1B-NB	-2.11	1.35	1.37
18	B	822	CLA	MG-NB	-2.11	2.01	2.05
17	2	606	CHL	C4B-NB	-2.10	1.35	1.37
22	K	205	BCR	C11-C12	2.10	1.40	1.34
19	2	617	XAT	C32-C33	-2.10	1.41	1.45
18	3	612	CLA	CHC-C1C	2.10	1.42	1.38
18	2	612	CLA	MG-NB	-2.10	2.01	2.05
18	L	302	CLA	CMB-C2B	-2.10	1.46	1.50
19	4	617	XAT	C12-C13	-2.10	1.41	1.45
18	3	601	CLA	MG-NB	-2.10	2.01	2.05
18	3	603	CLA	MG-NB	-2.10	2.01	2.05
18	A	842	CLA	CHC-C1C	2.10	1.42	1.38
18	4	603	CLA	MG-NB	-2.10	2.01	2.05
18	2	603	CLA	MG-NB	-2.09	2.01	2.05
22	L	306	BCR	C19-C18	-2.09	1.41	1.45
22	A	852	BCR	C11-C12	2.09	1.40	1.34
22	B	843	BCR	C12-C13	-2.09	1.41	1.45
17	4	605	CHL	C1B-NB	-2.09	1.35	1.37
17	4	607	CHL	C1B-NB	-2.09	1.35	1.37
18	B	823	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	828	CLA	CMD-C2D	-2.09	1.46	1.50
18	K	201	CLA	MG-NB	-2.09	2.01	2.05
18	A	818	CLA	MG-NB	-2.09	2.01	2.05
18	B	825	CLA	MG-NB	-2.08	2.01	2.05
21	1	616	LUT	C32-C33	-2.08	1.41	1.45
17	3	606	CHL	C1B-NB	-2.08	1.35	1.37
18	L	302	CLA	MG-NB	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	608	CLA	MG-NB	-2.08	2.01	2.05
19	1	614	XAT	O24-C25	-2.08	1.43	1.46
22	B	844	BCR	C20-C19	2.08	1.39	1.34
18	B	817	CLA	CMB-C2B	-2.08	1.46	1.50
17	1	606	CHL	C1D-ND	-2.08	1.35	1.37
18	2	609	CLA	MG-NB	-2.08	2.01	2.05
18	B	839	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	839	CLA	MG-NB	-2.07	2.01	2.05
18	B	809	CLA	MG-NB	-2.07	2.01	2.05
18	1	610	CLA	MG-NB	-2.07	2.01	2.05
18	B	819	CLA	MG-NB	-2.07	2.01	2.05
18	4	612	CLA	MG-NB	-2.07	2.01	2.05
19	2	617	XAT	C12-C13	-2.07	1.41	1.45
18	B	829	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	820	CLA	MG-NB	-2.07	2.01	2.05
18	2	609	CLA	CMD-C2D	-2.07	1.46	1.50
18	G	203	CLA	MG-NB	-2.07	2.01	2.05
18	3	612	CLA	CMD-C2D	-2.07	1.46	1.50
18	4	614	CLA	MG-NB	-2.07	2.01	2.05
18	4	610	CLA	MG-NB	-2.07	2.01	2.05
18	2	613	CLA	MG-NB	-2.07	2.01	2.05
18	4	613	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	851	BCR	C20-C19	2.06	1.39	1.34
18	2	610	CLA	MG-NB	-2.06	2.01	2.05
18	B	813	CLA	MG-NB	-2.06	2.01	2.05
18	K	206	CLA	MG-NB	-2.06	2.01	2.05
22	F	304	BCR	C19-C18	-2.06	1.41	1.45
18	1	609	CLA	CHC-C1C	2.06	1.42	1.38
18	4	611	CLA	CMD-C2D	-2.06	1.46	1.50
17	2	605	CHL	C4B-NB	-2.06	1.35	1.37
18	B	830	CLA	MG-NB	-2.06	2.01	2.05
18	B	839	CLA	MG-NB	-2.06	2.01	2.05
18	3	602	CLA	MG-NB	-2.06	2.01	2.05
18	A	838	CLA	MG-NB	-2.06	2.01	2.05
18	3	611	CLA	CBD-CAD	2.06	1.56	1.51
18	4	604	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	821	CLA	MG-NB	-2.06	2.01	2.05
18	F	302	CLA	MG-NB	-2.06	2.01	2.05
18	1	612	CLA	CHC-C1C	2.06	1.42	1.38
18	4	603	CLA	CMD-C2D	-2.06	1.46	1.50
18	K	204	CLA	CMC-C2C	-2.06	1.46	1.50
18	3	605	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	810	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	812	CLA	MG-NB	-2.05	2.01	2.05
18	A	804	CLA	MG-NB	-2.05	2.01	2.05
17	2	606	CHL	C1B-NB	-2.05	1.35	1.37
18	4	602	CLA	MG-NB	-2.05	2.01	2.05
18	B	819	CLA	CMB-C2B	-2.05	1.46	1.50
18	B	823	CLA	MG-NB	-2.05	2.01	2.05
18	A	802	CLA	MG-NB	-2.05	2.01	2.05
22	L	306	BCR	C12-C13	-2.05	1.41	1.45
18	3	609	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	810	CLA	MG-NB	-2.05	2.01	2.05
18	A	829	CLA	MG-NB	-2.05	2.01	2.05
18	B	827	CLA	MG-NB	-2.05	2.01	2.05
18	B	817	CLA	MG-NB	-2.05	2.01	2.05
18	2	611	CLA	MG-NB	-2.04	2.01	2.05
18	B	807	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	829	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	829	CLA	MG-NB	-2.04	2.01	2.05
18	A	811	CLA	CMD-C2D	-2.04	1.46	1.50
18	1	613	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	824	CLA	MG-NB	-2.04	2.01	2.05
18	F	301	CLA	MG-NB	-2.04	2.01	2.05
18	1	613	CLA	MG-NB	-2.04	2.01	2.05
18	A	816	CLA	MG-NB	-2.04	2.01	2.05
18	B	841	CLA	MG-NB	-2.04	2.01	2.05
18	1	608	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	822	CLA	MG-NB	-2.04	2.01	2.05
18	A	819	CLA	CMC-C2C	-2.04	1.46	1.50
18	3	608	CLA	MG-NB	-2.04	2.01	2.05
18	A	815	CLA	MG-NB	-2.04	2.01	2.05
18	B	803	CLA	CMC-C2C	-2.04	1.46	1.50
18	3	611	CLA	MG-NB	-2.03	2.01	2.05
18	3	610	CLA	MG-NB	-2.03	2.01	2.05
18	2	602	CLA	MG-NB	-2.03	2.01	2.05
18	H	201	CLA	MG-NB	-2.03	2.01	2.05
18	K	204	CLA	MG-NB	-2.03	2.01	2.05
18	B	822	CLA	CMB-C2B	-2.03	1.46	1.50
18	3	609	CLA	MG-NB	-2.03	2.01	2.05
18	A	841	CLA	MG-NB	-2.03	2.01	2.05
18	B	818	CLA	MG-NB	-2.03	2.01	2.05
18	2	612	CLA	CMD-C2D	-2.03	1.46	1.50
18	3	609	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	836	CLA	CMD-C2D	-2.03	1.46	1.50
17	4	615	CHL	C4B-NB	-2.03	1.35	1.37
18	4	608	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	838	CLA	CMB-C2B	-2.03	1.46	1.50
17	2	607	CHL	C1D-ND	-2.03	1.35	1.37
18	A	810	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	836	CLA	MG-NB	-2.03	2.01	2.05
18	B	826	CLA	CMD-C2D	-2.03	1.46	1.50
18	1	611	CLA	MG-NB	-2.03	2.01	2.05
18	4	611	CLA	MG-NB	-2.03	2.01	2.05
18	3	607	CLA	CMD-C2D	-2.02	1.46	1.50
18	4	603	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	810	CLA	CMD-C2D	-2.02	1.46	1.50
18	1	609	CLA	MG-NB	-2.02	2.01	2.05
18	A	813	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	840	CLA	CMB-C2B	-2.02	1.46	1.50
17	2	607	CHL	C4B-NB	-2.02	1.35	1.37
18	A	834	CLA	MG-NB	-2.02	2.01	2.05
18	B	804	CLA	MG-NB	-2.02	2.01	2.05
18	A	828	CLA	CMC-C2C	-2.02	1.46	1.50
18	1	603	CLA	CMD-C2D	-2.02	1.46	1.50
18	1	603	CLA	MG-NB	-2.02	2.01	2.05
18	3	604	CLA	MG-NB	-2.02	2.01	2.05
18	B	811	CLA	MG-NB	-2.02	2.01	2.05
18	3	601	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	815	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	811	CLA	MG-NB	-2.02	2.01	2.05
18	3	604	CLA	CMD-C2D	-2.02	1.46	1.50
18	4	609	CLA	MG-NB	-2.02	2.01	2.05
18	B	834	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	805	CLA	MG-NB	-2.02	2.01	2.05
18	A	844	CLA	CMB-C2B	-2.02	1.46	1.50
18	K	203	CLA	MG-NB	-2.02	2.01	2.05
18	B	816	CLA	MG-NB	-2.02	2.01	2.05
18	B	806	CLA	MG-NB	-2.02	2.01	2.05
18	A	802	CLA	CMD-C2D	-2.02	1.46	1.50
18	G	202	CLA	CMD-C2D	-2.02	1.46	1.50
18	4	608	CLA	MG-NB	-2.02	2.01	2.05
18	1	604	CLA	MG-NB	-2.01	2.01	2.05
18	A	806	CLA	MG-NB	-2.01	2.01	2.05
18	1	605	CLA	MG-NB	-2.01	2.01	2.05
18	B	830	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	840	CLA	CMD-C2D	-2.01	1.46	1.50
18	1	602	CLA	MG-NB	-2.01	2.01	2.05
18	A	824	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	835	CLA	MG-NB	-2.01	2.01	2.05
18	B	820	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	837	CLA	MG-NB	-2.01	2.01	2.05
18	4	609	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	835	CLA	MG-NB	-2.01	2.01	2.05
18	B	803	CLA	MG-NB	-2.01	2.01	2.05
18	1	612	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	830	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	817	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	845	CLA	MG-NB	-2.01	2.01	2.05
18	2	611	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	828	CLA	MG-NB	-2.01	2.01	2.05
18	3	605	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	813	CLA	CMD-C2D	-2.01	1.46	1.50
18	2	613	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	807	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	812	CLA	CMB-C2B	-2.01	1.46	1.50
18	G	202	CLA	MG-NB	-2.01	2.01	2.05
18	1	612	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	805	CLA	CMD-C2D	-2.01	1.46	1.50
18	2	602	CLA	CMD-C2D	-2.00	1.46	1.50
18	A	816	CLA	CMD-C2D	-2.00	1.46	1.50
18	K	204	CLA	CMB-C2B	-2.00	1.46	1.50
18	2	604	CLA	CMD-C2D	-2.00	1.46	1.50
18	B	838	CLA	CMD-C2D	-2.00	1.46	1.50
18	A	827	CLA	MG-NB	-2.00	2.01	2.05
18	A	833	CLA	MG-NB	-2.00	2.01	2.05
18	B	840	CLA	MG-NB	-2.00	2.01	2.05
22	A	851	BCR	C12-C13	-2.00	1.41	1.45
18	A	822	CLA	CMB-C2B	-2.00	1.46	1.50
18	B	835	CLA	CMD-C2D	-2.00	1.46	1.50
18	A	809	CLA	MG-NB	-2.00	2.01	2.05
18	B	831	CLA	MG-NB	-2.00	2.01	2.05
18	A	806	CLA	CMC-C2C	-2.00	1.46	1.50
18	F	303	CLA	CMB-C2B	-2.00	1.46	1.50
18	A	808	CLA	MG-NB	-2.00	2.01	2.05
18	1	612	CLA	MG-NB	-2.00	2.01	2.05
18	A	836	CLA	MG-NB	-2.00	2.01	2.05
18	A	832	CLA	CMD-C2D	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	613	CLA	MG-NB	-2.00	2.01	2.05
18	B	837	CLA	MG-NB	-2.00	2.01	2.05

All (1557) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	818	CLA	O2D-CGD-CBD	26.04	157.54	111.27
18	A	818	CLA	O2D-CGD-O1D	-25.22	74.53	123.84
18	A	818	CLA	O1D-CGD-CBD	-20.27	83.01	124.48
18	B	836	CLA	C5-C3-C4	-16.66	77.79	114.60
24	A	801	CL0	C2B-C1B-NB	15.14	120.38	110.23
18	B	836	CLA	C4-C3-C2	-13.89	82.51	122.65
18	B	836	CLA	C5-C3-C2	13.03	160.30	122.65
24	A	801	CL0	C4A-NA-C1A	-11.97	101.33	106.71
19	1	614	XAT	O4-C5-C4	11.64	122.12	113.38
24	A	801	CL0	C2C-C1C-NC	10.78	120.08	109.97
17	4	615	CHL	C2B-C1B-NB	9.86	116.84	110.23
24	A	801	CL0	CHA-C4D-C3D	-9.77	108.54	125.26
17	4	606	CHL	C2B-C1B-NB	9.67	116.72	110.23
17	3	606	CHL	C2B-C1B-NB	9.65	116.70	110.23
17	4	607	CHL	C2B-C1B-NB	9.46	116.58	110.23
17	2	615	CHL	C2B-C1B-NB	9.39	116.53	110.23
17	4	605	CHL	C2B-C1B-NB	9.27	116.45	110.23
17	2	605	CHL	C2B-C1B-NB	9.22	116.41	110.23
19	1	614	XAT	C38-C25-C26	-9.20	106.84	122.26
19	1	614	XAT	O24-C25-C24	9.17	120.27	113.38
17	2	607	CHL	C2B-C1B-NB	9.16	116.37	110.23
17	1	601	CHL	C2B-C1B-NB	9.12	116.35	110.23
17	2	606	CHL	C2B-C1B-NB	9.05	116.30	110.23
17	2	601	CHL	C2B-C1B-NB	9.00	116.27	110.23
24	A	801	CL0	C3D-C2D-C1D	-8.74	98.73	107.08
17	4	605	CHL	CMD-C2D-C1D	8.42	139.54	124.71
24	A	801	CL0	CMD-C2D-C1D	8.41	139.53	124.71
17	3	606	CHL	CMD-C2D-C1D	8.33	139.40	124.71
17	4	615	CHL	CMD-C2D-C1D	8.30	139.34	124.71
17	2	615	CHL	CMD-C2D-C1D	8.26	139.28	124.71
17	4	607	CHL	CMD-C2D-C1D	8.25	139.25	124.71
17	2	606	CHL	CMD-C2D-C1D	8.22	139.19	124.71
17	1	601	CHL	CMD-C2D-C1D	8.21	139.19	124.71
17	2	601	CHL	CMD-C2D-C1D	8.21	139.18	124.71
17	1	606	CHL	C2B-C1B-NB	8.19	115.72	110.23
24	A	801	CL0	C3C-C4C-NC	8.17	119.73	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	605	CHL	CMD-C2D-C1D	8.16	139.09	124.71
17	2	607	CHL	CMD-C2D-C1D	8.15	139.07	124.71
17	1	606	CHL	CMD-C2D-C1D	8.10	138.99	124.71
17	4	606	CHL	CMD-C2D-C1D	8.03	138.87	124.71
22	B	843	BCR	C16-C15-C14	7.85	139.55	123.47
19	1	614	XAT	C18-C5-C6	-7.71	109.34	122.26
24	A	801	CL0	C3B-C4B-NB	7.53	117.50	110.52
17	4	615	CHL	C2C-C3C-C4C	-7.52	101.13	106.49
17	1	606	CHL	CHD-C1D-ND	-7.49	117.58	124.45
22	L	301	BCR	C16-C15-C14	7.45	138.73	123.47
17	4	607	CHL	C2C-C3C-C4C	-7.44	101.18	106.49
22	L	301	BCR	C15-C16-C17	7.41	138.65	123.47
17	2	615	CHL	C2C-C3C-C4C	-7.38	101.22	106.49
17	1	601	CHL	C2C-C3C-C4C	-7.27	101.30	106.49
17	2	605	CHL	C2C-C3C-C4C	-7.24	101.11	106.49
24	A	801	CL0	C2D-C1D-ND	7.21	115.42	110.10
18	1	609	CLA	C4A-NA-C1A	7.20	109.94	106.71
17	2	601	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
17	2	607	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
24	A	801	CL0	CHA-C4D-ND	7.11	130.99	124.45
17	2	606	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
18	2	611	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	A	849	BCR	C15-C16-C17	7.08	137.98	123.47
21	2	616	LUT	C15-C35-C34	7.07	137.95	123.47
18	1	612	CLA	C4A-NA-C1A	7.04	109.87	106.71
17	2	606	CHL	CHD-C1D-ND	-7.00	118.02	124.45
17	4	605	CHL	C2C-C3C-C4C	-7.00	101.30	106.49
18	4	614	CLA	C4A-NA-C1A	6.95	109.83	106.71
18	A	818	CLA	C4A-NA-C1A	6.95	109.83	106.71
18	A	830	CLA	C4A-NA-C1A	6.94	109.83	106.71
17	4	615	CHL	C1B-C2B-C3B	-6.94	100.44	107.03
18	A	828	CLA	C4A-NA-C1A	6.94	109.82	106.71
17	4	606	CHL	C1B-C2B-C3B	-6.92	100.46	107.03
18	A	819	CLA	C4A-NA-C1A	6.91	109.81	106.71
17	1	601	CHL	CHD-C1D-ND	-6.90	118.12	124.45
18	F	302	CLA	C4A-NA-C1A	6.90	109.81	106.71
17	1	606	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
17	2	615	CHL	CHD-C1D-ND	-6.89	118.12	124.45
18	A	813	CLA	C4A-NA-C1A	6.85	109.78	106.71
18	A	827	CLA	C4A-NA-C1A	6.84	109.78	106.71
18	B	841	CLA	C4A-NA-C1A	6.83	109.78	106.71
17	4	605	CHL	CHD-C1D-ND	-6.83	118.18	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	604	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	2	604	CLA	C4A-NA-C1A	6.82	109.77	106.71
21	3	613	LUT	C15-C35-C34	6.81	137.43	123.47
18	A	843	CLA	C4A-NA-C1A	6.81	109.77	106.71
18	B	807	CLA	C4A-NA-C1A	6.81	109.77	106.71
18	B	804	CLA	C4A-NA-C1A	6.79	109.76	106.71
18	B	811	CLA	C4A-NA-C1A	6.77	109.75	106.71
18	B	840	CLA	C4A-NA-C1A	6.77	109.75	106.71
18	K	204	CLA	C4A-NA-C1A	6.77	109.75	106.71
18	B	826	CLA	C4A-NA-C1A	6.76	109.75	106.71
18	B	809	CLA	C4A-NA-C1A	6.76	109.74	106.71
17	2	601	CHL	CHD-C1D-ND	-6.76	118.25	124.45
18	3	605	CLA	C4A-NA-C1A	6.75	109.74	106.71
18	H	201	CLA	C4A-NA-C1A	6.75	109.74	106.71
18	A	831	CLA	C4A-NA-C1A	6.75	109.74	106.71
18	A	808	CLA	C4A-NA-C1A	6.74	109.74	106.71
18	B	808	CLA	C4A-NA-C1A	6.74	109.73	106.71
18	B	819	CLA	C4A-NA-C1A	6.74	109.73	106.71
18	G	202	CLA	C4A-NA-C1A	6.74	109.73	106.71
18	2	613	CLA	C4A-NA-C1A	6.73	109.73	106.71
18	A	812	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	B	814	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	A	817	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	1	605	CLA	C4A-NA-C1A	6.72	109.72	106.71
18	4	602	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	4	601	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	A	839	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	L	302	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	2	608	CLA	C4A-NA-C1A	6.69	109.71	106.71
18	3	612	CLA	C4A-NA-C1A	6.69	109.71	106.71
17	2	607	CHL	CHD-C1D-ND	-6.69	118.31	124.45
18	4	613	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	A	806	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	B	818	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	B	837	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	B	815	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	1	603	CLA	C4A-NA-C1A	6.67	109.71	106.71
18	A	826	CLA	C4A-NA-C1A	6.67	109.71	106.71
18	A	829	CLA	C4A-NA-C1A	6.67	109.71	106.71
18	4	612	CLA	C4A-NA-C1A	6.67	109.70	106.71
18	L	304	CLA	C4A-NA-C1A	6.67	109.70	106.71
18	3	601	CLA	C4A-NA-C1A	6.65	109.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	825	CLA	C4A-NA-C1A	6.65	109.69	106.71
18	1	611	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	L	303	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	G	203	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	4	608	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	B	813	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	4	610	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	B	827	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	A	851	BCR	C8-C9-C10	6.63	129.11	118.94
18	A	840	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	3	609	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	B	831	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	J	101	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	B	816	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	1	607	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	A	804	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	A	842	CLA	C4A-NA-C1A	6.60	109.67	106.71
18	B	806	CLA	C4A-NA-C1A	6.60	109.67	106.71
17	2	605	CHL	CHD-C1D-ND	-6.60	118.39	124.45
18	A	805	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	A	825	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	4	603	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	A	816	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	A	841	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	B	834	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	A	838	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	1	614	XAT	O24-C25-C38	6.57	122.93	115.06
18	A	833	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	B	820	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	A	845	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	B	830	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	B	829	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	A	802	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	A	851	BCR	C16-C15-C14	6.56	136.91	123.47
18	A	832	CLA	C4A-NA-C1A	6.56	109.65	106.71
18	1	610	CLA	C4A-NA-C1A	6.54	109.65	106.71
18	B	824	CLA	C4A-NA-C1A	6.54	109.65	106.71
18	K	201	CLA	C4A-NA-C1A	6.54	109.64	106.71
18	A	836	CLA	C4A-NA-C1A	6.53	109.64	106.71
18	3	608	CLA	C4A-NA-C1A	6.53	109.64	106.71
17	4	607	CHL	CHD-C1D-ND	-6.53	118.45	124.45
18	B	839	CLA	C4A-NA-C1A	6.53	109.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	609	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	A	820	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	B	823	CLA	C4A-NA-C1A	6.51	109.64	106.71
18	2	612	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	A	850	BCR	C15-C16-C17	6.51	136.81	123.47
18	B	803	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	A	809	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	B	817	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	F	303	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	B	821	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	G	201	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	B	838	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	3	611	CLA	C4A-NA-C1A	6.49	109.63	106.71
18	2	603	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	B	805	CLA	C4A-NA-C1A	6.49	109.62	106.71
18	4	604	CLA	C4A-NA-C1A	6.47	109.62	106.71
18	A	811	CLA	C4A-NA-C1A	6.47	109.62	106.71
18	3	610	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	B	835	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	B	812	CLA	C4A-NA-C1A	6.46	109.61	106.71
17	3	606	CHL	CHD-C1D-ND	-6.45	118.52	124.45
18	1	602	CLA	C4A-NA-C1A	6.45	109.61	106.71
18	3	607	CLA	C4A-NA-C1A	6.45	109.61	106.71
18	A	834	CLA	C4A-NA-C1A	6.45	109.61	106.71
18	4	611	CLA	C4A-NA-C1A	6.45	109.60	106.71
18	A	823	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	B	802	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	A	824	CLA	C4A-NA-C1A	6.43	109.60	106.71
18	1	613	CLA	C4A-NA-C1A	6.43	109.60	106.71
18	A	821	CLA	C4A-NA-C1A	6.41	109.59	106.71
18	A	815	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	A	835	CLA	C4A-NA-C1A	6.38	109.57	106.71
18	A	837	CLA	C4A-NA-C1A	6.38	109.57	106.71
18	B	833	CLA	C4A-NA-C1A	6.38	109.57	106.71
18	A	822	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	B	810	CLA	C4A-NA-C1A	6.36	109.57	106.71
18	B	832	CLA	C4A-NA-C1A	6.36	109.57	106.71
18	3	602	CLA	C4A-NA-C1A	6.36	109.56	106.71
18	3	604	CLA	C4A-NA-C1A	6.35	109.56	106.71
18	F	301	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	A	801	CL0	CHD-C4C-C3C	-6.35	115.51	124.84
17	4	606	CHL	CHD-C1D-ND	-6.34	118.62	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	828	CLA	C4A-NA-C1A	6.33	109.55	106.71
17	4	615	CHL	CHD-C1D-ND	-6.33	118.64	124.45
18	1	608	CLA	C4A-NA-C1A	6.32	109.55	106.71
18	3	603	CLA	C4A-NA-C1A	6.32	109.55	106.71
18	K	203	CLA	C4A-NA-C1A	6.32	109.55	106.71
18	2	602	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	A	850	BCR	C16-C15-C14	6.32	136.41	123.47
18	K	206	CLA	C4A-NA-C1A	6.31	109.54	106.71
18	A	810	CLA	C4A-NA-C1A	6.27	109.53	106.71
18	B	822	CLA	C4A-NA-C1A	6.23	109.51	106.71
18	A	807	CLA	C4A-NA-C1A	6.19	109.49	106.71
18	B	836	CLA	C4A-NA-C1A	6.16	109.47	106.71
18	A	814	CLA	C4A-NA-C1A	6.08	109.44	106.71
18	4	609	CLA	C4A-NA-C1A	6.07	109.44	106.71
24	A	801	CL0	C3B-C2B-C1B	-6.07	99.84	107.16
19	2	617	XAT	C15-C35-C34	6.06	135.88	123.47
21	2	619	LUT	C15-C35-C34	5.84	135.44	123.47
19	2	617	XAT	C35-C15-C14	5.84	135.43	123.47
22	K	205	BCR	C15-C16-C17	5.78	135.32	123.47
17	1	606	CHL	CHB-C1B-NB	-5.73	118.19	124.26
18	A	803	CLA	C4A-NA-C1A	5.71	109.27	106.71
17	4	615	CHL	C3B-C4B-NB	5.62	114.00	110.23
18	A	844	CLA	C4A-NA-C1A	5.61	109.23	106.71
17	2	601	CHL	O2D-CGD-CBD	5.57	121.17	111.27
22	F	304	BCR	C15-C16-C17	5.54	134.82	123.47
22	A	851	BCR	C23-C22-C21	5.50	127.38	118.94
17	2	605	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
22	F	304	BCR	C24-C23-C22	5.44	134.45	126.23
17	4	607	CHL	C3B-C2B-C1B	-5.43	100.61	107.16
17	4	606	CHL	C3B-C4B-NB	5.41	113.86	110.23
17	2	607	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
17	2	606	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
17	3	606	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
17	2	601	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
17	2	615	CHL	C3B-C2B-C1B	-5.34	100.71	107.16
17	1	606	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
24	A	801	CL0	CHD-C1D-ND	-5.33	119.55	124.45
22	B	846	BCR	C16-C15-C14	5.27	134.27	123.47
17	4	605	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
22	A	851	BCR	C34-C9-C10	-5.22	115.61	122.92
17	1	601	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
22	B	849	BCR	C30-C25-C26	-5.22	115.27	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	801	CL0	C1C-C2C-C3C	-5.13	101.57	106.96
17	2	615	CHL	CHB-C1B-NB	-5.10	118.86	124.26
22	K	202	BCR	C16-C15-C14	5.09	133.90	123.47
24	A	801	CL0	C4D-CHA-C1A	-5.08	114.37	126.62
21	1	616	LUT	C15-C35-C34	5.02	133.76	123.47
17	4	615	CHL	C3C-C4C-NC	4.97	116.14	110.57
24	A	801	CL0	C1D-CHD-C4C	-4.96	115.36	126.06
22	A	851	BCR	C7-C8-C9	-4.95	118.76	126.23
17	4	607	CHL	C3C-C4C-NC	4.94	116.11	110.57
17	2	615	CHL	O2D-CGD-CBD	4.94	120.05	111.27
17	2	606	CHL	O2D-CGD-CBD	4.92	120.01	111.27
22	J	102	BCR	C16-C15-C14	4.90	133.50	123.47
17	2	605	CHL	CHB-C1B-NB	-4.88	119.09	124.26
22	B	845	BCR	C19-C18-C17	4.87	126.42	118.94
19	1	614	XAT	O4-C5-C18	4.87	120.89	115.06
17	4	606	CHL	C3C-C4C-NC	4.85	116.02	110.57
22	A	851	BCR	C37-C22-C21	-4.84	116.14	122.92
21	1	616	LUT	C30-C31-C32	4.82	138.26	123.22
17	2	605	CHL	O2D-CGD-CBD	4.78	119.76	111.27
22	B	847	BCR	C16-C15-C14	4.77	133.25	123.47
19	1	614	XAT	C35-C34-C33	-4.74	120.54	127.31
17	4	605	CHL	C3C-C4C-NC	4.70	115.70	110.57
17	2	605	CHL	C3C-C4C-NC	4.70	115.70	110.57
17	2	606	CHL	CHB-C1B-NB	-4.69	119.30	124.26
17	2	607	CHL	O2D-CGD-CBD	4.68	119.59	111.27
21	2	616	LUT	C7-C8-C9	4.68	133.30	126.23
17	2	607	CHL	C3C-C4C-NC	4.67	115.81	110.57
17	4	607	CHL	O2D-CGD-CBD	4.66	119.55	111.27
17	4	606	CHL	O2D-CGD-CBD	4.65	119.52	111.27
17	3	606	CHL	O2D-CGD-CBD	4.63	119.49	111.27
21	2	616	LUT	C19-C9-C10	-4.62	116.44	122.92
17	4	615	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
17	4	607	CHL	C3D-C2D-C1D	-4.60	99.55	105.83
21	2	616	LUT	C39-C29-C30	-4.60	116.48	122.92
22	L	306	BCR	C34-C9-C10	-4.59	116.49	122.92
17	3	606	CHL	C2C-C1C-NC	4.57	114.26	109.97
17	2	601	CHL	CHB-C1B-NB	-4.56	119.42	124.26
17	2	601	CHL	C3C-C4C-NC	4.55	115.68	110.57
17	3	606	CHL	C3D-C2D-C1D	-4.55	99.62	105.83
22	F	304	BCR	C16-C15-C14	4.55	132.79	123.47
17	1	601	CHL	C3C-C4C-NC	4.54	115.67	110.57
17	2	605	CHL	C3D-C2D-C1D	-4.51	99.67	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	607	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
17	3	606	CHL	C3C-C4C-NC	4.50	115.62	110.57
17	4	606	CHL	C3D-C2D-C1D	-4.50	99.69	105.83
21	3	613	LUT	C39-C29-C30	-4.50	116.62	122.92
17	1	601	CHL	CHB-C1B-NB	-4.50	119.50	124.26
22	B	843	BCR	C34-C9-C10	-4.49	116.64	122.92
17	1	601	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
21	2	619	LUT	C19-C9-C10	-4.48	116.64	122.92
17	2	615	CHL	C3D-C2D-C1D	-4.48	99.72	105.83
17	2	615	CHL	C3C-C4C-NC	4.46	115.58	110.57
22	A	853	BCR	C16-C15-C14	4.46	132.61	123.47
22	L	306	BCR	C16-C15-C14	4.45	132.58	123.47
22	K	202	BCR	C15-C16-C17	4.44	132.56	123.47
17	2	606	CHL	C3C-C4C-NC	4.43	115.54	110.57
17	2	606	CHL	C3D-C2D-C1D	-4.43	99.79	105.83
22	A	851	BCR	C11-C10-C9	4.42	133.62	127.31
17	2	601	CHL	C3D-C2D-C1D	-4.41	99.81	105.83
22	B	845	BCR	C36-C18-C17	-4.41	116.75	122.92
22	G	204	BCR	C15-C16-C17	4.41	132.50	123.47
22	K	205	BCR	C19-C18-C17	4.40	125.70	118.94
22	L	306	BCR	C37-C22-C21	-4.40	116.76	122.92
22	A	848	BCR	C15-C16-C17	4.39	132.46	123.47
17	4	606	CHL	C2C-C1C-NC	4.38	114.08	109.97
22	K	202	BCR	C34-C9-C10	-4.37	116.80	122.92
22	K	202	BCR	C37-C22-C21	-4.37	116.80	122.92
22	B	844	BCR	C37-C22-C21	-4.37	116.80	122.92
22	K	205	BCR	C37-C22-C21	-4.35	116.83	122.92
17	4	605	CHL	CHB-C1B-NB	-4.33	119.67	124.26
22	A	852	BCR	C37-C22-C21	-4.32	116.87	122.92
19	2	617	XAT	C39-C29-C30	-4.31	116.88	122.92
17	4	605	CHL	C3D-C2D-C1D	-4.31	99.95	105.83
19	4	617	XAT	C19-C9-C10	-4.31	116.89	122.92
22	J	102	BCR	C34-C9-C10	-4.30	116.89	122.92
22	B	846	BCR	C34-C9-C10	-4.30	116.90	122.92
22	B	801	BCR	C16-C15-C14	4.30	132.27	123.47
17	1	606	CHL	C3D-C2D-C1D	-4.29	99.98	105.83
22	A	850	BCR	C34-C9-C10	-4.29	116.92	122.92
22	L	301	BCR	C12-C13-C14	4.27	125.49	118.94
22	F	304	BCR	C34-C9-C10	-4.26	116.95	122.92
21	2	619	LUT	C39-C29-C30	-4.24	116.98	122.92
22	L	305	BCR	C37-C22-C21	-4.24	116.98	122.92
19	2	617	XAT	C19-C9-C10	-4.24	116.98	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	616	LUT	C19-C9-C10	-4.24	116.98	122.92
22	A	852	BCR	C16-C15-C14	4.24	132.16	123.47
22	L	301	BCR	C37-C22-C21	-4.24	116.98	122.92
22	F	304	BCR	C21-C20-C19	4.23	136.42	123.22
17	2	607	CHL	CHB-C1B-NB	-4.23	119.78	124.26
22	B	848	BCR	C15-C16-C17	4.23	132.13	123.47
22	B	849	BCR	C16-C15-C14	4.23	132.13	123.47
22	L	306	BCR	C8-C9-C10	4.21	125.41	118.94
22	K	205	BCR	C34-C9-C10	-4.21	117.03	122.92
22	K	205	BCR	C36-C18-C17	-4.21	117.03	122.92
22	4	618	BCR	C30-C25-C26	-4.19	116.71	122.61
22	B	844	BCR	C34-C9-C10	-4.17	117.09	122.92
22	B	844	BCR	C16-C15-C14	4.16	132.00	123.47
22	G	204	BCR	C37-C22-C21	-4.16	117.09	122.92
21	1	616	LUT	C31-C30-C29	4.16	133.25	127.31
21	1	616	LUT	C39-C29-C28	4.16	124.62	118.08
22	A	851	BCR	C15-C16-C17	4.13	131.94	123.47
22	L	301	BCR	C36-C18-C17	-4.13	117.14	122.92
22	B	849	BCR	C37-C22-C21	-4.12	117.15	122.92
22	B	801	BCR	C37-C22-C21	-4.12	117.15	122.92
22	A	851	BCR	C12-C13-C14	4.12	125.26	118.94
17	3	606	CHL	CHB-C1B-NB	-4.12	119.90	124.26
22	A	848	BCR	C37-C22-C21	-4.11	117.16	122.92
22	3	614	BCR	C34-C9-C10	-4.11	117.17	122.92
21	1	616	LUT	C32-C33-C34	4.10	125.24	118.94
17	4	607	CHL	CHD-C4C-C3C	-4.09	118.82	124.84
17	4	606	CHL	CHB-C1B-NB	-4.09	119.92	124.26
27	B	850	DGD	O2G-C1B-C2B	4.09	120.32	111.50
22	B	845	BCR	C34-C9-C10	-4.09	117.19	122.92
22	J	102	BCR	C37-C22-C21	-4.07	117.22	122.92
22	A	853	BCR	C37-C22-C21	-4.07	117.22	122.92
22	L	305	BCR	C34-C9-C10	-4.06	117.24	122.92
21	2	619	LUT	C8-C9-C10	4.05	125.16	118.94
17	4	615	CHL	CHD-C4C-C3C	-4.05	118.88	124.84
22	L	301	BCR	C34-C9-C10	-4.05	117.25	122.92
22	F	304	BCR	C12-C13-C14	4.05	125.16	118.94
22	L	301	BCR	C35-C13-C14	-4.05	117.25	122.92
17	4	606	CHL	C4C-C3C-C2C	-4.05	101.00	106.90
21	2	616	LUT	C28-C29-C30	4.04	125.14	118.94
19	4	617	XAT	C39-C29-C30	-4.03	117.28	122.92
22	B	847	BCR	C34-C9-C10	-4.03	117.28	122.92
22	A	848	BCR	C34-C9-C10	-4.01	117.30	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	202	BCR	C12-C13-C14	4.01	125.10	118.94
21	1	616	LUT	C40-C33-C34	-4.01	117.30	122.92
18	4	613	CLA	CAA-C2A-C3A	-4.01	101.81	112.78
17	1	606	CHL	C4A-NA-C1A	3.99	108.50	106.71
22	4	618	BCR	C34-C9-C10	-3.98	117.34	122.92
22	A	849	BCR	C34-C9-C10	-3.98	117.34	122.92
22	B	848	BCR	C37-C22-C21	-3.98	117.34	122.92
22	4	618	BCR	C37-C22-C21	-3.98	117.34	122.92
22	B	846	BCR	C37-C22-C21	-3.98	117.35	122.92
22	K	202	BCR	C35-C13-C14	-3.98	117.35	122.92
22	A	852	BCR	C34-C9-C10	-3.98	117.35	122.92
22	L	305	BCR	C16-C15-C14	3.98	131.62	123.47
22	I	101	BCR	C15-C16-C17	3.97	131.61	123.47
22	3	614	BCR	C16-C15-C14	3.96	131.59	123.47
22	B	843	BCR	C8-C9-C10	3.94	124.99	118.94
22	B	848	BCR	C34-C9-C10	-3.93	117.42	122.92
22	4	618	BCR	C16-C15-C14	3.92	131.51	123.47
22	B	847	BCR	C37-C22-C21	-3.92	117.43	122.92
22	A	849	BCR	C30-C25-C26	-3.92	117.09	122.61
22	3	614	BCR	C37-C22-C21	-3.92	117.44	122.92
22	F	304	BCR	C35-C13-C14	-3.91	117.44	122.92
22	I	101	BCR	C37-C22-C21	-3.91	117.44	122.92
22	B	844	BCR	C21-C20-C19	3.91	135.41	123.22
18	B	821	CLA	CAA-C2A-C3A	-3.90	102.11	112.78
17	4	606	CHL	CHD-C4C-C3C	-3.89	119.12	124.84
21	3	613	LUT	C28-C29-C30	3.89	124.91	118.94
22	B	843	BCR	C37-C22-C21	-3.88	117.49	122.92
22	G	204	BCR	C34-C9-C10	-3.88	117.49	122.92
22	A	850	BCR	C37-C22-C21	-3.88	117.49	122.92
20	1	615	LHG	O7-C7-C8	3.87	119.85	111.50
22	I	101	BCR	C34-C9-C10	-3.87	117.50	122.92
22	B	849	BCR	C34-C9-C10	-3.86	117.52	122.92
21	2	619	LUT	C40-C33-C34	-3.84	117.54	122.92
22	B	845	BCR	C1-C6-C5	-3.84	117.21	122.61
19	4	617	XAT	C15-C35-C34	3.84	131.33	123.47
22	A	852	BCR	C10-C11-C12	3.83	135.18	123.22
17	4	615	CHL	C2D-C1D-ND	3.83	112.93	110.10
22	F	304	BCR	C20-C21-C22	3.82	132.76	127.31
21	4	616	LUT	C19-C9-C10	-3.82	117.57	122.92
19	2	617	XAT	C28-C29-C30	3.82	124.80	118.94
17	1	606	CHL	C3C-C4C-NC	3.81	114.85	110.57
22	B	844	BCR	C15-C16-C17	3.81	131.28	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	619	LUT	C32-C33-C34	3.80	124.78	118.94
21	4	616	LUT	C39-C29-C30	-3.80	117.61	122.92
22	L	306	BCR	C35-C13-C14	-3.77	117.64	122.92
17	3	606	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
17	4	607	CHL	C2D-C1D-ND	3.77	112.88	110.10
22	A	849	BCR	C21-C20-C19	3.75	134.94	123.22
22	B	801	BCR	C8-C9-C10	3.75	124.69	118.94
22	L	306	BCR	C23-C22-C21	3.75	124.69	118.94
17	4	615	CHL	CHB-C1B-NB	-3.74	120.29	124.26
22	L	305	BCR	C15-C16-C17	3.74	131.14	123.47
22	B	846	BCR	C35-C13-C14	-3.74	117.68	122.92
22	L	306	BCR	C12-C13-C14	3.74	124.68	118.94
22	L	301	BCR	C21-C20-C19	3.74	134.87	123.22
22	A	852	BCR	C35-C13-C14	-3.73	117.69	122.92
22	A	852	BCR	C19-C18-C17	3.73	124.67	118.94
22	B	845	BCR	C20-C21-C22	3.72	132.62	127.31
17	3	606	CHL	C3B-C4B-NB	3.71	113.95	110.52
17	4	606	CHL	C2D-C1D-ND	3.70	112.83	110.10
22	J	102	BCR	C35-C13-C14	-3.70	117.74	122.92
17	4	607	CHL	CHB-C1B-NB	-3.69	120.35	124.26
17	1	601	CHL	C6-C5-C3	-3.68	108.60	114.62
22	B	846	BCR	C12-C13-C14	3.68	124.59	118.94
17	2	607	CHL	CHD-C4C-C3C	-3.67	119.45	124.84
22	B	801	BCR	C10-C11-C12	3.66	134.64	123.22
22	A	852	BCR	C23-C22-C21	3.66	124.56	118.94
22	A	852	BCR	C36-C18-C17	-3.66	117.80	122.92
22	J	102	BCR	C8-C9-C10	3.65	124.54	118.94
17	3	606	CHL	C4C-C3C-C2C	-3.64	101.60	106.90
22	B	844	BCR	C36-C18-C17	-3.63	117.83	122.92
17	3	606	CHL	CAC-C3C-C4C	3.62	129.50	124.81
22	J	102	BCR	C12-C13-C14	3.61	124.48	118.94
22	K	205	BCR	C10-C11-C12	3.60	134.46	123.22
22	A	853	BCR	C10-C11-C12	3.59	134.41	123.22
17	3	606	CHL	C2D-C1D-ND	3.59	112.75	110.10
24	A	801	CL0	C4C-C3C-C2C	-3.58	101.67	106.90
17	4	607	CHL	CAC-C3C-C4C	3.58	129.45	124.81
22	A	853	BCR	C35-C13-C14	-3.57	117.92	122.92
22	K	202	BCR	C8-C9-C10	3.57	124.41	118.94
21	4	616	LUT	C15-C35-C34	3.57	130.78	123.47
18	B	813	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
17	4	615	CHL	C1D-ND-C4D	-3.56	103.81	106.33
17	1	601	CHL	CHD-C4C-C3C	-3.56	119.61	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	844	BCR	C23-C22-C21	3.55	124.39	118.94
24	A	801	CL0	C1-C2-C3	-3.54	119.92	126.04
22	K	202	BCR	C36-C18-C17	-3.53	117.97	122.92
22	L	306	BCR	C15-C16-C17	3.53	130.71	123.47
22	G	204	BCR	C36-C18-C17	-3.53	117.98	122.92
22	B	844	BCR	C35-C13-C14	-3.52	117.99	122.92
17	2	607	CHL	CAC-C3C-C4C	3.52	129.38	124.81
17	4	606	CHL	CAC-C3C-C4C	3.52	129.37	124.81
22	L	305	BCR	C36-C18-C17	-3.51	118.01	122.92
22	L	306	BCR	C36-C18-C17	-3.50	118.02	122.92
22	B	847	BCR	C35-C13-C14	-3.50	118.02	122.92
18	A	804	CLA	O2D-CGD-O1D	-3.49	117.00	123.84
22	A	848	BCR	C36-C18-C17	-3.49	118.03	122.92
18	B	811	CLA	C3B-C4B-NB	-3.49	107.89	110.23
17	2	601	CHL	CHD-C4C-C3C	-3.49	119.71	124.84
18	1	613	CLA	C3B-C4B-NB	-3.49	107.89	110.23
18	1	608	CLA	C3B-C4B-NB	-3.48	107.90	110.23
22	A	853	BCR	C11-C10-C9	3.48	132.28	127.31
18	1	612	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
22	L	305	BCR	C35-C13-C14	-3.47	118.06	122.92
18	A	804	CLA	CAA-C2A-C3A	-3.47	103.28	112.78
22	B	801	BCR	C35-C13-C14	-3.47	118.07	122.92
17	4	605	CHL	C3D-C4D-ND	3.46	115.84	110.24
17	4	615	CHL	CAC-C3C-C4C	3.46	129.30	124.81
18	1	610	CLA	C3B-C4B-NB	-3.46	107.92	110.23
21	1	616	LUT	C20-C13-C14	-3.45	118.09	122.92
19	4	617	XAT	C35-C15-C14	3.45	130.54	123.47
22	K	205	BCR	C35-C13-C14	-3.45	118.09	122.92
22	K	202	BCR	C19-C18-C17	3.44	124.22	118.94
18	3	605	CLA	C3B-C4B-NB	-3.44	107.92	110.23
18	A	813	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
18	4	604	CLA	C3B-C4B-NB	-3.44	107.93	110.23
22	B	849	BCR	C35-C13-C14	-3.44	118.11	122.92
22	K	205	BCR	C23-C22-C21	3.44	124.21	118.94
17	2	605	CHL	CHD-C4C-C3C	-3.41	119.65	124.98
18	2	610	CLA	C3B-C4B-NB	-3.41	107.94	110.23
21	1	616	LUT	C39-C29-C30	-3.41	118.15	122.92
17	4	605	CHL	CHD-C4C-C3C	-3.41	119.66	124.98
17	2	615	CHL	CAC-C3C-C4C	3.41	129.23	124.81
17	2	606	CHL	CAC-C3C-C4C	3.40	129.23	124.81
22	A	853	BCR	C12-C13-C14	3.40	124.16	118.94
17	4	607	CHL	C1D-ND-C4D	-3.39	103.92	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	607	CHL	C2D-C1D-ND	3.39	112.60	110.10
17	1	606	CHL	CAC-C3C-C4C	3.38	129.20	124.81
22	B	845	BCR	C21-C20-C19	3.38	133.76	123.22
17	2	615	CHL	CHD-C4C-C3C	-3.37	119.88	124.84
17	4	615	CHL	C3D-C4D-ND	3.37	115.69	110.24
17	1	601	CHL	CAC-C3C-C4C	3.37	129.18	124.81
22	A	852	BCR	C15-C16-C17	3.37	130.38	123.47
17	3	606	CHL	C3D-C4D-ND	3.37	115.69	110.24
22	4	618	BCR	C15-C16-C17	3.37	130.37	123.47
22	4	618	BCR	C35-C13-C14	-3.36	118.22	122.92
17	4	605	CHL	C3B-C4B-NB	3.35	113.63	110.52
19	4	617	XAT	C20-C13-C14	-3.35	118.23	122.92
17	4	607	CHL	C3D-C4D-ND	3.35	115.65	110.24
18	4	614	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
22	K	202	BCR	C23-C22-C21	3.34	124.07	118.94
17	1	606	CHL	CHC-C4B-NB	-3.34	120.72	124.26
22	A	851	BCR	C35-C13-C14	-3.34	118.25	122.92
22	B	845	BCR	C35-C13-C14	-3.33	118.26	122.92
24	A	801	CL0	CHC-C1C-C2C	-3.33	117.48	126.73
17	4	606	CHL	C3D-C4D-ND	3.33	115.62	110.24
17	1	601	CHL	C3D-C4D-ND	3.33	115.62	110.24
17	4	606	CHL	C1D-ND-C4D	-3.32	103.97	106.33
22	B	848	BCR	C36-C18-C17	-3.32	118.27	122.92
22	B	849	BCR	C15-C16-C17	3.32	130.28	123.47
18	3	605	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
22	3	614	BCR	C35-C13-C14	-3.32	118.27	122.92
17	2	606	CHL	CHD-C4C-C3C	-3.32	119.96	124.84
17	2	606	CHL	C3D-C4D-ND	3.32	115.61	110.24
17	3	606	CHL	C1D-ND-C4D	-3.32	103.98	106.33
18	4	603	CLA	C3B-C4B-NB	-3.31	108.01	110.23
22	A	851	BCR	C36-C18-C17	-3.31	118.28	122.92
22	B	849	BCR	C12-C13-C14	3.31	124.02	118.94
17	2	601	CHL	C3D-C4D-ND	3.31	115.59	110.24
17	1	601	CHL	C2D-C1D-ND	3.30	112.54	110.10
22	A	849	BCR	C1-C6-C5	-3.30	117.97	122.61
19	4	617	XAT	C40-C33-C34	-3.29	118.32	122.92
22	B	847	BCR	C12-C13-C14	3.29	123.98	118.94
22	B	844	BCR	C12-C13-C14	3.28	123.97	118.94
22	F	304	BCR	C37-C22-C21	-3.28	118.33	122.92
22	A	849	BCR	C20-C21-C22	3.28	131.99	127.31
17	2	605	CHL	C2D-C1D-ND	3.28	112.52	110.10
21	1	616	LUT	C12-C13-C14	3.28	123.97	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	601	CHL	C1-C2-C3	-3.28	120.38	126.04
19	2	617	XAT	C32-C33-C34	3.27	123.97	118.94
17	2	601	CHL	CAC-C3C-C4C	3.27	129.06	124.81
22	B	849	BCR	C36-C18-C17	-3.27	118.34	122.92
22	F	304	BCR	C1-C6-C5	-3.27	118.00	122.61
17	2	607	CHL	C3D-C4D-ND	3.27	115.52	110.24
22	G	204	BCR	C19-C18-C17	3.26	123.95	118.94
22	L	306	BCR	C19-C18-C17	3.26	123.95	118.94
22	L	305	BCR	C19-C18-C17	3.26	123.94	118.94
22	B	801	BCR	C36-C18-C17	-3.26	118.36	122.92
22	L	301	BCR	C19-C18-C17	3.25	123.93	118.94
22	L	305	BCR	C12-C13-C14	3.25	123.93	118.94
21	1	616	LUT	C35-C15-C14	3.25	130.13	123.47
22	A	848	BCR	C19-C18-C17	3.25	123.92	118.94
18	A	814	CLA	C3B-C4B-NB	-3.25	107.50	110.52
22	I	101	BCR	C36-C18-C17	-3.24	118.38	122.92
17	2	607	CHL	C1-C2-C3	-3.23	121.52	126.75
21	2	616	LUT	C35-C34-C33	3.22	131.91	127.31
17	4	605	CHL	C2D-C1D-ND	3.22	112.48	110.10
18	A	803	CLA	C3B-C4B-NB	-3.22	107.53	110.52
18	L	303	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
18	A	835	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
22	F	304	BCR	C10-C11-C12	3.21	133.23	123.22
22	B	846	BCR	C8-C9-C10	3.21	123.86	118.94
17	2	601	CHL	C2D-C1D-ND	3.20	112.46	110.10
22	B	801	BCR	C12-C13-C14	3.20	123.85	118.94
24	A	801	CL0	CHB-C1B-C2B	-3.20	118.20	127.24
17	2	615	CHL	C2D-C1D-ND	3.20	112.46	110.10
17	4	607	CHL	C3B-C4B-NB	3.19	113.48	110.52
22	B	843	BCR	C15-C14-C13	3.19	131.86	127.31
18	A	844	CLA	C3B-C4B-NB	-3.19	107.56	110.52
17	2	606	CHL	C3B-C4B-NB	3.19	113.47	110.52
18	A	810	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
21	3	613	LUT	C19-C9-C10	-3.18	118.47	122.92
22	3	614	BCR	C15-C16-C17	3.18	129.98	123.47
22	3	614	BCR	C36-C18-C17	-3.17	118.48	122.92
22	J	102	BCR	C36-C18-C17	-3.17	118.49	122.92
22	4	618	BCR	C36-C18-C17	-3.17	118.49	122.92
22	G	204	BCR	C35-C13-C14	-3.16	118.49	122.92
17	4	605	CHL	C1D-ND-C4D	-3.16	104.09	106.33
18	B	825	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
18	B	822	CLA	CAA-C2A-C3A	-3.16	104.13	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	606	CHL	C2D-C1D-ND	3.16	112.43	110.10
17	2	615	CHL	CHC-C4B-NB	-3.15	120.92	124.26
22	A	850	BCR	C16-C17-C18	3.15	131.81	127.31
22	A	853	BCR	C36-C18-C17	-3.15	118.51	122.92
18	B	827	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
22	A	848	BCR	C35-C13-C14	-3.14	118.52	122.92
17	2	615	CHL	C3B-C4B-NB	3.13	113.42	110.52
21	4	616	LUT	C40-C33-C34	-3.13	118.54	122.92
18	B	814	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
18	B	837	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
17	4	605	CHL	CMB-C2B-C1B	3.12	130.12	125.37
21	2	616	LUT	C20-C13-C14	-3.12	118.56	122.92
18	B	822	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
17	2	615	CHL	C3D-C4D-ND	3.11	115.26	110.24
17	1	606	CHL	C3D-C4D-ND	3.10	115.26	110.24
22	F	304	BCR	C8-C9-C10	3.10	123.70	118.94
22	B	801	BCR	C7-C8-C9	-3.10	121.55	126.23
18	B	808	CLA	C3B-C4B-NB	-3.10	107.64	110.52
22	A	849	BCR	C35-C13-C14	-3.10	118.58	122.92
17	2	601	CHL	C3B-C4B-NB	3.09	113.38	110.52
17	4	605	CHL	CMD-C2D-C3D	-3.09	120.50	127.61
22	K	205	BCR	C21-C20-C19	3.09	132.85	123.22
18	B	804	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
22	B	801	BCR	C11-C10-C9	3.09	131.71	127.31
22	A	850	BCR	C15-C14-C13	3.08	131.71	127.31
24	A	801	CL0	O2A-CGA-CBA	3.08	121.57	111.91
18	B	832	CLA	C3B-C4B-NB	-3.08	107.66	110.52
18	F	301	CLA	C3B-C4B-NB	-3.07	107.66	110.52
18	B	828	CLA	C3B-C4B-NB	-3.07	107.67	110.52
18	A	802	CLA	CHB-C4A-NA	3.07	128.76	124.51
18	4	601	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
18	4	609	CLA	C3B-C4B-NB	-3.07	107.67	110.52
22	B	801	BCR	C15-C16-C17	3.07	129.75	123.47
17	4	607	CHL	CMB-C2B-C1B	3.06	130.03	125.37
22	B	845	BCR	C12-C13-C14	3.06	123.64	118.94
22	A	849	BCR	C37-C22-C21	-3.06	118.64	122.92
18	B	819	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	A	850	BCR	C8-C9-C10	3.06	123.63	118.94
17	2	605	CHL	C3D-C4D-ND	3.06	115.18	110.24
24	A	801	CL0	CAC-C3C-C4C	3.06	128.77	124.81
22	B	801	BCR	C34-C9-C10	-3.05	118.64	122.92
22	A	851	BCR	C20-C21-C22	3.05	131.67	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	2	617	XAT	C40-C33-C34	-3.05	118.66	122.92
19	4	617	XAT	C8-C9-C10	3.05	123.62	118.94
18	B	805	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
18	A	809	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
18	B	826	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
18	B	803	CLA	CHB-C4A-NA	3.03	128.70	124.51
22	4	618	BCR	C12-C13-C14	3.03	123.59	118.94
18	A	840	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	B	849	BCR	C19-C18-C17	3.03	123.58	118.94
18	B	841	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
22	I	101	BCR	C35-C13-C14	-3.02	118.69	122.92
18	A	810	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
18	B	818	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
22	A	849	BCR	C16-C17-C18	3.02	131.62	127.31
18	B	833	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
18	B	812	CLA	C3B-C4B-NB	-3.02	107.72	110.52
21	4	616	LUT	C35-C15-C14	3.02	129.65	123.47
22	B	846	BCR	C36-C18-C17	-3.01	118.70	122.92
18	A	830	CLA	CHB-C4A-NA	3.01	128.68	124.51
17	1	601	CHL	CHC-C4B-NB	-3.01	121.07	124.26
18	A	838	CLA	C3B-C4B-NB	-3.01	107.73	110.52
22	A	853	BCR	C15-C16-C17	3.01	129.63	123.47
18	3	608	CLA	CAA-C2A-C3A	-3.01	109.09	116.10
19	2	617	XAT	C20-C13-C14	-3.00	118.72	122.92
18	1	608	CLA	CAA-C2A-C3A	-3.00	109.11	116.10
22	B	848	BCR	C35-C13-C14	-3.00	118.73	122.92
22	B	843	BCR	C36-C18-C17	-2.99	118.73	122.92
18	G	201	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
24	A	801	CL0	CMC-C2C-C1C	2.99	129.59	125.04
21	3	613	LUT	C8-C9-C10	2.98	123.52	118.94
18	1	609	CLA	CHB-C4A-NA	2.98	128.64	124.51
18	H	201	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
18	B	807	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
18	3	607	CLA	C3B-C4B-NB	-2.98	107.75	110.52
17	2	606	CHL	CMB-C2B-C1B	2.98	129.90	125.37
17	1	601	CHL	C3B-C4B-NB	2.97	113.27	110.52
22	F	304	BCR	C19-C18-C17	2.97	123.50	118.94
18	A	810	CLA	C1-C2-C3	-2.97	121.94	126.75
18	K	204	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
21	2	619	LUT	C28-C29-C30	2.97	123.50	118.94
18	B	832	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	B	848	BCR	C19-C18-C17	2.97	123.50	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	616	LUT	C20-C13-C14	-2.97	118.76	122.92
18	B	836	CLA	C3B-C4B-NB	-2.97	107.76	110.52
17	2	607	CHL	CMB-C2B-C1B	2.97	129.89	125.37
18	2	610	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
18	B	838	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
19	1	614	XAT	C27-C28-C29	-2.97	120.92	125.53
19	1	614	XAT	C15-C14-C13	-2.97	123.08	127.31
18	A	826	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
18	F	303	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
18	B	805	CLA	C3B-C4B-NB	-2.97	107.76	110.52
18	B	815	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
17	4	606	CHL	CMB-C2B-C1B	2.96	129.88	125.37
18	A	810	CLA	C3B-C4B-NB	-2.96	107.77	110.52
22	A	853	BCR	C34-C9-C10	-2.96	118.77	122.92
22	B	847	BCR	C36-C18-C17	-2.96	118.77	122.92
18	K	203	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
19	4	617	XAT	C12-C13-C14	2.96	123.48	118.94
22	L	305	BCR	C23-C22-C21	2.96	123.48	118.94
21	2	616	LUT	C30-C31-C32	2.96	132.45	123.22
18	A	834	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
18	B	820	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	A	815	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	B	823	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	2	602	CLA	C3B-C4B-NB	-2.95	107.78	110.52
18	A	844	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
18	B	811	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
18	4	613	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
17	4	615	CHL	CMB-C2B-C1B	2.95	129.86	125.37
22	A	852	BCR	C1-C6-C5	-2.95	118.46	122.61
18	2	612	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
19	2	617	XAT	C30-C31-C32	2.95	132.42	123.22
19	2	617	XAT	C12-C13-C14	2.95	123.46	118.94
18	4	612	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
17	2	607	CHL	C3B-C4B-NB	2.95	113.25	110.52
22	L	306	BCR	C10-C11-C12	2.94	132.40	123.22
17	1	601	CHL	C1D-ND-C4D	-2.93	104.25	106.33
18	A	832	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	A	821	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	A	838	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
21	3	613	LUT	C20-C13-C14	-2.93	118.82	122.92
18	A	833	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	B	836	CLA	O2D-CGD-O1D	-2.93	118.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	614	BCR	C12-C13-C14	2.93	123.43	118.94
18	2	604	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
17	1	601	CHL	CMB-C2B-C1B	2.92	129.81	125.37
18	A	820	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
18	L	302	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
18	L	302	CLA	C3B-C4B-NB	-2.91	107.81	110.52
18	2	602	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
18	A	823	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
18	1	603	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
18	4	601	CLA	C3B-C4B-NB	-2.90	107.82	110.52
18	1	611	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
18	A	845	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
18	3	601	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
18	4	602	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	4	617	XAT	C32-C33-C34	2.90	123.39	118.94
18	A	842	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
18	A	807	CLA	C3B-C4B-NB	-2.90	107.83	110.52
21	1	616	LUT	C8-C9-C10	2.90	123.39	118.94
18	2	604	CLA	C3B-C4B-NB	-2.89	107.83	110.52
18	1	604	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	A	851	BCR	C19-C18-C17	2.89	123.38	118.94
17	3	606	CHL	CMB-C2B-C1B	2.89	129.78	125.37
18	B	840	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	B	817	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	A	827	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	4	611	CLA	C3B-C4B-NB	-2.89	107.84	110.52
18	4	613	CLA	CHB-C4A-NA	2.89	128.50	124.51
17	2	605	CHL	CMB-C2B-C1B	2.89	129.77	125.37
18	A	808	CLA	C3B-C4B-NB	-2.89	107.84	110.52
18	B	802	CLA	C3B-C4B-NB	-2.89	107.84	110.52
17	3	606	CHL	CMD-C2D-C3D	-2.88	120.98	127.61
18	B	830	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
18	B	824	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
18	3	604	CLA	C3B-C4B-NB	-2.88	107.84	110.52
24	A	801	CL0	C2A-C1A-CHA	-2.88	117.24	123.39
18	B	816	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
17	1	601	CHL	O2A-CGA-CBA	2.87	120.93	111.91
24	A	801	CL0	C4-C3-C5	2.87	120.11	115.27
18	A	819	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
18	A	837	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
18	3	608	CLA	CMA-C3A-C2A	-2.87	109.39	116.10
17	2	615	CHL	CMD-C2D-C3D	-2.87	121.00	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	836	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	L	306	BCR	C7-C8-C9	2.87	130.57	126.23
17	2	601	CHL	CMD-C2D-C3D	-2.87	121.01	127.61
18	4	610	CLA	C3B-C4B-NB	-2.87	107.85	110.52
17	2	606	CHL	CMD-C2D-C3D	-2.87	121.01	127.61
21	2	616	LUT	C12-C13-C14	2.87	123.34	118.94
18	A	840	CLA	C3B-C4B-NB	-2.87	107.86	110.52
17	2	615	CHL	CMB-C2B-C1B	2.86	129.73	125.37
18	A	837	CLA	C3B-C4B-NB	-2.86	107.86	110.52
18	B	810	CLA	C3B-C4B-NB	-2.86	107.86	110.52
18	A	805	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	A	802	CLA	C3B-C4B-NB	-2.86	107.86	110.52
22	A	848	BCR	C16-C15-C14	2.86	129.33	123.47
17	1	606	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
18	1	602	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	2	607	CHL	O2A-CGA-CBA	2.86	120.88	111.91
18	3	611	CLA	C3B-C4B-NB	-2.86	107.86	110.52
18	A	812	CLA	C3B-C4B-NB	-2.86	107.86	110.52
18	A	828	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	2	607	CHL	C1D-ND-C4D	-2.86	104.30	106.33
18	B	810	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
18	A	816	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
18	B	817	CLA	C3B-C4B-NB	-2.86	107.86	110.52
18	A	806	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
18	3	602	CLA	C3B-C4B-NB	-2.85	107.87	110.52
18	3	607	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	F	304	BCR	C36-C18-C17	-2.85	118.93	122.92
18	B	821	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	A	801	CL0	C4D-C3D-C2D	2.85	109.09	106.75
18	1	609	CLA	C3B-C4B-NB	-2.85	107.87	110.52
18	A	835	CLA	C3B-C4B-NB	-2.85	107.87	110.52
18	B	802	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	A	825	CLA	C3B-C4B-NB	-2.85	107.87	110.52
18	A	839	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	J	101	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
17	4	605	CHL	CAC-C3C-C4C	2.85	129.37	125.04
18	A	807	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	A	811	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	A	822	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	A	813	CLA	C3B-C4B-NB	-2.84	107.88	110.52
18	A	831	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
18	B	831	CLA	O2D-CGD-O1D	-2.84	118.28	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	603	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
18	A	819	CLA	C3B-C4B-NB	-2.84	107.88	110.52
18	B	813	CLA	O2D-CGD-CBD	2.84	116.32	111.27
22	A	851	BCR	C24-C23-C22	-2.84	121.94	126.23
18	B	834	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
18	B	804	CLA	CAA-C2A-C3A	-2.84	109.48	116.10
21	3	613	LUT	C35-C34-C33	2.84	131.36	127.31
18	J	101	CLA	C3B-C4B-NB	-2.83	107.89	110.52
18	A	836	CLA	C3B-C4B-NB	-2.83	107.89	110.52
17	2	605	CHL	CAC-C3C-C4C	2.83	129.35	125.04
17	2	605	CHL	C3B-C4B-NB	2.83	113.14	110.52
18	B	808	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
18	1	604	CLA	C3B-C4B-NB	-2.83	107.89	110.52
18	B	823	CLA	C3B-C4B-NB	-2.83	107.89	110.52
17	1	601	CHL	CMD-C2D-C3D	-2.83	121.11	127.61
18	A	824	CLA	C3B-C4B-NB	-2.83	107.89	110.52
27	B	850	DGD	C2G-O2G-C1B	-2.83	110.83	117.79
18	B	812	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
18	4	608	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
18	B	835	CLA	C3B-C4B-NB	-2.83	107.89	110.52
17	4	615	CHL	CMD-C2D-C3D	-2.82	121.12	127.61
18	3	610	CLA	C3B-C4B-NB	-2.82	107.89	110.52
18	2	613	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	3	612	CLA	C3B-C4B-NB	-2.82	107.90	110.52
18	B	840	CLA	C3B-C4B-NB	-2.82	107.90	110.52
18	4	604	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	G	203	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	1	608	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	G	204	BCR	C16-C15-C14	2.82	129.24	123.47
18	G	202	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	A	814	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
22	I	101	BCR	C19-C18-C17	2.81	123.26	118.94
18	B	827	CLA	C3B-C4B-NB	-2.81	107.91	110.52
17	1	606	CHL	CMB-C2B-C1B	2.81	129.65	125.37
18	B	803	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
18	K	201	CLA	C3B-C4B-NB	-2.81	107.91	110.52
18	B	828	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
18	B	803	CLA	C3B-C4B-NB	-2.81	107.91	110.52
18	4	610	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	I	101	BCR	C16-C15-C14	2.81	129.23	123.47
19	1	614	XAT	C26-C27-C28	-2.81	120.05	125.99
18	A	824	CLA	O2D-CGD-O1D	-2.81	118.35	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	835	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	B	801	BCR	C19-C18-C17	2.81	123.25	118.94
18	A	822	CLA	C3B-C4B-NB	-2.81	107.91	110.52
18	A	804	CLA	CHB-C4A-NA	2.80	128.39	124.51
18	4	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
17	2	601	CHL	CMB-C2B-C1B	2.80	129.63	125.37
18	A	841	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
18	B	839	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
17	2	601	CHL	C1D-ND-C4D	-2.80	104.35	106.33
18	A	817	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	L	301	BCR	C23-C22-C21	2.80	123.23	118.94
18	B	824	CLA	C3B-C4B-NB	-2.80	107.92	110.52
18	1	610	CLA	CAA-C2A-C3A	-2.80	109.58	116.10
18	1	611	CLA	C3B-C4B-NB	-2.79	107.92	110.52
18	A	829	CLA	C3B-C4B-NB	-2.79	107.92	110.52
18	A	814	CLA	CHB-C4A-NA	2.79	128.37	124.51
18	A	802	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	1	607	CLA	C3B-C4B-NB	-2.79	107.93	110.52
18	B	834	CLA	C3B-C4B-NB	-2.79	107.93	110.52
18	A	819	CLA	CHB-C4A-NA	2.79	128.37	124.51
21	2	619	LUT	C20-C13-C14	-2.79	119.02	122.92
17	4	607	CHL	CMD-C2D-C3D	-2.79	121.20	127.61
18	A	825	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
18	3	609	CLA	C3B-C4B-NB	-2.79	107.93	110.52
18	A	828	CLA	C3B-C4B-NB	-2.79	107.93	110.52
18	F	302	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	F	304	BCR	C37-C22-C23	2.79	122.47	118.08
18	A	821	CLA	C3B-C4B-NB	-2.78	107.93	110.52
18	F	302	CLA	C3B-C4B-NB	-2.78	107.93	110.52
18	3	602	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
18	F	301	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
18	2	610	CLA	C1A-CHA-C4D	-2.78	121.83	125.72
18	F	303	CLA	CAA-C2A-C3A	-2.78	109.62	116.10
18	B	811	CLA	CHB-C4A-NA	2.77	128.35	124.51
18	4	608	CLA	C3B-C4B-NB	-2.77	107.94	110.52
18	4	614	CLA	C3B-C4B-NB	-2.77	107.94	110.52
17	2	605	CHL	CMD-C2D-C3D	-2.77	121.23	127.61
18	A	834	CLA	C3B-C4B-NB	-2.77	107.94	110.52
18	1	604	CLA	CHB-C4A-NA	2.77	128.34	124.51
18	A	843	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
18	F	303	CLA	C3B-C4B-NB	-2.77	107.94	110.52
18	4	614	CLA	CHB-C4A-NA	2.77	128.34	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	825	CLA	CHB-C4A-NA	2.77	128.34	124.51
18	B	819	CLA	C3B-C4B-NB	-2.77	107.95	110.52
18	1	605	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
18	A	839	CLA	C3B-C4B-NB	-2.77	107.95	110.52
21	3	613	LUT	C35-C15-C14	2.77	129.14	123.47
22	J	102	BCR	C15-C16-C17	2.77	129.14	123.47
17	2	607	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
22	B	844	BCR	C30-C25-C26	-2.76	118.72	122.61
18	B	839	CLA	C3B-C4B-NB	-2.76	107.95	110.52
21	2	616	LUT	C19-C9-C8	2.76	122.43	118.08
18	K	204	CLA	C3B-C4B-NB	-2.76	107.95	110.52
17	2	606	CHL	C1D-ND-C4D	-2.76	104.38	106.33
18	2	604	CLA	CHB-C4A-NA	2.76	128.33	124.51
18	A	830	CLA	CAA-C2A-C3A	-2.76	105.23	112.78
18	L	303	CLA	C3B-C4B-NB	-2.76	107.96	110.52
18	B	829	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
18	B	834	CLA	CHB-C4A-NA	2.75	128.32	124.51
18	A	842	CLA	CHB-C4A-NA	2.75	128.31	124.51
18	A	829	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
18	A	828	CLA	CHB-C4A-NA	2.75	128.31	124.51
18	B	807	CLA	C3B-C4B-NB	-2.75	107.97	110.52
18	2	609	CLA	CHB-C4A-NA	2.75	128.31	124.51
18	A	824	CLA	CAA-C2A-C3A	-2.75	109.69	116.10
18	4	609	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	B	816	CLA	C3B-C4B-NB	-2.74	107.97	110.52
18	2	608	CLA	CHB-C4A-NA	2.74	128.30	124.51
18	B	822	CLA	C1-C2-C3	-2.74	121.30	126.04
18	2	613	CLA	C3B-C4B-NB	-2.74	107.97	110.52
18	A	816	CLA	C3B-C4B-NB	-2.74	107.97	110.52
18	B	838	CLA	C3B-C4B-NB	-2.74	107.98	110.52
18	K	206	CLA	C3B-C4B-NB	-2.73	107.98	110.52
18	A	830	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
18	3	607	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	L	303	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	A	817	CLA	C3B-C4B-NB	-2.73	107.98	110.52
18	4	601	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	L	304	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
18	G	201	CLA	C3B-C4B-NB	-2.73	107.98	110.52
18	1	612	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	A	803	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
18	B	806	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
18	1	602	CLA	C3B-C4B-NB	-2.72	107.99	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	822	CLA	CHB-C4A-NA	2.72	128.28	124.51
18	L	304	CLA	CHB-C4A-NA	2.72	128.28	124.51
18	A	802	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
18	B	821	CLA	CHB-C4A-NA	2.72	128.28	124.51
18	G	202	CLA	C3B-C4B-NB	-2.72	107.99	110.52
18	A	805	CLA	CHB-C4A-NA	2.72	128.27	124.51
18	B	809	CLA	CHB-C4A-NA	2.72	128.27	124.51
18	2	608	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	3	608	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	K	202	BCR	C10-C11-C12	2.72	131.70	123.22
18	3	612	CLA	CAA-C2A-C3A	-2.72	109.75	116.10
18	B	809	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
17	4	605	CHL	CHC-C4B-NB	-2.72	121.38	124.26
18	3	612	CLA	O2D-CGD-O1D	-2.72	117.92	124.09
18	1	605	CLA	C3B-C4B-NB	-2.72	108.00	110.52
18	2	609	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
18	A	835	CLA	CHB-C4A-NA	2.71	128.26	124.51
21	2	619	LUT	C7-C8-C9	-2.71	122.14	126.23
22	B	844	BCR	C8-C9-C10	2.71	123.09	118.94
18	B	804	CLA	C3B-C4B-NB	-2.70	108.01	110.52
18	4	609	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	B	848	BCR	C16-C15-C14	2.70	129.01	123.47
18	2	611	CLA	CHB-C4A-NA	2.70	128.25	124.51
18	A	845	CLA	C3B-C4B-NB	-2.70	108.01	110.52
18	B	841	CLA	CHB-C4A-NA	2.70	128.24	124.51
17	2	601	CHL	O2D-CGD-O1D	-2.70	118.56	123.84
18	A	812	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
18	A	808	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
18	A	809	CLA	CHB-C4A-NA	2.70	128.24	124.51
18	B	833	CLA	CAA-C2A-C3A	-2.70	105.40	112.78
18	A	843	CLA	CHB-C4A-NA	2.69	128.24	124.51
24	A	801	CL0	CHB-C1B-NB	-2.69	121.41	124.26
18	B	822	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	4	618	BCR	C19-C18-C17	2.69	123.07	118.94
18	A	813	CLA	CHB-C4A-NA	2.69	128.23	124.51
18	A	832	CLA	C3B-C4B-NB	-2.69	108.02	110.52
18	H	201	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	A	853	BCR	C19-C18-C17	2.69	123.07	118.94
22	B	844	BCR	C19-C18-C17	2.69	123.06	118.94
18	K	206	CLA	CBD-CHA-C1A	2.69	131.67	128.50
17	2	605	CHL	CHC-C4B-NB	-2.69	121.41	124.26
18	A	815	CLA	C3B-C4B-NB	-2.69	108.02	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	613	CLA	CAA-C2A-C3A	-2.69	109.83	116.10
18	3	611	CLA	CAA-C2A-C3A	-2.69	109.83	116.10
18	3	612	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	A	852	BCR	C12-C13-C14	2.68	123.06	118.94
24	A	801	CL0	CMD-C2D-C3D	-2.68	121.73	128.30
17	4	606	CHL	CMD-C2D-C3D	-2.68	121.44	127.61
18	4	608	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	B	813	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	B	806	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	B	804	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	A	836	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	A	832	CLA	CHB-C4A-NA	2.68	128.21	124.51
18	B	814	CLA	C3B-C4B-NB	-2.68	108.03	110.52
18	A	829	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	B	839	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	2	602	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	J	102	BCR	C19-C18-C17	2.67	123.04	118.94
18	B	841	CLA	C3B-C4B-NB	-2.67	108.04	110.52
18	A	808	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	A	849	BCR	C36-C18-C17	-2.67	119.18	122.92
18	3	608	CLA	CHB-C4A-NA	2.67	128.20	124.51
18	3	610	CLA	CAA-C2A-C3A	-2.67	109.88	116.10
18	A	833	CLA	CHB-C4A-NA	2.67	128.20	124.51
24	A	801	CL0	CHC-C4B-NB	-2.67	121.44	124.26
22	B	845	BCR	C16-C17-C18	2.67	131.11	127.31
18	A	844	CLA	CHB-C4A-NA	2.66	128.20	124.51
18	B	808	CLA	CHB-C4A-NA	2.66	128.20	124.51
18	A	818	CLA	CHB-C4A-NA	2.66	128.20	124.51
18	A	811	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	B	845	BCR	C37-C22-C21	-2.66	119.19	122.92
18	A	841	CLA	C3B-C4B-NB	-2.66	108.05	110.52
18	1	612	CLA	O2D-CGD-CBD	2.66	116.00	111.27
18	1	603	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	B	827	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	B	840	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	A	834	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	A	812	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	4	610	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	A	849	BCR	C19-C18-C17	2.66	123.02	118.94
22	B	843	BCR	C35-C13-C14	-2.66	119.20	122.92
18	B	818	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	K	201	CLA	CAA-C2A-C3A	-2.66	109.90	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	815	CLA	C3B-C4B-NB	-2.65	108.05	110.52
21	3	613	LUT	C30-C31-C32	2.65	131.50	123.22
21	3	613	LUT	C32-C33-C34	2.65	123.01	118.94
18	B	810	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	A	852	BCR	C21-C20-C19	2.65	131.49	123.22
18	B	837	CLA	C3B-C4B-NB	-2.65	108.06	110.52
18	K	203	CLA	C3B-C4B-NB	-2.65	108.06	110.52
18	B	819	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	A	831	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	B	820	CLA	C1-C2-C3	-2.64	122.47	126.75
18	1	609	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
18	B	833	CLA	C3B-C4B-NB	-2.64	108.06	110.52
18	3	601	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	G	202	CLA	CHB-C4A-NA	2.64	128.17	124.51
17	2	601	CHL	CHC-C4B-NB	-2.64	121.46	124.26
18	A	806	CLA	C3B-C4B-NB	-2.64	108.06	110.52
18	3	610	CLA	O2D-CGD-O1D	-2.64	118.09	124.09
18	B	830	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	4	602	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	B	817	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	A	804	CLA	C3B-C4B-NB	-2.64	108.07	110.52
18	B	837	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	B	813	CLA	C3B-C4B-NB	-2.64	108.07	110.52
18	3	603	CLA	CHB-C4A-NA	2.63	128.16	124.51
22	A	849	BCR	C16-C15-C14	2.63	128.86	123.47
18	B	824	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	A	840	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	B	831	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	1	602	CLA	CHB-C4A-NA	2.63	128.14	124.51
22	A	848	BCR	C12-C13-C14	2.63	122.97	118.94
18	B	829	CLA	C3B-C4B-NB	-2.63	108.08	110.52
18	1	607	CLA	CHB-C4A-NA	2.63	128.14	124.51
18	A	813	CLA	O2D-CGD-CBD	2.62	115.93	111.27
22	3	614	BCR	C19-C18-C17	2.62	122.97	118.94
18	A	827	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	B	828	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	A	821	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	4	604	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	A	805	CLA	C3B-C4B-NB	-2.62	108.08	110.52
18	B	830	CLA	C3B-C4B-NB	-2.62	108.08	110.52
18	3	605	CLA	CHB-C4A-NA	2.62	128.13	124.51
18	4	602	CLA	C3B-C4B-NB	-2.62	108.09	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	820	CLA	CHB-C4A-NA	2.62	128.13	124.51
18	A	833	CLA	C3B-C4B-NB	-2.62	108.09	110.52
18	2	610	CLA	CAB-C3B-C2B	2.61	130.36	123.59
18	2	603	CLA	C3B-C4B-NB	-2.61	108.09	110.52
18	A	825	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	A	841	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	1	603	CLA	C3B-C4B-NB	-2.61	108.09	110.52
18	4	611	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	G	203	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	3	603	CLA	C3B-C4B-NB	-2.61	108.09	110.52
24	A	801	CL0	CMB-C2B-C1B	2.61	129.34	125.37
18	3	601	CLA	C3B-C4B-NB	-2.61	108.10	110.52
17	2	605	CHL	C1D-ND-C4D	-2.61	104.48	106.33
18	2	603	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	B	814	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	B	812	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	B	815	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	G	201	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	B	821	CLA	C3B-C4B-NB	-2.60	108.10	110.52
18	B	807	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	1	610	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	B	838	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	K	203	CLA	CHB-C4A-NA	2.60	128.10	124.51
18	1	613	CLA	CHB-C4A-NA	2.60	128.10	124.51
18	A	816	CLA	CHB-C4A-NA	2.60	128.10	124.51
18	2	609	CLA	C3B-C4B-NB	-2.59	108.11	110.52
18	B	831	CLA	C3B-C4B-NB	-2.59	108.11	110.52
18	3	608	CLA	C3B-C4B-NB	-2.59	108.11	110.52
18	A	827	CLA	C3B-C4B-NB	-2.59	108.11	110.52
18	1	608	CLA	CHB-C4A-NA	2.59	128.10	124.51
18	B	826	CLA	CHB-C4A-NA	2.59	128.10	124.51
17	2	615	CHL	C1D-ND-C4D	-2.59	104.49	106.33
18	4	612	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	A	809	CLA	C3B-C4B-NB	-2.59	108.11	110.52
18	A	811	CLA	C3B-C4B-NB	-2.59	108.11	110.52
18	B	825	CLA	C3B-C4B-NB	-2.59	108.11	110.52
18	A	845	CLA	CHB-C4A-NA	2.58	128.09	124.51
18	B	816	CLA	CHB-C4A-NA	2.58	128.08	124.51
18	4	613	CLA	C3B-C4B-NB	-2.58	108.12	110.52
18	A	820	CLA	C3B-C4B-NB	-2.58	108.12	110.52
18	B	826	CLA	C3B-C4B-NB	-2.58	108.12	110.52
18	A	838	CLA	CHB-C4A-NA	2.58	128.08	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	616	LUT	C32-C33-C34	2.58	122.90	118.94
18	A	826	CLA	CHB-C4A-NA	2.58	128.08	124.51
18	A	826	CLA	C3B-C4B-NB	-2.58	108.12	110.52
18	A	806	CLA	CHB-C4A-NA	2.58	128.07	124.51
18	K	201	CLA	CHB-C4A-NA	2.58	128.07	124.51
22	B	849	BCR	C23-C22-C21	2.57	122.89	118.94
18	B	832	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	B	836	CLA	C1-C2-C3	-2.57	122.59	126.75
18	A	839	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	B	833	CLA	CHB-C4A-NA	2.57	128.07	124.51
21	3	613	LUT	C40-C33-C34	-2.57	119.32	122.92
18	A	842	CLA	CMB-C2B-C1B	-2.57	121.45	125.37
18	J	101	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	2	612	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	A	822	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	F	303	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	L	302	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	K	206	CLA	O2D-CGD-O1D	-2.56	118.27	124.09
19	1	614	XAT	C6-C7-C8	-2.56	120.57	125.99
18	A	815	CLA	CHB-C4A-NA	2.56	128.06	124.51
18	A	803	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	A	837	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	1	613	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
18	A	810	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	H	201	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	F	304	BCR	C16-C17-C18	2.56	130.96	127.31
22	A	850	BCR	C35-C13-C14	-2.56	119.34	122.92
18	A	824	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	1	611	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	B	808	CLA	O2A-CGA-O1A	-2.55	117.14	123.59
21	2	616	LUT	C35-C15-C14	2.55	128.70	123.47
18	1	612	CLA	C3B-C4B-NB	-2.55	108.15	110.52
18	A	823	CLA	CHB-C4A-NA	2.55	128.03	124.51
18	B	829	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	G	204	BCR	C12-C13-C14	2.55	122.85	118.94
18	A	832	CLA	C1-C2-C3	-2.55	122.63	126.75
21	3	613	LUT	C11-C10-C9	2.54	130.94	127.31
18	B	835	CLA	CHB-C4A-NA	2.54	128.03	124.51
18	2	611	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
18	2	608	CLA	C3B-C4B-NB	-2.54	108.16	110.52
18	2	613	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	B	805	CLA	CHB-C4A-NA	2.54	128.02	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	606	CHL	CHD-C4C-C3C	-2.53	121.11	124.84
18	A	820	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	B	802	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	A	849	BCR	C12-C13-C14	2.53	122.83	118.94
18	B	806	CLA	C3B-C4B-NB	-2.53	108.17	110.52
18	B	820	CLA	C3B-C4B-NB	-2.53	108.17	110.52
18	3	610	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	2	603	CLA	O2D-CGD-O1D	-2.53	118.35	124.09
17	2	606	CHL	CHC-C4B-NB	-2.53	121.58	124.26
18	A	807	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	1	605	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	3	609	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	A	818	CLA	C3B-C4B-NB	-2.52	108.18	110.52
18	3	604	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	G	203	CLA	C3B-C4B-NB	-2.52	108.18	110.52
18	L	304	CLA	C3B-C4B-NB	-2.51	108.18	110.52
18	A	823	CLA	C3B-C4B-NB	-2.51	108.18	110.52
22	B	846	BCR	C15-C16-C17	2.51	128.62	123.47
18	3	611	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	L	301	BCR	C10-C11-C12	2.51	131.05	123.22
18	3	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	1	607	CLA	O2D-CGD-O1D	-2.50	118.41	124.09
18	3	609	CLA	O2D-CGD-O1D	-2.50	118.41	124.09
18	4	611	CLA	O2D-CGD-O1D	-2.50	118.41	124.09
18	A	831	CLA	C3B-C4B-NB	-2.50	108.19	110.52
18	A	817	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	2	617	XAT	C35-C34-C33	2.50	130.88	127.31
18	3	604	CLA	O2D-CGD-O1D	-2.50	118.42	124.09
18	K	203	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
22	A	850	BCR	C12-C13-C14	2.50	122.77	118.94
18	1	610	CLA	O2D-CGD-O1D	-2.49	118.43	124.09
18	A	843	CLA	C3B-C4B-NB	-2.49	108.21	110.52
21	4	616	LUT	C19-C9-C8	2.49	122.00	118.08
18	4	603	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	B	801	BCR	C23-C22-C21	2.49	122.76	118.94
18	K	204	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	F	301	CLA	CHB-C4A-NA	2.48	127.95	124.51
18	B	836	CLA	CHB-C4A-NA	2.48	127.95	124.51
18	B	809	CLA	C3B-C4B-NB	-2.48	108.21	110.52
27	B	850	DGD	O1G-C1A-C2A	2.48	119.69	111.91
21	4	616	LUT	C39-C29-C28	2.47	121.97	118.08
18	2	612	CLA	C3B-C4B-NB	-2.47	108.22	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	603	CLA	CAB-C3B-C2B	2.47	129.98	123.59
18	1	613	CLA	CAB-C3B-C2B	2.47	129.98	123.59
18	1	610	CLA	CAB-C3B-C2B	2.46	129.95	123.59
18	B	823	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	G	204	BCR	C23-C22-C21	2.45	122.70	118.94
18	1	608	CLA	CAB-C3B-C2B	2.45	129.94	123.59
18	4	612	CLA	C3B-C4B-NB	-2.45	108.25	110.52
18	B	811	CLA	CAB-C3B-C2B	2.44	129.91	123.59
21	3	613	LUT	C10-C11-C12	2.44	130.82	123.22
17	1	601	CHL	C4-C3-C5	2.44	119.37	115.27
17	1	606	CHL	CHD-C1D-C2D	2.44	130.59	125.48
18	2	611	CLA	C3B-C4B-NB	-2.43	108.26	110.52
18	B	818	CLA	C3B-C4B-NB	-2.43	108.26	110.52
19	2	617	XAT	C8-C9-C10	2.43	122.67	118.94
22	B	849	BCR	C30-C25-C24	2.43	122.66	115.78
18	B	816	CLA	C1-C2-C3	-2.43	121.84	126.04
18	3	605	CLA	CAB-C3B-C2B	2.43	129.88	123.59
18	1	608	CLA	CMB-C2B-C3B	2.43	129.88	123.59
22	K	202	BCR	C30-C25-C24	2.43	122.64	115.78
22	B	846	BCR	C10-C11-C12	2.42	130.76	123.22
22	K	205	BCR	C8-C9-C10	2.42	122.65	118.94
17	2	605	CHL	OMC-CMC-C2C	-2.42	120.22	125.69
22	B	847	BCR	C15-C16-C17	2.41	128.42	123.47
22	G	204	BCR	C30-C25-C26	-2.41	119.22	122.61
18	B	818	CLA	C1-C2-C3	-2.41	121.88	126.04
22	A	851	BCR	C15-C14-C13	2.41	130.75	127.31
19	2	617	XAT	C15-C14-C13	2.40	130.74	127.31
18	1	613	CLA	CMB-C2B-C3B	2.40	129.82	123.59
18	A	814	CLA	CHB-C1B-NB	2.40	126.80	124.26
18	F	302	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
22	B	843	BCR	C1-C6-C7	2.40	122.56	115.78
18	B	811	CLA	CMB-C2B-C3B	2.40	129.81	123.59
17	2	607	CHL	C5-C3-C4	2.40	119.90	114.60
18	A	844	CLA	CHB-C1B-NB	2.40	126.79	124.26
22	I	101	BCR	C12-C13-C14	2.39	122.61	118.94
22	K	202	BCR	C30-C25-C26	-2.39	119.25	122.61
22	A	851	BCR	C30-C25-C26	-2.38	119.26	122.61
22	J	102	BCR	C1-C6-C5	-2.38	119.26	122.61
18	4	614	CLA	O2D-CGD-CBD	2.38	115.50	111.27
18	B	821	CLA	CAA-CBA-CGA	-2.38	106.30	113.25
18	2	610	CLA	CMB-C2B-C3B	2.37	129.74	123.59
18	4	604	CLA	CAB-C3B-C2B	2.37	129.72	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	606	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
22	L	306	BCR	C1-C6-C5	-2.37	119.28	122.61
18	1	610	CLA	CMB-C2B-C3B	2.36	129.72	123.59
22	B	846	BCR	C19-C18-C17	2.36	122.57	118.94
18	A	830	CLA	C3B-C4B-NB	-2.36	108.32	110.52
22	J	102	BCR	C10-C11-C12	2.36	130.58	123.22
17	2	606	CHL	C1C-C2C-C3C	-2.36	105.24	107.11
22	K	205	BCR	C16-C15-C14	2.36	128.31	123.47
17	4	615	CHL	CMB-C2B-C3B	2.36	129.70	123.59
22	K	205	BCR	C1-C6-C5	-2.35	119.30	122.61
24	A	801	CL0	C2A-C3A-C4A	-2.35	98.07	101.87
24	A	801	CL0	C4B-CHC-C1C	-2.35	120.77	126.34
17	1	606	CHL	C3B-C4B-NB	2.35	112.69	110.52
17	1	606	CHL	C2D-C1D-ND	2.35	111.83	110.10
22	B	843	BCR	C1-C6-C5	-2.34	119.31	122.61
17	4	606	CHL	CMB-C2B-C3B	2.34	129.66	123.59
18	3	605	CLA	CMB-C2B-C3B	2.34	129.65	123.59
18	A	820	CLA	CMB-C2B-C1B	-2.33	121.81	125.37
22	B	848	BCR	C12-C13-C14	2.33	122.52	118.94
21	3	613	LUT	C12-C13-C14	2.33	122.52	118.94
22	A	850	BCR	C36-C18-C17	-2.33	119.66	122.92
22	B	843	BCR	C12-C13-C14	2.33	122.52	118.94
21	2	616	LUT	C40-C33-C34	-2.33	119.66	122.92
22	K	205	BCR	C30-C25-C26	-2.33	119.33	122.61
18	A	844	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
17	1	601	CHL	O2D-CGD-O1D	-2.32	118.82	124.09
21	4	616	LUT	C12-C13-C14	2.32	122.50	118.94
18	K	206	CLA	CHB-C4A-NA	2.31	127.71	124.51
18	4	609	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
22	B	849	BCR	C34-C9-C8	2.31	121.72	118.08
17	2	615	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
17	2	601	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
22	B	847	BCR	C19-C18-C17	2.31	122.48	118.94
19	2	617	XAT	C27-C28-C29	-2.31	121.95	125.53
18	3	607	CLA	CHB-C1B-NB	2.30	126.70	124.26
18	A	808	CLA	C1-C2-C3	-2.30	123.02	126.75
22	A	851	BCR	C30-C25-C24	2.30	122.29	115.78
18	A	830	CLA	C1-C2-C3	2.30	130.02	126.04
22	J	102	BCR	C23-C22-C21	2.30	122.47	118.94
22	A	851	BCR	C11-C12-C13	2.30	132.87	126.42
18	B	834	CLA	CHD-C1D-ND	-2.29	122.35	124.45
18	4	603	CLA	CMB-C2B-C3B	2.28	129.51	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	828	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
22	I	101	BCR	C34-C9-C8	2.28	121.67	118.08
18	A	842	CLA	C3B-C4B-NB	-2.28	108.40	110.52
21	2	619	LUT	C30-C31-C32	2.28	130.32	123.22
18	A	810	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
18	4	604	CLA	CMB-C2B-C3B	2.27	129.47	123.59
17	4	615	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
17	2	607	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
17	4	605	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
18	A	841	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
18	B	819	CLA	C1-C2-C3	-2.26	122.13	126.04
22	B	843	BCR	C19-C18-C17	2.26	122.41	118.94
20	1	615	LHG	O8-C23-C24	2.26	119.00	111.91
22	A	853	BCR	C30-C25-C24	2.26	122.17	115.78
22	A	853	BCR	C30-C25-C26	-2.26	119.43	122.61
22	B	848	BCR	C30-C25-C24	2.26	122.16	115.78
17	2	605	CHL	O2D-CGD-O1D	-2.26	119.43	123.84
22	L	305	BCR	C30-C25-C24	2.25	122.16	115.78
18	A	845	CLA	C1-C2-C3	-2.25	123.11	126.75
22	A	848	BCR	C23-C22-C21	2.25	122.39	118.94
22	L	305	BCR	C1-C6-C7	2.25	122.14	115.78
18	4	614	CLA	C1-C2-C3	-2.25	123.11	126.75
17	1	601	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
22	L	306	BCR	C21-C20-C19	2.25	130.23	123.22
18	B	828	CLA	CHB-C1B-NB	2.25	126.64	124.26
18	4	602	CLA	CMB-C2B-C1B	-2.24	121.95	125.37
18	B	832	CLA	CHB-C1B-NB	2.24	126.63	124.26
18	B	812	CLA	CHB-C1B-NB	2.24	126.63	124.26
18	A	804	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
22	J	102	BCR	C1-C6-C7	2.24	122.11	115.78
21	2	619	LUT	C15-C14-C13	2.24	130.50	127.31
18	B	818	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
18	B	832	CLA	CHD-C1D-ND	-2.23	122.40	124.45
18	4	609	CLA	C1-C2-C3	-2.23	122.18	126.04
18	A	803	CLA	CHD-C1D-ND	-2.23	122.40	124.45
17	3	606	CHL	O2D-CGD-O1D	-2.23	119.48	123.84
22	L	301	BCR	C8-C9-C10	2.23	122.36	118.94
18	B	821	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
18	B	841	CLA	O2D-CGD-CBD	2.22	115.21	111.27
18	2	609	CLA	CHD-C1D-ND	-2.22	122.41	124.45
22	A	848	BCR	C30-C25-C24	2.22	122.06	115.78
22	K	205	BCR	C30-C25-C24	2.22	122.06	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	835	CLA	O2D-CGD-CBD	2.22	115.21	111.27
17	2	607	CHL	C1C-C2C-C3C	-2.22	105.35	107.11
22	K	205	BCR	C1-C6-C7	2.21	122.04	115.78
17	4	615	CHL	C2A-C1A-CHA	-2.21	119.99	123.86
17	4	605	CHL	C2A-C1A-CHA	-2.21	119.99	123.86
18	A	803	CLA	CHB-C1B-NB	2.21	126.60	124.26
18	B	825	CLA	CMB-C2B-C1B	-2.21	122.01	125.37
18	A	814	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
18	A	810	CLA	CHD-C1D-ND	-2.21	122.43	124.45
22	B	849	BCR	C7-C8-C9	2.21	129.57	126.23
17	4	606	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
21	2	619	LUT	C11-C10-C9	2.20	130.46	127.31
22	B	845	BCR	C8-C9-C10	2.20	122.32	118.94
20	1	615	LHG	C5-O7-C7	-2.20	112.37	117.79
22	B	843	BCR	C16-C17-C18	2.20	130.45	127.31
22	L	305	BCR	C1-C6-C5	-2.20	119.52	122.61
24	A	801	CL0	CHB-C4A-NA	2.20	127.55	124.51
22	J	102	BCR	C7-C8-C9	2.19	129.55	126.23
17	1	606	CHL	O2D-CGD-O1D	-2.19	119.11	124.09
17	4	607	CHL	C2A-C1A-CHA	-2.19	120.03	123.86
18	B	805	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
18	4	609	CLA	CHB-C1B-NB	2.19	126.58	124.26
18	A	844	CLA	CHD-C1D-ND	-2.19	122.44	124.45
18	A	819	CLA	CHD-C1D-ND	-2.19	122.44	124.45
17	4	607	CHL	O2D-CGD-O1D	-2.18	119.57	123.84
18	A	827	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
22	A	852	BCR	C24-C23-C22	2.18	129.53	126.23
18	A	810	CLA	CHB-C1B-NB	2.18	126.57	124.26
18	3	602	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
18	B	839	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
22	K	205	BCR	C12-C13-C14	2.18	122.28	118.94
18	B	816	CLA	CHD-C1D-ND	-2.18	122.45	124.45
18	2	612	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
22	G	204	BCR	C34-C9-C8	2.17	121.50	118.08
18	B	816	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
18	B	836	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
22	A	850	BCR	C19-C18-C17	2.17	122.26	118.94
18	B	808	CLA	C1-C2-C3	-2.16	122.30	126.04
22	L	305	BCR	C8-C9-C10	2.16	122.26	118.94
17	2	615	CHL	OMC-CMC-C2C	-2.16	120.81	125.69
22	K	202	BCR	C21-C20-C19	2.16	129.94	123.22
22	B	848	BCR	C34-C9-C8	2.15	121.47	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	615	CHL	O2D-CGD-O1D	-2.15	119.20	124.09
18	A	821	CLA	CHB-C1B-NB	2.15	126.54	124.26
17	4	607	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
22	A	850	BCR	C1-C6-C7	2.15	121.86	115.78
22	A	848	BCR	C30-C25-C26	-2.15	119.59	122.61
18	K	204	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	B	835	CLA	CHB-C1B-NB	2.15	126.53	124.26
18	A	807	CLA	CHB-C1B-NB	2.15	126.53	124.26
22	B	847	BCR	C8-C9-C10	2.15	122.23	118.94
18	4	609	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	B	814	CLA	CHD-C1D-ND	-2.14	122.48	124.45
18	A	804	CLA	O2D-CGD-CBD	2.14	115.07	111.27
22	L	305	BCR	C30-C25-C26	-2.14	119.60	122.61
18	B	813	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
18	2	609	CLA	CMB-C2B-C1B	-2.14	122.12	125.37
18	B	838	CLA	CHD-C1D-ND	-2.13	122.49	124.45
17	1	601	CHL	C4A-NA-C1A	2.13	107.66	106.71
17	1	606	CHL	C1C-C2C-C3C	-2.13	105.42	107.11
18	A	809	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	L	306	BCR	C1-C6-C7	2.13	121.80	115.78
18	B	837	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	I	101	BCR	C37-C22-C23	2.13	121.43	118.08
18	1	613	CLA	CHD-C1D-ND	-2.13	122.50	124.45
18	A	808	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	A	801	CL0	O2A-CGA-O1A	-2.13	118.22	123.59
18	A	807	CLA	CHD-C1D-ND	-2.13	122.50	124.45
18	L	302	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	B	822	CLA	CHB-C1B-NB	2.12	126.51	124.26
22	A	853	BCR	C1-C6-C5	-2.12	119.62	122.61
18	A	838	CLA	C1-C2-C3	-2.12	122.37	126.04
18	A	841	CLA	C1-C2-C3	-2.12	122.37	126.04
18	B	820	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
21	4	616	LUT	C7-C8-C9	2.12	129.44	126.23
19	1	614	XAT	O24-C25-C26	-2.12	57.20	58.96
18	B	834	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
18	2	611	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
18	A	841	CLA	CHD-C1D-ND	-2.12	122.51	124.45
19	1	614	XAT	C35-C15-C14	-2.12	119.14	123.47
18	B	833	CLA	CHD-C1D-ND	-2.11	122.51	124.45
18	B	826	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
18	B	825	CLA	C1-C2-C3	-2.11	122.39	126.04
18	A	829	CLA	O2A-CGA-O1A	-2.11	118.26	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	614	BCR	C30-C25-C24	2.11	121.75	115.78
22	A	853	BCR	C23-C22-C21	2.11	122.18	118.94
18	B	805	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	F	301	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	B	809	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
19	1	614	XAT	C31-C30-C29	-2.11	124.30	127.31
18	B	814	CLA	O2D-CGD-CBD	2.11	115.01	111.27
18	B	827	CLA	O2D-CGD-CBD	2.11	115.01	111.27
18	A	836	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	2	602	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
18	B	825	CLA	O2D-CGD-CBD	2.10	115.01	111.27
27	B	850	DGD	O2G-C1B-O1B	-2.10	118.62	123.70
18	B	822	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
18	L	303	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	L	303	CLA	O2D-CGD-CBD	2.10	115.00	111.27
18	3	601	CLA	C1-C2-C3	-2.10	122.41	126.04
18	L	302	CLA	CHD-C1D-ND	-2.10	122.53	124.45
18	A	825	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
18	L	304	CLA	CHD-C1D-ND	-2.10	122.53	124.45
17	4	607	CHL	CHB-C4A-NA	2.10	127.41	124.51
18	B	819	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
18	B	829	CLA	CHD-C1D-ND	-2.10	122.53	124.45
18	A	808	CLA	CHB-C1B-NB	2.09	126.47	124.26
17	4	605	CHL	O2D-CGD-O1D	-2.09	119.33	124.09
22	B	843	BCR	C10-C11-C12	2.09	129.75	123.22
18	B	805	CLA	CHD-C1D-ND	-2.09	122.53	124.45
18	B	824	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
17	2	607	CHL	CHC-C4B-NB	-2.09	122.05	124.26
22	3	614	BCR	C8-C9-C10	2.09	122.15	118.94
18	A	834	CLA	CHD-C1D-ND	-2.09	122.53	124.45
18	A	839	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
18	B	803	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
18	B	810	CLA	C1-C2-C3	-2.09	122.43	126.04
22	B	845	BCR	C24-C23-C22	-2.09	123.08	126.23
18	1	604	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
18	B	836	CLA	CHB-C1B-NB	2.08	126.46	124.26
17	4	615	CHL	CHB-C4A-NA	2.08	127.39	124.51
22	3	614	BCR	C37-C22-C23	2.08	121.36	118.08
17	2	606	CHL	C4A-NA-C1A	2.08	107.64	106.71
18	3	608	CLA	CHD-C1D-ND	-2.08	122.54	124.45
18	A	812	CLA	CHD-C1D-ND	-2.08	122.54	124.45
18	A	825	CLA	C1-C2-C3	-2.08	122.44	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	833	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
22	B	845	BCR	C16-C15-C14	2.08	127.73	123.47
18	A	838	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
18	A	802	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	B	831	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	B	829	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
18	B	836	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	B	826	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
18	1	607	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	A	820	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	B	822	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
18	J	101	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
18	2	602	CLA	CHB-C1B-NB	2.07	126.45	124.26
18	4	612	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
18	F	303	CLA	CHB-C1B-NB	2.07	126.45	124.26
17	2	615	CHL	C1C-C2C-C3C	-2.07	105.47	107.11
18	3	603	CLA	CHB-C1B-NB	2.07	126.45	124.26
18	3	604	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	A	810	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
20	2	618	LHG	O7-C7-C8	2.07	115.95	111.50
18	A	822	CLA	CHB-C1B-NB	2.07	126.44	124.26
17	2	601	CHL	O1D-CGD-CBD	-2.06	120.26	124.48
19	1	614	XAT	O4-C5-C6	-2.06	57.25	58.96
17	4	605	CHL	OMC-CMC-C2C	-2.06	121.03	125.69
18	A	831	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
18	B	838	CLA	CHB-C1B-NB	2.06	126.44	124.26
17	2	615	CHL	C4A-NA-C1A	2.06	107.63	106.71
18	A	842	CLA	CHB-C1B-NB	2.06	126.44	124.26
18	1	602	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
18	B	817	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
19	1	614	XAT	C7-C8-C9	-2.06	122.34	125.53
18	2	610	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	4	617	XAT	C28-C29-C30	2.06	122.10	118.94
18	B	828	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
18	1	603	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
18	3	609	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	A	818	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	B	843	BCR	C7-C8-C9	-2.05	123.14	126.23
22	4	618	BCR	C8-C9-C10	2.05	122.09	118.94
19	4	617	XAT	C16-C1-C2	-2.05	105.42	108.98
18	3	601	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
17	4	607	CHL	OMC-CMC-C2C	-2.05	121.06	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	611	CLA	CHB-C1B-NB	2.05	126.42	124.26
18	B	807	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
18	A	837	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	B	806	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	F	301	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
18	K	201	CLA	CHB-C1B-NB	2.04	126.42	124.26
18	B	814	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
17	2	605	CHL	CAA-C2A-C3A	-2.04	109.16	114.26
18	A	834	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
18	B	830	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	K	206	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	B	825	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
18	B	835	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	K	203	CLA	CHD-C1D-ND	-2.04	122.58	124.45
17	2	615	CHL	CAA-C2A-C3A	-2.04	109.17	114.26
18	A	827	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	A	840	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
18	B	838	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
18	A	808	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	A	824	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	A	817	CLA	CHD-C1D-ND	-2.04	122.58	124.45
18	B	817	CLA	CHD-C1D-ND	-2.03	122.58	124.45
18	B	806	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	B	802	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	F	302	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	1	605	CLA	CHB-C1B-NB	2.03	126.41	124.26
18	1	604	CLA	CHD-C1D-ND	-2.03	122.59	124.45
18	3	609	CLA	CHB-C1B-NB	2.03	126.41	124.26
18	4	613	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
18	A	813	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
18	A	842	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
18	A	832	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	L	306	BCR	C24-C23-C22	2.03	129.30	126.23
18	2	602	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	2	601	CHL	O2A-CGA-CBA	2.03	120.24	112.23
18	B	837	CLA	O2D-CGD-CBD	2.03	114.87	111.27
18	A	830	CLA	C2A-C1A-CHA	2.03	127.40	123.86
18	J	101	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	B	848	BCR	C37-C22-C23	2.03	121.27	118.08
18	B	811	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	A	850	BCR	C1-C6-C5	-2.02	119.76	122.61
18	B	809	CLA	O2A-CGA-O1A	-2.02	118.48	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	828	CLA	CMB-C2B-C3B	2.02	131.49	126.59
19	1	614	XAT	C10-C11-C12	-2.02	116.90	123.22
18	F	302	CLA	CHB-C1B-NB	2.02	126.40	124.26
22	A	852	BCR	C30-C25-C24	2.02	121.50	115.78
18	4	602	CLA	CMB-C2B-C3B	2.02	131.48	126.59
18	B	840	CLA	CHD-C1D-ND	-2.02	122.60	124.45
19	1	614	XAT	C40-C33-C34	-2.02	120.10	122.92
18	J	101	CLA	CHB-C1B-NB	2.02	126.39	124.26
22	3	614	BCR	C30-C25-C26	-2.02	119.77	122.61
18	4	602	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
17	1	606	CHL	OMC-CMC-C2C	-2.02	121.13	125.69
18	3	609	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
18	A	831	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
18	2	612	CLA	CHB-C1B-NB	2.01	126.39	124.26
18	A	807	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
18	L	303	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
22	B	847	BCR	C37-C22-C23	2.01	121.25	118.08
18	3	603	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
18	2	613	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	B	837	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	A	822	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	A	802	CLA	CHB-C1B-NB	2.01	126.39	124.26
18	B	825	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	A	824	CLA	CHB-C1B-NB	2.01	126.38	124.26
18	A	838	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	B	813	CLA	C1-C2-C3	-2.01	122.57	126.04
17	4	615	CHL	C4B-C3B-C2B	-2.01	105.12	107.03
22	A	851	BCR	C10-C11-C12	-2.01	116.95	123.22
18	A	832	CLA	CHD-C1D-ND	-2.01	122.61	124.45
17	2	607	CHL	OMC-CMC-C2C	-2.01	121.15	125.69
18	A	838	CLA	CHB-C1B-NB	2.01	126.38	124.26
18	4	612	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
18	1	603	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	B	813	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
18	A	822	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
22	B	845	BCR	C30-C25-C26	-2.00	119.79	122.61
18	B	834	CLA	C1-C2-C3	-2.00	122.58	126.04
18	A	820	CLA	CHB-C1B-NB	2.00	126.38	124.26
18	A	842	CLA	C2D-C1D-ND	-2.00	108.63	110.10
18	A	830	CLA	O2A-C1-C2	2.00	113.90	108.64
18	A	845	CLA	CHD-C1D-ND	-2.00	122.61	124.45
18	B	825	CLA	CMB-C2B-C3B	2.00	131.44	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	810	CLA	O2D-CGD-CBD	2.00	114.82	111.27
18	A	816	CLA	CHD-C1D-ND	-2.00	122.61	124.45
18	B	823	CLA	CHD-C1D-ND	-2.00	122.61	124.45
17	3	606	CHL	CMC-C2C-C1C	2.00	128.09	125.04
18	A	811	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
18	A	820	CLA	CMB-C2B-C3B	2.00	131.43	126.59
19	4	617	XAT	C10-C11-C12	2.00	129.46	123.22
18	3	607	CLA	CHD-C1D-ND	-2.00	122.62	124.45
18	A	830	CLA	CHD-C1D-ND	-2.00	122.62	124.45

There are no chirality outliers.

All (1560) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	2	605	CHL	C3C-C2C-CMC-OMC
17	2	601	CHL	C1A-C2A-CAA-CBA
17	2	601	CHL	C3A-C2A-CAA-CBA
17	2	601	CHL	CHA-CBD-CGD-O1D
17	2	601	CHL	CHA-CBD-CGD-O2D
17	3	606	CHL	CHA-CBD-CGD-O1D
17	3	606	CHL	CHA-CBD-CGD-O2D
17	3	606	CHL	CBD-CGD-O2D-CED
17	4	605	CHL	C1A-C2A-CAA-CBA
18	1	604	CLA	C1A-C2A-CAA-CBA
18	1	604	CLA	CHA-CBD-CGD-O1D
18	1	604	CLA	CHA-CBD-CGD-O2D
18	1	605	CLA	C1A-C2A-CAA-CBA
18	1	605	CLA	C3A-C2A-CAA-CBA
18	1	605	CLA	CBA-CGA-O2A-C1
18	1	607	CLA	C1A-C2A-CAA-CBA
18	1	607	CLA	C3A-C2A-CAA-CBA
18	1	608	CLA	CBD-CGD-O2D-CED
18	1	609	CLA	CBD-CGD-O2D-CED
18	2	612	CLA	CHA-CBD-CGD-O1D
18	2	612	CLA	CHA-CBD-CGD-O2D
18	2	612	CLA	C11-C12-C13-C14
18	2	602	CLA	C2-C3-C5-C6
18	2	602	CLA	C4-C3-C5-C6
18	2	613	CLA	C2B-C3B-CAB-CBB
18	2	613	CLA	C4B-C3B-CAB-CBB
18	2	613	CLA	CBD-CGD-O2D-CED
18	2	610	CLA	CMA-C3A-C4A-CHB

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Mol	Chain	Res	Type	Atoms
18	2	608	CLA	C3A-C2A-CAA-CBA
18	3	605	CLA	C1A-C2A-CAA-CBA
18	3	605	CLA	C3A-C2A-CAA-CBA
18	3	605	CLA	CAD-CBD-CGD-O1D
18	3	603	CLA	C1A-C2A-CAA-CBA
18	3	603	CLA	C3A-C2A-CAA-CBA
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
18	4	609	CLA	CBD-CGD-O2D-CED
18	4	613	CLA	C1A-C2A-CAA-CBA
18	4	612	CLA	CBD-CGD-O2D-CED
18	4	612	CLA	C6-C7-C8-C9
18	4	604	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	822	CLA	C1A-C2A-CAA-CBA
18	A	818	CLA	CBD-CGD-O2D-CED
18	A	825	CLA	C1A-C2A-CAA-CBA
18	A	825	CLA	C3A-C2A-CAA-CBA
18	A	825	CLA	CHA-CBD-CGD-O1D
18	A	825	CLA	CHA-CBD-CGD-O2D
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	C1A-C2A-CAA-CBA
18	A	806	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O1D
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	CAD-CBD-CGD-O1D
18	A	804	CLA	CAD-CBD-CGD-O2D
18	A	804	CLA	C11-C10-C8-C9
18	A	811	CLA	CBD-CGD-O2D-CED
18	A	823	CLA	C1A-C2A-CAA-CBA
18	A	823	CLA	C3A-C2A-CAA-CBA
18	A	826	CLA	C11-C12-C13-C14
18	A	802	CLA	C1A-C2A-CAA-CBA
18	A	802	CLA	C3A-C2A-CAA-CBA
18	A	802	CLA	CBD-CGD-O2D-CED
18	A	830	CLA	C1A-C2A-CAA-CBA
18	A	830	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
18	A	840	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O2D
18	A	845	CLA	C3A-C2A-CAA-CBA
18	A	845	CLA	C2B-C3B-CAB-CBB
18	A	845	CLA	C4B-C3B-CAB-CBB
18	A	845	CLA	CHA-CBD-CGD-O1D
18	A	845	CLA	CHA-CBD-CGD-O2D
18	A	835	CLA	CHA-CBD-CGD-O1D
18	A	835	CLA	CHA-CBD-CGD-O2D
18	A	842	CLA	C1A-C2A-CAA-CBA
18	A	842	CLA	C3A-C2A-CAA-CBA
18	A	841	CLA	C1A-C2A-CAA-CBA
18	A	841	CLA	C3A-C2A-CAA-CBA
18	A	841	CLA	CBD-CGD-O2D-CED
18	A	817	CLA	C1A-C2A-CAA-CBA
18	A	817	CLA	C3A-C2A-CAA-CBA
18	A	814	CLA	C1A-C2A-CAA-CBA
18	A	814	CLA	C3A-C2A-CAA-CBA
18	A	827	CLA	C3A-C2A-CAA-CBA
18	A	812	CLA	C2B-C3B-CAB-CBB
18	A	812	CLA	C4B-C3B-CAB-CBB
18	A	829	CLA	CHA-CBD-CGD-O1D
18	A	829	CLA	CHA-CBD-CGD-O2D
18	A	836	CLA	C1A-C2A-CAA-CBA
18	A	838	CLA	C2A-CAA-CBA-CGA
18	A	837	CLA	CHA-CBD-CGD-O1D
18	A	837	CLA	CHA-CBD-CGD-O2D
18	B	818	CLA	C3A-C2A-CAA-CBA
18	B	830	CLA	CBD-CGD-O2D-CED
18	B	821	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C3A-C2A-CAA-CBA
18	B	805	CLA	C6-C7-C8-C9
18	B	826	CLA	C1A-C2A-CAA-CBA
18	B	835	CLA	C3A-C2A-CAA-CBA
18	B	834	CLA	C1A-C2A-CAA-CBA
18	B	834	CLA	C3A-C2A-CAA-CBA
18	B	823	CLA	C1A-C2A-CAA-CBA
18	B	823	CLA	C3A-C2A-CAA-CBA
18	B	819	CLA	C1A-C2A-CAA-CBA
18	B	819	CLA	C3A-C2A-CAA-CBA
18	B	819	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	B	819	CLA	C4B-C3B-CAB-CBB
18	B	809	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	C1A-C2A-CAA-CBA
18	B	814	CLA	C2-C3-C5-C6
18	B	814	CLA	C4-C3-C5-C6
18	B	814	CLA	C11-C10-C8-C9
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C11-C12-C13-C15
18	B	828	CLA	C1A-C2A-CAA-CBA
18	B	828	CLA	C3A-C2A-CAA-CBA
18	B	813	CLA	CAD-CBD-CGD-O2D
18	B	824	CLA	C2-C3-C5-C6
18	B	824	CLA	C4-C3-C5-C6
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	825	CLA	C3A-C2A-CAA-CBA
18	B	825	CLA	CHA-CBD-CGD-O1D
18	B	825	CLA	CHA-CBD-CGD-O2D
18	B	825	CLA	C11-C12-C13-C14
18	B	832	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C3A-C2A-CAA-CBA
18	B	802	CLA	C3A-C2A-CAA-CBA
18	B	802	CLA	CBD-CGD-O2D-CED
18	B	820	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C3A-C2A-CAA-CBA
18	B	803	CLA	CHA-CBD-CGD-O1D
18	B	803	CLA	CHA-CBD-CGD-O2D
18	B	803	CLA	CBD-CGD-O2D-CED
18	B	803	CLA	O1D-CGD-O2D-CED
18	B	817	CLA	C2B-C3B-CAB-CBB
18	B	817	CLA	C4B-C3B-CAB-CBB
18	B	822	CLA	C1A-C2A-CAA-CBA
18	B	822	CLA	CHA-CBD-CGD-O1D
18	B	822	CLA	CHA-CBD-CGD-O2D
18	B	840	CLA	C1A-C2A-CAA-CBA
18	B	840	CLA	C3A-C2A-CAA-CBA
18	B	840	CLA	C6-C7-C8-C9
18	F	301	CLA	CBD-CGD-O2D-CED
18	F	301	CLA	C2-C3-C5-C6
18	F	301	CLA	C4-C3-C5-C6
18	F	302	CLA	CBD-CGD-O2D-CED
18	G	201	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	G	201	CLA	CHA-CBD-CGD-O2D
18	G	202	CLA	C1A-C2A-CAA-CBA
18	G	202	CLA	C3A-C2A-CAA-CBA
18	H	201	CLA	C2A-CAA-CBA-CGA
18	H	201	CLA	CBD-CGD-O2D-CED
18	K	204	CLA	C1A-C2A-CAA-CBA
18	K	204	CLA	CBD-CGD-O2D-CED
18	K	203	CLA	C1A-C2A-CAA-CBA
18	L	304	CLA	C2B-C3B-CAB-CBB
18	L	304	CLA	C4B-C3B-CAB-CBB
19	1	614	XAT	C5-C6-C7-C8
19	1	614	XAT	O4-C6-C7-C8
19	1	614	XAT	C7-C8-C9-C10
19	1	614	XAT	C7-C8-C9-C19
19	1	614	XAT	C11-C12-C13-C14
19	1	614	XAT	C11-C12-C13-C20
19	1	614	XAT	O24-C26-C27-C28
19	2	617	XAT	O4-C6-C7-C8
19	2	617	XAT	C11-C10-C9-C19
19	2	617	XAT	C10-C11-C12-C13
19	2	617	XAT	C13-C14-C15-C35
19	2	617	XAT	O24-C26-C27-C28
19	2	617	XAT	C28-C29-C30-C31
19	2	617	XAT	C39-C29-C30-C31
19	2	617	XAT	C33-C34-C35-C15
19	4	617	XAT	C7-C8-C9-C10
19	4	617	XAT	C7-C8-C9-C19
20	1	615	LHG	C1-C2-C3-O3
20	1	615	LHG	C2-C3-O3-P
20	1	615	LHG	C3-O3-P-O4
20	1	615	LHG	C4-O6-P-O5
20	1	615	LHG	O7-C5-C6-O8
20	2	618	LHG	C3-O3-P-O5
20	2	618	LHG	O9-C7-O7-C5
20	2	618	LHG	C8-C7-O7-C5
20	2	618	LHG	O10-C23-O8-C6
20	2	618	LHG	C24-C23-O8-C6
20	A	846	LHG	O10-C23-O8-C6
20	A	846	LHG	C24-C23-O8-C6
20	B	851	LHG	C8-C7-O7-C5
20	B	852	LHG	C2-C3-O3-P
20	B	852	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
20	B	852	LHG	C4-O6-P-O3
21	2	619	LUT	C5-C6-C7-C8
21	3	613	LUT	C9-C10-C11-C12
21	3	613	LUT	C21-C26-C27-C28
21	3	613	LUT	C25-C26-C27-C28
22	3	614	BCR	C21-C22-C23-C24
22	3	614	BCR	C37-C22-C23-C24
22	4	618	BCR	C23-C24-C25-C26
22	A	849	BCR	C23-C24-C25-C26
22	A	849	BCR	C23-C24-C25-C30
22	A	852	BCR	C35-C13-C14-C15
22	A	852	BCR	C14-C15-C16-C17
22	A	852	BCR	C16-C17-C18-C19
22	A	852	BCR	C16-C17-C18-C36
22	A	852	BCR	C21-C22-C23-C24
22	A	852	BCR	C37-C22-C23-C24
22	A	850	BCR	C7-C8-C9-C10
22	A	850	BCR	C7-C8-C9-C34
22	A	851	BCR	C11-C12-C13-C14
22	A	851	BCR	C11-C12-C13-C35
22	B	846	BCR	C7-C8-C9-C10
22	B	846	BCR	C7-C8-C9-C34
22	B	846	BCR	C23-C24-C25-C26
22	B	846	BCR	C23-C24-C25-C30
22	B	844	BCR	C12-C13-C14-C15
22	B	844	BCR	C35-C13-C14-C15
22	B	844	BCR	C18-C19-C20-C21
22	B	801	BCR	C1-C6-C7-C8
22	B	801	BCR	C5-C6-C7-C8
22	B	845	BCR	C17-C18-C19-C20
22	B	845	BCR	C36-C18-C19-C20
22	B	845	BCR	C21-C22-C23-C24
22	B	845	BCR	C37-C22-C23-C24
22	B	849	BCR	C22-C23-C24-C25
22	F	304	BCR	C11-C12-C13-C14
22	F	304	BCR	C11-C12-C13-C35
22	F	304	BCR	C15-C16-C17-C18
22	J	102	BCR	C7-C8-C9-C10
22	J	102	BCR	C7-C8-C9-C34
27	B	850	DGD	O2G-C2G-C3G-O3G
18	2	609	CLA	O1D-CGD-O2D-CED
18	4	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	B	802	CLA	O1D-CGD-O2D-CED
18	H	201	CLA	O1D-CGD-O2D-CED
18	1	608	CLA	O1D-CGD-O2D-CED
18	3	608	CLA	O1D-CGD-O2D-CED
18	4	609	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	O1D-CGD-O2D-CED
18	A	829	CLA	O1D-CGD-O2D-CED
18	K	204	CLA	O1D-CGD-O2D-CED
18	1	605	CLA	CBD-CGD-O2D-CED
18	2	612	CLA	CBD-CGD-O2D-CED
18	2	609	CLA	CBD-CGD-O2D-CED
18	2	608	CLA	CBD-CGD-O2D-CED
18	3	605	CLA	CBD-CGD-O2D-CED
18	3	608	CLA	CBD-CGD-O2D-CED
18	3	607	CLA	CBD-CGD-O2D-CED
18	4	614	CLA	CBD-CGD-O2D-CED
18	A	813	CLA	CBD-CGD-O2D-CED
18	A	803	CLA	CBD-CGD-O2D-CED
18	A	829	CLA	CBD-CGD-O2D-CED
18	B	816	CLA	CBD-CGD-O2D-CED
18	B	822	CLA	CBD-CGD-O2D-CED
18	G	201	CLA	CBD-CGD-O2D-CED
18	3	602	CLA	O1A-CGA-O2A-C1
18	A	803	CLA	O1A-CGA-O2A-C1
18	A	830	CLA	O1A-CGA-O2A-C1
18	A	835	CLA	O1A-CGA-O2A-C1
18	B	802	CLA	O1A-CGA-O2A-C1
18	B	836	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	O1D-CGD-O2D-CED
18	F	302	CLA	O1D-CGD-O2D-CED
18	1	609	CLA	O1D-CGD-O2D-CED
18	2	613	CLA	O1D-CGD-O2D-CED
18	A	811	CLA	O1D-CGD-O2D-CED
18	B	830	CLA	O1D-CGD-O2D-CED
18	G	201	CLA	O1D-CGD-O2D-CED
18	3	602	CLA	CBA-CGA-O2A-C1
18	A	803	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	CBA-CGA-O2A-C1
17	2	607	CHL	CBD-CGD-O2D-CED
17	4	607	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	2	604	CLA	CBD-CGD-O2D-CED
18	A	806	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	CBD-CGD-O2D-CED
18	B	835	CLA	CBD-CGD-O2D-CED
18	B	819	CLA	CBD-CGD-O2D-CED
18	B	809	CLA	CBD-CGD-O2D-CED
18	B	827	CLA	CBD-CGD-O2D-CED
18	1	603	CLA	O1A-CGA-O2A-C1
18	2	609	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	O1A-CGA-O2A-C1
18	1	605	CLA	O1A-CGA-O2A-C1
18	4	612	CLA	O1D-CGD-O2D-CED
18	A	841	CLA	O1D-CGD-O2D-CED
18	F	301	CLA	O1D-CGD-O2D-CED
17	2	601	CHL	CBD-CGD-O2D-CED
18	3	603	CLA	CBD-CGD-O2D-CED
18	B	840	CLA	CBD-CGD-O2D-CED
17	3	606	CHL	O1D-CGD-O2D-CED
20	B	851	LHG	O9-C7-O7-C5
18	B	827	CLA	O1A-CGA-O2A-C1
18	3	602	CLA	C3-C5-C6-C7
18	A	819	CLA	C3-C5-C6-C7
18	A	807	CLA	C3-C5-C6-C7
18	A	818	CLA	C3-C5-C6-C7
18	A	803	CLA	C3-C5-C6-C7
18	A	834	CLA	C3-C5-C6-C7
18	A	843	CLA	C3-C5-C6-C7
18	A	844	CLA	C3-C5-C6-C7
18	A	841	CLA	C3-C5-C6-C7
18	A	814	CLA	C3-C5-C6-C7
18	A	828	CLA	C3-C5-C6-C7
18	B	805	CLA	C3-C5-C6-C7
18	B	841	CLA	C3-C5-C6-C7
18	B	814	CLA	C3-C5-C6-C7
18	B	806	CLA	C3-C5-C6-C7
18	B	840	CLA	C3-C5-C6-C7
18	H	201	CLA	C3-C5-C6-C7
18	B	802	CLA	CBA-CGA-O2A-C1
18	B	836	CLA	CBA-CGA-O2A-C1
17	4	606	CHL	CBD-CGD-O2D-CED
18	3	602	CLA	CBD-CGD-O2D-CED
18	A	839	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	820	CLA	C4-C3-C5-C6
18	A	839	CLA	C4-C3-C5-C6
18	B	809	CLA	C4-C3-C5-C6
18	A	820	CLA	C2-C3-C5-C6
18	A	839	CLA	C2-C3-C5-C6
18	1	602	CLA	CBD-CGD-O2D-CED
18	4	603	CLA	CBD-CGD-O2D-CED
18	B	813	CLA	CBD-CGD-O2D-CED
18	J	101	CLA	CBD-CGD-O2D-CED
17	2	601	CHL	C2A-CAA-CBA-CGA
17	2	607	CHL	C2A-CAA-CBA-CGA
17	3	606	CHL	C2A-CAA-CBA-CGA
18	1	605	CLA	C2A-CAA-CBA-CGA
18	2	611	CLA	C2A-CAA-CBA-CGA
18	2	608	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	C2A-CAA-CBA-CGA
18	A	843	CLA	C2A-CAA-CBA-CGA
18	A	832	CLA	C2A-CAA-CBA-CGA
18	B	813	CLA	C2A-CAA-CBA-CGA
18	B	839	CLA	C2A-CAA-CBA-CGA
18	B	802	CLA	C2A-CAA-CBA-CGA
18	A	833	CLA	C3-C5-C6-C7
18	B	829	CLA	C3-C5-C6-C7
18	1	603	CLA	CBA-CGA-O2A-C1
18	2	609	CLA	CBA-CGA-O2A-C1
18	B	814	CLA	CBA-CGA-O2A-C1
18	B	827	CLA	CBA-CGA-O2A-C1
17	2	606	CHL	CBD-CGD-O2D-CED
18	4	614	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	O1A-CGA-O2A-C1
18	A	820	CLA	O1A-CGA-O2A-C1
18	A	811	CLA	O1A-CGA-O2A-C1
18	A	839	CLA	O1A-CGA-O2A-C1
18	L	303	CLA	O1A-CGA-O2A-C1
21	1	616	LUT	C29-C30-C31-C32
21	2	616	LUT	C33-C34-C35-C15
21	3	613	LUT	C33-C34-C35-C15
22	A	849	BCR	C15-C16-C17-C18
22	A	849	BCR	C19-C20-C21-C22
22	A	853	BCR	C9-C10-C11-C12
22	A	850	BCR	C13-C14-C15-C16
22	A	850	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	A	851	BCR	C13-C14-C15-C16
22	B	801	BCR	C9-C10-C11-C12
22	B	843	BCR	C13-C14-C15-C16
22	B	845	BCR	C19-C20-C21-C22
22	F	304	BCR	C19-C20-C21-C22
18	1	612	CLA	CBD-CGD-O2D-CED
18	2	610	CLA	CBD-CGD-O2D-CED
18	3	601	CLA	CBD-CGD-O2D-CED
18	B	834	CLA	CBD-CGD-O2D-CED
18	A	813	CLA	O1D-CGD-O2D-CED
20	1	615	LHG	O2-C2-C3-O3
18	B	827	CLA	C3-C5-C6-C7
18	L	303	CLA	C3-C5-C6-C7
24	A	801	CL0	C3-C5-C6-C7
18	A	818	CLA	CBA-CGA-O2A-C1
18	A	839	CLA	CBA-CGA-O2A-C1
18	L	303	CLA	CBA-CGA-O2A-C1
18	1	605	CLA	O1D-CGD-O2D-CED
18	2	612	CLA	O1D-CGD-O2D-CED
18	A	803	CLA	O1D-CGD-O2D-CED
18	K	203	CLA	CBD-CGD-O2D-CED
18	2	608	CLA	O1D-CGD-O2D-CED
18	4	602	CLA	C3-C5-C6-C7
18	B	803	CLA	C3-C5-C6-C7
18	B	822	CLA	C3-C5-C6-C7
18	A	820	CLA	CBA-CGA-O2A-C1
18	A	811	CLA	CBA-CGA-O2A-C1
20	1	615	LHG	C26-C27-C28-C29
18	A	833	CLA	C4-C3-C5-C6
25	B	842	PQN	C14-C13-C15-C16
18	A	833	CLA	C2-C3-C5-C6
25	B	842	PQN	C12-C13-C15-C16
18	A	822	CLA	C2A-CAA-CBA-CGA
18	G	203	CLA	C2A-CAA-CBA-CGA
18	B	816	CLA	O1D-CGD-O2D-CED
18	A	842	CLA	CBA-CGA-O2A-C1
18	A	838	CLA	CBA-CGA-O2A-C1
18	B	841	CLA	CBD-CGD-O2D-CED
18	3	605	CLA	O1D-CGD-O2D-CED
18	3	607	CLA	O1D-CGD-O2D-CED
18	A	834	CLA	O1D-CGD-O2D-CED
17	2	607	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	4	607	CHL	O1D-CGD-O2D-CED
17	2	615	CHL	CBD-CGD-O2D-CED
18	A	809	CLA	CBD-CGD-O2D-CED
18	A	842	CLA	O1A-CGA-O2A-C1
18	A	838	CLA	O1A-CGA-O2A-C1
17	1	601	CHL	CBA-CGA-O2A-C1
18	A	825	CLA	CBA-CGA-O2A-C1
18	A	802	CLA	CBA-CGA-O2A-C1
18	A	845	CLA	CBA-CGA-O2A-C1
18	B	822	CLA	CBA-CGA-O2A-C1
18	F	301	CLA	CBA-CGA-O2A-C1
18	A	819	CLA	CBD-CGD-O2D-CED
18	B	808	CLA	CBD-CGD-O2D-CED
18	A	812	CLA	C5-C6-C7-C8
18	4	602	CLA	C5-C6-C7-C8
18	A	828	CLA	C15-C16-C17-C18
18	B	822	CLA	O1A-CGA-O2A-C1
18	B	809	CLA	C2-C3-C5-C6
18	3	601	CLA	C11-C10-C8-C9
18	4	612	CLA	C11-C10-C8-C9
18	A	819	CLA	C6-C7-C8-C9
18	A	807	CLA	C11-C10-C8-C9
18	A	820	CLA	C11-C10-C8-C9
18	A	806	CLA	C11-C10-C8-C9
18	A	811	CLA	C14-C13-C15-C16
18	A	826	CLA	C11-C10-C8-C9
18	A	802	CLA	C11-C12-C13-C14
18	A	835	CLA	C11-C10-C8-C9
18	A	841	CLA	C14-C13-C15-C16
18	A	812	CLA	C6-C7-C8-C9
18	B	805	CLA	C11-C10-C8-C9
18	B	808	CLA	C6-C7-C8-C9
18	B	808	CLA	C14-C13-C15-C16
18	B	809	CLA	C11-C10-C8-C9
18	B	828	CLA	C14-C13-C15-C16
18	B	825	CLA	C14-C13-C15-C16
18	B	802	CLA	C11-C12-C13-C14
18	B	803	CLA	C11-C10-C8-C9
18	B	840	CLA	C14-C13-C15-C16
18	F	301	CLA	C6-C7-C8-C9
18	H	201	CLA	C6-C7-C8-C9
18	2	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	B	809	CLA	O1D-CGD-O2D-CED
18	A	816	CLA	CBD-CGD-O2D-CED
19	2	617	XAT	C31-C32-C33-C40
21	2	616	LUT	C31-C32-C33-C40
22	4	618	BCR	C7-C8-C9-C34
22	A	853	BCR	C11-C12-C13-C35
22	B	846	BCR	C37-C22-C23-C24
22	K	205	BCR	C7-C8-C9-C34
22	K	205	BCR	C36-C18-C19-C20
22	L	306	BCR	C7-C8-C9-C34
22	L	306	BCR	C37-C22-C23-C24
21	2	616	LUT	C31-C32-C33-C34
22	A	853	BCR	C11-C12-C13-C14
22	L	306	BCR	C7-C8-C9-C10
22	L	306	BCR	C21-C22-C23-C24
18	A	806	CLA	C13-C15-C16-C17
18	A	832	CLA	CBA-CGA-O2A-C1
18	A	822	CLA	C15-C16-C17-C18
18	A	806	CLA	C10-C11-C12-C13
18	A	835	CLA	C15-C16-C17-C18
18	A	842	CLA	C13-C15-C16-C17
18	A	812	CLA	C10-C11-C12-C13
18	B	814	CLA	C5-C6-C7-C8
18	B	835	CLA	O1D-CGD-O2D-CED
20	1	615	LHG	C34-C35-C36-C37
18	2	602	CLA	C5-C6-C7-C8
18	A	819	CLA	C5-C6-C7-C8
18	A	820	CLA	C5-C6-C7-C8
18	A	804	CLA	C8-C10-C11-C12
18	A	831	CLA	C13-C15-C16-C17
18	A	828	CLA	C8-C10-C11-C12
18	A	812	CLA	C8-C10-C11-C12
18	B	805	CLA	C10-C11-C12-C13
18	B	826	CLA	C8-C10-C11-C12
18	B	808	CLA	C13-C15-C16-C17
18	B	806	CLA	C10-C11-C12-C13
18	B	822	CLA	C13-C15-C16-C17
20	1	615	LHG	C7-C8-C9-C10
18	A	835	CLA	C8-C10-C11-C12
18	B	837	CLA	C5-C6-C7-C8
18	B	819	CLA	O1D-CGD-O2D-CED
18	A	843	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
18	2	602	CLA	C15-C16-C17-C18
18	A	844	CLA	C5-C6-C7-C8
20	1	615	LHG	C5-C4-O6-P
18	H	201	CLA	C8-C10-C11-C12
18	A	804	CLA	C6-C7-C8-C10
18	A	803	CLA	C11-C12-C13-C15
18	A	835	CLA	C11-C10-C8-C7
18	A	829	CLA	C11-C10-C8-C7
18	B	805	CLA	C6-C7-C8-C10
18	B	834	CLA	C6-C7-C8-C10
18	B	810	CLA	C6-C7-C8-C10
18	B	841	CLA	C11-C10-C8-C7
18	B	841	CLA	C12-C13-C15-C16
18	B	802	CLA	C11-C12-C13-C15
18	2	612	CLA	C3-C5-C6-C7
18	B	802	CLA	C3-C5-C6-C7
17	1	601	CHL	O1A-CGA-O2A-C1
18	A	802	CLA	O1A-CGA-O2A-C1
18	A	845	CLA	O1A-CGA-O2A-C1
18	1	603	CLA	C2A-CAA-CBA-CGA
18	1	607	CLA	C2A-CAA-CBA-CGA
18	2	609	CLA	C2A-CAA-CBA-CGA
18	2	603	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C2A-CAA-CBA-CGA
18	B	832	CLA	C2A-CAA-CBA-CGA
18	A	806	CLA	O1D-CGD-O2D-CED
18	B	827	CLA	O1D-CGD-O2D-CED
18	B	840	CLA	O1D-CGD-O2D-CED
18	A	828	CLA	C5-C6-C7-C8
18	H	201	CLA	C5-C6-C7-C8
18	F	301	CLA	O1A-CGA-O2A-C1
18	A	836	CLA	CBD-CGD-O2D-CED
18	A	804	CLA	C5-C6-C7-C8
19	2	617	XAT	C30-C31-C32-C33
22	B	849	BCR	C10-C11-C12-C13
22	K	205	BCR	C10-C11-C12-C13
22	K	205	BCR	C18-C19-C20-C21
18	A	828	CLA	C13-C15-C16-C17
18	A	829	CLA	C8-C10-C11-C12
18	B	813	CLA	C13-C15-C16-C17
18	B	841	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	3	602	CLA	O1D-CGD-O2D-CED
18	A	825	CLA	O1A-CGA-O2A-C1
18	3	601	CLA	C8-C10-C11-C12
18	A	806	CLA	C8-C10-C11-C12
18	A	829	CLA	C15-C16-C17-C18
18	B	814	CLA	C8-C10-C11-C12
18	B	817	CLA	C5-C6-C7-C8
18	B	840	CLA	C5-C6-C7-C8
18	3	603	CLA	O1D-CGD-O2D-CED
18	A	832	CLA	O1A-CGA-O2A-C1
17	2	601	CHL	O1D-CGD-O2D-CED
18	A	839	CLA	O1D-CGD-O2D-CED
18	A	807	CLA	C5-C6-C7-C8
18	A	842	CLA	C8-C10-C11-C12
18	B	806	CLA	C5-C6-C7-C8
20	1	615	LHG	C3-O3-P-O6
18	B	808	CLA	C3-C5-C6-C7
18	A	813	CLA	CBA-CGA-O2A-C1
18	J	101	CLA	CBA-CGA-O2A-C1
17	4	606	CHL	O1D-CGD-O2D-CED
18	A	840	CLA	C4-C3-C5-C6
18	B	832	CLA	C15-C16-C17-C18
24	A	801	CL0	C10-C11-C12-C13
18	1	602	CLA	O1D-CGD-O2D-CED
18	3	602	CLA	C2A-CAA-CBA-CGA
18	4	604	CLA	C2A-CAA-CBA-CGA
18	A	819	CLA	C2A-CAA-CBA-CGA
18	A	830	CLA	C2A-CAA-CBA-CGA
18	B	817	CLA	C2A-CAA-CBA-CGA
18	G	201	CLA	C2A-CAA-CBA-CGA
18	A	839	CLA	C6-C7-C8-C10
18	A	830	CLA	C3-C5-C6-C7
18	A	843	CLA	CBA-CGA-O2A-C1
18	B	811	CLA	CBA-CGA-O2A-C1
18	4	602	CLA	C10-C11-C12-C13
18	A	811	CLA	C8-C10-C11-C12
18	B	839	CLA	C13-C15-C16-C17
18	J	101	CLA	O1D-CGD-O2D-CED
20	1	615	LHG	C13-C14-C15-C16
17	2	606	CHL	O1D-CGD-O2D-CED
18	4	603	CLA	O1D-CGD-O2D-CED
19	2	617	XAT	C20-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
21	3	613	LUT	C11-C10-C9-C19
22	A	849	BCR	C20-C21-C22-C37
22	B	844	BCR	C16-C17-C18-C36
22	B	849	BCR	C11-C10-C9-C34
22	F	304	BCR	C35-C13-C14-C15
22	K	205	BCR	C20-C21-C22-C37
18	1	603	CLA	C5-C6-C7-C8
18	B	828	CLA	C16-C17-C18-C20
18	B	824	CLA	C16-C17-C18-C19
18	B	813	CLA	CBA-CGA-O2A-C1
18	B	817	CLA	CBA-CGA-O2A-C1
18	3	601	CLA	O1D-CGD-O2D-CED
20	1	615	LHG	C15-C16-C17-C18
18	B	813	CLA	O1D-CGD-O2D-CED
19	2	617	XAT	C11-C10-C9-C8
22	A	852	BCR	C12-C13-C14-C15
22	B	844	BCR	C16-C17-C18-C19
22	B	849	BCR	C11-C10-C9-C8
22	K	205	BCR	C20-C21-C22-C23
18	A	819	CLA	CBA-CGA-O2A-C1
20	1	615	LHG	C25-C26-C27-C28
18	2	612	CLA	C10-C11-C12-C13
18	A	813	CLA	O1A-CGA-O2A-C1
18	A	843	CLA	O1A-CGA-O2A-C1
18	B	816	CLA	C6-C7-C8-C10
18	B	824	CLA	C16-C17-C18-C20
18	B	822	CLA	C16-C17-C18-C19
18	A	822	CLA	C4-C3-C5-C6
18	A	835	CLA	C4-C3-C5-C6
18	B	805	CLA	C11-C12-C13-C14
18	B	810	CLA	C14-C13-C15-C16
18	B	839	CLA	C6-C7-C8-C9
18	B	802	CLA	C11-C10-C8-C9
20	1	615	LHG	C23-C24-C25-C26
20	1	615	LHG	C27-C28-C29-C30
18	B	805	CLA	C5-C6-C7-C8
18	A	829	CLA	C2A-CAA-CBA-CGA
18	B	826	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C3-C5-C6-C7
18	B	809	CLA	C8-C10-C11-C12
20	1	615	LHG	C11-C10-C9-C8
27	B	850	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
18	2	604	CLA	C4B-C3B-CAB-CBB
18	4	610	CLA	C4B-C3B-CAB-CBB
18	A	819	CLA	C4B-C3B-CAB-CBB
18	A	825	CLA	C4B-C3B-CAB-CBB
18	A	803	CLA	C4B-C3B-CAB-CBB
18	A	834	CLA	C4B-C3B-CAB-CBB
18	A	838	CLA	C4B-C3B-CAB-CBB
18	B	823	CLA	C4B-C3B-CAB-CBB
18	2	612	CLA	C16-C17-C18-C20
18	A	839	CLA	C6-C7-C8-C9
18	2	610	CLA	O1D-CGD-O2D-CED
18	B	811	CLA	O1A-CGA-O2A-C1
18	B	841	CLA	O1A-CGA-O2A-C1
18	4	612	CLA	C8-C10-C11-C12
23	4	620	LMG	C29-C28-O8-C9
20	1	615	LHG	C12-C13-C14-C15
18	B	834	CLA	O1D-CGD-O2D-CED
18	1	604	CLA	C3A-C2A-CAA-CBA
18	1	612	CLA	C3A-C2A-CAA-CBA
18	2	611	CLA	C3A-C2A-CAA-CBA
18	A	810	CLA	C3A-C2A-CAA-CBA
18	A	830	CLA	C3A-C2A-CAA-CBA
18	A	815	CLA	C3A-C2A-CAA-CBA
18	B	826	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	C3A-C2A-CAA-CBA
18	B	809	CLA	C3A-C2A-CAA-CBA
18	B	810	CLA	C3A-C2A-CAA-CBA
18	B	811	CLA	C3A-C2A-CAA-CBA
18	B	824	CLA	C3A-C2A-CAA-CBA
18	B	815	CLA	C3A-C2A-CAA-CBA
18	G	201	CLA	C3A-C2A-CAA-CBA
18	K	203	CLA	C3A-C2A-CAA-CBA
18	B	837	CLA	C8-C10-C11-C12
18	4	601	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	O1D-CGD-O2D-CED
18	J	101	CLA	O1A-CGA-O2A-C1
18	B	827	CLA	C10-C11-C12-C13
18	B	811	CLA	CBD-CGD-O2D-CED
20	1	615	LHG	C10-C11-C12-C13
22	B	844	BCR	C14-C15-C16-C17
18	2	602	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	3	609	CLA	C4-C3-C5-C6
18	B	828	CLA	C4-C3-C5-C6
18	A	834	CLA	CBA-CGA-O2A-C1
18	3	609	CLA	C2-C3-C5-C6
18	B	817	CLA	O1A-CGA-O2A-C1
18	B	816	CLA	C6-C7-C8-C9
18	2	604	CLA	C2B-C3B-CAB-CBB
18	4	610	CLA	C2B-C3B-CAB-CBB
18	A	819	CLA	C2B-C3B-CAB-CBB
18	A	825	CLA	C2B-C3B-CAB-CBB
18	A	803	CLA	C2B-C3B-CAB-CBB
18	A	834	CLA	C2B-C3B-CAB-CBB
18	A	838	CLA	C2B-C3B-CAB-CBB
18	B	823	CLA	C2B-C3B-CAB-CBB
18	B	839	CLA	C2B-C3B-CAB-CBB
18	L	303	CLA	C8-C10-C11-C12
25	A	855	PQN	C25-C26-C27-C28
18	A	802	CLA	C3-C5-C6-C7
20	1	615	LHG	C18-C19-C20-C21
18	2	602	CLA	C13-C15-C16-C17
18	B	841	CLA	C13-C15-C16-C17
18	B	813	CLA	O1A-CGA-O2A-C1
20	B	851	LHG	C23-C24-C25-C26
21	2	619	LUT	C1-C6-C7-C8
21	4	616	LUT	C1-C6-C7-C8
21	4	616	LUT	C5-C6-C7-C8
22	4	618	BCR	C23-C24-C25-C30
22	B	844	BCR	C23-C24-C25-C26
22	B	844	BCR	C23-C24-C25-C30
22	B	845	BCR	C5-C6-C7-C8
22	B	849	BCR	C23-C24-C25-C26
22	F	304	BCR	C1-C6-C7-C8
22	F	304	BCR	C5-C6-C7-C8
18	2	613	CLA	C2A-CAA-CBA-CGA
18	B	840	CLA	CBA-CGA-O2A-C1
18	A	834	CLA	C13-C15-C16-C17
18	A	819	CLA	O1A-CGA-O2A-C1
18	2	602	CLA	C6-C7-C8-C10
18	3	601	CLA	C2-C3-C5-C6
18	A	819	CLA	C6-C7-C8-C10
18	A	807	CLA	C2-C3-C5-C6
18	A	807	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
18	A	822	CLA	C2-C3-C5-C6
18	A	806	CLA	C11-C10-C8-C7
18	A	826	CLA	C11-C10-C8-C7
18	A	835	CLA	C2-C3-C5-C6
18	B	808	CLA	C6-C7-C8-C10
18	B	810	CLA	C12-C13-C15-C16
18	B	828	CLA	C2-C3-C5-C6
18	B	806	CLA	C12-C13-C15-C16
18	B	839	CLA	C6-C7-C8-C10
18	B	802	CLA	C11-C10-C8-C7
18	B	840	CLA	C12-C13-C15-C16
18	A	834	CLA	O1A-CGA-O2A-C1
18	A	812	CLA	C16-C17-C18-C20
18	3	609	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C2A-CAA-CBA-CGA
18	A	802	CLA	C2A-CAA-CBA-CGA
27	B	850	DGD	CCB-CDB-CEB-CFB
18	4	609	CLA	C5-C6-C7-C8
21	2	616	LUT	C6-C7-C8-C9
18	B	820	CLA	CBA-CGA-O2A-C1
18	B	822	CLA	C16-C17-C18-C20
18	B	805	CLA	C8-C10-C11-C12
18	K	203	CLA	O1D-CGD-O2D-CED
27	B	850	DGD	C2B-C1B-O2G-C2G
22	F	304	BCR	C10-C11-C12-C13
18	B	823	CLA	CBD-CGD-O2D-CED
27	B	850	DGD	O1B-C1B-O2G-C2G
23	4	619	LMG	C2-C1-O1-C7
20	1	615	LHG	C17-C18-C19-C20
18	B	828	CLA	C16-C17-C18-C19
18	3	601	CLA	C4-C3-C5-C6
18	A	830	CLA	C4-C3-C5-C6
18	A	840	CLA	C2-C3-C5-C6
18	A	818	CLA	C6-C7-C8-C9
18	A	803	CLA	C11-C12-C13-C14
18	A	831	CLA	C11-C10-C8-C9
18	A	828	CLA	C11-C10-C8-C9
18	A	829	CLA	C11-C10-C8-C9
18	B	834	CLA	C6-C7-C8-C9
18	B	841	CLA	C11-C10-C8-C9
18	B	806	CLA	C14-C13-C15-C16
17	2	615	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	809	CLA	O1D-CGD-O2D-CED
18	B	818	CLA	C3-C5-C6-C7
18	A	806	CLA	C2A-CAA-CBA-CGA
18	A	813	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	C2A-CAA-CBA-CGA
23	4	619	LMG	O6-C5-C6-O5
18	B	840	CLA	O1A-CGA-O2A-C1
23	4	620	LMG	O10-C28-O8-C9
18	1	609	CLA	C1A-C2A-CAA-CBA
18	1	612	CLA	C1A-C2A-CAA-CBA
18	2	611	CLA	C1A-C2A-CAA-CBA
18	2	604	CLA	C1A-C2A-CAA-CBA
18	2	608	CLA	C1A-C2A-CAA-CBA
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C1A-C2A-CAA-CBA
18	A	845	CLA	C1A-C2A-CAA-CBA
18	A	815	CLA	C1A-C2A-CAA-CBA
18	A	827	CLA	C1A-C2A-CAA-CBA
18	A	833	CLA	C1A-C2A-CAA-CBA
18	A	812	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C1A-C2A-CAA-CBA
18	B	833	CLA	C1A-C2A-CAA-CBA
18	B	810	CLA	C1A-C2A-CAA-CBA
18	B	824	CLA	C1A-C2A-CAA-CBA
18	B	802	CLA	C1A-C2A-CAA-CBA
18	B	815	CLA	C1A-C2A-CAA-CBA
18	F	302	CLA	C1A-C2A-CAA-CBA
18	G	201	CLA	C1A-C2A-CAA-CBA
18	2	612	CLA	C16-C17-C18-C19
18	2	612	CLA	C5-C6-C7-C8
20	2	618	LHG	C3-O3-P-O6
18	A	805	CLA	CBA-CGA-O2A-C1
18	A	803	CLA	C10-C11-C12-C13
18	B	808	CLA	C5-C6-C7-C8
18	B	802	CLA	C8-C10-C11-C12
18	B	808	CLA	O1D-CGD-O2D-CED
18	A	807	CLA	C4-C3-C5-C6
18	4	611	CLA	C3A-C2A-CAA-CBA
18	A	831	CLA	C5-C6-C7-C8
18	B	840	CLA	C16-C17-C18-C20
18	B	841	CLA	O1D-CGD-O2D-CED
18	B	832	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	1	615	LHG	C4-C5-C6-O8
27	B	850	DGD	C1G-C2G-C3G-O3G
18	B	817	CLA	C11-C12-C13-C14
18	A	819	CLA	O1D-CGD-O2D-CED
18	A	816	CLA	O1D-CGD-O2D-CED
27	B	850	DGD	CCA-CDA-CEA-CFA
18	B	828	CLA	C13-C15-C16-C17
21	2	619	LUT	C11-C10-C9-C19
22	F	304	BCR	C11-C10-C9-C34
18	A	803	CLA	C4-C3-C5-C6
18	B	820	CLA	O1A-CGA-O2A-C1
18	B	828	CLA	CBA-CGA-O2A-C1
18	B	829	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	C10-C11-C12-C13
18	L	303	CLA	C10-C11-C12-C13
20	2	618	LHG	C6-C5-O7-C7
18	3	603	CLA	C2A-CAA-CBA-CGA
18	A	820	CLA	C13-C15-C16-C17
18	A	812	CLA	C2-C1-O2A-CGA
23	4	619	LMG	C30-C31-C32-C33
18	B	807	CLA	CBA-CGA-O2A-C1
18	B	841	CLA	C8-C10-C11-C12
18	A	805	CLA	O1A-CGA-O2A-C1
18	A	822	CLA	CBD-CGD-O2D-CED
19	2	617	XAT	C12-C13-C14-C15
22	F	304	BCR	C12-C13-C14-C15
23	4	620	LMG	C2-C1-O1-C7
18	B	810	CLA	C5-C6-C7-C8
18	1	603	CLA	C4-C3-C5-C6
18	B	810	CLA	C4-C3-C5-C6
18	B	827	CLA	C4-C3-C5-C6
18	B	813	CLA	C4-C3-C5-C6
18	3	601	CLA	C11-C10-C8-C7
18	A	809	CLA	C11-C10-C8-C7
18	A	804	CLA	C11-C12-C13-C15
18	A	804	CLA	C12-C13-C15-C16
18	A	811	CLA	C11-C12-C13-C15
18	A	811	CLA	C12-C13-C15-C16
18	A	802	CLA	C6-C7-C8-C10
18	A	802	CLA	C11-C12-C13-C15
18	A	802	CLA	C12-C13-C15-C16
18	A	831	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
18	A	831	CLA	C12-C13-C15-C16
18	A	842	CLA	C11-C10-C8-C7
18	A	844	CLA	C6-C7-C8-C10
18	A	844	CLA	C12-C13-C15-C16
18	A	828	CLA	C11-C12-C13-C15
18	B	805	CLA	C11-C12-C13-C15
18	B	808	CLA	C11-C12-C13-C15
18	B	809	CLA	C11-C10-C8-C7
18	B	809	CLA	C12-C13-C15-C16
18	B	827	CLA	C12-C13-C15-C16
18	B	828	CLA	C12-C13-C15-C16
18	B	813	CLA	C11-C12-C13-C15
18	B	806	CLA	C11-C10-C8-C7
18	B	806	CLA	C11-C12-C13-C15
18	B	825	CLA	C12-C13-C15-C16
18	H	201	CLA	C6-C7-C8-C10
18	H	201	CLA	C11-C10-C8-C7
18	B	837	CLA	C3-C5-C6-C7
20	1	615	LHG	C19-C20-C21-C22
18	A	806	CLA	C14-C13-C15-C16
18	A	809	CLA	C11-C10-C8-C9
18	A	804	CLA	C6-C7-C8-C9
18	A	804	CLA	C14-C13-C15-C16
18	A	811	CLA	C11-C12-C13-C14
18	A	803	CLA	C6-C7-C8-C9
18	A	802	CLA	C6-C7-C8-C9
18	A	802	CLA	C14-C13-C15-C16
18	A	843	CLA	C6-C7-C8-C9
18	A	844	CLA	C14-C13-C15-C16
18	A	812	CLA	C14-C13-C15-C16
18	A	829	CLA	C6-C7-C8-C9
18	B	808	CLA	C11-C12-C13-C14
18	B	809	CLA	C14-C13-C15-C16
18	B	841	CLA	C6-C7-C8-C9
18	B	806	CLA	C11-C12-C13-C14
18	B	824	CLA	C14-C13-C15-C16
18	B	817	CLA	C6-C7-C8-C9
18	H	201	CLA	C11-C10-C8-C9
18	B	822	CLA	C2A-CAA-CBA-CGA
18	B	825	CLA	C10-C11-C12-C13
18	B	840	CLA	C16-C17-C18-C19
22	K	205	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
20	B	852	LHG	C8-C7-O7-C5
18	A	819	CLA	C11-C12-C13-C14
18	A	807	CLA	C15-C16-C17-C18
18	A	812	CLA	C13-C15-C16-C17
18	A	812	CLA	C15-C16-C17-C18
18	1	603	CLA	C6-C7-C8-C9
20	A	846	LHG	C27-C28-C29-C30
18	1	604	CLA	C4B-C3B-CAB-CBB
18	3	612	CLA	C4B-C3B-CAB-CBB
18	4	608	CLA	C4B-C3B-CAB-CBB
18	4	614	CLA	C4B-C3B-CAB-CBB
18	A	824	CLA	C4B-C3B-CAB-CBB
18	A	844	CLA	C4B-C3B-CAB-CBB
18	A	829	CLA	C4B-C3B-CAB-CBB
18	A	836	CLA	C4B-C3B-CAB-CBB
18	B	827	CLA	C4B-C3B-CAB-CBB
18	B	839	CLA	C4B-C3B-CAB-CBB
18	B	836	CLA	C4B-C3B-CAB-CBB
18	H	201	CLA	C4B-C3B-CAB-CBB
18	J	101	CLA	C4B-C3B-CAB-CBB
18	A	807	CLA	C8-C10-C11-C12
20	1	615	LHG	O6-C4-C5-C6
18	1	603	CLA	C3-C5-C6-C7
18	B	813	CLA	C15-C16-C17-C18
18	A	836	CLA	O1D-CGD-O2D-CED
18	A	803	CLA	C2-C3-C5-C6
18	B	810	CLA	C2-C3-C5-C6
18	B	827	CLA	C2-C3-C5-C6
18	B	813	CLA	C2-C3-C5-C6
18	4	612	CLA	C5-C6-C7-C8
20	A	847	LHG	C5-C6-O8-C23
18	3	601	CLA	C3-C5-C6-C7
18	B	824	CLA	C3-C5-C6-C7
18	A	834	CLA	C5-C6-C7-C8
18	B	819	CLA	C2A-CAA-CBA-CGA
18	A	814	CLA	CAA-CBA-CGA-O2A
18	B	829	CLA	O1A-CGA-O2A-C1
18	2	604	CLA	C3A-C2A-CAA-CBA
18	A	822	CLA	C3A-C2A-CAA-CBA
18	A	833	CLA	C3A-C2A-CAA-CBA
18	A	836	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	K	204	CLA	C3A-C2A-CAA-CBA
18	B	803	CLA	C15-C16-C17-C18
20	1	615	LHG	C14-C15-C16-C17
18	B	841	CLA	C16-C17-C18-C20
17	1	601	CHL	C3-C5-C6-C7
18	A	841	CLA	C5-C6-C7-C8
20	B	852	LHG	C4-C5-C6-O8
23	4	620	LMG	C7-C8-C9-O8
18	B	828	CLA	O1A-CGA-O2A-C1
18	A	812	CLA	C16-C17-C18-C19
18	B	811	CLA	C5-C6-C7-C8
18	B	811	CLA	O1D-CGD-O2D-CED
18	B	841	CLA	C2A-CAA-CBA-CGA
18	B	820	CLA	C2A-CAA-CBA-CGA
20	1	615	LHG	O6-C4-C5-O7
18	1	604	CLA	C2B-C3B-CAB-CBB
18	3	612	CLA	C2B-C3B-CAB-CBB
18	4	608	CLA	C2B-C3B-CAB-CBB
18	4	614	CLA	C2B-C3B-CAB-CBB
18	A	824	CLA	C2B-C3B-CAB-CBB
18	A	836	CLA	C2B-C3B-CAB-CBB
18	B	836	CLA	C2B-C3B-CAB-CBB
18	H	201	CLA	C2B-C3B-CAB-CBB
18	J	101	CLA	C2B-C3B-CAB-CBB
18	B	827	CLA	C15-C16-C17-C18
18	B	807	CLA	O1A-CGA-O2A-C1
18	A	831	CLA	C3-C5-C6-C7
18	A	822	CLA	C2-C1-O2A-CGA
18	A	809	CLA	C2-C1-O2A-CGA
18	A	830	CLA	C2-C1-O2A-CGA
18	B	817	CLA	C2-C1-O2A-CGA
18	A	835	CLA	C11-C12-C13-C14
18	A	842	CLA	C11-C10-C8-C9
18	A	814	CLA	C14-C13-C15-C16
18	B	809	CLA	C6-C7-C8-C9
18	B	814	CLA	C11-C12-C13-C14
18	B	827	CLA	C14-C13-C15-C16
18	B	806	CLA	C6-C7-C8-C9
18	B	837	CLA	C15-C16-C17-C18
20	2	618	LHG	C2-C3-O3-P
20	B	852	LHG	C5-C4-O6-P
18	B	828	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	B	807	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C3-C5-C6-C7
22	B	845	BCR	C1-C6-C7-C8
18	4	611	CLA	C1A-C2A-CAA-CBA
18	B	835	CLA	C1A-C2A-CAA-CBA
19	2	617	XAT	C31-C32-C33-C34
22	4	618	BCR	C7-C8-C9-C10
22	K	205	BCR	C17-C18-C19-C20
18	B	841	CLA	C15-C16-C17-C18
18	B	827	CLA	C8-C10-C11-C12
22	F	304	BCR	C14-C15-C16-C17
18	B	832	CLA	C16-C17-C18-C19
18	A	806	CLA	C15-C16-C17-C18
18	2	612	CLA	C12-C13-C15-C16
18	A	806	CLA	C12-C13-C15-C16
18	A	804	CLA	C11-C10-C8-C7
18	A	826	CLA	C11-C12-C13-C15
18	A	831	CLA	C11-C12-C13-C15
18	A	835	CLA	C11-C12-C13-C15
18	A	842	CLA	C11-C12-C13-C15
18	A	843	CLA	C6-C7-C8-C10
18	A	841	CLA	C12-C13-C15-C16
18	A	814	CLA	C12-C13-C15-C16
18	A	812	CLA	C12-C13-C15-C16
18	A	829	CLA	C6-C7-C8-C10
18	B	818	CLA	C11-C10-C8-C7
18	B	841	CLA	C6-C7-C8-C10
18	B	814	CLA	C11-C10-C8-C7
18	B	814	CLA	C11-C12-C13-C15
18	B	806	CLA	C6-C7-C8-C10
18	B	824	CLA	C12-C13-C15-C16
18	B	803	CLA	C11-C10-C8-C7
18	B	817	CLA	C6-C7-C8-C10
18	B	840	CLA	C6-C7-C8-C10
18	F	301	CLA	C6-C7-C8-C10
18	A	831	CLA	C10-C11-C12-C13
18	A	833	CLA	CBD-CGD-O2D-CED
18	A	802	CLA	C15-C16-C17-C18
18	A	829	CLA	C13-C15-C16-C17
18	B	840	CLA	C15-C16-C17-C18
18	A	841	CLA	C2A-CAA-CBA-CGA
19	2	617	XAT	C40-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
18	1	609	CLA	C2A-CAA-CBA-CGA
18	B	841	CLA	C16-C17-C18-C19
18	A	820	CLA	C8-C10-C11-C12
18	2	602	CLA	CBA-CGA-O2A-C1
18	4	612	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	CBA-CGA-O2A-C1
18	A	826	CLA	C8-C10-C11-C12
18	1	602	CLA	CAD-CBD-CGD-O2D
18	1	605	CLA	CAD-CBD-CGD-O2D
18	2	610	CLA	CAD-CBD-CGD-O2D
18	3	608	CLA	CAD-CBD-CGD-O2D
18	3	607	CLA	CAD-CBD-CGD-O2D
18	4	603	CLA	CAD-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O2D
18	A	811	CLA	CAD-CBD-CGD-O2D
18	A	810	CLA	CAD-CBD-CGD-O2D
18	A	842	CLA	CAD-CBD-CGD-O2D
18	A	827	CLA	CAD-CBD-CGD-O2D
18	B	814	CLA	CAD-CBD-CGD-O2D
18	B	832	CLA	CAD-CBD-CGD-O2D
18	B	839	CLA	CAD-CBD-CGD-O2D
18	B	802	CLA	CAD-CBD-CGD-O2D
18	L	304	CLA	CAD-CBD-CGD-O2D
18	L	303	CLA	CAD-CBD-CGD-O2D
22	B	849	BCR	C6-C7-C8-C9
22	K	205	BCR	C22-C23-C24-C25
18	A	809	CLA	CBA-CGA-O2A-C1
20	1	615	LHG	C35-C36-C37-C38
18	A	818	CLA	C5-C6-C7-C8
18	B	837	CLA	C10-C11-C12-C13
18	L	303	CLA	C15-C16-C17-C18
18	4	603	CLA	C2A-CAA-CBA-CGA
18	A	841	CLA	C8-C10-C11-C12
18	A	824	CLA	CBD-CGD-O2D-CED
18	B	832	CLA	C16-C17-C18-C20
18	1	611	CLA	CHA-CBD-CGD-O1D
18	1	611	CLA	CHA-CBD-CGD-O2D
18	2	602	CLA	CHA-CBD-CGD-O1D
18	2	602	CLA	CHA-CBD-CGD-O2D
18	2	604	CLA	CHA-CBD-CGD-O1D
18	2	604	CLA	CHA-CBD-CGD-O2D
18	4	601	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	4	601	CLA	CHA-CBD-CGD-O2D
18	4	612	CLA	CHA-CBD-CGD-O1D
18	4	612	CLA	CHA-CBD-CGD-O2D
18	4	614	CLA	CHA-CBD-CGD-O1D
18	4	614	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	813	CLA	CHA-CBD-CGD-O1D
18	A	813	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	CHA-CBD-CGD-O1D
18	A	841	CLA	CHA-CBD-CGD-O2D
18	B	837	CLA	CHA-CBD-CGD-O1D
18	B	833	CLA	CHA-CBD-CGD-O1D
18	B	833	CLA	CHA-CBD-CGD-O2D
18	B	819	CLA	CHA-CBD-CGD-O1D
18	B	819	CLA	CHA-CBD-CGD-O2D
18	B	811	CLA	CHA-CBD-CGD-O1D
18	B	811	CLA	CHA-CBD-CGD-O2D
18	B	836	CLA	CHA-CBD-CGD-O1D
18	H	201	CLA	CHA-CBD-CGD-O1D
21	3	613	LUT	C11-C10-C9-C8
22	A	849	BCR	C20-C21-C22-C23
22	F	304	BCR	C11-C10-C9-C8
20	1	615	LHG	O1-C1-C2-O2
18	B	823	CLA	O1D-CGD-O2D-CED
18	B	834	CLA	C3-C5-C6-C7
18	4	601	CLA	O1A-CGA-O2A-C1
18	2	602	CLA	C14-C13-C15-C16
18	B	827	CLA	C11-C12-C13-C14
17	1	601	CHL	C2A-CAA-CBA-CGA
18	F	301	CLA	C3-C5-C6-C7
17	4	605	CHL	CHA-CBD-CGD-O2D
18	4	611	CLA	CHA-CBD-CGD-O2D
18	A	844	CLA	C16-C17-C18-C20
18	B	819	CLA	C6-C7-C8-C10
18	B	826	CLA	C5-C6-C7-C8
20	2	618	LHG	C4-O6-P-O3
20	B	852	LHG	C3-O3-P-O6
18	A	822	CLA	O1D-CGD-O2D-CED
17	1	601	CHL	C4-C3-C5-C6
20	2	618	LHG	C5-C4-O6-P

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Mol	Chain	Res	Type	Atoms
18	A	842	CLA	C2C-C3C-CAC-CBC
18	2	602	CLA	O1A-CGA-O2A-C1
18	4	612	CLA	O1A-CGA-O2A-C1
18	A	809	CLA	O1A-CGA-O2A-C1
17	2	607	CHL	C4B-C3B-CAB-CBB
18	1	607	CLA	C4B-C3B-CAB-CBB
18	1	611	CLA	C4B-C3B-CAB-CBB
18	1	612	CLA	C4B-C3B-CAB-CBB
18	3	611	CLA	C4B-C3B-CAB-CBB
18	3	609	CLA	C4B-C3B-CAB-CBB
18	3	604	CLA	C4B-C3B-CAB-CBB
18	3	610	CLA	C4B-C3B-CAB-CBB
18	3	602	CLA	C4B-C3B-CAB-CBB
18	4	601	CLA	C4B-C3B-CAB-CBB
18	4	611	CLA	C4B-C3B-CAB-CBB
18	A	813	CLA	C4B-C3B-CAB-CBB
18	A	808	CLA	C4B-C3B-CAB-CBB
18	A	810	CLA	C4B-C3B-CAB-CBB
18	A	840	CLA	C4B-C3B-CAB-CBB
18	A	817	CLA	C4B-C3B-CAB-CBB
18	A	837	CLA	C4B-C3B-CAB-CBB
18	B	835	CLA	C4B-C3B-CAB-CBB
18	B	834	CLA	C4B-C3B-CAB-CBB
18	B	808	CLA	C4B-C3B-CAB-CBB
18	B	840	CLA	C4B-C3B-CAB-CBB
18	F	303	CLA	C4B-C3B-CAB-CBB
18	F	301	CLA	C4B-C3B-CAB-CBB
18	G	201	CLA	C4B-C3B-CAB-CBB
18	G	202	CLA	C4B-C3B-CAB-CBB
18	K	201	CLA	C4B-C3B-CAB-CBB
18	K	204	CLA	C4B-C3B-CAB-CBB
18	L	302	CLA	C4B-C3B-CAB-CBB
20	1	615	LHG	C3-O3-P-O5
20	B	852	LHG	C4-O6-P-O4
18	A	812	CLA	CBA-CGA-O2A-C1
18	B	839	CLA	CBA-CGA-O2A-C1
18	A	841	CLA	CAD-CBD-CGD-O1D
18	B	813	CLA	CAD-CBD-CGD-O1D
18	B	822	CLA	CAD-CBD-CGD-O1D
18	F	302	CLA	CAD-CBD-CGD-O1D
18	B	837	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	A	808	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	C16-C17-C18-C20
18	2	602	CLA	C12-C13-C15-C16
18	A	830	CLA	C2-C3-C5-C6
18	A	812	CLA	C6-C7-C8-C10
18	B	805	CLA	C11-C10-C8-C7
18	B	808	CLA	C12-C13-C15-C16
18	B	814	CLA	C6-C7-C8-C10
18	F	301	CLA	C11-C10-C8-C7
25	B	842	PQN	C16-C17-C18-C20
25	B	842	PQN	C22-C23-C25-C26
20	1	615	LHG	C8-C7-O7-C5
18	4	614	CLA	C2A-CAA-CBA-CGA
24	A	801	CL0	C2A-CAA-CBA-CGA
18	4	601	CLA	CAA-CBA-CGA-O2A
17	1	601	CHL	CAD-CBD-CGD-O1D
17	2	605	CHL	C1C-C2C-CMC-OMC
18	3	609	CLA	CAD-CBD-CGD-O1D
23	4	620	LMG	O7-C8-C9-O8
27	B	850	DGD	CBB-CCB-CDB-CEB
18	A	812	CLA	O1A-CGA-O2A-C1
18	B	839	CLA	O1A-CGA-O2A-C1
18	4	609	CLA	C4-C3-C5-C6
18	1	602	CLA	CBA-CGA-O2A-C1
18	A	814	CLA	C13-C15-C16-C17
18	2	612	CLA	C14-C13-C15-C16
18	A	820	CLA	C6-C7-C8-C9
18	A	802	CLA	C11-C10-C8-C9
18	A	831	CLA	C11-C12-C13-C14
18	A	831	CLA	C14-C13-C15-C16
18	A	842	CLA	C11-C12-C13-C14
18	B	818	CLA	C11-C10-C8-C9
18	B	805	CLA	C14-C13-C15-C16
18	B	808	CLA	C11-C10-C8-C9
18	B	810	CLA	C6-C7-C8-C9
18	1	602	CLA	O1A-CGA-O2A-C1
18	A	841	CLA	CAA-CBA-CGA-O2A
22	A	852	BCR	C10-C11-C12-C13
22	L	301	BCR	C18-C19-C20-C21
18	B	808	CLA	C16-C17-C18-C20
22	B	846	BCR	C21-C22-C23-C24
18	1	607	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	1	611	CLA	C2B-C3B-CAB-CBB
18	1	612	CLA	C2B-C3B-CAB-CBB
18	3	611	CLA	C2B-C3B-CAB-CBB
18	3	604	CLA	C2B-C3B-CAB-CBB
18	3	610	CLA	C2B-C3B-CAB-CBB
18	3	602	CLA	C2B-C3B-CAB-CBB
18	4	609	CLA	C2B-C3B-CAB-CBB
18	4	611	CLA	C2B-C3B-CAB-CBB
18	A	808	CLA	C2B-C3B-CAB-CBB
18	A	810	CLA	C2B-C3B-CAB-CBB
18	A	835	CLA	C2B-C3B-CAB-CBB
18	A	844	CLA	C2B-C3B-CAB-CBB
18	A	829	CLA	C2B-C3B-CAB-CBB
18	A	837	CLA	C2B-C3B-CAB-CBB
18	B	835	CLA	C2B-C3B-CAB-CBB
18	B	834	CLA	C2B-C3B-CAB-CBB
18	B	808	CLA	C2B-C3B-CAB-CBB
18	B	827	CLA	C2B-C3B-CAB-CBB
18	B	840	CLA	C2B-C3B-CAB-CBB
18	F	301	CLA	C2B-C3B-CAB-CBB
18	G	201	CLA	C2B-C3B-CAB-CBB
18	K	201	CLA	C2B-C3B-CAB-CBB
18	K	204	CLA	C2B-C3B-CAB-CBB
18	L	302	CLA	C2B-C3B-CAB-CBB
20	1	615	LHG	O9-C7-O7-C5
20	B	851	LHG	C26-C27-C28-C29
27	B	850	DGD	C6B-C7B-C8B-C9B
18	2	612	CLA	C15-C16-C17-C18
18	1	604	CLA	C1-C2-C3-C4
18	3	601	CLA	C2A-CAA-CBA-CGA
18	4	612	CLA	C2A-CAA-CBA-CGA
18	A	808	CLA	O1A-CGA-O2A-C1
18	A	833	CLA	O1D-CGD-O2D-CED
17	1	601	CHL	C2-C1-O2A-CGA
18	A	842	CLA	C2-C1-O2A-CGA
18	B	827	CLA	C2-C1-O2A-CGA
18	A	844	CLA	C16-C17-C18-C19
18	A	824	CLA	O1D-CGD-O2D-CED
18	L	303	CLA	C13-C15-C16-C17
18	B	832	CLA	C13-C15-C16-C17
18	2	610	CLA	CMA-C3A-C4A-NA
18	4	614	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	818	CLA	C4-C3-C5-C6
18	1	603	CLA	C2-C3-C5-C6
20	B	852	LHG	O9-C7-O7-C5
18	B	826	CLA	C10-C11-C12-C13
18	A	822	CLA	CBA-CGA-O2A-C1
18	A	819	CLA	CAA-CBA-CGA-O2A
23	4	620	LMG	O7-C10-C11-C12
24	A	801	CL0	CAA-CBA-CGA-O2A
18	K	204	CLA	CBA-CGA-O2A-C1
21	2	619	LUT	C11-C10-C9-C8
22	L	301	BCR	C11-C10-C9-C8
20	B	852	LHG	O7-C5-C6-O8
20	A	847	LHG	C4-O6-P-O3
20	A	846	LHG	C3-O3-P-O6
18	A	842	CLA	C4C-C3C-CAC-CBC
17	2	605	CHL	O1D-CGD-O2D-CED
18	A	828	CLA	C11-C10-C8-C7
18	A	804	CLA	C11-C12-C13-C14
18	A	844	CLA	C6-C7-C8-C9
18	B	841	CLA	C14-C13-C15-C16
18	B	813	CLA	C11-C12-C13-C14
18	A	814	CLA	C10-C11-C12-C13
19	1	614	XAT	C33-C34-C35-C15
18	4	614	CLA	CBA-CGA-O2A-C1
18	A	839	CLA	C2A-CAA-CBA-CGA
18	A	822	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C31-C32-C33-C34
20	1	615	LHG	C32-C33-C34-C35
18	A	829	CLA	C16-C17-C18-C20
18	B	819	CLA	C6-C7-C8-C9
18	B	824	CLA	CBA-CGA-O2A-C1
18	B	832	CLA	CBA-CGA-O2A-C1
18	B	832	CLA	O1A-CGA-O2A-C1
18	2	602	CLA	C4B-C3B-CAB-CBB
18	4	609	CLA	C4B-C3B-CAB-CBB
18	A	835	CLA	C4B-C3B-CAB-CBB
18	B	803	CLA	C4B-C3B-CAB-CBB
18	B	805	CLA	O1A-CGA-O2A-C1
18	B	824	CLA	O1A-CGA-O2A-C1
18	3	602	CLA	C2-C1-O2A-CGA
18	B	836	CLA	C2-C1-O2A-CGA
18	A	835	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	B	808	CLA	C16-C17-C18-C19
18	1	607	CLA	CAA-CBA-CGA-O2A
18	1	602	CLA	C2A-CAA-CBA-CGA
18	A	814	CLA	C2A-CAA-CBA-CGA
18	B	816	CLA	C2A-CAA-CBA-CGA
18	4	613	CLA	C3A-C2A-CAA-CBA
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	813	CLA	C3A-C2A-CAA-CBA
18	A	843	CLA	C3A-C2A-CAA-CBA
18	B	821	CLA	C3A-C2A-CAA-CBA
18	H	201	CLA	C3A-C2A-CAA-CBA
18	A	831	CLA	C6-C7-C8-C9
18	B	825	CLA	C11-C10-C8-C9
18	L	303	CLA	C11-C12-C13-C14
25	B	842	PQN	C24-C23-C25-C26
18	1	607	CLA	CAA-CBA-CGA-O1A
22	A	852	BCR	C11-C10-C9-C34
22	A	851	BCR	C11-C10-C9-C34
22	A	851	BCR	C20-C21-C22-C37
22	B	845	BCR	C16-C17-C18-C36
22	K	202	BCR	C16-C17-C18-C36
22	L	305	BCR	C16-C17-C18-C36
22	L	301	BCR	C11-C10-C9-C34
18	1	611	CLA	CAA-CBA-CGA-O1A
18	2	611	CLA	CAA-CBA-CGA-O1A
18	2	608	CLA	CAA-CBA-CGA-O1A
18	B	809	CLA	C5-C6-C7-C8
18	B	805	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	O1D-CGD-O2D-CED
18	1	611	CLA	CAA-CBA-CGA-O2A
18	A	830	CLA	CBD-CGD-O2D-CED
20	B	851	LHG	C4-C5-O7-C7
18	A	818	CLA	C8-C10-C11-C12
18	B	841	CLA	C4-C3-C5-C6
18	2	609	CLA	C1A-C2A-CAA-CBA
18	4	604	CLA	C1A-C2A-CAA-CBA
18	A	813	CLA	C1A-C2A-CAA-CBA
18	A	843	CLA	C1A-C2A-CAA-CBA
18	B	803	CLA	C1A-C2A-CAA-CBA
18	H	201	CLA	C1A-C2A-CAA-CBA
18	4	612	CLA	C11-C10-C8-C7
18	B	828	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	B	813	CLA	C11-C10-C8-C7
18	B	840	CLA	C11-C10-C8-C7
24	A	801	CL0	C11-C12-C13-C15
18	B	816	CLA	C5-C6-C7-C8
18	3	603	CLA	CAA-CBA-CGA-O2A
24	A	801	CL0	CBA-CGA-O2A-C1
24	A	801	CL0	O1A-CGA-O2A-C1
18	3	603	CLA	CAA-CBA-CGA-O1A
18	G	203	CLA	CAA-CBA-CGA-O1A
18	1	604	CLA	C2A-CAA-CBA-CGA
18	A	836	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C11-C12-C13-C14
17	2	607	CHL	C2B-C3B-CAB-CBB
18	3	609	CLA	C2B-C3B-CAB-CBB
18	4	601	CLA	C2B-C3B-CAB-CBB
18	A	813	CLA	C2B-C3B-CAB-CBB
18	A	840	CLA	C2B-C3B-CAB-CBB
18	A	817	CLA	C2B-C3B-CAB-CBB
18	A	816	CLA	C2B-C3B-CAB-CBB
18	B	807	CLA	C2B-C3B-CAB-CBB
18	F	303	CLA	C2B-C3B-CAB-CBB
18	G	202	CLA	C2B-C3B-CAB-CBB
18	B	839	CLA	C15-C16-C17-C18
17	2	605	CHL	CBD-CGD-O2D-CED
19	2	617	XAT	C32-C33-C34-C35
22	A	852	BCR	C11-C10-C9-C8
22	A	851	BCR	C11-C10-C9-C8
22	A	851	BCR	C20-C21-C22-C23
22	B	845	BCR	C16-C17-C18-C19
22	K	202	BCR	C16-C17-C18-C19
22	L	305	BCR	C16-C17-C18-C19
18	4	603	CLA	CAA-CBA-CGA-O1A
18	A	809	CLA	C16-C17-C18-C20
18	2	611	CLA	CAA-CBA-CGA-O2A
18	B	818	CLA	C4-C3-C5-C6
18	A	803	CLA	C2-C1-O2A-CGA
18	A	832	CLA	C2-C1-O2A-CGA
18	B	841	CLA	C2-C1-O2A-CGA
18	B	817	CLA	CAA-CBA-CGA-O2A
18	F	301	CLA	C11-C10-C8-C9
18	2	608	CLA	CAA-CBA-CGA-O2A
18	B	805	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	2	612	CLA	C2A-CAA-CBA-CGA
18	K	204	CLA	C2A-CAA-CBA-CGA
18	L	303	CLA	C16-C17-C18-C20
22	A	852	BCR	C1-C6-C7-C8
22	A	852	BCR	C5-C6-C7-C8
22	B	849	BCR	C23-C24-C25-C30
18	A	819	CLA	C4-C3-C5-C6
18	A	829	CLA	C16-C17-C18-C19
18	A	835	CLA	CBD-CGD-O2D-CED
18	2	603	CLA	CAA-CBA-CGA-O2A
18	4	603	CLA	CAA-CBA-CGA-O2A
18	G	203	CLA	CAA-CBA-CGA-O2A
18	3	601	CLA	C11-C12-C13-C14
18	A	802	CLA	C5-C6-C7-C8
27	B	850	DGD	C1B-C2B-C3B-C4B
18	A	815	CLA	CAA-CBA-CGA-O2A
18	K	203	CLA	CAA-CBA-CGA-O2A
18	B	828	CLA	C3-C5-C6-C7
18	A	816	CLA	C4B-C3B-CAB-CBB
18	A	832	CLA	C4B-C3B-CAB-CBB
18	B	807	CLA	C4B-C3B-CAB-CBB
18	B	821	CLA	CAA-CBA-CGA-O2A
17	1	601	CHL	C2-C3-C5-C6
18	A	820	CLA	C11-C10-C8-C7
18	A	803	CLA	C6-C7-C8-C10
18	A	803	CLA	C11-C10-C8-C7
18	B	808	CLA	C11-C10-C8-C7
18	B	841	CLA	C2-C3-C5-C6
18	A	843	CLA	C5-C6-C7-C8
18	K	203	CLA	CAA-CBA-CGA-O1A
18	3	602	CLA	CAA-CBA-CGA-O2A
18	B	827	CLA	C16-C17-C18-C20
22	3	614	BCR	C20-C21-C22-C37
22	B	844	BCR	C11-C10-C9-C34
24	A	801	CL0	C4-C3-C5-C6
17	4	607	CHL	CAA-CBA-CGA-O2A
18	B	809	CLA	CAA-CBA-CGA-O2A
18	A	818	CLA	C11-C10-C8-C9
18	B	814	CLA	C6-C7-C8-C9
18	B	828	CLA	C6-C7-C8-C9
18	B	813	CLA	C11-C10-C8-C9
18	B	832	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	842	PQN	C16-C17-C18-C19
18	3	607	CLA	C3A-C2A-CAA-CBA
18	A	803	CLA	C3A-C2A-CAA-CBA
18	B	837	CLA	C3A-C2A-CAA-CBA
18	B	803	CLA	C3A-C2A-CAA-CBA
18	F	302	CLA	C3A-C2A-CAA-CBA
18	A	826	CLA	CAA-CBA-CGA-O2A
18	2	613	CLA	CAD-CBD-CGD-O2D
18	3	605	CLA	CAD-CBD-CGD-O2D
18	4	602	CLA	CAD-CBD-CGD-O2D
18	4	609	CLA	CAD-CBD-CGD-O2D
18	A	807	CLA	CAD-CBD-CGD-O2D
18	A	826	CLA	CAD-CBD-CGD-O2D
18	A	803	CLA	CAD-CBD-CGD-O2D
18	A	817	CLA	CAD-CBD-CGD-O2D
18	A	815	CLA	CAD-CBD-CGD-O2D
18	A	832	CLA	CAD-CBD-CGD-O2D
18	B	808	CLA	CAD-CBD-CGD-O2D
18	B	810	CLA	CAD-CBD-CGD-O2D
18	B	841	CLA	CAD-CBD-CGD-O2D
18	B	812	CLA	CAD-CBD-CGD-O2D
18	B	824	CLA	CAD-CBD-CGD-O2D
18	B	829	CLA	CAD-CBD-CGD-O2D
18	B	838	CLA	CAD-CBD-CGD-O2D
18	G	202	CLA	CAD-CBD-CGD-O2D
18	J	101	CLA	CAD-CBD-CGD-O2D
18	L	302	CLA	CAD-CBD-CGD-O2D
18	2	612	CLA	C8-C10-C11-C12
22	B	844	BCR	C15-C16-C17-C18
18	A	821	CLA	C2A-CAA-CBA-CGA
18	A	806	CLA	CBA-CGA-O2A-C1
18	2	603	CLA	CAA-CBA-CGA-O1A
18	A	815	CLA	CAA-CBA-CGA-O1A
17	1	601	CHL	CAA-CBA-CGA-O2A
17	2	607	CHL	CAA-CBA-CGA-O2A
18	3	609	CLA	CAA-CBA-CGA-O2A
18	A	807	CLA	CAA-CBA-CGA-O2A
19	4	617	XAT	O4-C6-C7-C8
18	A	814	CLA	CAA-CBA-CGA-O1A
20	B	852	LHG	C30-C31-C32-C33
18	B	828	CLA	C15-C16-C17-C18
18	B	832	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	4	604	CLA	CAA-CBA-CGA-O2A
18	A	826	CLA	O2A-C1-C2-C3
18	B	832	CLA	O2A-C1-C2-C3
18	F	301	CLA	O2A-C1-C2-C3
18	H	201	CLA	O2A-C1-C2-C3
18	J	101	CLA	O2A-C1-C2-C3
18	A	825	CLA	C2A-CAA-CBA-CGA
18	J	101	CLA	C2A-CAA-CBA-CGA
18	B	841	CLA	CAA-CBA-CGA-O2A
18	4	604	CLA	CAA-CBA-CGA-O1A
18	B	809	CLA	C16-C17-C18-C20
18	3	603	CLA	CHA-CBD-CGD-O1D
18	3	601	CLA	CHA-CBD-CGD-O1D
18	3	601	CLA	CHA-CBD-CGD-O2D
18	4	610	CLA	CHA-CBD-CGD-O1D
18	4	610	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	CHA-CBD-CGD-O2D
18	A	820	CLA	CHA-CBD-CGD-O2D
18	A	823	CLA	CHA-CBD-CGD-O1D
18	A	823	CLA	CHA-CBD-CGD-O2D
18	A	839	CLA	CHA-CBD-CGD-O1D
18	A	839	CLA	CHA-CBD-CGD-O2D
18	A	836	CLA	CHA-CBD-CGD-O1D
18	A	838	CLA	CHA-CBD-CGD-O2D
18	B	837	CLA	CHA-CBD-CGD-O2D
18	B	823	CLA	CHA-CBD-CGD-O1D
18	B	823	CLA	CHA-CBD-CGD-O2D
18	B	828	CLA	CHA-CBD-CGD-O1D
18	B	828	CLA	CHA-CBD-CGD-O2D
18	B	807	CLA	CHA-CBD-CGD-O1D
18	B	807	CLA	CHA-CBD-CGD-O2D
18	B	804	CLA	CHA-CBD-CGD-O1D
18	B	804	CLA	CHA-CBD-CGD-O2D
18	B	836	CLA	CHA-CBD-CGD-O2D
18	H	201	CLA	CHA-CBD-CGD-O2D
18	K	204	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O2D
18	4	608	CLA	CAA-CBA-CGA-O2A
18	B	811	CLA	CAA-CBA-CGA-O2A
22	B	844	BCR	C11-C10-C9-C8
17	4	607	CHL	CAA-CBA-CGA-O1A
18	A	804	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	A	806	CLA	O1A-CGA-O2A-C1
18	A	840	CLA	CAA-CBA-CGA-O2A
18	A	842	CLA	CAA-CBA-CGA-O2A
18	A	807	CLA	CBA-CGA-O2A-C1
23	4	619	LMG	C8-C9-O8-C28
18	2	609	CLA	C2-C1-O2A-CGA
18	4	609	CLA	C2-C3-C5-C6
18	4	612	CLA	C6-C7-C8-C10
18	A	804	CLA	C2-C3-C5-C6
18	B	837	CLA	C16-C17-C18-C20
18	A	803	CLA	C11-C10-C8-C9
18	A	843	CLA	C8-C10-C11-C12
18	A	809	CLA	C16-C17-C18-C19
18	A	842	CLA	C16-C17-C18-C20
18	B	827	CLA	C16-C17-C18-C19
18	L	303	CLA	C16-C17-C18-C19
18	A	807	CLA	O1A-CGA-O2A-C1
18	B	818	CLA	C2A-CAA-CBA-CGA
17	2	607	CHL	CAA-CBA-CGA-O1A
18	3	609	CLA	CAA-CBA-CGA-O1A
18	A	807	CLA	CAA-CBA-CGA-O1A
18	A	818	CLA	C2-C3-C5-C6
18	A	805	CLA	C3-C5-C6-C7
23	4	619	LMG	C29-C28-O8-C9
18	K	204	CLA	O1A-CGA-O2A-C1
18	1	610	CLA	CHA-CBD-CGD-O2D
18	A	803	CLA	C1A-C2A-CAA-CBA
18	B	837	CLA	C1A-C2A-CAA-CBA
18	3	602	CLA	CAA-CBA-CGA-O1A
20	B	852	LHG	O7-C7-C8-C9
18	B	811	CLA	CAA-CBA-CGA-O1A
20	B	852	LHG	C11-C12-C13-C14
18	2	602	CLA	C2A-CAA-CBA-CGA
18	4	602	CLA	C2A-CAA-CBA-CGA
18	A	815	CLA	C2A-CAA-CBA-CGA
18	B	824	CLA	C2A-CAA-CBA-CGA
18	2	602	CLA	C16-C17-C18-C19
18	B	809	CLA	CAA-CBA-CGA-O1A
17	4	607	CHL	C4B-C3B-CAB-CBB
18	B	810	CLA	C4B-C3B-CAB-CBB
20	1	615	LHG	C4-O6-P-O4
20	A	846	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
18	A	840	CLA	CAA-CBA-CGA-O1A
22	4	618	BCR	C1-C6-C7-C8
22	4	618	BCR	C5-C6-C7-C8
22	B	846	BCR	C1-C6-C7-C8
22	B	846	BCR	C5-C6-C7-C8
22	B	847	BCR	C1-C6-C7-C8
22	B	847	BCR	C5-C6-C7-C8
22	G	204	BCR	C1-C6-C7-C8
22	G	204	BCR	C5-C6-C7-C8
22	L	306	BCR	C5-C6-C7-C8
20	B	852	LHG	O9-C7-C8-C9
18	4	602	CLA	CAA-CBA-CGA-O2A
18	4	614	CLA	CAA-CBA-CGA-O2A
18	4	608	CLA	CAA-CBA-CGA-O1A
18	A	804	CLA	C2A-CAA-CBA-CGA
18	A	826	CLA	CAA-CBA-CGA-O1A
18	3	601	CLA	CAA-CBA-CGA-O2A
20	2	618	LHG	O7-C7-C8-C9
27	B	850	DGD	CFB-CGB-CHB-CIB
18	A	809	CLA	C4C-C3C-CAC-CBC
18	4	613	CLA	CAD-CBD-CGD-O1D
18	A	844	CLA	CAD-CBD-CGD-O1D
18	B	837	CLA	CAD-CBD-CGD-O1D
18	B	827	CLA	CAD-CBD-CGD-O1D
18	A	804	CLA	O1A-CGA-O2A-C1
18	B	832	CLA	CAA-CBA-CGA-O1A
18	B	806	CLA	CAA-CBA-CGA-O2A
18	B	828	CLA	C5-C6-C7-C8
18	2	602	CLA	C6-C7-C8-C9
18	A	820	CLA	C11-C12-C13-C14
18	B	810	CLA	C11-C12-C13-C14
18	B	840	CLA	C11-C10-C8-C9
23	4	620	LMG	C8-C9-O8-C28
18	K	204	CLA	CAA-CBA-CGA-O2A
18	B	822	CLA	C8-C10-C11-C12
18	2	612	CLA	CAA-CBA-CGA-O2A
18	A	830	CLA	C8-C10-C11-C12
18	A	842	CLA	CAA-CBA-CGA-O1A
18	A	804	CLA	C4-C3-C5-C6
17	1	601	CHL	CAD-CBD-CGD-O2D
18	1	607	CLA	CHA-CBD-CGD-O1D
18	2	612	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	3	609	CLA	CAD-CBD-CGD-O2D
18	3	610	CLA	CAD-CBD-CGD-O2D
18	4	611	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	C6-C7-C8-C10
18	B	825	CLA	C11-C12-C13-C15
21	2	619	LUT	C25-C26-C27-C28
18	2	609	CLA	CAA-CBA-CGA-O2A
18	A	837	CLA	CAA-CBA-CGA-O2A
22	A	852	BCR	C13-C14-C15-C16
18	B	824	CLA	CAA-CBA-CGA-O2A
18	F	301	CLA	CAA-CBA-CGA-O2A
18	2	609	CLA	CAA-CBA-CGA-O1A
18	B	806	CLA	CAA-CBA-CGA-O1A
18	B	802	CLA	C5-C6-C7-C8
18	1	604	CLA	O1D-CGD-O2D-CED
18	B	814	CLA	C10-C11-C12-C13
18	4	613	CLA	C2A-CAA-CBA-CGA
18	A	844	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	C2C-C3C-CAC-CBC
18	F	301	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

164 monomers are involved in 464 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	843	CLA	2	0
18	A	825	CLA	3	0
18	B	833	CLA	1	0
19	2	617	XAT	7	0
18	A	810	CLA	1	0
18	3	601	CLA	4	0
18	2	602	CLA	8	0
17	4	615	CHL	1	0
21	3	613	LUT	6	0
18	A	835	CLA	5	0
23	4	620	LMG	1	0
18	2	612	CLA	4	0
18	A	806	CLA	3	0
18	A	812	CLA	6	0
18	B	836	CLA	2	0
18	4	613	CLA	2	0
18	4	603	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	841	CLA	2	0
18	A	826	CLA	2	0
18	B	813	CLA	4	0
18	4	602	CLA	5	0
18	H	201	CLA	2	0
17	1	601	CHL	10	0
18	A	820	CLA	4	0
18	2	609	CLA	5	0
22	B	845	BCR	8	0
18	A	819	CLA	4	0
18	A	830	CLA	4	0
18	B	821	CLA	1	0
22	B	846	BCR	7	0
17	2	601	CHL	1	0
17	2	607	CHL	2	0
18	3	607	CLA	3	0
18	1	604	CLA	3	0
18	B	831	CLA	1	0
19	4	617	XAT	5	0
22	A	853	BCR	7	0
17	3	606	CHL	1	0
18	B	818	CLA	4	0
18	A	809	CLA	9	0
18	A	829	CLA	6	0
18	B	837	CLA	2	0
18	4	612	CLA	2	0
27	B	850	DGD	5	0
18	A	844	CLA	4	0
18	A	815	CLA	1	0
18	A	813	CLA	4	0
22	A	851	BCR	8	0
18	A	823	CLA	1	0
18	B	814	CLA	3	0
19	1	614	XAT	18	0
18	G	201	CLA	1	0
22	L	301	BCR	4	0
18	A	804	CLA	6	0
22	L	306	BCR	5	0
18	B	832	CLA	6	0
18	B	802	CLA	4	0
17	2	606	CHL	1	0
18	1	605	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	609	CLA	7	0
22	B	847	BCR	4	0
20	B	852	LHG	3	0
17	4	607	CHL	2	0
18	B	812	CLA	1	0
20	2	618	LHG	3	0
18	B	820	CLA	2	0
18	4	614	CLA	2	0
18	B	840	CLA	6	0
18	B	819	CLA	1	0
18	A	836	CLA	1	0
18	B	838	CLA	2	0
18	A	805	CLA	3	0
18	A	814	CLA	2	0
18	B	822	CLA	8	0
18	B	817	CLA	3	0
25	A	855	PQN	3	0
18	K	201	CLA	1	0
18	A	842	CLA	5	0
18	B	803	CLA	4	0
21	2	616	LUT	4	0
18	1	608	CLA	1	0
18	L	302	CLA	2	0
20	1	615	LHG	13	0
18	1	603	CLA	1	0
21	4	616	LUT	4	0
18	A	845	CLA	1	0
18	3	612	CLA	1	0
18	A	808	CLA	2	0
17	2	605	CHL	3	0
18	B	825	CLA	2	0
18	A	802	CLA	3	0
18	3	605	CLA	1	0
22	4	618	BCR	4	0
21	1	616	LUT	3	0
18	A	831	CLA	1	0
17	2	615	CHL	5	0
18	A	827	CLA	1	0
18	A	828	CLA	1	0
22	B	844	BCR	2	0
18	1	607	CLA	1	0
18	A	817	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	821	CLA	2	0
18	B	804	CLA	1	0
18	F	302	CLA	5	0
22	L	305	BCR	9	0
21	2	619	LUT	6	0
22	B	801	BCR	10	0
18	B	830	CLA	1	0
18	1	612	CLA	1	0
18	2	604	CLA	5	0
18	3	609	CLA	1	0
18	F	301	CLA	1	0
18	2	613	CLA	1	0
22	A	849	BCR	2	0
22	J	102	BCR	6	0
18	4	609	CLA	4	0
18	A	818	CLA	1	0
22	3	614	BCR	4	0
18	B	808	CLA	5	0
18	J	101	CLA	2	0
18	A	807	CLA	3	0
20	A	846	LHG	6	0
18	B	823	CLA	2	0
18	B	827	CLA	5	0
22	F	304	BCR	2	0
18	A	834	CLA	3	0
25	B	842	PQN	2	0
18	B	828	CLA	6	0
22	K	202	BCR	3	0
18	1	602	CLA	8	0
18	2	608	CLA	2	0
18	B	826	CLA	3	0
18	L	303	CLA	5	0
18	B	824	CLA	6	0
18	B	809	CLA	4	0
18	A	832	CLA	1	0
18	A	833	CLA	3	0
18	A	841	CLA	6	0
17	4	605	CHL	1	0
18	A	840	CLA	1	0
18	3	602	CLA	2	0
18	1	611	CLA	1	0
20	B	851	LHG	2	0

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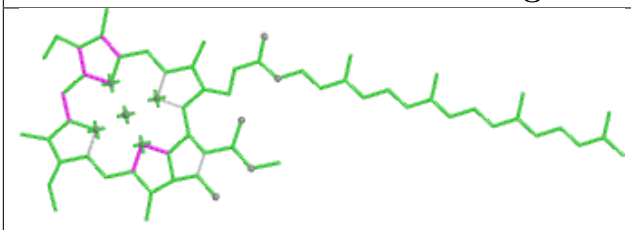
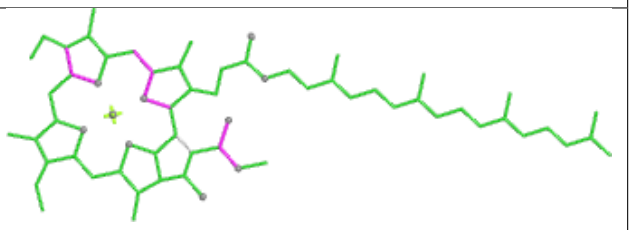
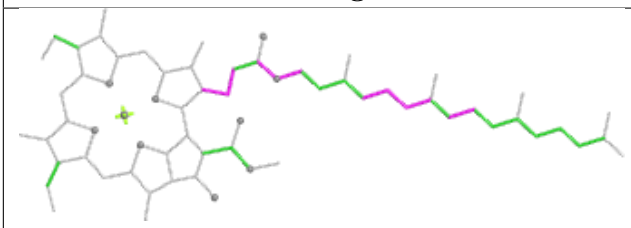
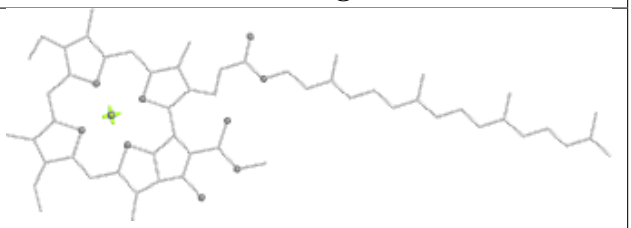
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	K	205	BCR	4	0
18	A	839	CLA	1	0
22	B	849	BCR	4	0
22	I	101	BCR	1	0
18	K	204	CLA	1	0
22	B	843	BCR	4	0
18	A	822	CLA	4	0
18	4	608	CLA	2	0
18	3	603	CLA	2	0
22	A	850	BCR	5	0
18	4	610	CLA	1	0
18	A	803	CLA	3	0
18	B	806	CLA	3	0
18	A	811	CLA	3	0
24	A	801	CL0	5	0
18	B	834	CLA	1	0
18	B	805	CLA	6	0
22	A	848	BCR	3	0
22	B	848	BCR	5	0
22	A	852	BCR	2	0
22	G	204	BCR	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 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

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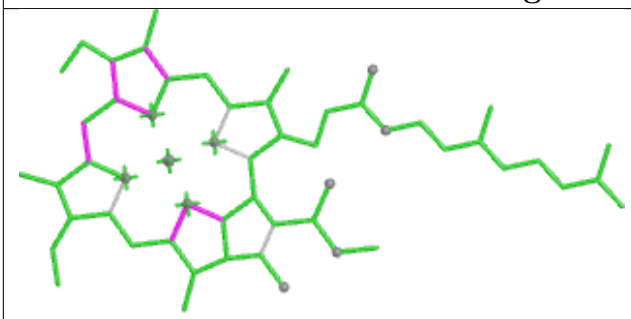
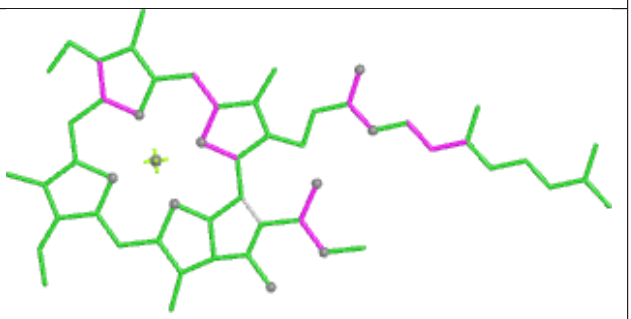
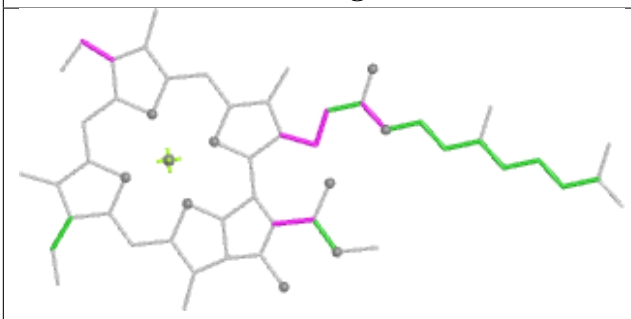
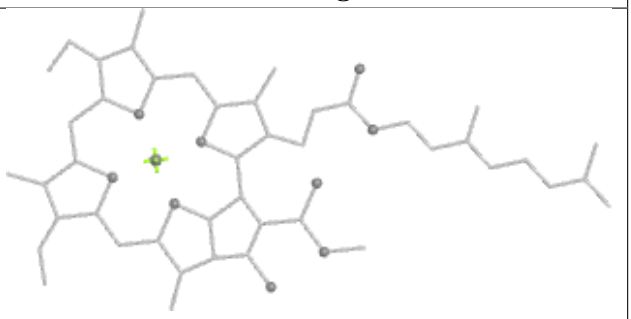
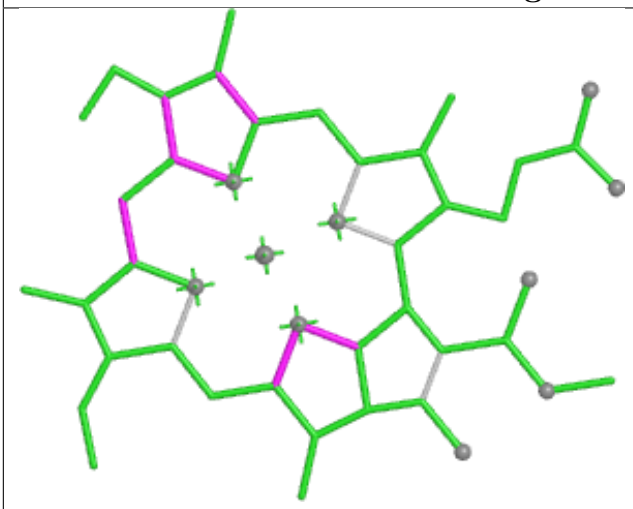
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 833



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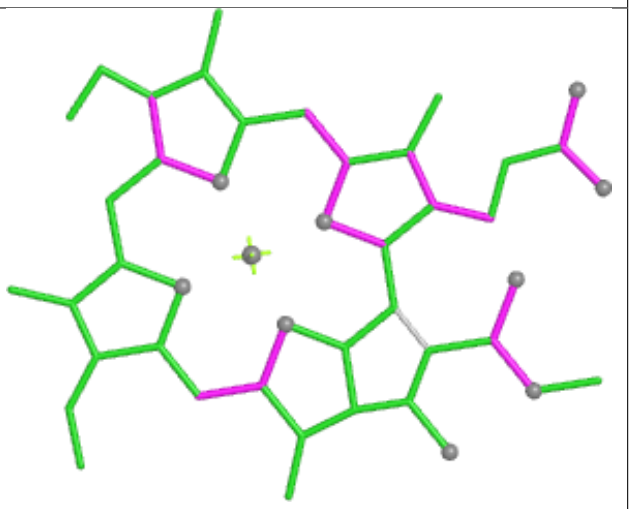

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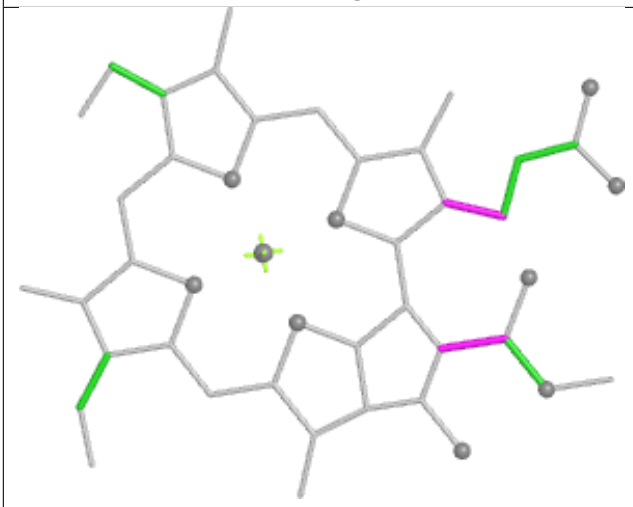
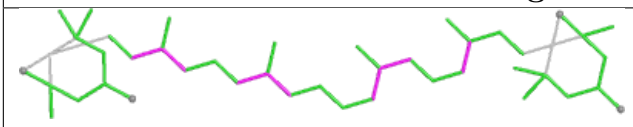


Torsions

Rings

Ligand XAT 2 617



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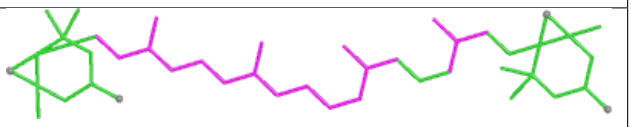

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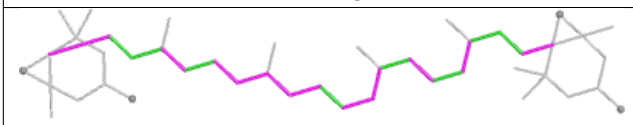

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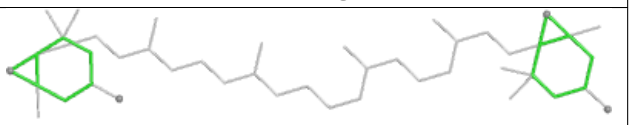
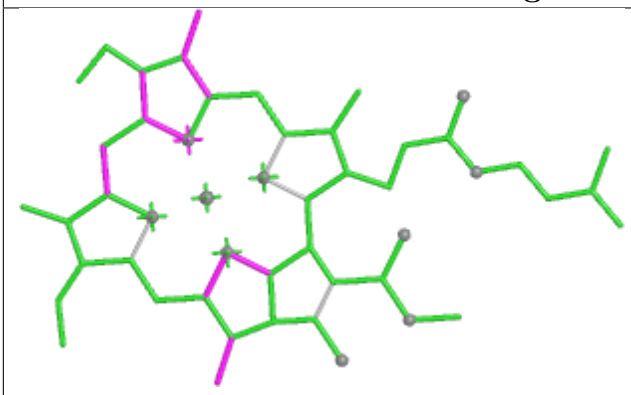


Rings

Ligand CLA A 810



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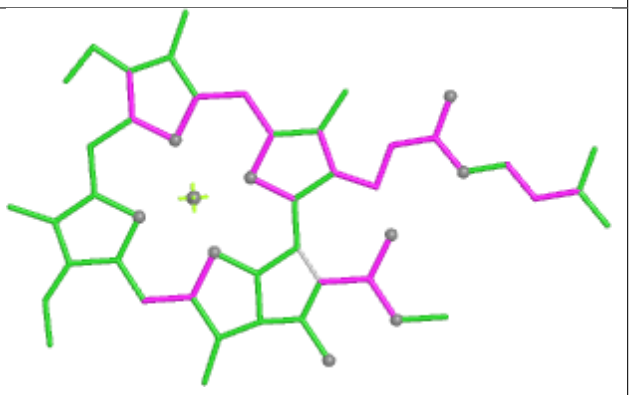

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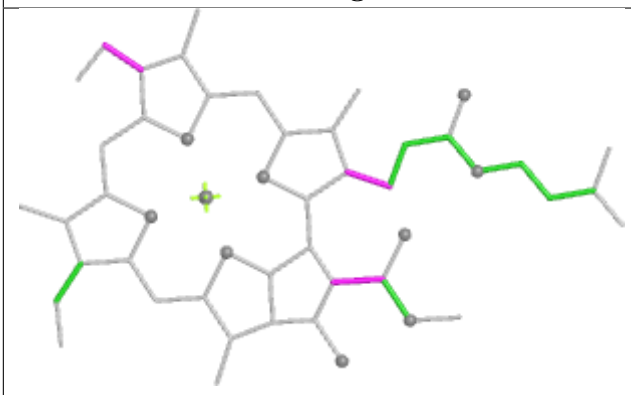

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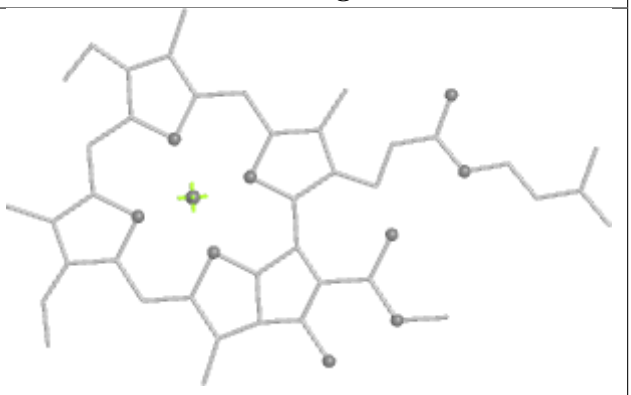
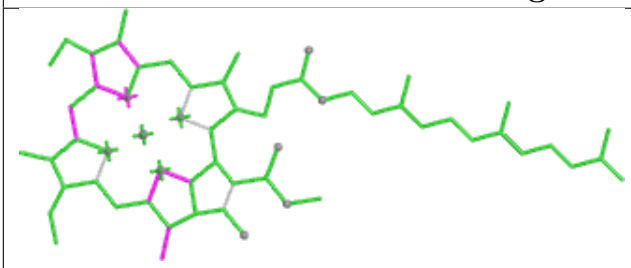


Rings

Ligand CLA 3 601



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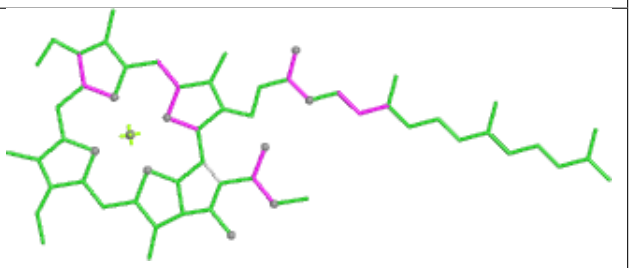

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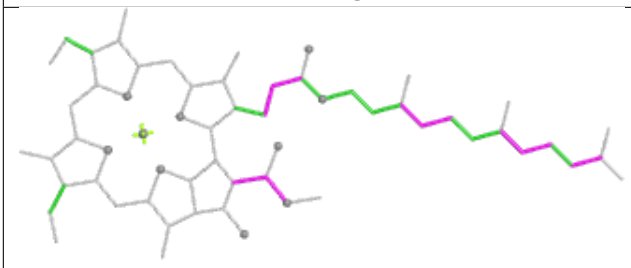

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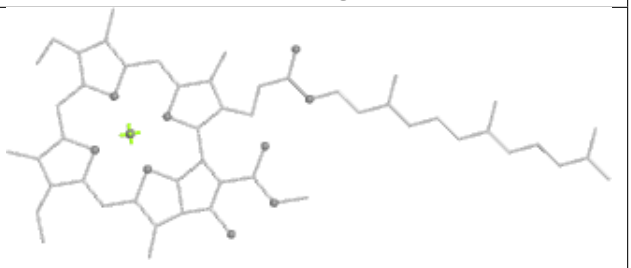
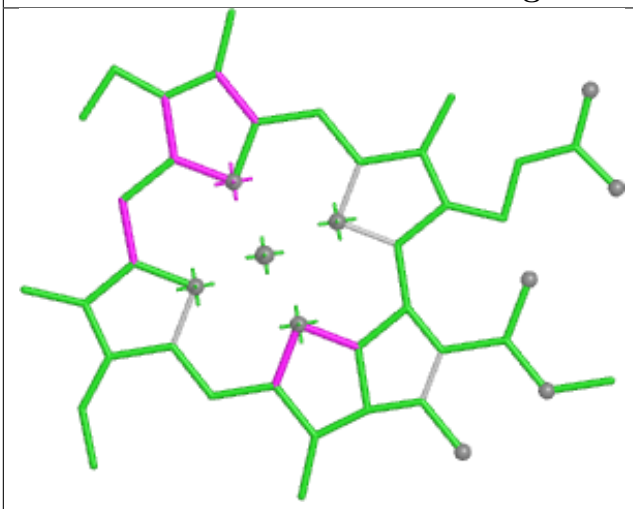


Rings

Ligand CLA G 203



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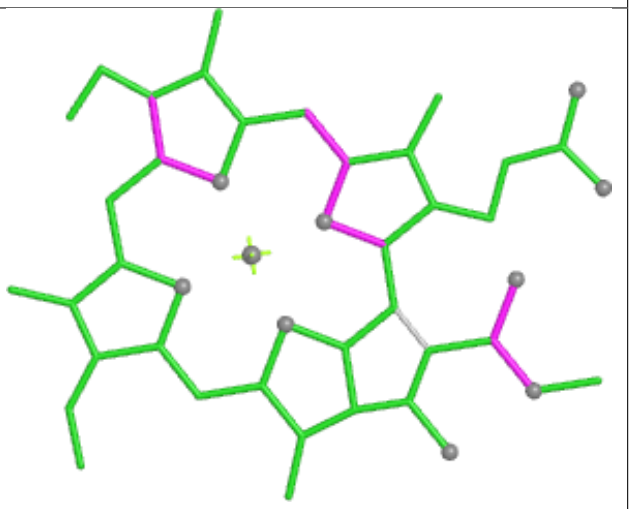

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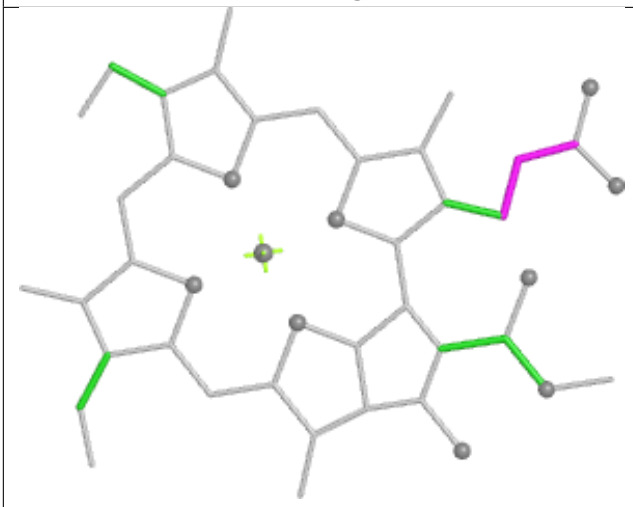
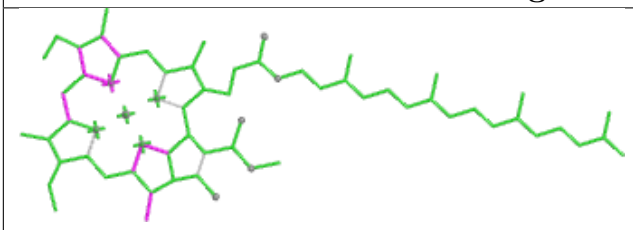


Torsions

Rings

Ligand CLA 2 602



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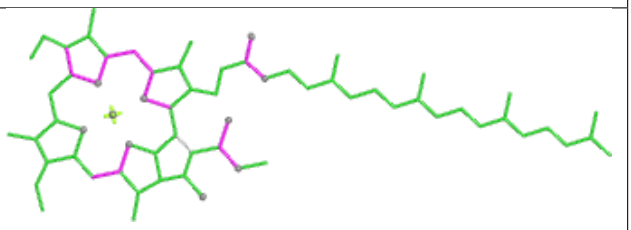

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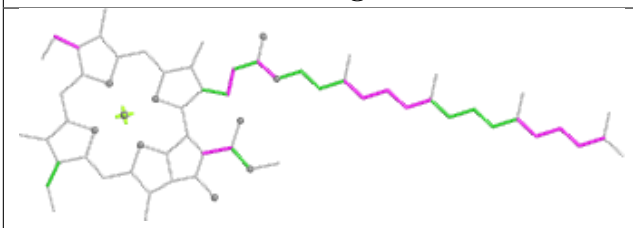
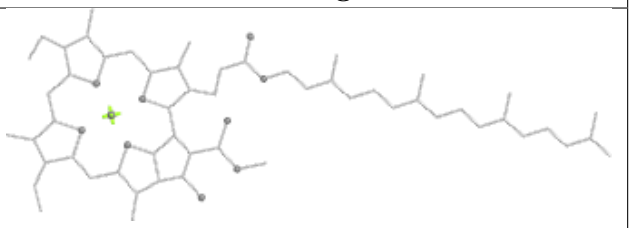
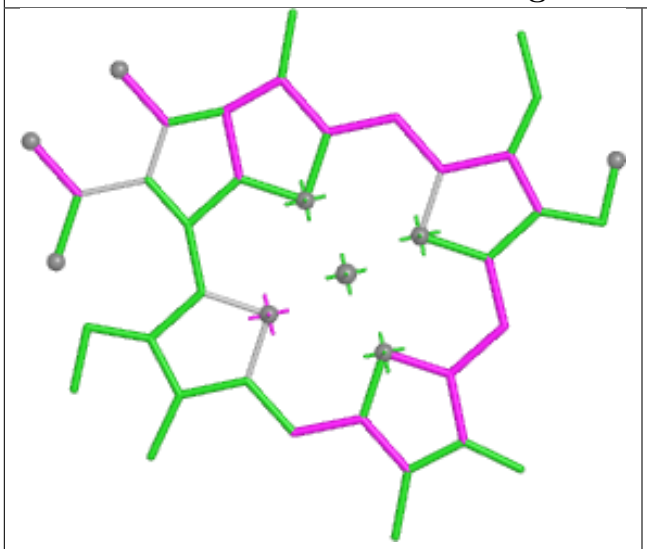


Torsions



Rings

Ligand CHL 4 615



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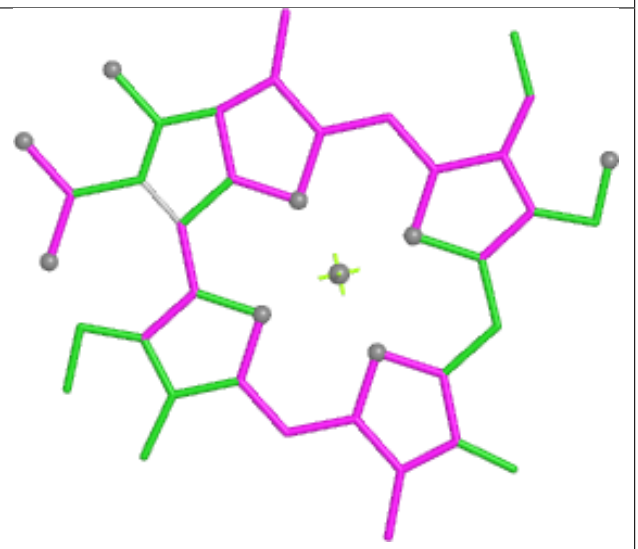

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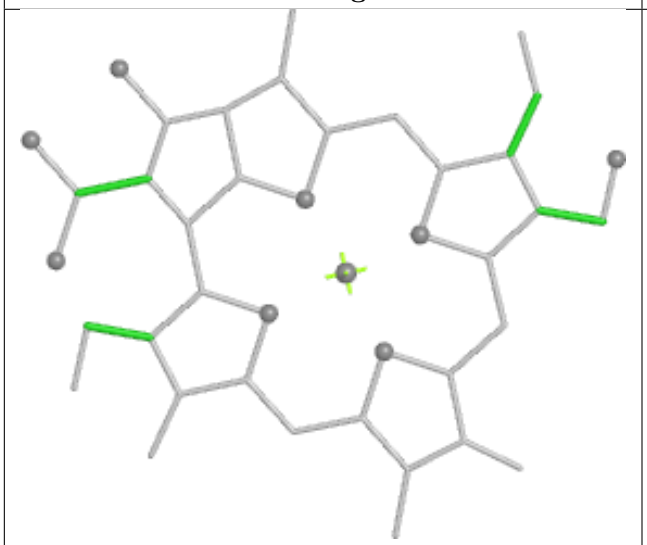

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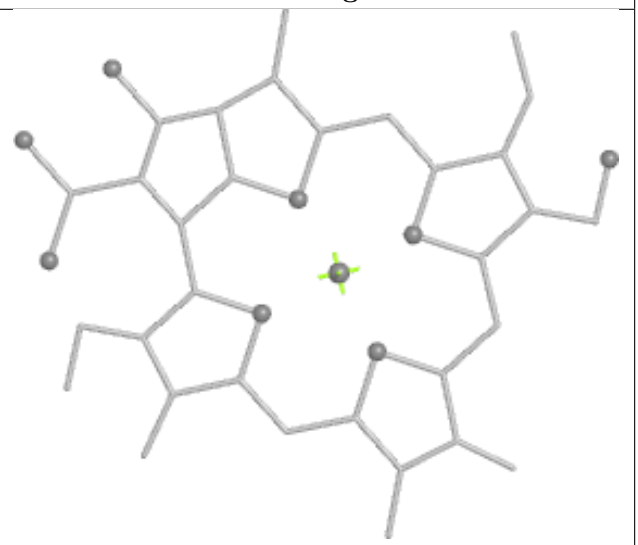

Rings

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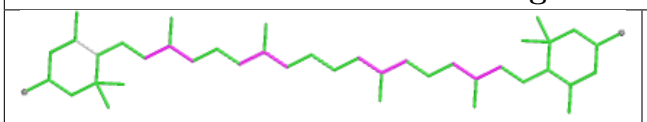

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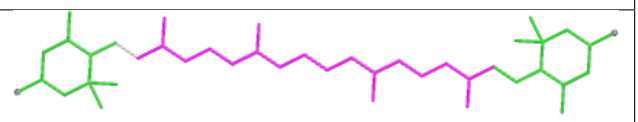

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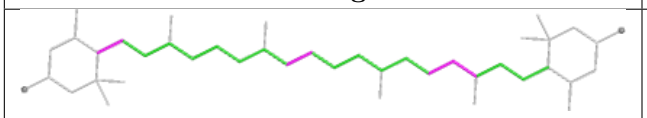

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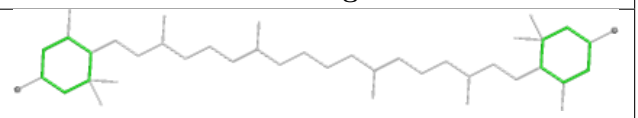
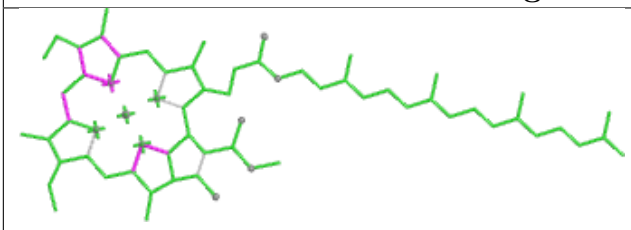


Rings

Ligand CLA A 835



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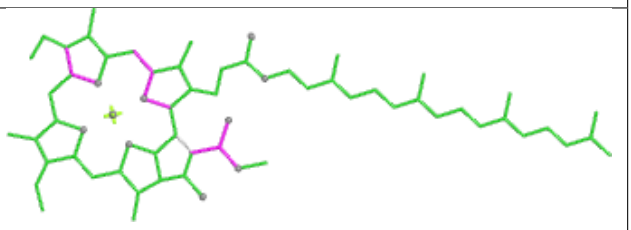

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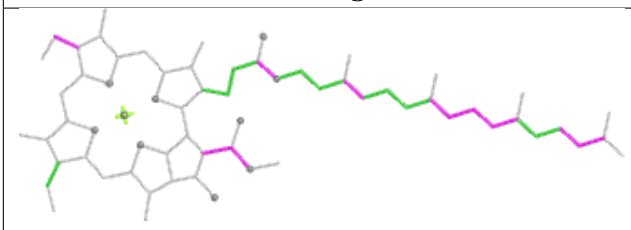

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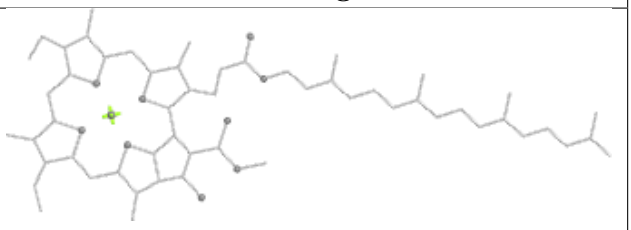
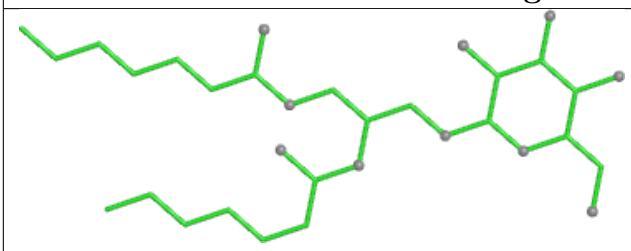


Rings

Ligand LMG 4 620



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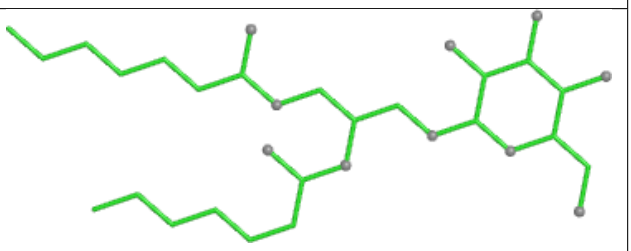
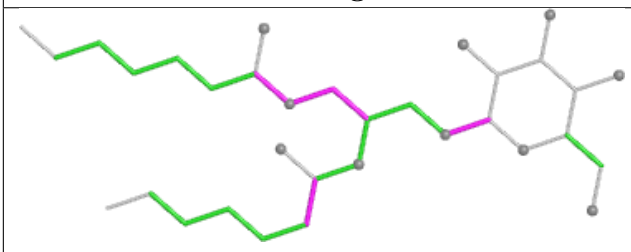


Bond angles



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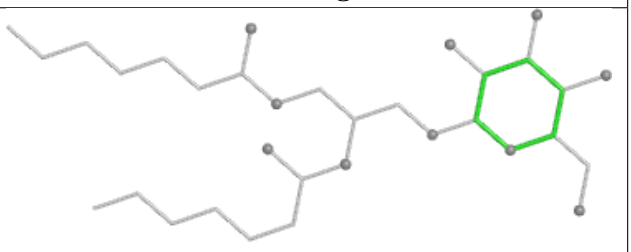
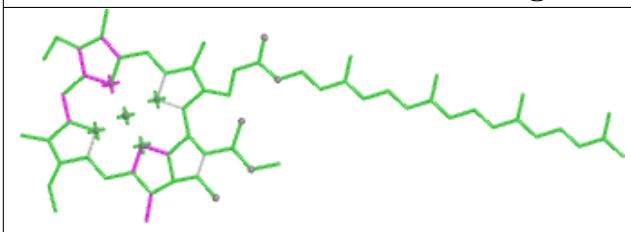


Rings

Ligand CLA 2 612



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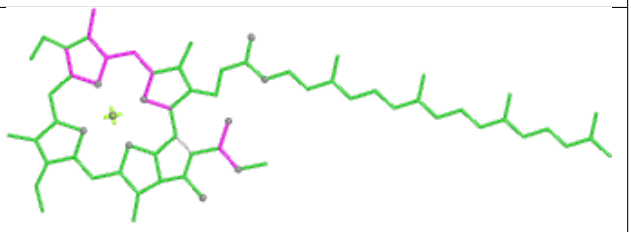
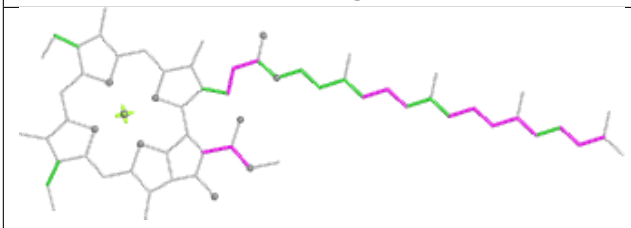


Bond angles



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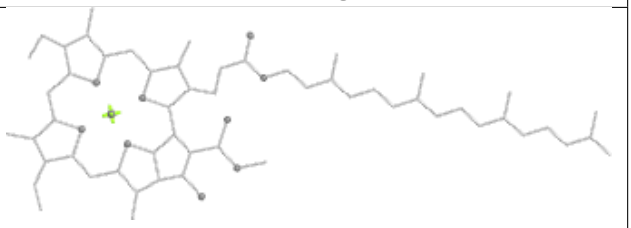
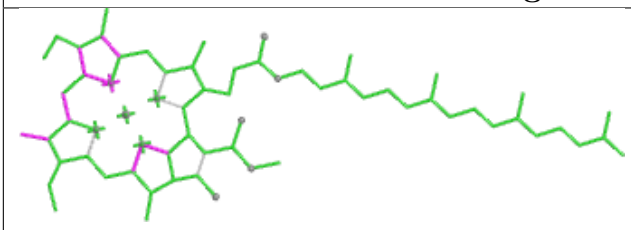


Rings

Ligand CLA A 806



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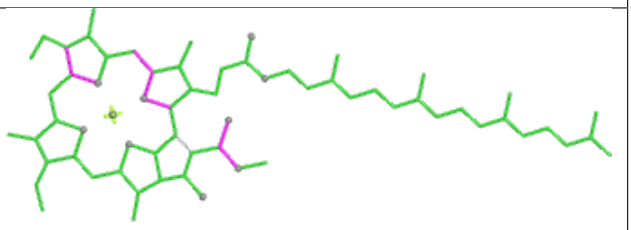
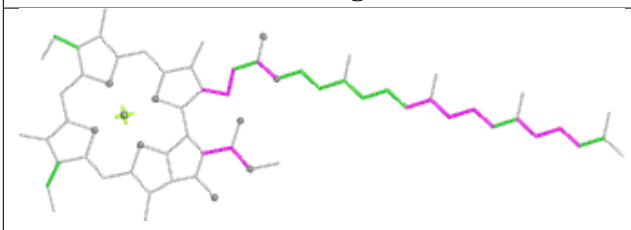
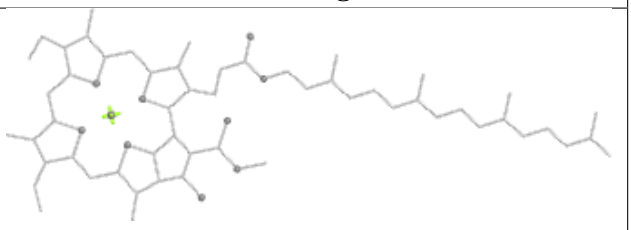


Bond angles

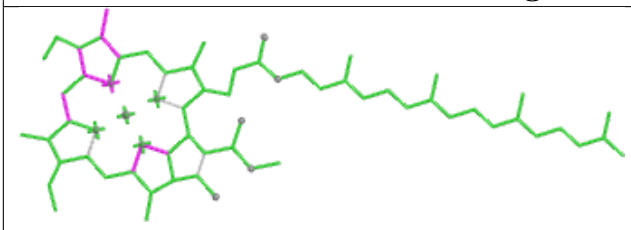


Torsions

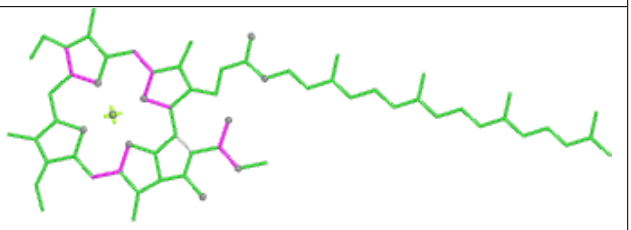


Rings

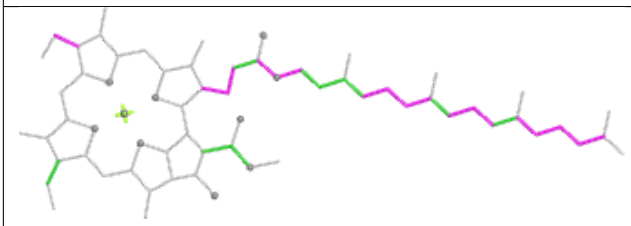
Ligand CLA A 812



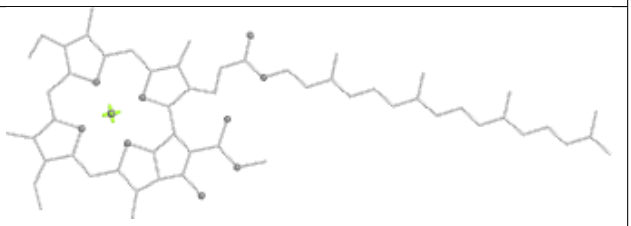
Bond lengths



Bond angles

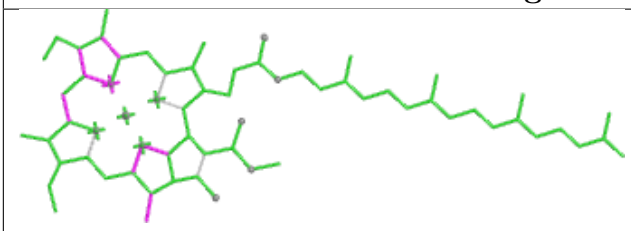


Torsions

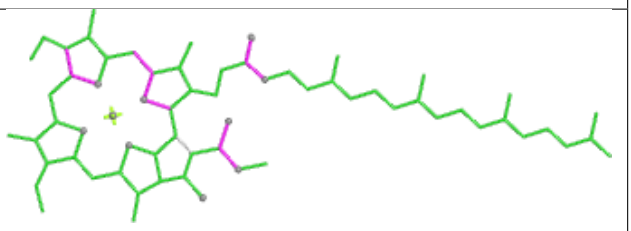


Rings

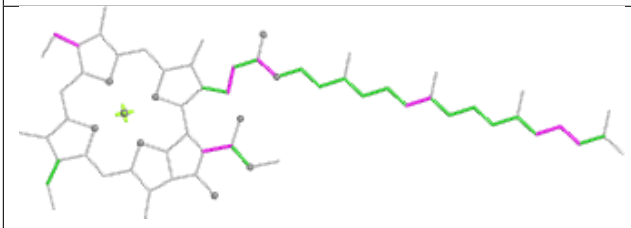
Ligand CLA B 839



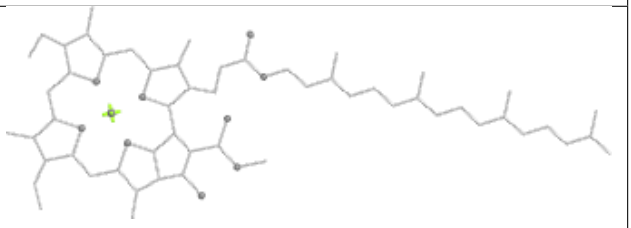
Bond lengths



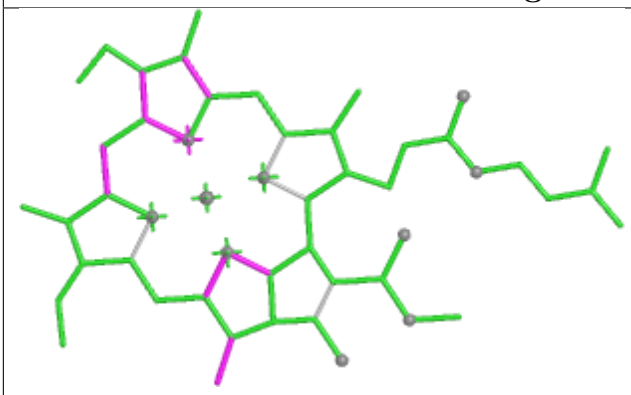
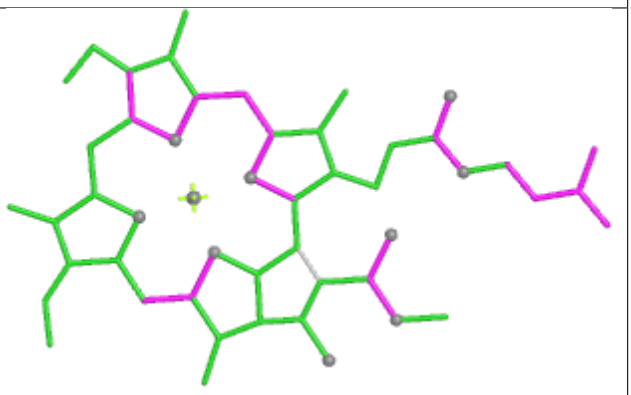
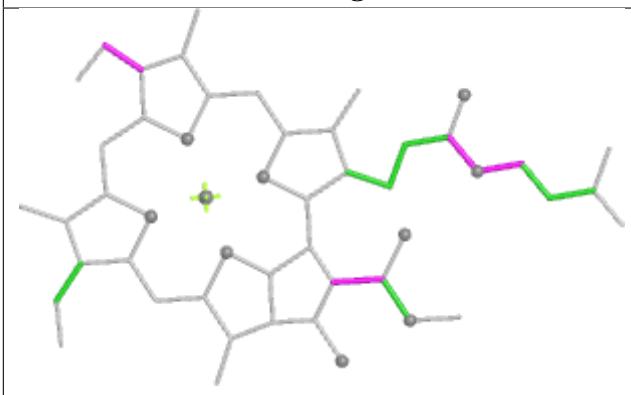
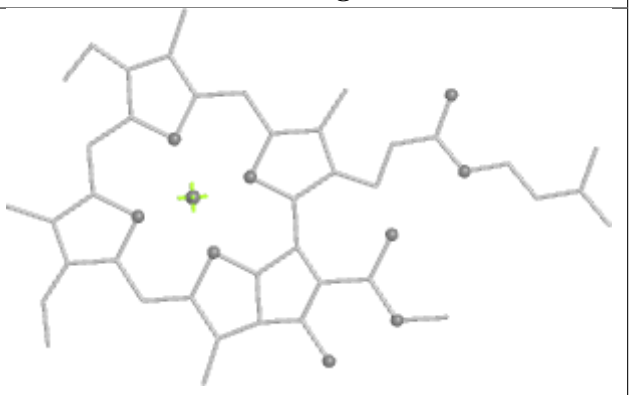
Bond angles



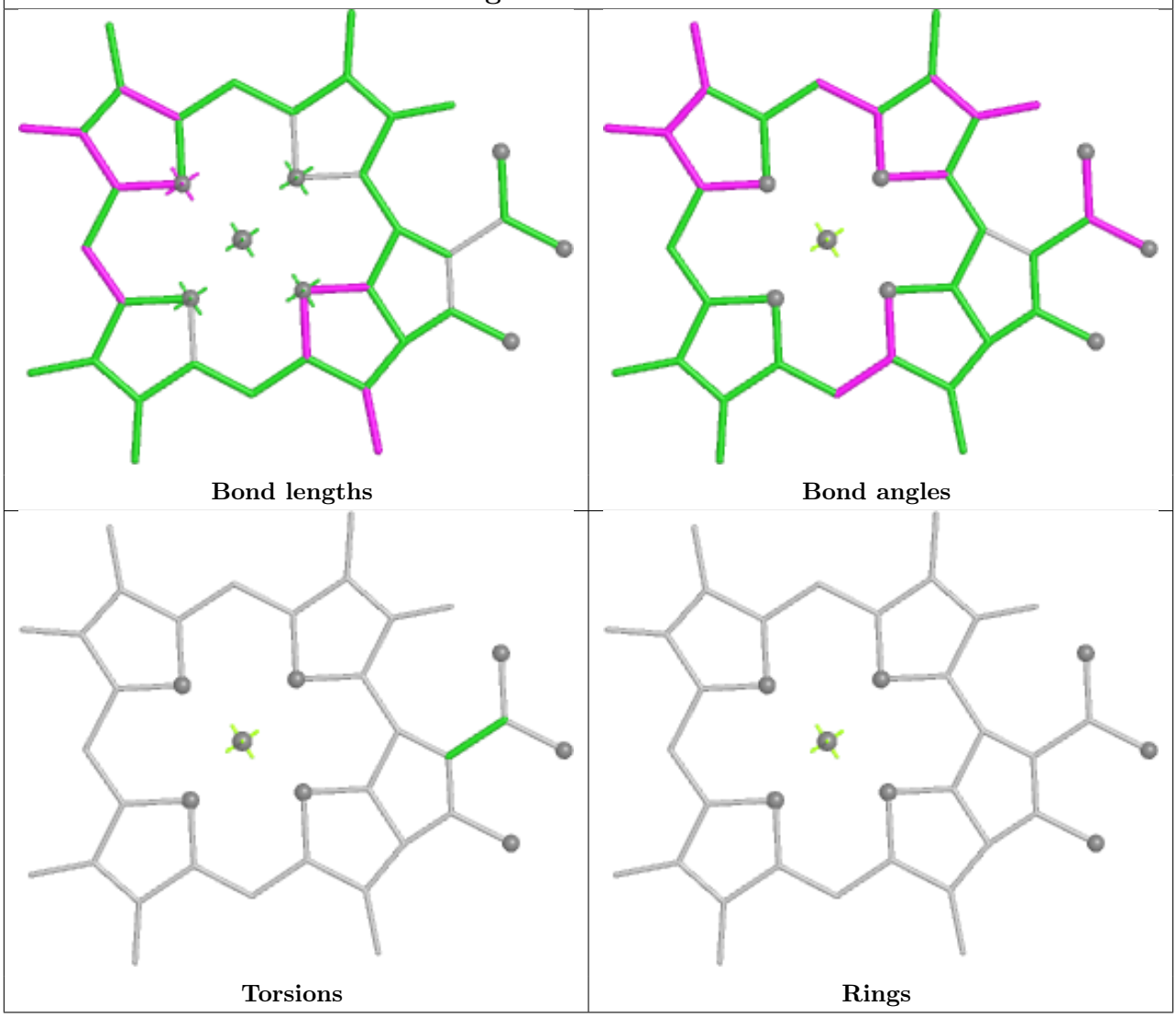
Torsions



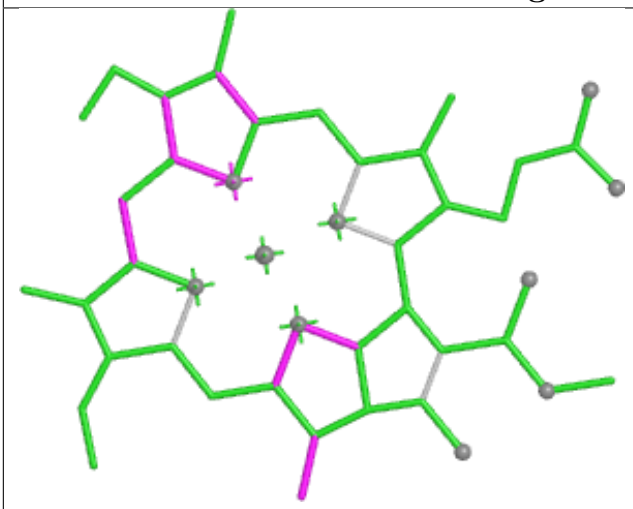
Rings

Ligand CLA B 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

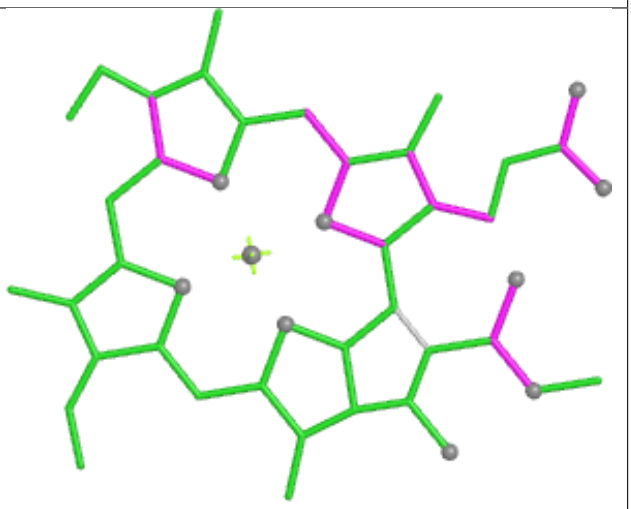
Ligand CLA 1 613



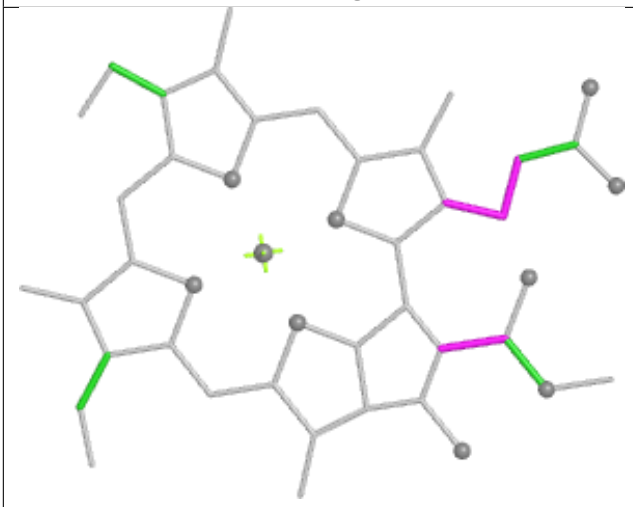
Ligand CLA 4 613



Bond lengths



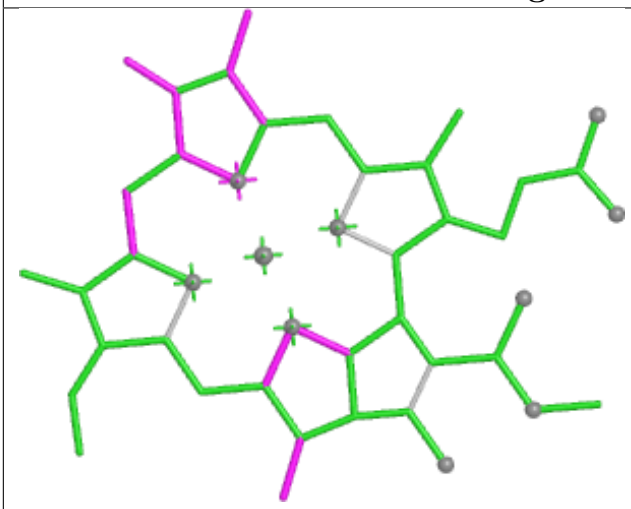
Bond angles



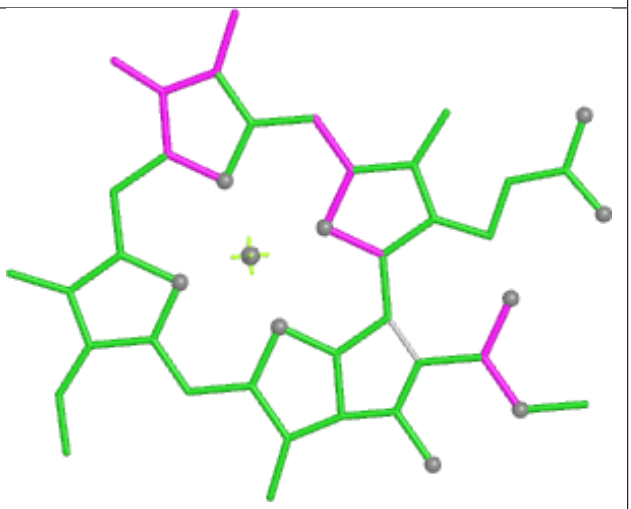
Torsions

Rings

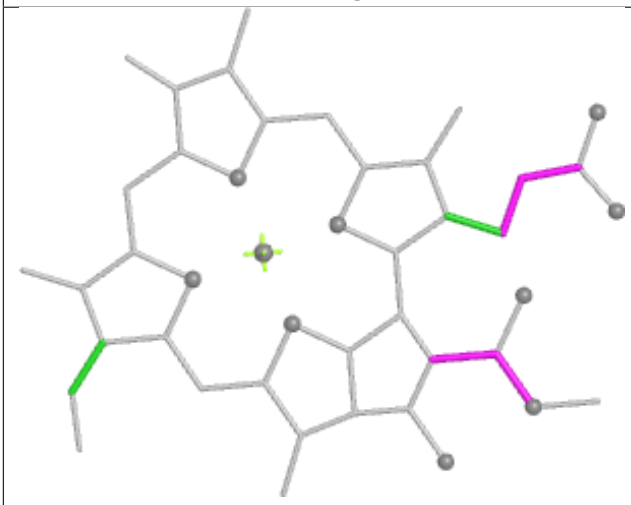
Ligand CLA 4 603



Bond lengths



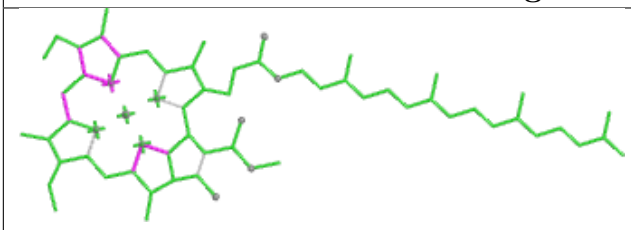
Bond angles



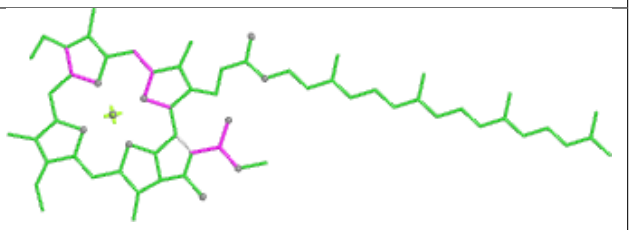
Torsions

Rings

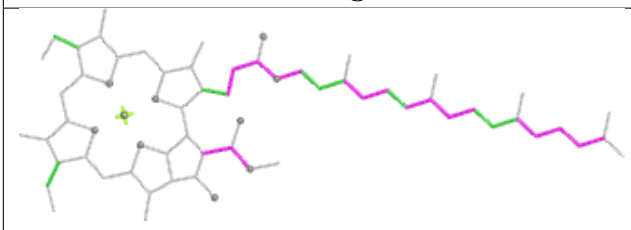
Ligand CLA B 841



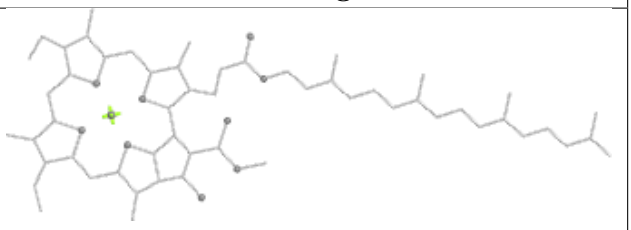
Bond lengths



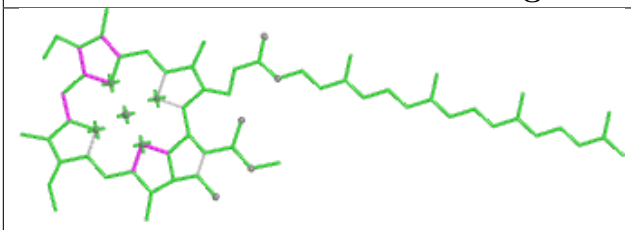
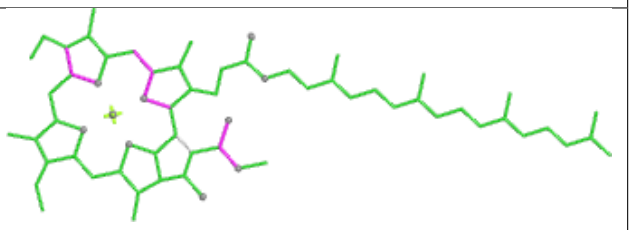
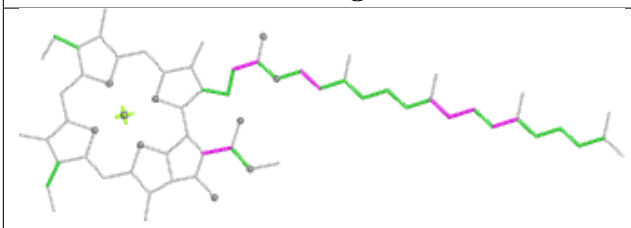
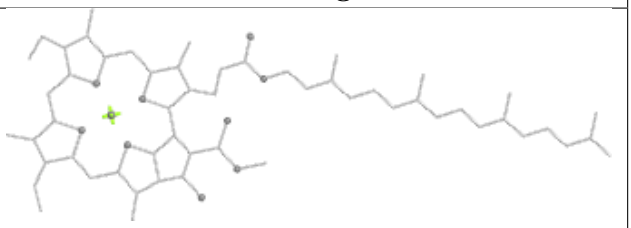
Bond angles

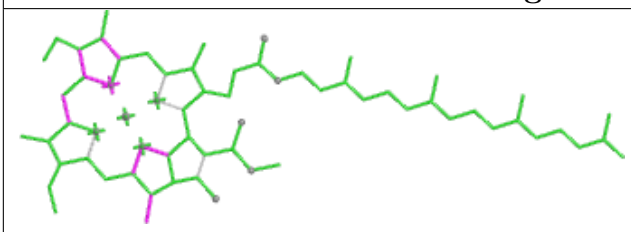
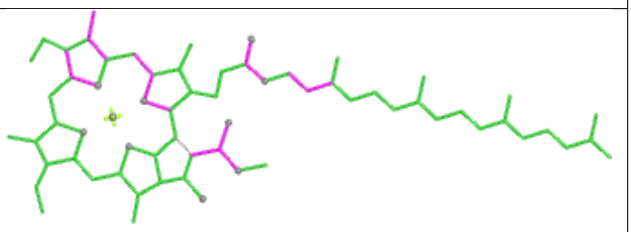
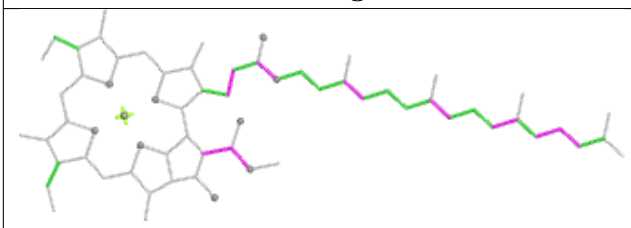
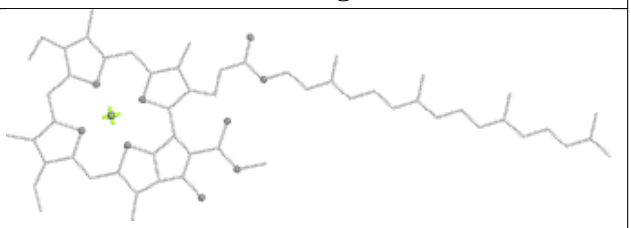


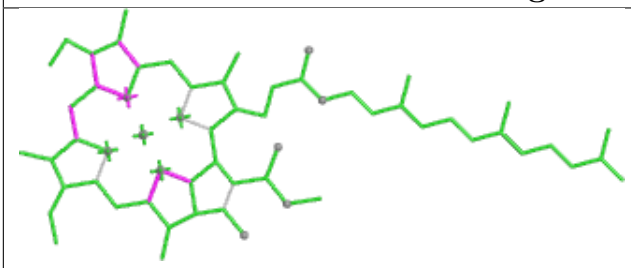
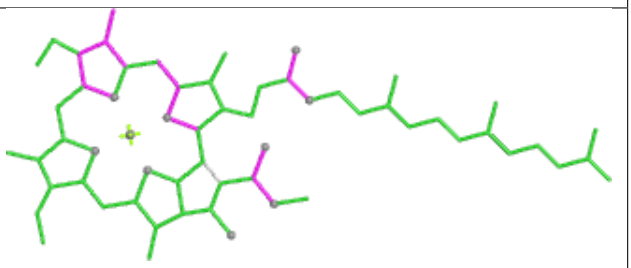
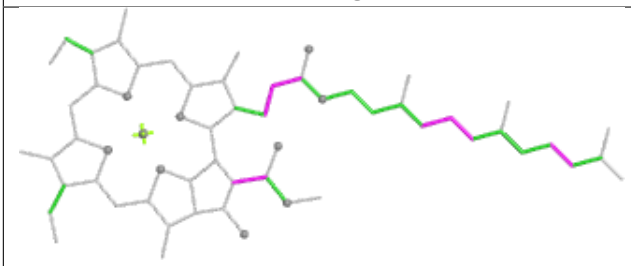
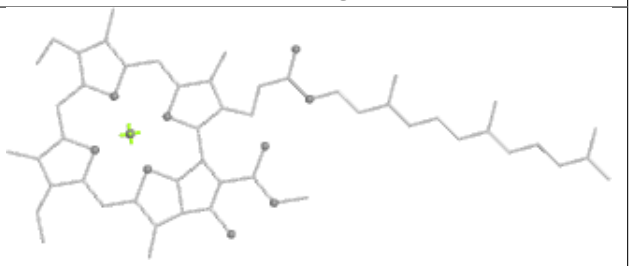
Torsions

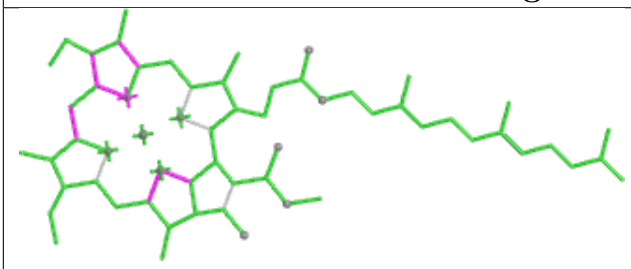
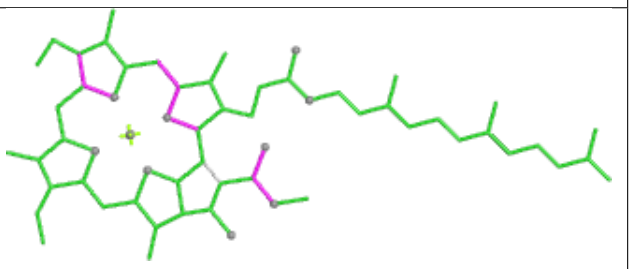
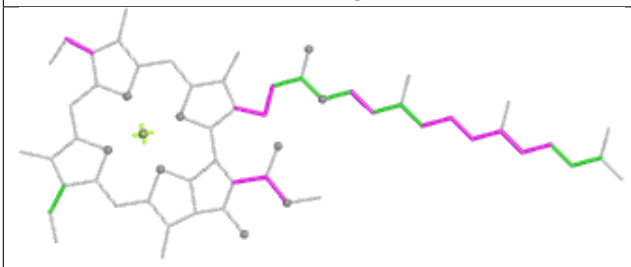
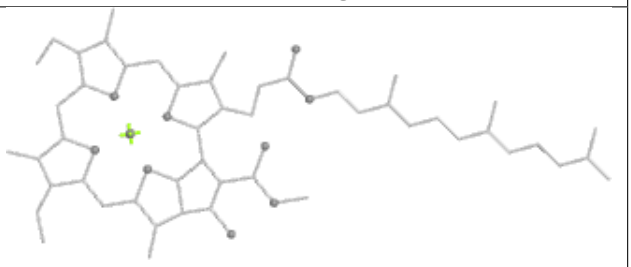


Rings

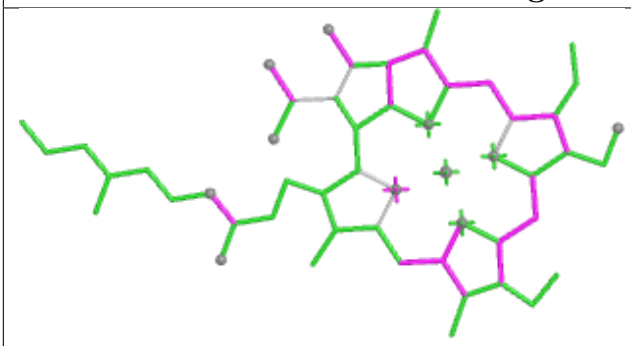
Ligand CLA A 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

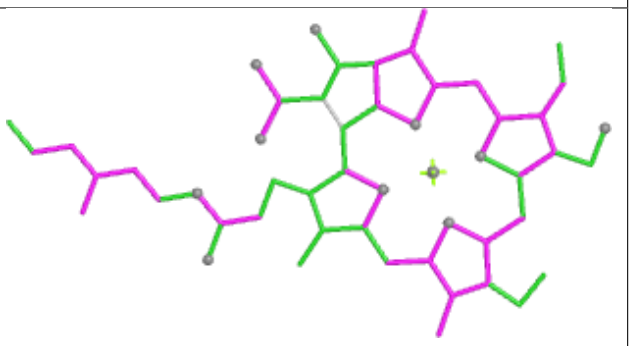
Ligand CLA 4 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

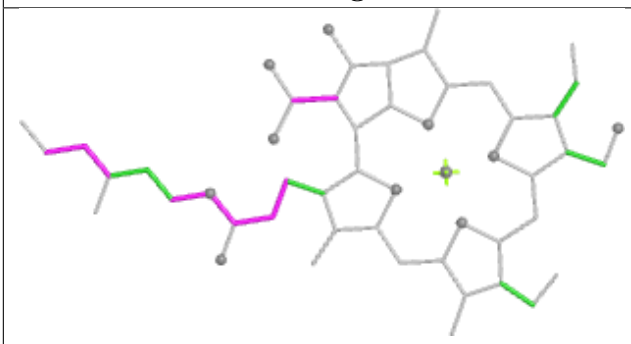
Ligand CHL 1 601



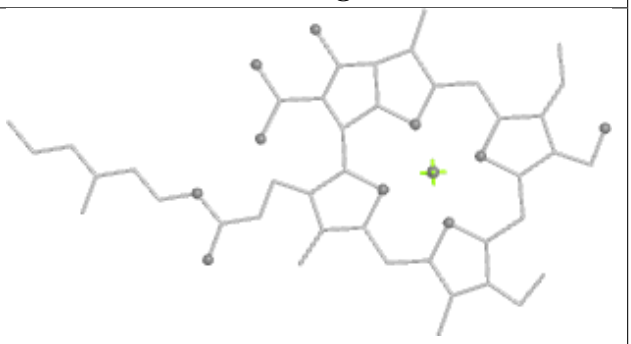
Bond lengths



Bond angles

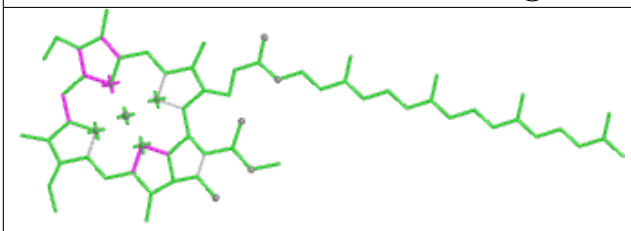


Torsions



Rings

Ligand CLA A 820



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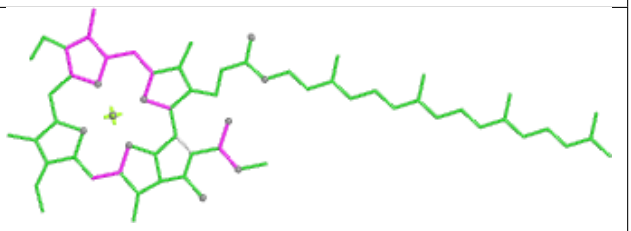
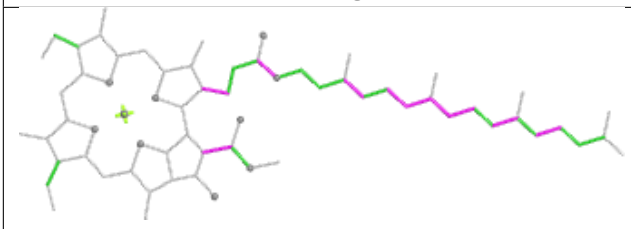
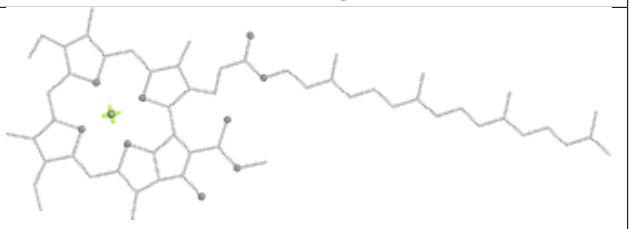


Bond angles

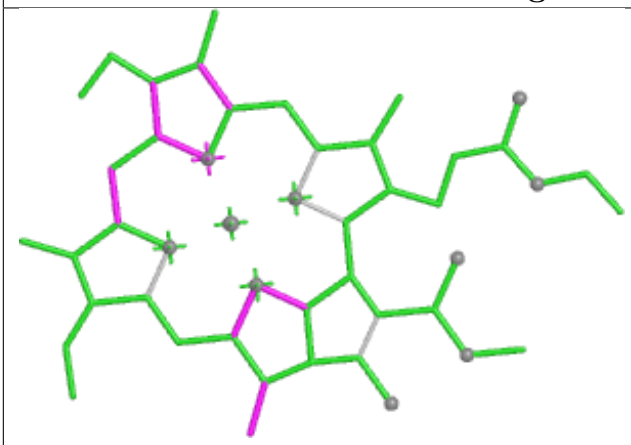


Torsions

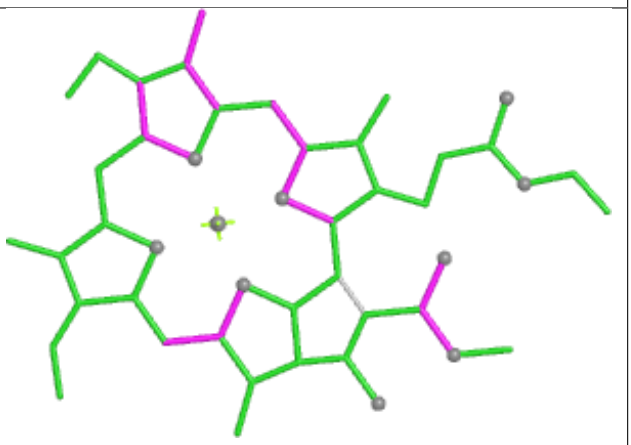


Rings

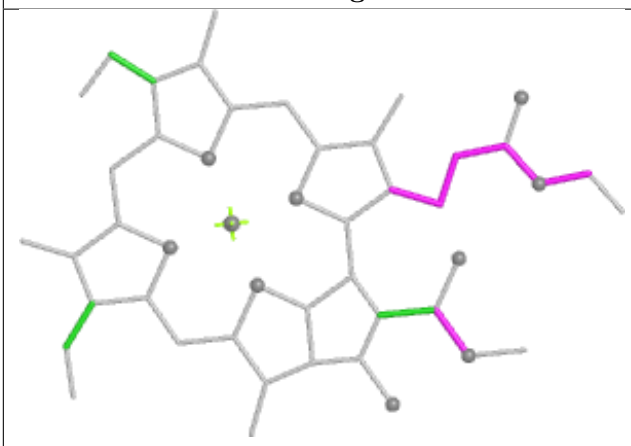
Ligand CLA 2 609



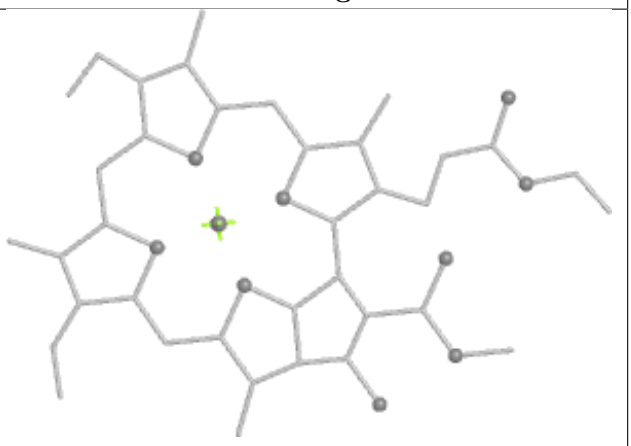
Bond lengths



Bond angles

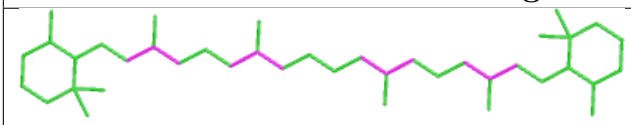


Torsions

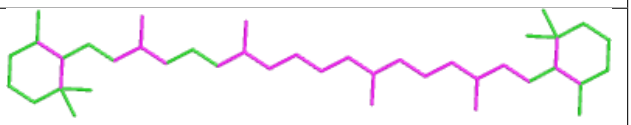


Rings

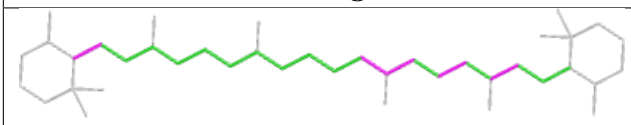
Ligand BCR B 845



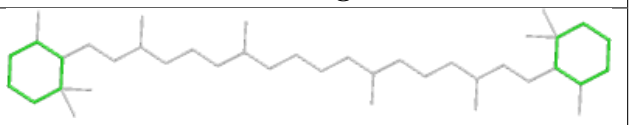
Bond lengths



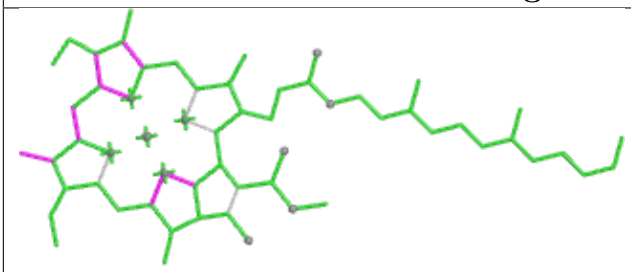
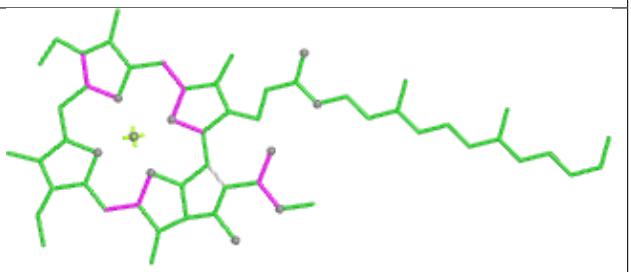
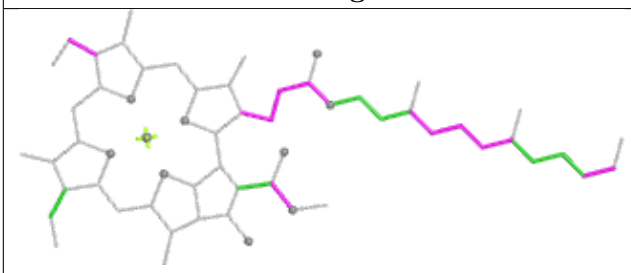
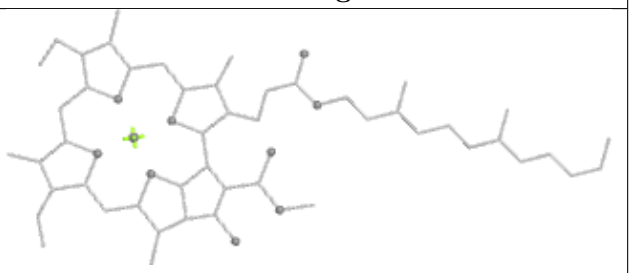
Bond angles



Torsions



Rings

Ligand CLA A 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

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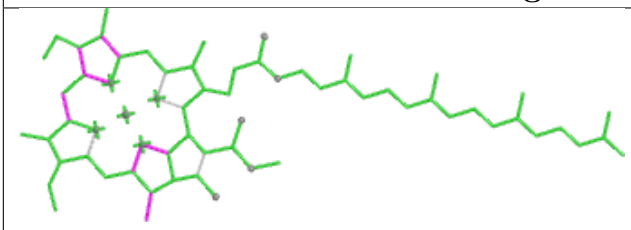
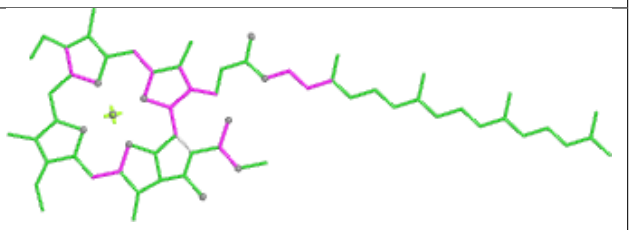
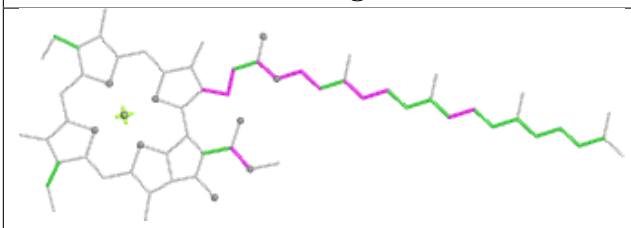
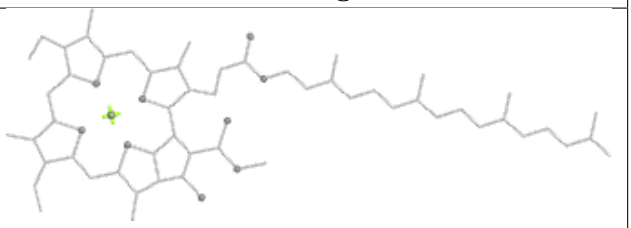
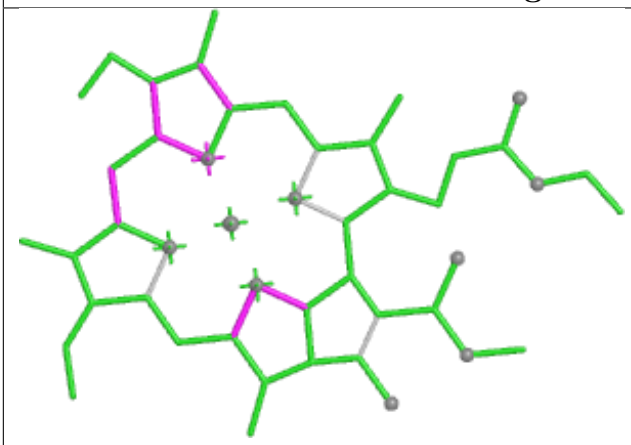
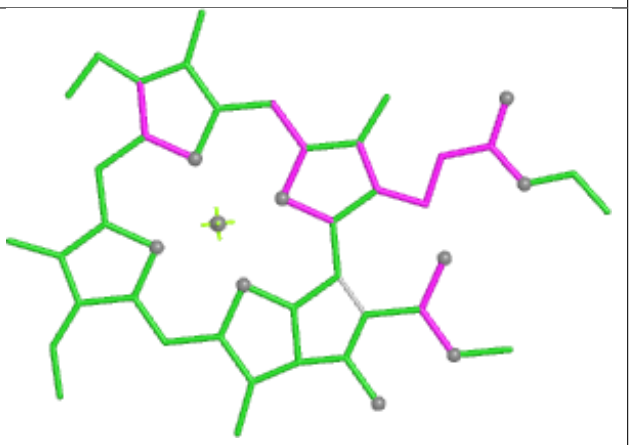
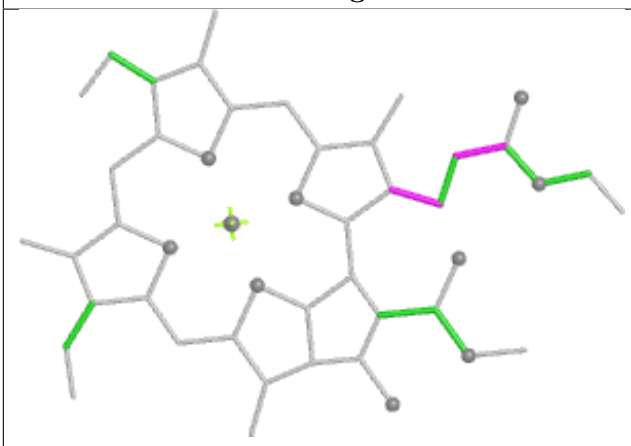
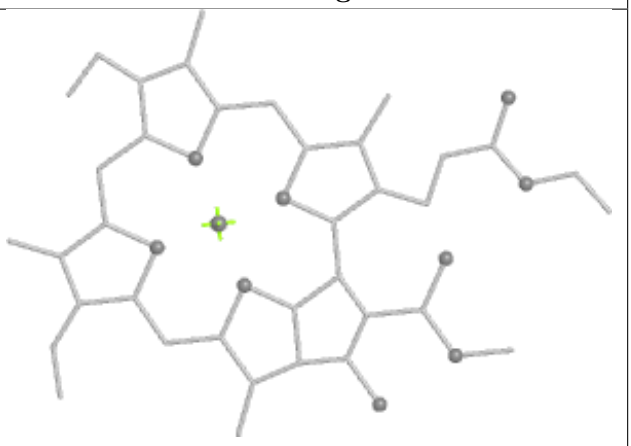
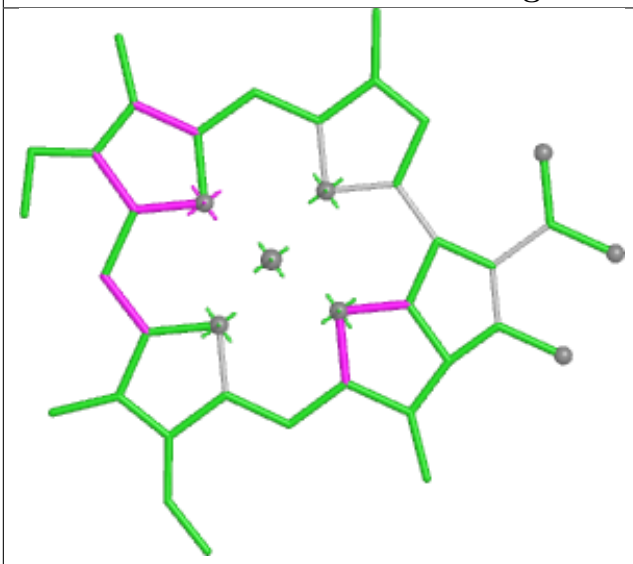
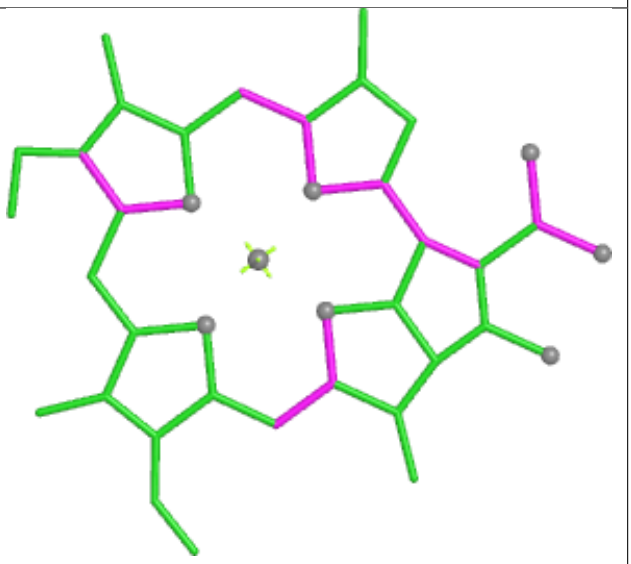
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

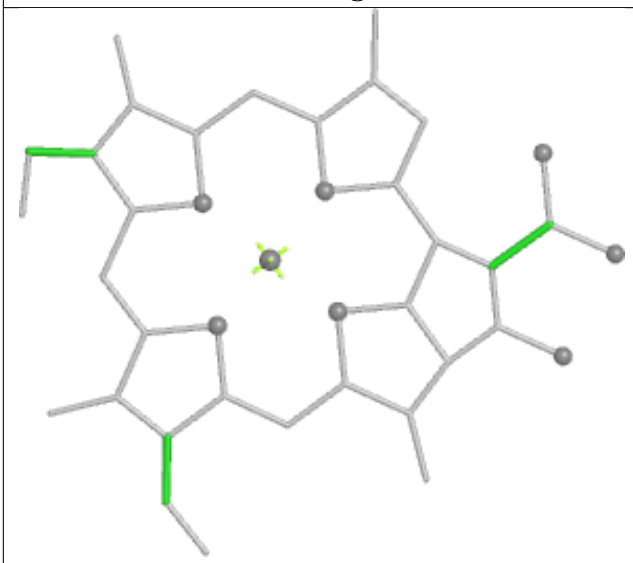
Ligand CLA K 206



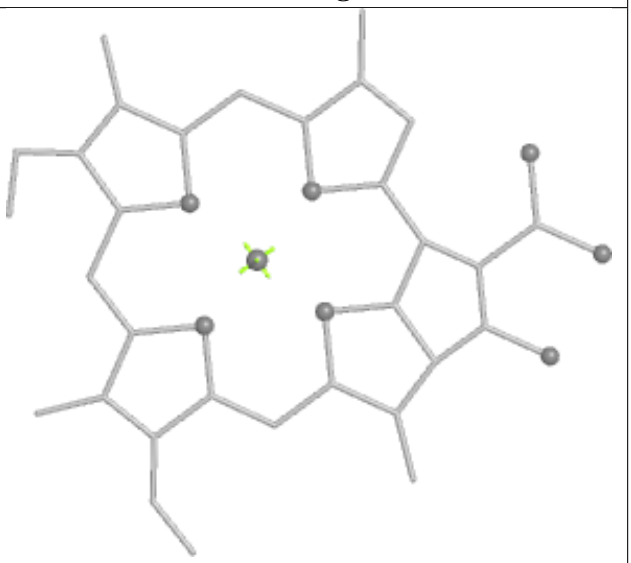
Bond lengths



Bond angles

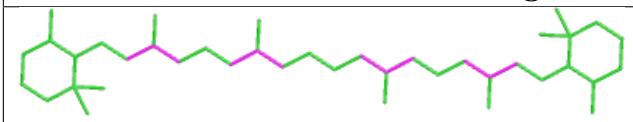


Torsions

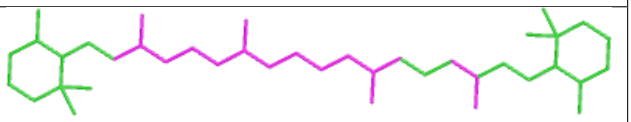


Rings

Ligand BCR B 846

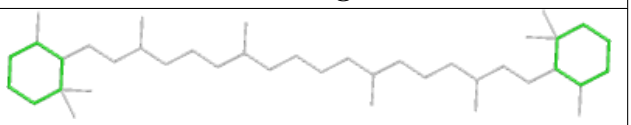


Bond lengths

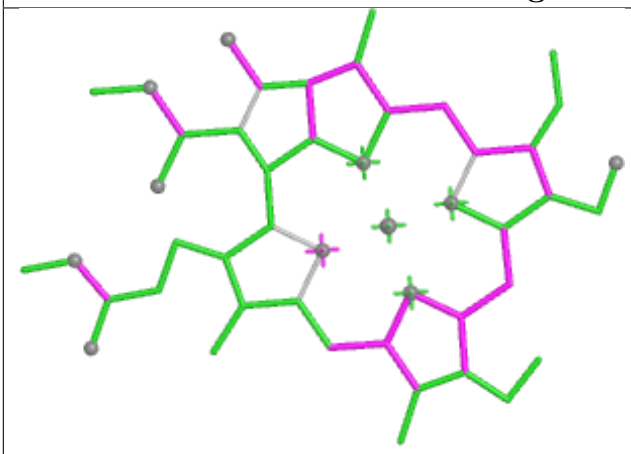
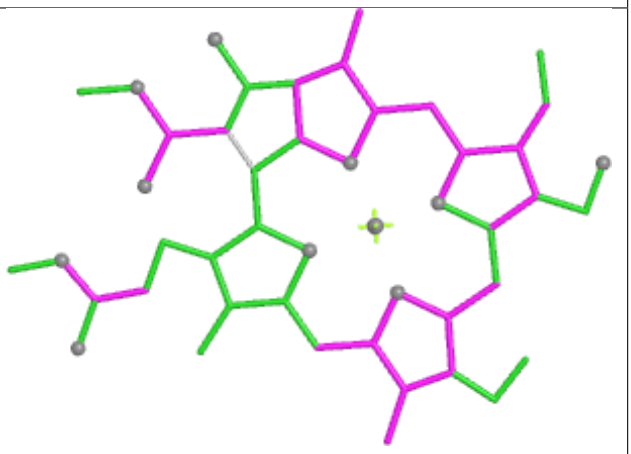
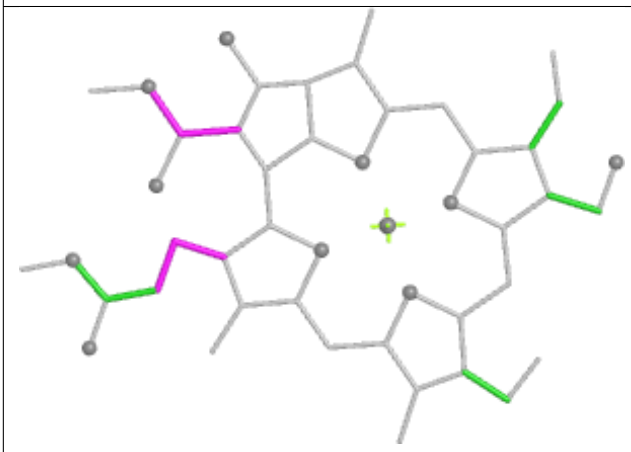
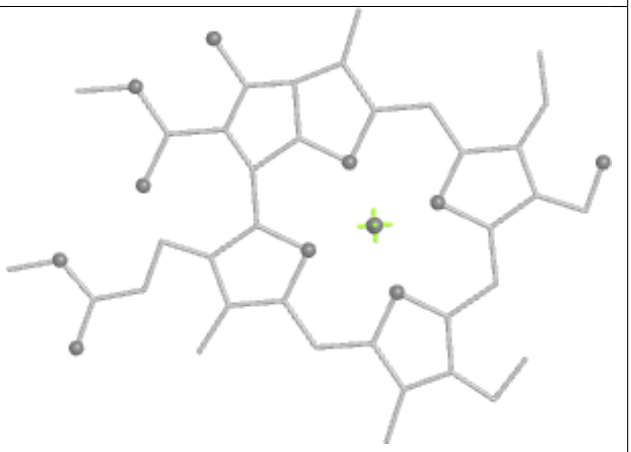


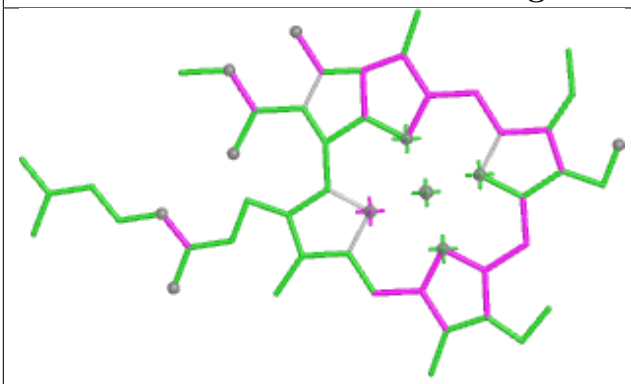
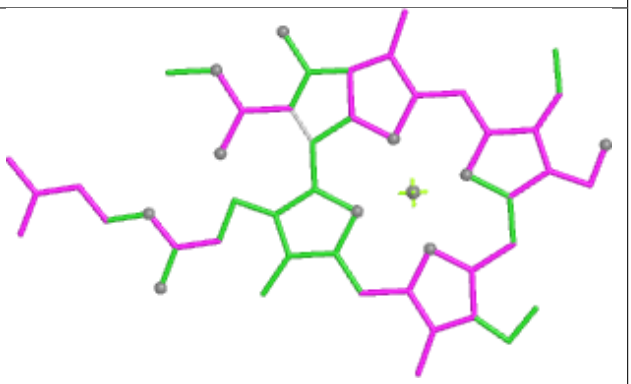
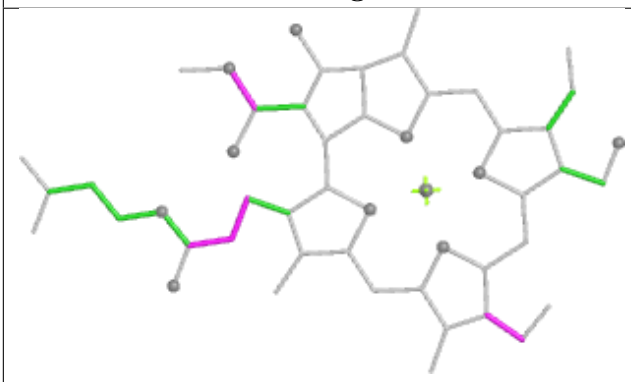
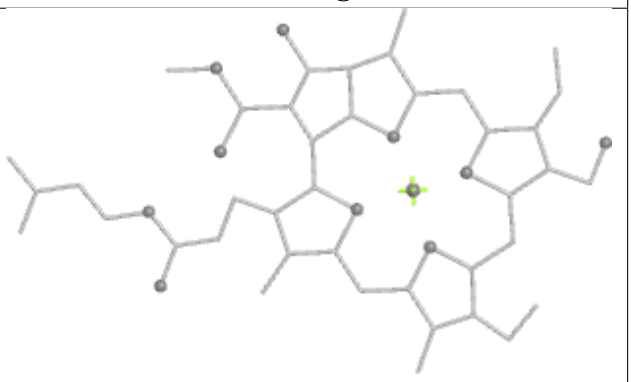
Bond angles

Torsions

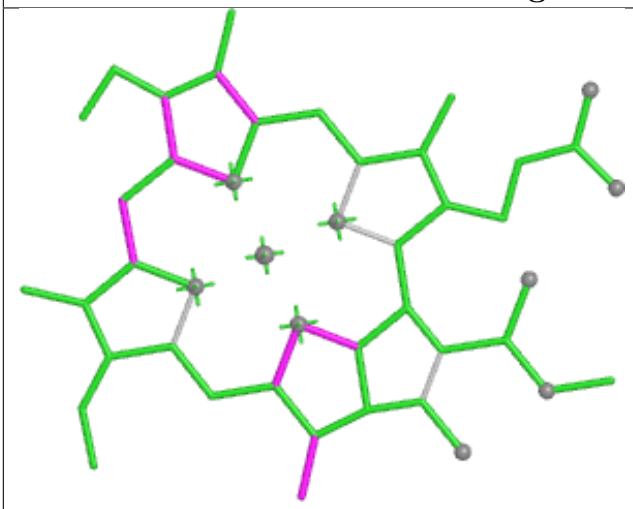


Rings

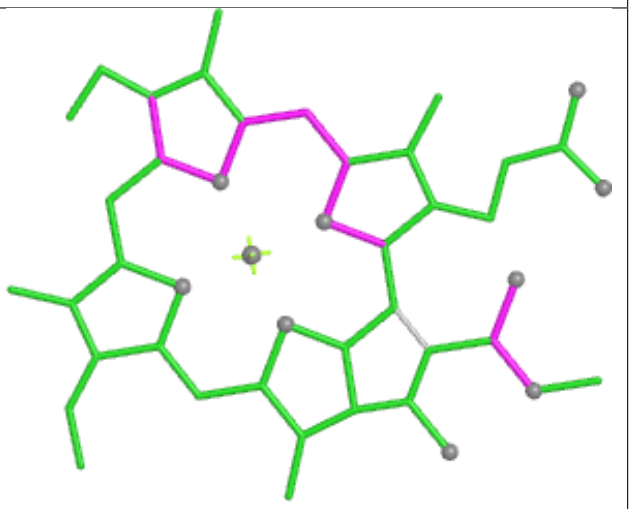
Ligand CHL 2 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 2 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

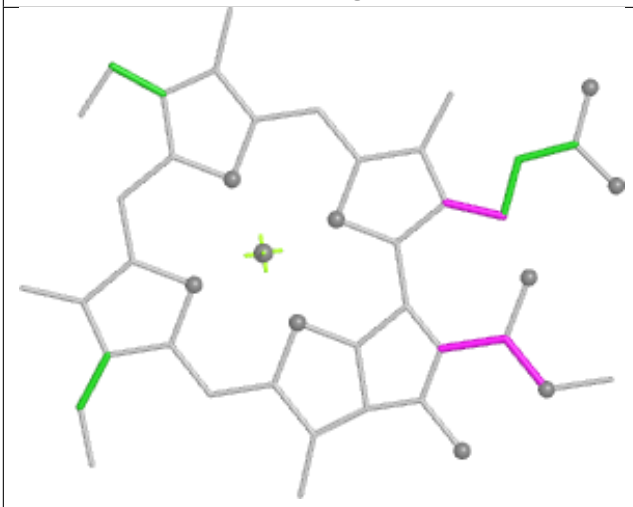
Ligand CLA 3 607



Bond lengths

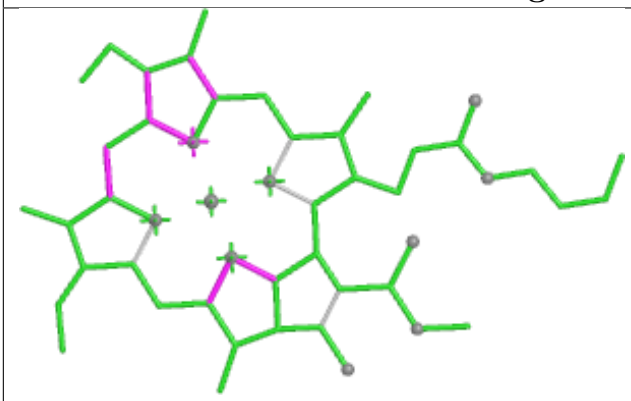
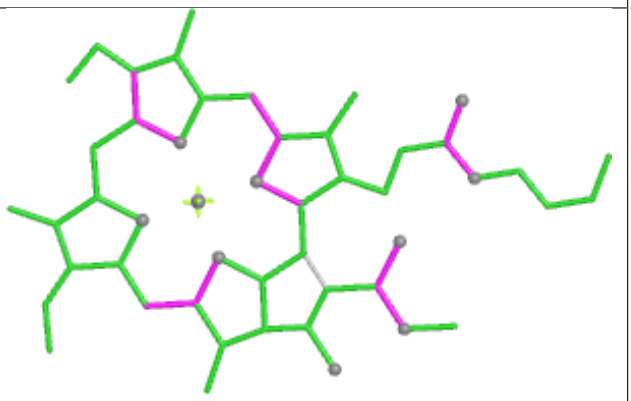
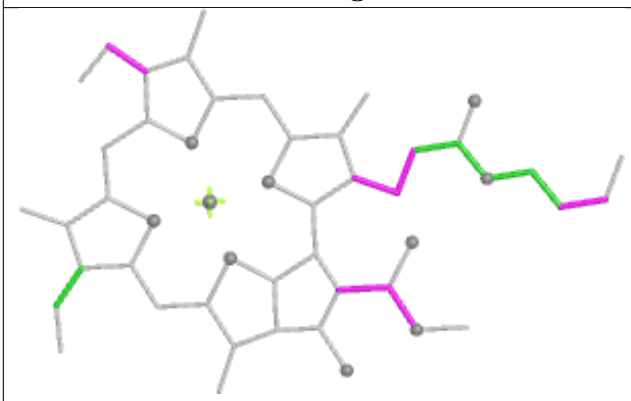
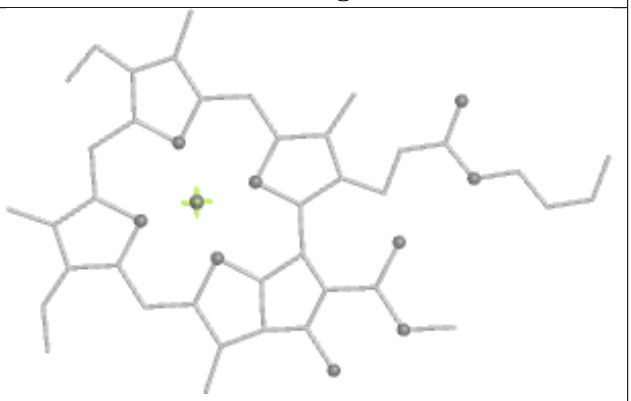


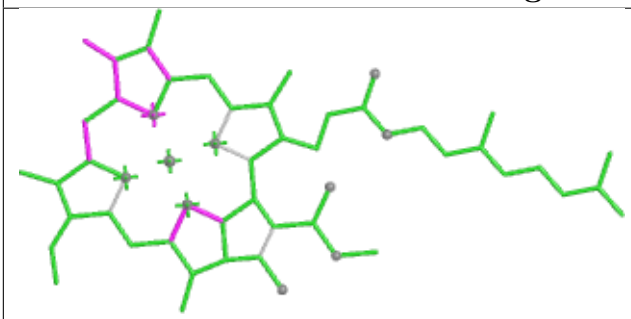
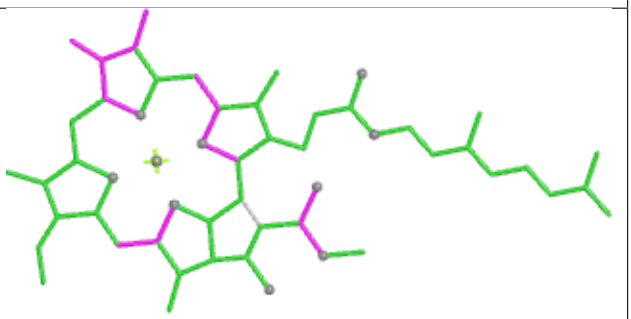
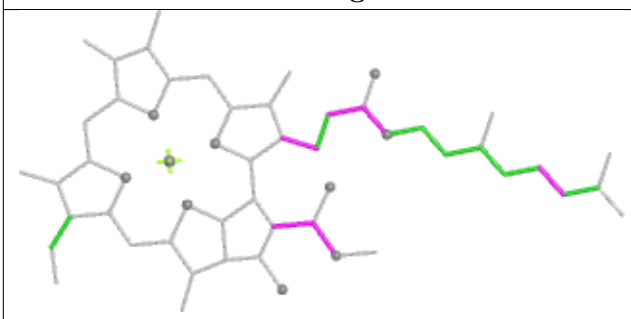
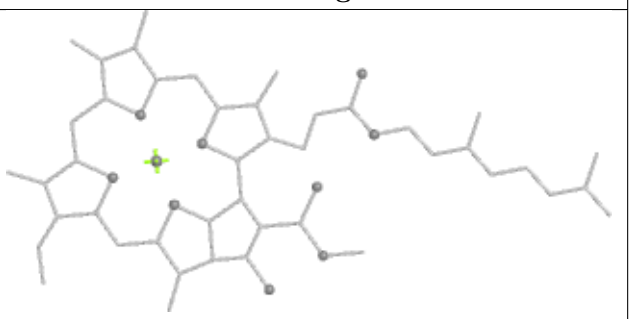
Bond angles



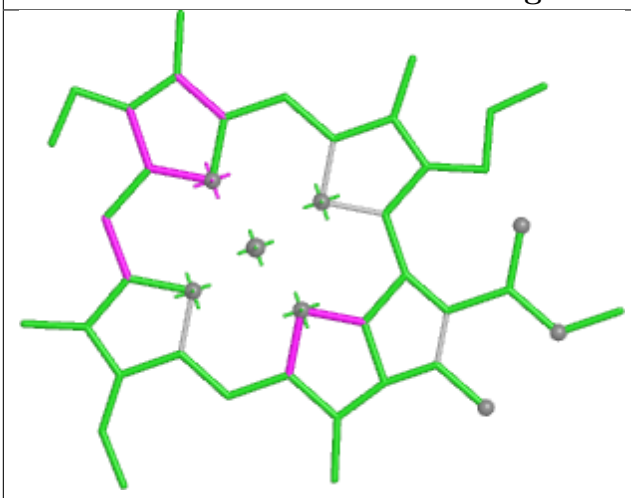
Torsions

Rings

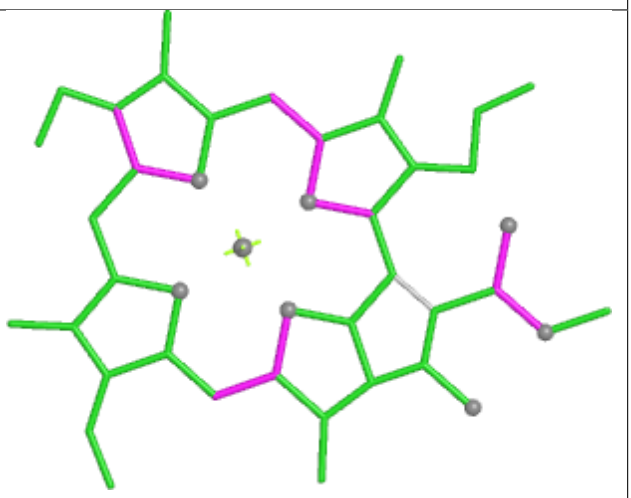
Ligand CLA 1 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

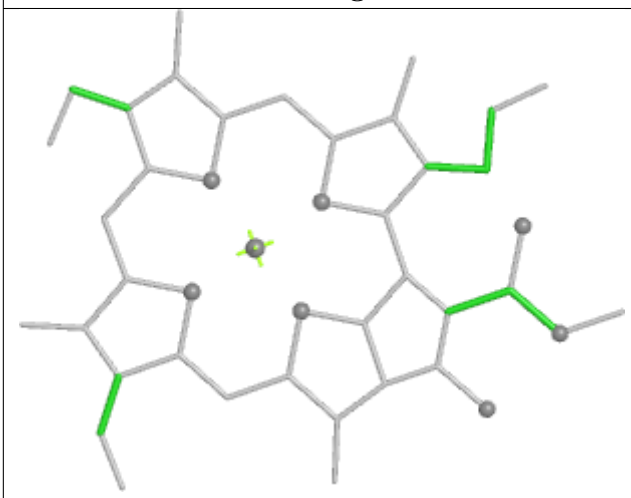
Ligand CLA B 831



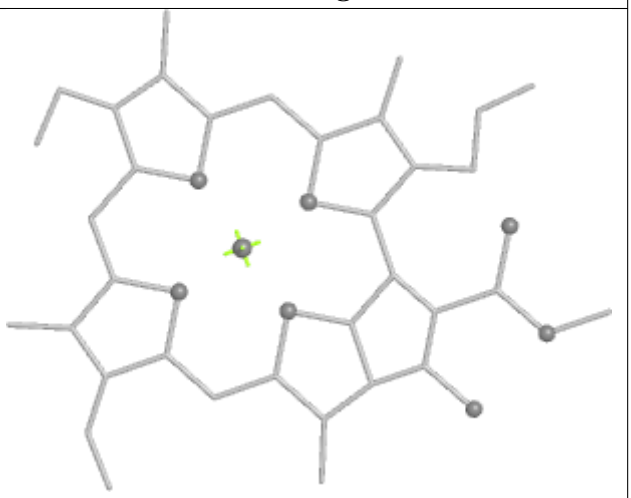
Bond lengths



Bond angles

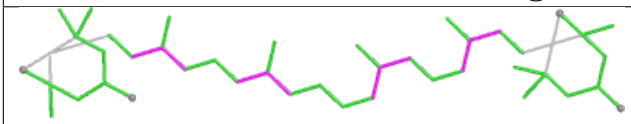


Torsions

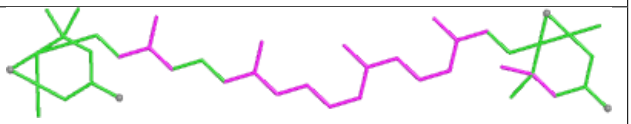


Rings

Ligand XAT 4 617

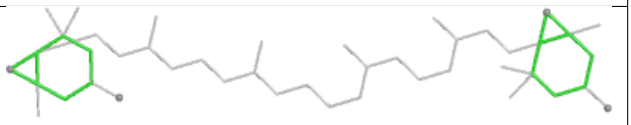


Bond lengths



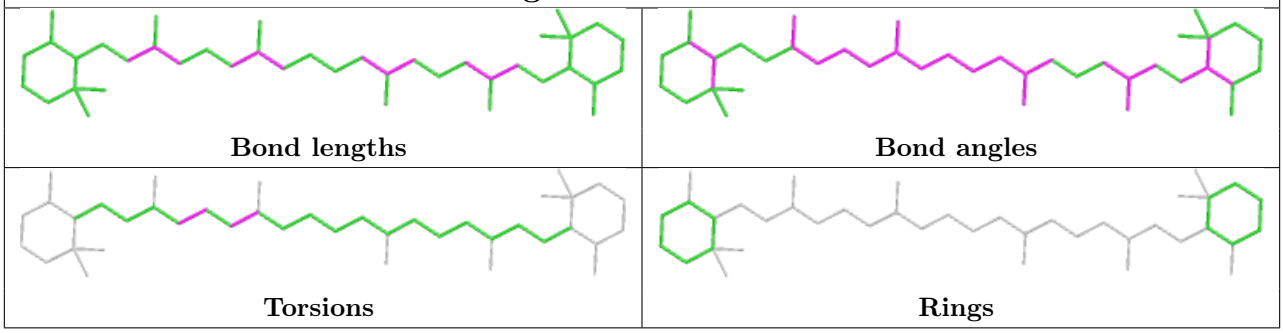
Bond angles

Torsions

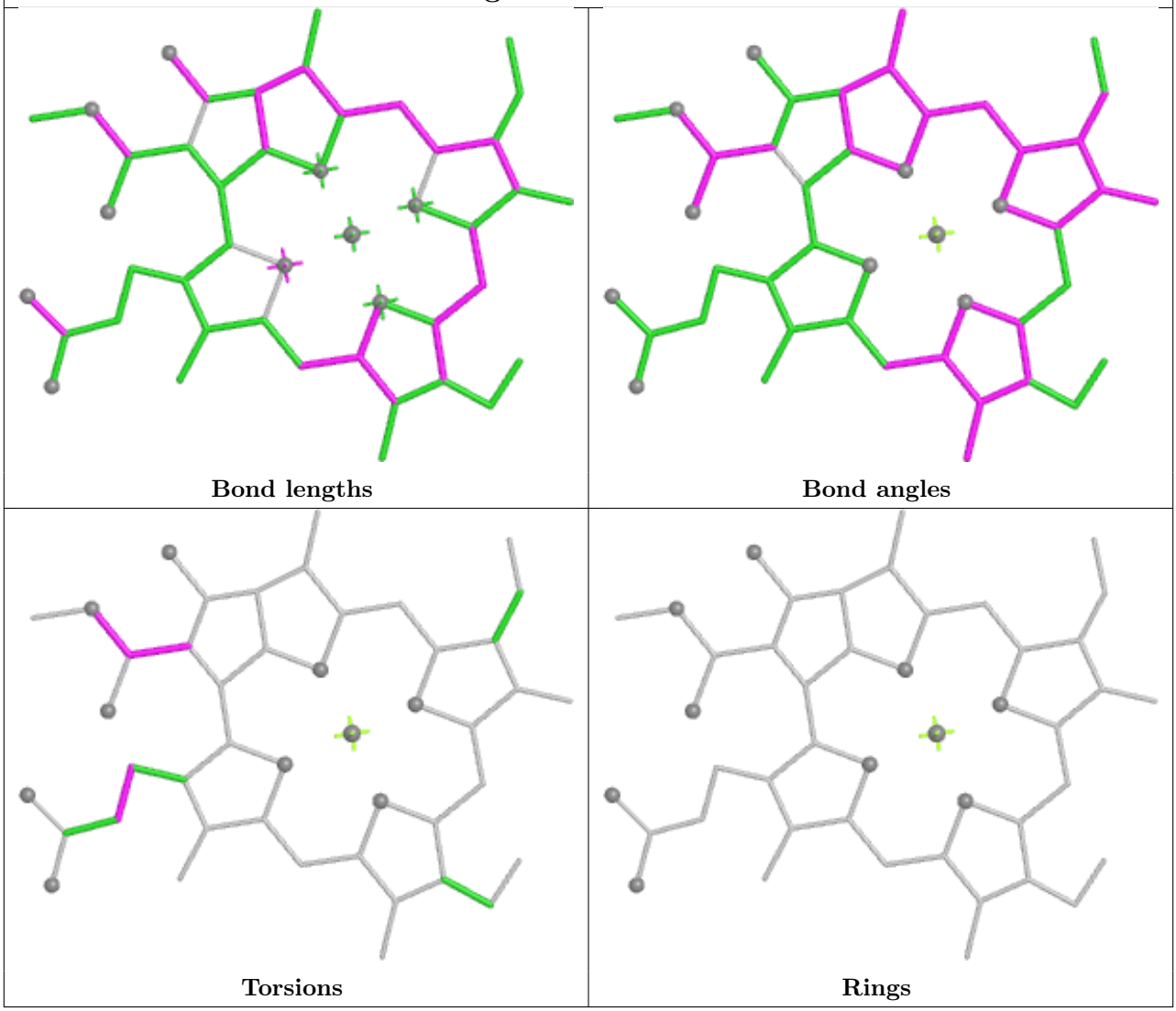


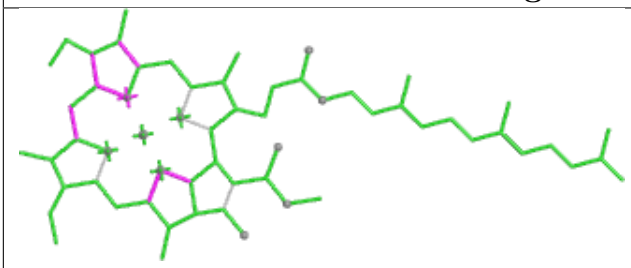
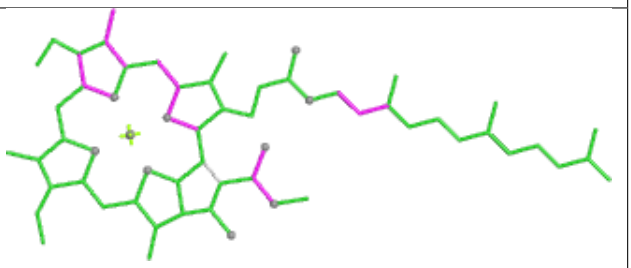
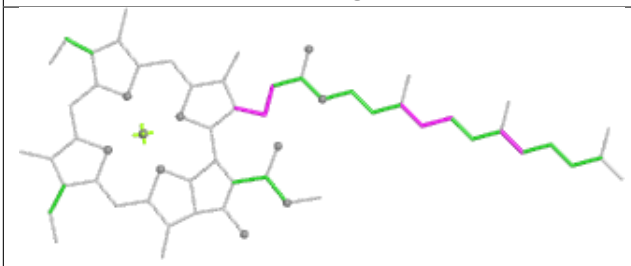
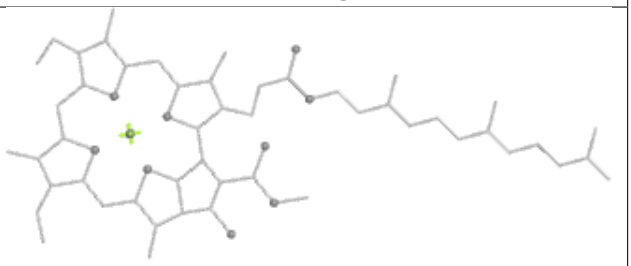
Rings

Ligand BCR A 853



Ligand CHL 3 606



Ligand CLA B 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

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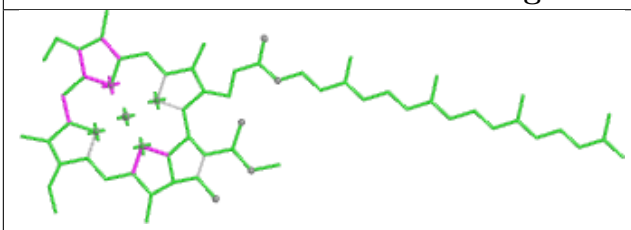
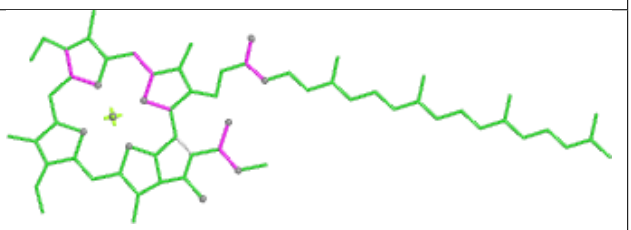
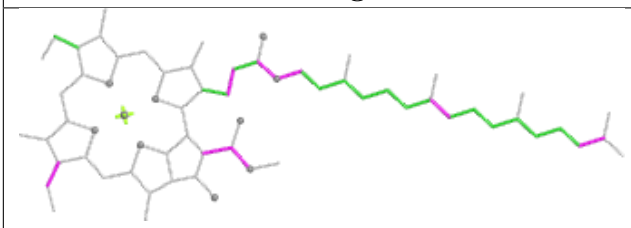
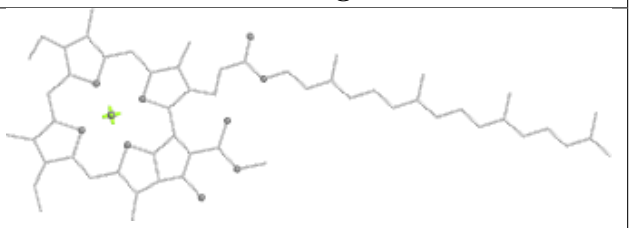
 Bond lengths	 Bond angles
 Torsions	 Rings

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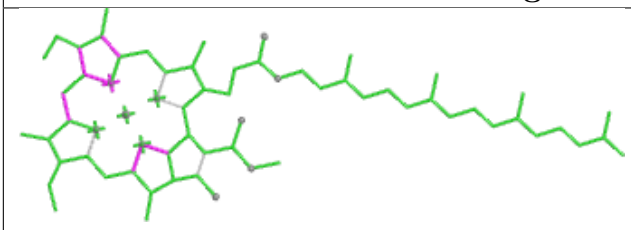
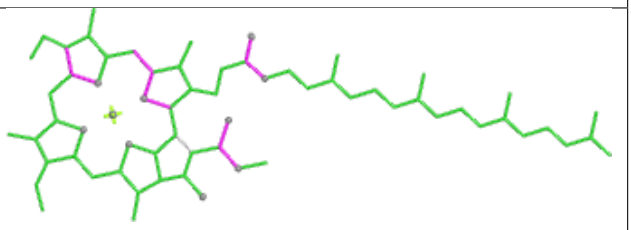
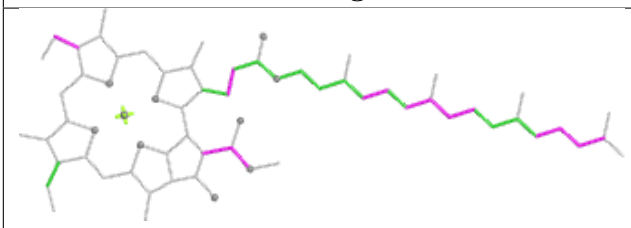
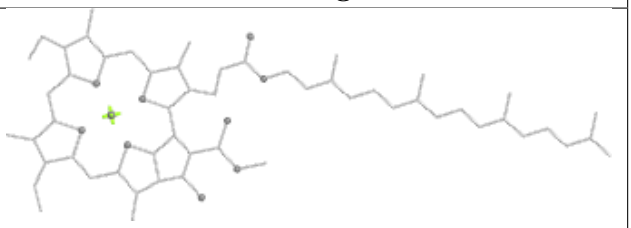
 Bond lengths	 Bond angles
 Torsions	 Rings

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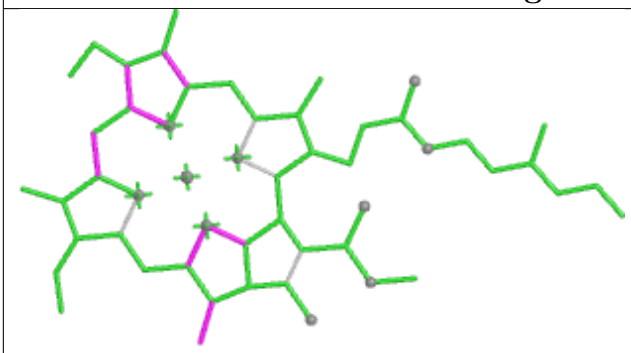
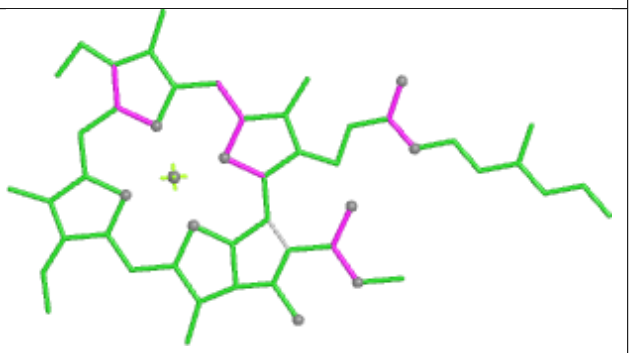
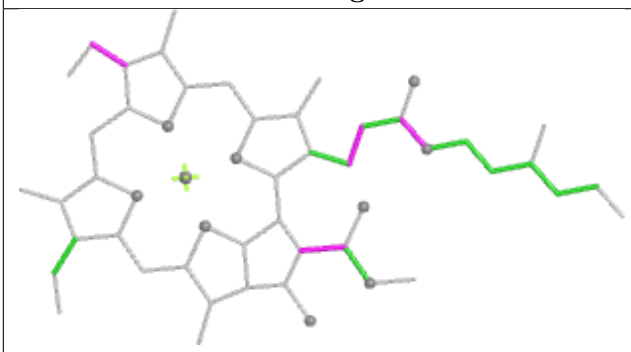
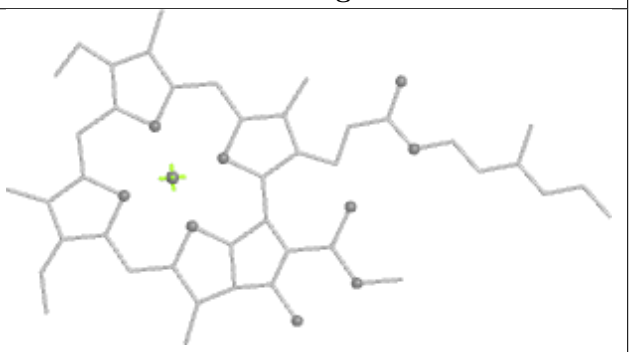
 Bond lengths	 Bond angles
 Torsions	 Rings

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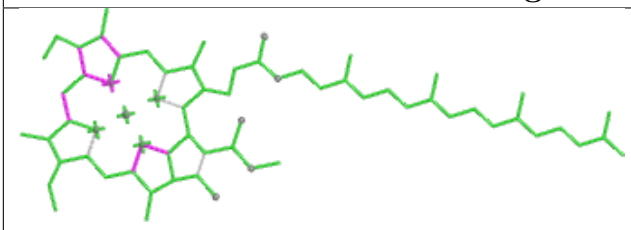
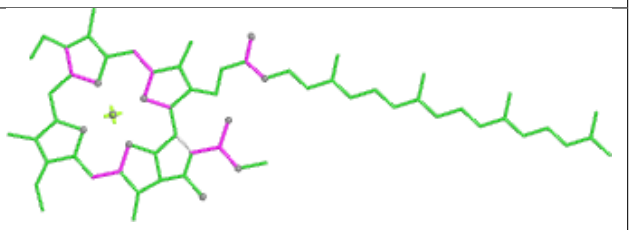
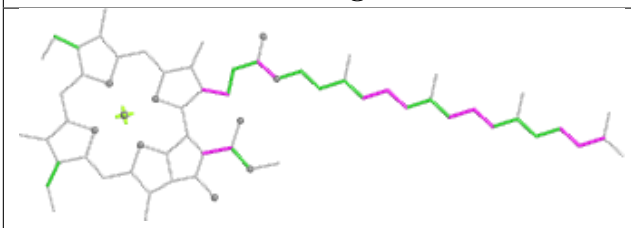
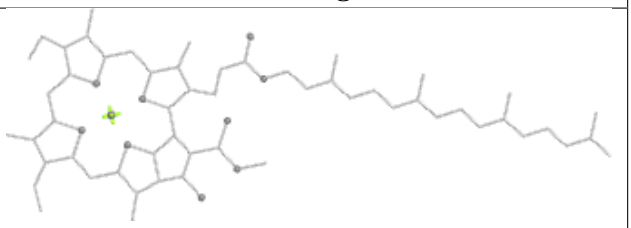
 Bond lengths	 Bond angles
 Torsions	 Rings

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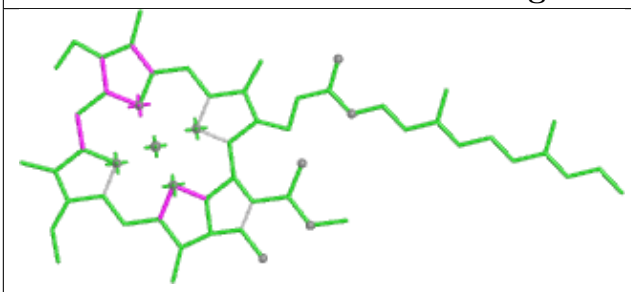
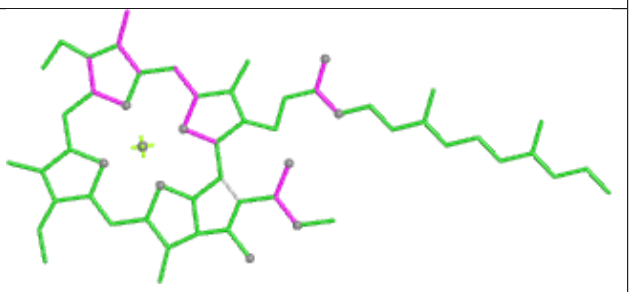
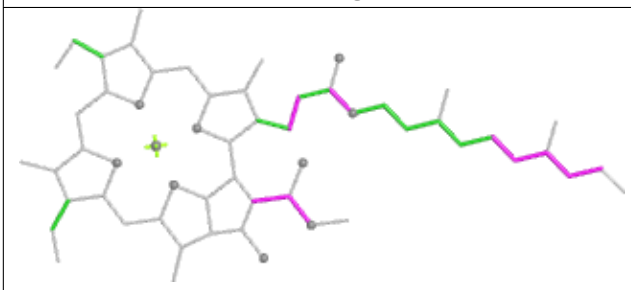
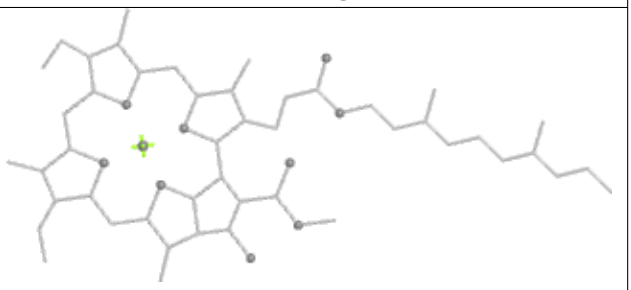
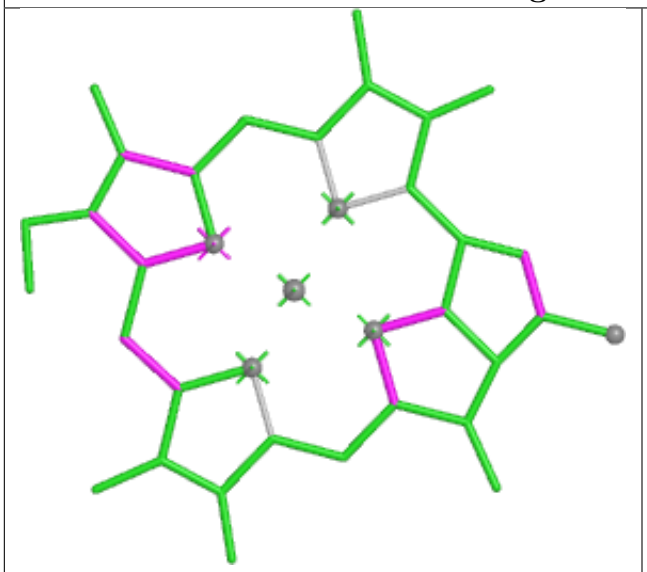
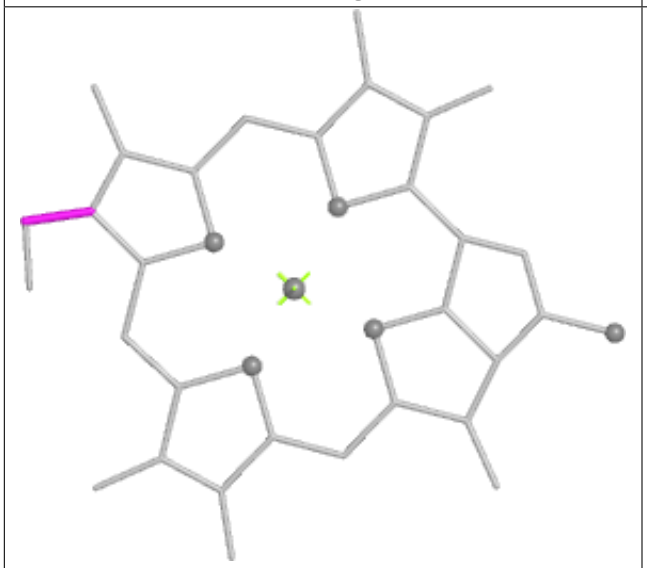
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 611

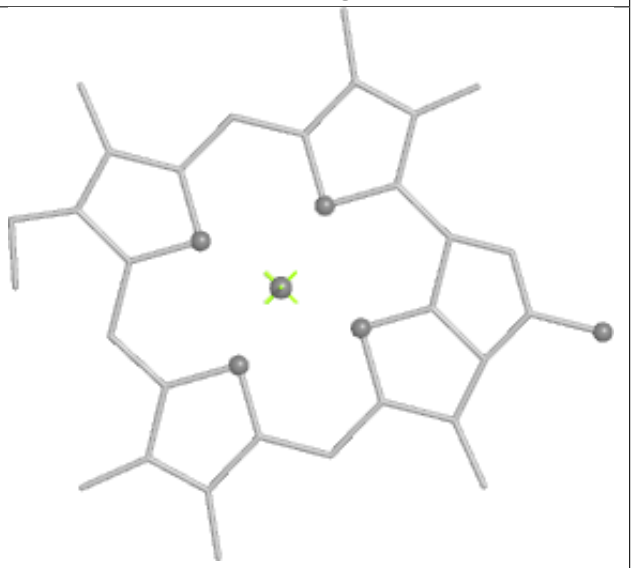


Bond lengths

Bond angles

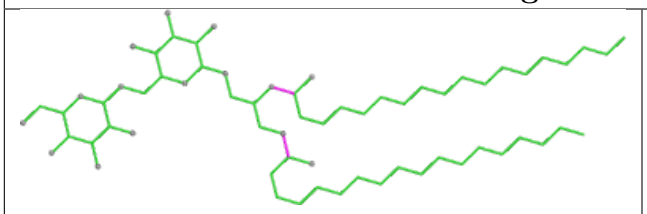


Torsions



Rings

Ligand DGD B 850



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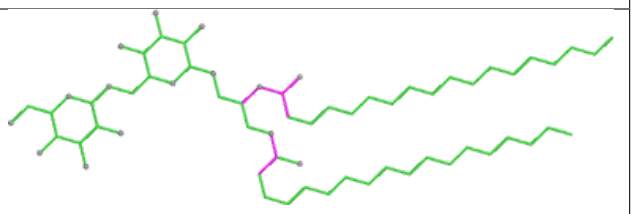
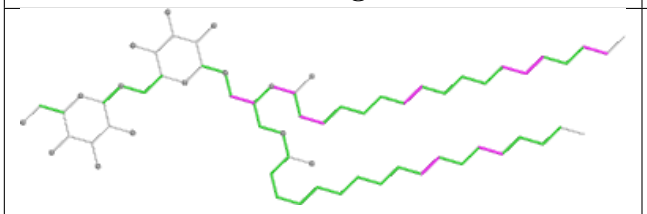


Bond angles



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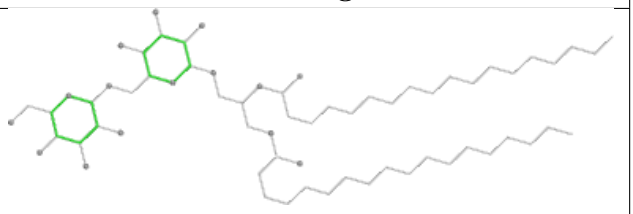
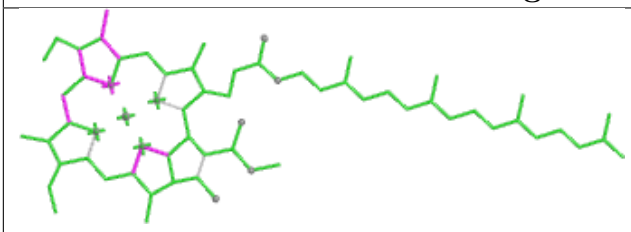


Rings

Ligand CLA A 844



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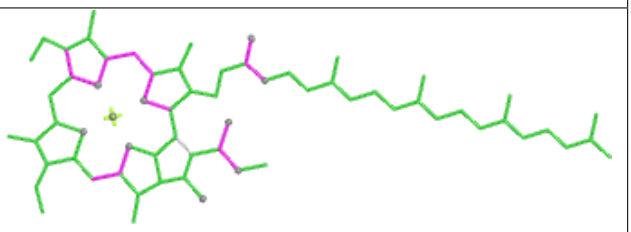
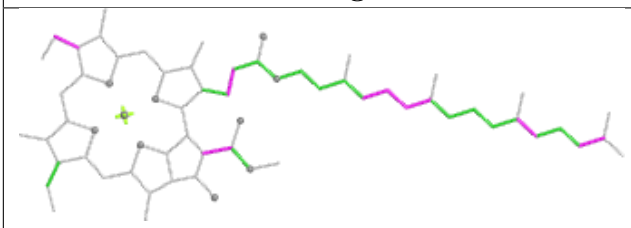


Bond angles



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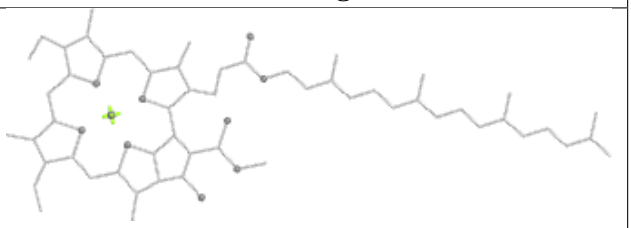
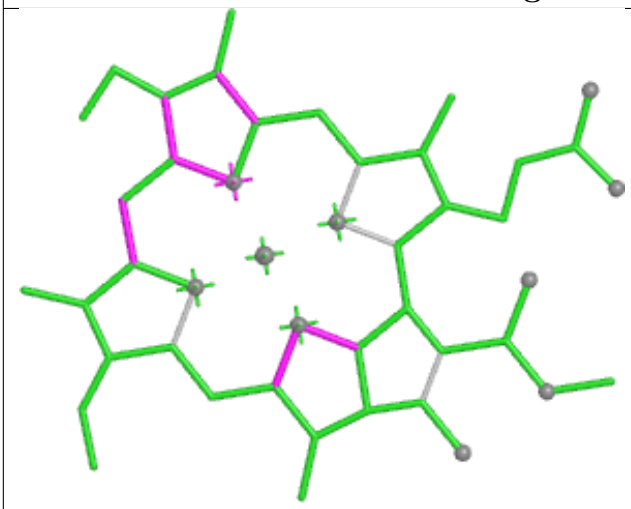


Rings

Ligand CLA A 815



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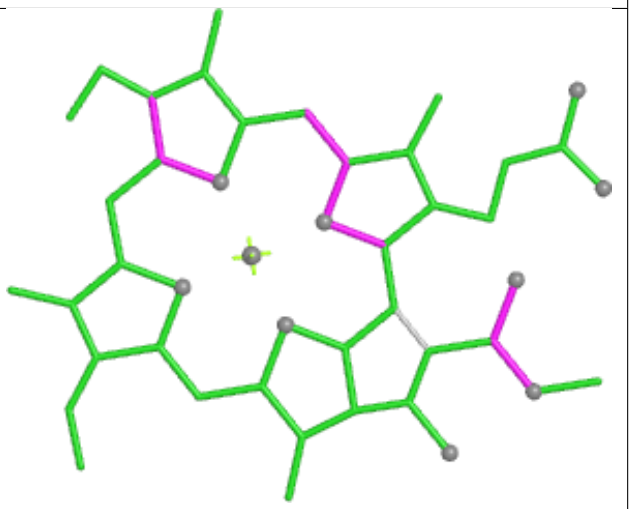
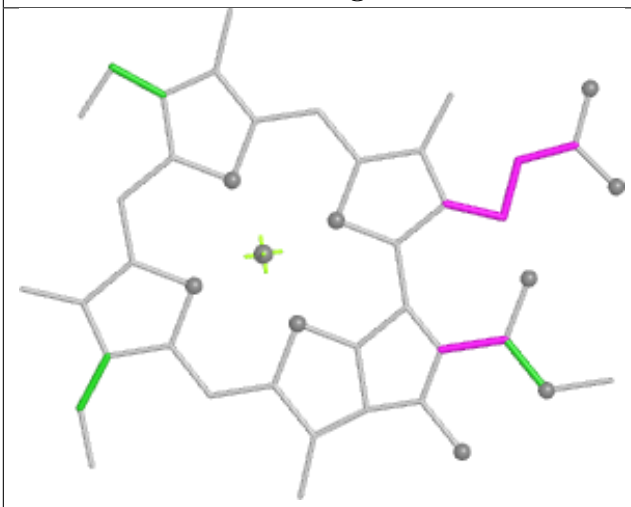


Bond angles



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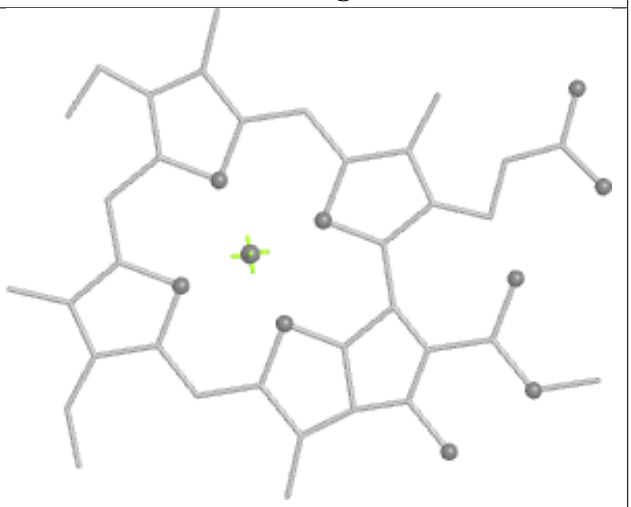
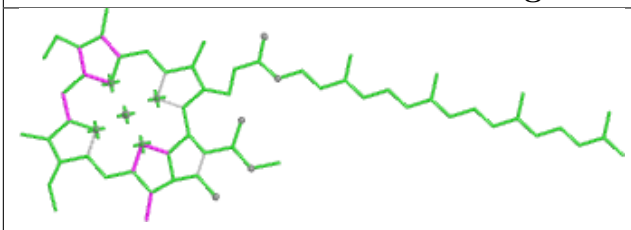


Rings

Ligand CLA B 810



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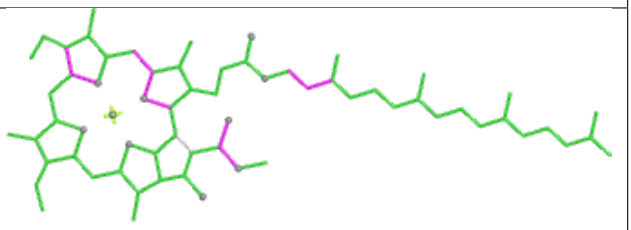

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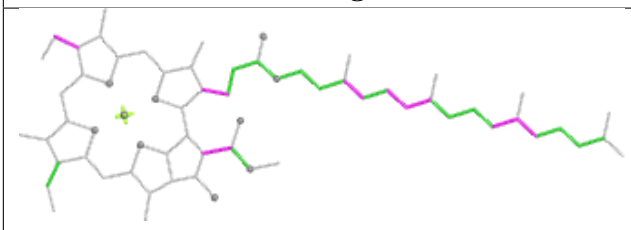

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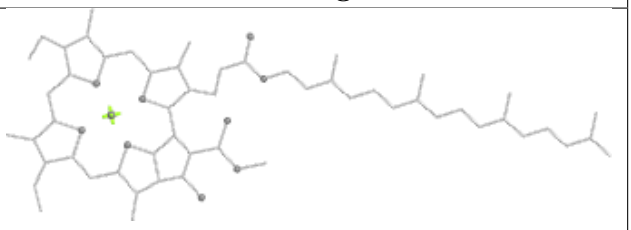
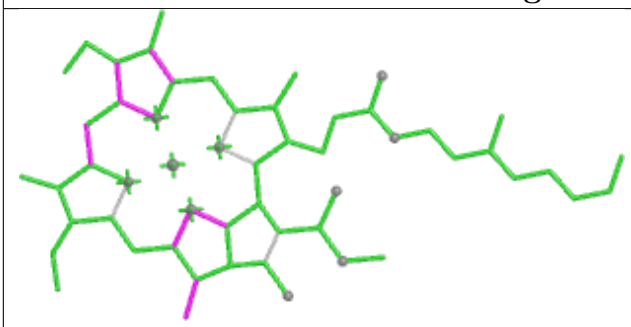


Rings

Ligand CLA A 813



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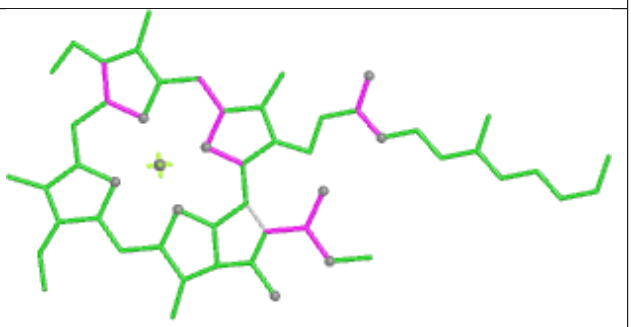

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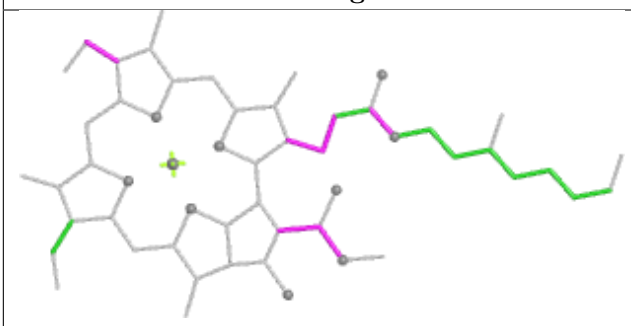

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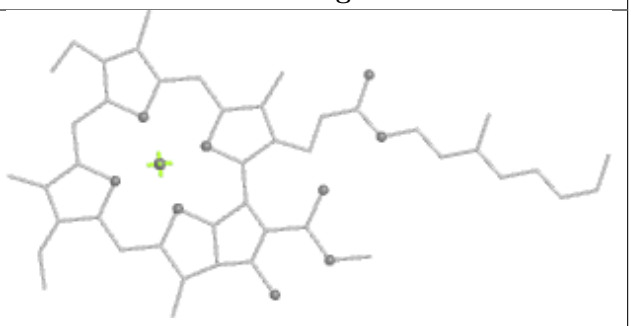
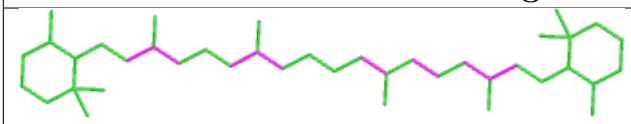


Rings

Ligand BCR A 851



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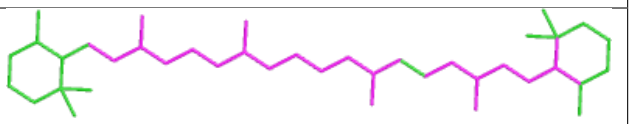

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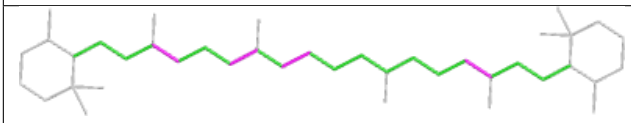

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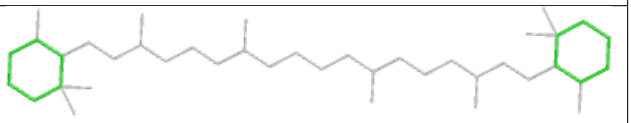
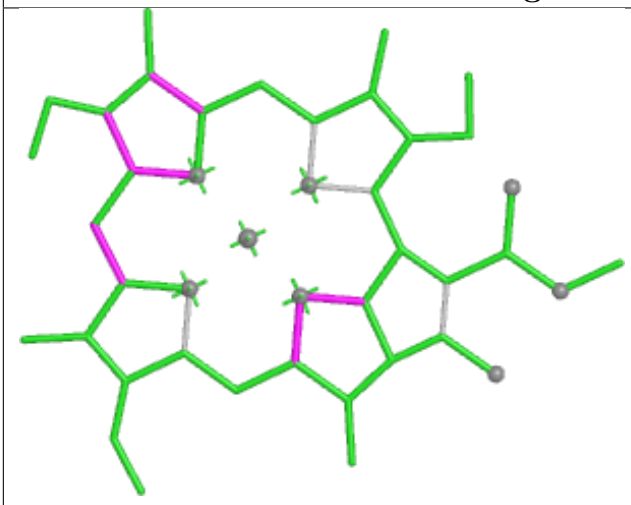


Rings

Ligand CLA A 823



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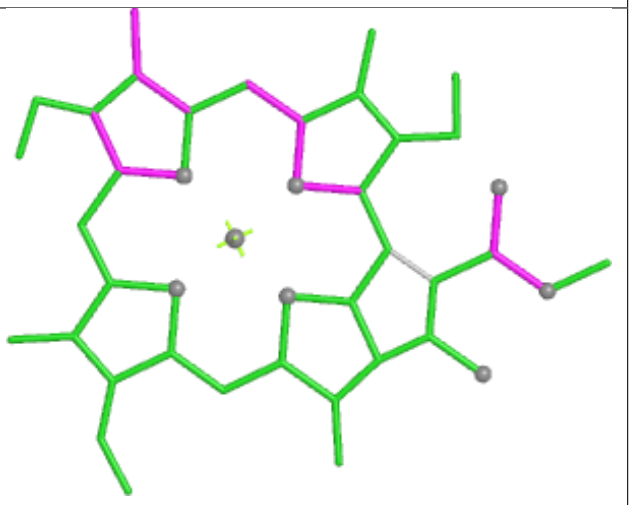
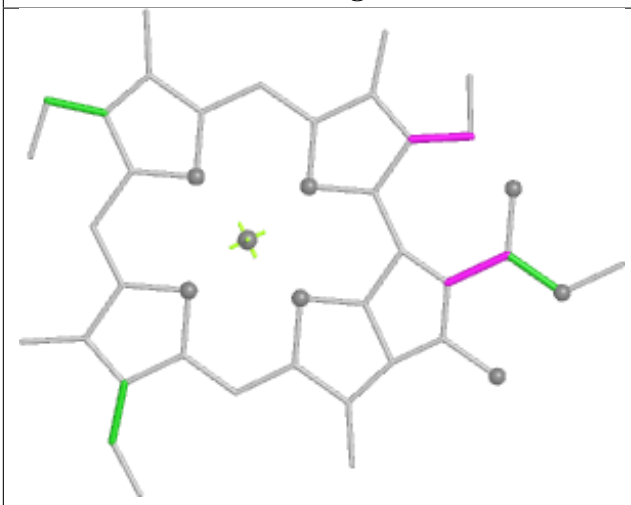


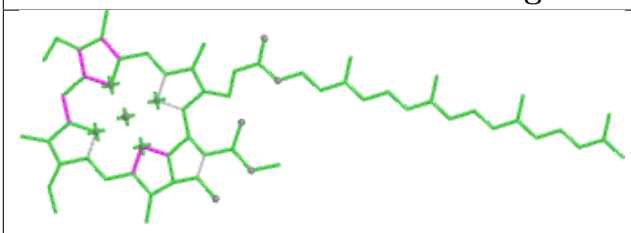
Bond angles



Torsions

Rings

Ligand CLA B 814



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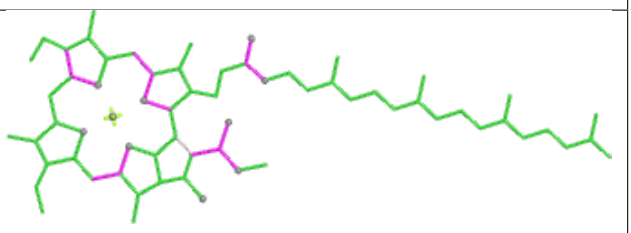
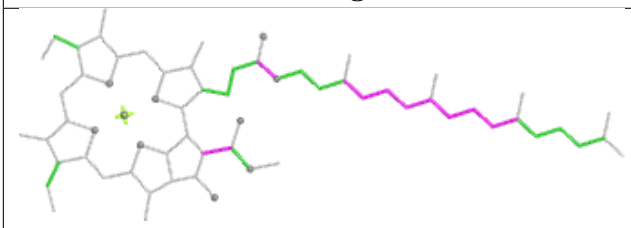
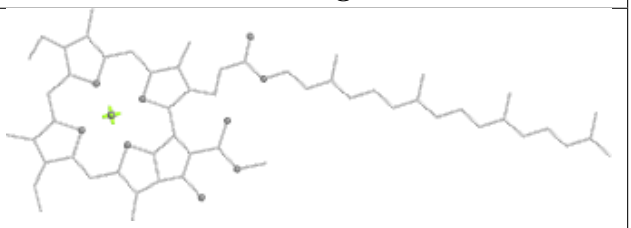


Bond angles

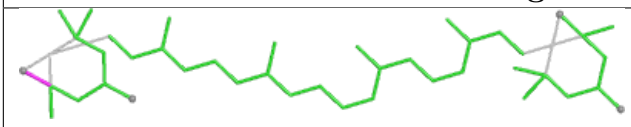


Torsions

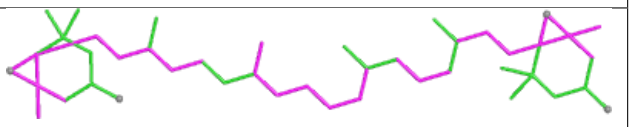


Rings

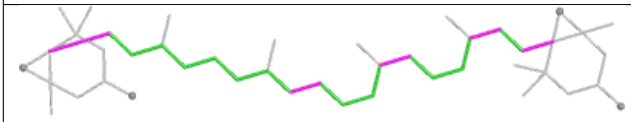
Ligand XAT 1 614



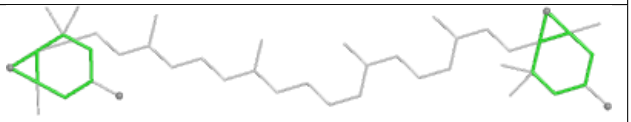
Bond lengths



Bond angles

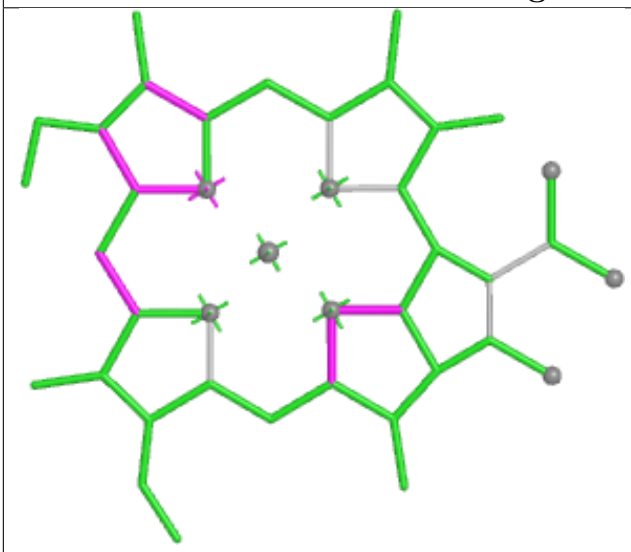


Torsions



Rings

Ligand CLA 3 610



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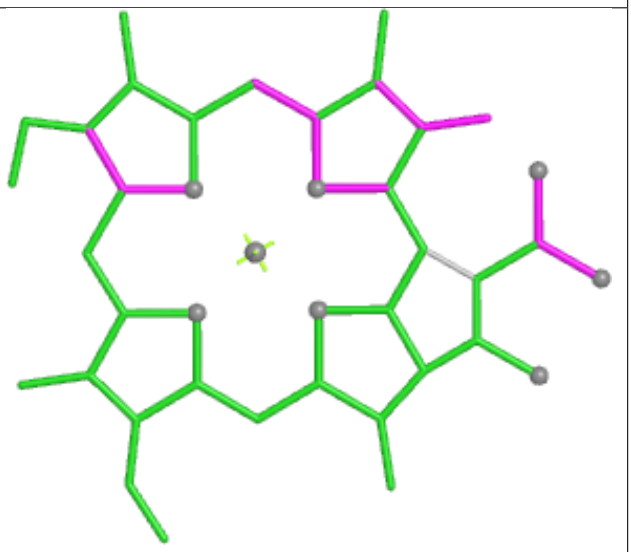
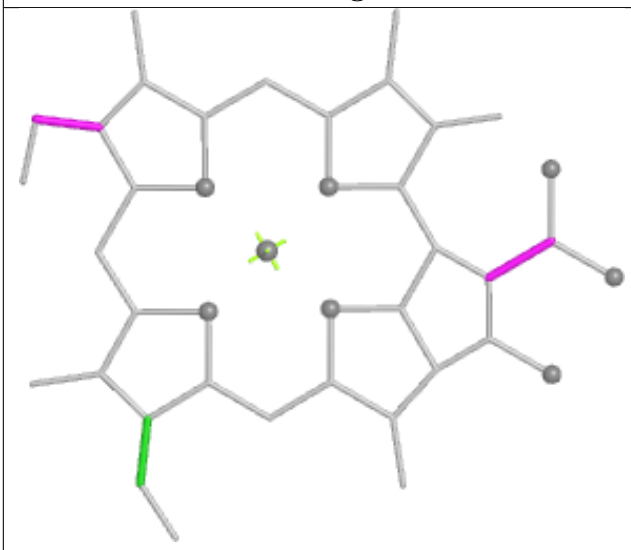
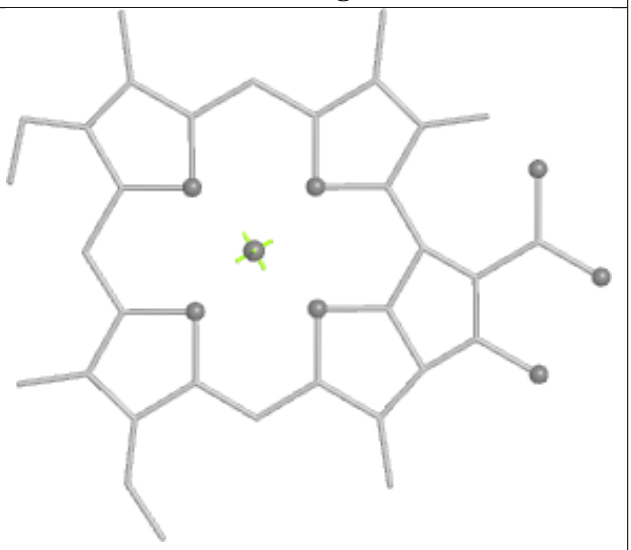


Bond angles

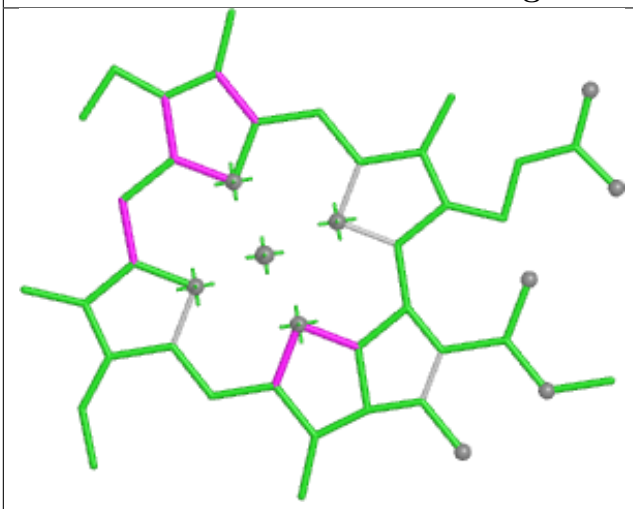


Torsions



Rings

Ligand CLA G 201



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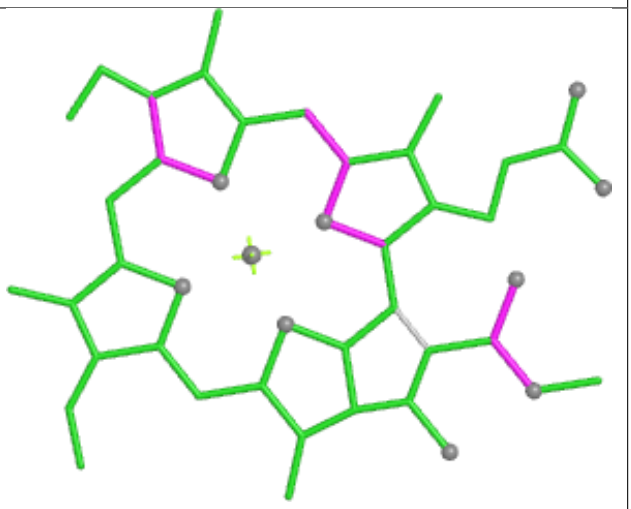
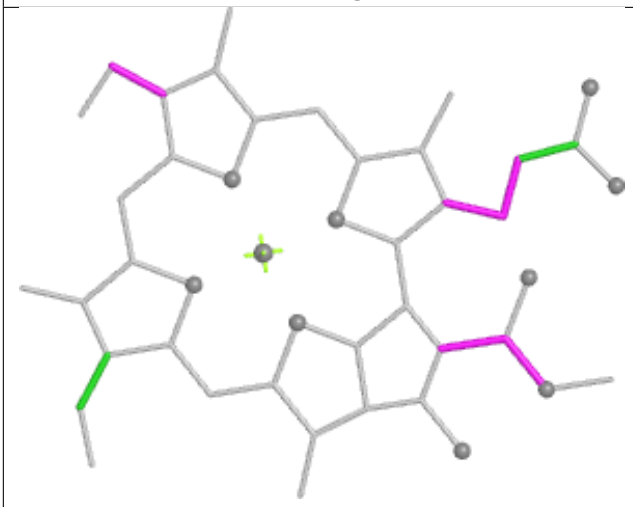


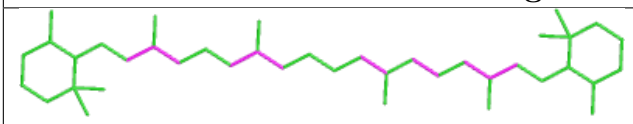
Bond angles



Torsions

Rings

Ligand BCR L 301



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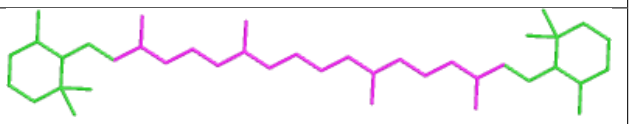
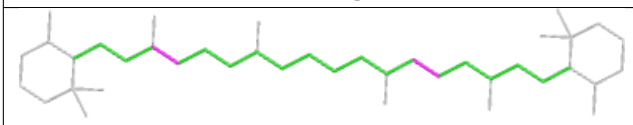
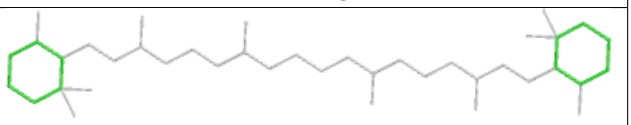


Bond angles

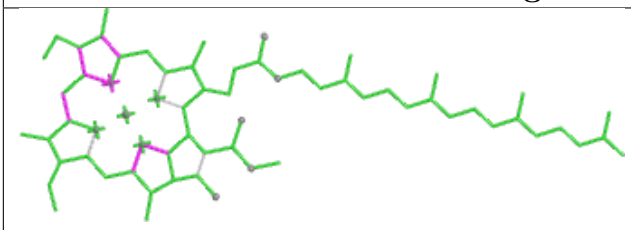


Torsions

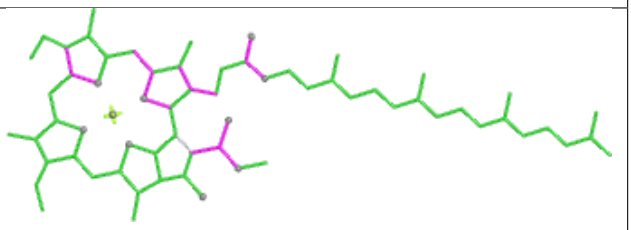


Rings

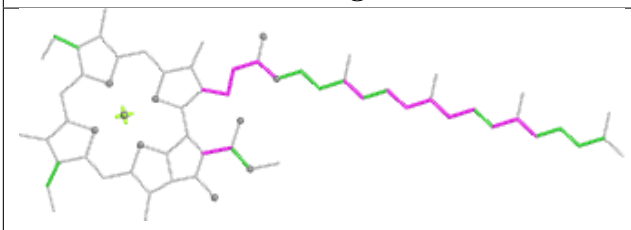
Ligand CLA A 804



Bond lengths



Bond angles



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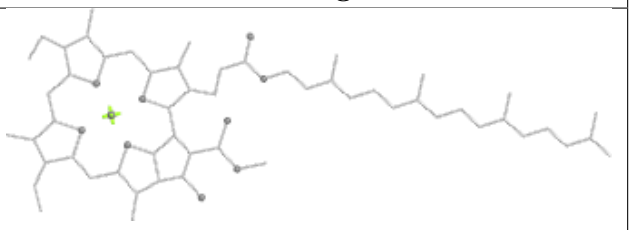
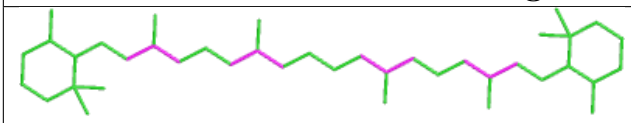
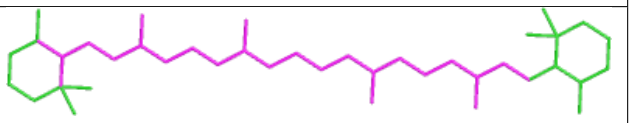


Rings

Ligand BCR L 306

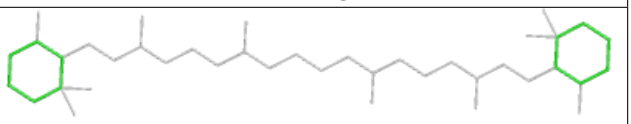


Bond lengths



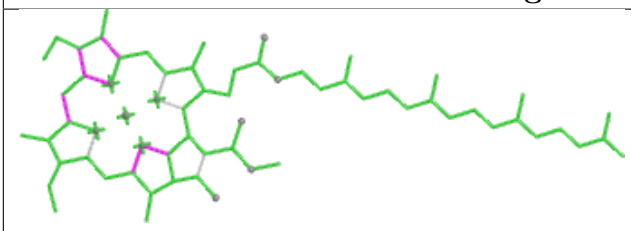
Bond angles

Torsions

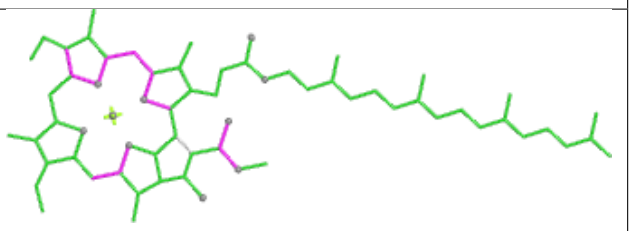


Rings

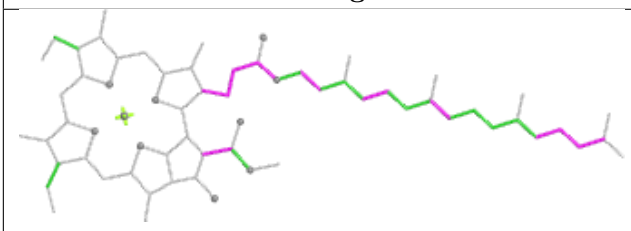
Ligand CLA B 832



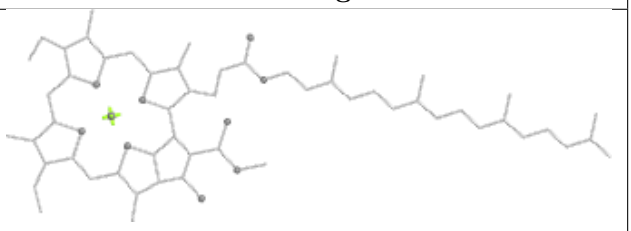
Bond lengths



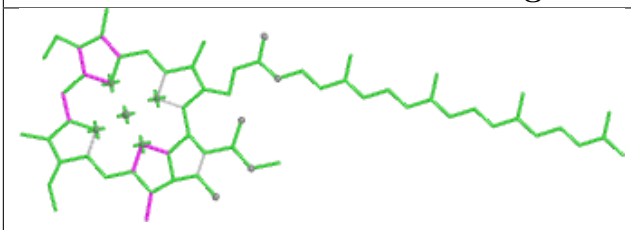
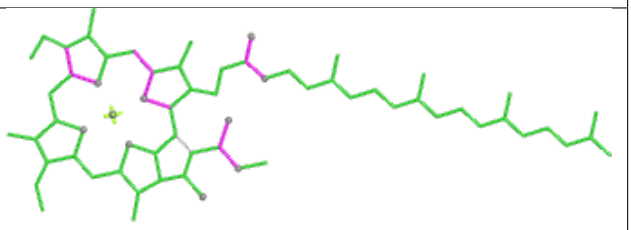
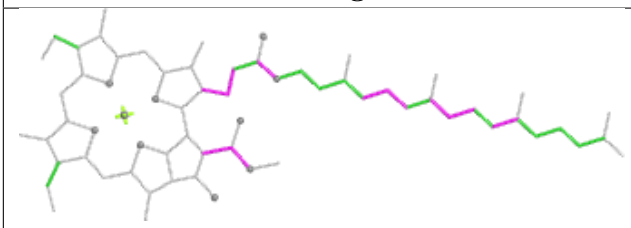
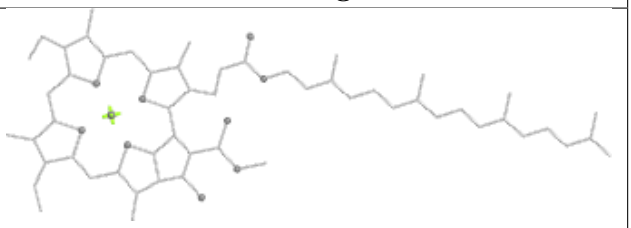
Bond angles

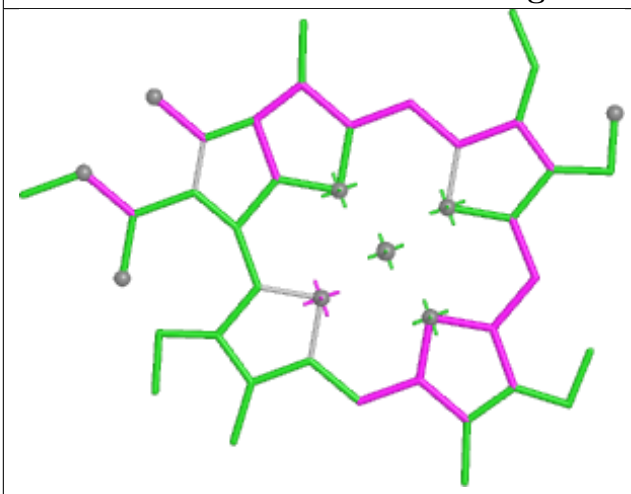
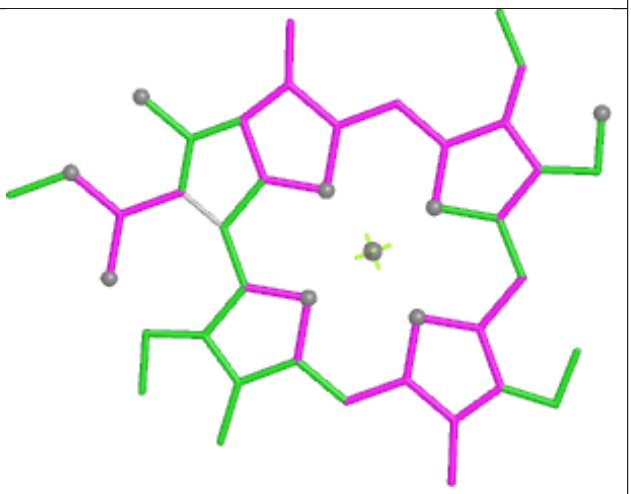
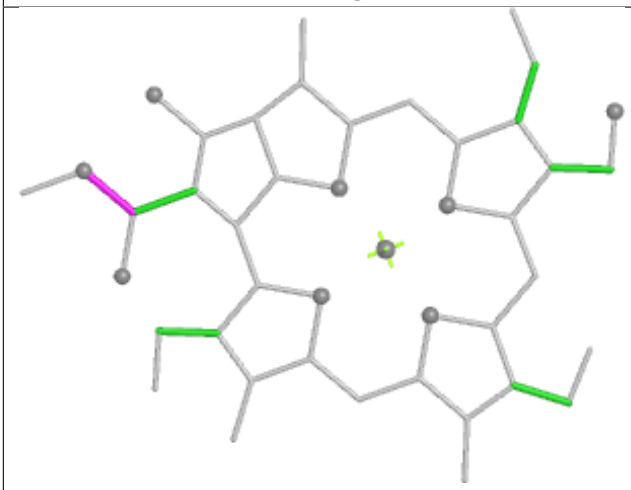


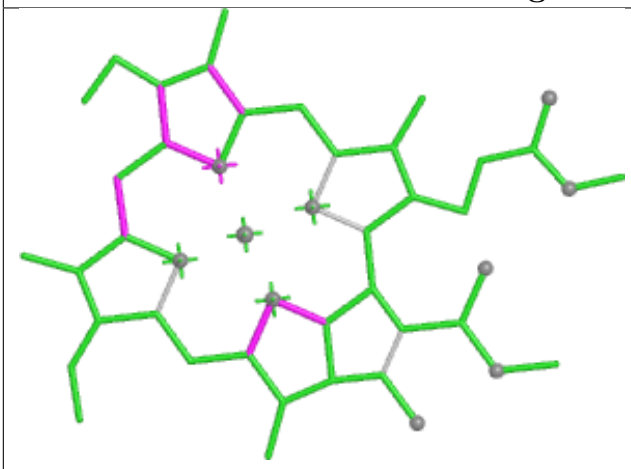
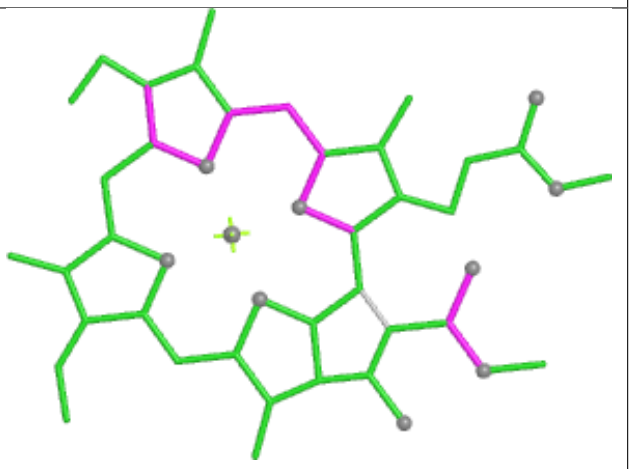
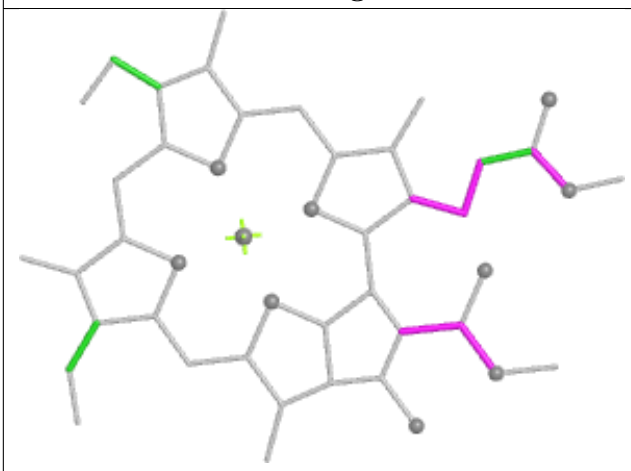
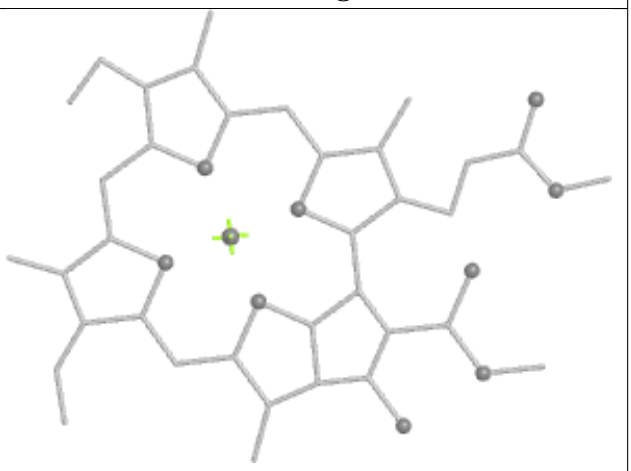
Torsions



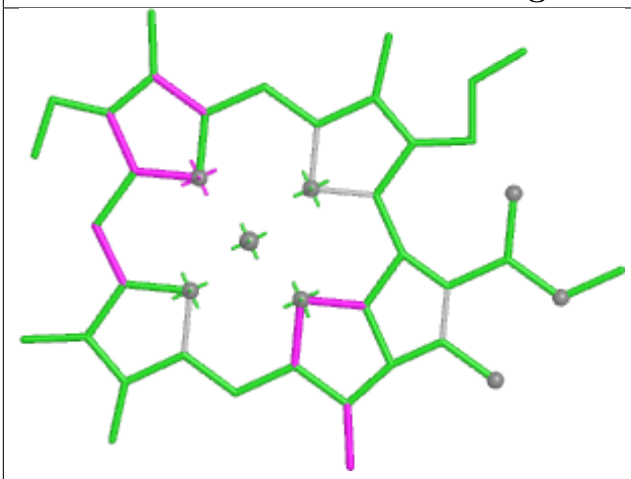
Rings

Ligand CLA B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

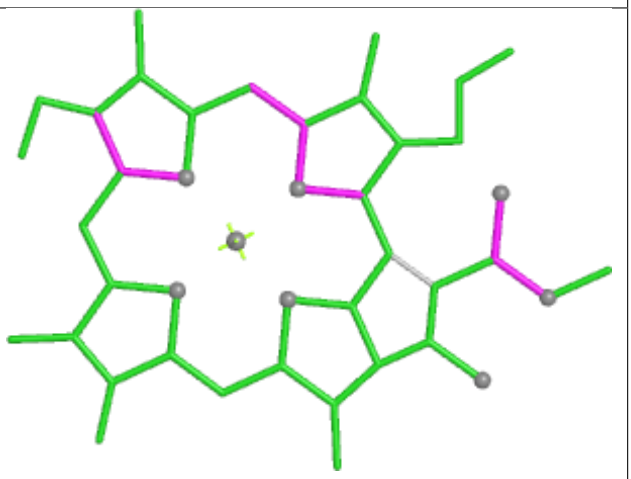
Ligand CHL 2 606	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA 1 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

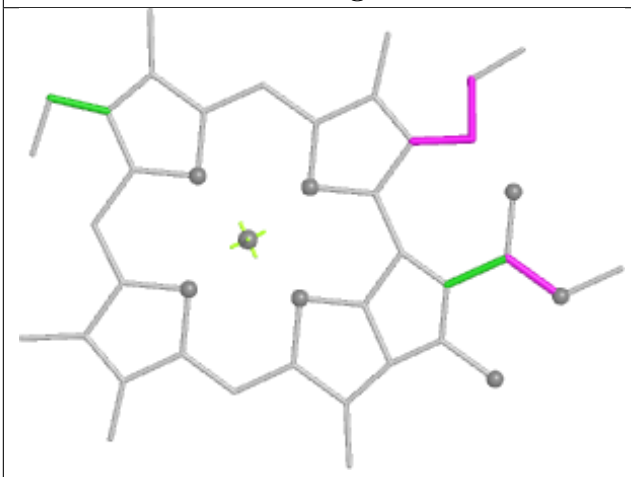
Ligand CLA 1 609



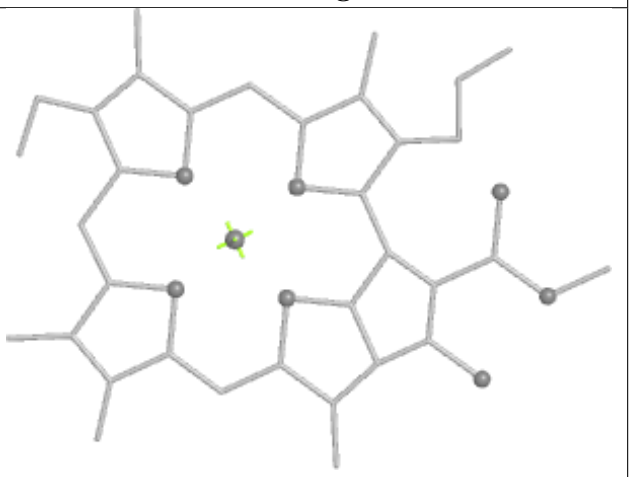
Bond lengths



Bond angles

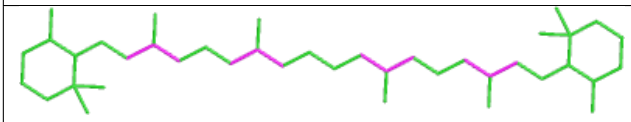


Torsions

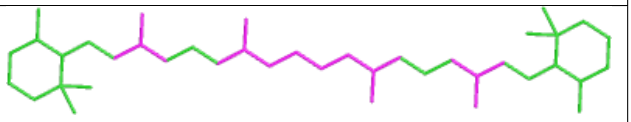


Rings

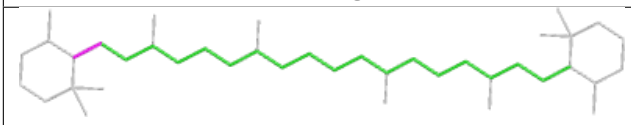
Ligand BCR B 847



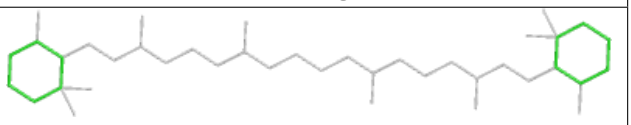
Bond lengths



Bond angles

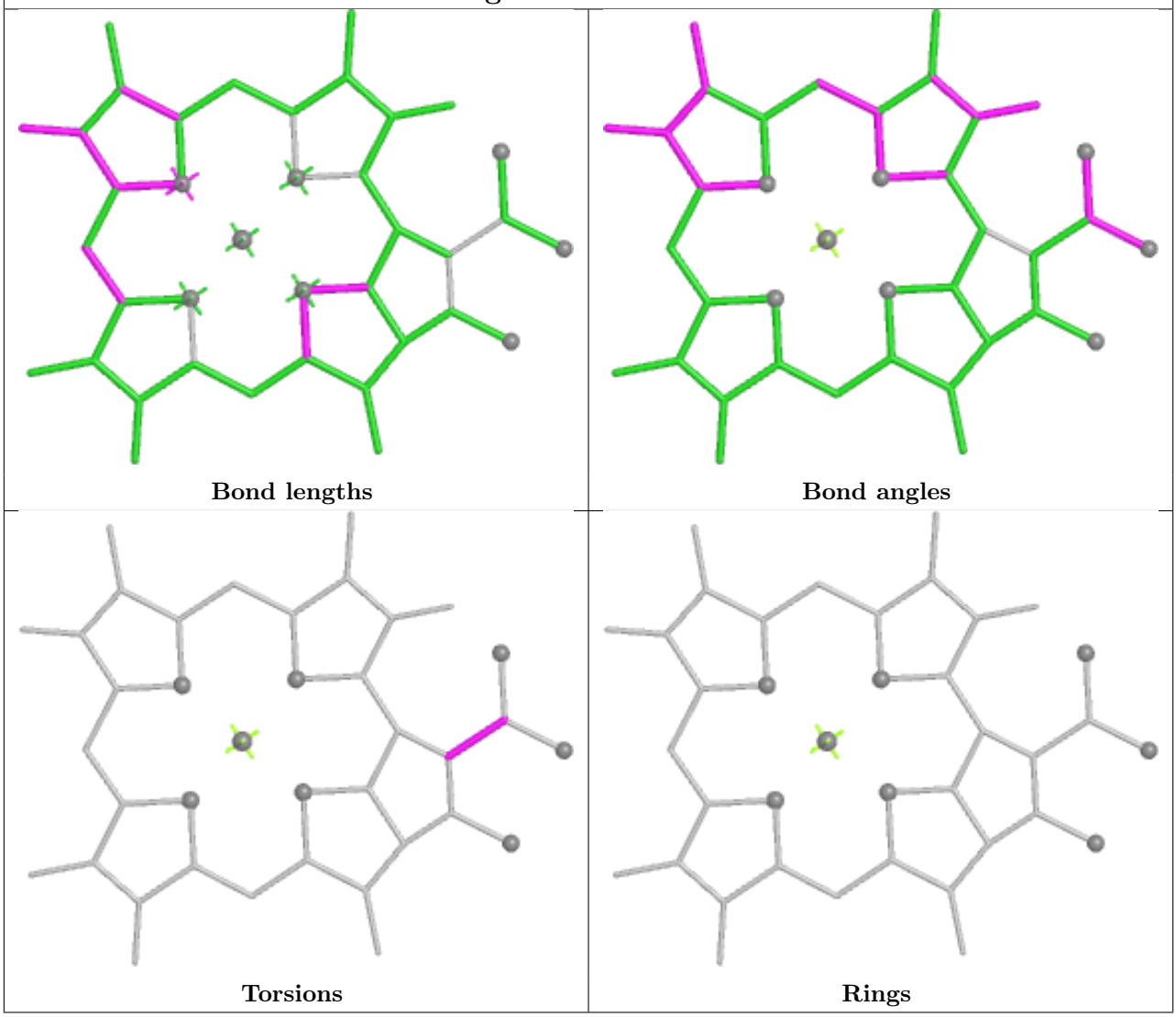


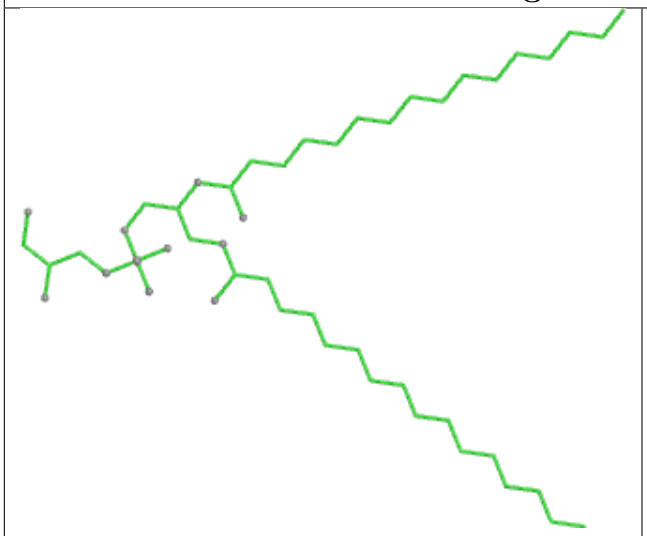
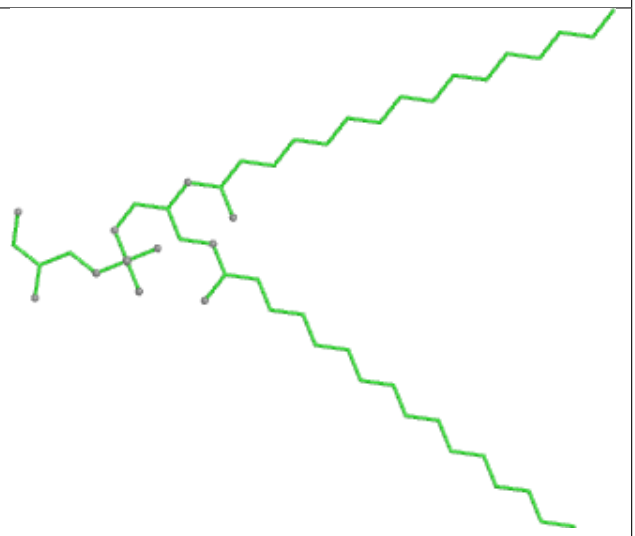
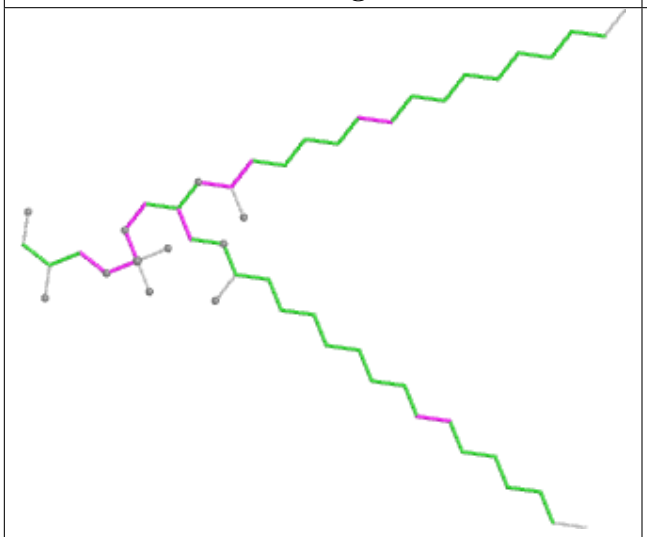
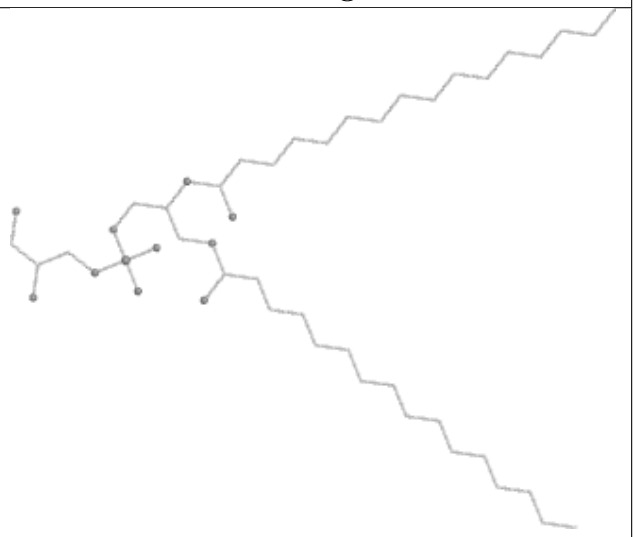
Torsions



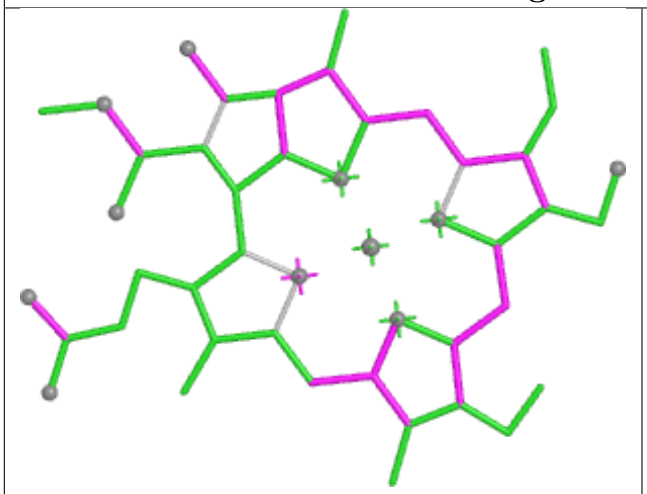
Rings

Ligand CLA 1 610

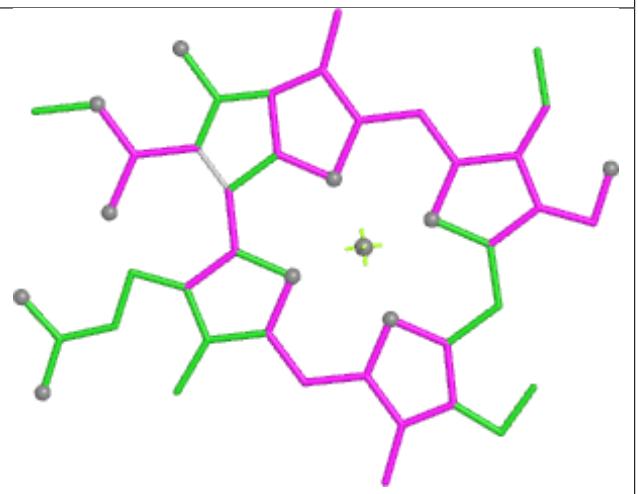


Ligand LHG B 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

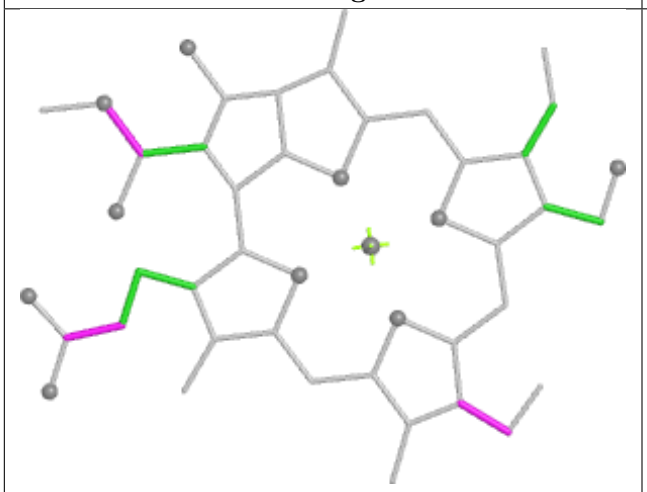
Ligand CHL 4 607



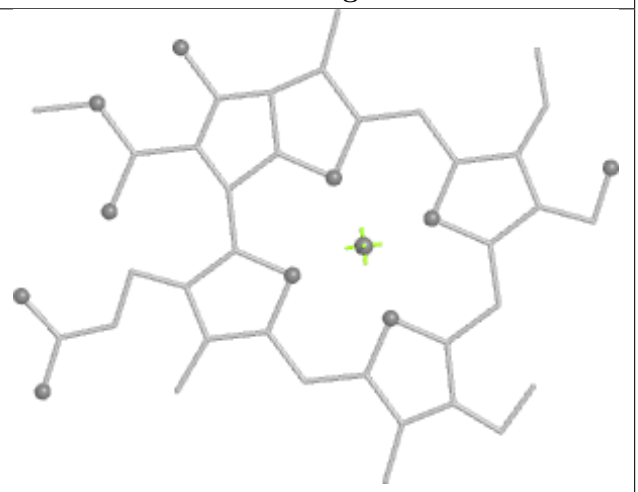
Bond lengths



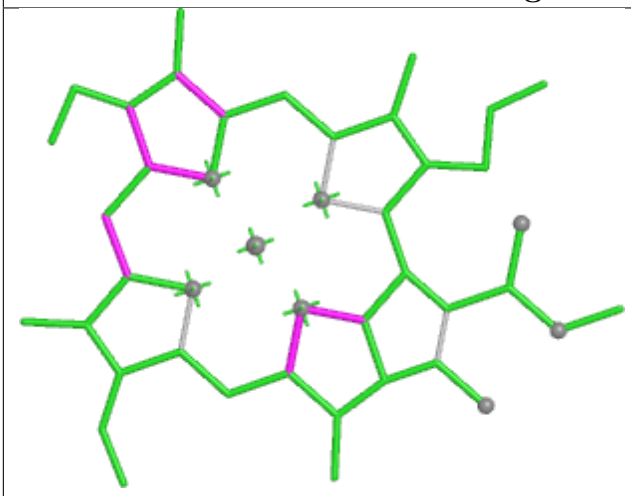
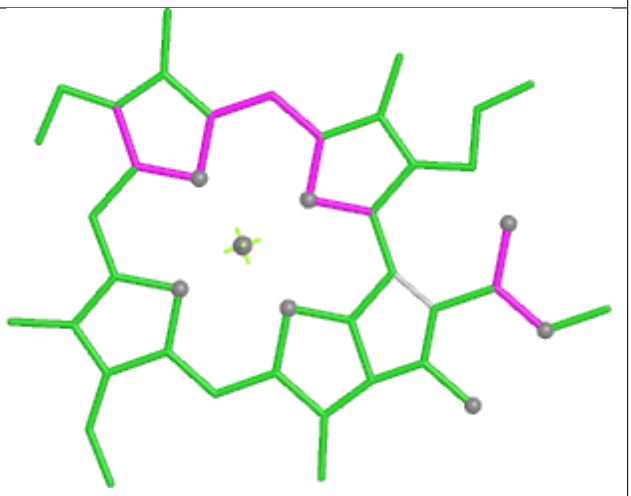
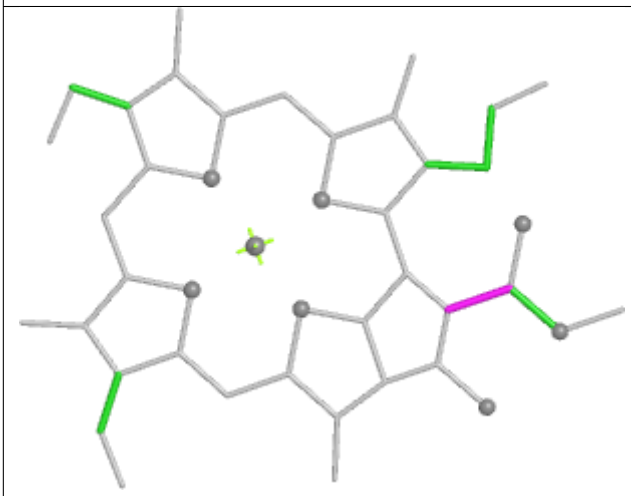
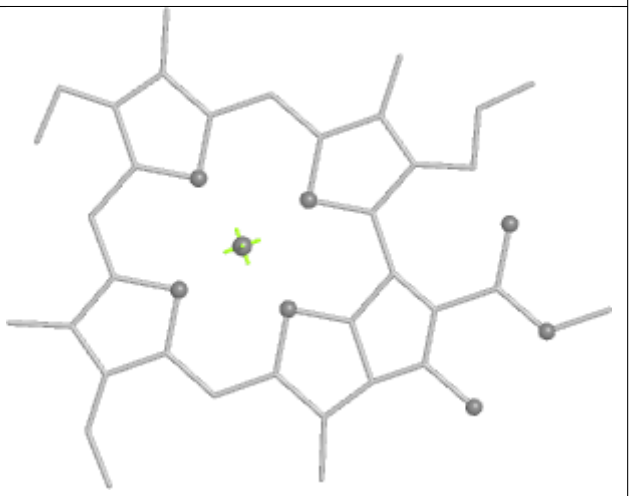
Bond angles

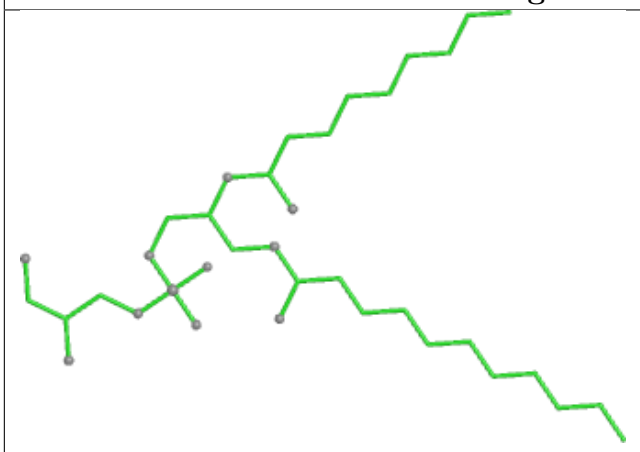
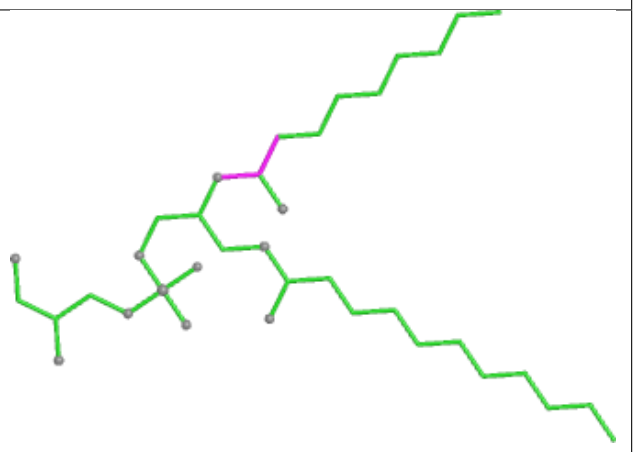
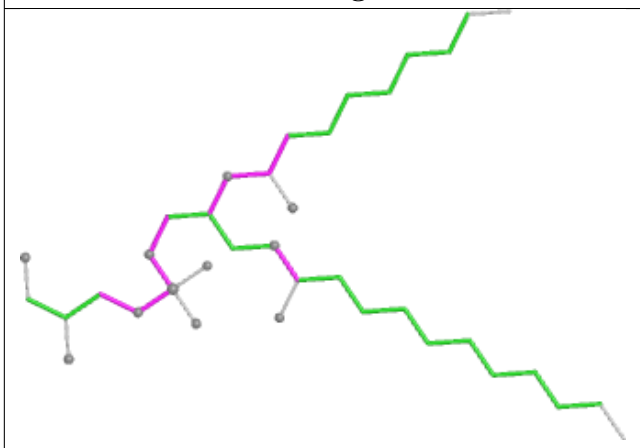
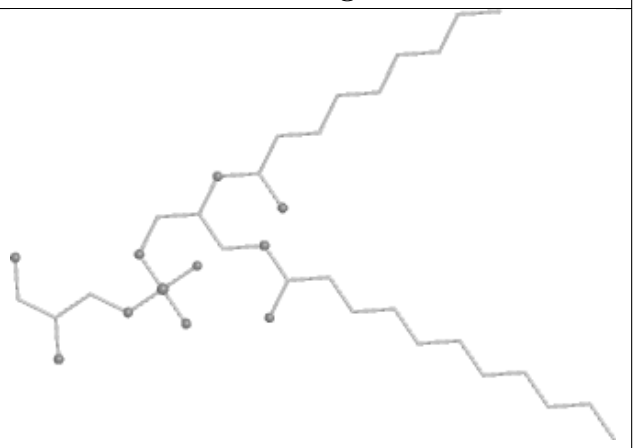


Torsions



Rings

Ligand CLA B 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 2 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

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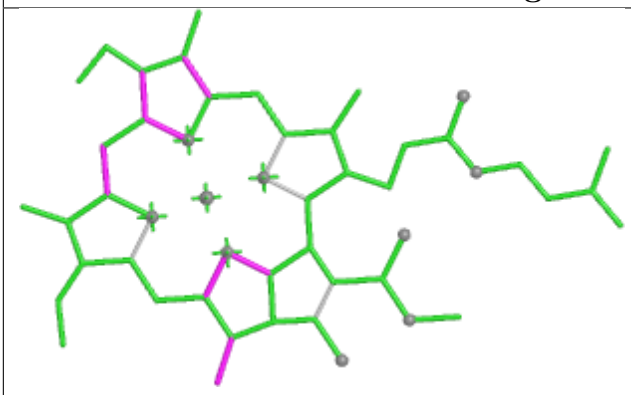
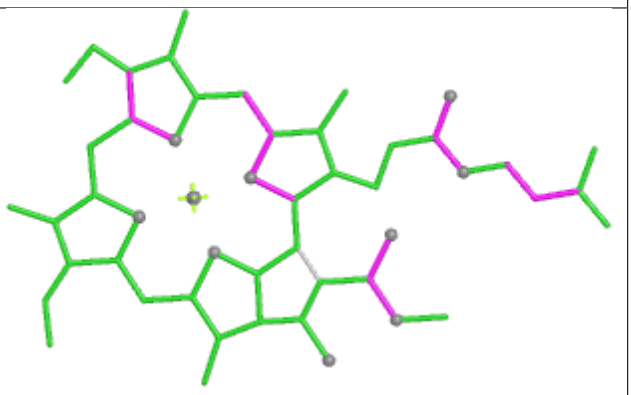
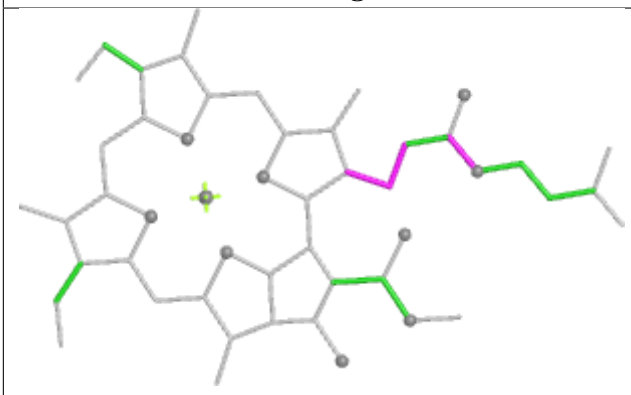
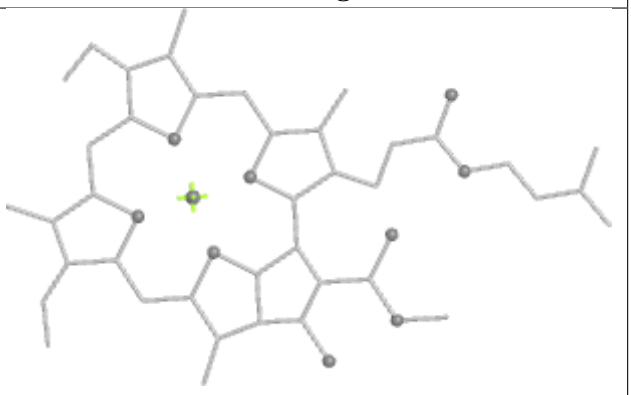
 Bond lengths	 Bond angles
 Torsions	 Rings

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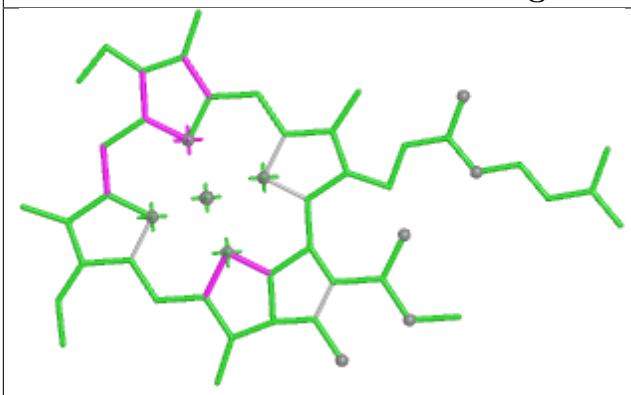
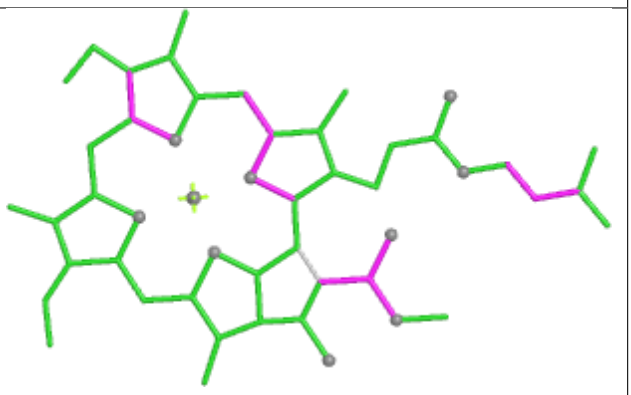
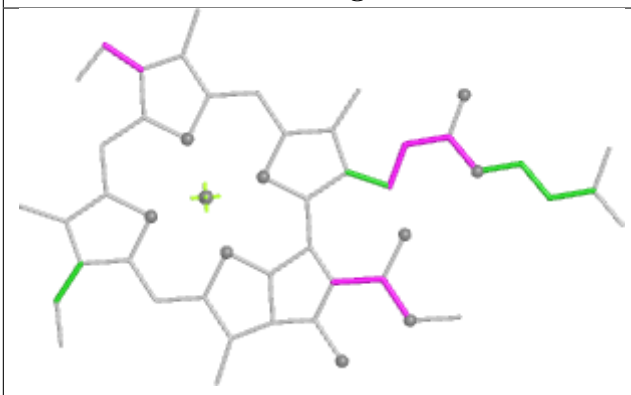
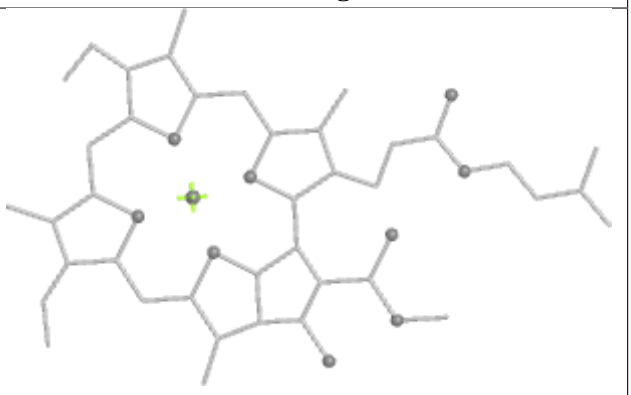
 Bond lengths	 Bond angles
 Torsions	 Rings

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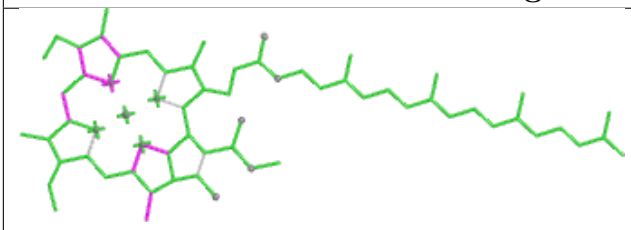
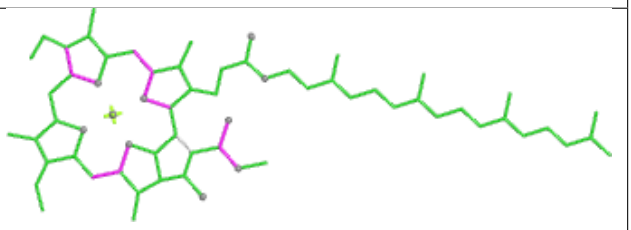
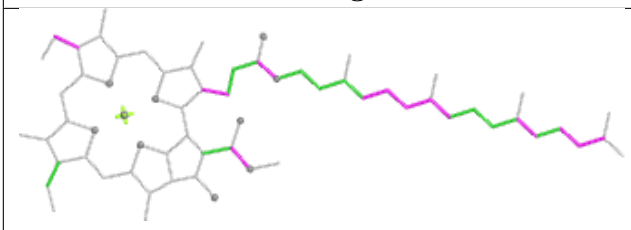
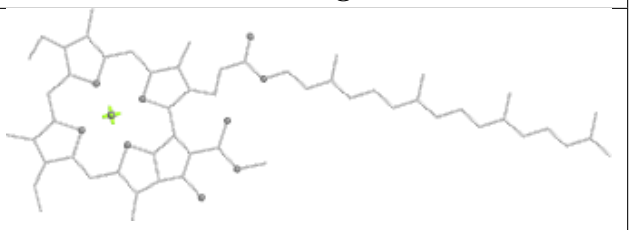
 Bond lengths	 Bond angles
 Torsions	 Rings

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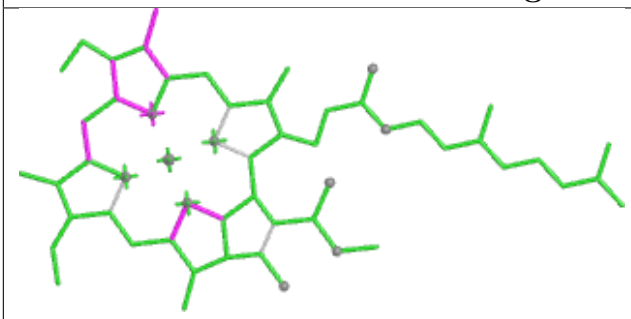
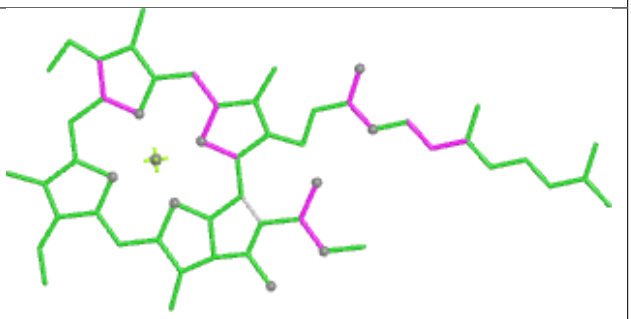
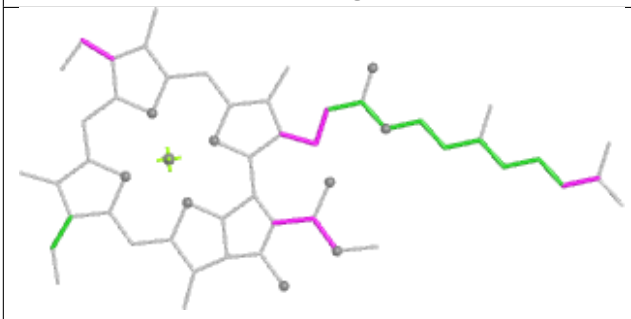
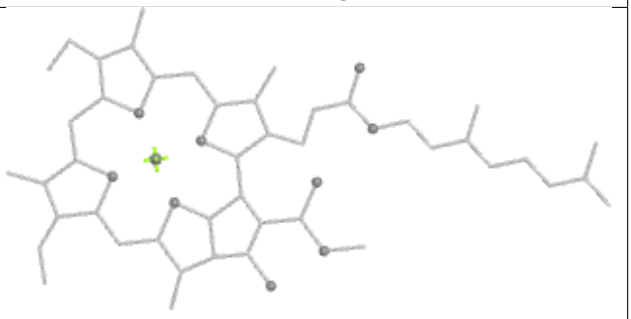
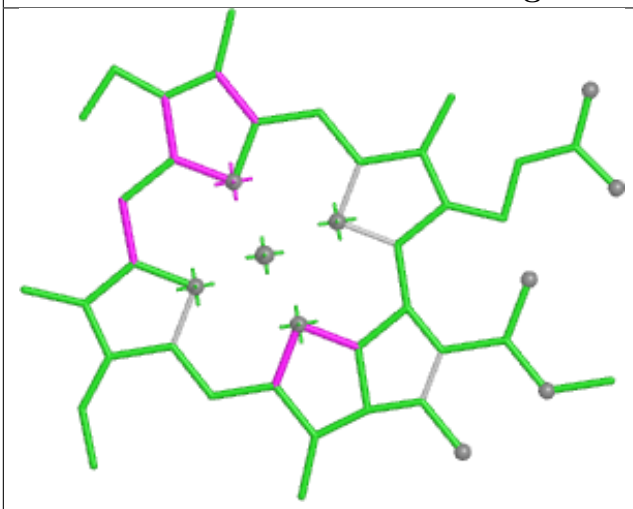
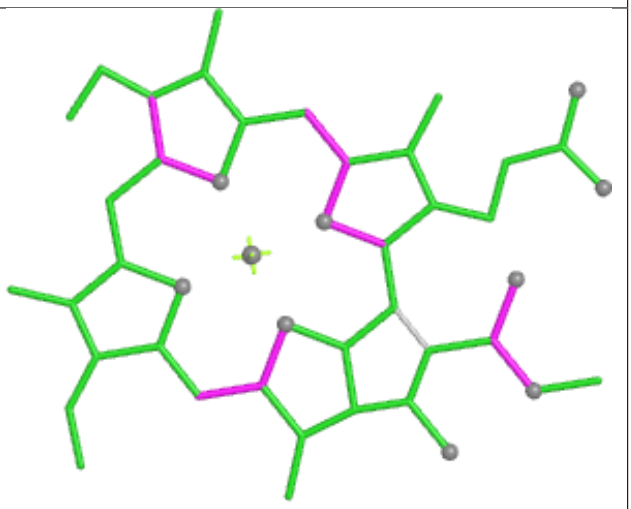
 Bond lengths	 Bond angles
 Torsions	 Rings

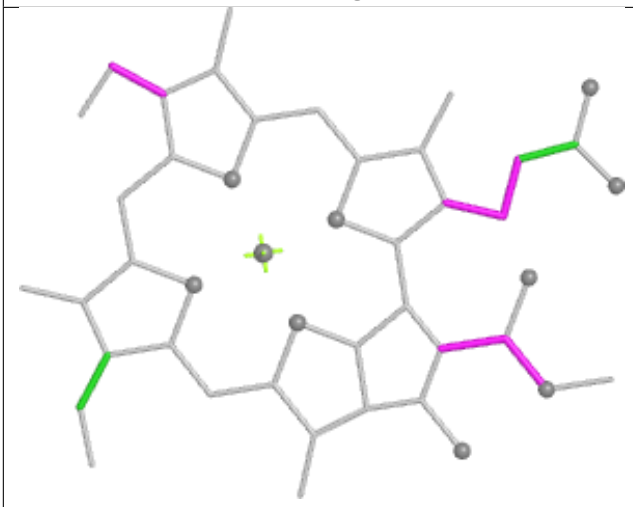
Ligand CLA A 836



Bond lengths

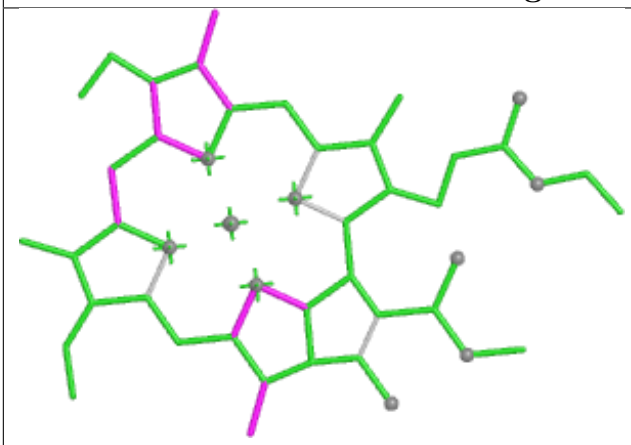
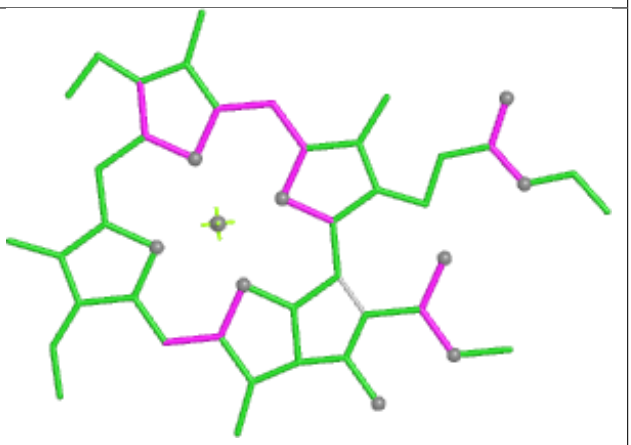
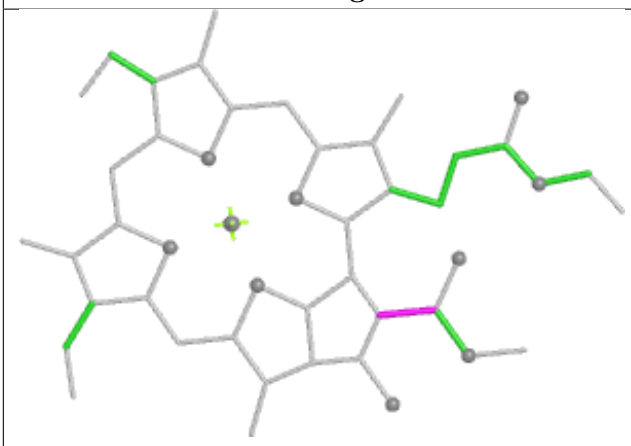
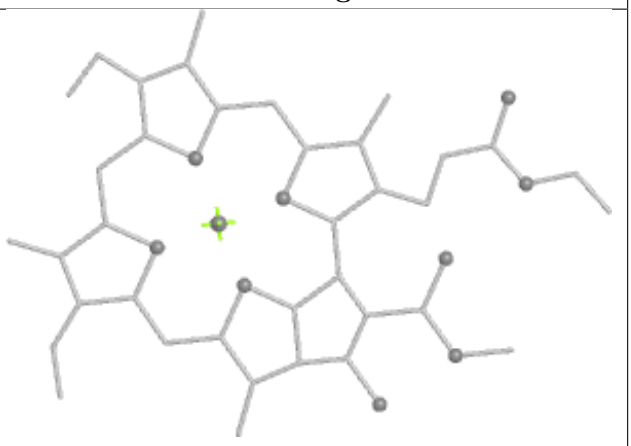


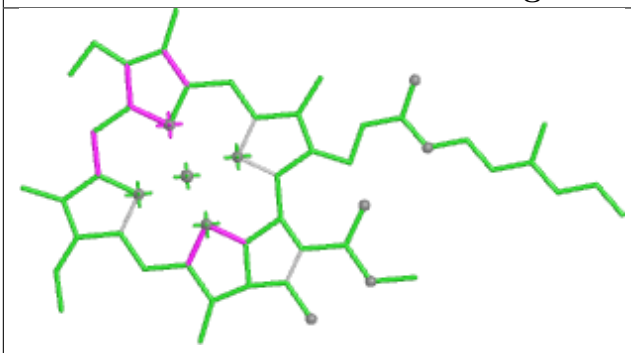
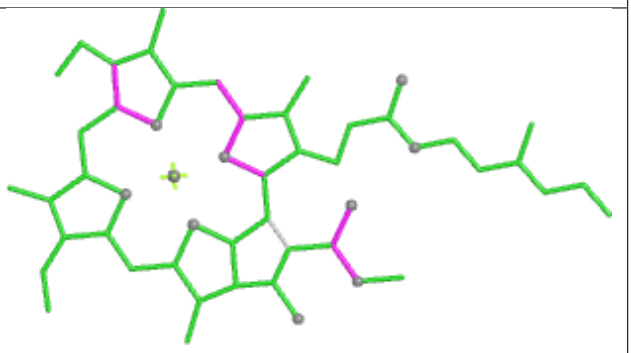
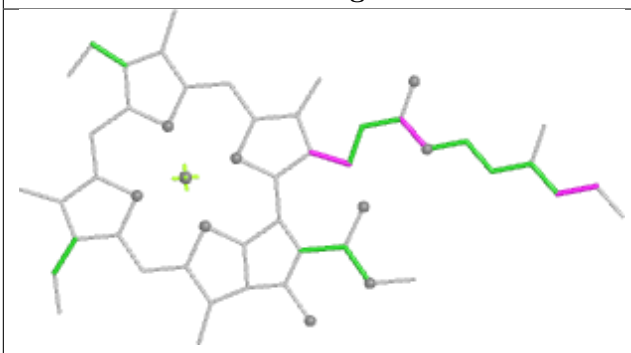
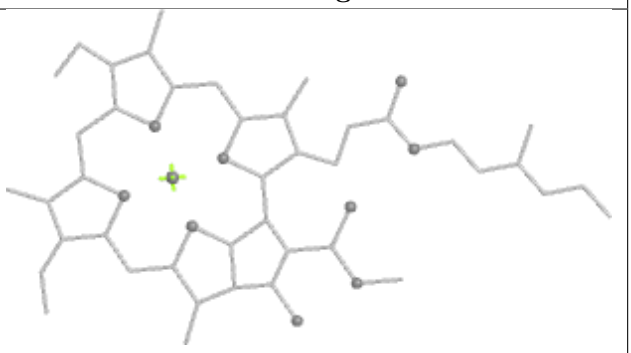
Bond angles

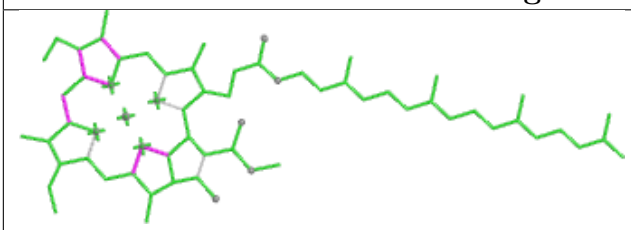
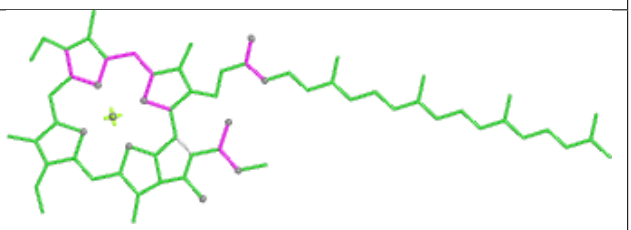
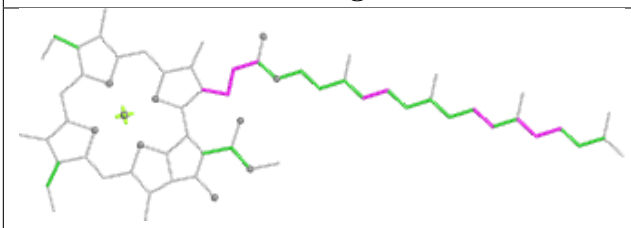
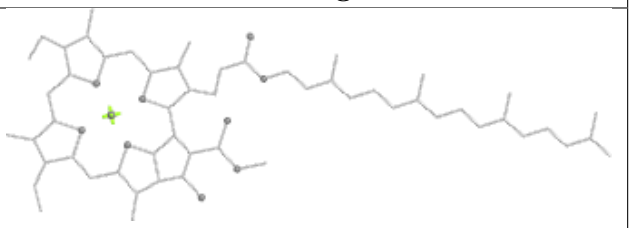


Torsions

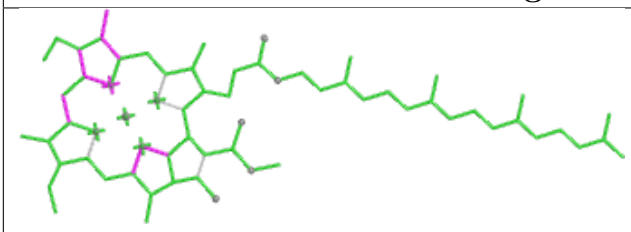
Rings

Ligand CLA B 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

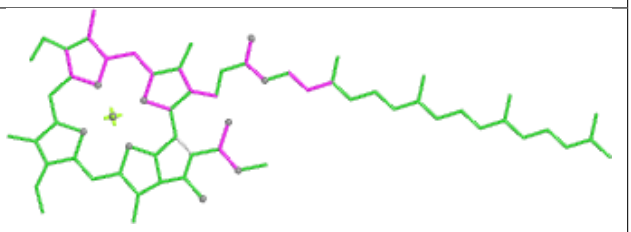
Ligand CLA A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

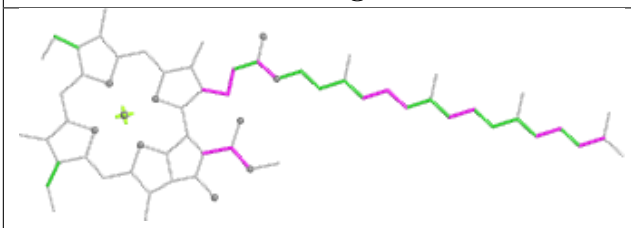
Ligand CLA B 822



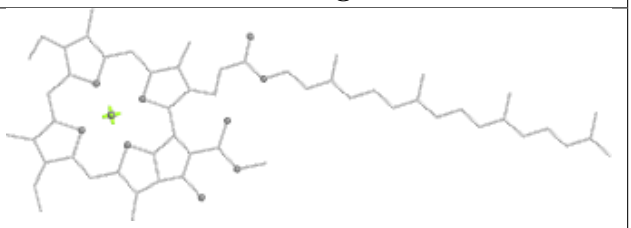
Bond lengths



Bond angles

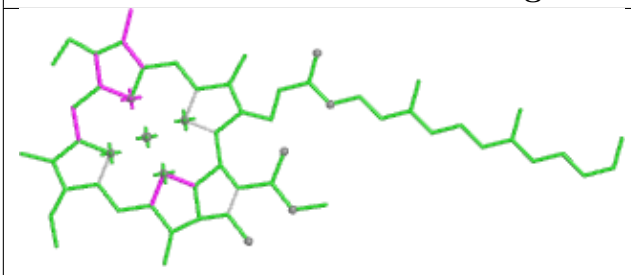


Torsions



Rings

Ligand CLA B 817



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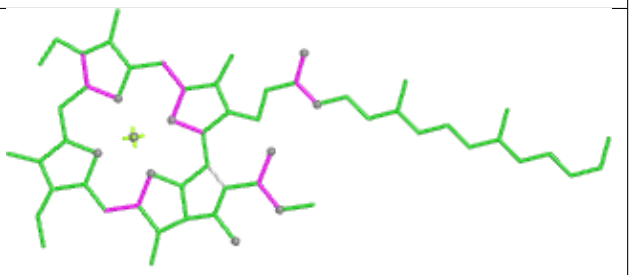
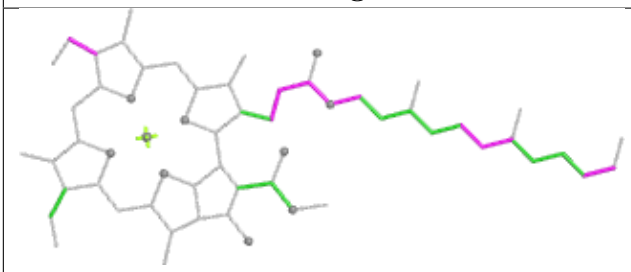
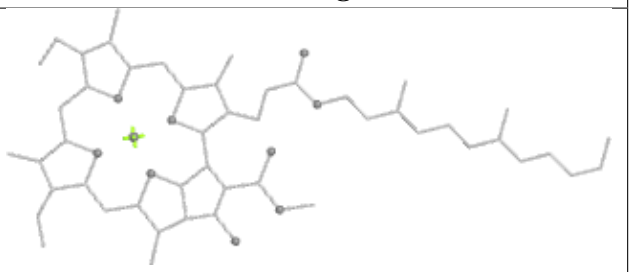


Bond angles

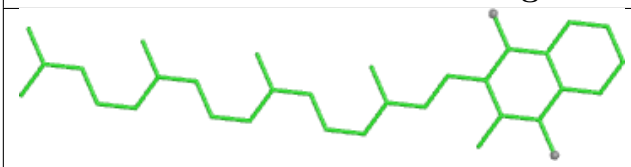


Torsions

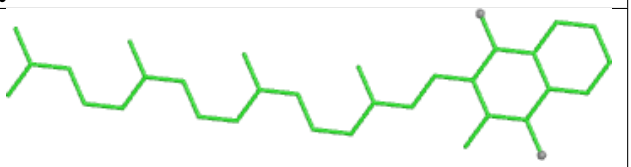


Rings

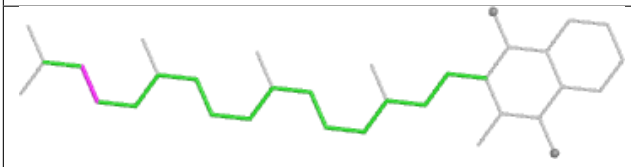
Ligand PQN A 855



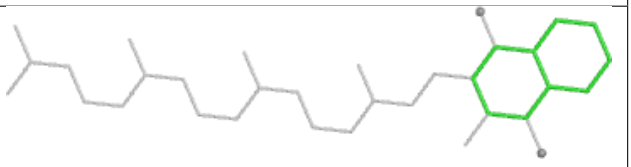
Bond lengths



Bond angles

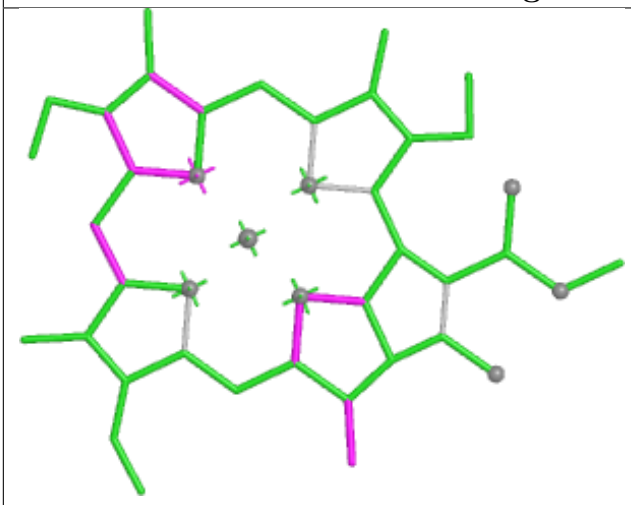


Torsions

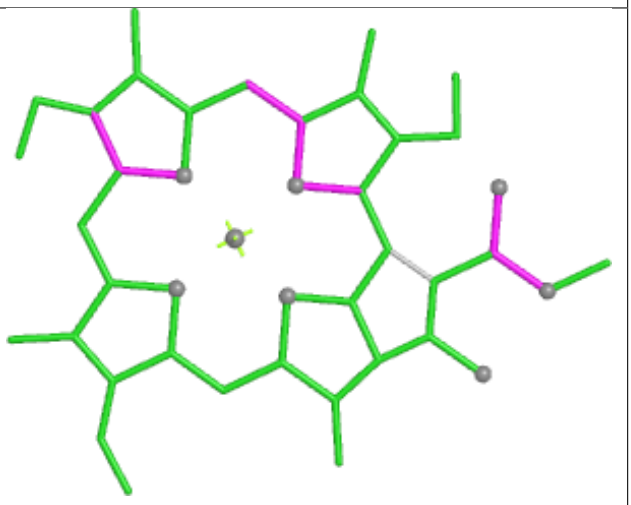


Rings

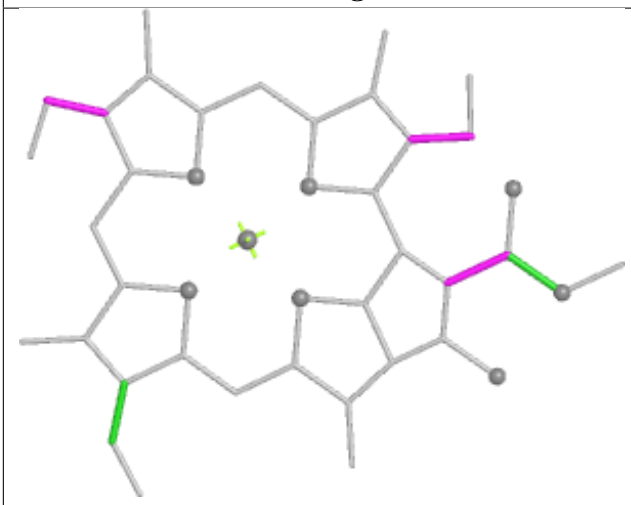
Ligand CLA G 202



Bond lengths



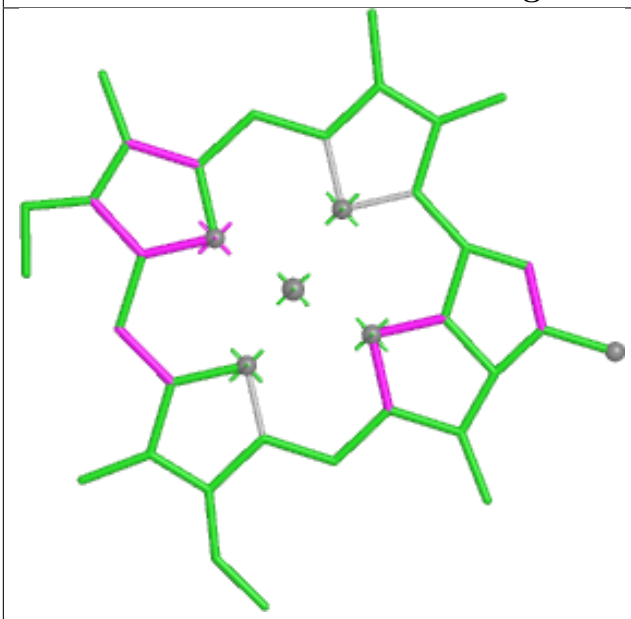
Bond angles



Torsions

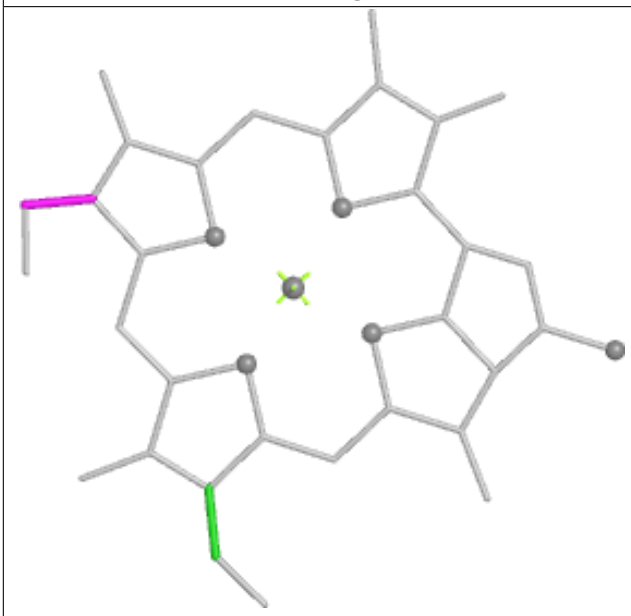
Rings

Ligand CLA K 201

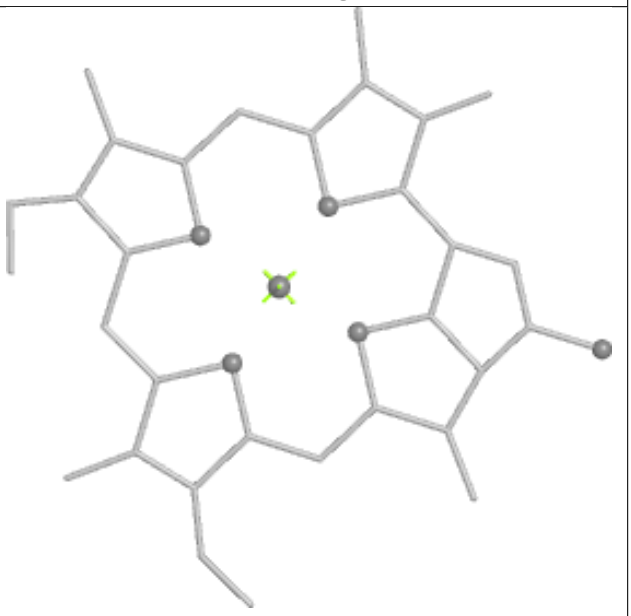


Bond lengths

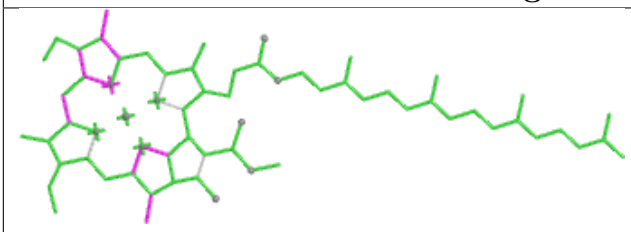
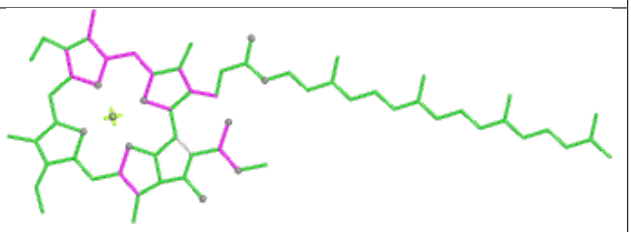
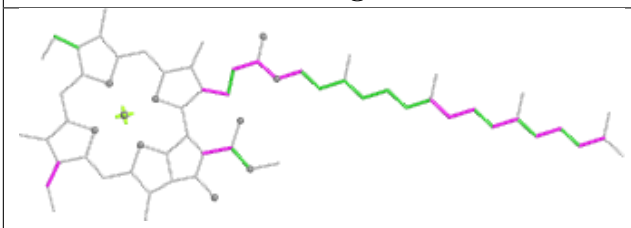
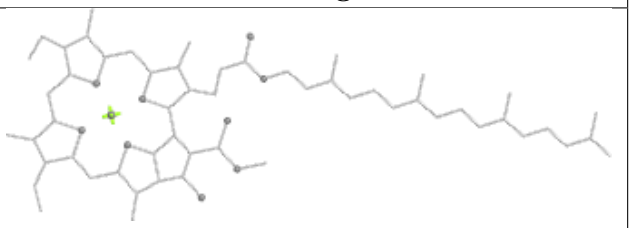
Bond angles

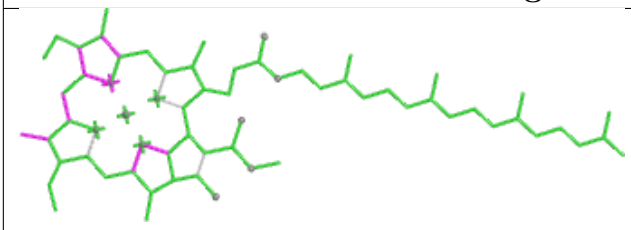
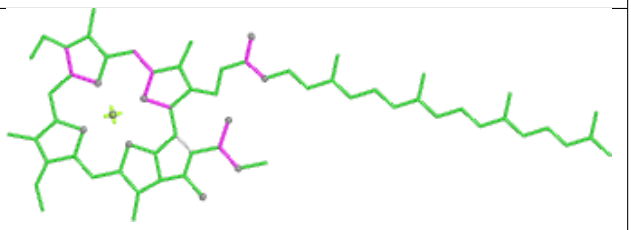
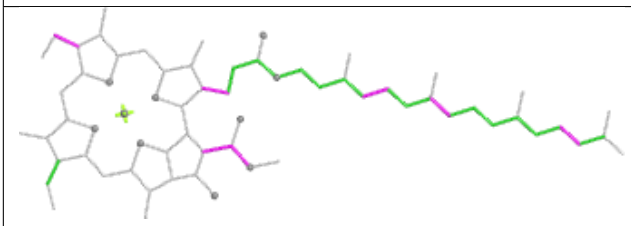
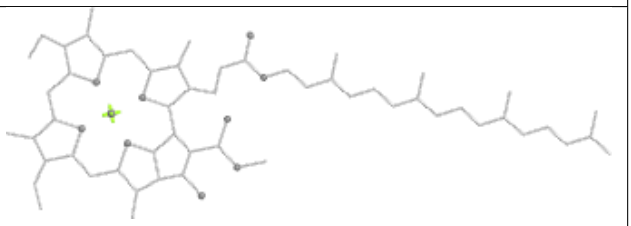


Torsions

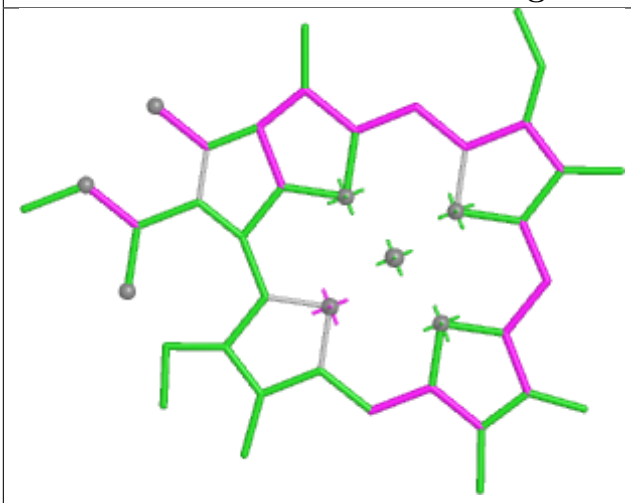


Rings

Ligand CLA A 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 4 606



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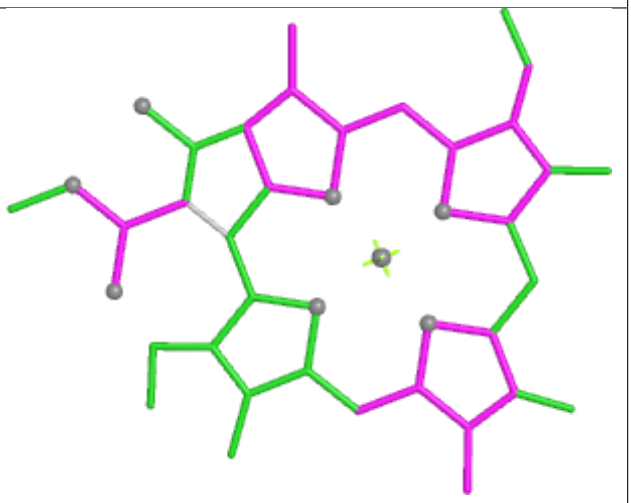
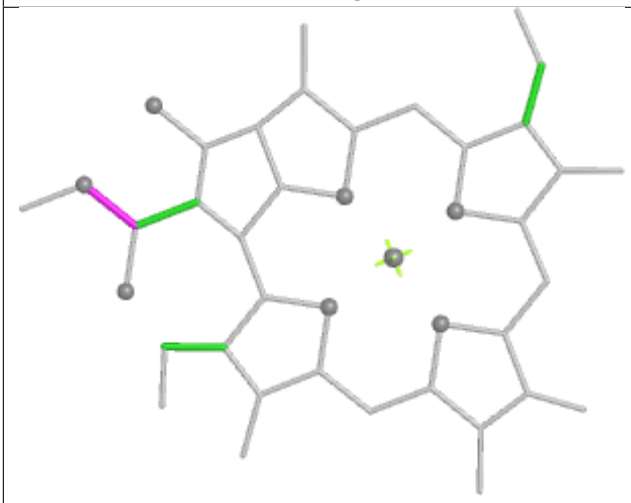


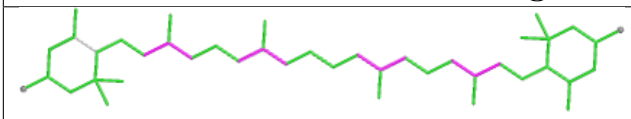
Bond angles



Torsions

Rings

Ligand LUT 2 616



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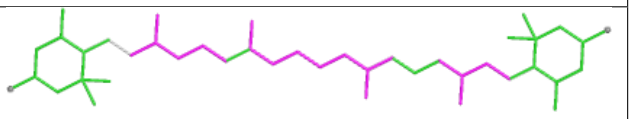

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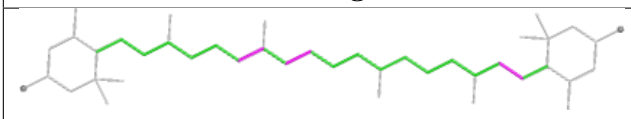
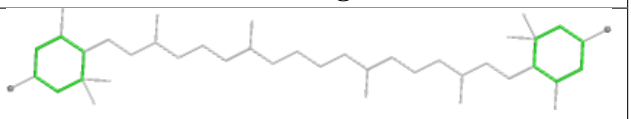
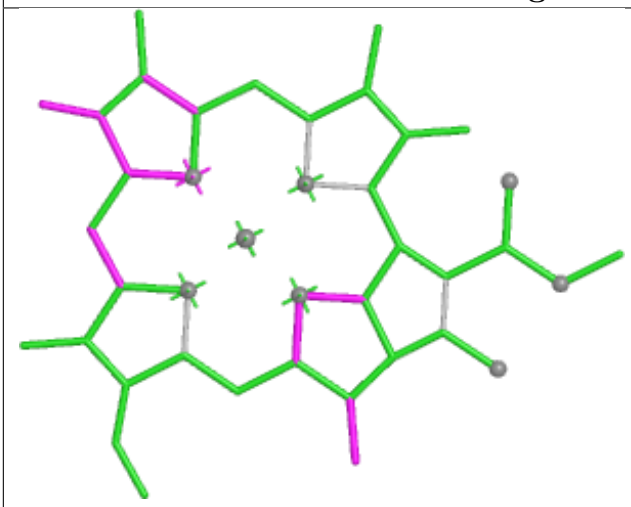


Torsions



Rings

Ligand CLA 1 608



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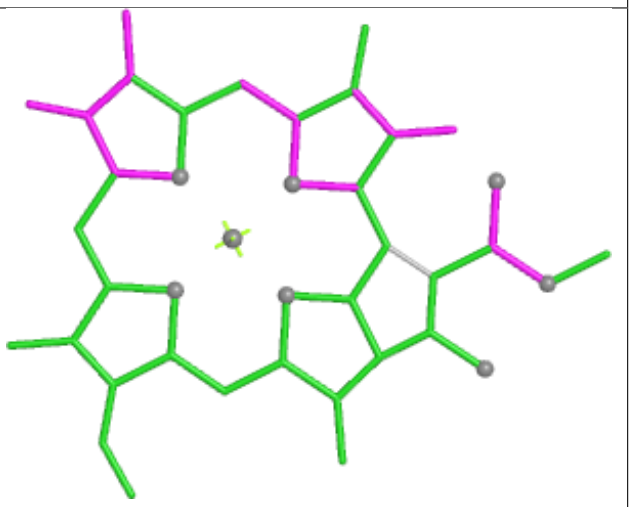
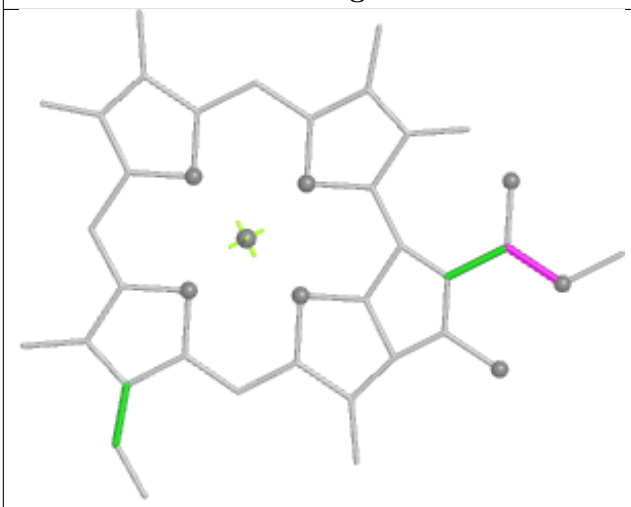


Bond angles



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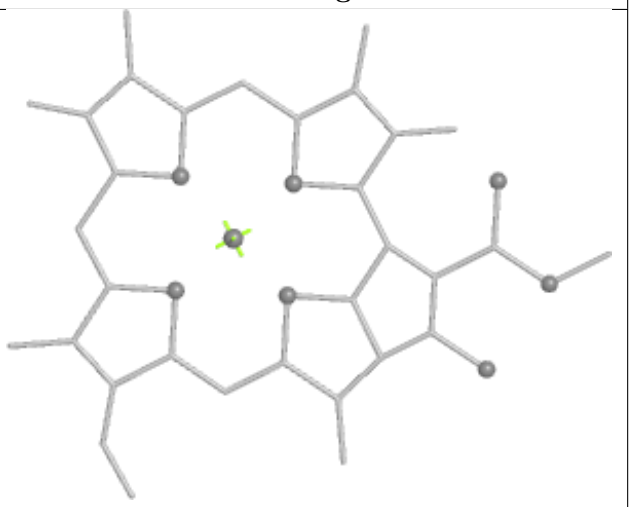
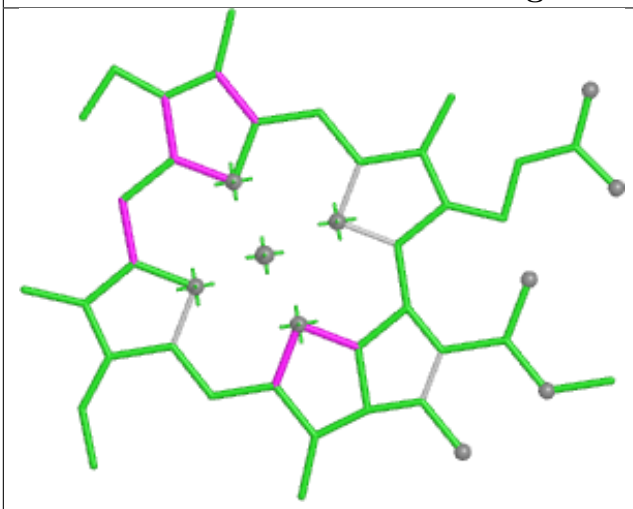


Rings

Ligand CLA L 304



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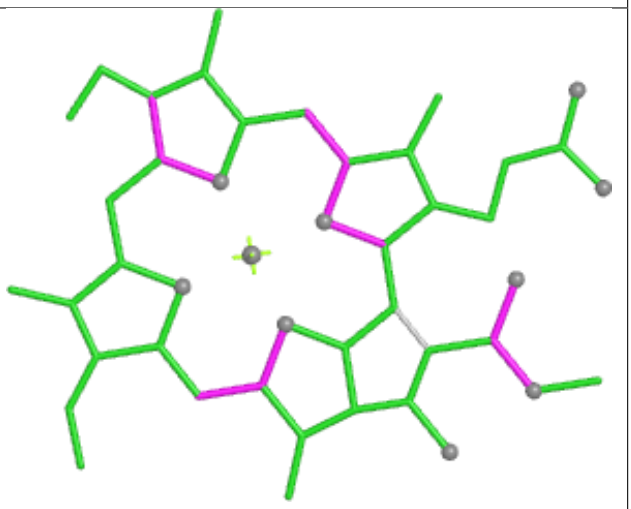
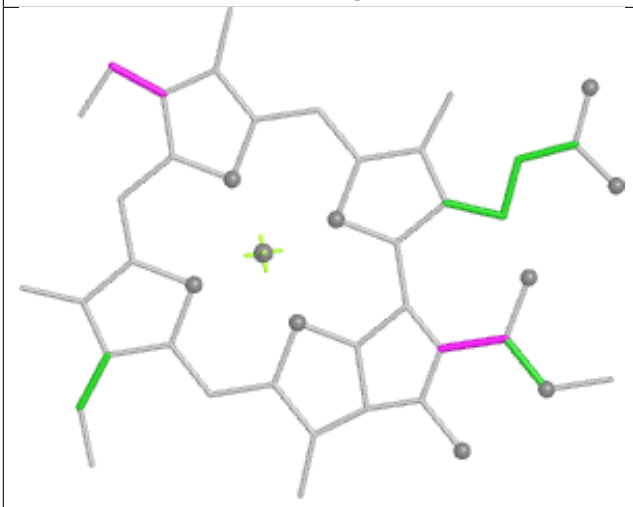


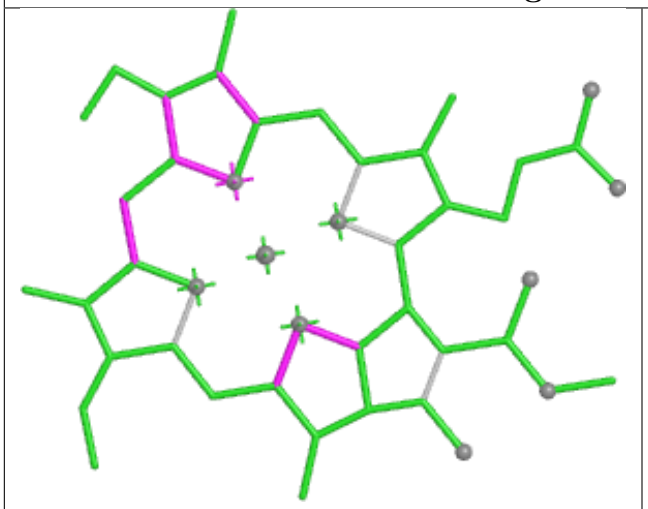
Bond angles



Torsions

Rings

Ligand CLA A 837



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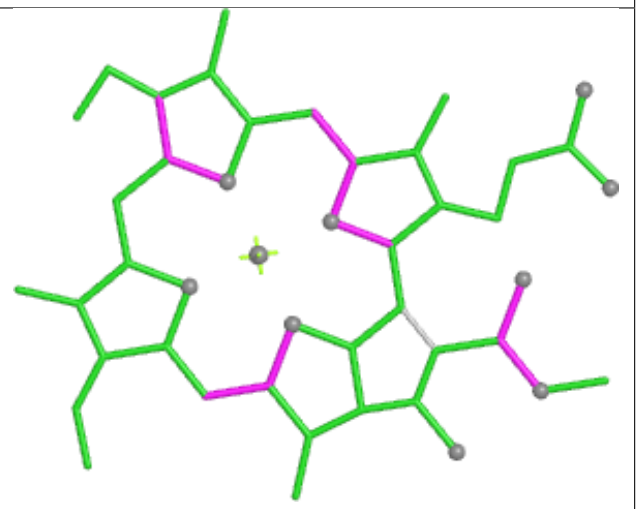
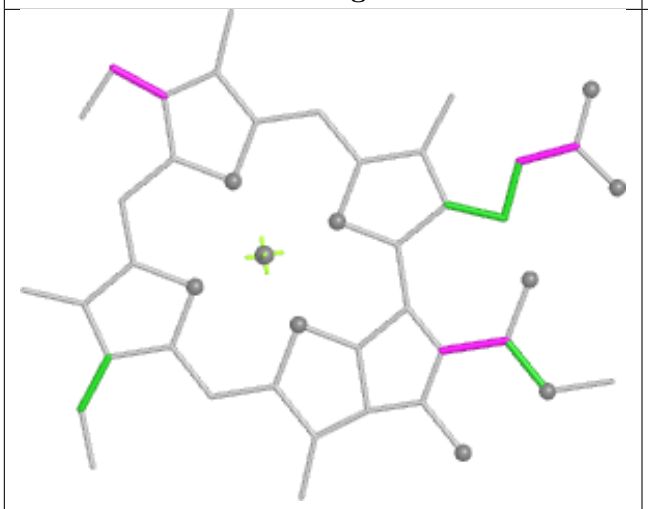


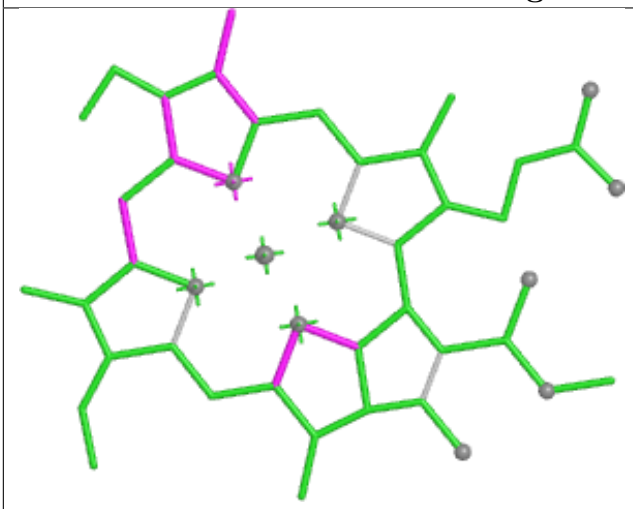
Bond angles



Torsions

Rings

Ligand CLA L 302



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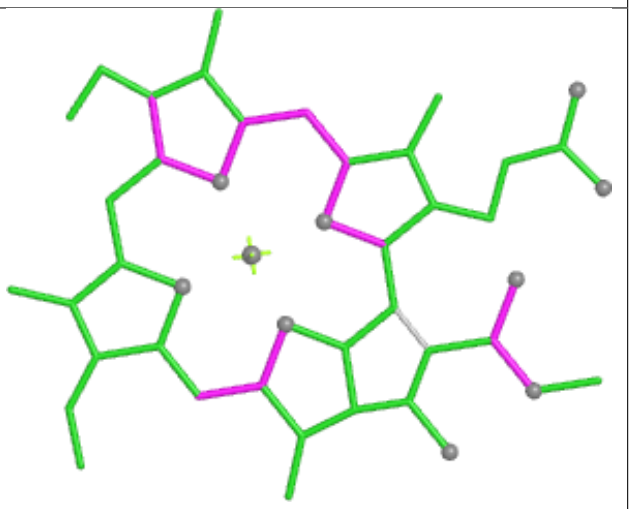
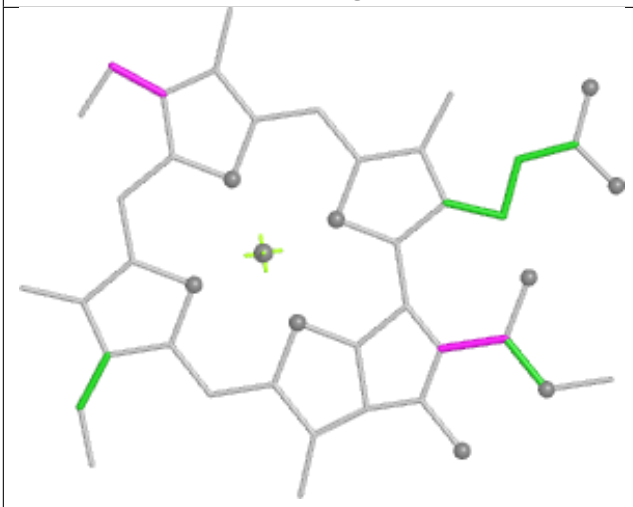


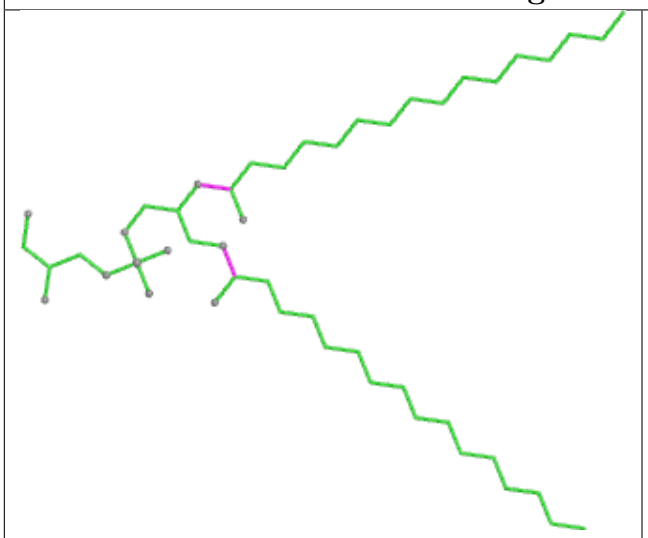
Bond angles



Torsions

Rings

Ligand LHG 1 615



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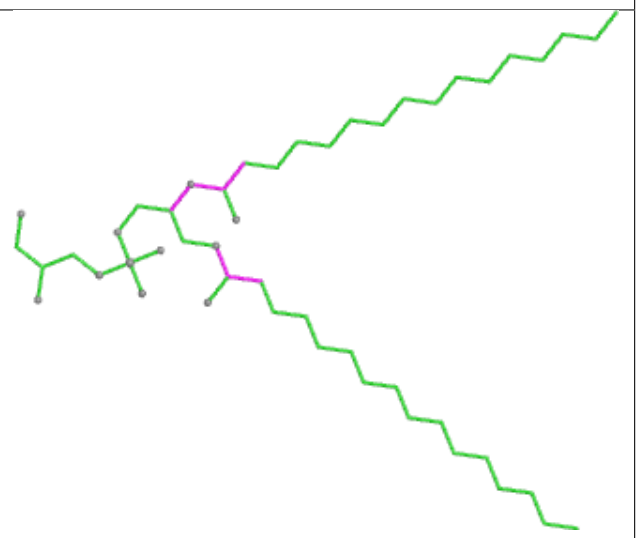
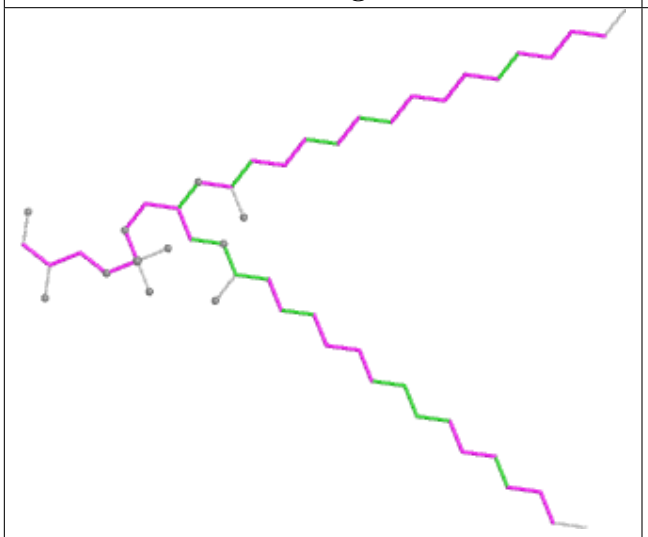
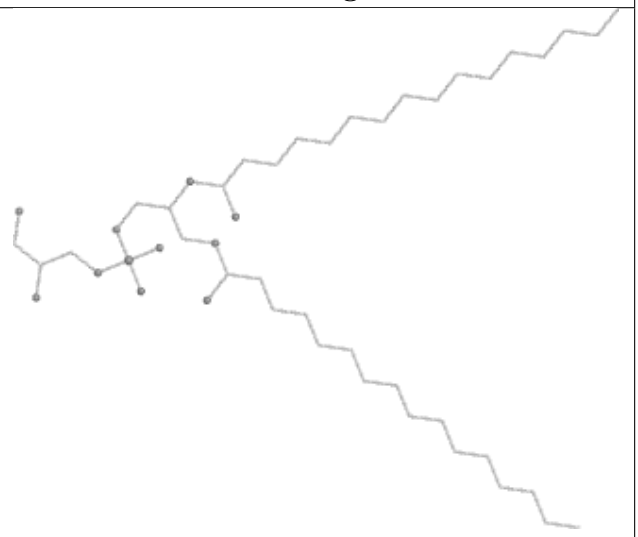


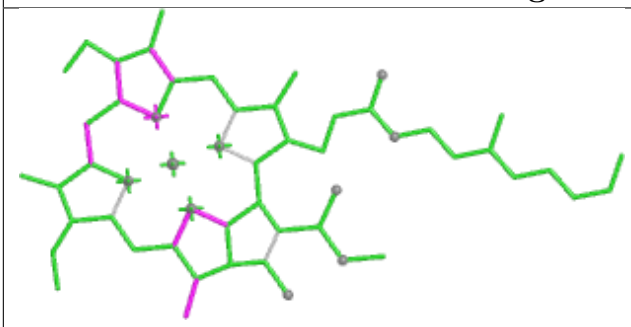
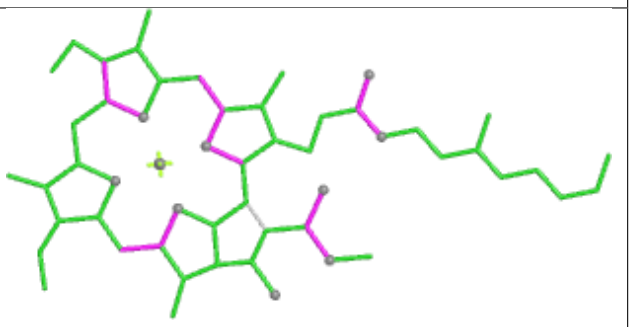
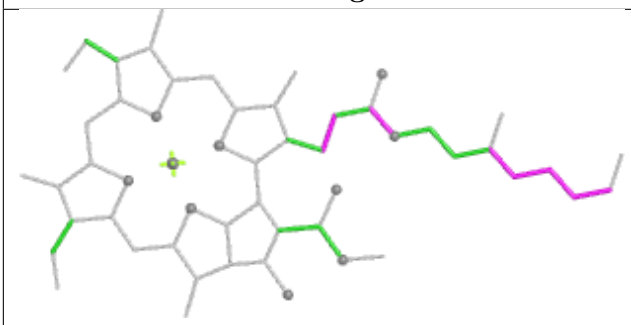
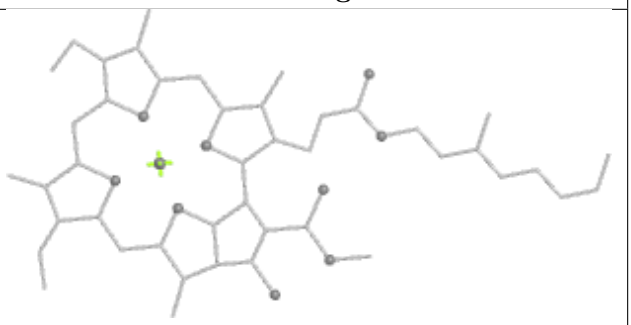
Bond angles

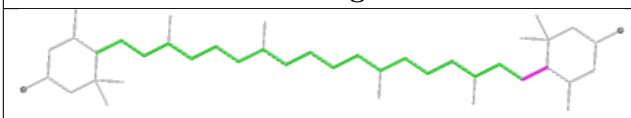
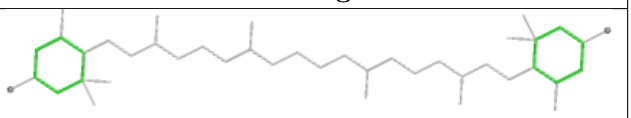


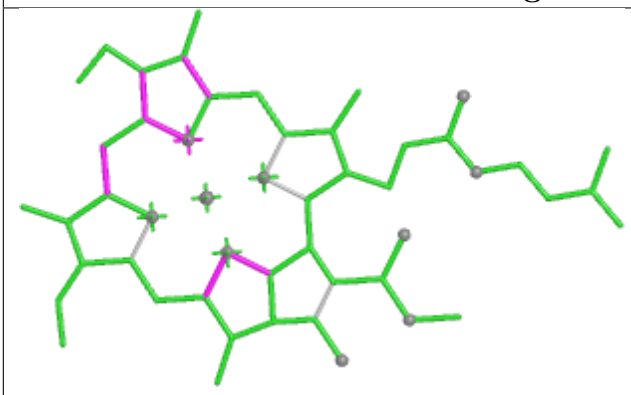
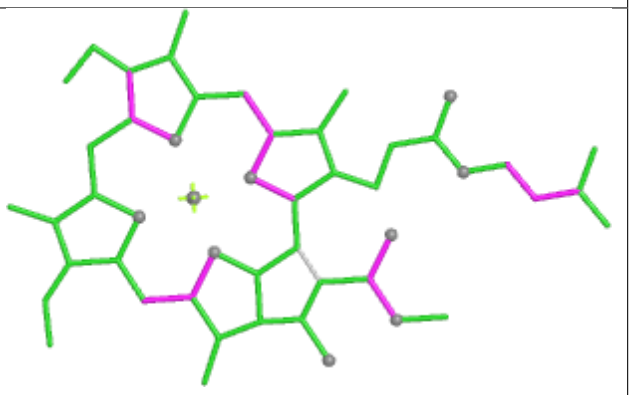
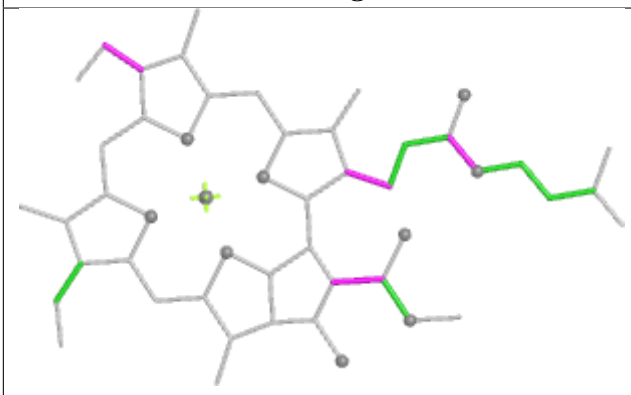
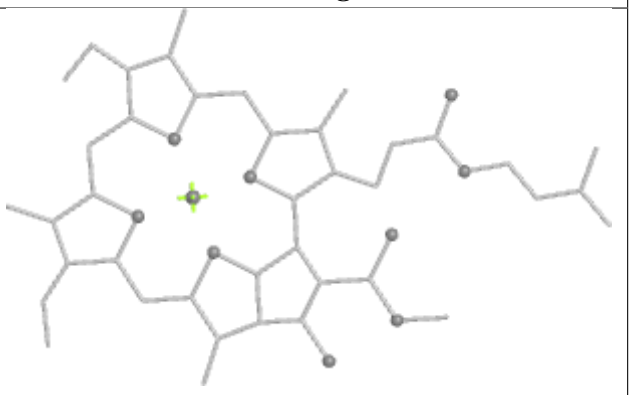
Torsions



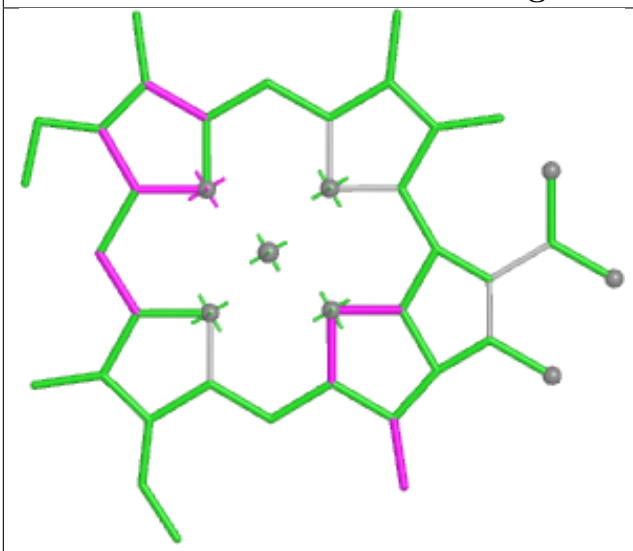
Rings

Ligand CLA 1 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

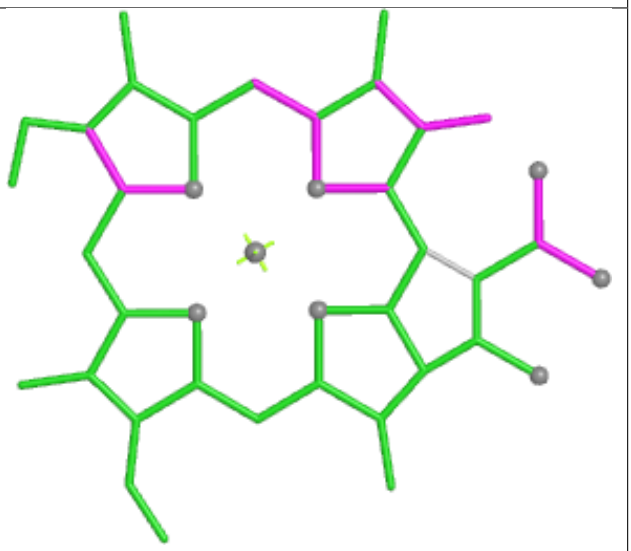
Ligand LUT 4 616	
Bond lengths	Bond angles
 Torsions	 Rings

Ligand CLA A 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

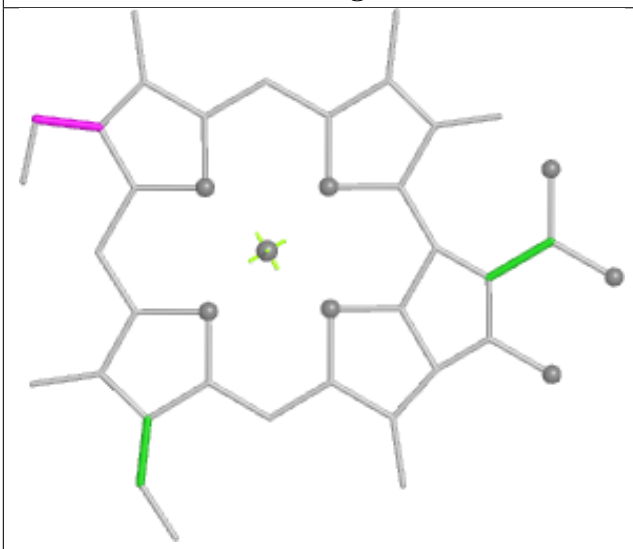
Ligand CLA 3 612



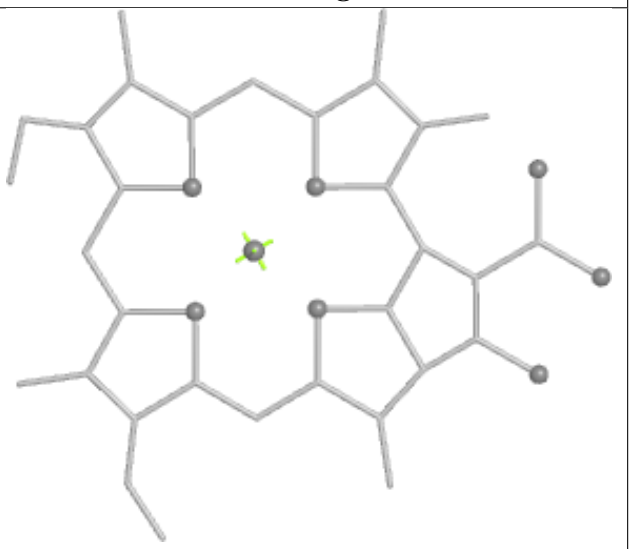
Bond lengths



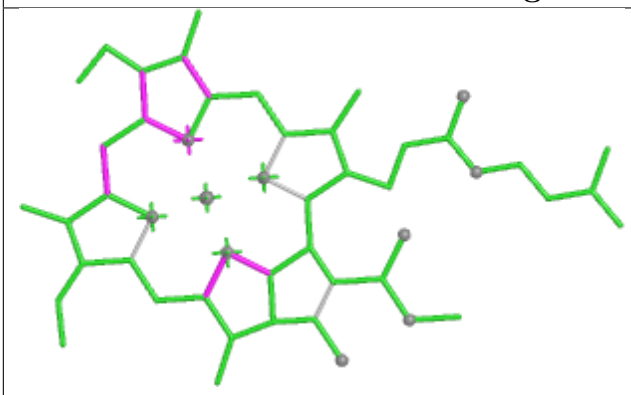
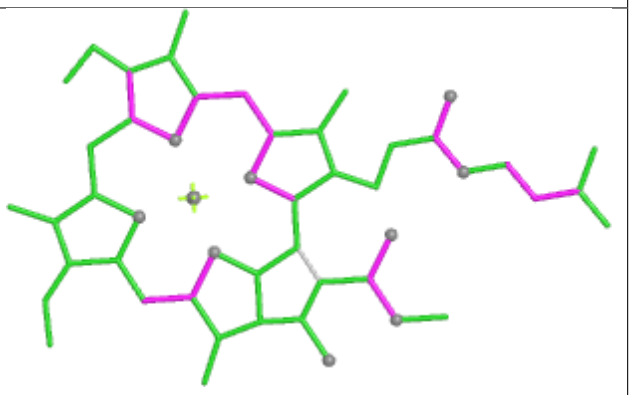
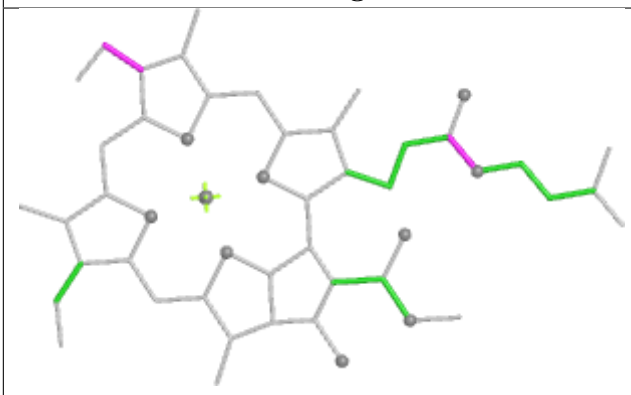
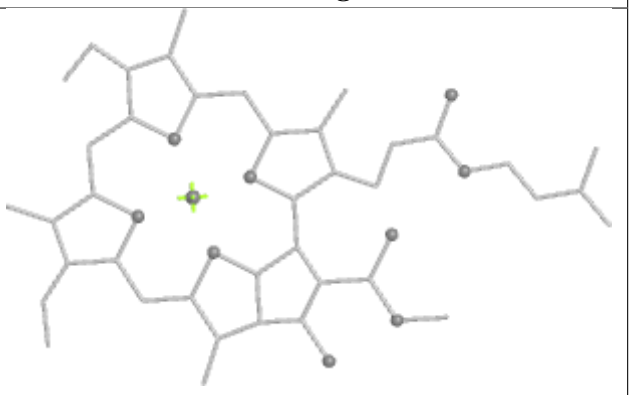
Bond angles



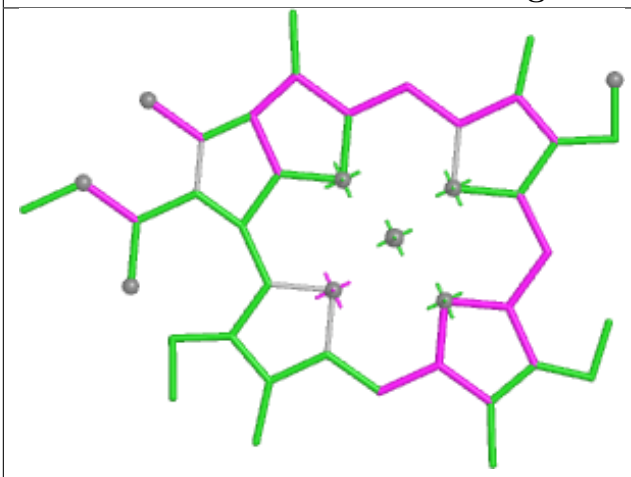
Torsions



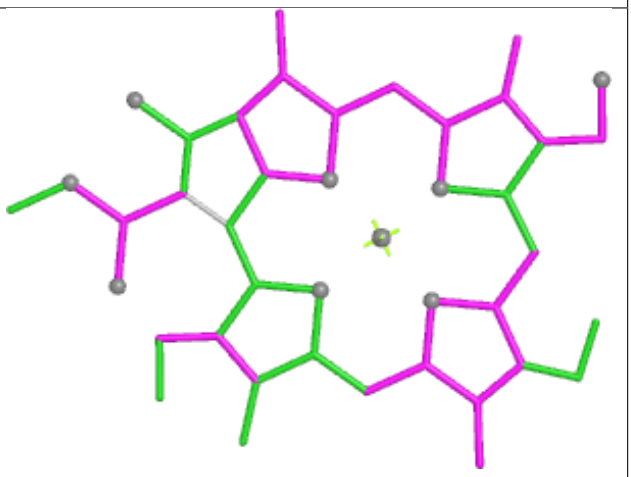
Rings

Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

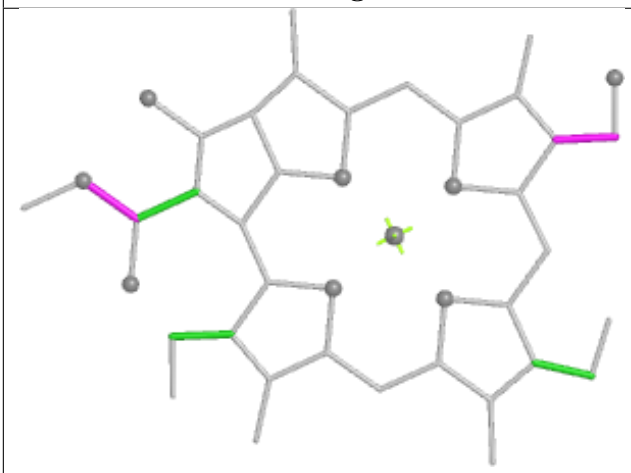
Ligand CHL 2 605



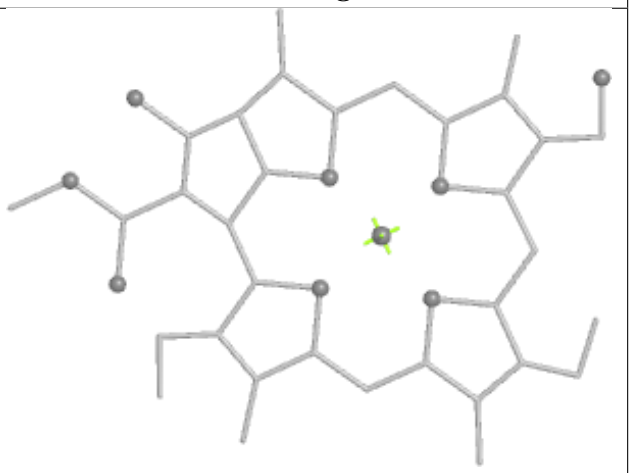
Bond lengths



Bond angles

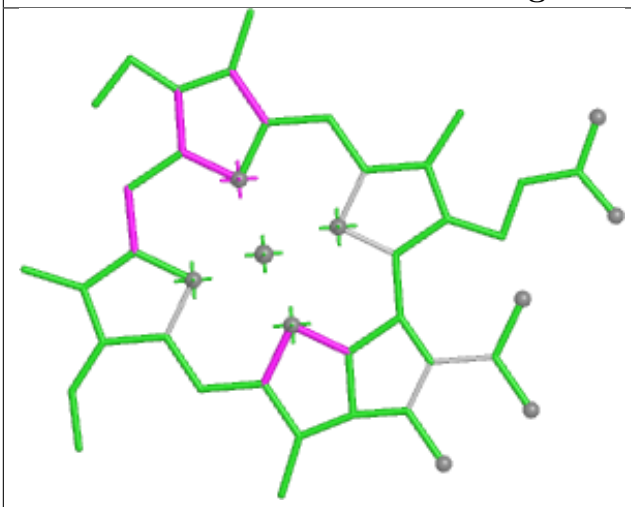


Torsions

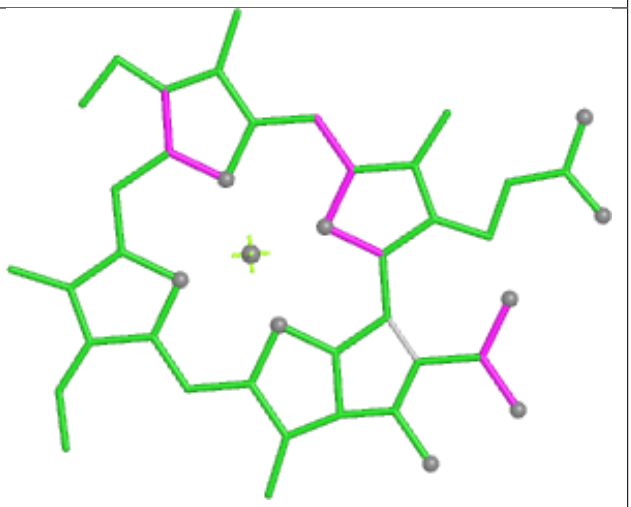


Rings

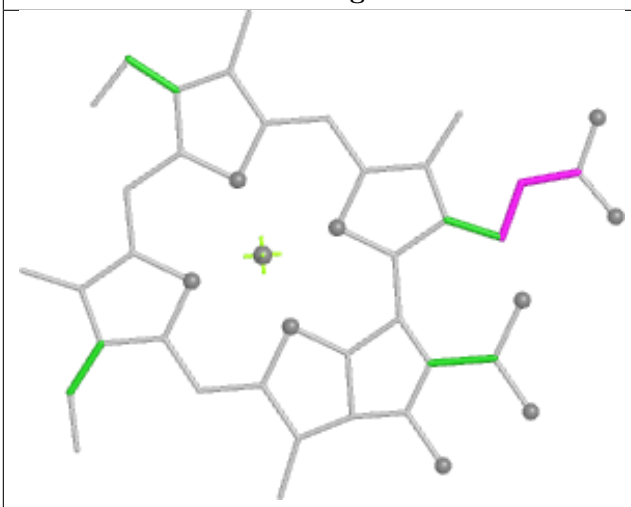
Ligand CLA 2 603



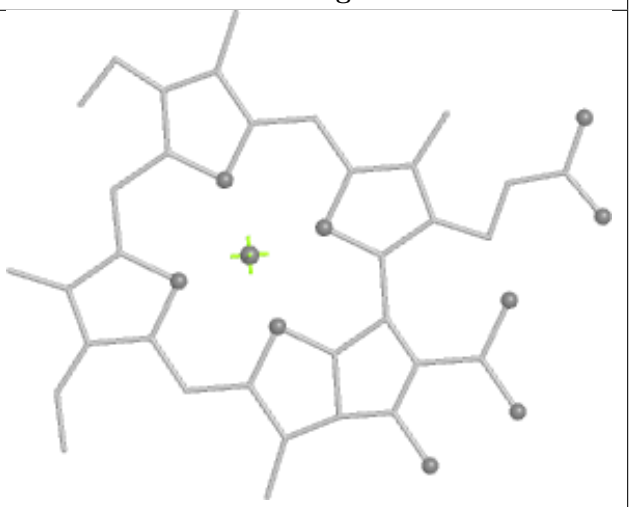
Bond lengths



Bond angles

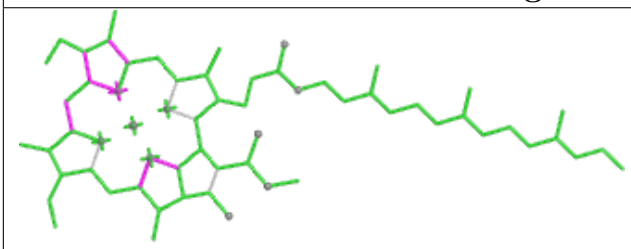


Torsions

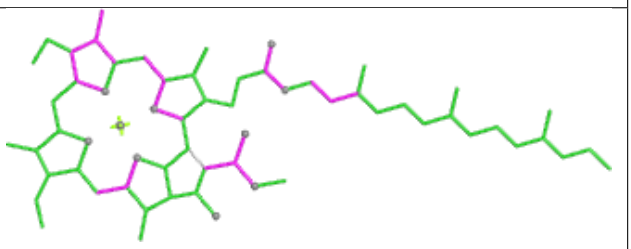


Rings

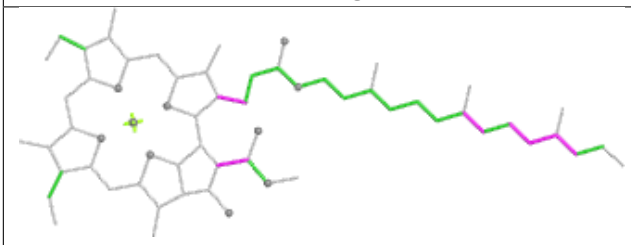
Ligand CLA B 825



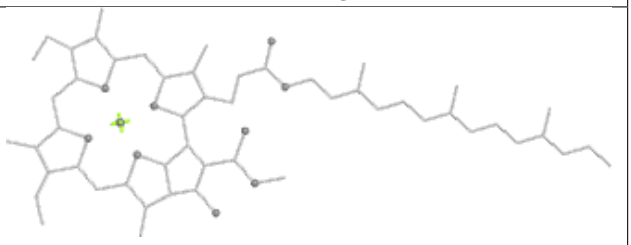
Bond lengths



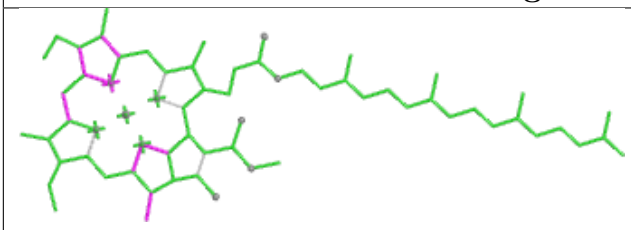
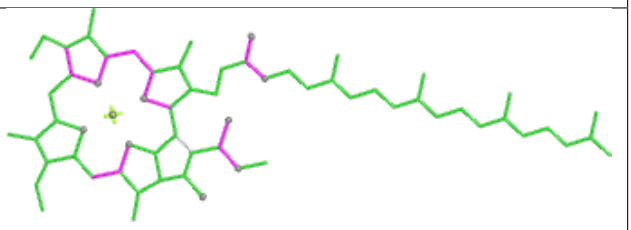
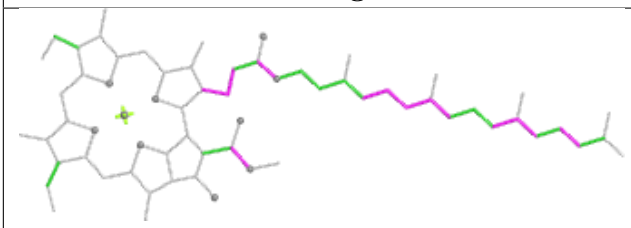
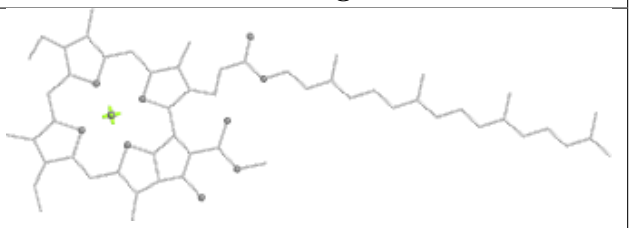
Bond angles

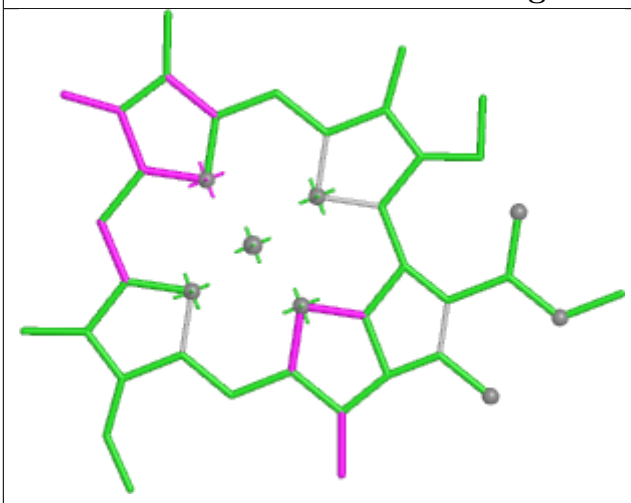
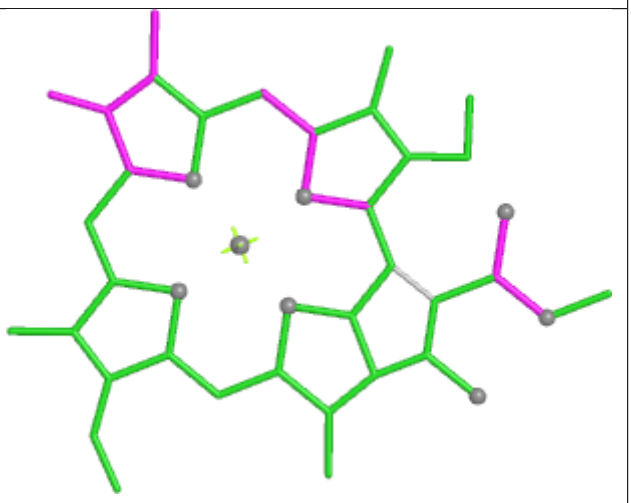
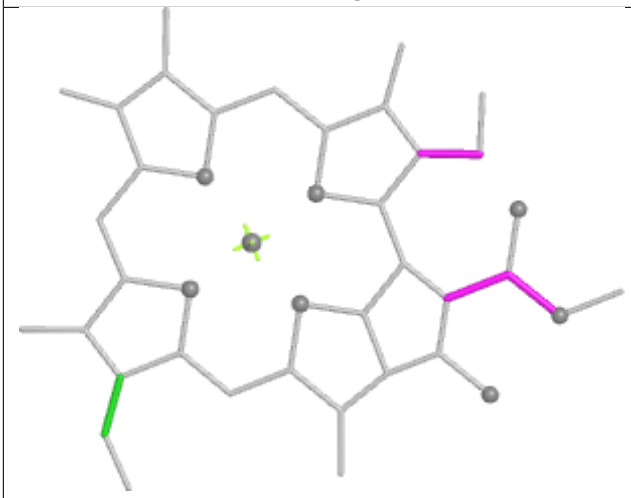
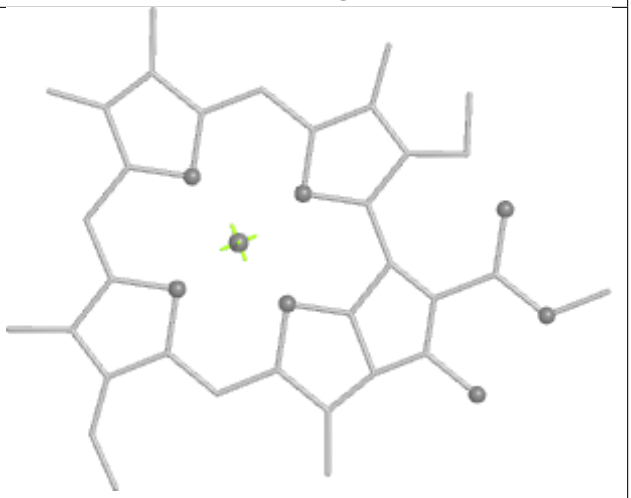


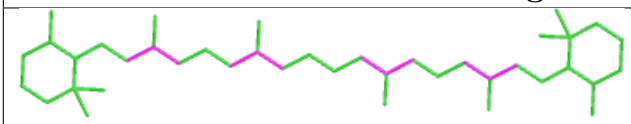
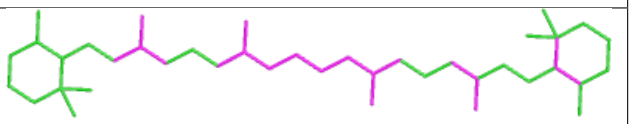
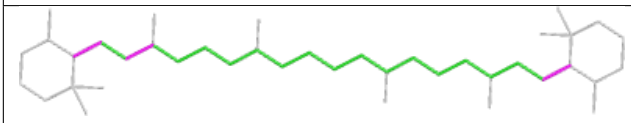
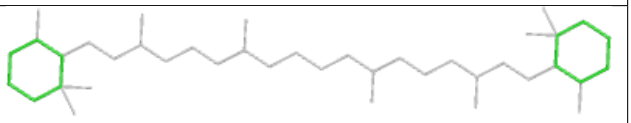
Torsions

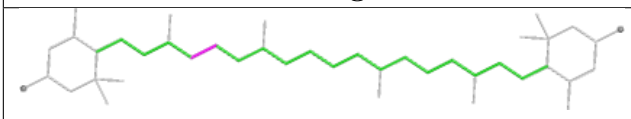
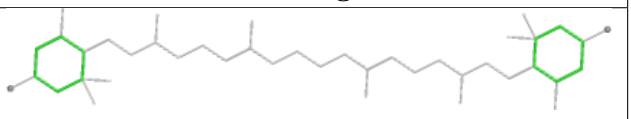


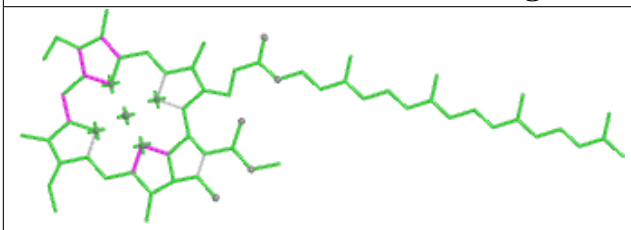
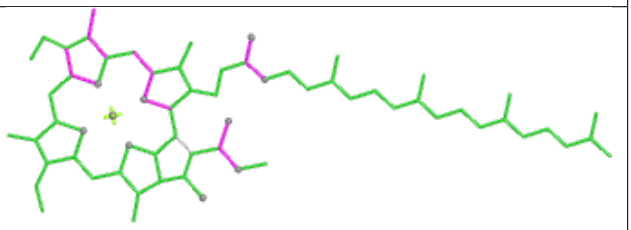
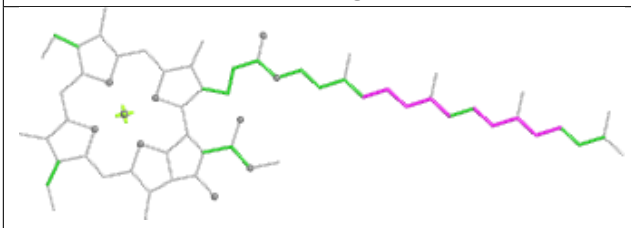
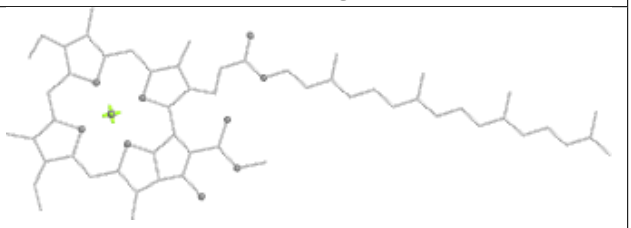
Rings

Ligand CLA A 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

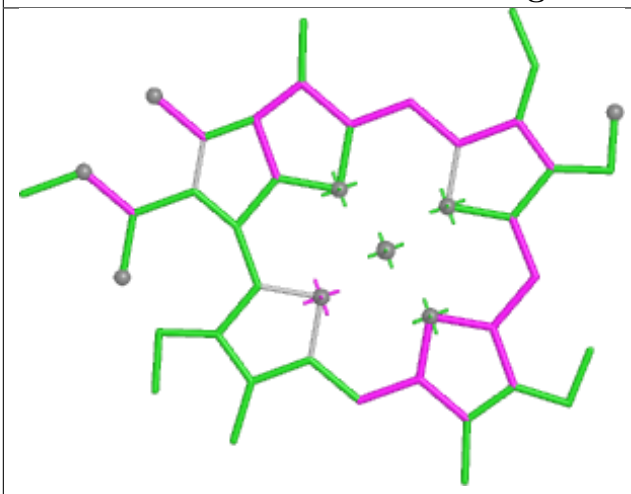
Ligand CLA 3 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR 4 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

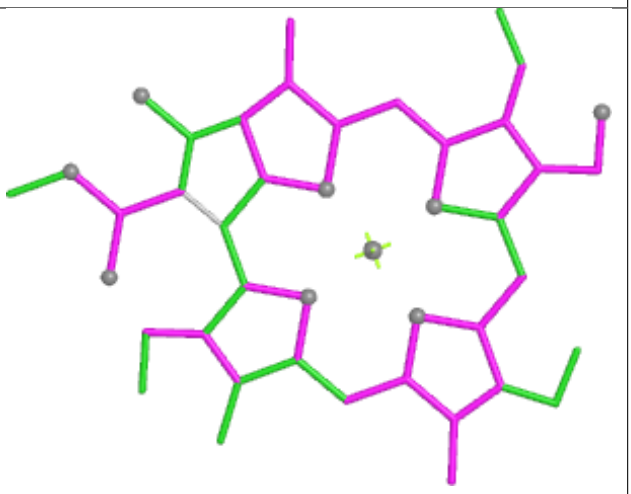
Ligand LUT 1 616	
Bond lengths	Bond angles
 Torsions	 Rings

Ligand CLA A 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

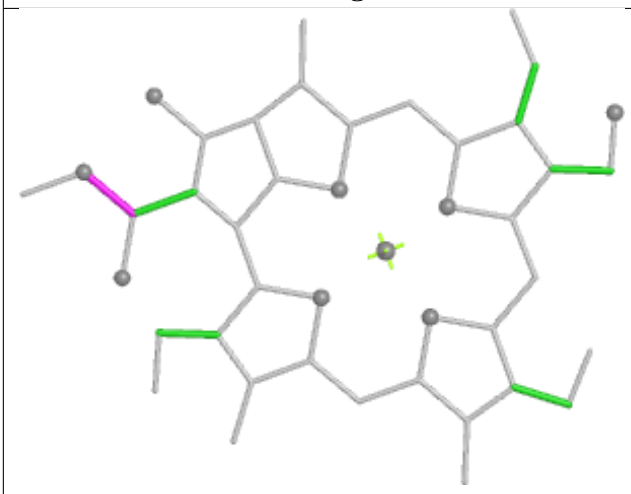
Ligand CHL 2 615



Bond lengths



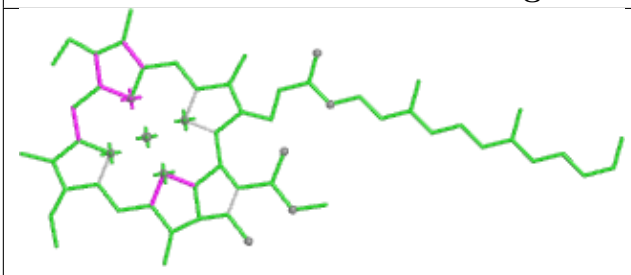
Bond angles



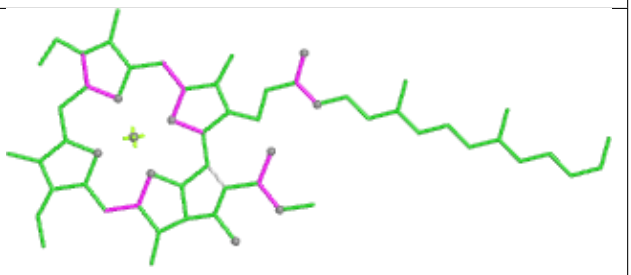
Torsions

Rings

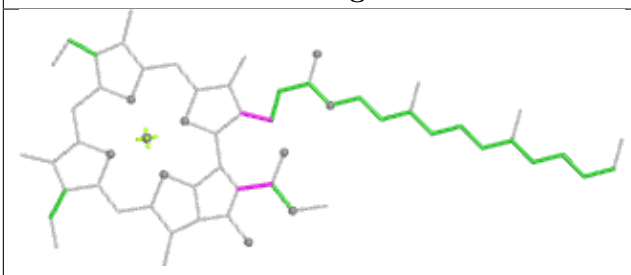
Ligand CLA A 827



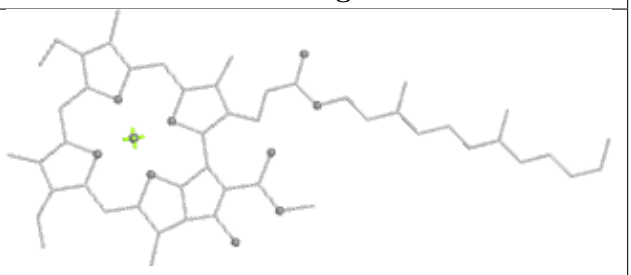
Bond lengths



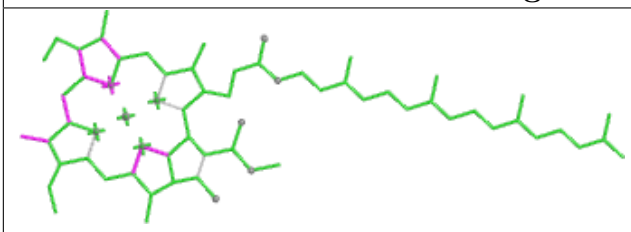
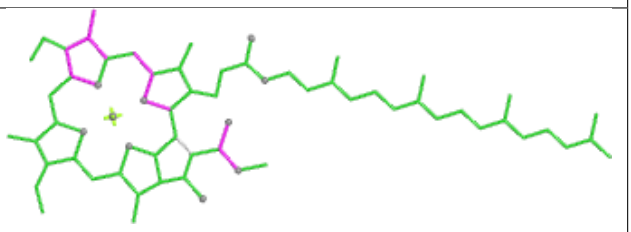
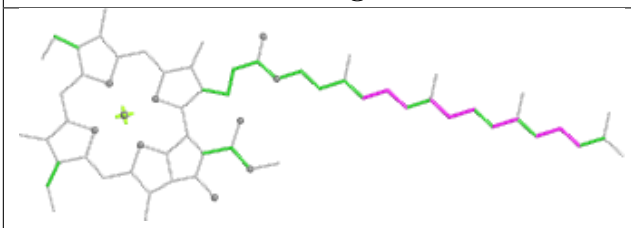
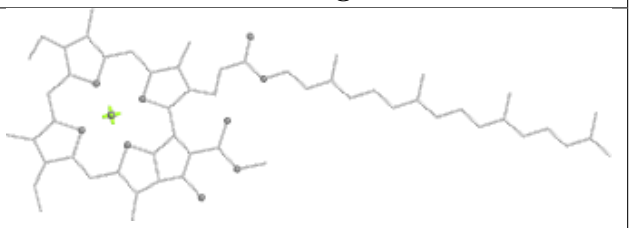
Bond angles

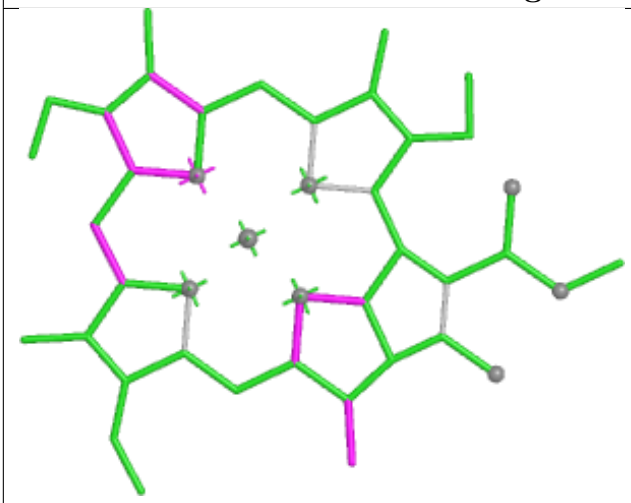
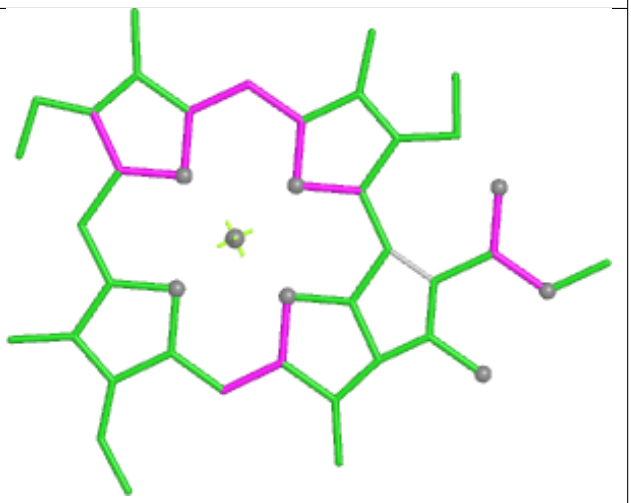
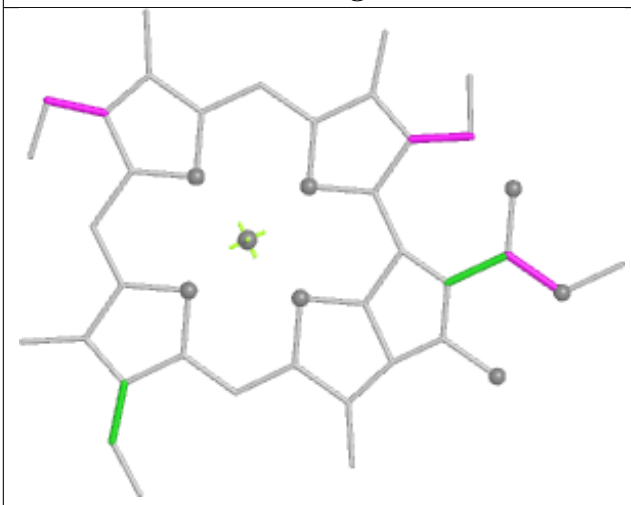
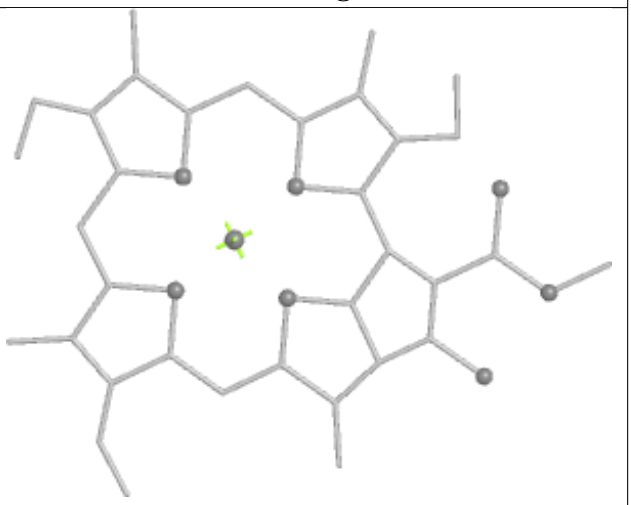


Torsions



Rings

Ligand CLA A 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

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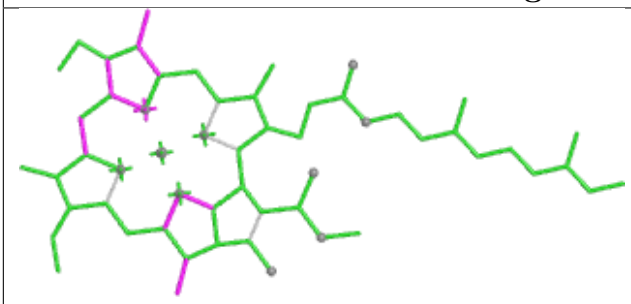
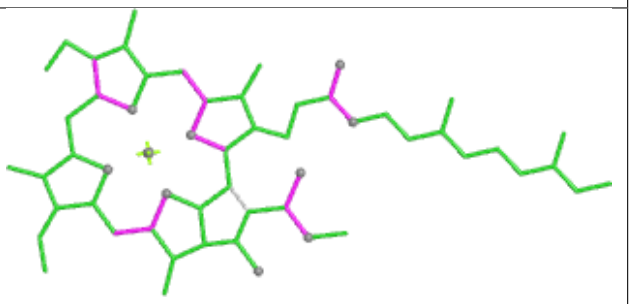
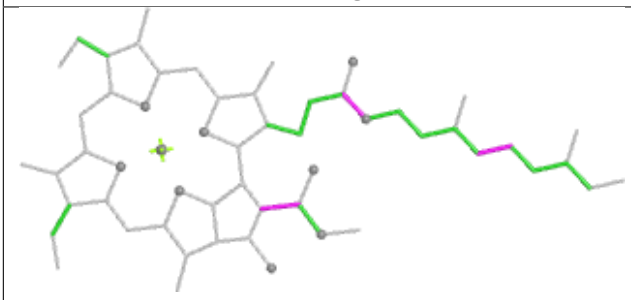
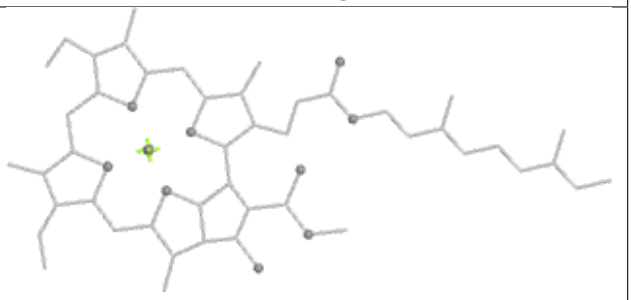
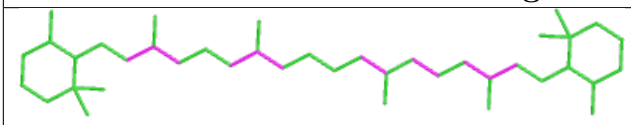
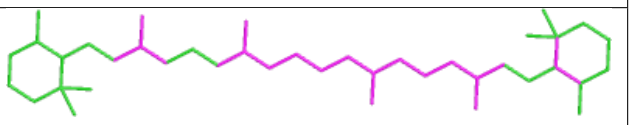
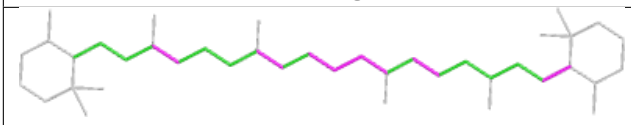
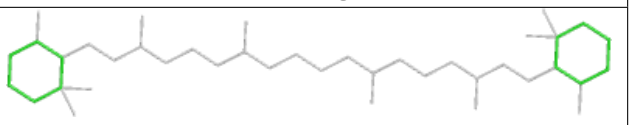
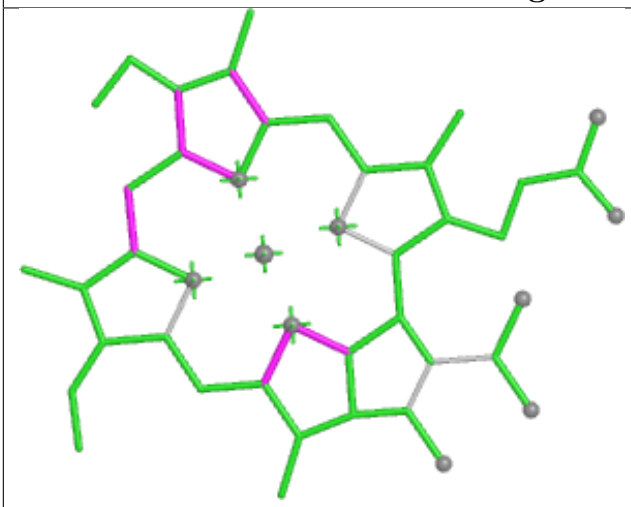
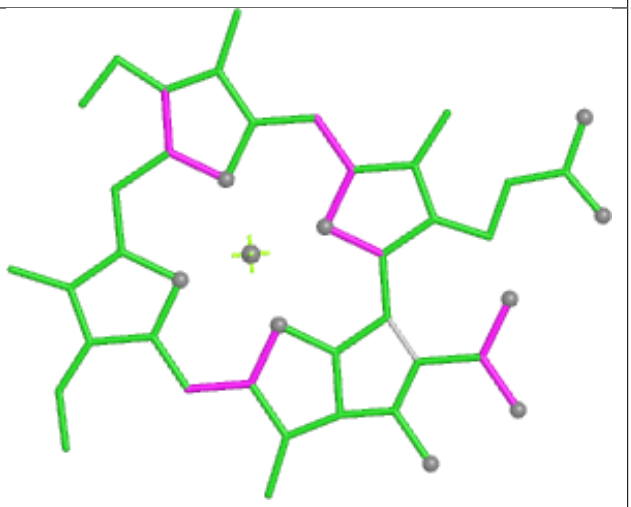
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

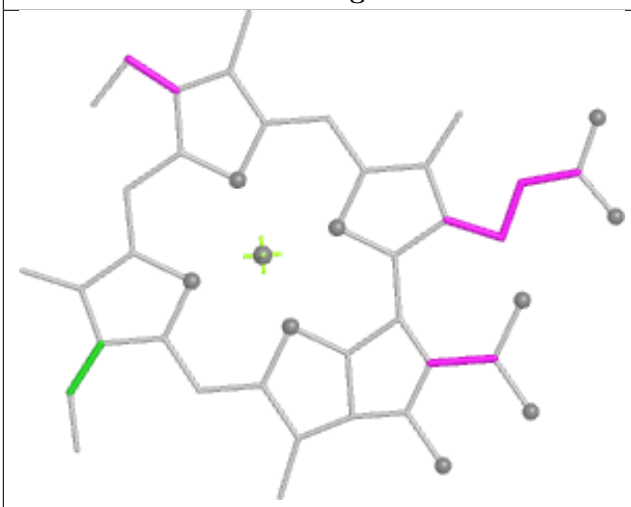
Ligand CLA 1 607



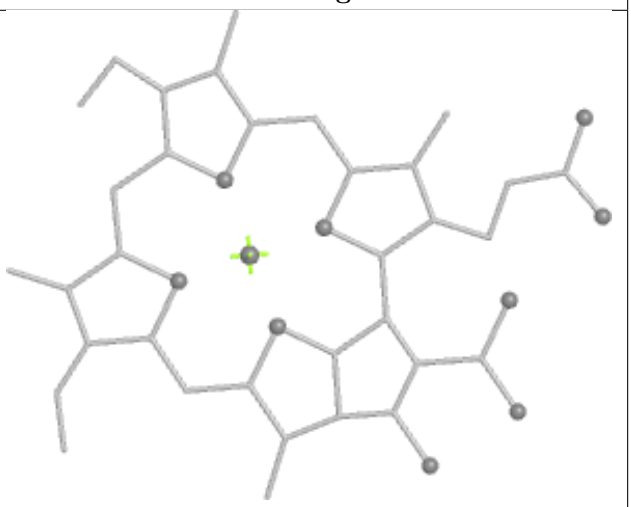
Bond lengths



Bond angles

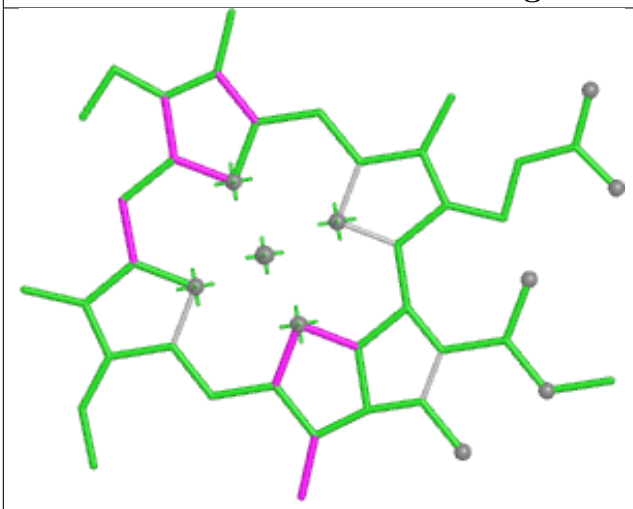


Torsions

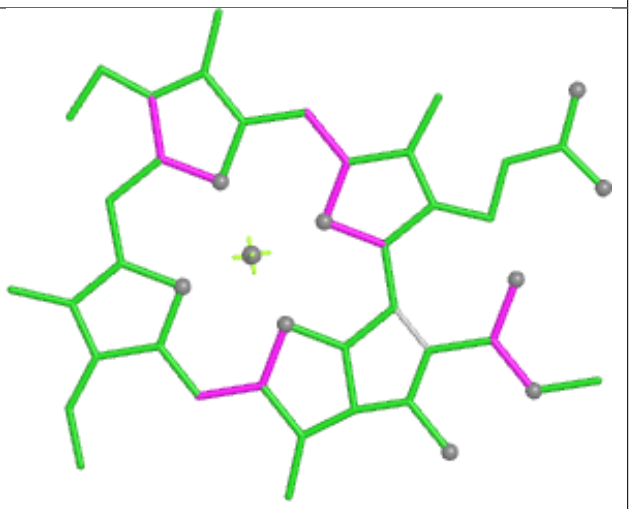


Rings

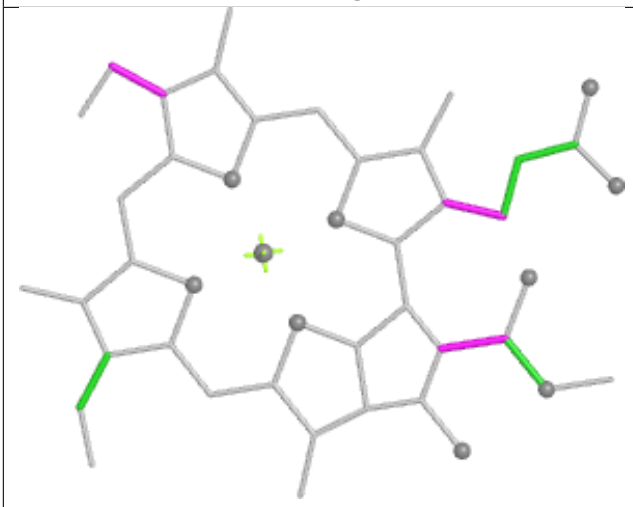
Ligand CLA A 817



Bond lengths



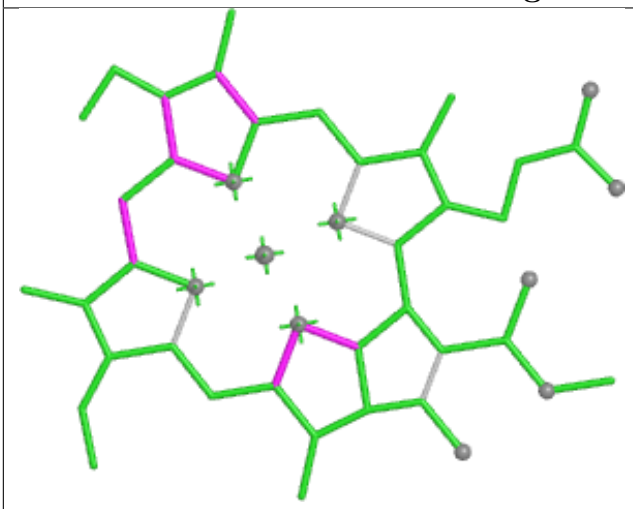
Bond angles



Torsions

Rings

Ligand CLA A 821



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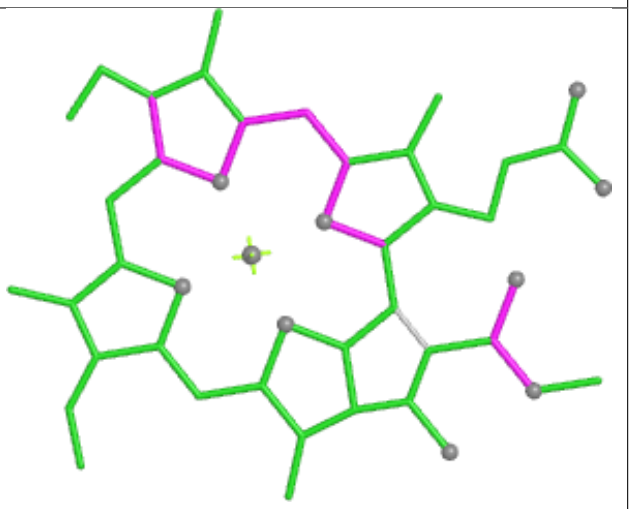
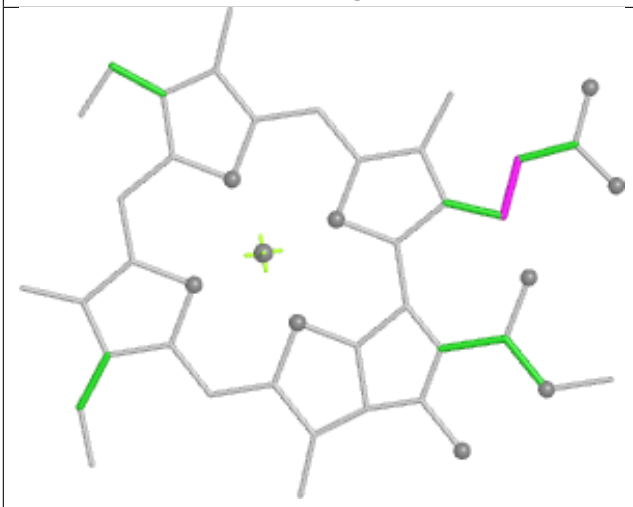


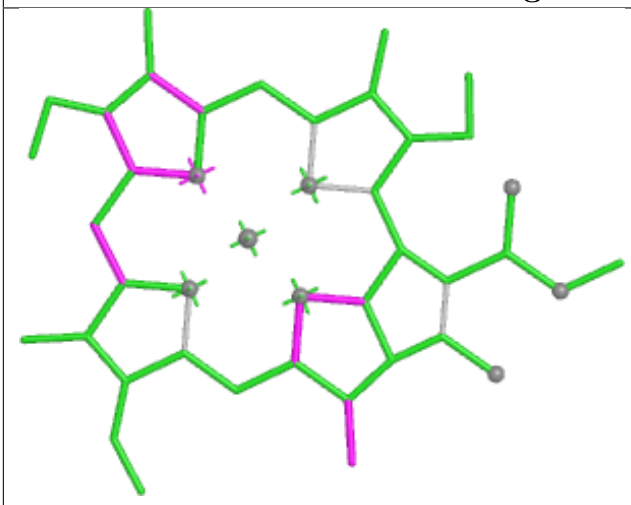
Bond angles



Torsions

Rings

Ligand CLA A 816



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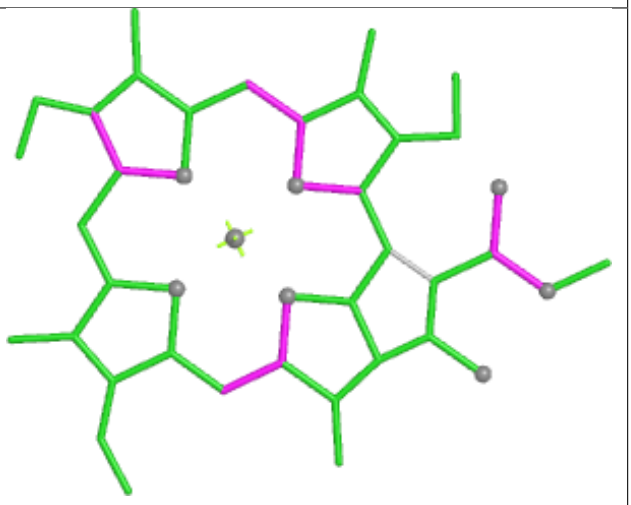
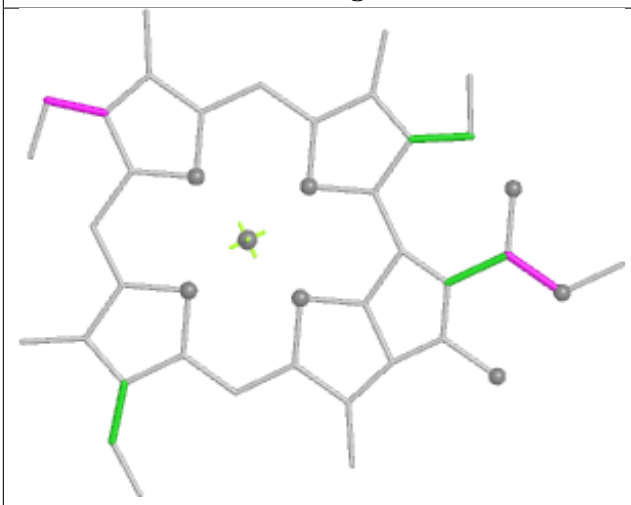


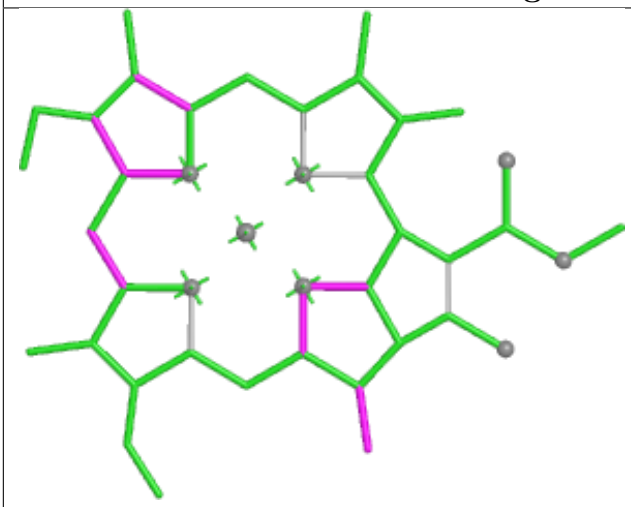
Bond angles



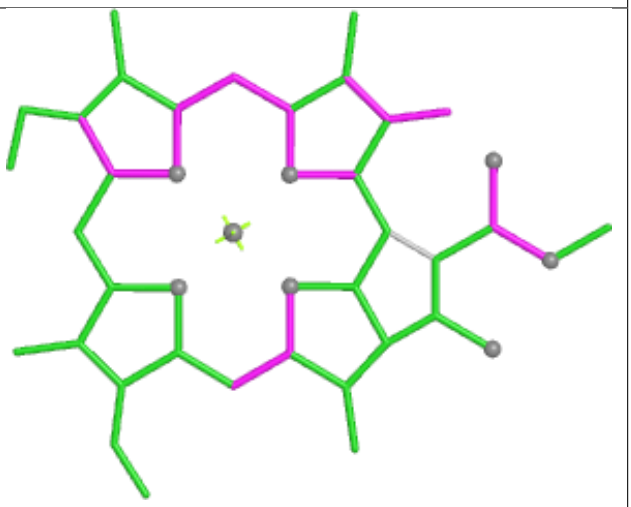
Torsions

Rings

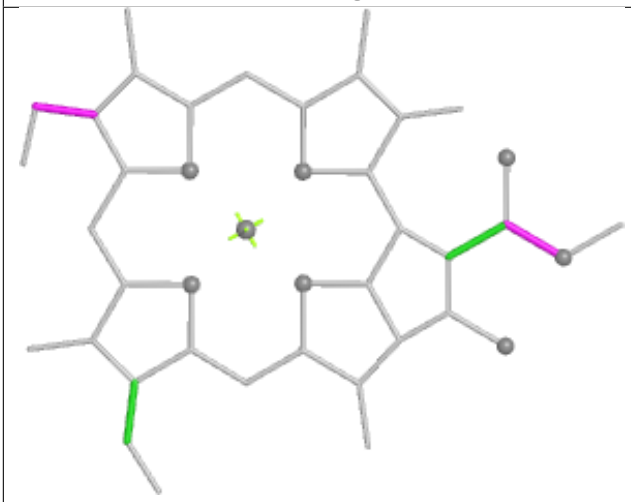
Ligand CLA A 824



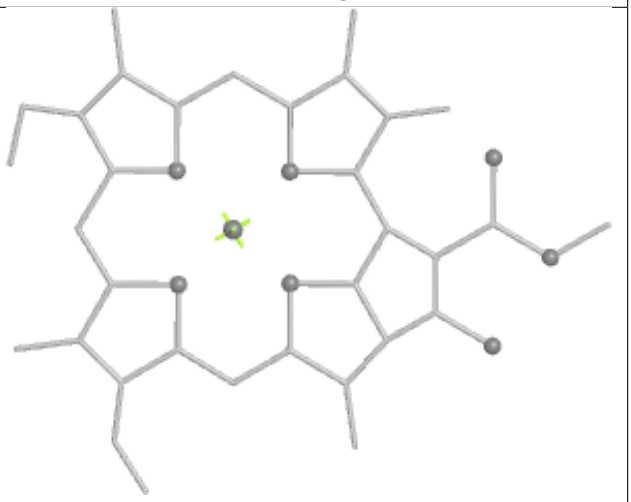
Bond lengths



Bond angles

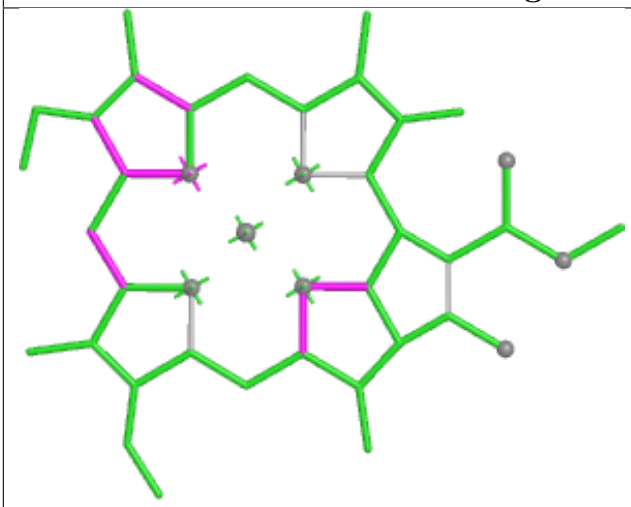


Torsions



Rings

Ligand CLA B 804



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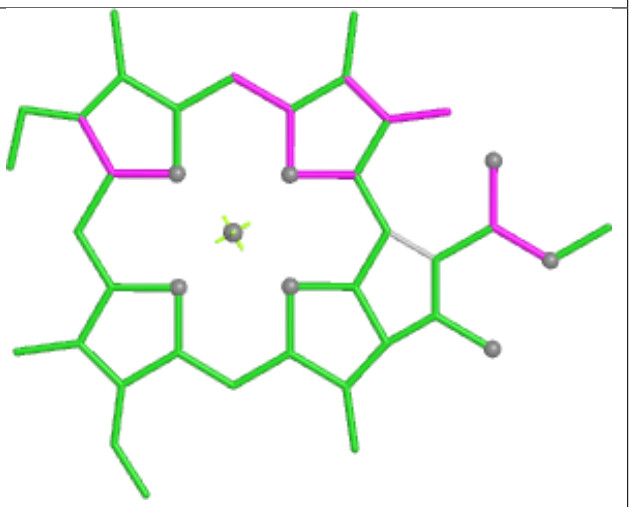
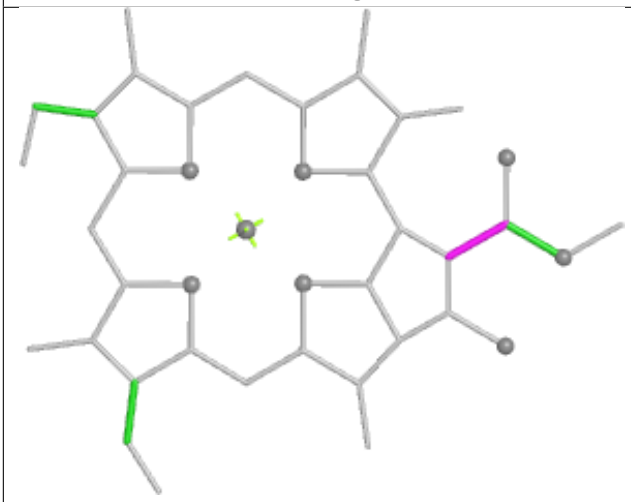


Bond angles



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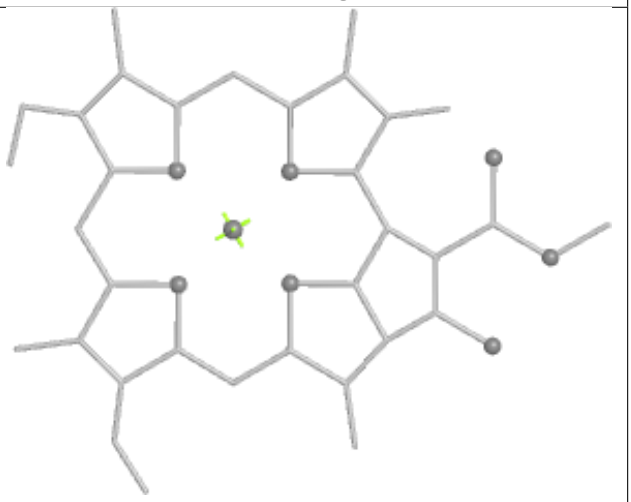
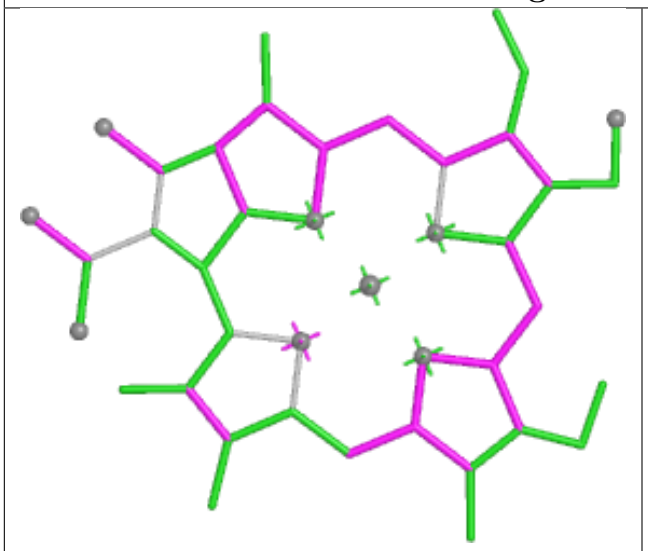


Rings

Ligand CHL 1 606



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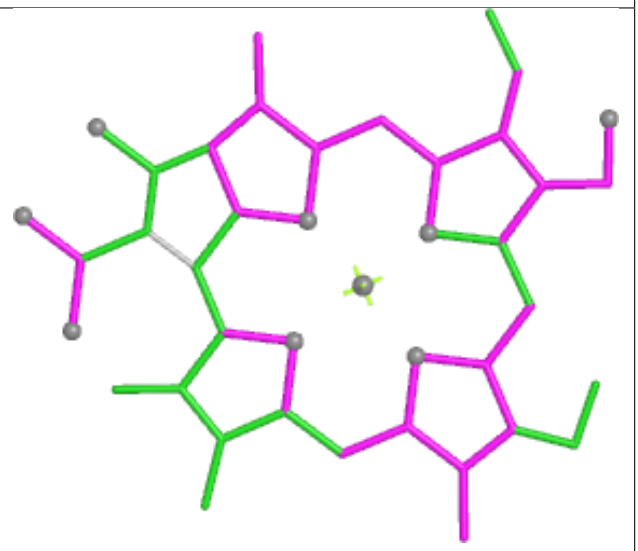
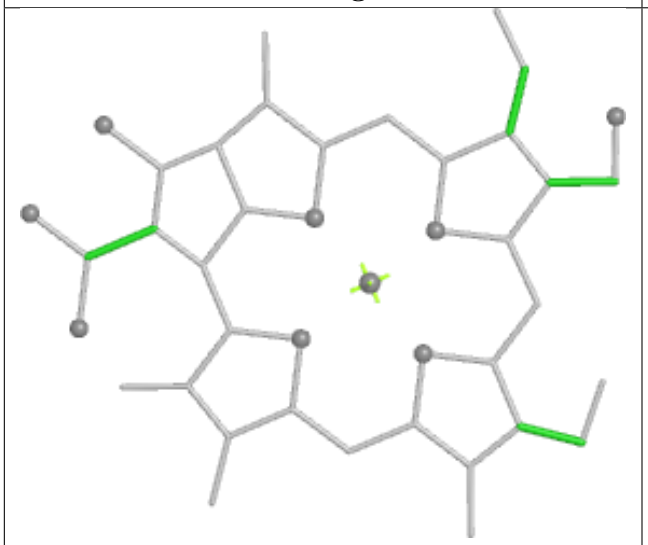


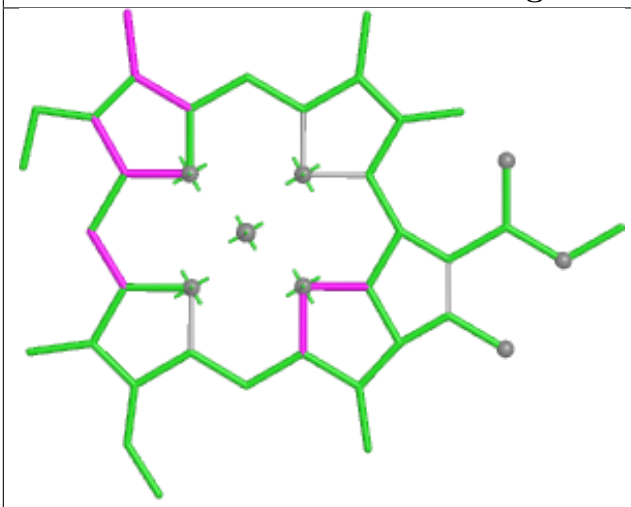
Bond angles



Torsions

Rings

Ligand CLA F 303



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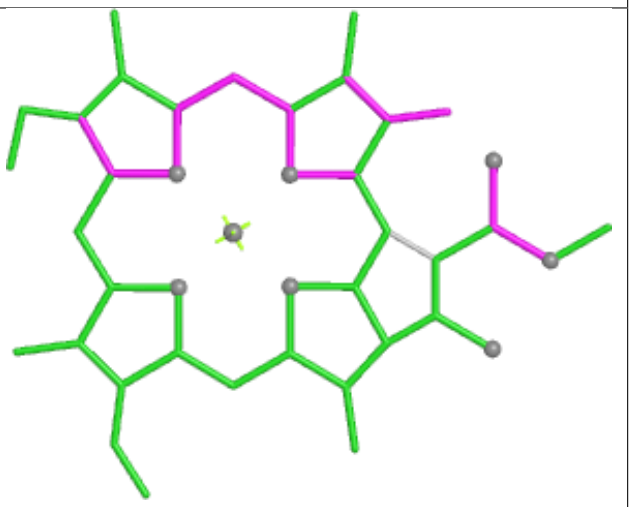
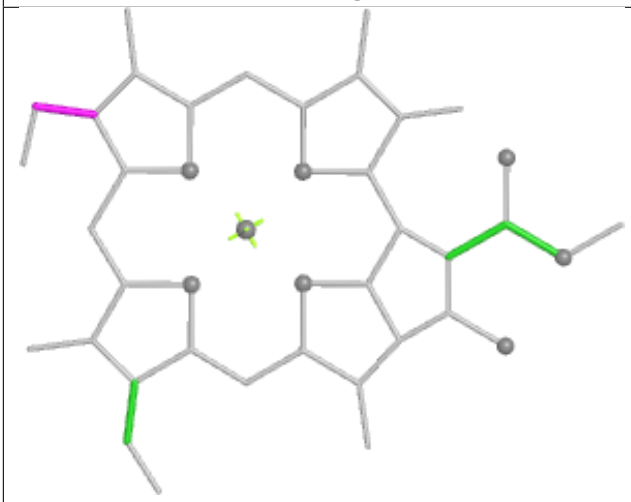


Bond angles



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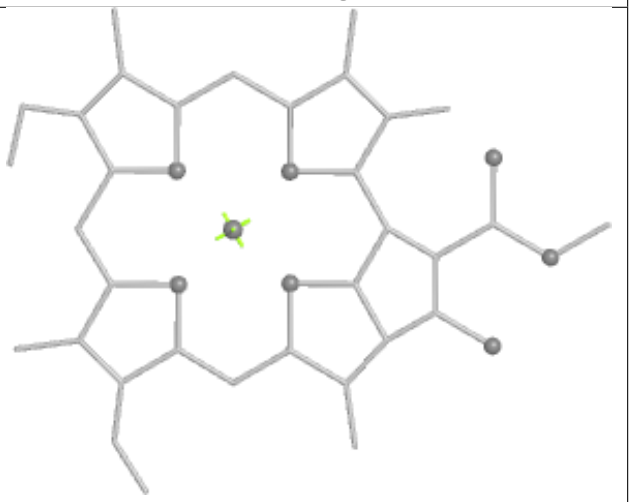

Rings

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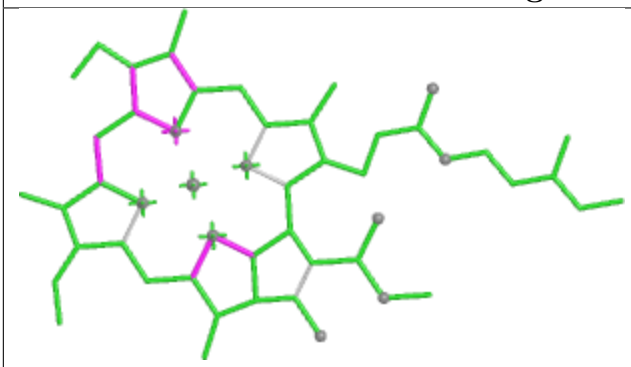

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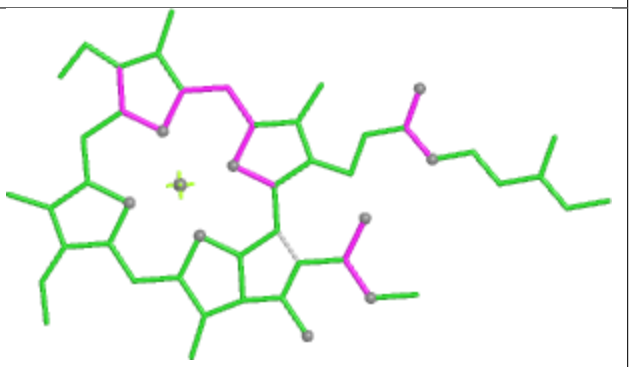
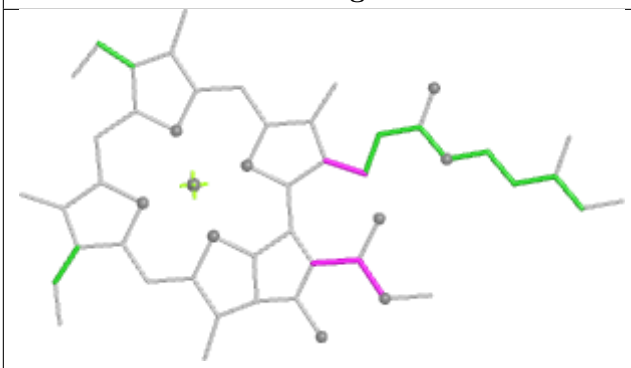


Bond angles



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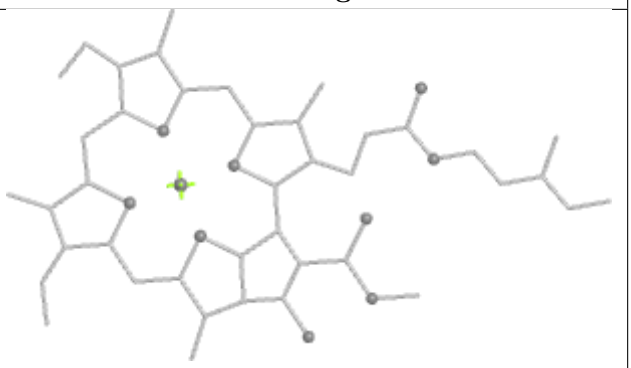
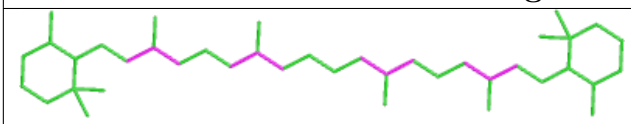


Rings

Ligand BCR L 305



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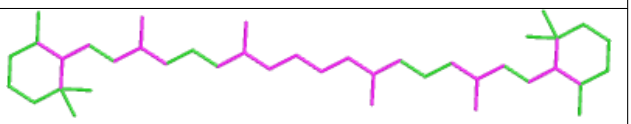
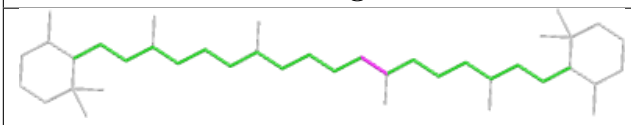


Bond angles



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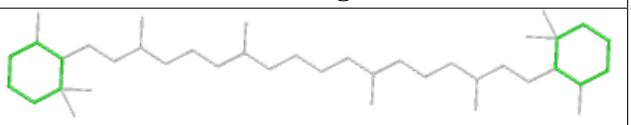
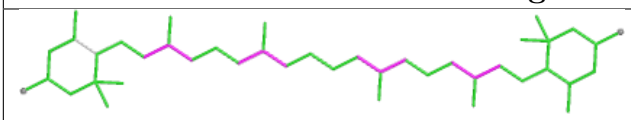


Rings

Ligand LUT 2 619



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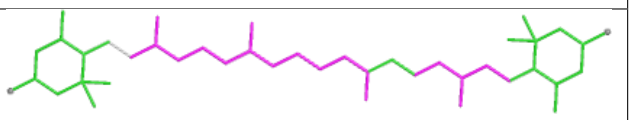
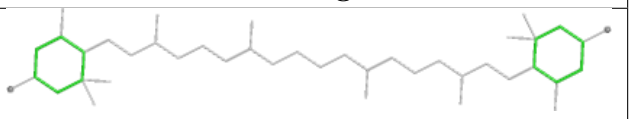


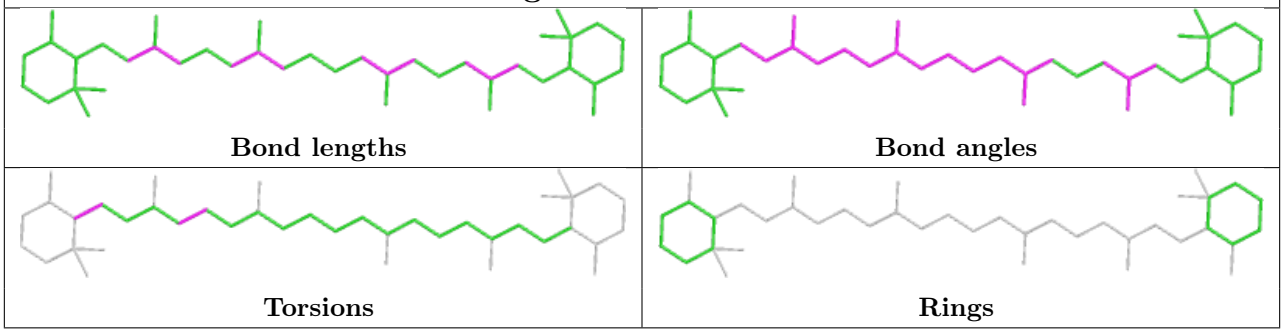
Bond angles

Torsions

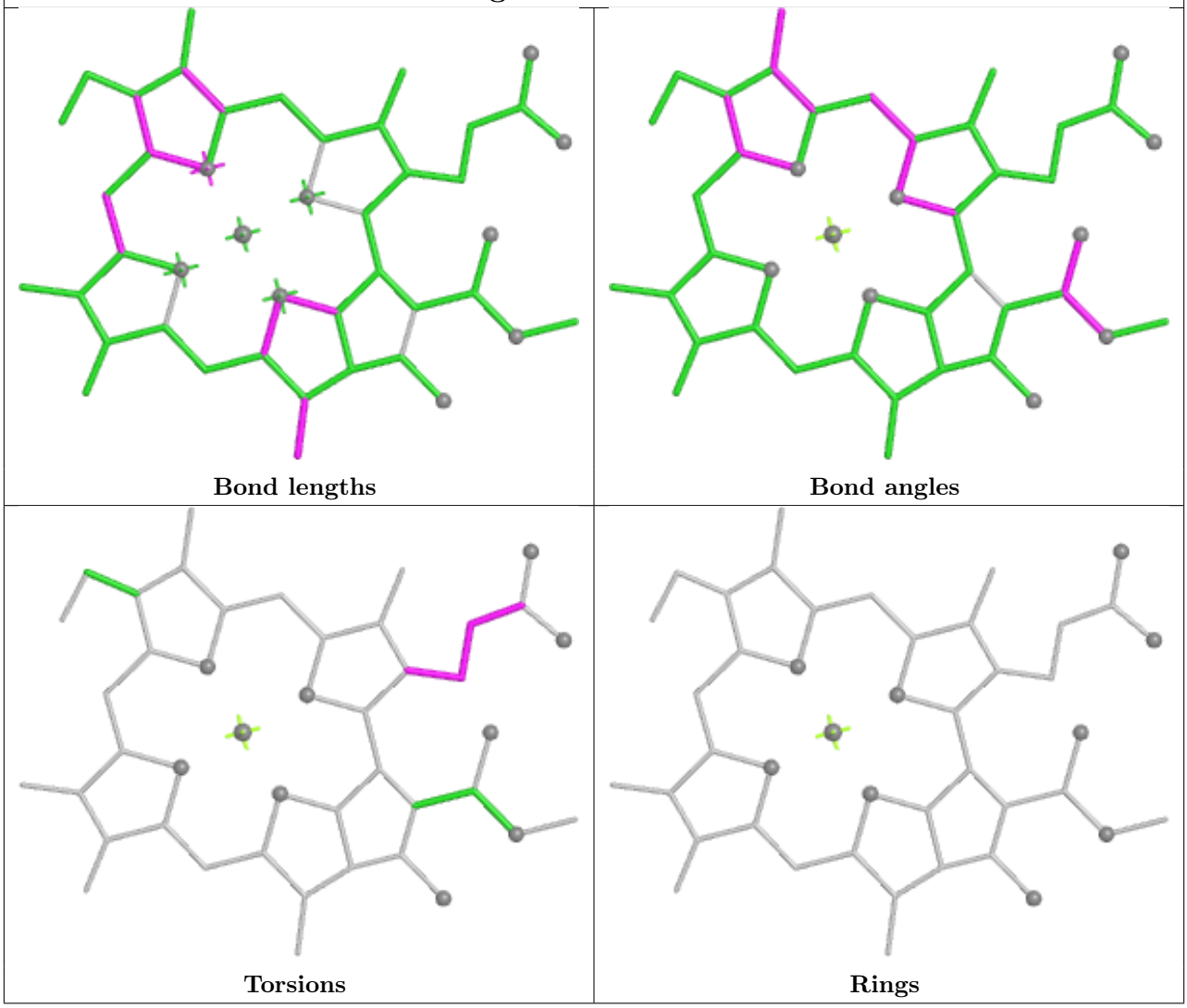


Rings

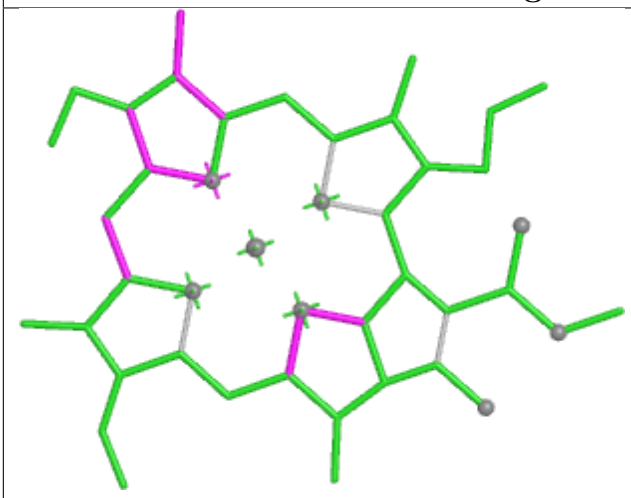
Ligand BCR B 801



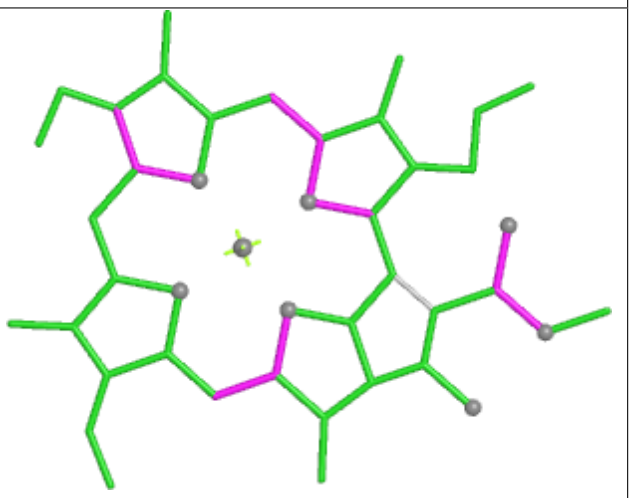
Ligand CLA 2 611



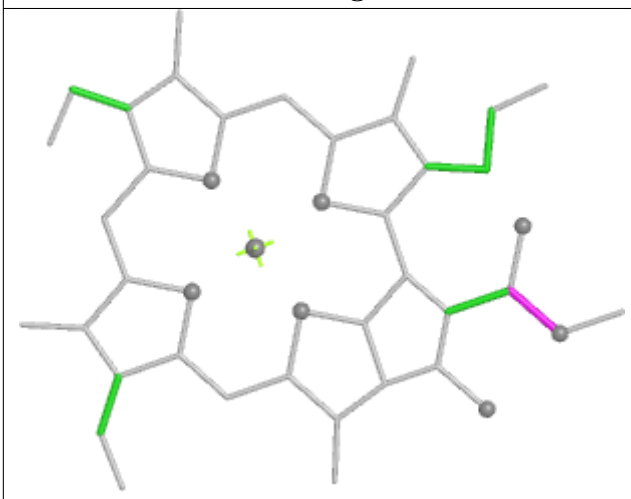
Ligand CLA B 830



Bond lengths



Bond angles



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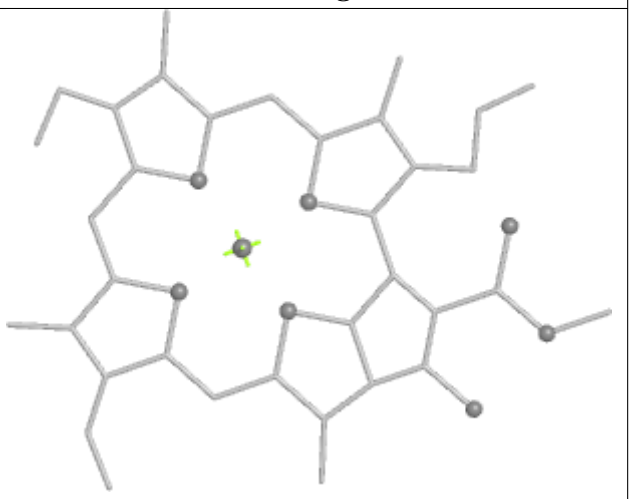
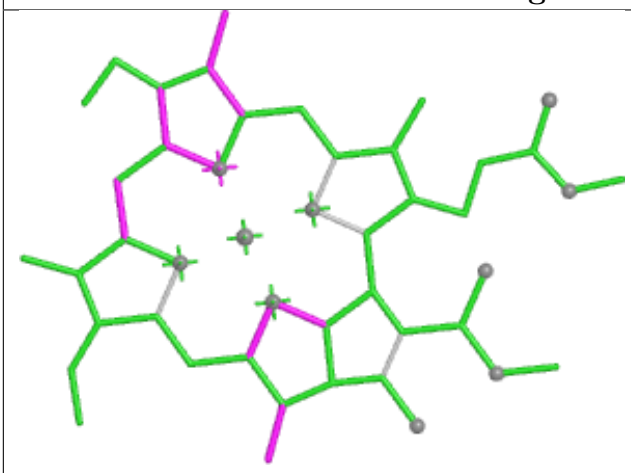


Rings

Ligand CLA 1 612



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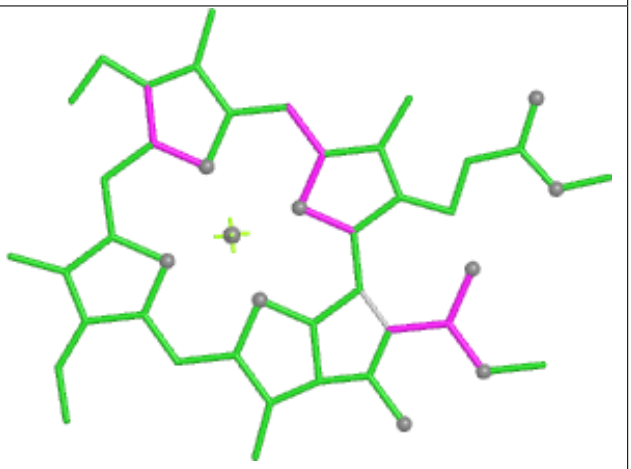
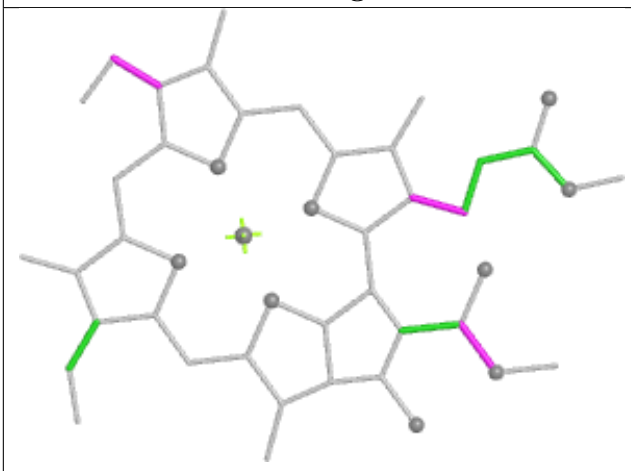
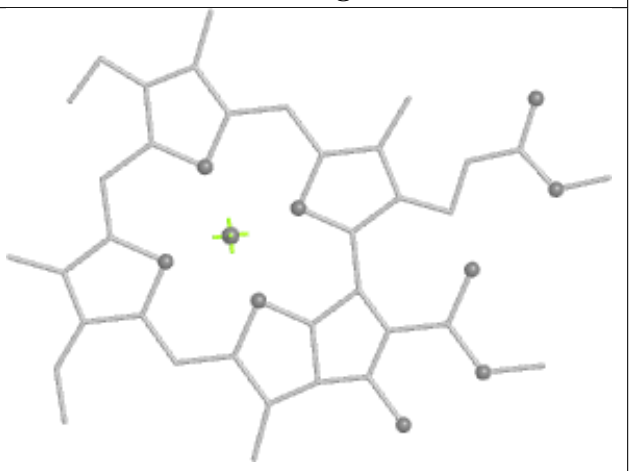


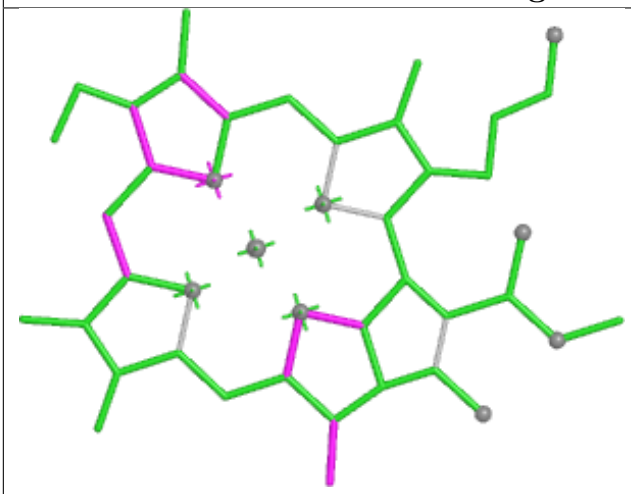
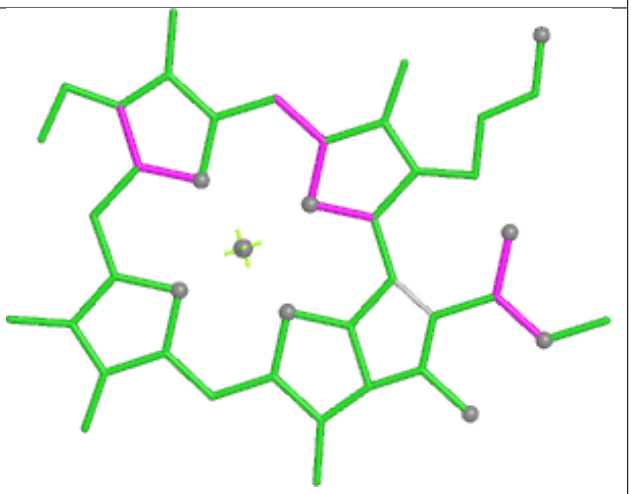
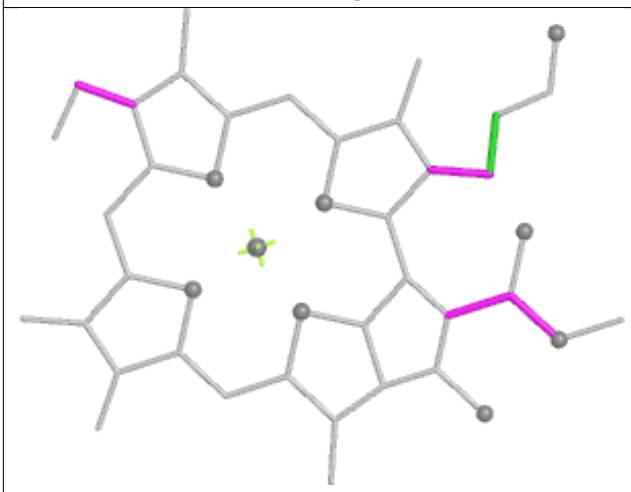
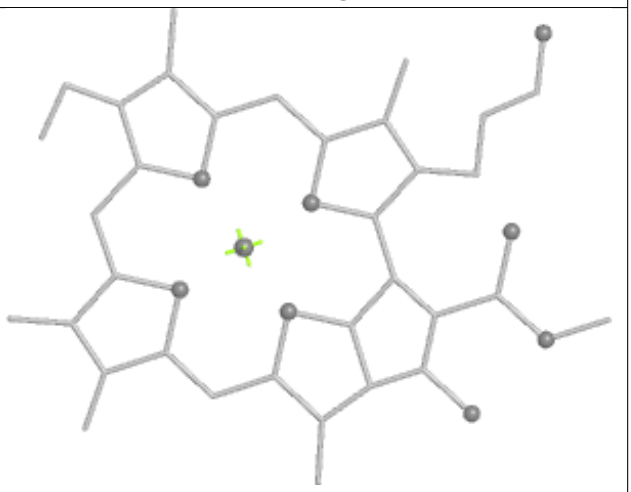
Bond angles



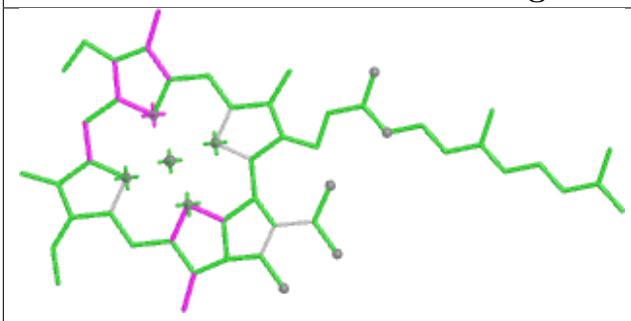
Torsions



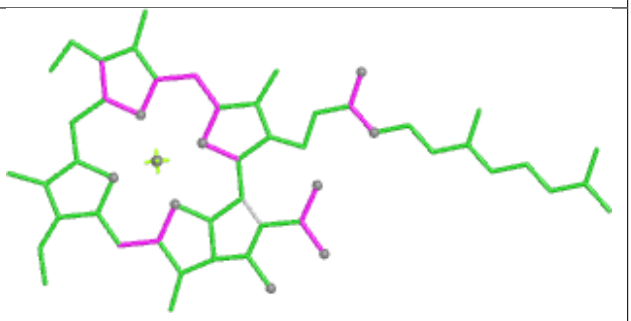
Rings

Ligand CLA 2 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

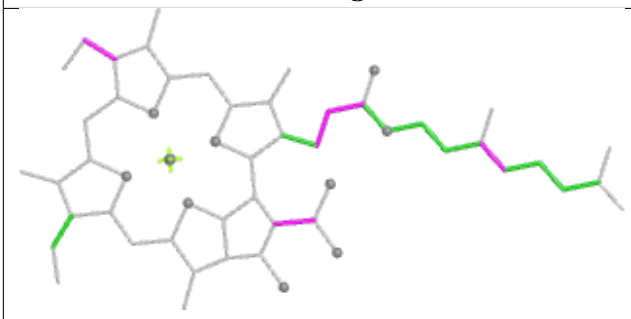
Ligand CLA 3 609



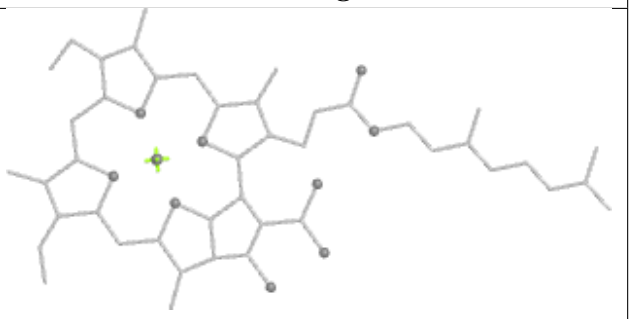
Bond lengths



Bond angles

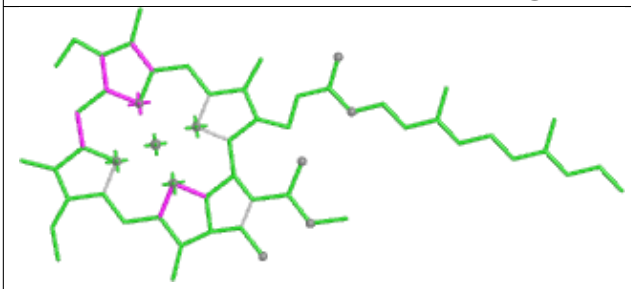


Torsions

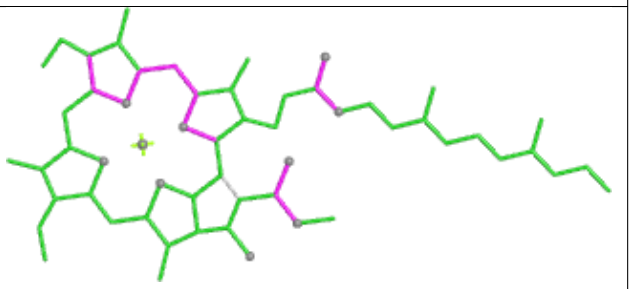


Rings

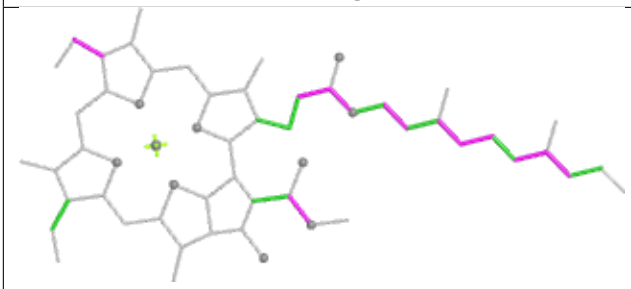
Ligand CLA F 301



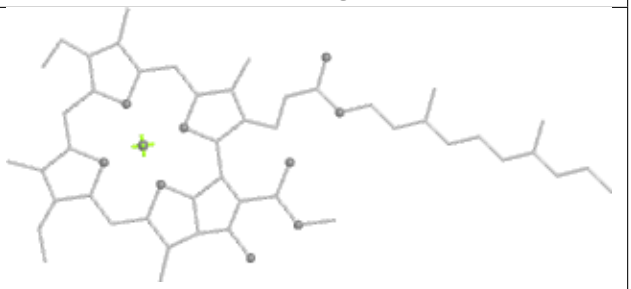
Bond lengths



Bond angles

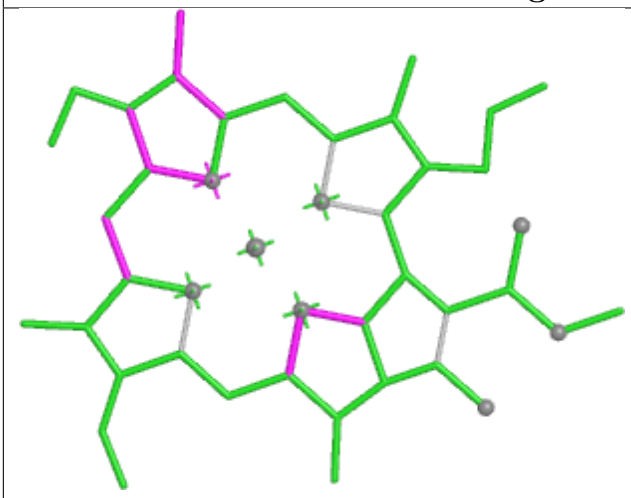


Torsions

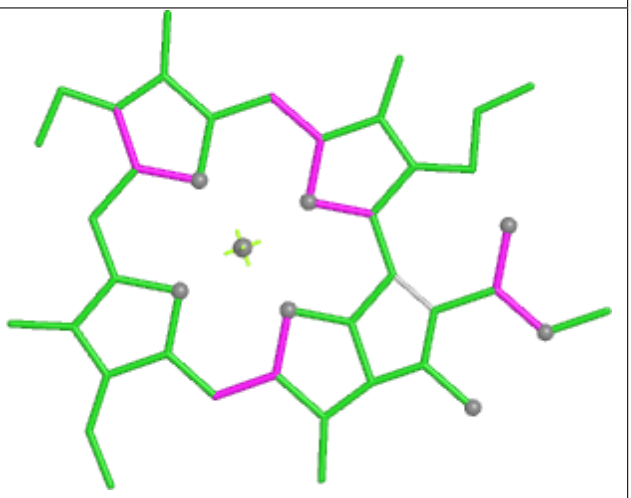


Rings

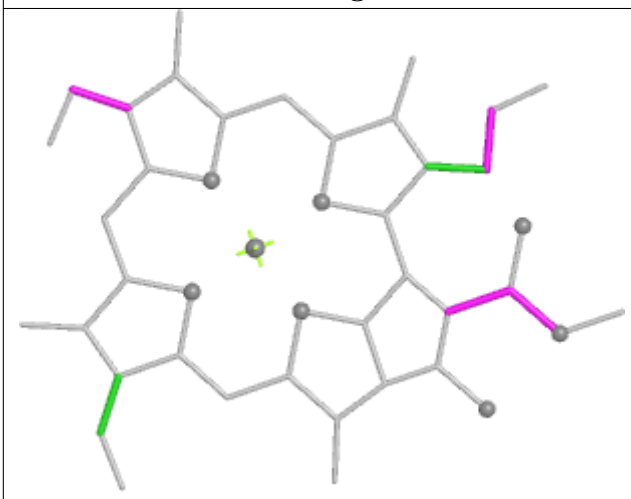
Ligand CLA 2 613



Bond lengths



Bond angles



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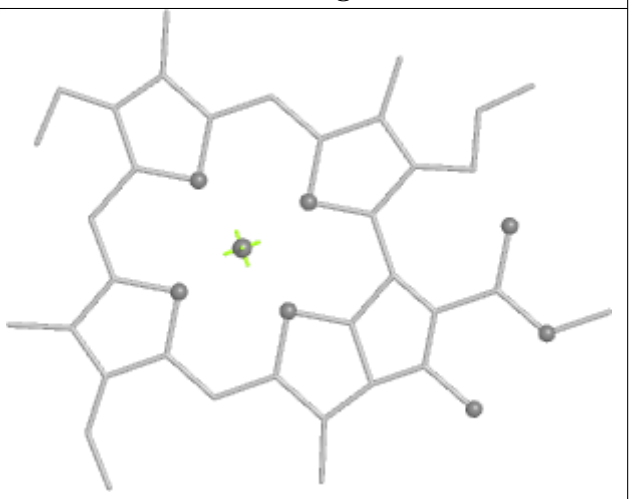
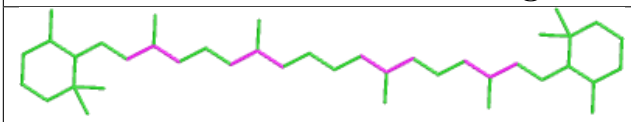
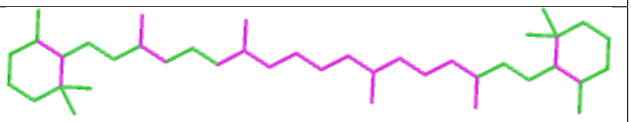


Rings

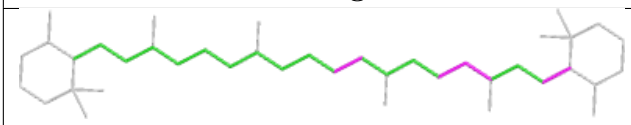
Ligand BCR A 849



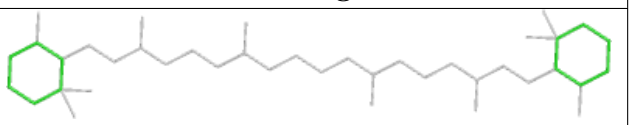
Bond lengths



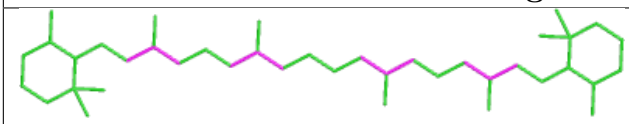
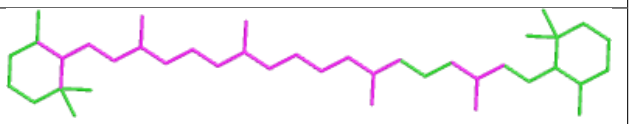
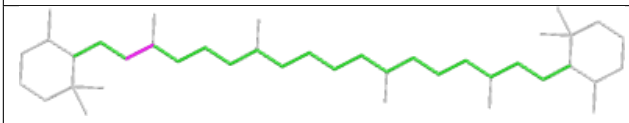
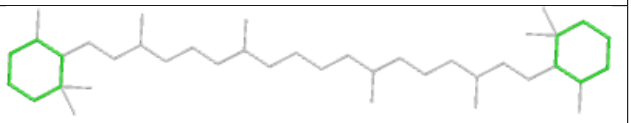
Bond angles

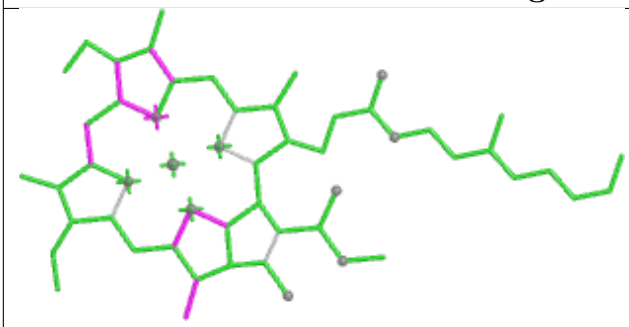
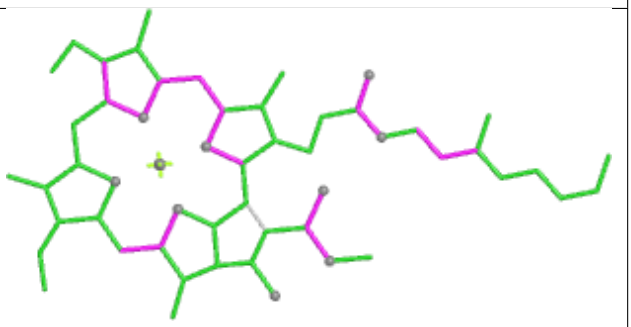
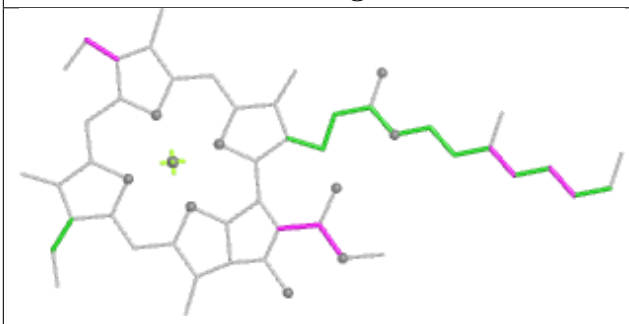
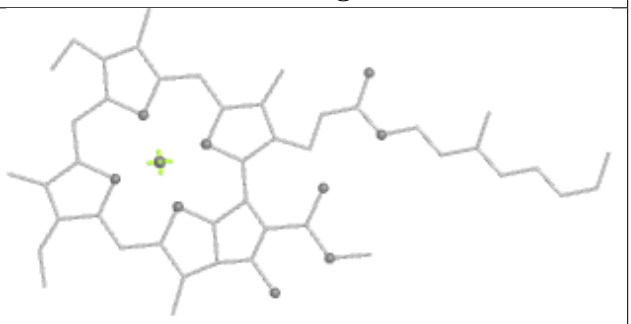


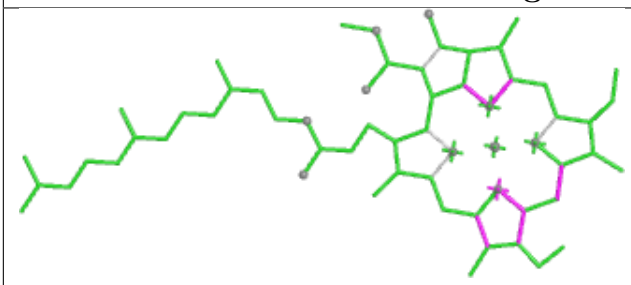
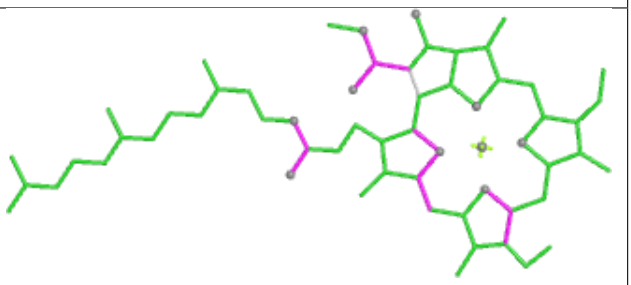
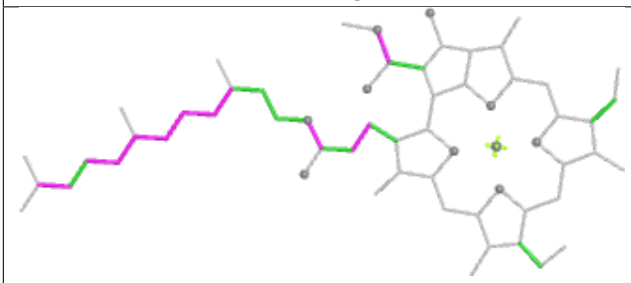
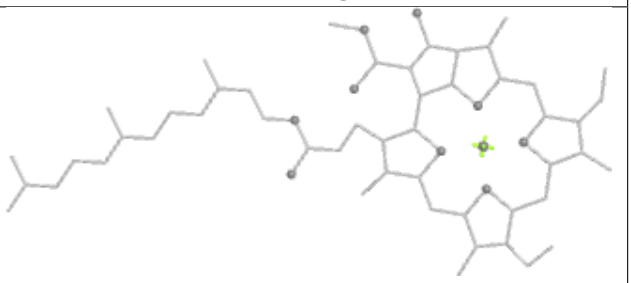
Torsions



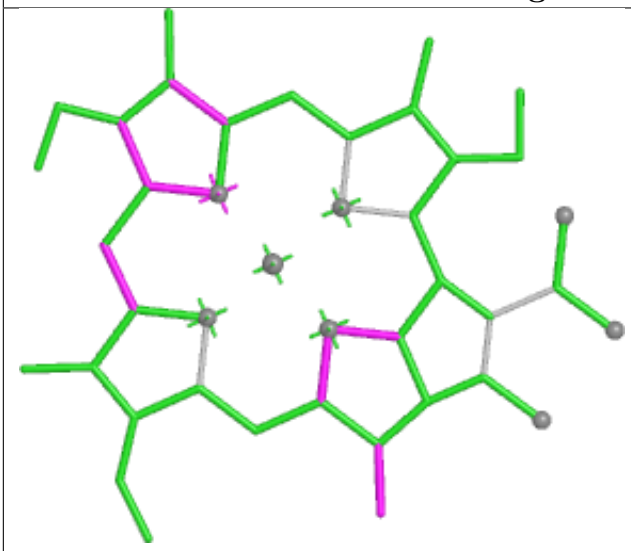
Rings

Ligand BCR J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

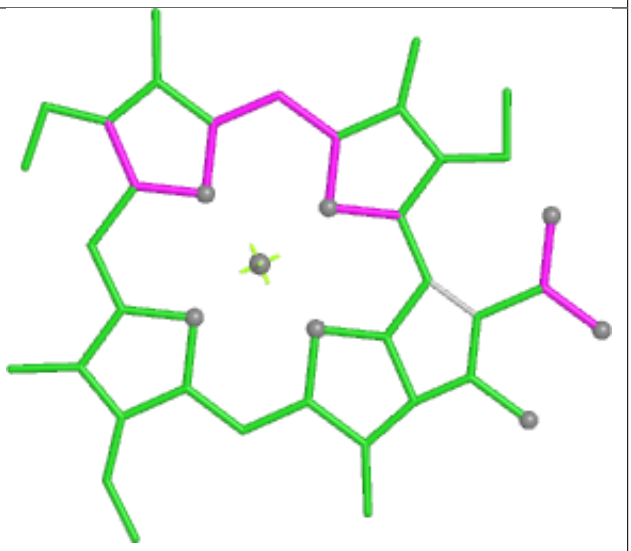
Ligand CLA 4 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

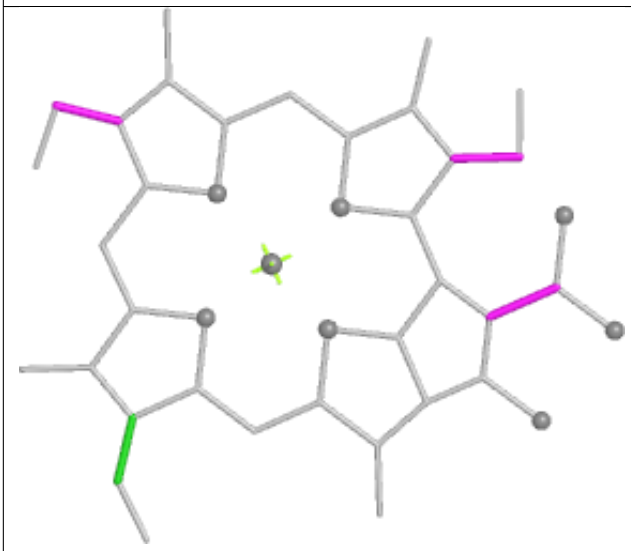
Ligand CLA 4 611



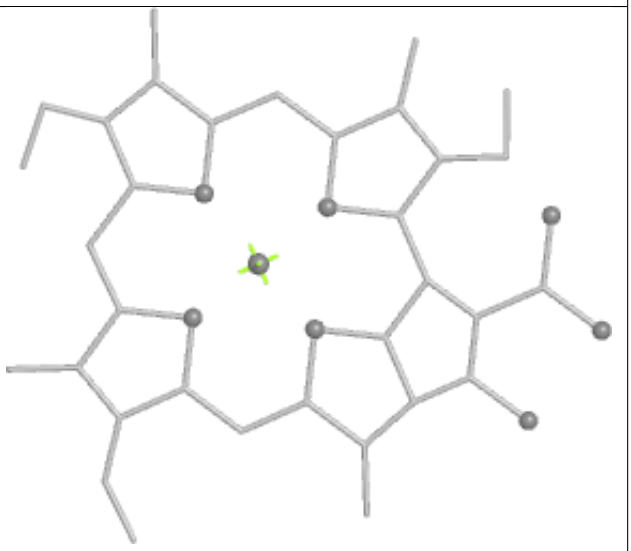
Bond lengths



Bond angles

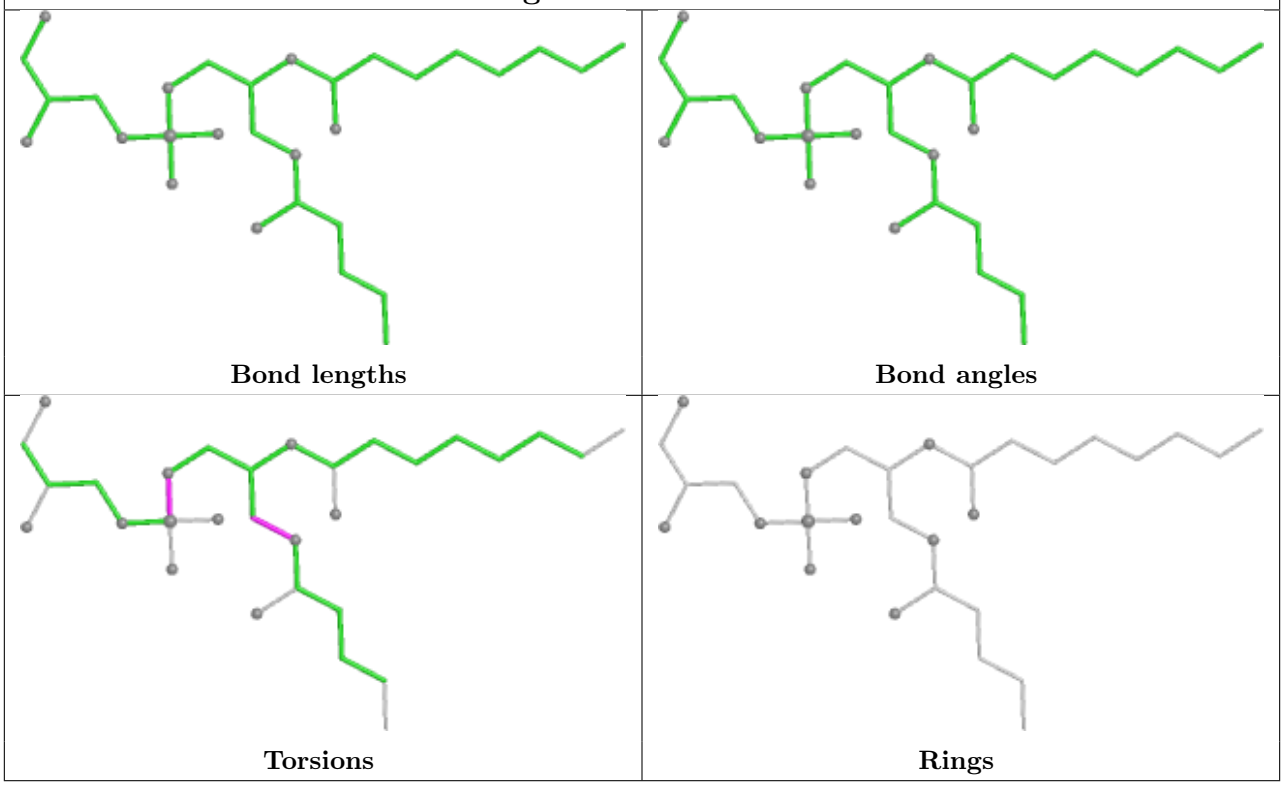


Torsions

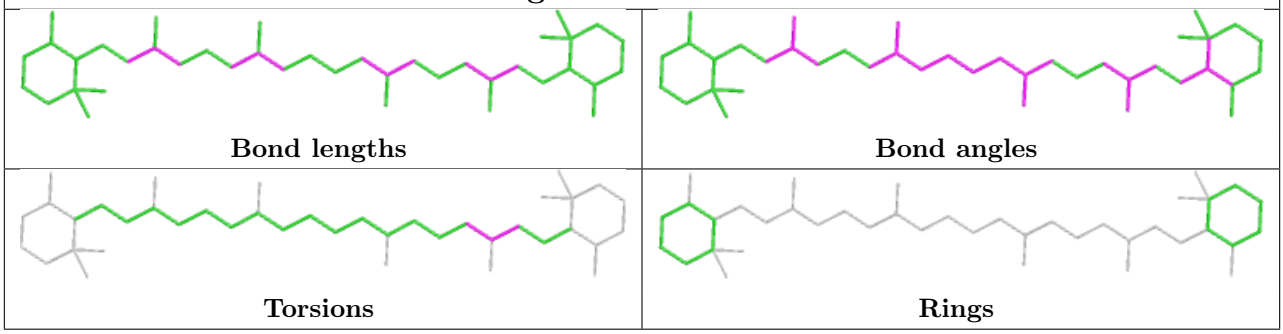


Rings

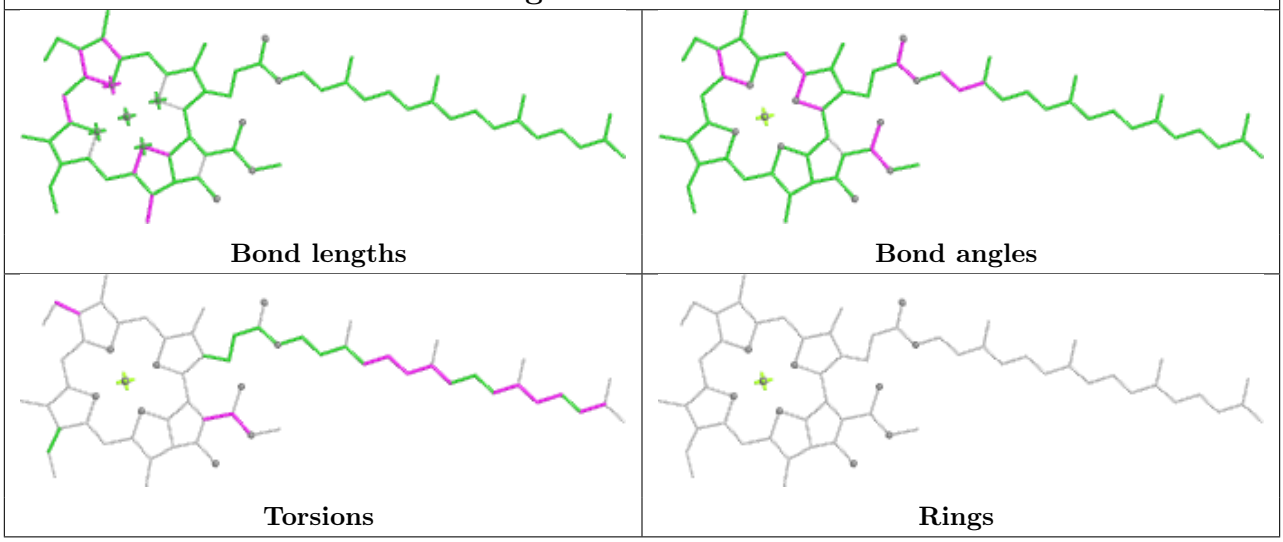
Ligand LHG A 847

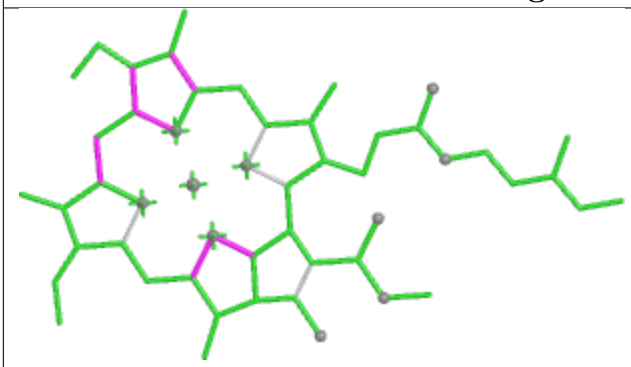
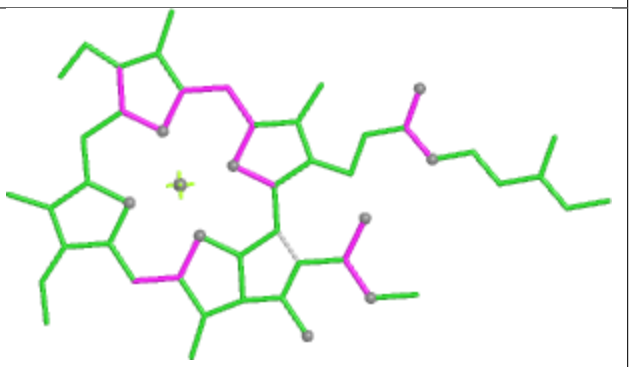
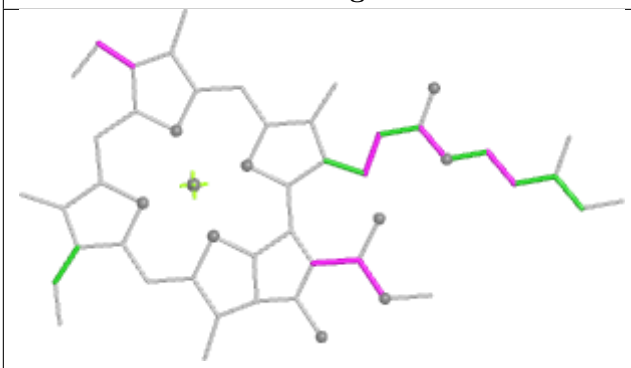
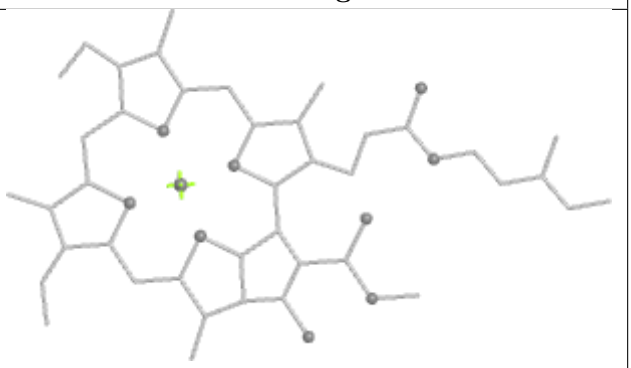


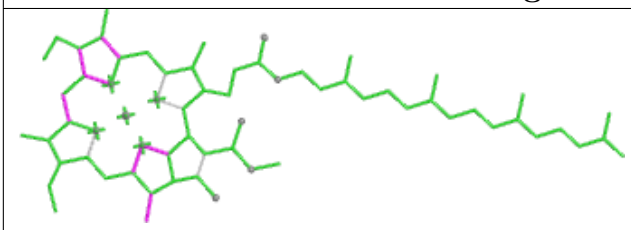
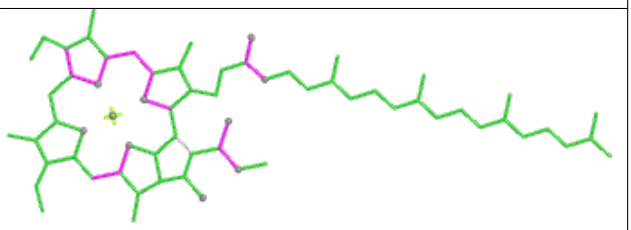
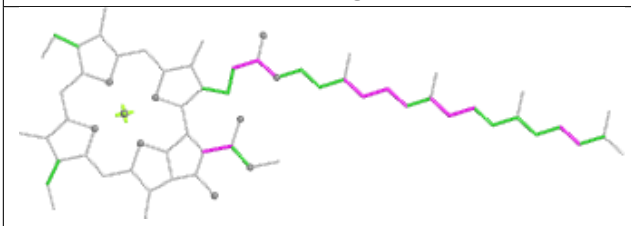
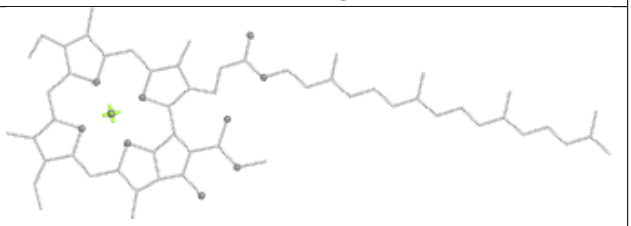
Ligand BCR 3 614

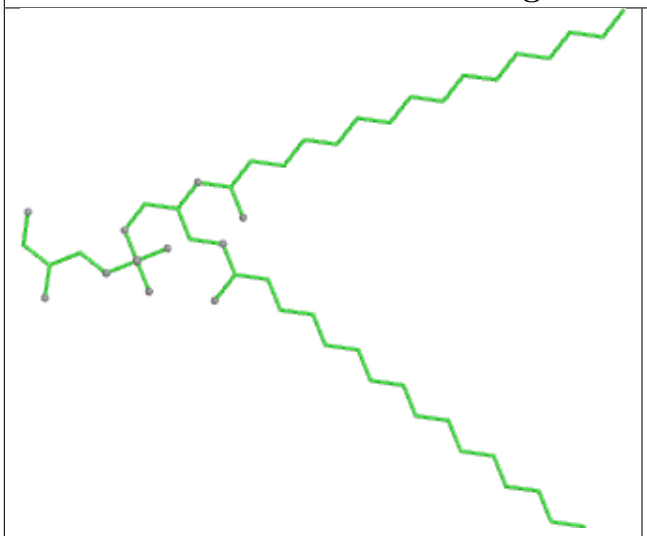
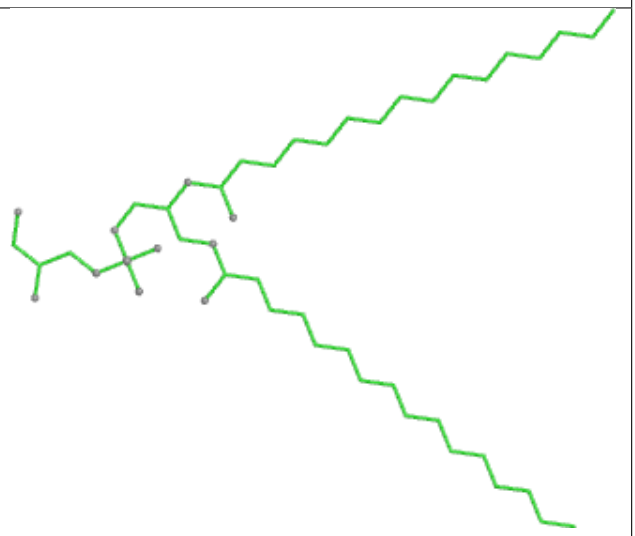
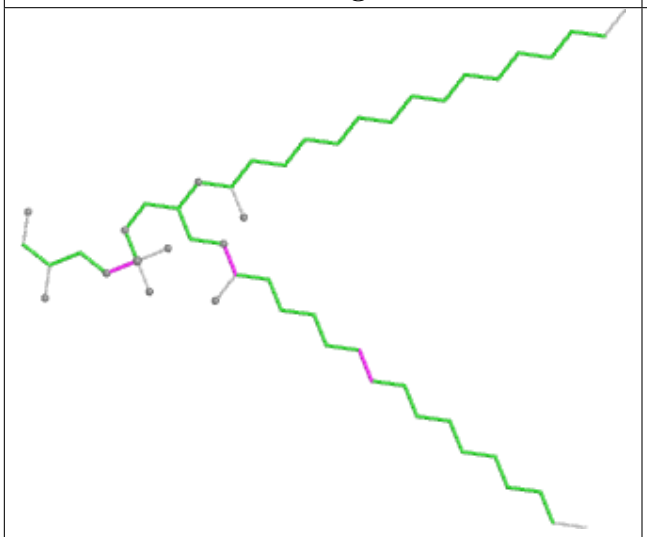
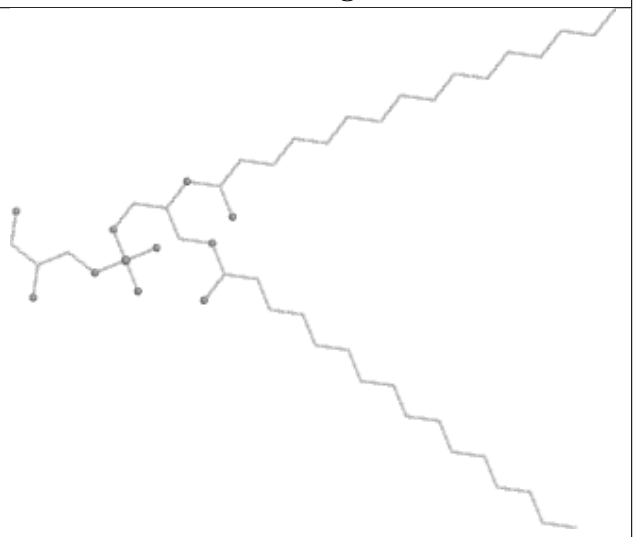


Ligand CLA B 808

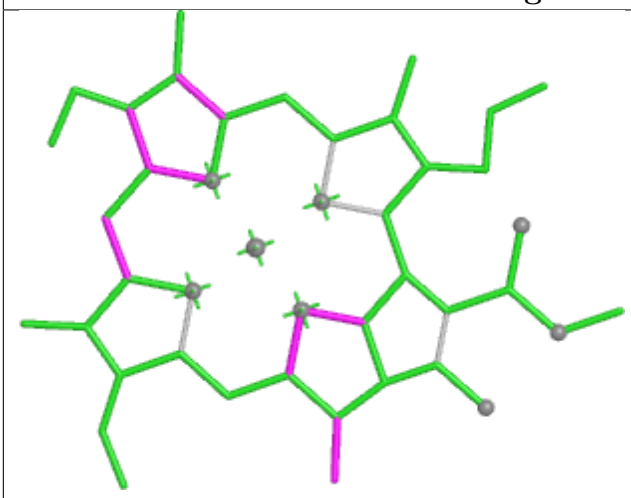


Ligand CLA J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

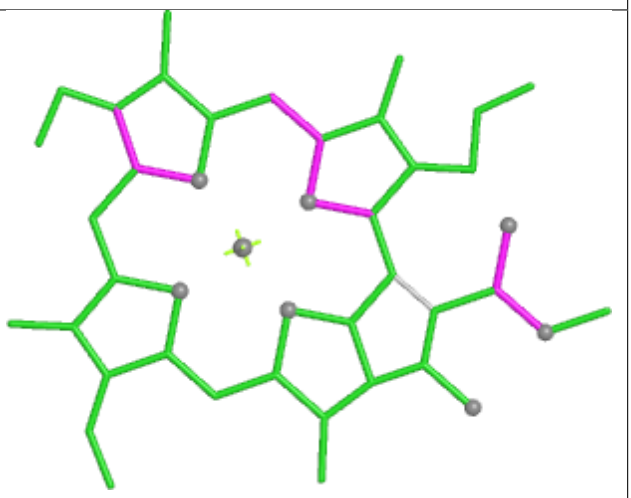
Ligand CLA A 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

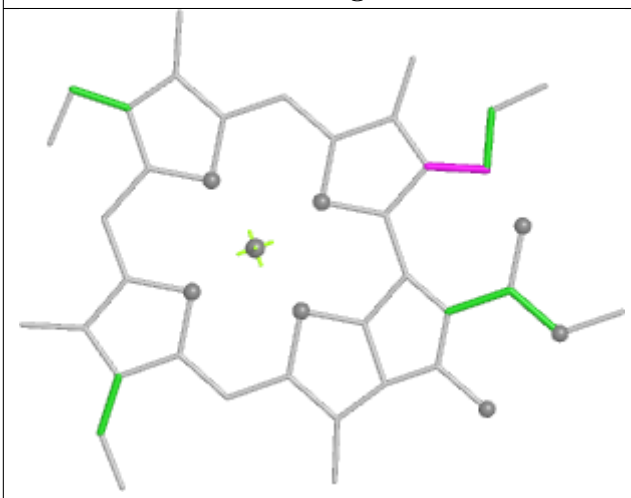
Ligand CLA B 815



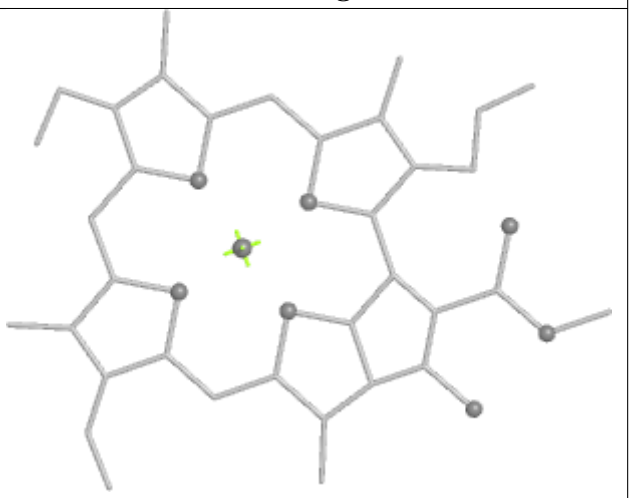
Bond lengths



Bond angles

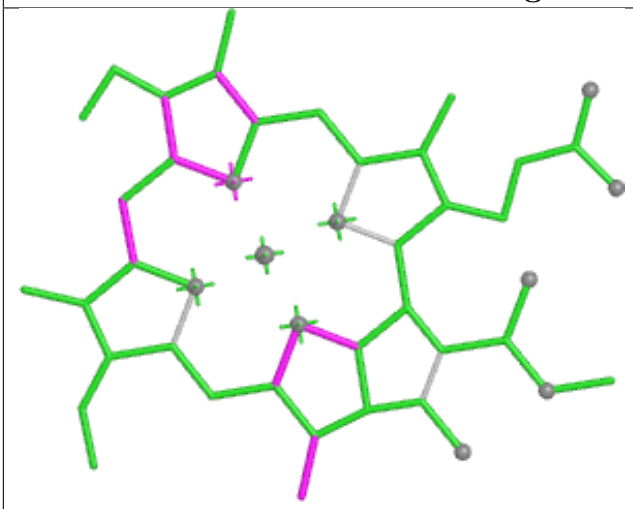


Torsions

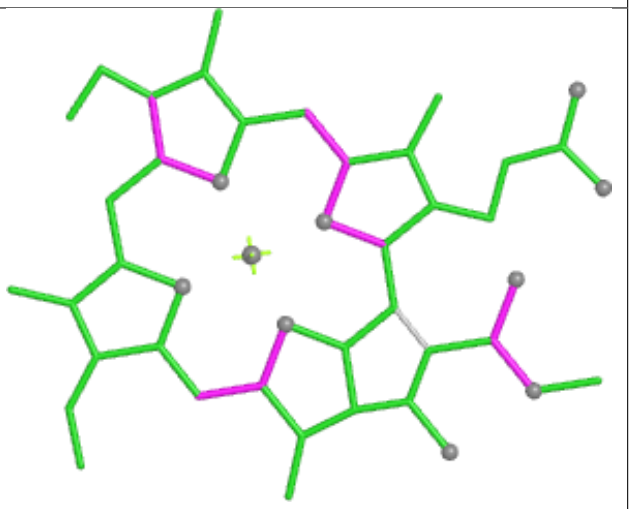


Rings

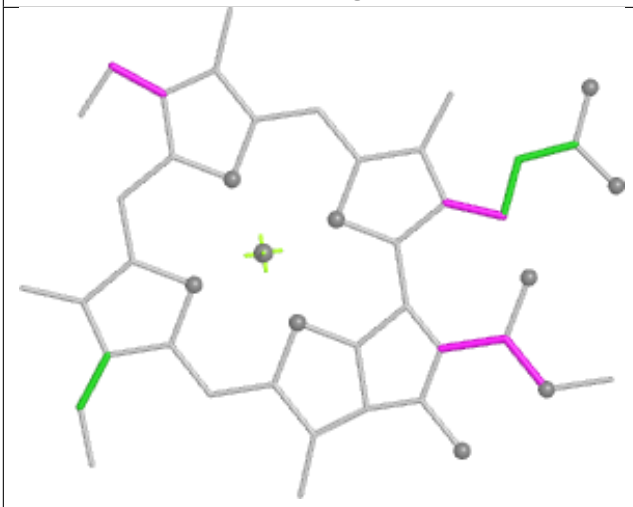
Ligand CLA B 823



Bond lengths



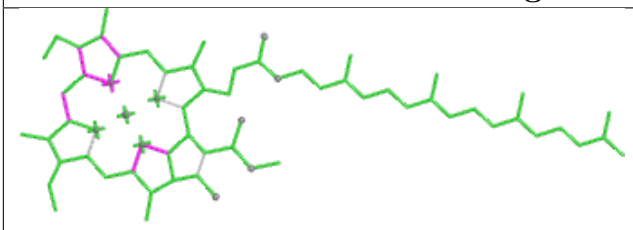
Bond angles



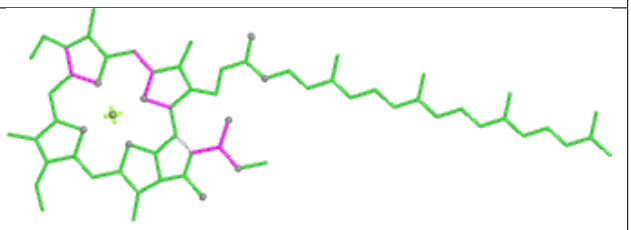
Torsions

Rings

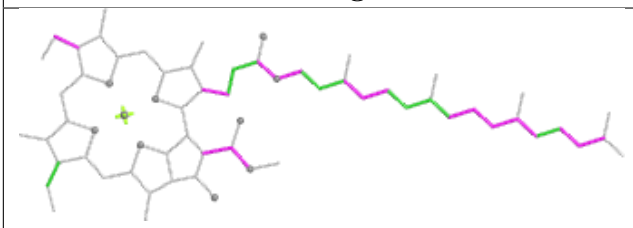
Ligand CLA B 827



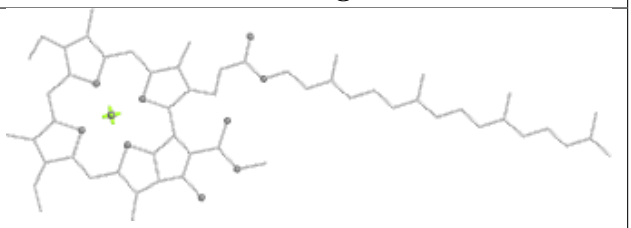
Bond lengths



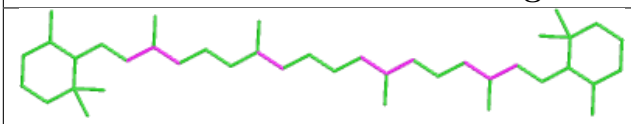
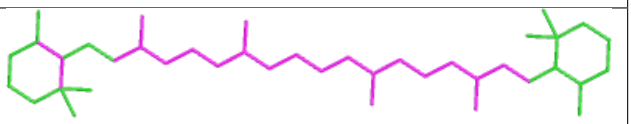
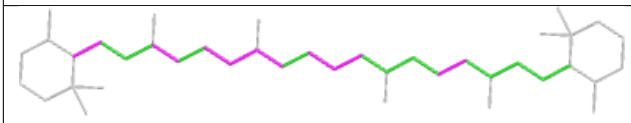
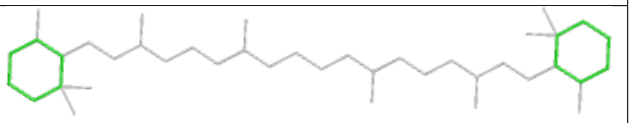
Bond angles

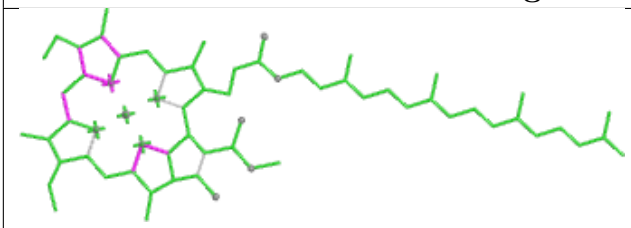
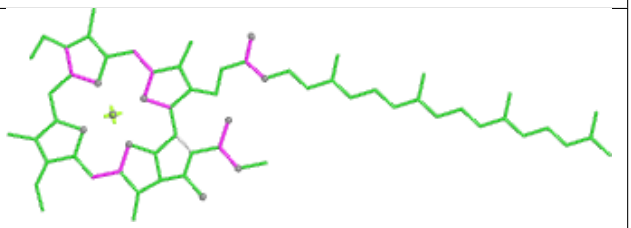
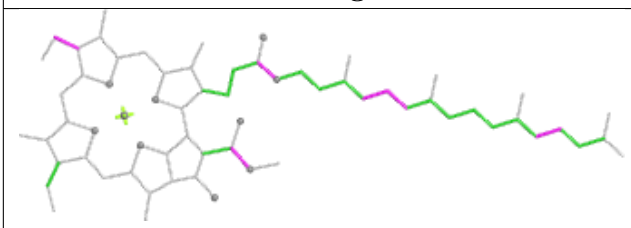
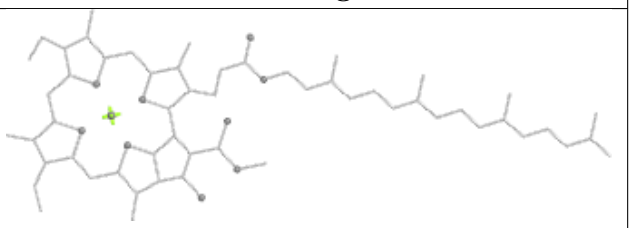


Torsions

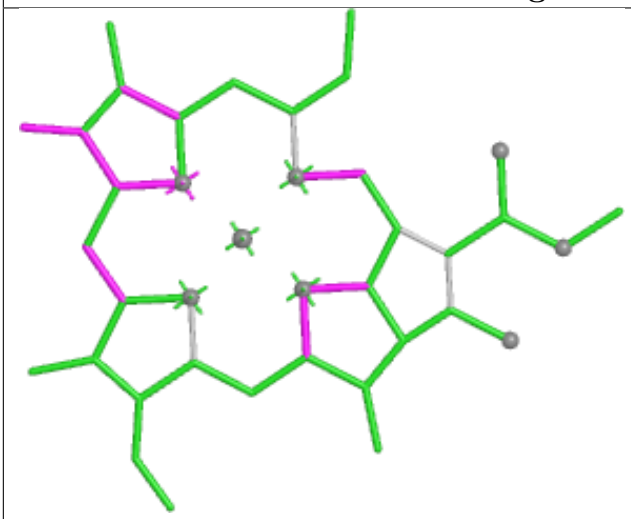


Rings

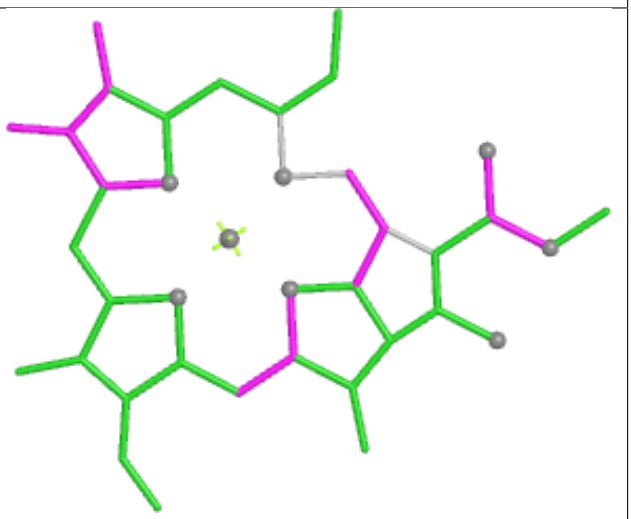
Ligand BCR F 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

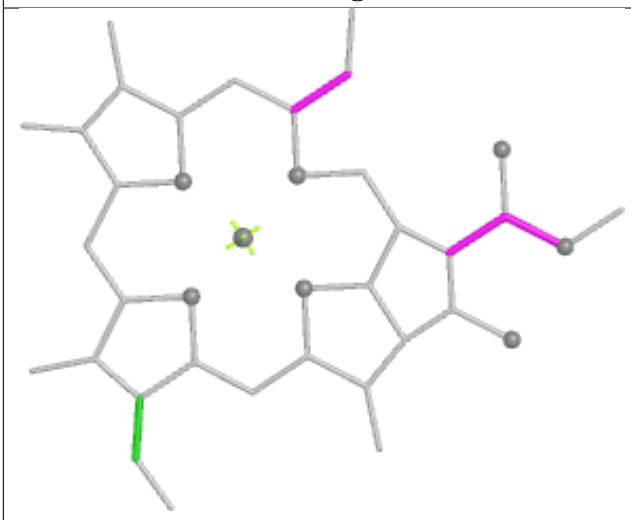
Ligand CLA 2 610



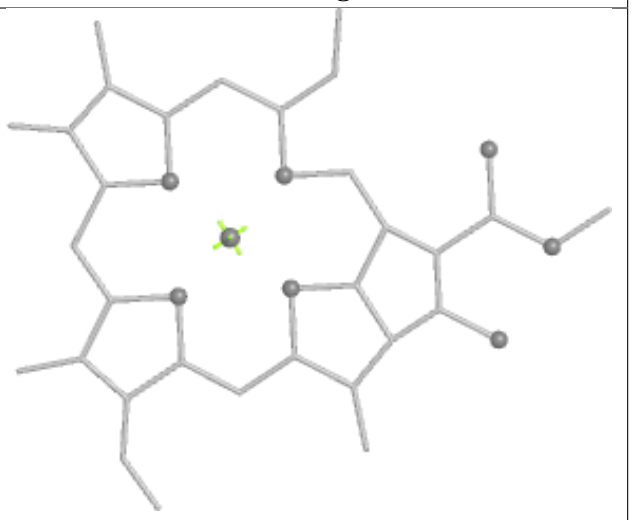
Bond lengths



Bond angles

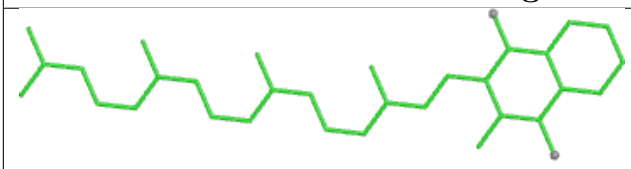


Torsions



Rings

Ligand PQN B 842



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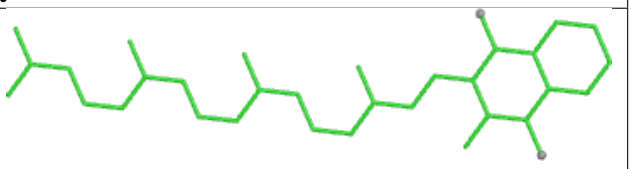
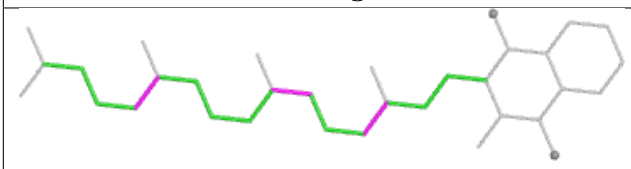
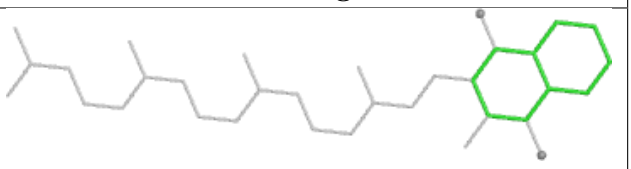


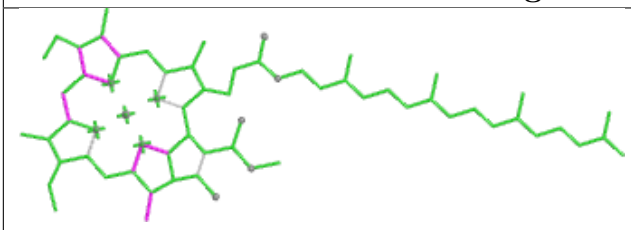
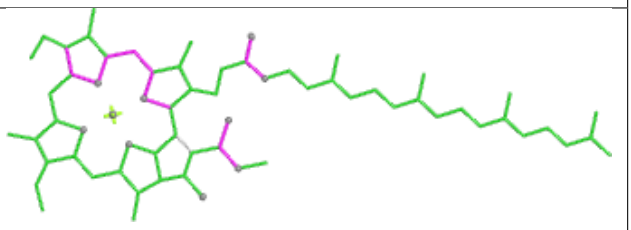
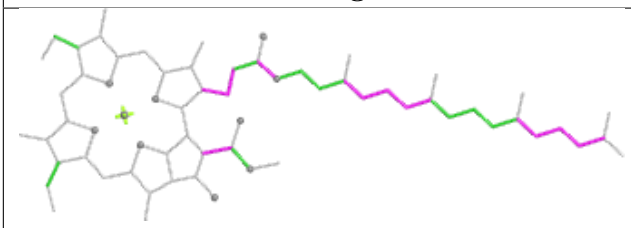
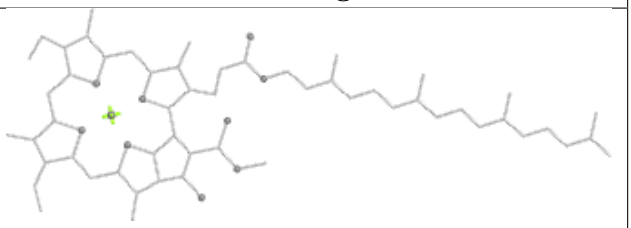
Bond angles

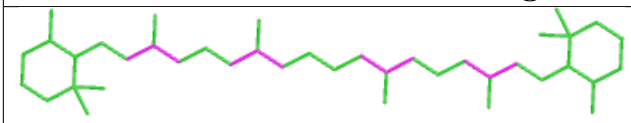
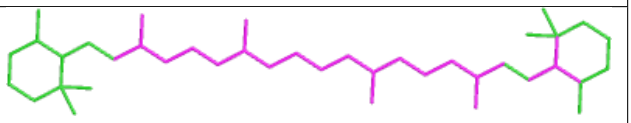
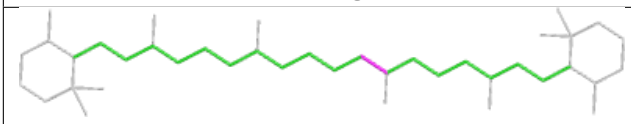
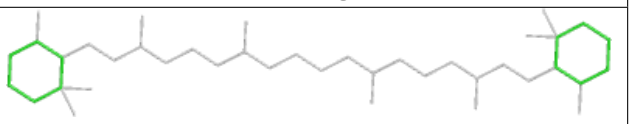


Torsions

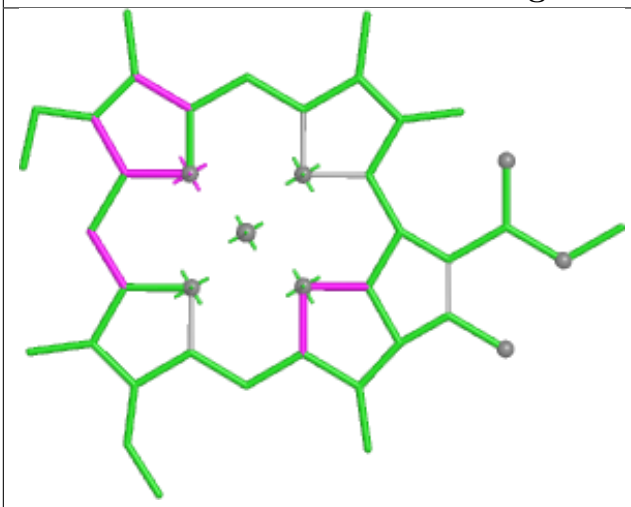


Rings

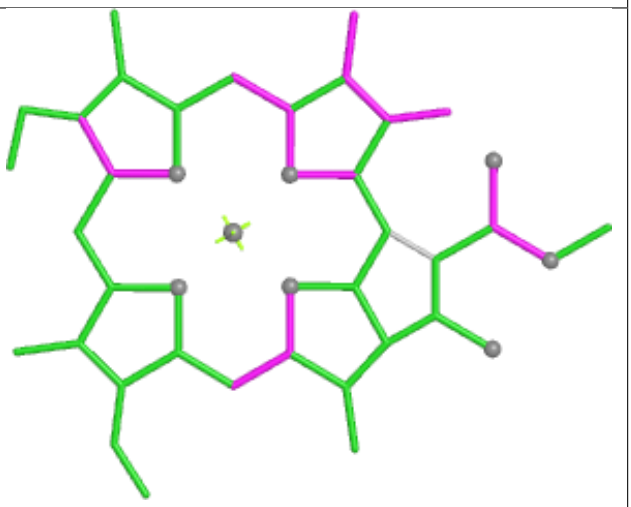
Ligand CLA B 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR K 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

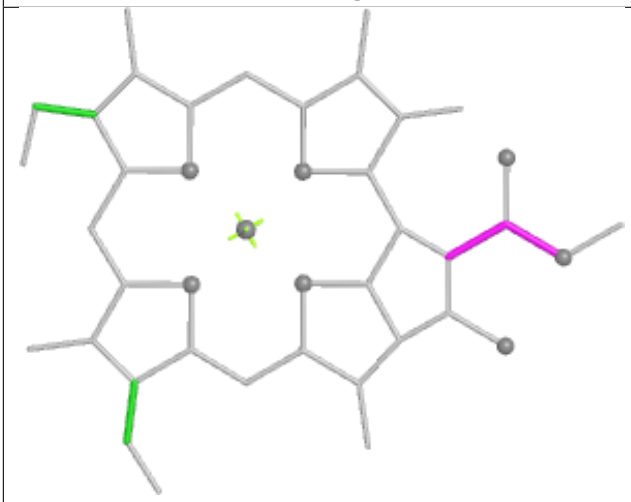
Ligand CLA 3 608



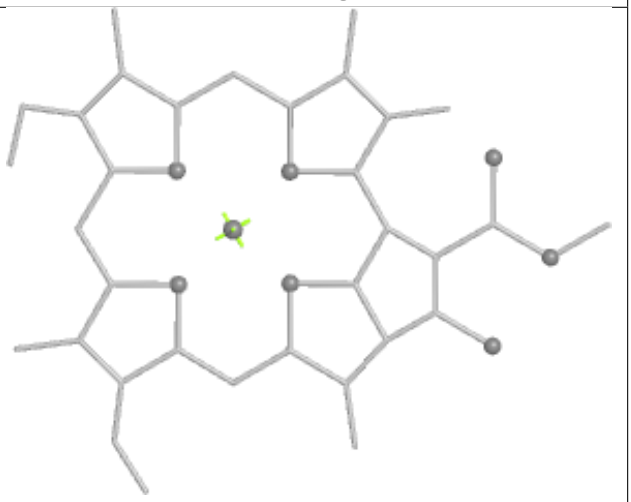
Bond lengths



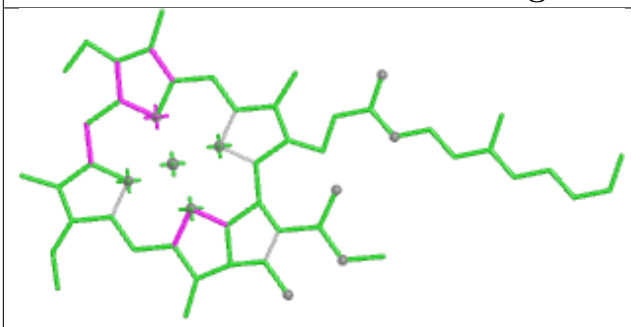
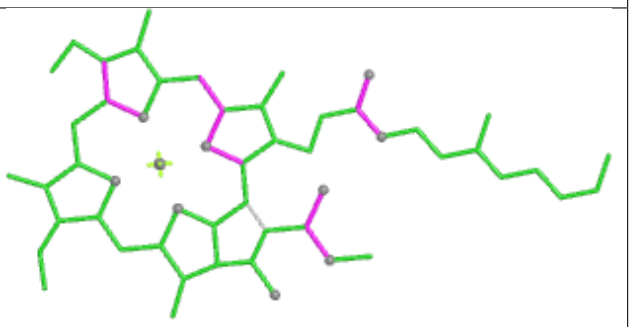
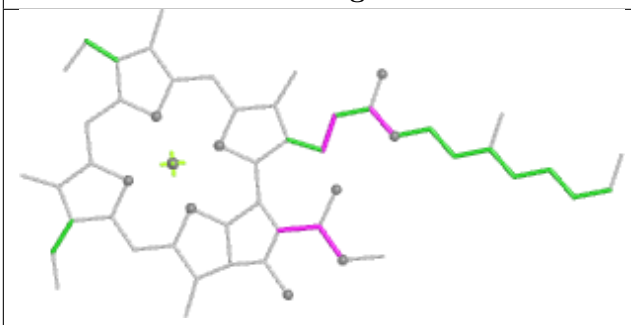
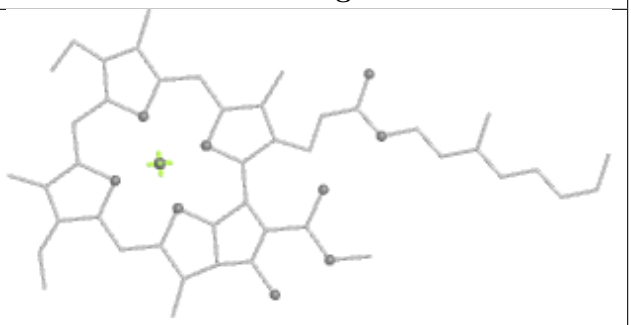
Bond angles



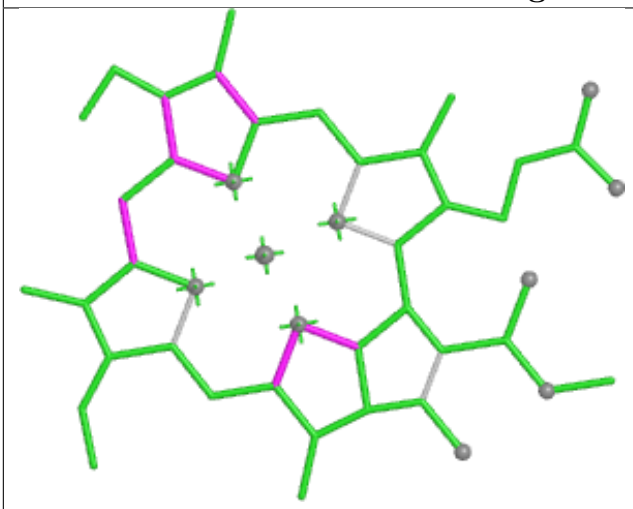
Torsions



Rings

Ligand CLA 1 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 608



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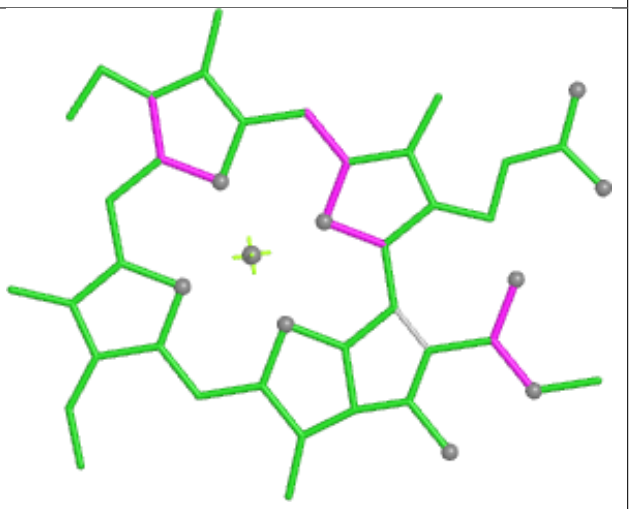
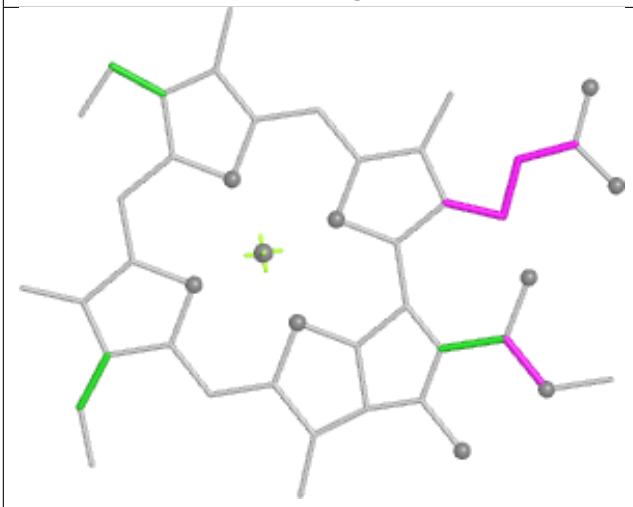


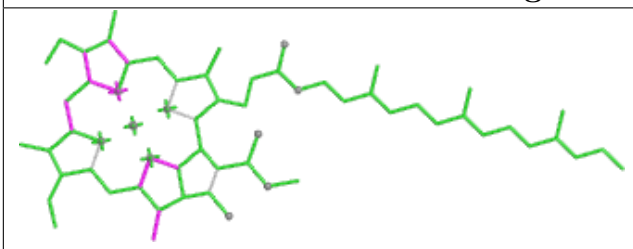
Bond angles



Torsions

Rings

Ligand CLA B 826



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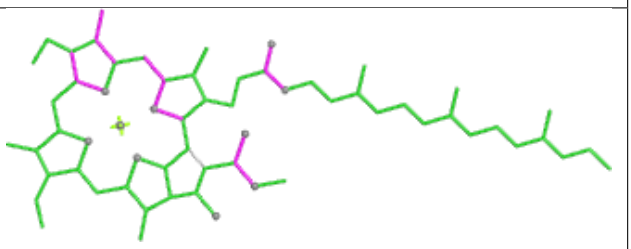
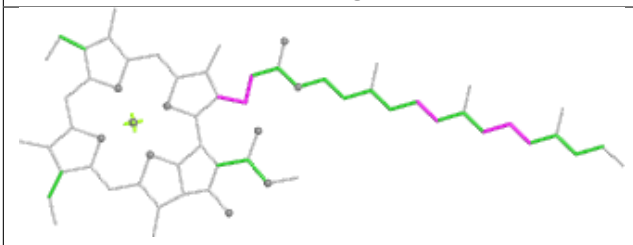
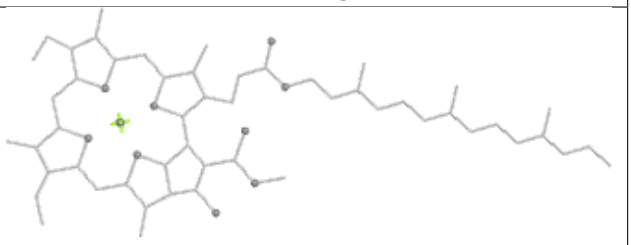


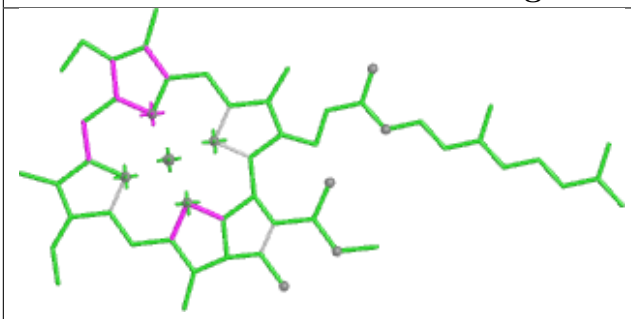
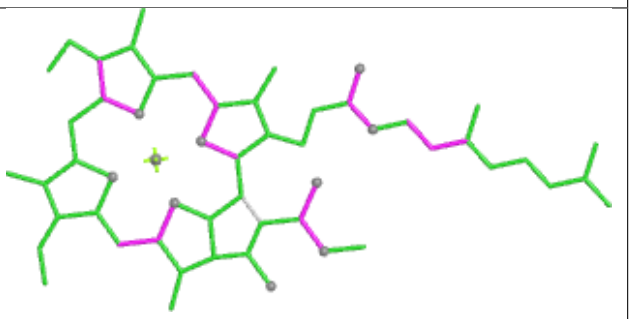
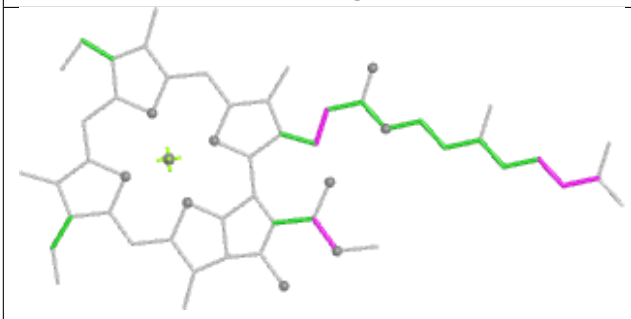
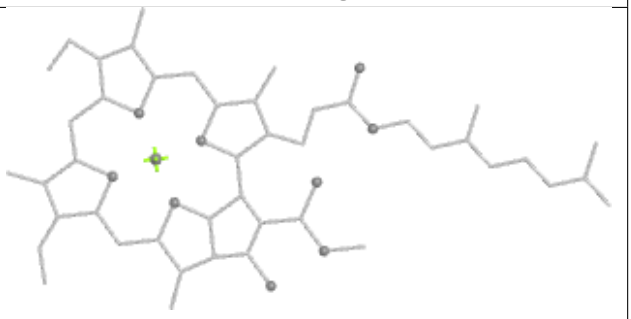
Bond angles

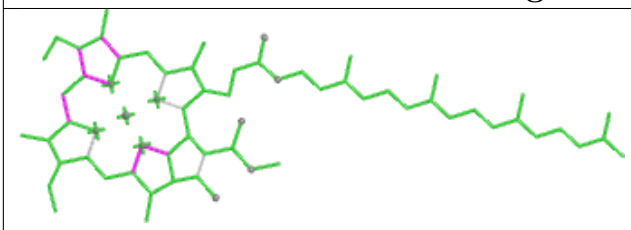
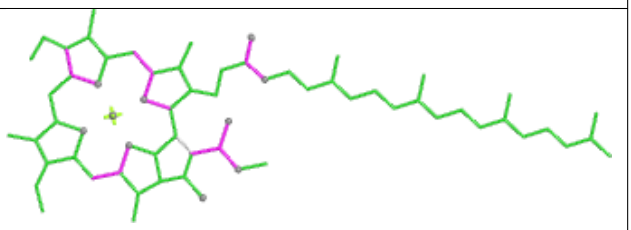
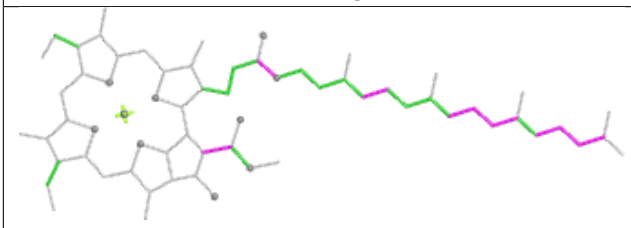
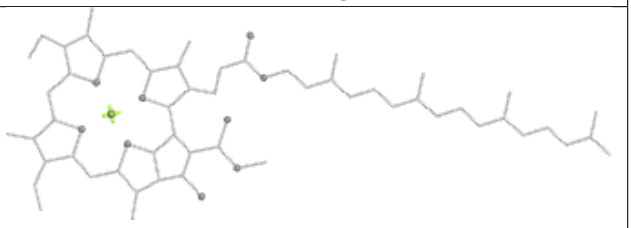


Torsions



Rings

Ligand CLA B 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

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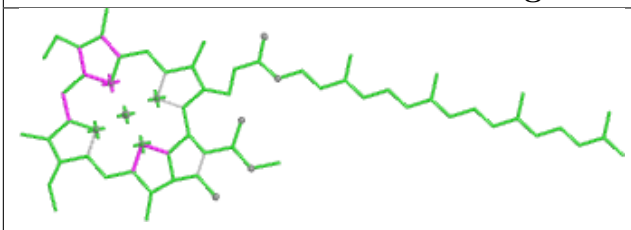
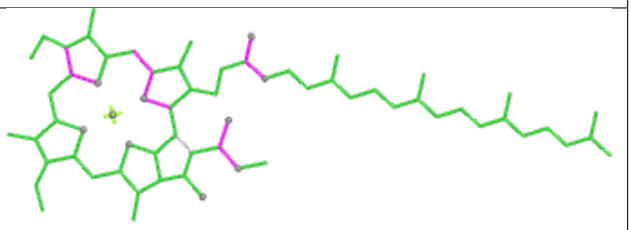
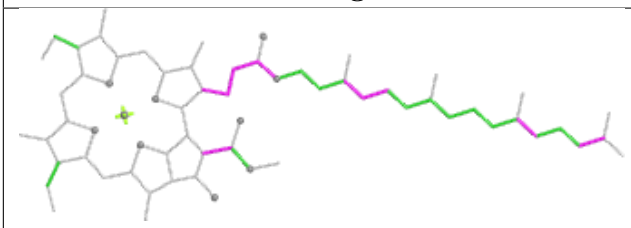
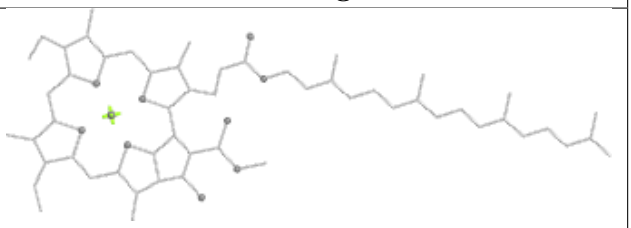
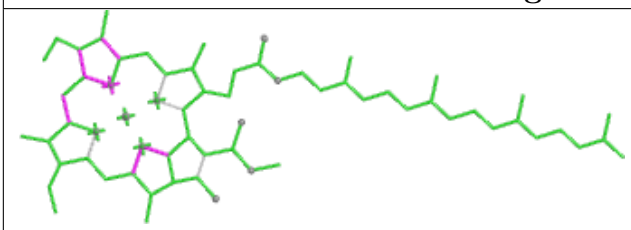
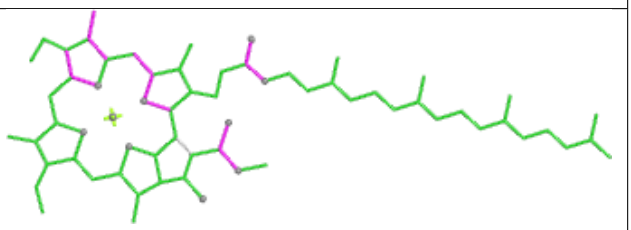
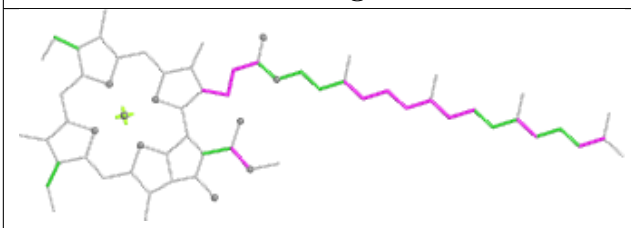
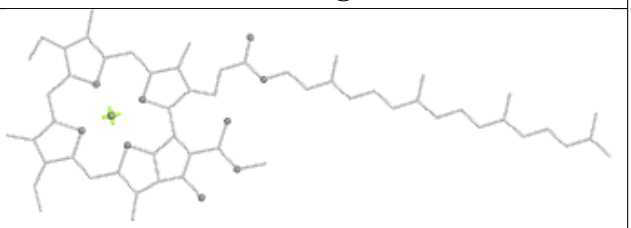
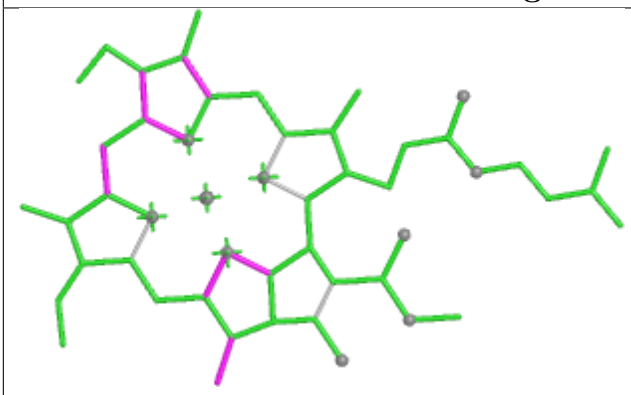
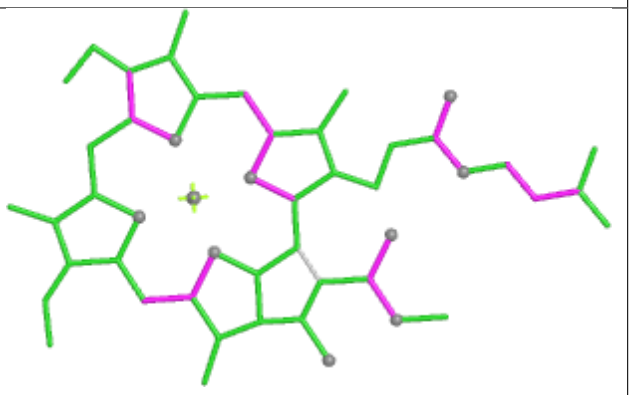
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

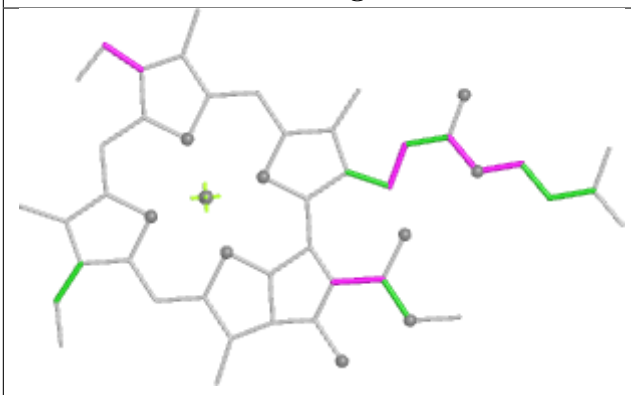
Ligand CLA A 832



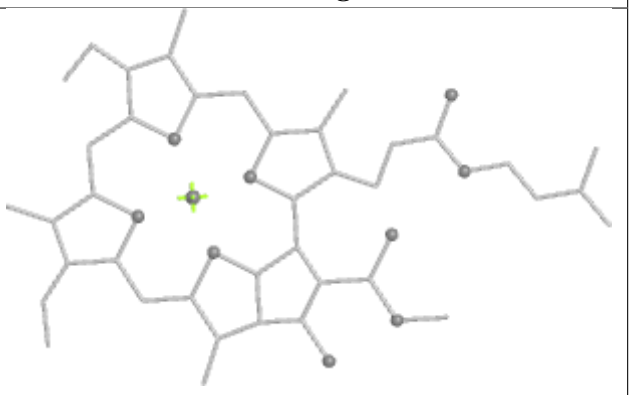
Bond lengths



Bond angles

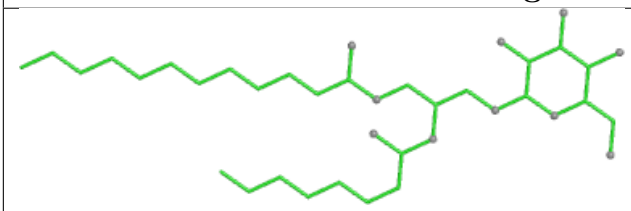


Torsions



Rings

Ligand LMG 4 619



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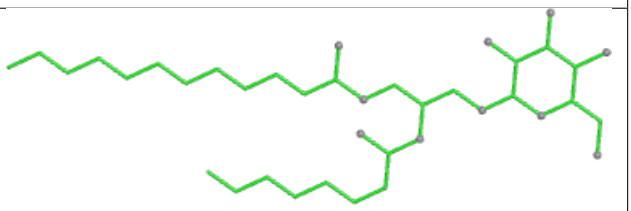
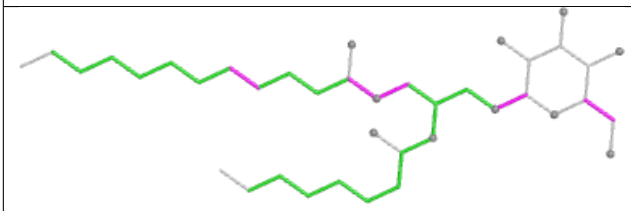
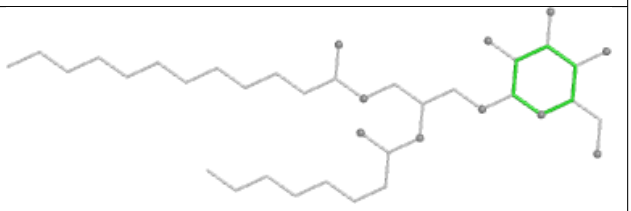


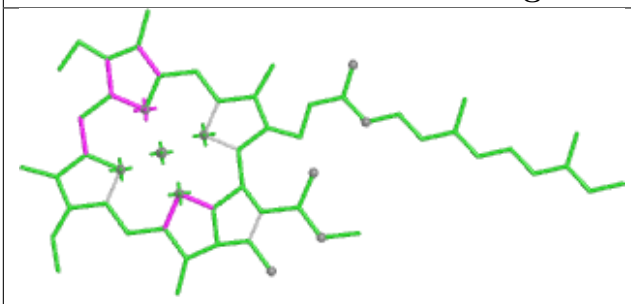
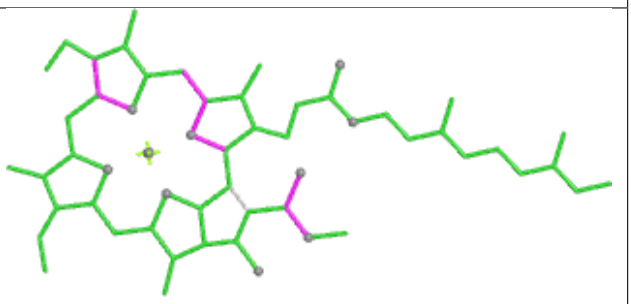
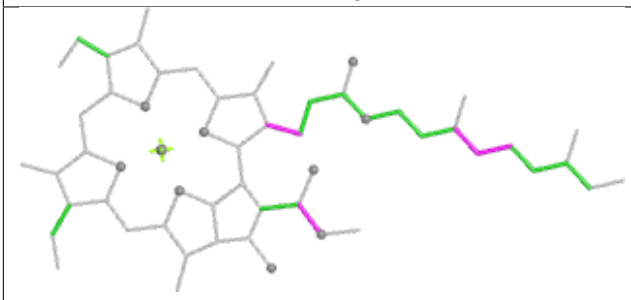
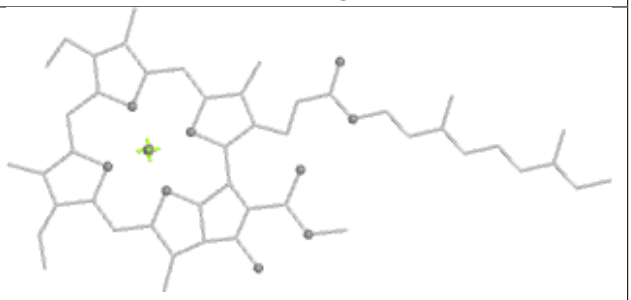
Bond angles



Torsions



Rings

Ligand CLA A 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

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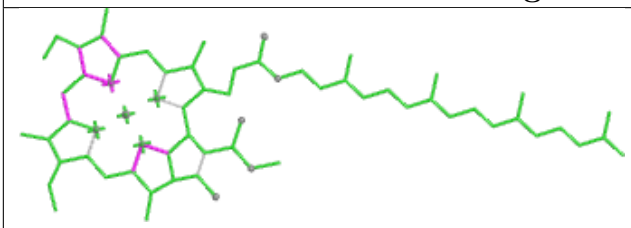
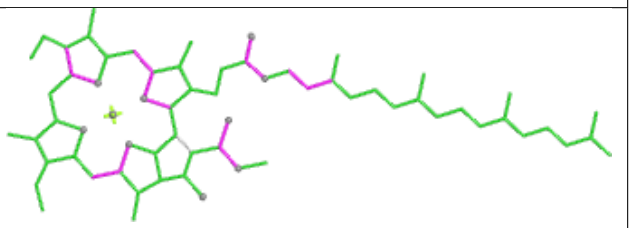
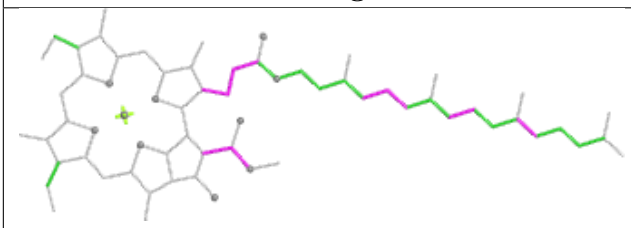
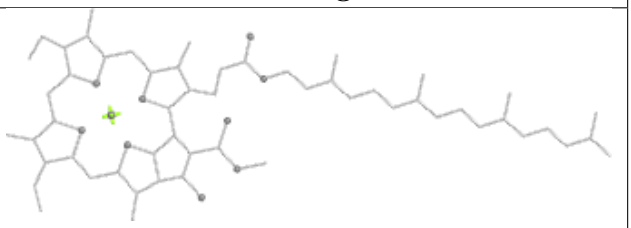
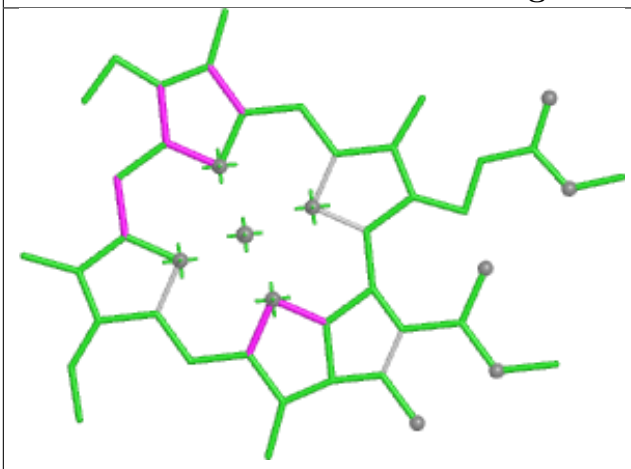
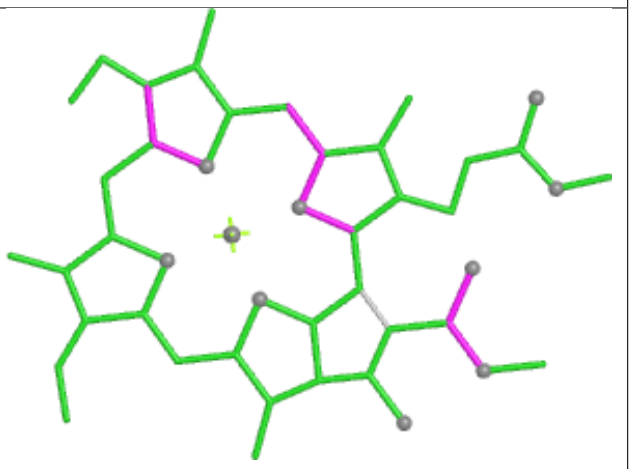
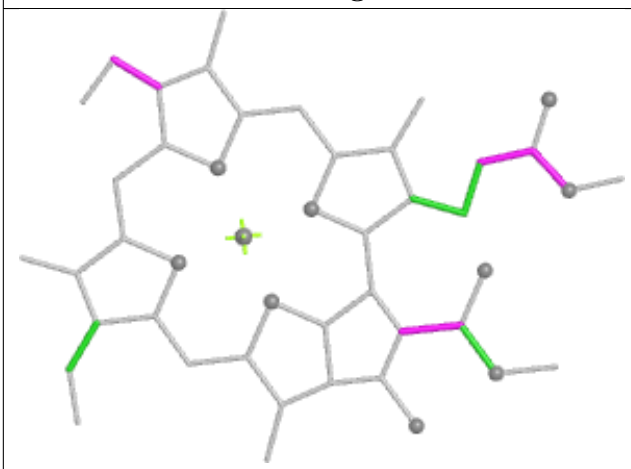
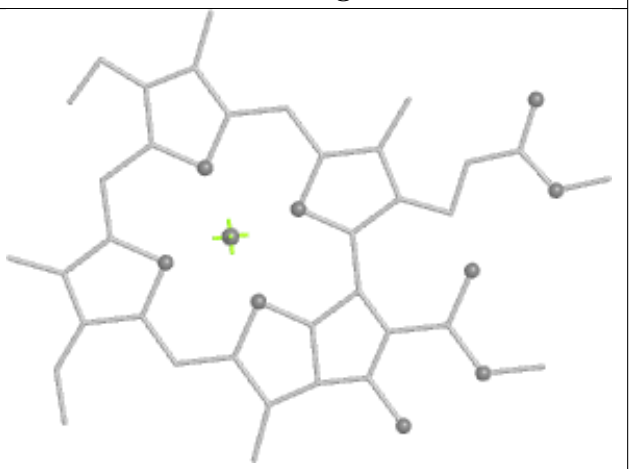
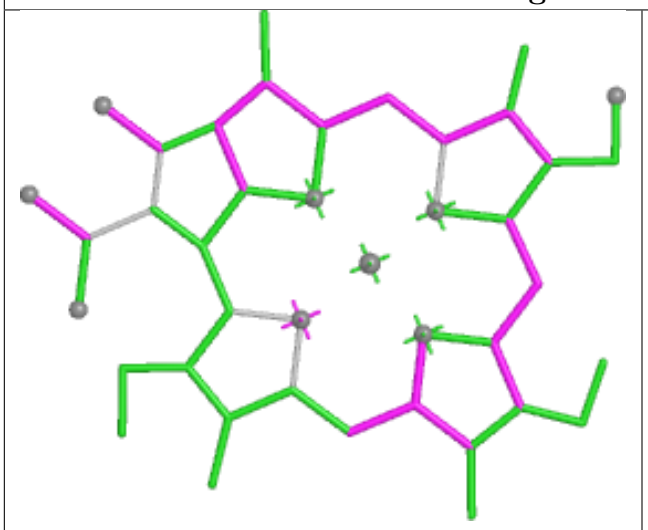
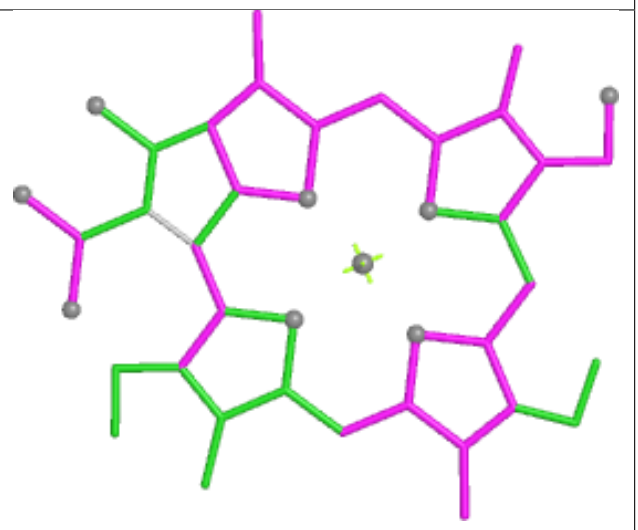
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

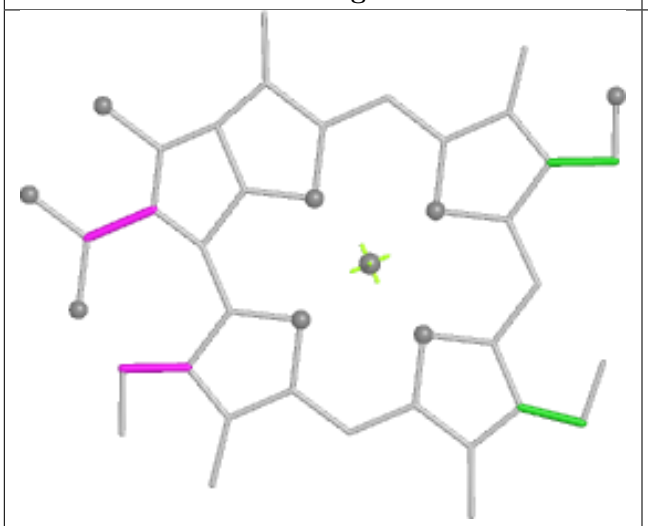
Ligand CHL 4 605



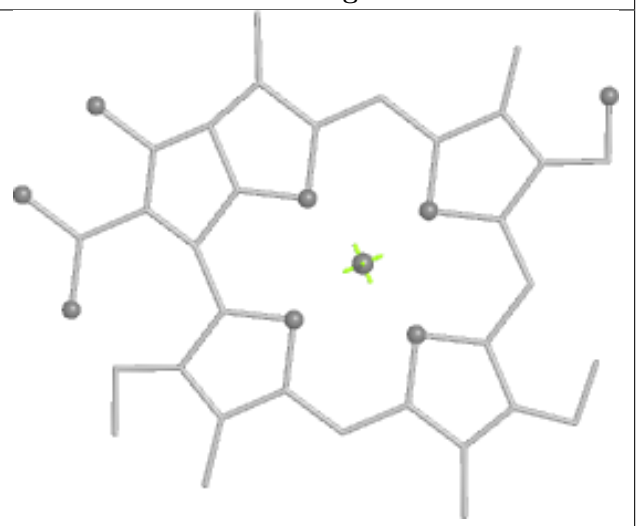
Bond lengths



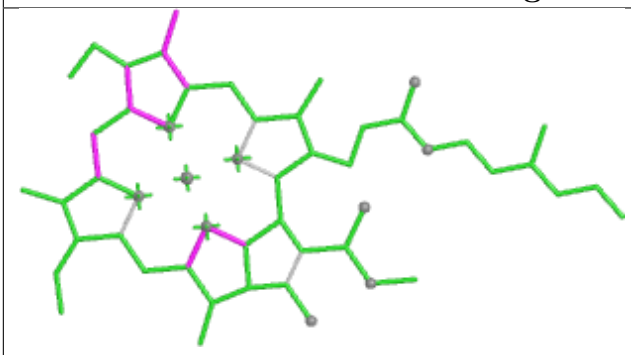
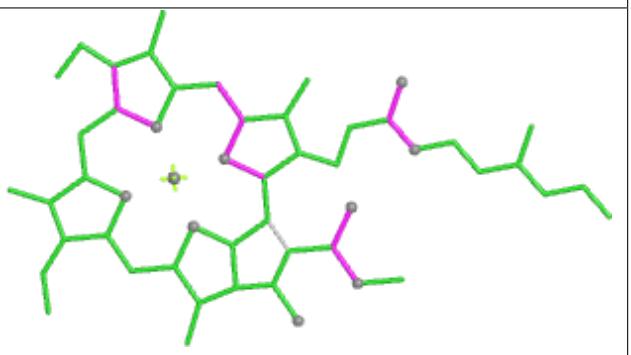
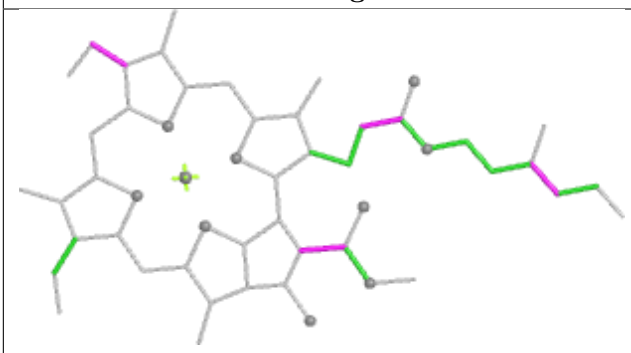
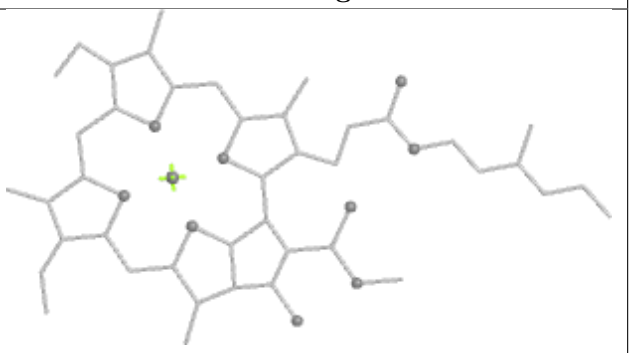
Bond angles

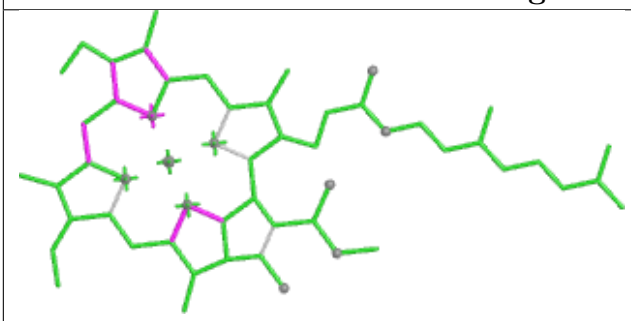
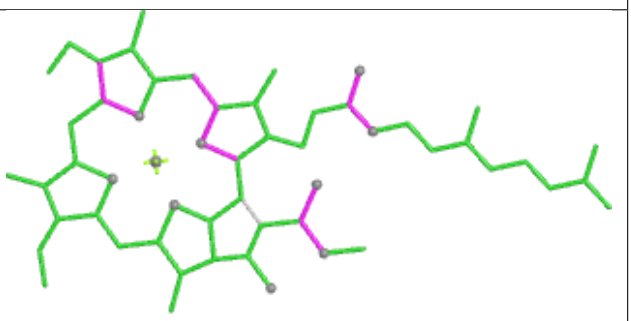
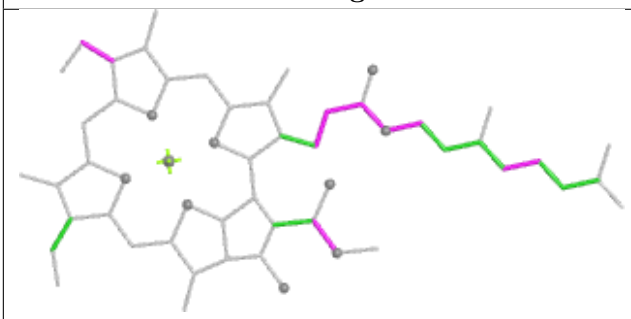
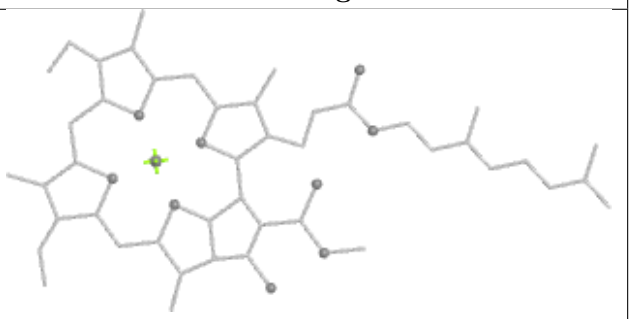


Torsions

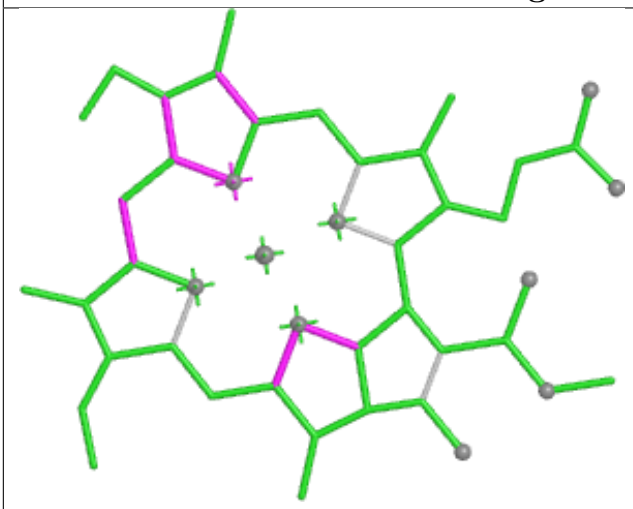


Rings

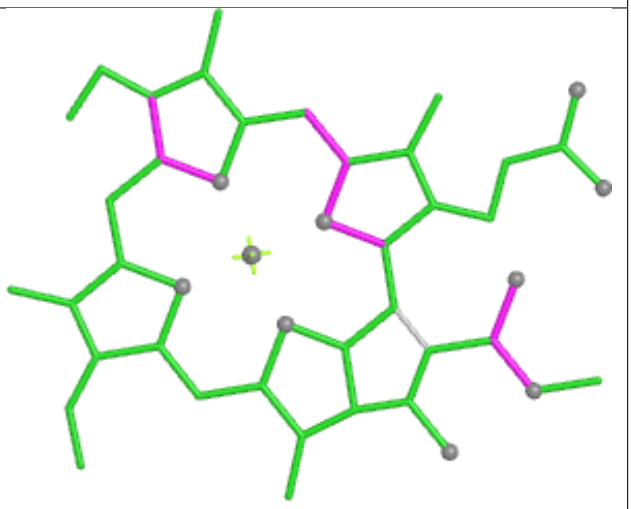
Ligand CLA A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

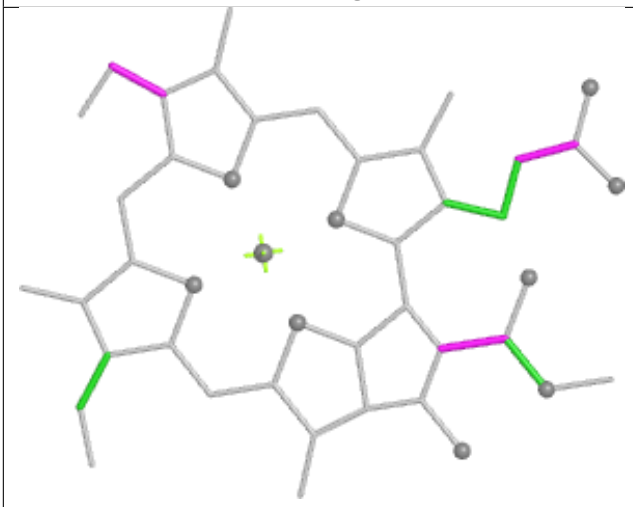
Ligand CLA 1 611



Bond lengths



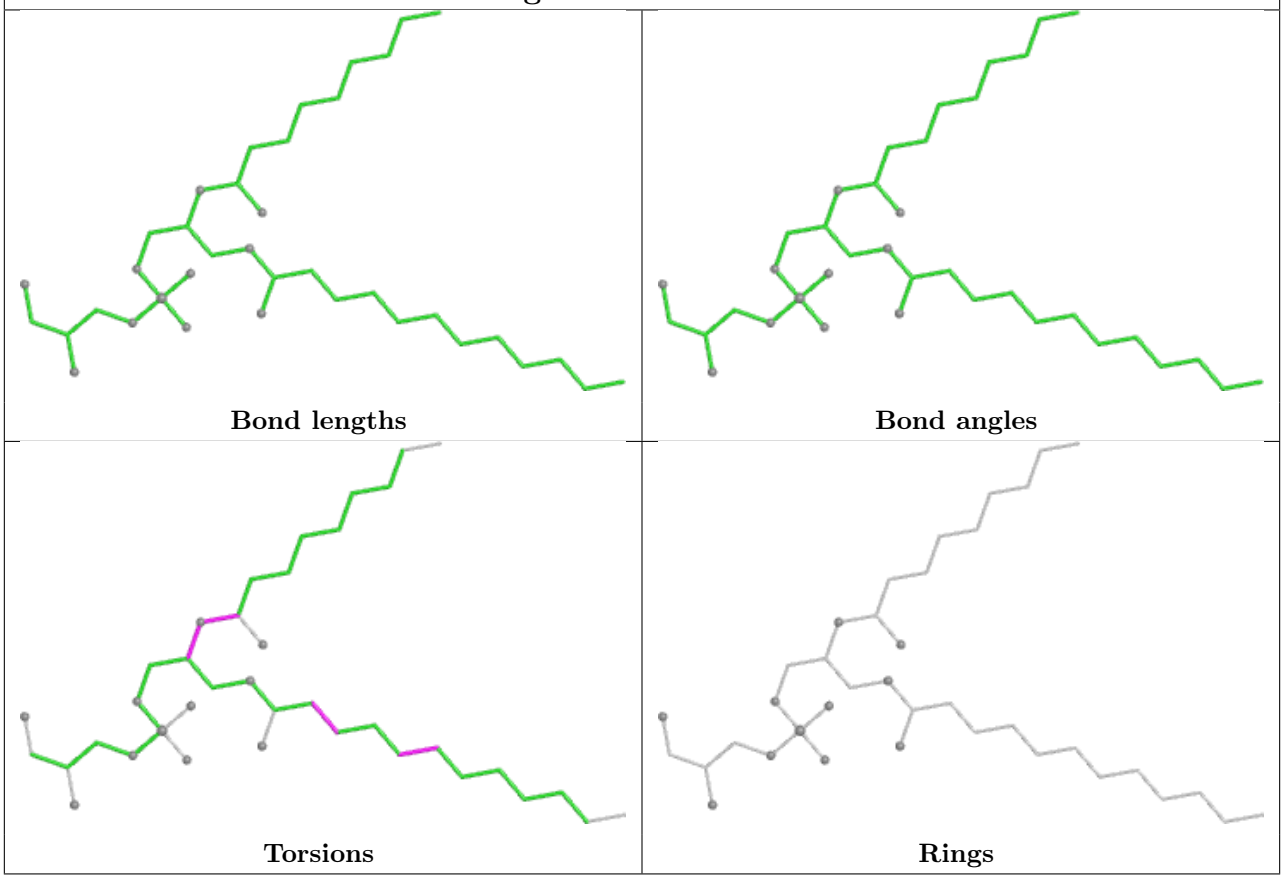
Bond angles



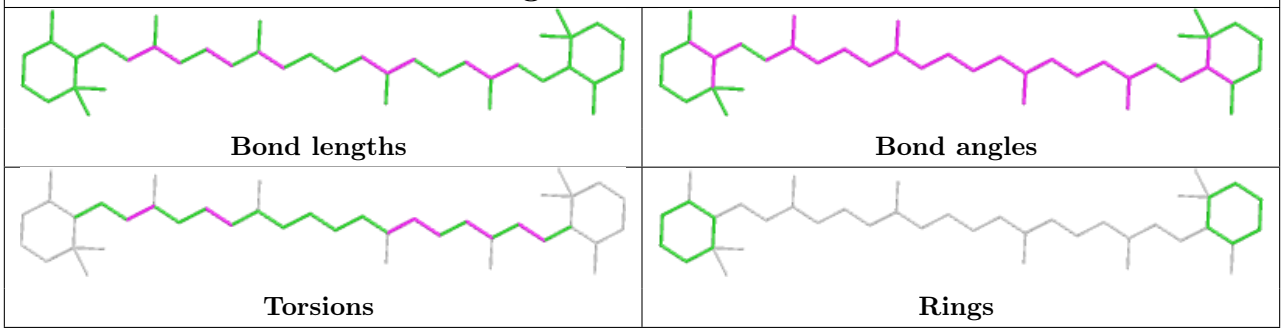
Torsions

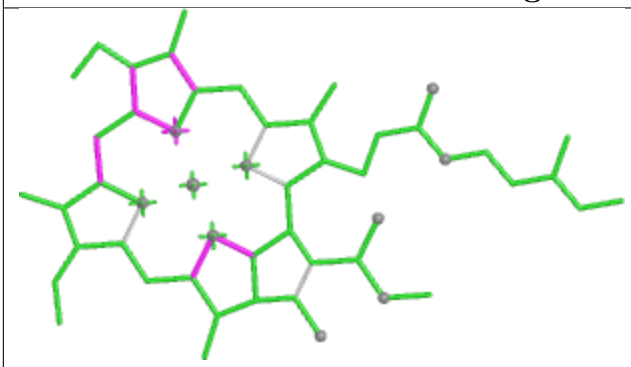
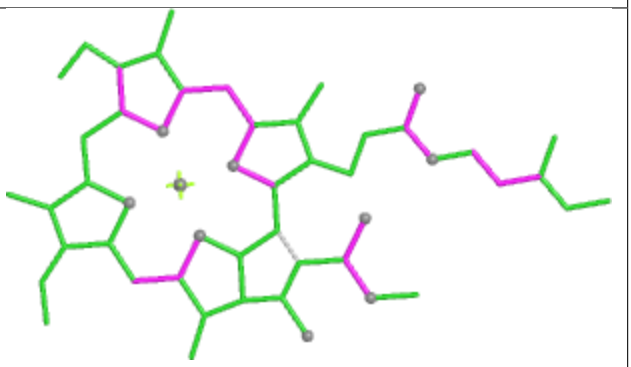
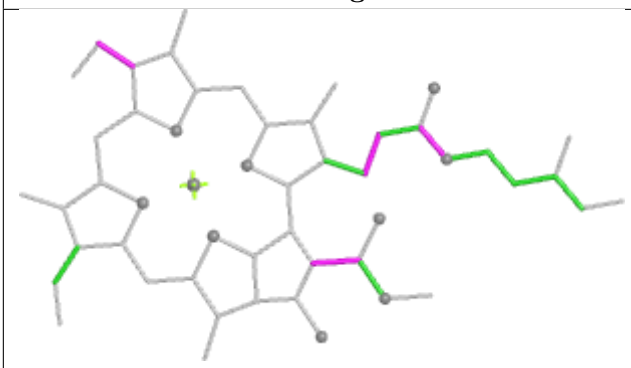
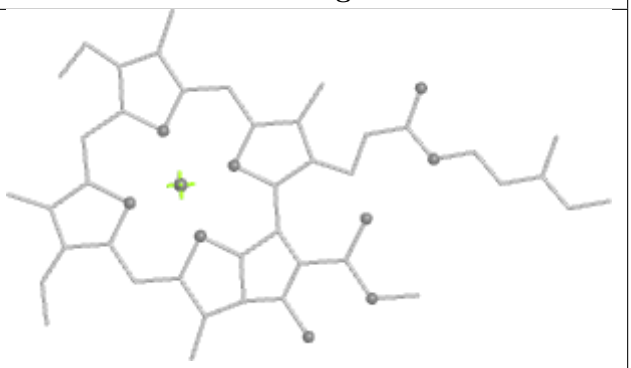
Rings

Ligand LHG B 851

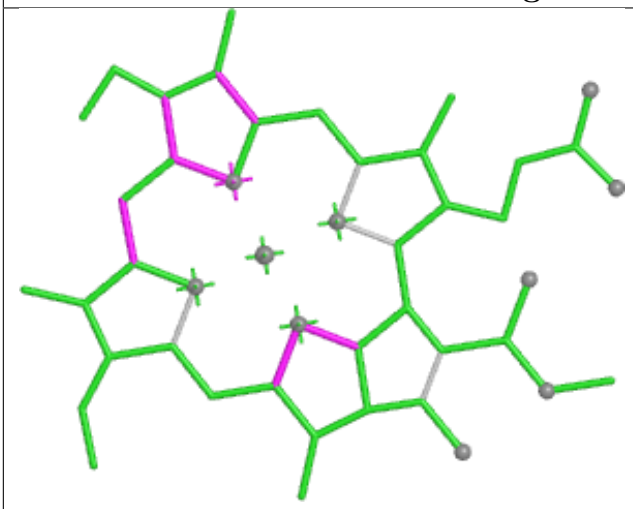


Ligand BCR K 205

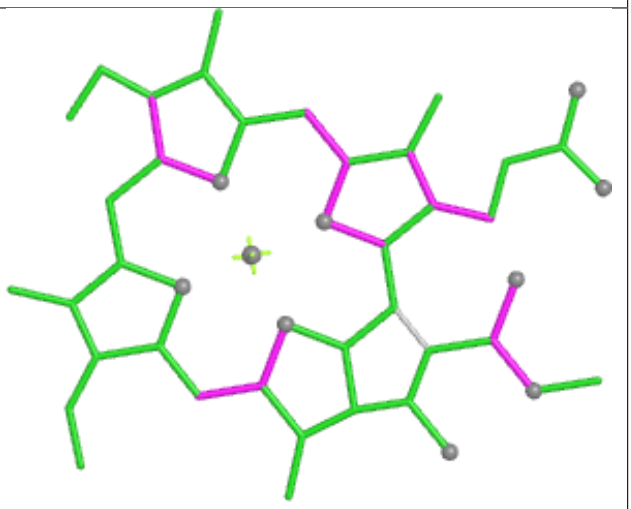


Ligand CLA A 838	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

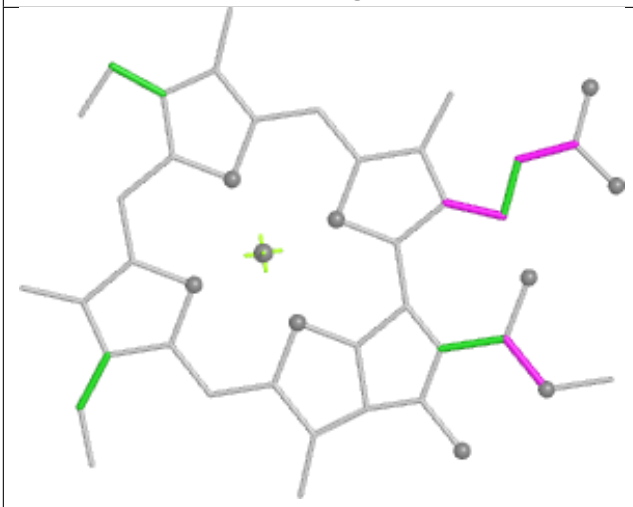
Ligand CLA K 203



Bond lengths



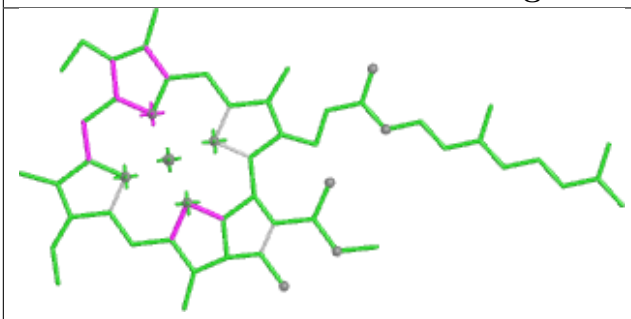
Bond angles



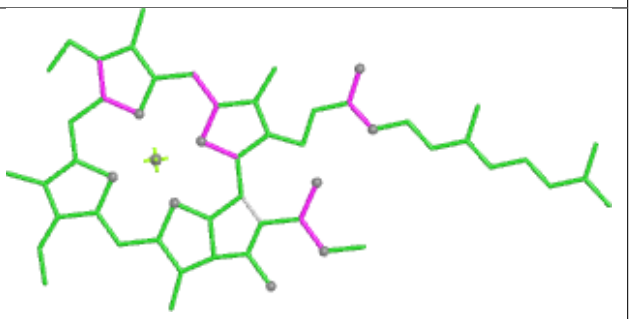
Torsions

Rings

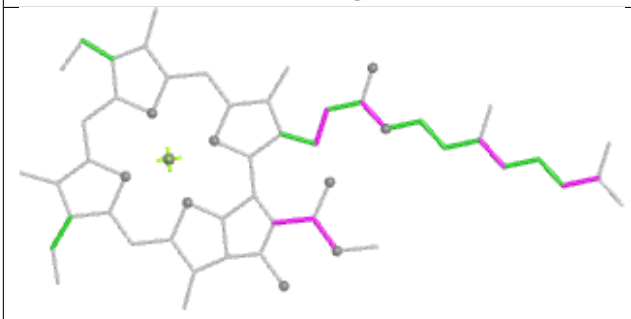
Ligand CLA A 839



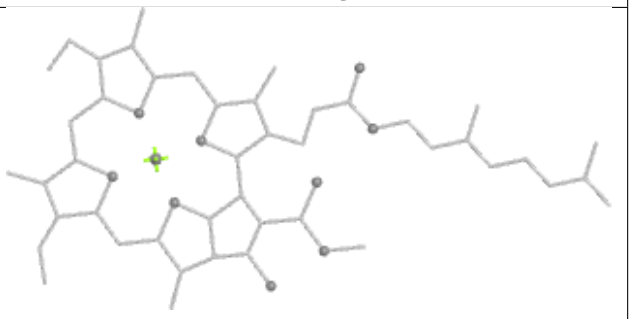
Bond lengths



Bond angles

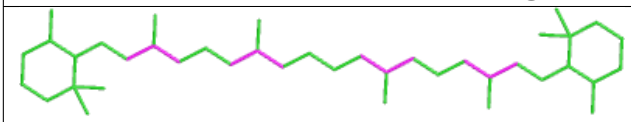


Torsions

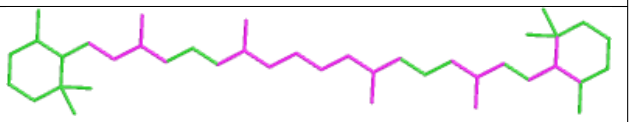


Rings

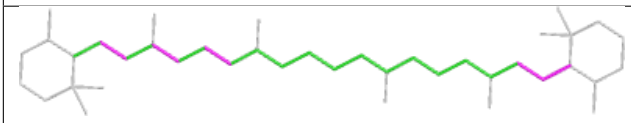
Ligand BCR B 849



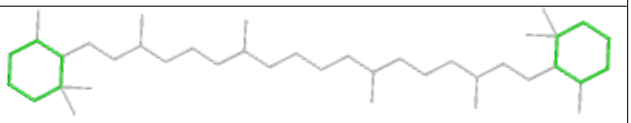
Bond lengths



Bond angles

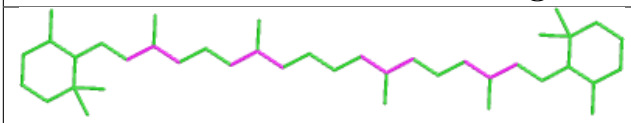


Torsions

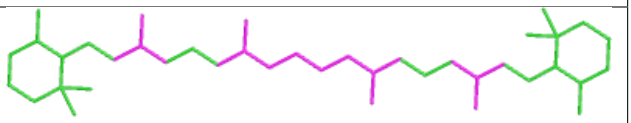


Rings

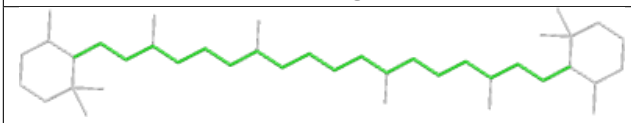
Ligand BCR I 101



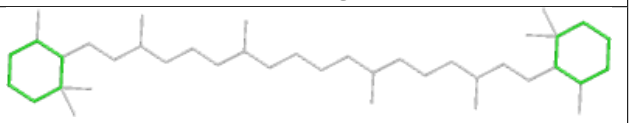
Bond lengths



Bond angles

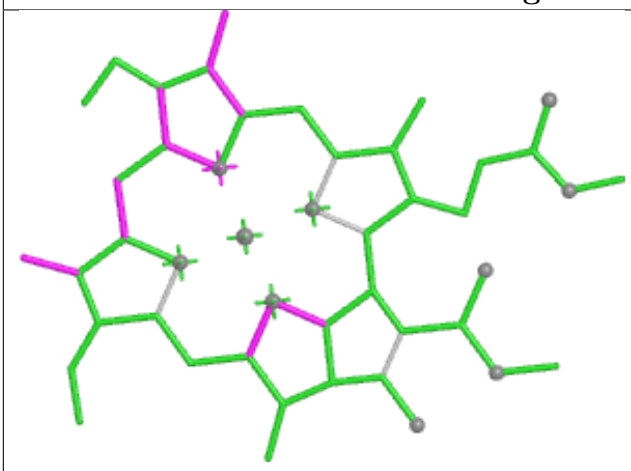


Torsions



Rings

Ligand CLA K 204



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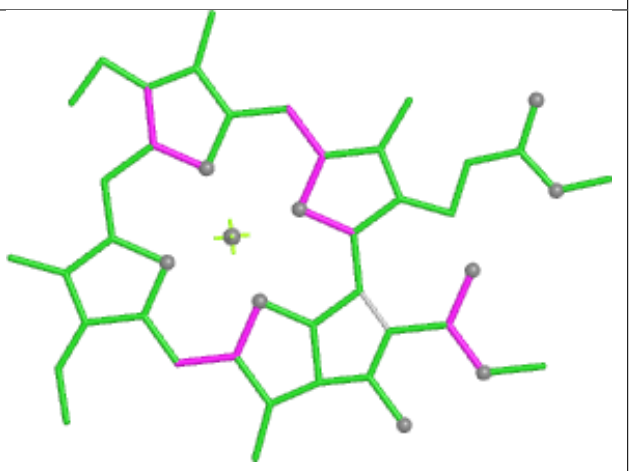

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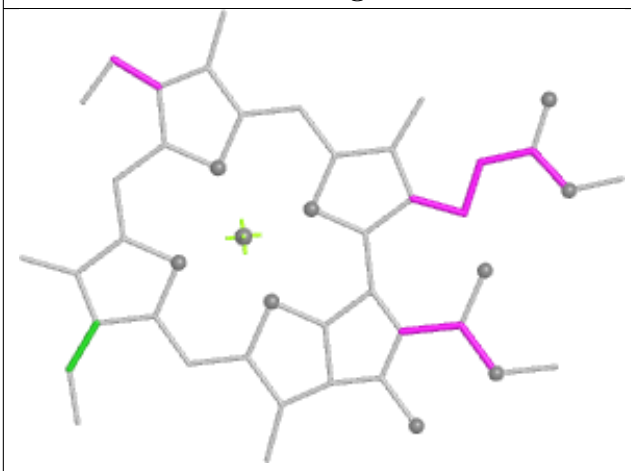

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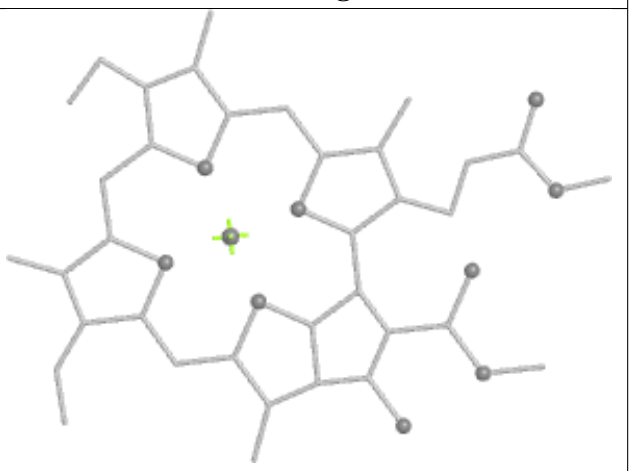
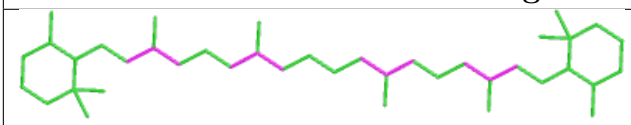


Rings

Ligand BCR B 843



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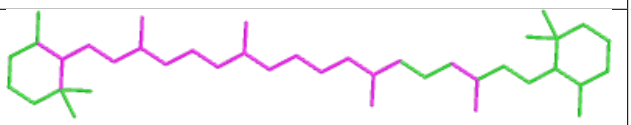

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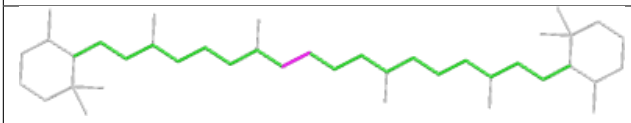

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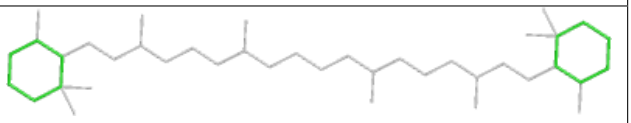
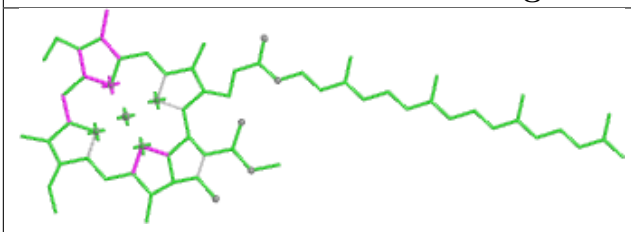


Rings

Ligand CLA A 822



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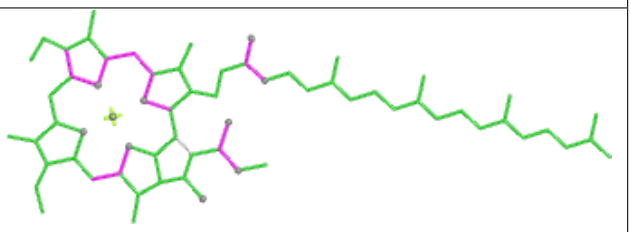

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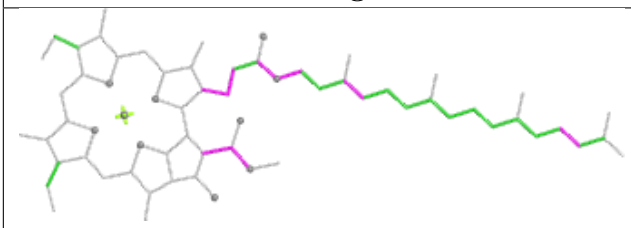

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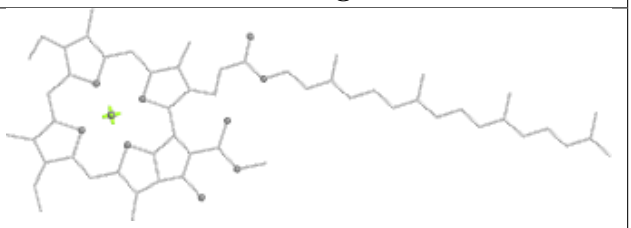
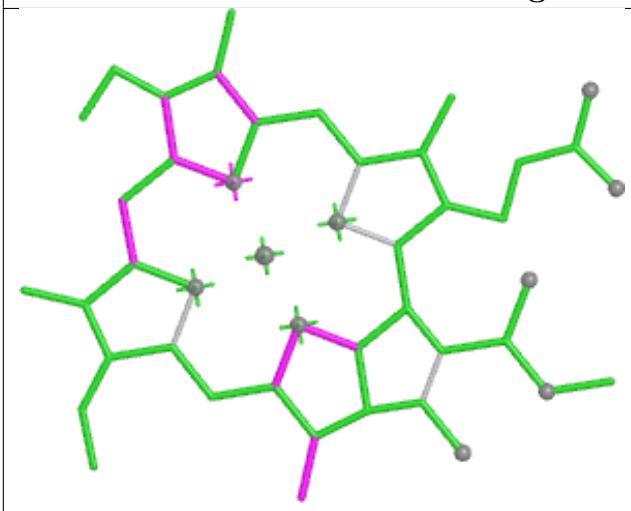


Rings

Ligand CLA 4 608



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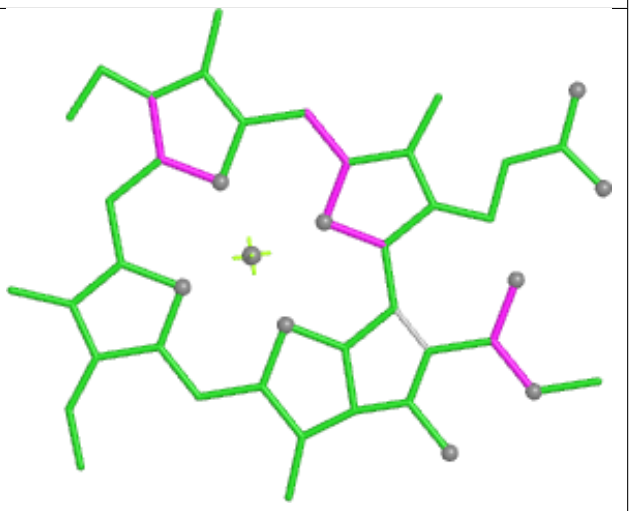

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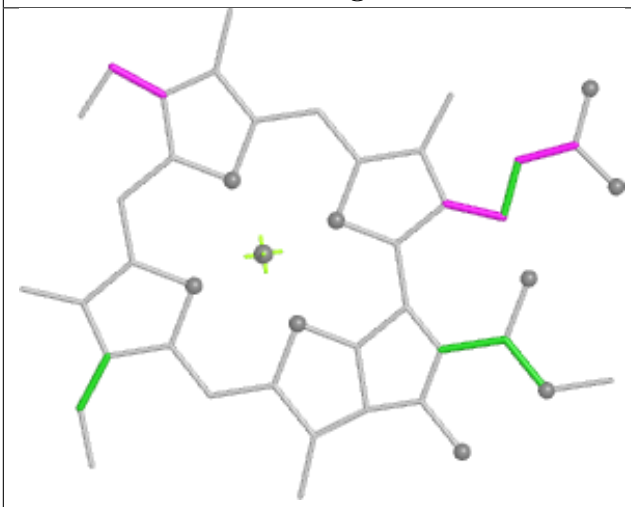

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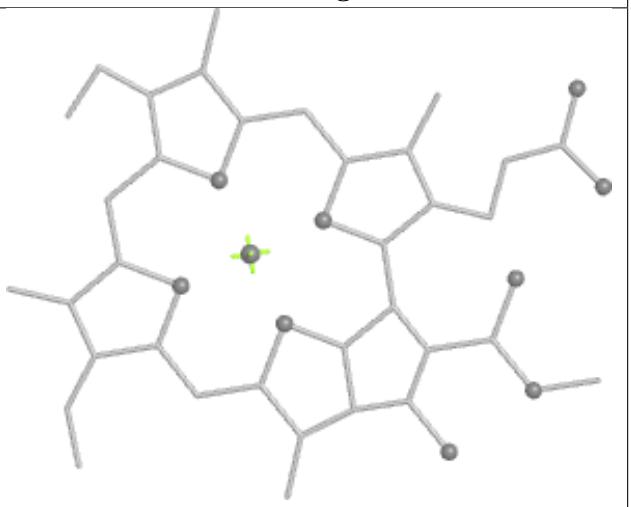
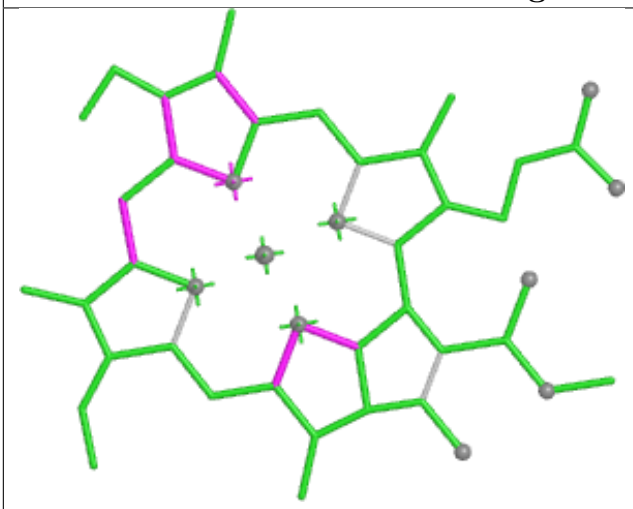


Rings

Ligand CLA 3 603



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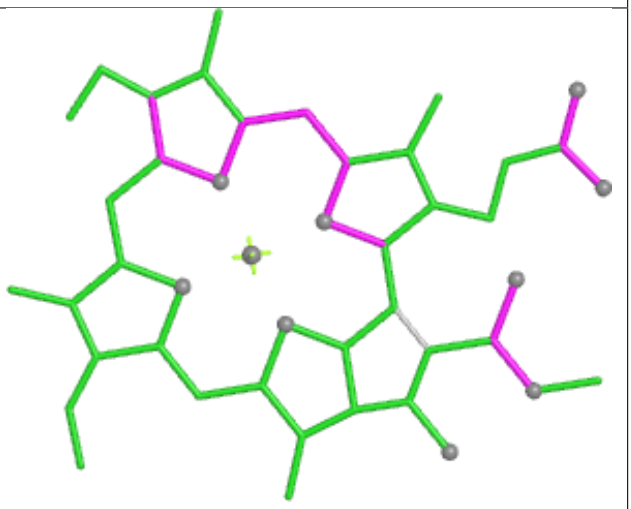

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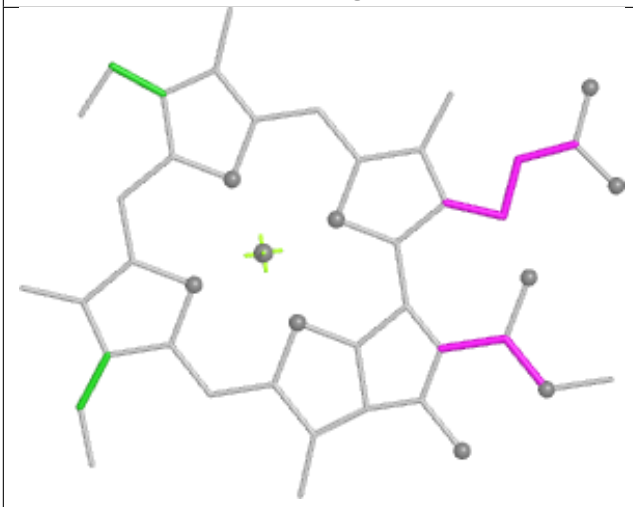
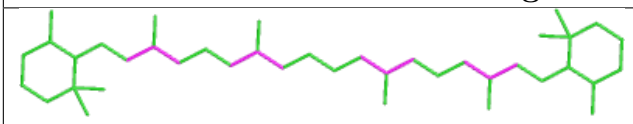


Torsions

Rings

Ligand BCR A 850



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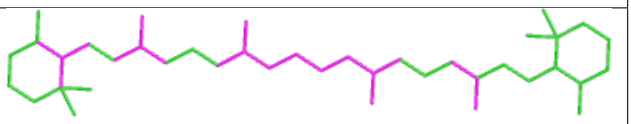

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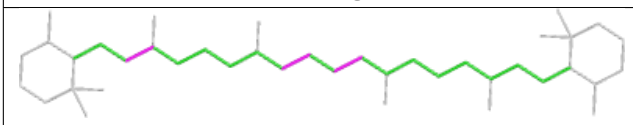

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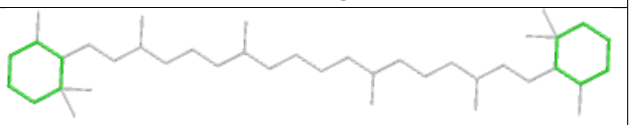
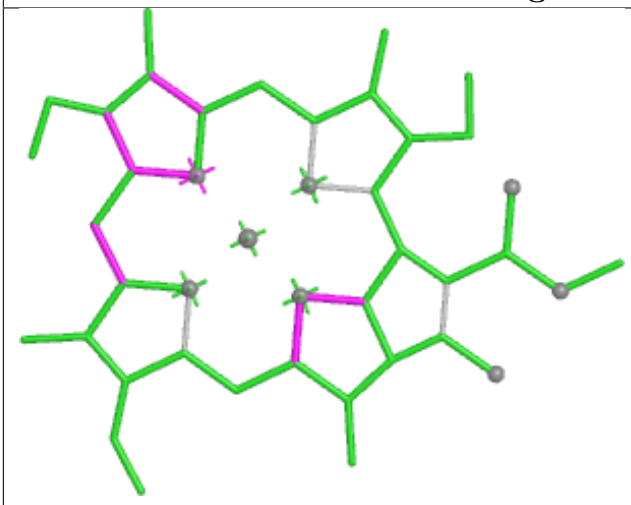


Rings

Ligand CLA 4 610



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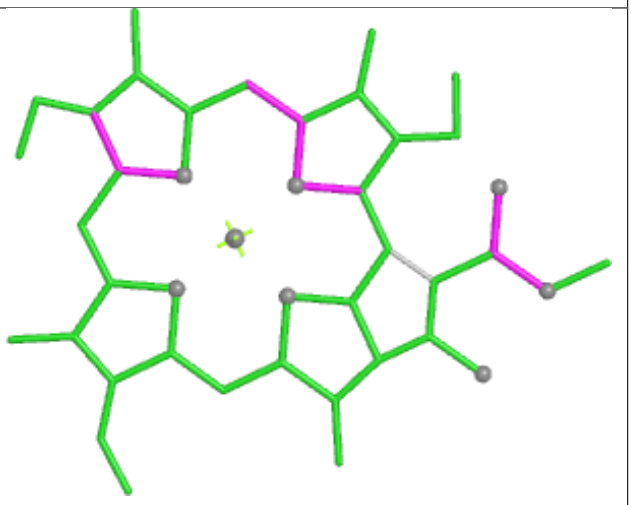

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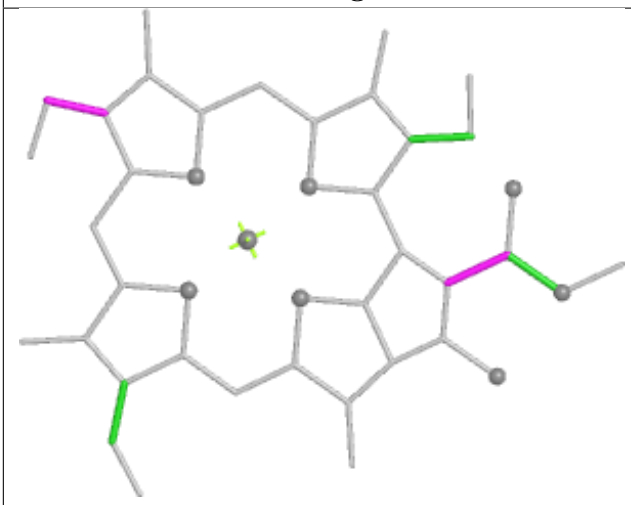
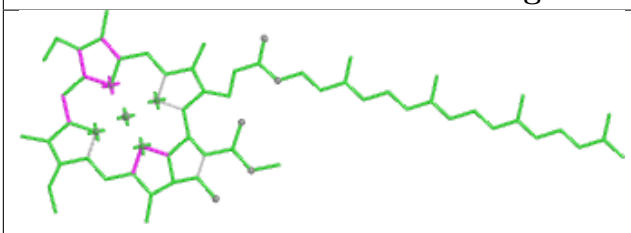


Torsions

Rings

Ligand CLA A 803



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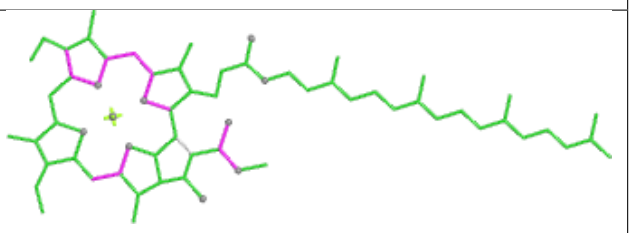

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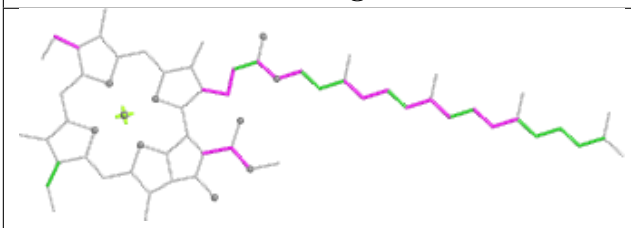

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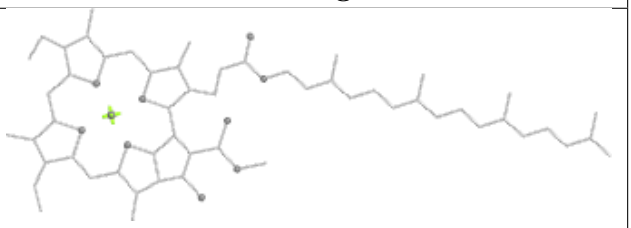
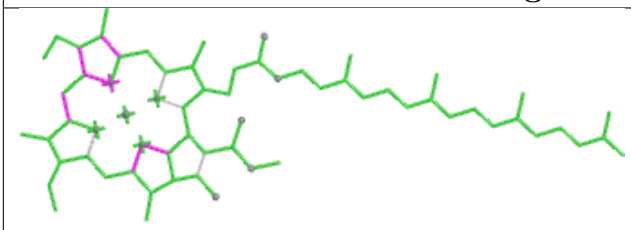


Rings

Ligand CLA B 806



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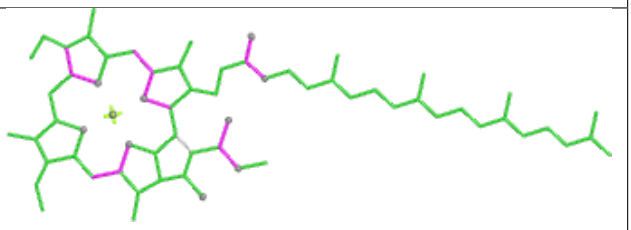

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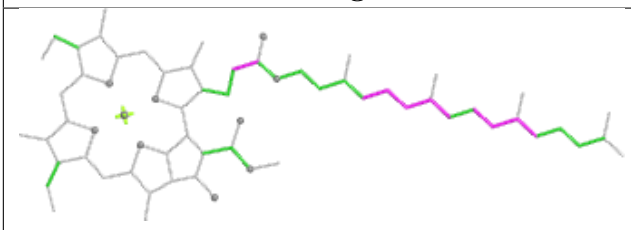

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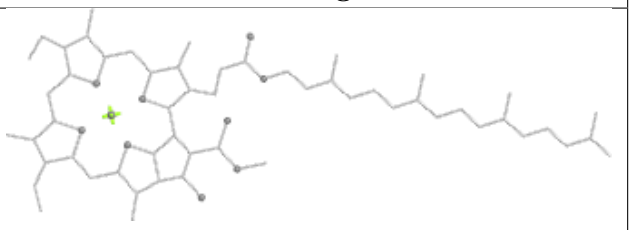
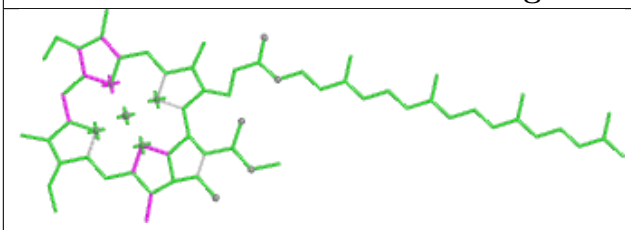


Rings

Ligand CLA A 811



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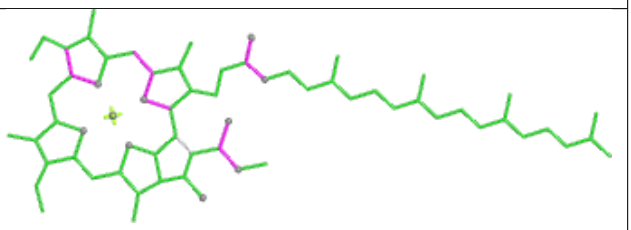
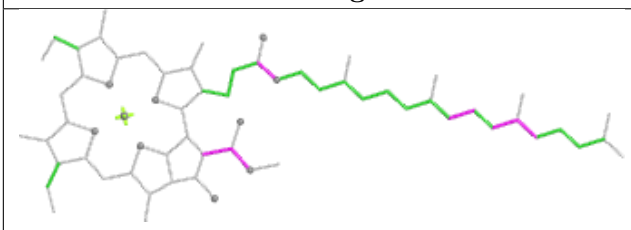


Bond angles



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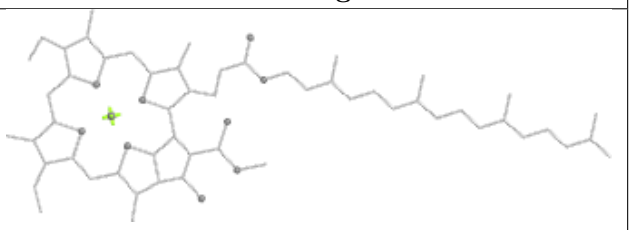
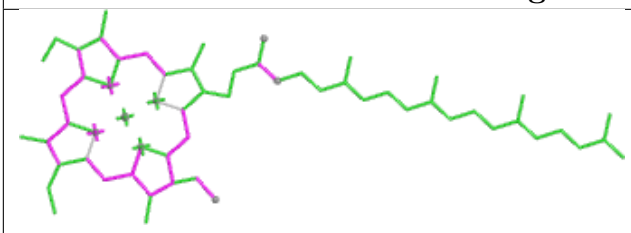


Rings

Ligand CL0 A 801



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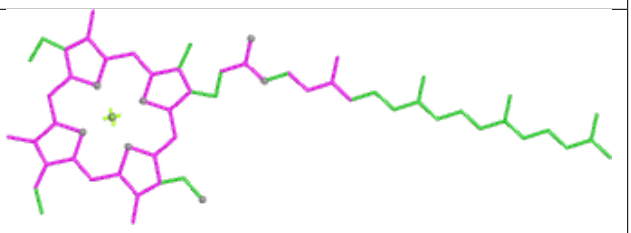

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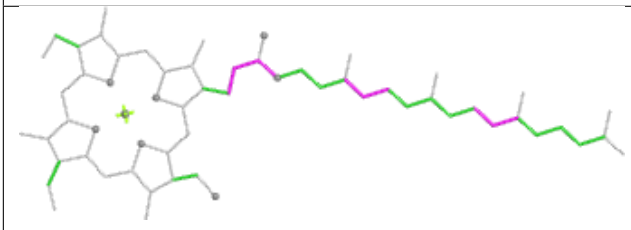

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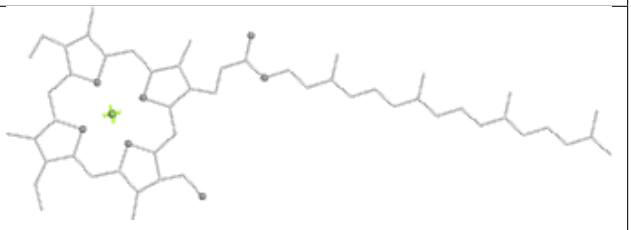
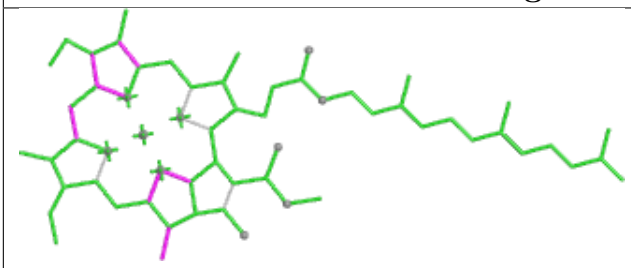
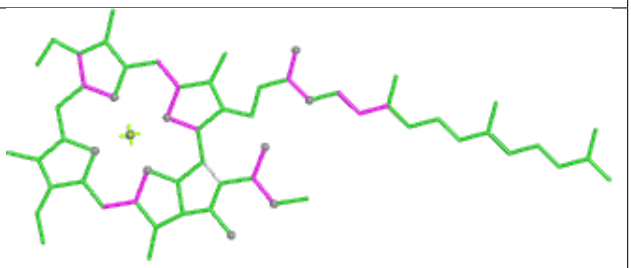
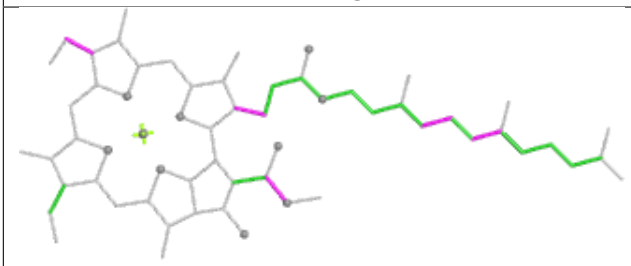
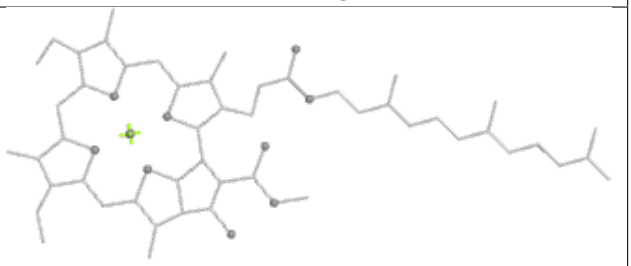
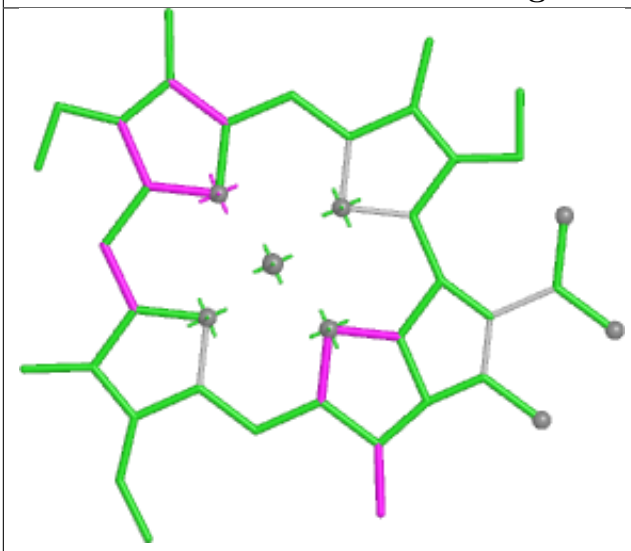


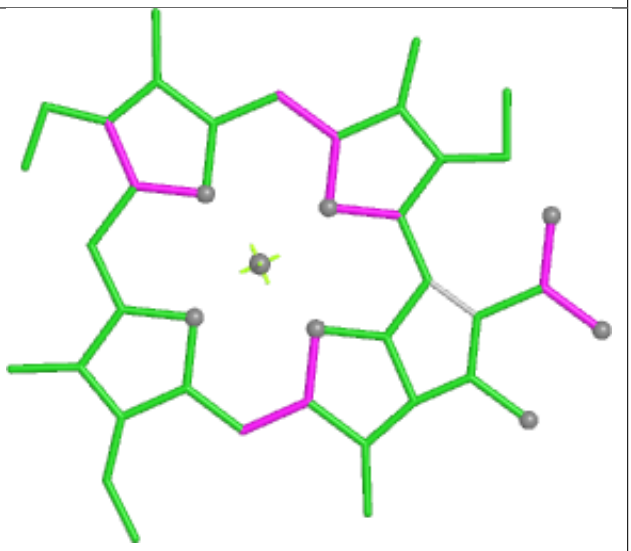
Rings

Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

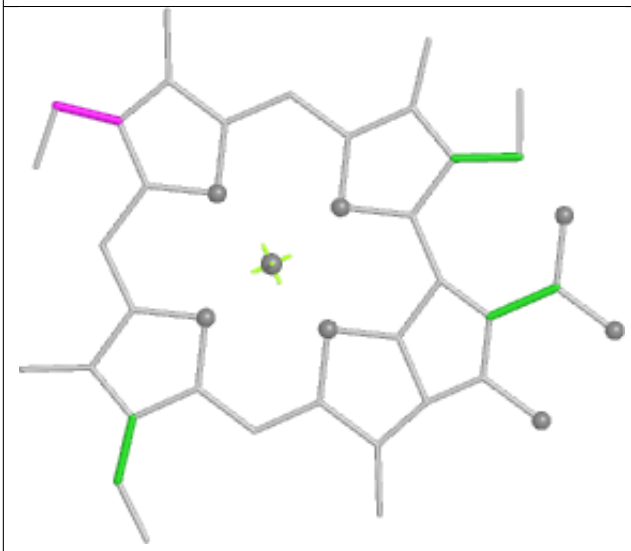
Ligand CLA 3 604



Bond lengths



Bond angles



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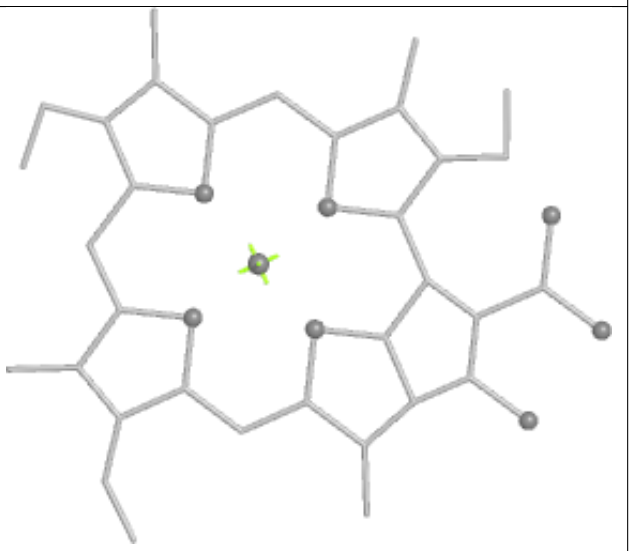
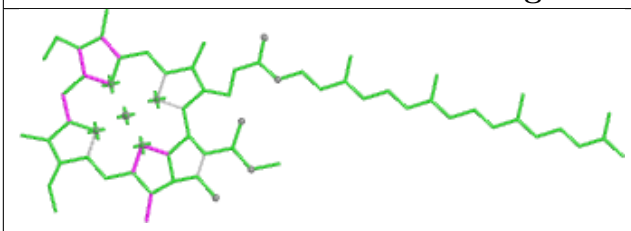


Rings

Ligand CLA B 805



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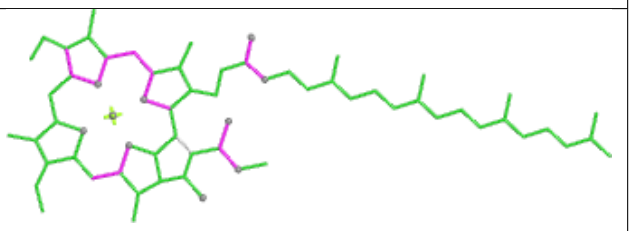
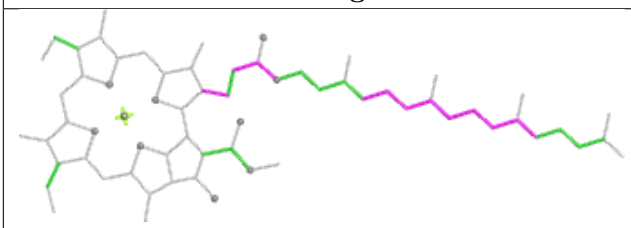
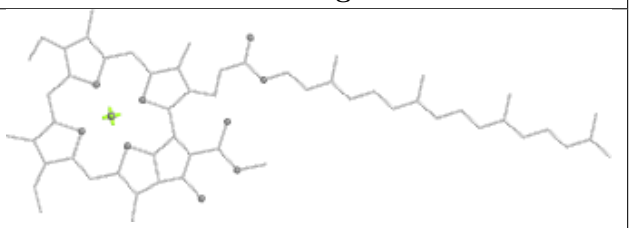


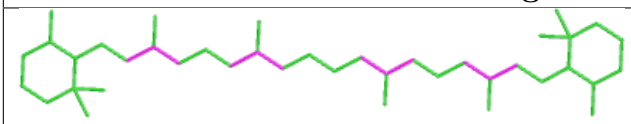
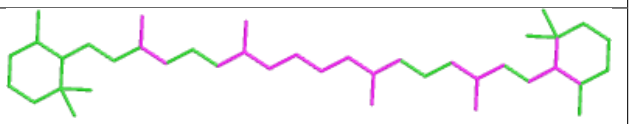
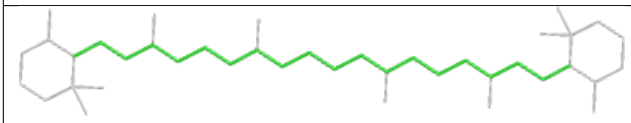
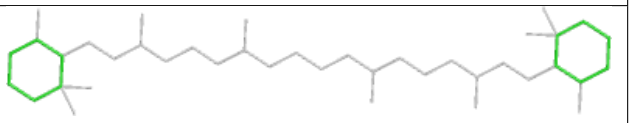
Bond angles

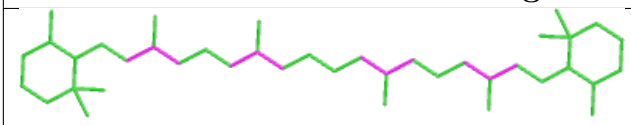
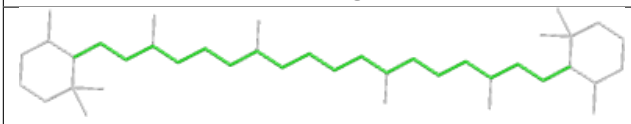
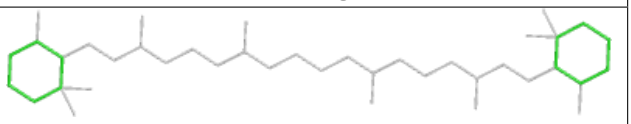


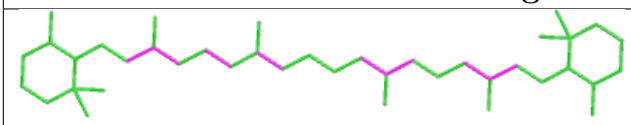
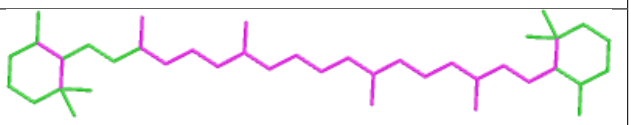
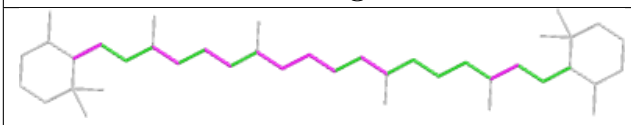
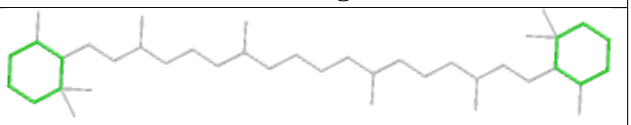
Torsions

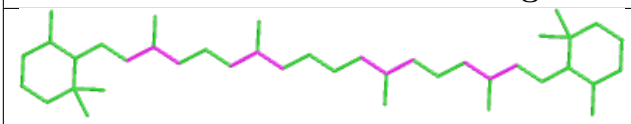
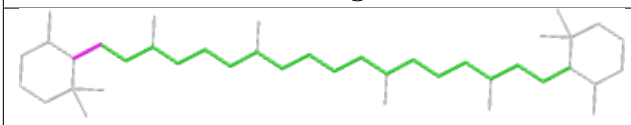
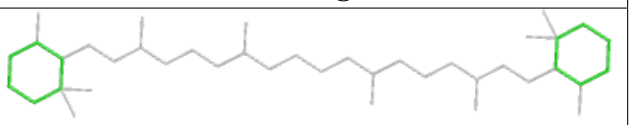


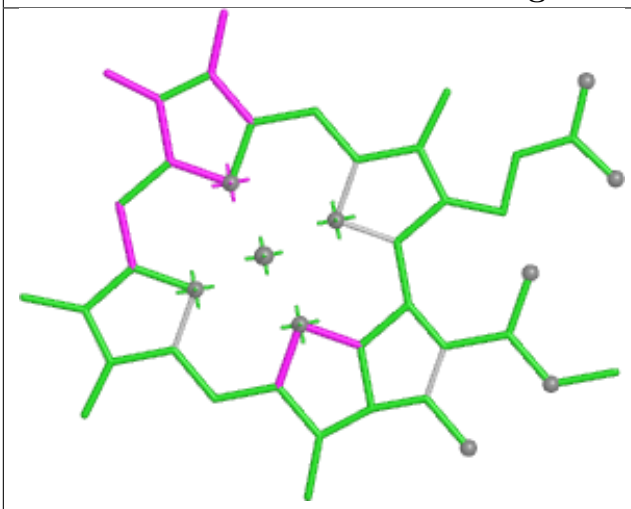
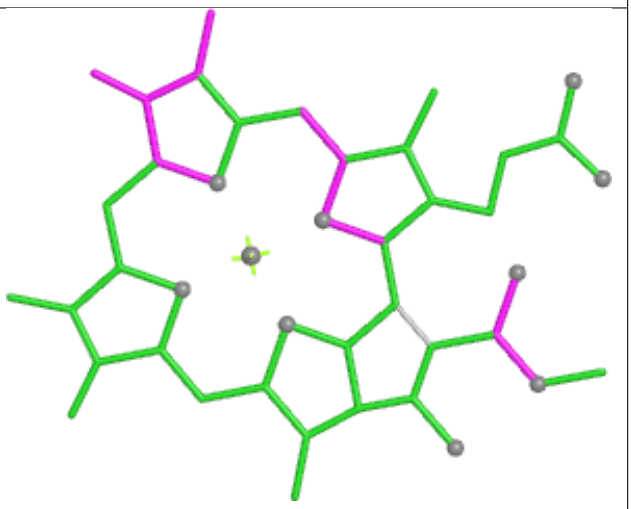
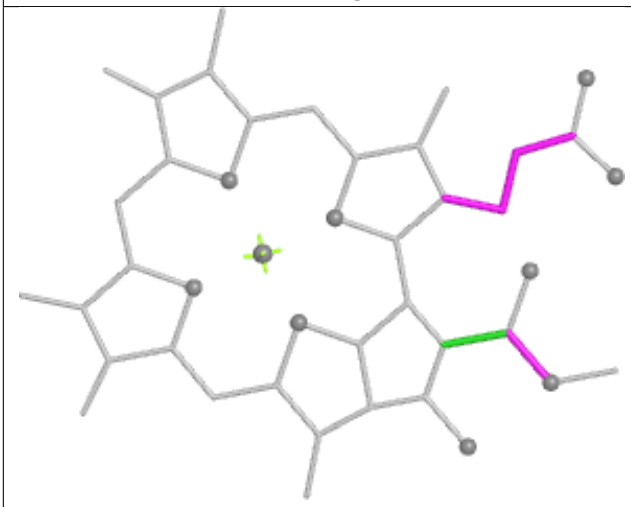
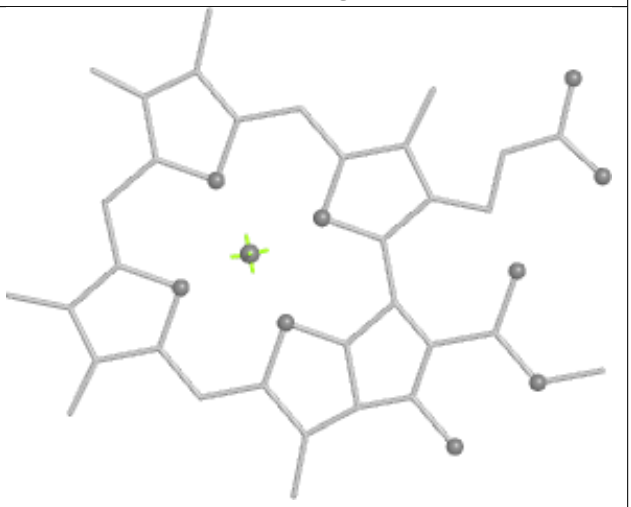
Rings

Ligand BCR A 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 848	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand BCR A 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR G 204	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand CLA 4 604	
 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.

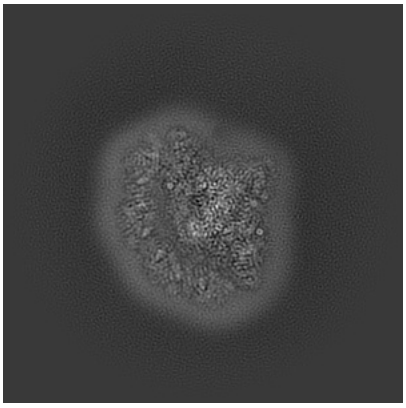
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-36037. These allow visual inspection of the internal detail of the map and identification of artifacts.

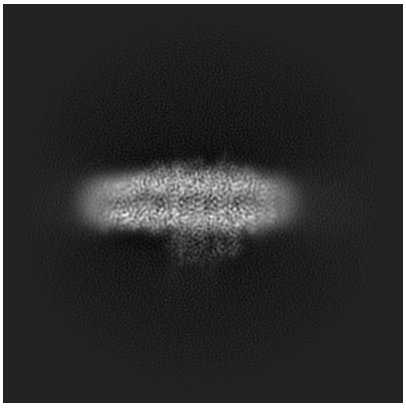
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

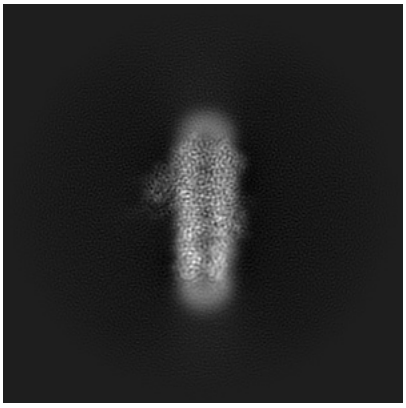
6.1.1 Primary map



X



Y

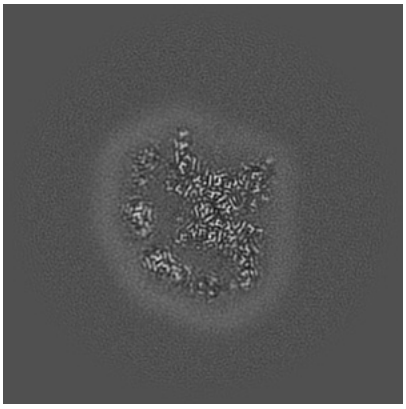


Z

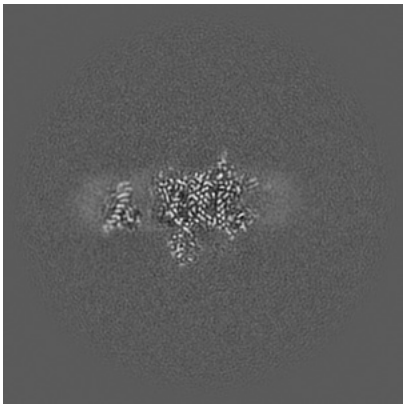
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

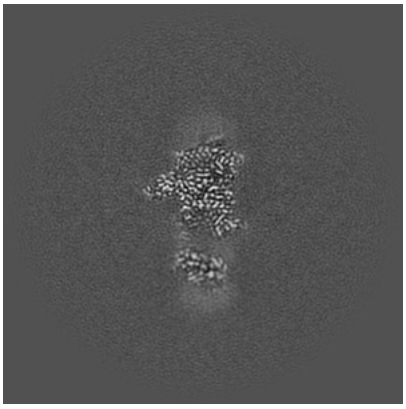
6.2.1 Primary map



X Index: 168



Y Index: 168

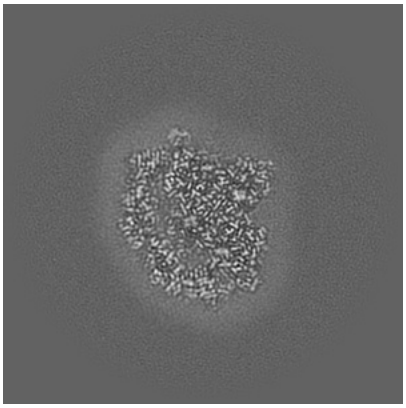


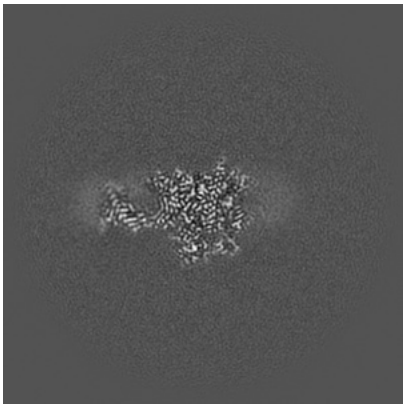
Z Index: 168

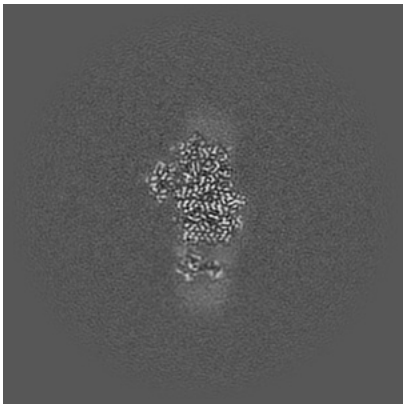
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 157

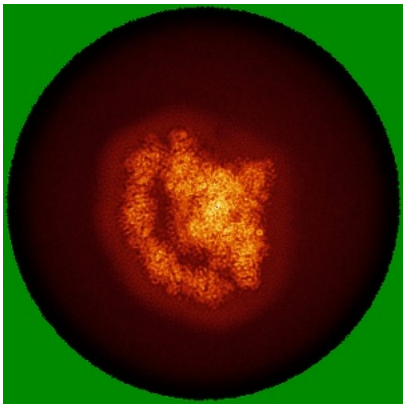

Y Index: 174

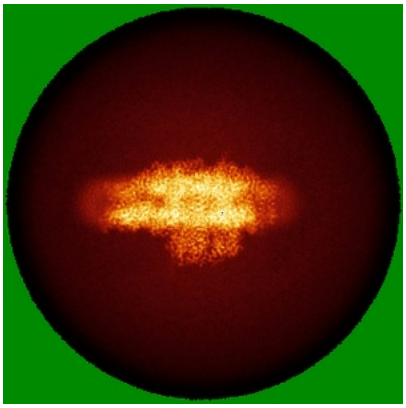

Z Index: 182

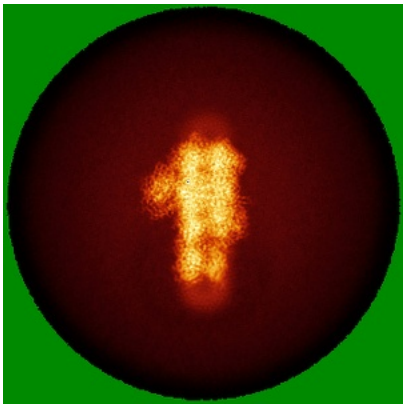
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

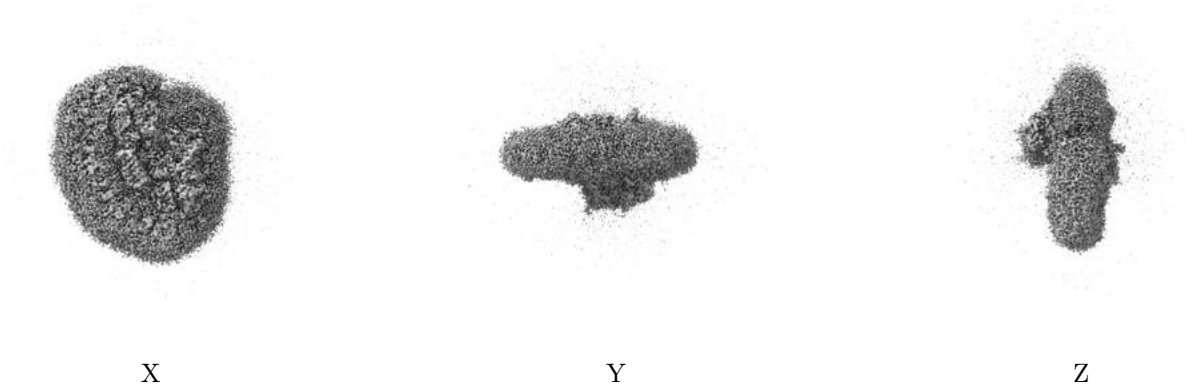

Y


Z

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 3.21. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

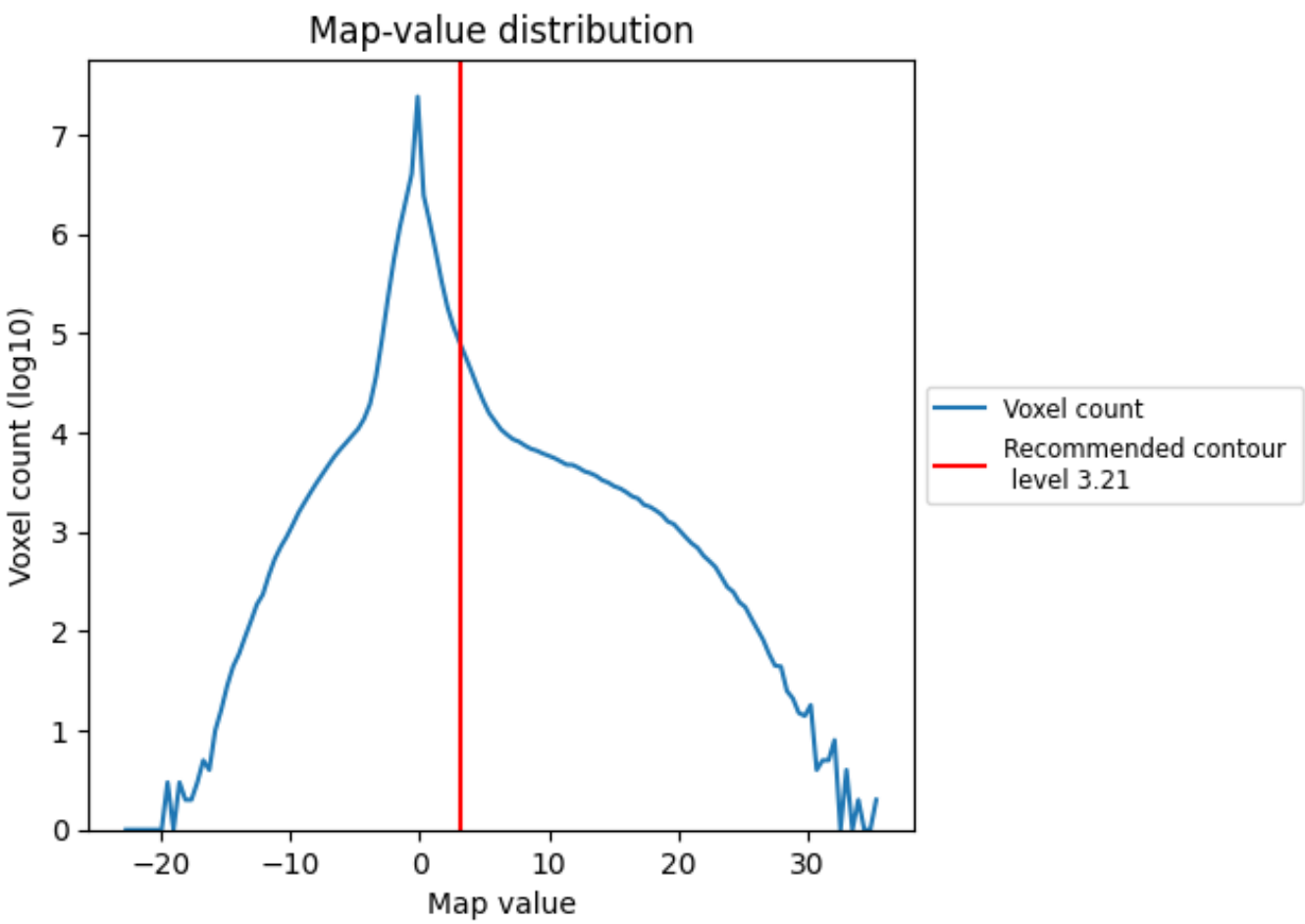
6.6 Mask visualisation (i)

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

7 Map analysis (i)

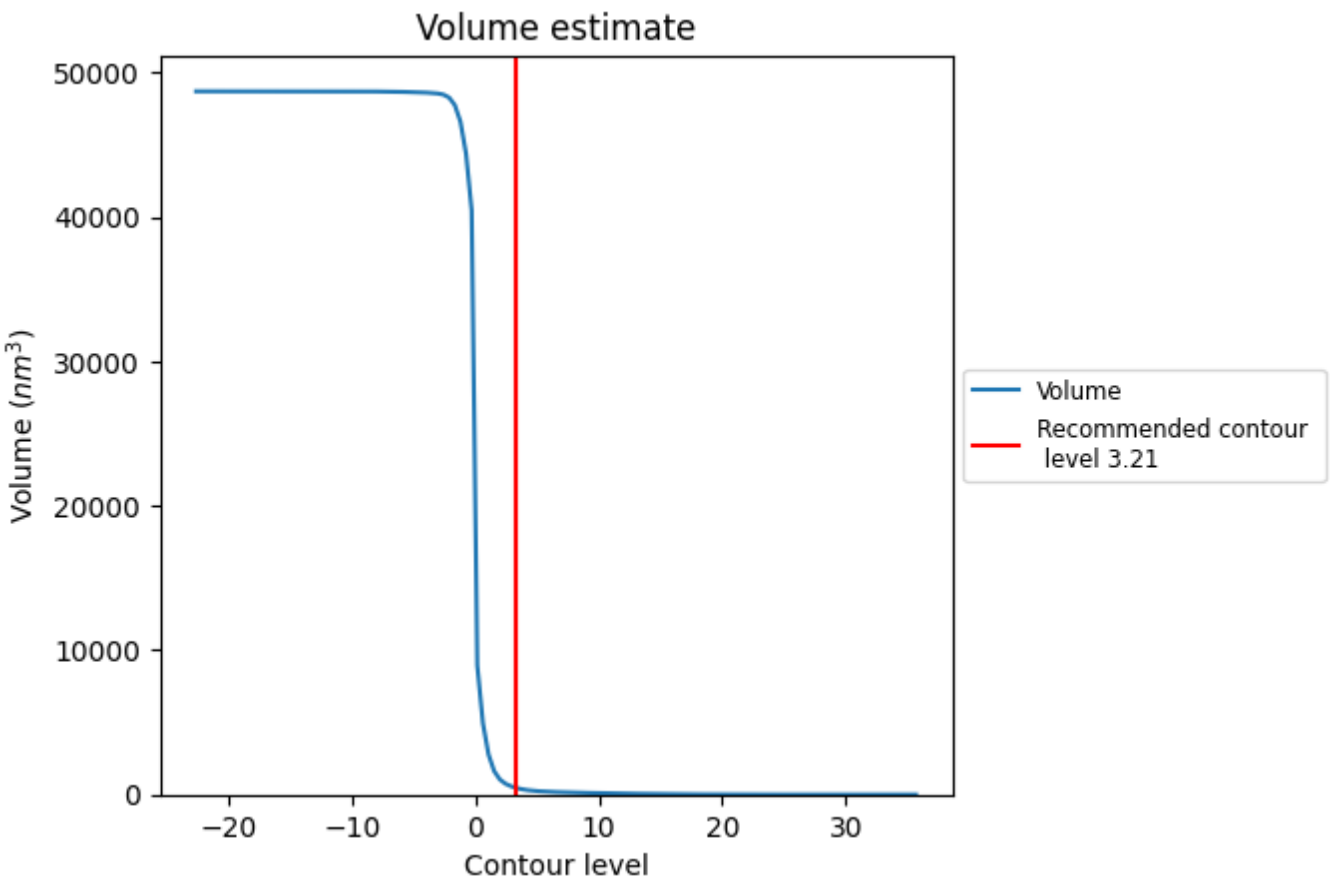
This section contains the results of statistical analysis of the map.

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.

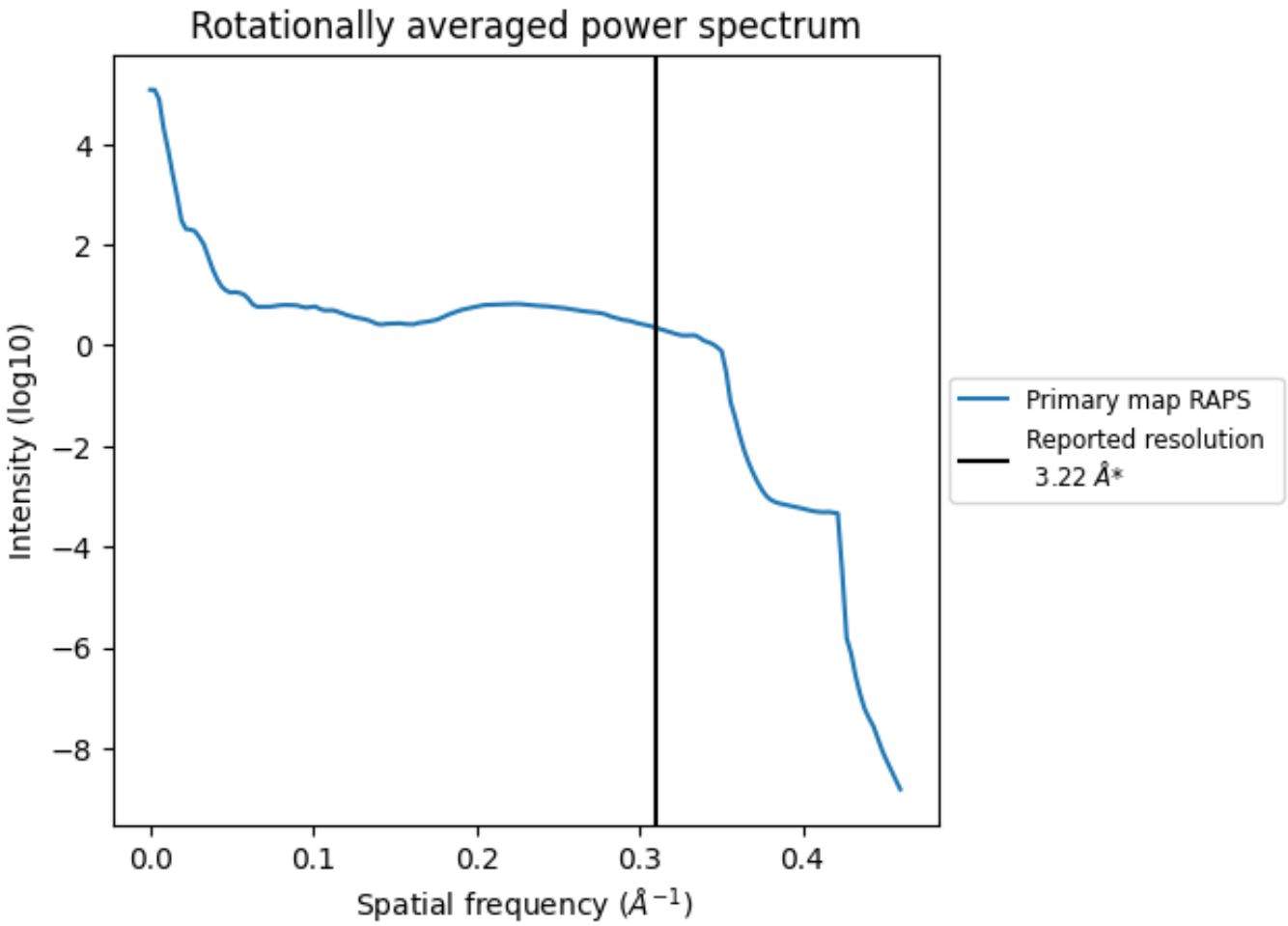
7.2 Volume estimate (i)



The volume at the recommended contour level is 489 nm^3; this corresponds to an approximate mass of 442 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 0.311 Å^{-1}

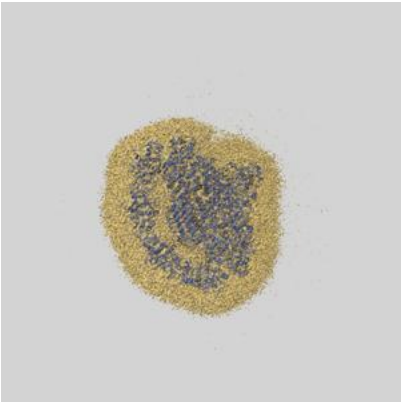
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

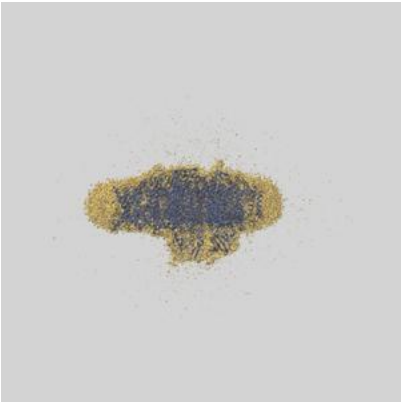
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-36037 and PDB model 8J7B. Per-residue inclusion information can be found in section 3 on page 22.

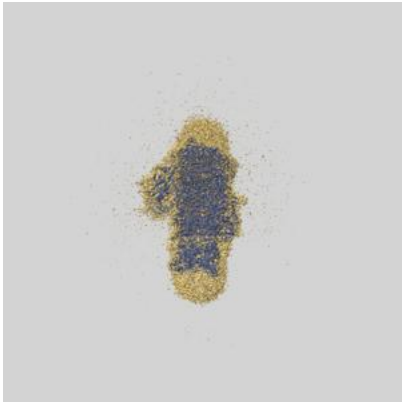
9.1 Map-model overlay (i)



X



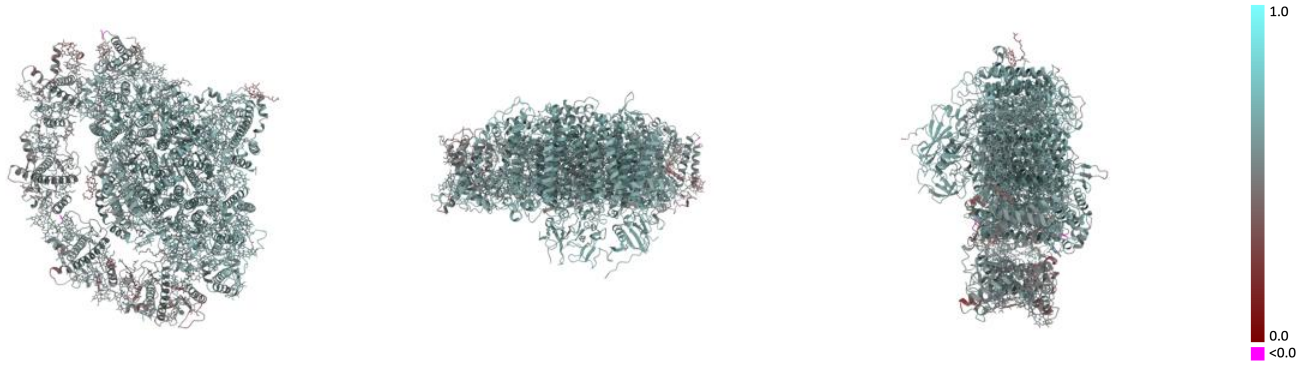
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.21 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.

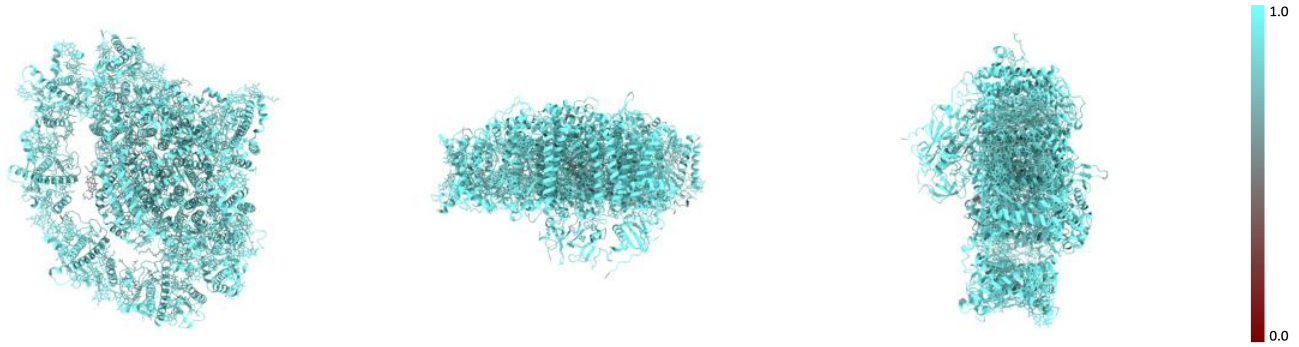
9.2 Q-score mapped to coordinate model (i)



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.

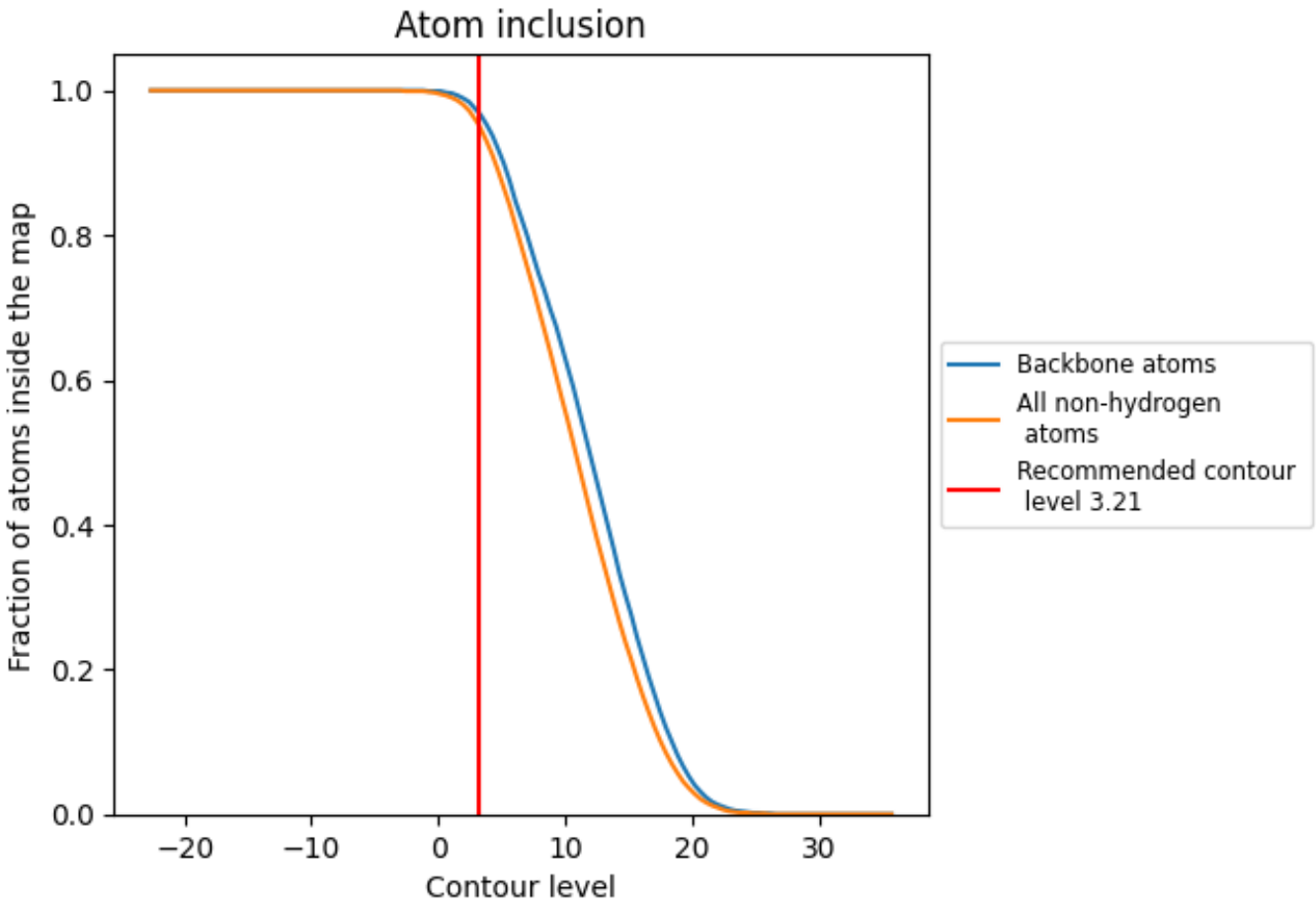
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.21).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (3.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.5760
1	0.9220	0.4980
2	0.9450	0.5180
3	0.9450	0.5120
4	0.9520	0.5350
A	0.9570	0.6050
B	0.9670	0.6150
C	0.9810	0.6130
D	0.9770	0.6080
E	0.9760	0.6050
F	0.9210	0.5690
G	0.9520	0.5730
H	0.9350	0.5650
I	0.9790	0.6000
J	0.8600	0.5340
K	0.8620	0.4680
L	0.9610	0.5960