Full wwPDB EM Validation Report (i)

Sep 15, 2026 – 12:16 AM JST

PDB ID	:	8J7A / pdb_00008j7a
EMDB ID	:	EMD-36036
Title	:	Coordinates of Cryo-EM structure of the Arabidopsis thaliana PSI in state 1 (PSI-ST1)
Authors	:	Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on	:	2023-04-27
Resolution	:	3.06 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:

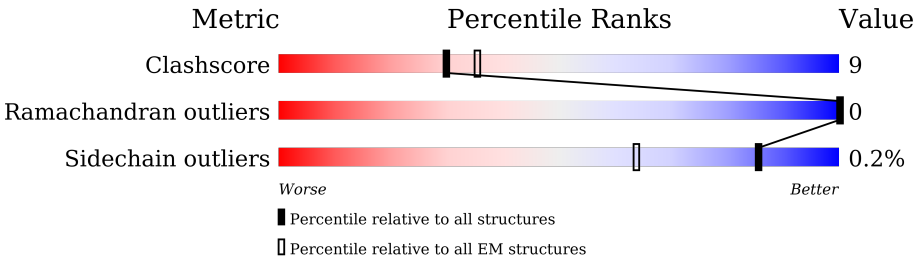
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

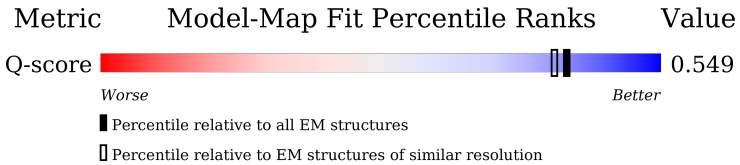
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.06 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	13976 (2.56 - 3.56)

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	51% 17% 31%
2	2	257	69% 9% 22%
3	3	273	73% 7% 21%
4	4	251	65% 13% 22%

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Mol	Chain	Length	Quality of chain
5	A	750	86% 8% 5%
6	B	734	90% 9%
7	C	81	83% 16%
8	D	204	66% 30%
9	E	143	41% 55%
10	F	221	62% 6% 33%
11	G	160	51% 6% 43%
12	H	145	54% 6% 41%
13	I	37	81% 16%
14	J	44	70% 23% 7%
15	K	130	37% 6% 57%
16	L	219	67% 6% 27%

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 34246 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	166	1296	844	215	232	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	217	1661	1085	269	302	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	709	5582	3662	946	956	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	149	1183	773	203	204	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	86	660	431	104	125	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

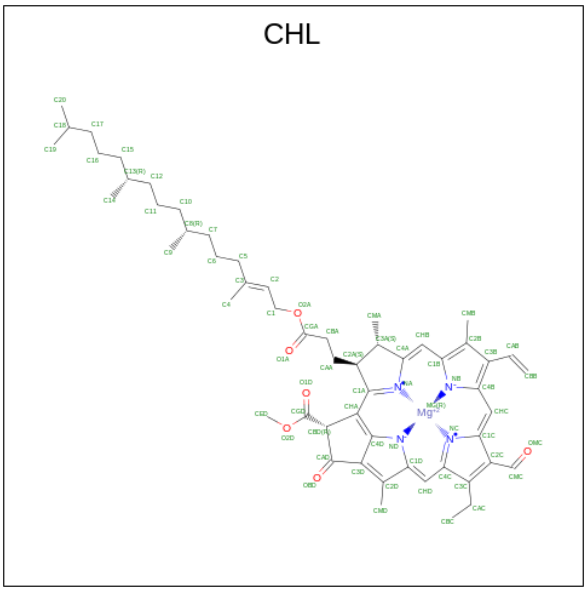
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K	56	397	256	64	74	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	159	1200	795	190	213	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	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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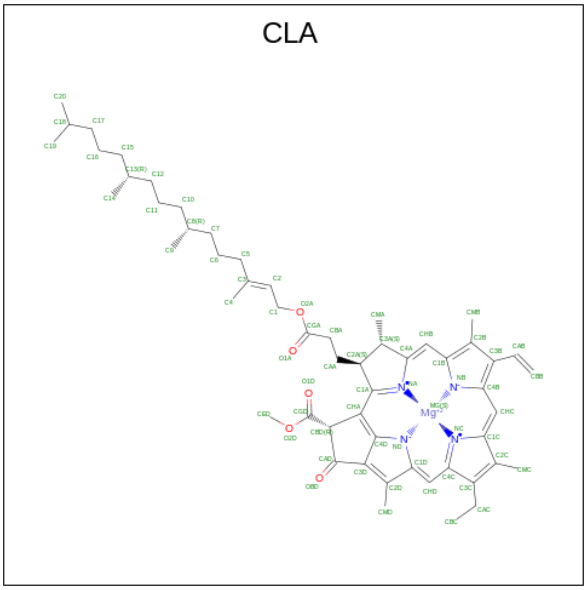
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	2	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
17	2	1	47	36	1	4	6	0
			Total	C	Mg	N	O	
17	2	1	42	33	1	4	4	0
			Total	C	Mg	N	O	
17	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	4	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	4	1	41	32	1	4	4	0
			Total	C	Mg	N	O	
17	4	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	43	34	1	4	4	0
			Total	C	Mg	N	O	
18	2	1	65	55	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	35	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	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	47	37	1	4	5	0
			Total	C	Mg	N	O	
18	2	1	45	35	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	54	44	1	4	5	0
			Total	C	Mg	N	O	
18	3	1	55	45	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	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	3	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
18	3	1	60	50	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	41	33	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	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	4	1	44	34	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	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	4	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
18	4	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	4	1	50	40	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	57	47	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	45	35	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	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	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	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	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	59	49	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	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	55	45	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	55	45	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	52	42	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	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	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	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	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	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	41	33	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

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Mol	Chain	Residues	Atoms					AltConf
			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	55	45	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	62	52	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	52	42	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	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	59	49	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	43	35	1	4	3	0
			Total	C	Mg	N	O	
18	B	1	56	46	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	43	35	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			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	65	55	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	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	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	60	50	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	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	54	44	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	F	1	51	41	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	G	1	42	34	1	4	3	0

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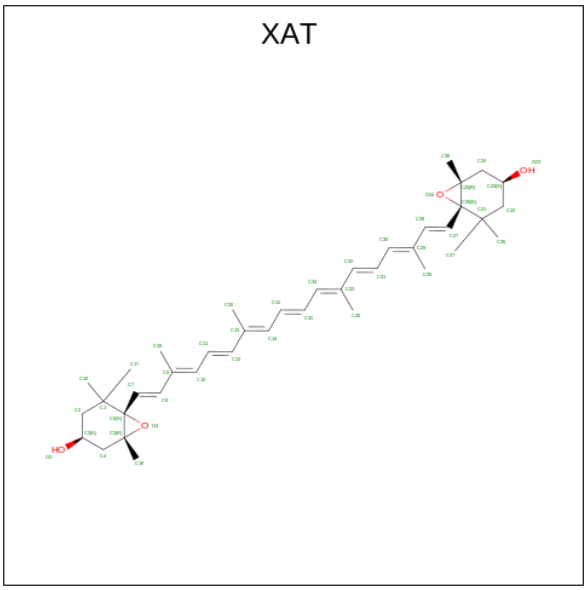
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	G	1	45	35	1	4	5	0
18	G	1	45	35	1	4	5	0
18	H	1	60	50	1	4	5	0
18	K	1	46	36	1	4	5	0
18	K	1	45	35	1	4	5	0
18	K	1	37	31	1	4	1	0
18	L	1	45	35	1	4	5	0
18	L	1	65	55	1	4	5	0
18	L	1	45	35	1	4	5	0

- 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

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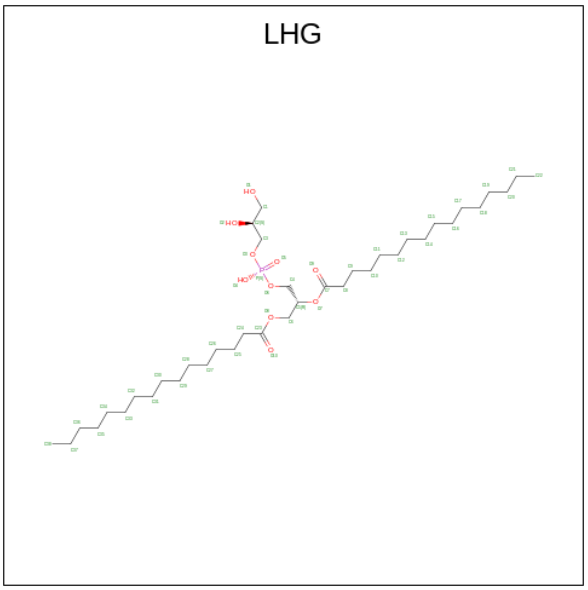
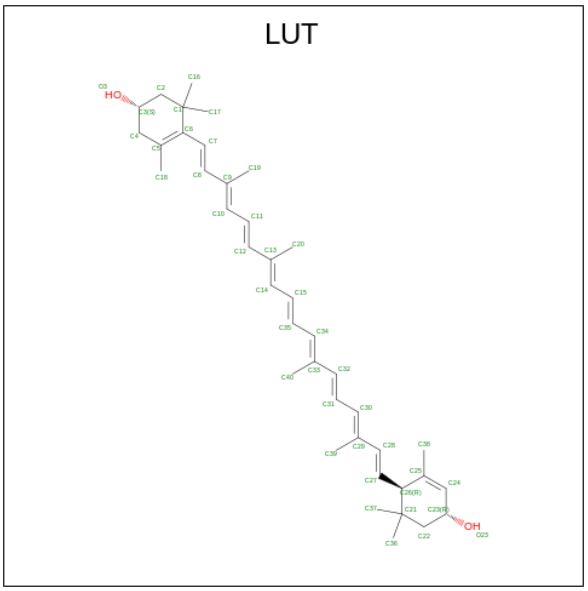
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
19	4	1	44	40	4	0

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



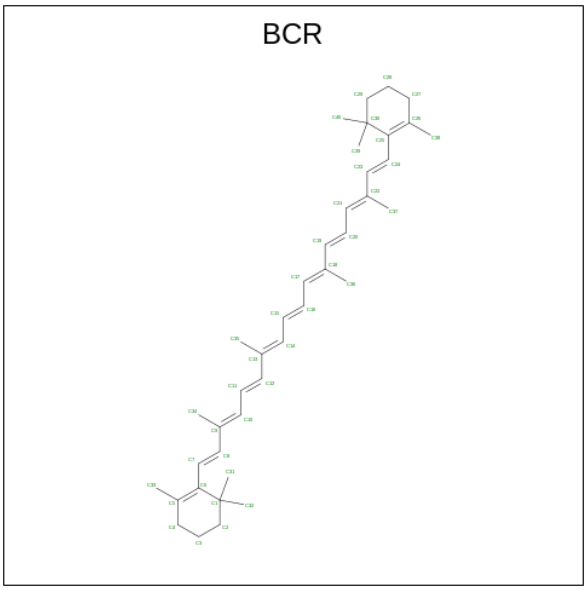
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	1	1	49	38	10	1	0
			Total	C	O	P	
20	2	1	37	26	10	1	0
			Total	C	O	P	
20	A	1	30	19	10	1	0
			Total	C	O	P	
20	A	1	49	38	10	1	0
			Total	C	O	P	
20	B	1	38	27	10	1	0
			Total	C	O	P	
20	B	1	49	38	10	1	0

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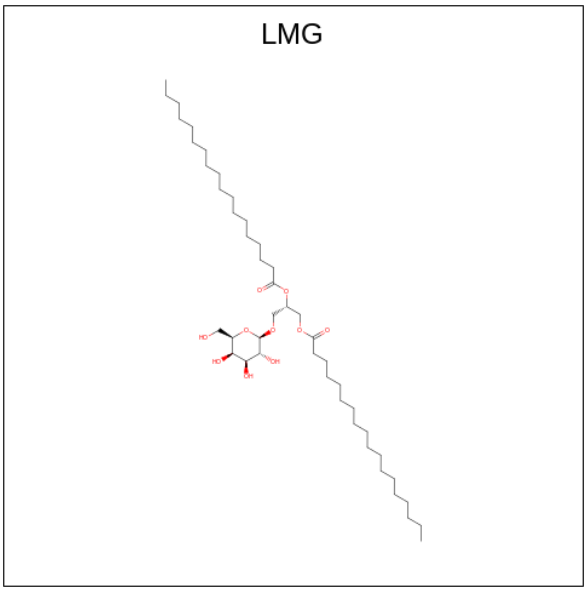
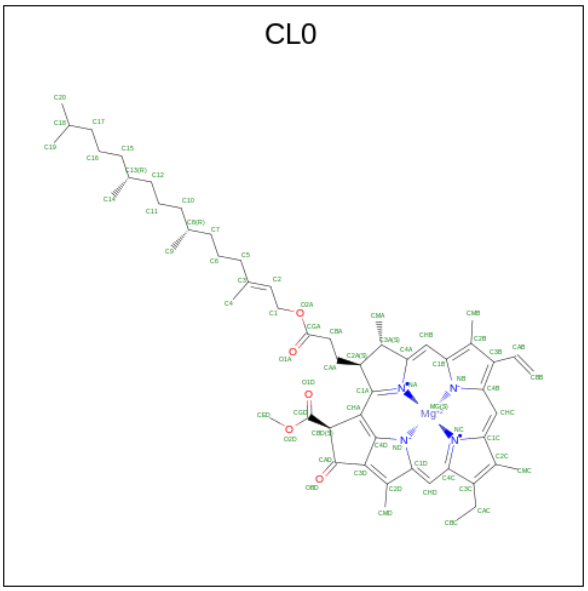
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
22	L	1	40	40	0
			Total	C	
22	L	1	40	40	0
			Total	C	
22	L	1	40	40	0

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



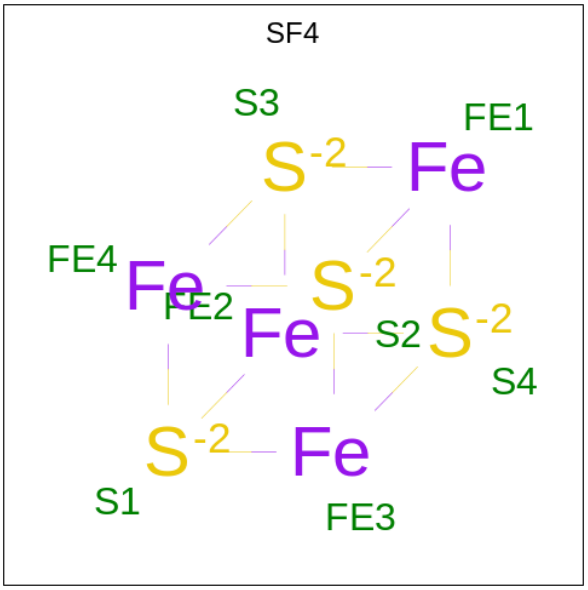
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	4	1	33	23	10	0
			Total	C	O	
23	4	1	39	29	10	0

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



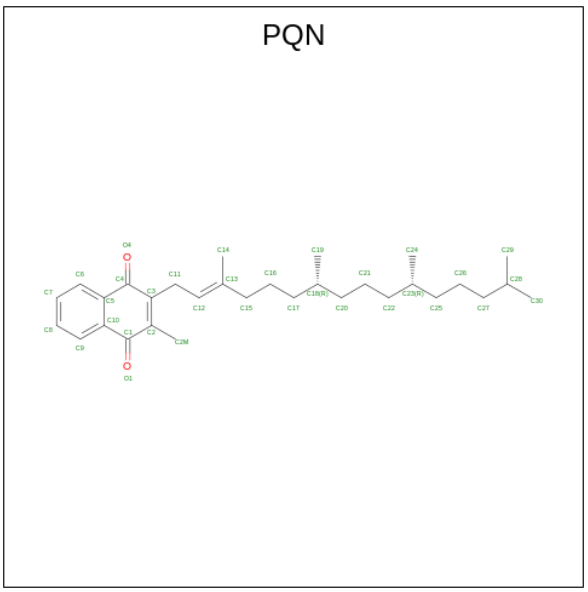
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	A	1	60	52	1	4	3	0

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



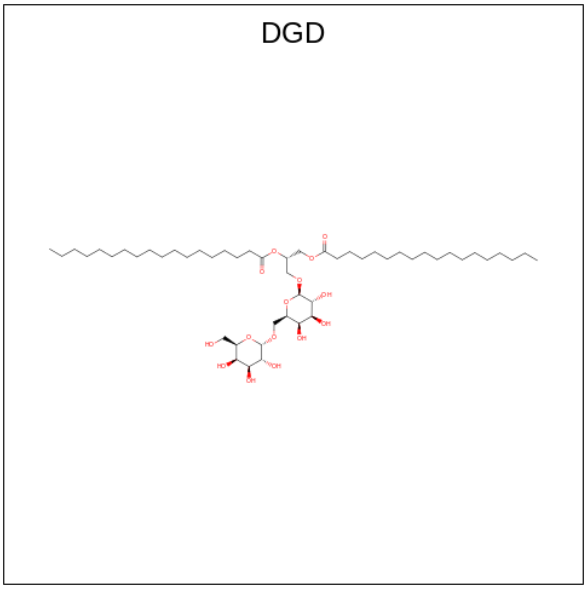
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
25	A	1	8	4	4	0
25	C	1	8	4	4	0
25	C	1	8	4	4	0

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

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



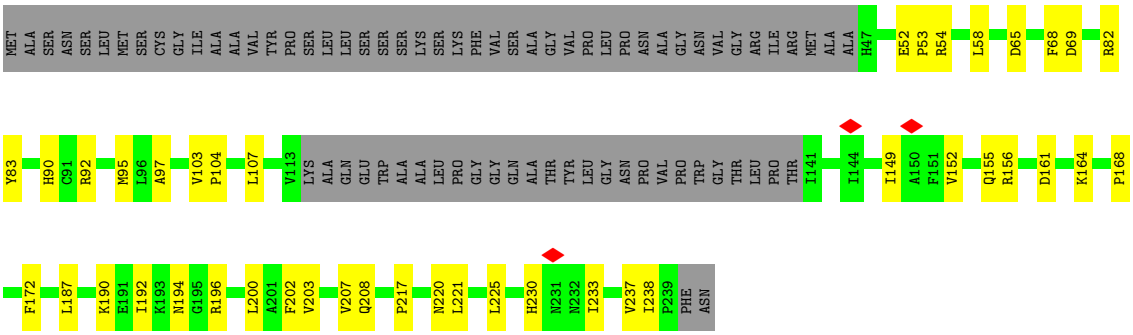
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	B	1	66	51	15	0

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.

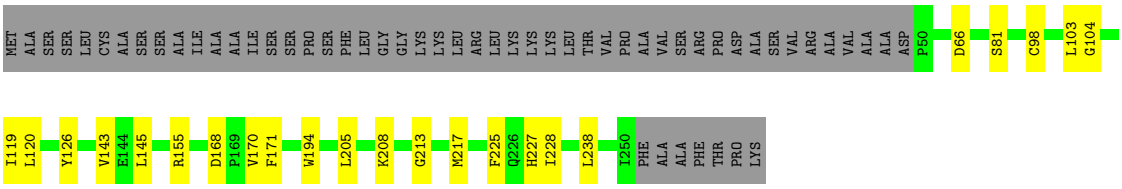
• Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic

Chain 1:



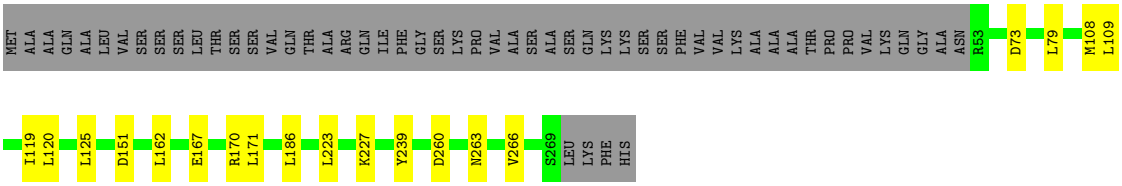
• Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

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: 65% 13% 22%

MET ALA THR VAL THR THR HIS ALA SER ALA SER ILE PHE ARG PRO CYS THR SER LYS PRO ARG PHE LEU THR GLY SER SER GLY ARG LEU ASN ARG ASP LEU SER PHE THR SER ILE GLY SER SER ALA LYS THR SER SER PHE LYS VAL GLU ALA LYS K54 F77 L82 K90

Q94 G100 R101 W102 A103 M104 I121 I122 D129 K132 S140 T141 I145 I148 L149 E154 R157 Q175 L193 N194 L206 M213 L214 Q222 K228 E232 Q236 H237 L238 S239 D240 N244 T245 I246 T249 PHE ASN

- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 86% 8% 5%

MET ILE ILE ARG SER PRO GLU PRO GLU VAL LYS ILE LEU VAL ASP ARG ASP PRO ILE LYS THR SER PHE GLU GLU TRP ALA LYS PRO GLY HIS PHE SER ARG THR ILE ALA LYS GLY PRO D41 S61 S72 F90 H91 G92 S96 Q113 W175 Y178 H197

H213 L236 E239 H294 A297 F302 A305 R310 T311 N312 H317 F330 H335 L338 A348 N353 L360 T361 A365 P373 T379 T389 H390 H391 H392 W393 L505 G508 L512 V515 V519 A520 L521 L522 P523 I536

F571 C582 S585 D588 W596 I605 V616 I620 V626 I657 F671 H675 A679 G688 I699 L717 R723 W739 V749 GLY

- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 90% 9%

MET ALA L3 S9 I25 A26 D36 R41 L54 A55 I56 I57 D80 H83 I91 K92 D93 P112 V120 W124 L129 R174 L182 H276 I280 R292 T293 N294 L304 A307 T325 L338 A339 I382 N403 M411

H432 G435 D441 L444 E450 E456 Q461 W462 I463 K469 F509 D516 F517 H521 A522 I523 P548 D549 D569 I570 S571 D574 W582 Y593 M617 R621 W648 M649 F652 L655 V656 T659 M662 W667 L678

R684 D695 K696 P697 Q704 A705 R706 L707 S714 G734

- Molecule 7: Photosystem I iron-sulfur center

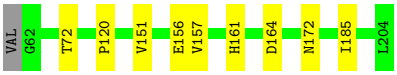
Chain C: 83% 16%

MET S2 H3 D9 T15 D24 M28 T60 D61 F62 R66 E72 M77 Y81

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

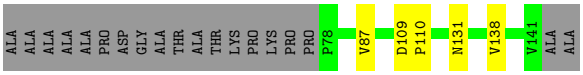
Chain D: 66% 30%

MET ALA THR GLN ALA ALA GLY ILE PHE SER PRO ALA ILE THR THR THR THR SER ALA VAL LYS LYS LEU HIS LEU PHE SER SER SER HIS ARG PRO LYS SER LEU SER PHE THR LYS THR ALA ILE ARG ALA GLU LYS THR GLU SER SER SER ALA ALA PRO ALA VAL LYS GLU ALA PRO



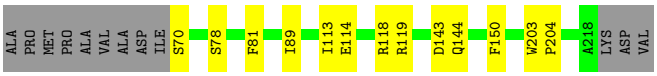
• Molecule 9: Photosystem I reaction center subunit IV A, chloroplastic

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: 70% 23% 7%

M1 R2 V10 A11 P12 L22 L25 L26 I29 F33 A36 L37 T38 F41 PHE SER PHE

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

Chain K: 37% 6% 57%

MET ALA SER THR MET MET THR THR LEU PRO GLN PHE ASN GLY LEU ARG ALA THR LYS ILE SER ALA ALA PRO VAL GLN GLY LEU ALA SER VAL GLN PRO MET ARG ARG LYS GLY ASN GLY ALA LEU GLY ALA LYS CYS D47 M57 F70 GLY LEU ALA PRO SER ALA ASN ARG LYS

ALA THR ALA GLY LEU ARG LEU GLU ALA ARG ASP SER GLY LEU GLN THR G96 T102 L103 A104 A108 T111 V112 I115 I116 G117 I127 GLY ALA ILE

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

Chain L: 67% 6% 27%

MET ALA ALA SER ALA SER PRO MET ALA SER GLN LEU ARG SER SER PHE SER SER ALA SER LEU SER GLN ARG LEU ALA VAL PRO LYS GLY ILE SER GLY ALA PRO PHE GLY VAL SER PRO THR LYS ARG VAL SER SER PHE THR VAL ARG ALA VAL LYS SER ASP LYS THR THR F59

I65 E75 N90 V98 V107 L137 V144 I152 Y153 S168 L169 T170 L171 T172 L209 F217 VAL LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	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	48.607	Depositor
Minimum map value	-26.329	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.028	Depositor
Recommended contour level	2.57	Depositor
Map size (Å)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: DGD, CL0, BCR, LMG, CLA, SF4, PQN, XAT, LHG, LUT, CHL

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	0.17	0/1336	0.38	1/1816 (0.1%)
2	2	0.14	0/1622	0.28	0/2219
3	3	0.14	0/1712	0.28	0/2329
4	4	0.14	0/1599	0.27	0/2178
5	A	0.15	0/5772	0.26	0/7878
6	B	0.16	0/6065	0.27	0/8279
7	C	0.16	0/629	0.32	0/852
8	D	0.13	0/1157	0.27	0/1563
9	E	0.12	0/528	0.21	0/715
10	F	0.12	0/1213	0.24	0/1637
11	G	0.19	0/724	0.48	1/981 (0.1%)
12	H	0.12	0/680	0.24	0/927
13	I	0.14	0/245	0.28	0/333
14	J	0.19	0/336	0.40	0/458
15	K	0.14	0/401	0.30	0/542
16	L	0.13	0/1237	0.28	0/1690
All	All	0.15	0/25256	0.29	2/34397 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	64	PRO	CA-N-CD	-11.01	96.59	112.00
1	1	104	PRO	CA-N-CD	-9.12	99.23	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1296	0	1277	38	0
2	2	1566	0	1519	20	0
3	3	1661	0	1625	18	0
4	4	1551	0	1508	41	0
5	A	5582	0	5436	52	0
6	B	5854	0	5646	64	0
7	C	616	0	600	13	0
8	D	1128	0	1134	6	0
9	E	517	0	526	3	0
10	F	1183	0	1215	8	0
11	G	708	0	700	9	0
12	H	660	0	650	5	0
13	I	239	0	258	1	0
14	J	327	0	342	12	0
15	K	397	0	409	5	0
16	L	1200	0	1202	12	0
17	1	93	0	62	7	0
17	2	226	0	150	5	0
17	3	45	0	30	0	0
17	4	169	0	100	4	0
18	1	496	0	354	26	0
18	2	434	0	352	22	0
18	3	498	0	377	10	0
18	4	527	0	412	22	0
18	A	2483	0	2456	114	0
18	B	2284	0	2242	79	0
18	F	149	0	123	8	0
18	G	132	0	97	1	0
18	H	60	0	59	1	0
18	K	128	0	91	1	0
18	L	155	0	138	6	0
19	1	44	0	56	9	0
19	2	44	0	56	6	0
19	4	44	0	52	18	0
20	1	49	0	74	20	0
20	2	37	0	44	0	0
20	A	79	0	104	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	87	0	120	1	0
21	1	42	0	56	9	0
21	2	84	0	112	12	0
21	3	42	0	56	7	0
21	4	42	0	56	3	0
22	3	40	0	56	2	0
22	4	40	0	56	8	0
22	A	240	0	336	31	0
22	B	320	0	448	49	0
22	F	40	0	56	1	0
22	G	40	0	56	3	0
22	I	40	0	56	2	0
22	J	40	0	56	4	0
22	K	80	0	112	9	0
22	L	120	0	168	14	0
23	4	72	0	84	1	0
24	A	60	0	68	7	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	A	33	0	46	5	0
26	B	33	0	46	1	0
27	B	66	0	96	8	0
All	All	34246	0	33616	620	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 (620) 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)
21:2:619:LUT:H8	21:2:619:LUT:H181	1.55	0.88
4:4:77:PHE:HE2	19:4:617:XAT:C38	1.88	0.85
6:B:54:LEU:HD12	18:B:813:CLA:HED1	1.65	0.79
18:1:604:CLA:HMB3	19:1:614:XAT:H162	1.65	0.78
2:2:143:VAL:HG22	18:4:613:CLA:HBA2	1.64	0.78
18:A:804:CLA:HBD	18:A:804:CLA:HBA2	1.64	0.77
22:4:618:BCR:H342	17:4:605:CHL:HHB	1.67	0.76
14:J:10:VAL:HG12	14:J:12:PRO:HD2	1.66	0.76
4:4:77:PHE:HE2	19:4:617:XAT:H383	1.50	0.76
18:A:829:CLA:H202	22:J:102:BCR:H19C	1.68	0.76
4:4:103:ALA:HB2	19:4:617:XAT:C20	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:25:ILE:HD11	22:L:305:BCR:H312	1.69	0.75
14:J:25:LEU:O	14:J:29:ILE:HD12	1.87	0.75
18:B:814:CLA:H3A	22:B:845:BCR:H393	1.68	0.74
22:A:853:BCR:H12C	22:A:853:BCR:H341	1.67	0.74
22:B:801:BCR:H12C	22:B:801:BCR:H341	1.67	0.74
17:1:601:CHL:HAA1	20:1:615:LHG:H142	1.69	0.74
18:B:832:CLA:HHC	18:B:832:CLA:HBB1	1.71	0.72
22:A:850:BCR:H16C	22:A:850:BCR:H351	1.70	0.72
4:4:103:ALA:HB2	19:4:617:XAT:H202	1.71	0.72
22:L:306:BCR:H321	22:L:306:BCR:HC8	1.70	0.72
21:4:616:LUT:H8	21:4:616:LUT:H171	1.72	0.71
5:A:311:THR:HG22	5:A:312:ASN:H	1.55	0.71
20:1:615:LHG:HC32	20:1:615:LHG:HC91	1.70	0.71
18:A:844:CLA:HMB2	18:B:802:CLA:H203	1.73	0.71
1:1:156:ARG:NH2	18:1:608:CLA:O1D	2.23	0.71
22:B:848:BCR:H403	22:B:848:BCR:H23C	1.72	0.71
15:K:111:THR:O	15:K:115:ILE:HD12	1.92	0.70
22:K:205:BCR:H321	22:K:205:BCR:HC8	1.74	0.70
1:1:237:VAL:HG13	1:1:238:ILE:HG12	1.72	0.69
22:3:614:BCR:H403	22:3:614:BCR:H23C	1.74	0.69
18:A:843:CLA:HMD3	22:B:848:BCR:H393	1.74	0.69
6:B:517:PHE:HA	18:B:837:CLA:HED1	1.75	0.68
22:J:102:BCR:HC8	22:J:102:BCR:H311	1.75	0.68
18:A:803:CLA:HBA2	6:B:655:LEU:HB2	1.75	0.68
20:1:615:LHG:H132	20:1:615:LHG:H281	1.74	0.68
21:3:613:LUT:H401	21:3:613:LUT:H15	1.76	0.68
4:4:121:ILE:HG22	4:4:122:ILE:HG23	1.75	0.68
4:4:82:LEU:HD13	18:4:602:CLA:H42	1.75	0.67
22:B:849:BCR:H373	10:F:150:PHE:HE1	1.58	0.67
22:L:305:BCR:H321	22:L:305:BCR:HC8	1.75	0.67
18:A:804:CLA:H161	18:A:809:CLA:H143	1.76	0.67
2:2:104:GLY:HA3	19:2:617:XAT:H192	1.77	0.66
20:1:615:LHG:H342	20:1:615:LHG:H201	1.77	0.66
5:A:585:SER:OG	5:A:588:ASP:OD2	2.14	0.66
18:A:830:CLA:HBD	18:A:830:CLA:HBA1	1.78	0.66
16:L:209:LEU:HD13	18:L:304:CLA:HED3	1.78	0.65
5:A:393:TRP:CD1	18:A:829:CLA:HAB	2.31	0.65
4:4:77:PHE:CE2	19:4:617:XAT:H383	2.31	0.65
19:2:617:XAT:H401	19:2:617:XAT:H15	1.79	0.64
16:L:65:ILE:HA	16:L:75:GLU:HG3	1.77	0.64
15:K:102:THR:HG22	15:K:104:ALA:H	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:612:CLA:H3A	21:1:616:LUT:H383	1.80	0.64
18:3:612:CLA:HAB	18:3:607:CLA:HBA1	1.80	0.64
22:B:801:BCR:HC8	22:B:801:BCR:H331	1.80	0.64
22:B:847:BCR:HC8	22:B:847:BCR:H311	1.80	0.63
18:4:604:CLA:C2B	19:4:617:XAT:H182	2.28	0.63
11:G:119:LEU:HA	11:G:128:ASN:ND2	2.13	0.63
18:B:813:CLA:H2	18:B:805:CLA:H52	1.81	0.63
18:B:841:CLA:HED1	18:B:822:CLA:HAB	1.80	0.63
18:1:604:CLA:HBA1	18:1:604:CLA:HBD	1.80	0.63
18:B:805:CLA:H2	18:B:805:CLA:H92	1.81	0.63
22:A:851:BCR:H16C	22:A:851:BCR:H351	1.80	0.63
5:A:335:HIS:HB3	5:A:338:LEU:HD12	1.79	0.63
1:1:103:VAL:HG13	1:1:107:LEU:HD13	1.81	0.62
18:A:802:CLA:H202	18:A:842:CLA:H2	1.81	0.62
4:4:77:PHE:HE2	19:4:617:XAT:H382	1.61	0.62
18:A:842:CLA:HBA2	20:A:846:LHG:H162	1.81	0.62
22:A:849:BCR:H383	22:A:849:BCR:H23C	1.81	0.62
18:2:602:CLA:HMC1	19:2:617:XAT:H31	1.80	0.62
22:B:845:BCR:H16C	22:B:845:BCR:H20C	1.81	0.62
4:4:175:GLN:OE1	4:4:175:GLN:N	2.24	0.62
22:4:618:BCR:HC8	22:4:618:BCR:H321	1.81	0.62
3:3:260:ASP:OD2	3:3:263:ASN:ND2	2.33	0.61
6:B:704:GLN:HG3	27:B:850:DGD:HA22	1.82	0.61
4:4:141:THR:O	4:4:145:ILE:HG13	1.99	0.61
18:A:812:CLA:H141	18:A:812:CLA:H203	1.81	0.61
22:A:853:BCR:HC8	22:A:853:BCR:H311	1.82	0.61
6:B:707:LEU:HD23	27:B:850:DGD:HA21	1.82	0.61
4:4:77:PHE:CE2	19:4:617:XAT:C38	2.78	0.61
18:1:604:CLA:C4A	18:1:604:CLA:H12	2.31	0.61
20:1:615:LHG:H362	18:4:614:CLA:HAA2	1.83	0.61
5:A:505:LEU:HB2	5:A:521:LEU:HD23	1.83	0.61
4:4:132:LYS:NZ	17:4:606:CHL:O1D	2.28	0.60
7:C:24:ASP:OD2	8:D:161:HIS:ND1	2.33	0.60
1:1:97:ALA:HB1	19:1:614:XAT:H181	1.82	0.60
1:1:187:LEU:HD13	18:1:609:CLA:HAA2	1.83	0.60
22:A:851:BCR:H23C	22:A:851:BCR:H403	1.83	0.60
22:B:843:BCR:H16C	22:B:843:BCR:H351	1.83	0.60
22:A:850:BCR:H311	22:A:850:BCR:HC8	1.84	0.60
6:B:571:SER:OG	6:B:574:ASP:OD2	2.17	0.60
8:D:151:VAL:HG22	8:D:157:VAL:HG12	1.83	0.60
22:K:205:BCR:H403	22:K:205:BCR:H23C	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:353:ASN:ND2	18:A:806:CLA:OBD	2.33	0.59
1:1:54:ARG:NH1	1:1:58:LEU:O	2.35	0.59
18:4:613:CLA:HBD	18:4:613:CLA:HBA1	1.83	0.59
22:A:848:BCR:H321	22:A:848:BCR:HC8	1.84	0.59
11:G:119:LEU:HA	11:G:128:ASN:HD21	1.67	0.59
22:B:846:BCR:HC8	22:B:846:BCR:H311	1.84	0.59
7:C:62:PHE:HD2	8:D:185:ILE:HG21	1.68	0.59
5:A:379:THR:HG21	5:A:515:VAL:HB	1.82	0.59
1:1:208:GLN:OE1	1:1:220:ASN:ND2	2.36	0.59
18:A:820:CLA:H91	18:A:820:CLA:H151	1.83	0.59
22:B:843:BCR:H311	22:B:843:BCR:HC8	1.85	0.58
3:3:109:LEU:HD22	18:3:603:CLA:HBC1	1.84	0.58
5:A:739:TRP:HH2	18:A:809:CLA:HBC2	1.67	0.58
21:1:616:LUT:H391	21:1:616:LUT:H32	1.85	0.58
1:1:217:PRO:O	21:1:616:LUT:O23	2.22	0.58
20:A:846:LHG:H182	18:A:831:CLA:H203	1.86	0.58
18:F:302:CLA:HBA1	14:J:26:LEU:HD21	1.85	0.58
22:G:204:BCR:HC8	22:G:204:BCR:H311	1.86	0.58
22:B:846:BCR:H323	20:B:852:LHG:H321	1.85	0.58
1:1:190:LYS:O	1:1:194:ASN:ND2	2.36	0.57
22:B:845:BCR:H362	18:B:828:CLA:H171	1.86	0.57
20:1:615:LHG:H192	20:1:615:LHG:H361	1.87	0.57
6:B:36:ASP:O	6:B:41:ARG:NH1	2.37	0.57
1:1:95:MET:SD	18:1:609:CLA:HAB	2.45	0.57
5:A:72:SER:OG	5:A:178:TYR:HB2	2.05	0.57
5:A:330:PHE:HD2	20:A:847:LHG:HC41	1.69	0.57
1:1:82:ARG:NH1	18:1:603:CLA:O1A	2.35	0.56
4:4:103:ALA:HB2	19:4:617:XAT:C13	2.35	0.56
6:B:523:ILE:HG21	18:B:836:CLA:HAB	1.87	0.56
2:2:155:ARG:NH2	18:2:608:CLA:O1D	2.35	0.56
16:L:170:THR:HG22	16:L:172:THR:H	1.71	0.56
18:2:604:CLA:HAB	17:2:605:CHL:C4C	2.35	0.56
18:A:804:CLA:H201	18:A:844:CLA:H203	1.87	0.56
1:1:172:PHE:HB3	18:1:609:CLA:HMD1	1.87	0.56
6:B:469:LYS:NZ	6:B:509:PHE:O	2.36	0.56
22:B:849:BCR:H311	14:J:33:PHE:HD2	1.71	0.56
18:2:604:CLA:HBB2	17:2:605:CHL:C2C	2.37	0.55
6:B:307:ALA:HB3	18:B:822:CLA:HED3	1.87	0.55
22:L:305:BCR:H402	22:L:305:BCR:H23C	1.89	0.55
5:A:361:THR:HA	18:A:830:CLA:HBC2	1.88	0.55
18:A:821:CLA:HAB	22:K:205:BCR:H341	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:809:CLA:H201	20:A:846:LHG:H211	1.88	0.55
21:2:616:LUT:H391	18:2:611:CLA:HAB	1.88	0.55
6:B:659:THR:HA	18:B:803:CLA:HAB	1.88	0.55
20:1:615:LHG:H101	22:4:618:BCR:H393	1.89	0.55
18:A:841:CLA:H72	18:B:832:CLA:H42	1.89	0.55
3:3:108:MET:HE1	18:3:608:CLA:HAB	1.89	0.54
5:A:699:ILE:HA	18:A:841:CLA:HED1	1.89	0.54
1:1:92:ARG:NH1	18:1:607:CLA:OBD	2.40	0.54
18:A:826:CLA:HBB1	18:A:822:CLA:H2	1.90	0.54
6:B:450:GLU:OE2	10:F:119:ARG:NH1	2.40	0.54
18:B:805:CLA:H43	22:B:844:BCR:H383	1.90	0.54
18:B:806:CLA:H2	18:B:806:CLA:HED3	1.88	0.54
22:K:202:BCR:H23C	22:K:202:BCR:H392	1.89	0.54
24:A:801:CL0:H14	18:B:802:CLA:C4A	2.37	0.54
18:2:602:CLA:CGA	18:2:602:CLA:H3A	2.38	0.54
3:3:79:LEU:HD13	18:A:813:CLA:H2	1.88	0.54
22:B:844:BCR:H361	22:B:844:BCR:H21C	1.90	0.54
1:1:230:HIS:NE2	4:4:145:ILE:HG12	2.23	0.54
1:1:233:ILE:HG13	18:1:612:CLA:HBC2	1.90	0.54
6:B:435:GLY:HA3	18:B:833:CLA:HAB	1.89	0.53
18:A:842:CLA:HBD	18:A:842:CLA:HBA1	1.89	0.53
18:A:832:CLA:CGA	18:A:832:CLA:H3A	2.38	0.53
18:A:814:CLA:HHC	18:A:814:CLA:HBB1	1.89	0.53
18:B:829:CLA:H102	27:B:850:DGD:HAG2	1.90	0.53
5:A:657:ILE:HD12	6:B:621:ARG:HG3	1.90	0.53
5:A:236:LEU:N	5:A:239:GLU:OE1	2.41	0.53
11:G:88:ARG:NH2	11:G:131:ASP:OD2	2.41	0.53
2:2:205:LEU:O	2:2:208:LYS:HG2	2.08	0.53
17:1:601:CHL:HHC	17:1:601:CHL:HBB1	1.91	0.53
22:K:205:BCR:H343	22:K:202:BCR:H14C	1.90	0.52
19:4:617:XAT:H242	19:4:617:XAT:H362	1.90	0.52
5:A:302:PHE:HE1	18:A:822:CLA:HAB	1.73	0.52
22:A:852:BCR:H403	22:A:852:BCR:H23C	1.91	0.52
17:2:607:CHL:H43	21:2:616:LUT:H173	1.91	0.52
2:2:81:SER:O	2:2:81:SER:OG	2.23	0.52
3:3:162:LEU:HB3	22:3:614:BCR:H363	1.91	0.52
12:H:80:SER:HB2	16:L:98:VAL:HG13	1.90	0.52
18:2:602:CLA:H42	18:2:602:CLA:C2B	2.39	0.52
22:A:848:BCR:H383	22:K:202:BCR:H10C	1.90	0.52
6:B:25:ILE:HG12	22:L:305:BCR:HC32	1.90	0.52
6:B:707:LEU:HD11	27:B:850:DGD:HB81	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:41:ASP:OD1	5:A:41:ASP:N	2.42	0.52
5:A:596:TRP:CH2	18:A:803:CLA:HAB	2.45	0.52
15:K:57:MET:HG2	15:K:117:GLY:HA3	1.91	0.52
17:2:615:CHL:HHC	17:2:615:CHL:HBB1	1.92	0.52
4:4:103:ALA:CB	19:4:617:XAT:H202	2.38	0.52
22:B:801:BCR:H341	22:B:801:BCR:C12	2.37	0.52
1:1:168:PRO:HG2	18:1:609:CLA:HMD2	1.92	0.52
4:4:194:ASN:O	4:4:194:ASN:ND2	2.39	0.52
18:4:609:CLA:CGA	18:4:609:CLA:H3A	2.40	0.52
5:A:348:ALA:HB1	22:A:850:BCR:H393	1.92	0.52
20:1:615:LHG:H211	4:4:148:ILE:HD11	1.91	0.51
21:3:613:LUT:H161	21:3:613:LUT:H8	1.91	0.51
18:A:806:CLA:H192	22:A:849:BCR:H363	1.91	0.51
6:B:93:ASP:H	12:H:129:ILE:HD13	1.73	0.51
6:B:456:GLU:OE1	6:B:461:GLN:NE2	2.39	0.51
22:B:844:BCR:H352	18:B:828:CLA:H172	1.91	0.51
8:D:156:GLU:OE1	8:D:156:GLU:N	2.43	0.51
5:A:512:LEU:HD11	5:A:519:VAL:HG13	1.91	0.51
6:B:695:ASP:OD1	6:B:695:ASP:N	2.42	0.51
12:H:83:ASN:ND2	18:H:201:CLA:HAC2	2.25	0.51
22:A:853:BCR:H23C	22:A:853:BCR:H393	1.93	0.51
6:B:25:ILE:HG21	27:B:850:DGD:HA72	1.92	0.51
17:1:601:CHL:C3B	20:1:615:LHG:H282	2.41	0.51
6:B:292:ARG:HD3	11:G:97:PRO:HD3	1.93	0.51
6:B:339:ALA:HB2	22:B:847:BCR:H372	1.92	0.51
10:F:70:SER:O	10:F:70:SER:OG	2.28	0.51
16:L:153:TYR:HB2	22:L:305:BCR:H361	1.93	0.51
2:2:66:ASP:OD1	2:2:66:ASP:N	2.34	0.50
6:B:120:VAL:HG21	18:B:808:CLA:HED1	1.91	0.50
18:B:838:CLA:HBB2	18:B:830:CLA:HAB	1.93	0.50
4:4:103:ALA:CA	19:4:617:XAT:H202	2.41	0.50
22:B:801:BCR:H312	18:B:832:CLA:CBB	2.41	0.50
18:A:825:CLA:H41	22:A:851:BCR:H15C	1.94	0.50
6:B:463:ILE:HD11	18:B:836:CLA:H11	1.93	0.50
5:A:717:LEU:HD21	26:A:855:PQN:H151	1.93	0.50
18:A:844:CLA:HAB	6:B:582:TRP:CH2	2.47	0.50
18:B:806:CLA:HAB	18:B:828:CLA:HBB1	1.94	0.50
22:B:849:BCR:C10	14:J:36:ALA:HB1	2.41	0.50
18:B:838:CLA:HMC3	18:B:831:CLA:HBC2	1.93	0.50
3:3:167:GLU:OE1	3:3:170:ARG:NH2	2.40	0.50
3:3:223:LEU:HD11	3:3:227:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:522:LEU:HD21	5:A:616:VAL:HA	1.92	0.50
6:B:57:ILE:HA	18:B:806:CLA:HBC3	1.94	0.50
10:F:114:GLU:O	10:F:118:ARG:HG3	2.11	0.50
4:4:100:GLY:HA2	4:4:213:MET:HE3	1.93	0.49
5:A:305:ALA:HB2	18:A:822:CLA:HBC2	1.94	0.49
18:A:835:CLA:HHB	18:A:834:CLA:HAB	1.93	0.49
26:A:855:PQN:H172	22:B:801:BCR:H382	1.94	0.49
4:4:103:ALA:N	19:4:617:XAT:H202	2.27	0.49
5:A:297:ALA:HB1	18:A:818:CLA:HBC2	1.93	0.49
5:A:389:THR:HG23	5:A:605:ILE:HG21	1.94	0.49
6:B:91:ILE:HB	6:B:112:PRO:HB2	1.94	0.49
22:B:801:BCR:HC31	22:B:849:BCR:H351	1.94	0.49
5:A:671:PHE:O	5:A:675:HIS:ND1	2.43	0.49
24:A:801:CL0:H59	24:A:801:CL0:H51	1.56	0.49
22:A:848:BCR:H323	18:A:806:CLA:H151	1.94	0.49
18:2:604:CLA:HED2	18:2:604:CLA:H2A	1.95	0.49
18:A:803:CLA:H2	6:B:655:LEU:HD22	1.93	0.49
6:B:9:SER:OG	27:B:850:DGD:O4E	2.24	0.49
21:2:616:LUT:H401	21:2:616:LUT:H15	1.95	0.49
3:3:151:ASP:OD1	3:3:151:ASP:N	2.46	0.49
22:B:849:BCR:H311	14:J:33:PHE:CD2	2.47	0.49
18:4:602:CLA:CGA	18:4:602:CLA:H3A	2.43	0.48
24:A:801:CL0:H14	18:B:802:CLA:NA	2.28	0.48
16:L:107:VAL:HA	18:L:303:CLA:HED1	1.94	0.48
17:1:601:CHL:C4A	20:1:615:LHG:H131	2.43	0.48
12:H:107:LEU:HD22	16:L:144:VAL:HG13	1.94	0.48
1:1:52:GLU:OE2	1:1:53:PRO:HD2	2.14	0.48
22:A:851:BCR:H351	22:A:851:BCR:C16	2.42	0.48
9:E:87:VAL:HB	9:E:138:VAL:HG13	1.94	0.48
15:K:115:ILE:HG22	18:K:203:CLA:HBC1	1.96	0.48
4:4:90:LYS:O	4:4:94:GLN:HG2	2.13	0.48
4:4:102:TRP:CE2	17:4:607:CHL:HED2	2.49	0.48
5:A:330:PHE:CD2	20:A:847:LHG:HC41	2.48	0.48
5:A:657:ILE:HA	6:B:617:MET:HE3	1.95	0.48
18:A:843:CLA:H93	18:A:843:CLA:HBB1	1.95	0.48
6:B:697:PRO:O	7:C:81:TYR:OH	2.24	0.48
1:1:155:GLN:HG3	18:1:607:CLA:HMC3	1.96	0.48
1:1:221:LEU:HD22	21:1:616:LUT:H363	1.96	0.48
5:A:294:HIS:HB2	18:A:819:CLA:C1B	2.44	0.48
6:B:649:MET:HE1	18:B:808:CLA:HBC3	1.95	0.48
22:4:618:BCR:H383	22:4:618:BCR:H23C	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:373:PRO:HG3	18:A:820:CLA:HBA1	1.95	0.48
18:A:841:CLA:H143	18:F:302:CLA:HBC1	1.96	0.48
1:1:168:PRO:HD2	18:1:609:CLA:HMD2	1.95	0.48
5:A:739:TRP:CH2	18:A:809:CLA:HBC2	2.48	0.48
18:A:809:CLA:H203	18:A:812:CLA:H191	1.96	0.48
8:D:164:ASP:OD2	8:D:172:ASN:ND2	2.44	0.48
1:1:156:ARG:HG3	18:1:607:CLA:CHD	2.44	0.48
2:2:119:ILE:HG22	2:2:120:LEU:HD12	1.94	0.48
6:B:548:PRO:HD2	7:C:62:PHE:CZ	2.49	0.48
18:4:602:CLA:H93	19:4:617:XAT:H30	1.95	0.48
18:A:802:CLA:H3A	18:A:802:CLA:O2A	2.13	0.48
22:B:801:BCR:H383	22:B:801:BCR:H23C	1.95	0.48
21:2:619:LUT:H172	18:4:610:CLA:HHC	1.96	0.47
18:A:802:CLA:H143	18:A:844:CLA:H151	1.95	0.47
22:A:852:BCR:H323	18:A:829:CLA:H11	1.95	0.47
17:1:601:CHL:C4C	20:1:615:LHG:HC92	2.45	0.47
20:1:615:LHG:H251	20:1:615:LHG:HC81	1.97	0.47
18:A:834:CLA:H162	18:A:834:CLA:H141	1.69	0.47
18:B:825:CLA:H142	18:B:825:CLA:H111	1.73	0.47
18:4:604:CLA:HAA1	18:4:604:CLA:HED3	1.96	0.47
1:1:69:ASP:HA	19:1:614:XAT:O23	2.15	0.47
1:1:83:TYR:CD2	18:1:602:CLA:H11	2.50	0.47
18:B:808:CLA:O1A	18:B:827:CLA:HBD	2.15	0.47
12:H:63:ASP:OD2	12:H:66:ASN:ND2	2.33	0.47
2:2:217:MET:HE1	18:2:602:CLA:HHC	1.96	0.47
18:2:608:CLA:H3A	18:2:608:CLA:HBA2	1.36	0.47
10:F:78:SER:HB3	10:F:81:PHE:HB2	1.97	0.47
1:1:68:PHE:CE2	19:1:614:XAT:H383	2.49	0.47
4:4:100:GLY:CA	4:4:213:MET:HE3	2.45	0.47
4:4:236:GLN:NE2	4:4:244:ASN:HD22	2.12	0.47
18:B:828:CLA:H112	18:B:828:CLA:H142	1.65	0.47
18:A:819:CLA:H62	18:A:819:CLA:H41	1.59	0.47
18:A:828:CLA:H93	18:A:828:CLA:H111	1.66	0.47
6:B:549:ASP:OD1	7:C:66:ARG:NH2	2.44	0.47
22:B:846:BCR:H403	22:B:846:BCR:H23C	1.96	0.47
18:B:840:CLA:H11	26:B:842:PQN:H272	1.96	0.47
21:1:616:LUT:H11	21:1:616:LUT:H191	1.82	0.46
5:A:360:LEU:HG	18:A:830:CLA:HBC1	1.97	0.46
18:A:806:CLA:H161	22:A:849:BCR:H353	1.97	0.46
18:A:842:CLA:HBC2	26:A:855:PQN:H192	1.96	0.46
22:A:852:BCR:H271	18:A:842:CLA:H141	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:830:CLA:HBA1	18:A:830:CLA:CHA	2.45	0.46
18:A:818:CLA:H92	18:A:818:CLA:H61	1.78	0.46
10:F:89:ILE:HD12	10:F:113:ILE:HG23	1.96	0.46
1:1:68:PHE:HE2	19:1:614:XAT:H383	1.80	0.46
2:2:170:VAL:HG23	2:2:171:PHE:CD2	2.51	0.46
5:A:620:ILE:HG12	5:A:626:VAL:HG22	1.96	0.46
22:F:304:BCR:H14C	22:F:304:BCR:H10C	1.97	0.46
18:1:607:CLA:H3A	18:1:607:CLA:HBA2	1.32	0.46
4:4:154:GLU:HG3	18:4:608:CLA:C4B	2.46	0.46
18:A:829:CLA:H72	18:A:829:CLA:H111	1.49	0.46
18:A:819:CLA:H91	18:A:819:CLA:H111	1.72	0.46
18:A:844:CLA:H3A	18:A:844:CLA:O1A	2.16	0.46
6:B:411:MET:HG3	22:B:846:BCR:H401	1.98	0.46
5:A:508:GLY:HA2	5:A:523:PRO:HB3	1.96	0.46
6:B:304:LEU:HA	18:B:822:CLA:HED1	1.96	0.46
14:J:29:ILE:HD12	14:J:29:ILE:H	1.80	0.46
18:A:844:CLA:H202	18:A:829:CLA:H121	1.98	0.46
22:B:843:BCR:H11C	22:B:843:BCR:H341	1.81	0.46
1:1:95:MET:HG2	21:1:616:LUT:C14	2.46	0.46
17:1:601:CHL:C3C	20:1:615:LHG:HC92	2.46	0.46
18:3:603:CLA:H3A	18:3:603:CLA:HBA1	1.38	0.46
22:A:848:BCR:H403	22:A:848:BCR:H23C	1.97	0.46
18:B:814:CLA:H41	18:B:814:CLA:H62	1.45	0.46
18:A:804:CLA:H91	18:A:804:CLA:H111	1.70	0.45
6:B:517:PHE:HE1	22:B:849:BCR:H381	1.81	0.45
22:I:101:BCR:H383	22:L:301:BCR:H363	1.98	0.45
20:1:615:LHG:H161	20:1:615:LHG:H301	1.96	0.45
18:B:809:CLA:H92	18:B:809:CLA:H62	1.71	0.45
7:C:60:THR:OG1	7:C:62:PHE:O	2.30	0.45
2:2:225:PHE:HA	2:2:228:ILE:HG22	1.98	0.45
21:2:616:LUT:H373	18:2:612:CLA:C2B	2.47	0.45
3:3:266:VAL:HG21	18:3:609:CLA:H11	1.98	0.45
5:A:582:CYS:HB2	6:B:667:TRP:HB3	1.99	0.45
6:B:124:TRP:HB3	6:B:129:LEU:HD12	1.98	0.45
1:1:221:LEU:O	1:1:225:LEU:HG	2.16	0.45
18:2:602:CLA:H3A	18:2:602:CLA:O1A	2.16	0.45
4:4:157:ARG:NH1	18:4:608:CLA:O1D	2.43	0.45
5:A:393:TRP:HD1	18:A:829:CLA:HAB	1.80	0.45
1:1:200:LEU:HD12	1:1:200:LEU:HA	1.79	0.45
20:1:615:LHG:H132	20:1:615:LHG:C28	2.43	0.45
4:4:132:LYS:HZ2	17:4:606:CHL:CGD	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:614:CLA:O2D	18:4:614:CLA:H2A	2.17	0.45
18:A:830:CLA:HBA1	18:A:830:CLA:CBD	2.45	0.45
18:B:811:CLA:H41	18:B:811:CLA:H61	1.74	0.45
18:A:806:CLA:H61	18:A:806:CLA:H2	1.69	0.45
6:B:26:ALA:O	18:B:829:CLA:H11	2.16	0.45
22:B:844:BCR:H382	22:B:844:BCR:H23C	1.97	0.45
2:2:126:TYR:HB2	2:2:227:HIS:CD2	2.52	0.45
4:4:129:ASP:OD1	4:4:129:ASP:N	2.47	0.45
15:K:108:ALA:O	15:K:112:VAL:HG23	2.17	0.45
22:L:305:BCR:H361	22:L:305:BCR:H20C	1.87	0.45
18:3:609:CLA:C2B	21:3:613:LUT:H373	2.46	0.45
18:A:830:CLA:H41	18:A:830:CLA:H62	1.55	0.45
18:B:827:CLA:H152	18:B:827:CLA:H111	1.39	0.45
22:B:846:BCR:H11C	22:B:846:BCR:H341	1.81	0.45
22:J:102:BCR:H341	22:J:102:BCR:H11C	1.79	0.45
22:L:301:BCR:H15C	22:L:301:BCR:H351	1.76	0.45
22:A:851:BCR:H331	22:A:851:BCR:C8	2.45	0.44
6:B:516:ASP:OD2	6:B:593:TYR:OH	2.35	0.44
18:B:808:CLA:H141	18:B:808:CLA:H162	1.65	0.44
18:B:824:CLA:H62	18:B:824:CLA:H41	1.57	0.44
11:G:68:ILE:HG21	11:G:147:LEU:HD21	1.99	0.44
21:2:616:LUT:H22	18:2:609:CLA:C2	2.47	0.44
18:A:825:CLA:HMB1	20:A:847:LHG:O6	2.17	0.44
18:B:825:CLA:HAA2	18:B:826:CLA:OBD	2.17	0.44
11:G:68:ILE:HD11	11:G:146:ILE:HB	1.99	0.44
1:1:207:VAL:HG21	18:1:612:CLA:HMD2	1.99	0.44
17:1:601:CHL:H61	17:1:601:CHL:H41	1.62	0.44
2:2:238:LEU:HB2	21:2:616:LUT:H24	1.99	0.44
4:4:193:LEU:HD12	21:4:616:LUT:H222	1.99	0.44
18:A:809:CLA:H202	18:A:809:CLA:H91	1.99	0.44
18:A:813:CLA:H3A	18:A:813:CLA:HBA2	1.65	0.44
18:B:809:CLA:H41	18:B:809:CLA:H61	1.56	0.44
1:1:90:HIS:CD2	18:1:608:CLA:HMD1	2.53	0.44
6:B:182:LEU:HD11	22:B:844:BCR:H363	1.99	0.44
6:B:652:PHE:O	6:B:656:VAL:HG23	2.17	0.44
18:B:802:CLA:H161	18:B:802:CLA:H121	1.72	0.44
22:B:801:BCR:H15C	22:B:801:BCR:H351	1.86	0.44
21:2:619:LUT:H181	21:2:619:LUT:C8	2.34	0.44
3:3:266:VAL:HG22	18:3:609:CLA:CAD	2.48	0.44
5:A:213:HIS:HB2	18:A:815:CLA:CHC	2.48	0.44
18:A:802:CLA:H3A	18:A:802:CLA:HBA1	1.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:806:CLA:HBA1	18:A:806:CLA:H3A	1.33	0.44
18:B:826:CLA:H142	18:B:826:CLA:H111	1.83	0.44
18:L:303:CLA:H112	18:L:303:CLA:H71	1.74	0.44
5:A:588:ASP:OD1	5:A:723:ARG:NH1	2.51	0.44
22:A:848:BCR:H24C	22:A:848:BCR:H371	1.86	0.44
18:A:842:CLA:H62	18:A:842:CLA:H102	1.69	0.44
18:A:809:CLA:H101	18:A:809:CLA:H13	1.77	0.44
18:A:820:CLA:HMB1	18:A:820:CLA:HBB1	2.00	0.44
7:C:2:SER:OG	7:C:3:HIS:N	2.49	0.44
9:E:109:ASP:OD1	9:E:110:PRO:HD2	2.17	0.44
1:1:164:LYS:HE3	1:1:164:LYS:HA	1.99	0.44
1:1:203:VAL:O	1:1:207:VAL:HG23	2.18	0.44
18:2:612:CLA:H141	18:2:612:CLA:H161	1.81	0.44
4:4:238:LEU:CD1	18:4:613:CLA:HAB	2.48	0.44
18:A:833:CLA:H41	18:A:833:CLA:H61	1.51	0.44
6:B:338:LEU:HD22	6:B:382:ILE:HG23	2.00	0.44
18:1:603:CLA:H41	18:1:603:CLA:H62	1.65	0.44
18:A:827:CLA:H62	18:A:827:CLA:H102	1.68	0.44
18:A:803:CLA:H142	6:B:648:TRP:HH2	1.83	0.44
18:B:822:CLA:HBA1	18:B:822:CLA:O1D	2.18	0.44
7:C:15:THR:HG22	7:C:28:MET:HG3	2.00	0.44
22:L:305:BCR:H331	22:L:305:BCR:HC7	1.80	0.44
18:2:602:CLA:H91	18:2:602:CLA:H111	1.79	0.44
18:2:609:CLA:CHA	18:2:609:CLA:HBA1	2.44	0.44
4:4:214:LEU:HD23	4:4:214:LEU:HA	1.87	0.44
22:4:618:BCR:H15C	22:4:618:BCR:H351	1.88	0.44
18:4:602:CLA:H93	18:4:602:CLA:H61	1.77	0.44
18:A:803:CLA:HBA1	18:A:803:CLA:H3A	1.57	0.44
21:3:613:LUT:H391	21:3:613:LUT:H31	1.78	0.43
18:A:809:CLA:H172	22:A:853:BCR:H372	2.01	0.43
22:A:851:BCR:H371	22:A:851:BCR:H24C	1.72	0.43
18:B:803:CLA:H202	18:B:803:CLA:H162	1.80	0.43
22:B:844:BCR:H371	22:B:844:BCR:H24C	1.72	0.43
8:D:72:THR:HG23	8:D:120:PRO:HB2	2.00	0.43
18:A:802:CLA:H92	18:A:802:CLA:H62	1.68	0.43
18:A:805:CLA:HBA2	18:A:805:CLA:H3A	1.59	0.43
6:B:174:ARG:HB2	18:B:813:CLA:HBC2	2.01	0.43
6:B:276:HIS:HB2	18:B:817:CLA:C1B	2.49	0.43
18:B:819:CLA:HBA1	18:B:819:CLA:H3A	1.80	0.43
18:B:825:CLA:H141	18:B:825:CLA:H162	1.73	0.43
18:2:604:CLA:C2C	19:2:617:XAT:H183	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:826:CLA:H111	18:A:826:CLA:H93	1.66	0.43
22:A:850:BCR:H20C	22:A:850:BCR:H361	1.91	0.43
16:L:90:ASN:HB3	18:L:302:CLA:HAC1	2.00	0.43
22:L:301:BCR:H361	22:L:301:BCR:C21	2.48	0.43
5:A:92:GLY:O	5:A:96:SER:OG	2.31	0.43
18:B:822:CLA:H91	18:B:822:CLA:H111	1.73	0.43
20:1:615:LHG:C10	22:4:618:BCR:H281	2.49	0.43
4:4:240:ASP:HB2	4:4:244:ASN:OD1	2.17	0.43
18:4:603:CLA:HMB3	19:4:617:XAT:C32	2.48	0.43
18:A:841:CLA:H43	18:B:832:CLA:HAA2	1.99	0.43
22:B:847:BCR:H351	22:B:847:BCR:H15C	1.84	0.43
18:F:302:CLA:CAD	14:J:22:LEU:HD21	2.48	0.43
18:A:804:CLA:HBA2	18:A:804:CLA:CBD	2.40	0.43
6:B:444:LEU:HD12	6:B:444:LEU:O	2.19	0.43
18:B:828:CLA:H3A	18:B:828:CLA:HBA2	1.27	0.43
22:J:102:BCR:H351	22:J:102:BCR:H15C	1.81	0.43
18:1:604:CLA:HBA2	18:1:605:CLA:HMA2	2.01	0.43
18:2:602:CLA:H162	18:2:602:CLA:H192	1.80	0.43
5:A:310:ARG:N	5:A:317:HIS:O	2.47	0.43
18:A:839:CLA:HMB3	18:A:839:CLA:HBB1	2.01	0.43
18:B:826:CLA:H13	22:B:847:BCR:H15C	2.00	0.43
7:C:72:GLU:OE1	7:C:77:MET:HE2	2.18	0.43
10:F:203:TRP:CD1	10:F:204:PRO:HD3	2.54	0.43
18:A:812:CLA:H13	18:A:812:CLA:H172	1.71	0.43
18:A:812:CLA:H91	18:A:812:CLA:H111	1.65	0.43
4:4:149:LEU:HD11	22:4:618:BCR:C16	2.49	0.43
19:4:617:XAT:C28	19:4:617:XAT:H381	2.26	0.43
18:A:804:CLA:HBB2	18:A:812:CLA:H143	2.01	0.43
6:B:56:ILE:HG22	18:B:806:CLA:HBC2	2.01	0.43
22:B:849:BCR:H10C	14:J:38:THR:O	2.19	0.43
21:2:616:LUT:H202	18:2:611:CLA:H3A	2.00	0.43
4:4:238:LEU:HD13	4:4:238:LEU:HA	1.92	0.43
18:A:836:CLA:HBA1	18:A:836:CLA:H3A	1.92	0.43
6:B:684:ARG:HA	6:B:684:ARG:HD3	1.85	0.43
2:2:227:HIS:O	2:2:227:HIS:ND1	2.51	0.42
22:A:848:BCR:H20C	22:A:848:BCR:H361	1.90	0.42
18:B:837:CLA:H3A	18:B:837:CLA:HBA2	1.71	0.42
22:B:845:BCR:H11C	22:B:845:BCR:H341	1.89	0.42
11:G:64:PRO:O	11:G:68:ILE:HG22	2.19	0.42
14:J:2:ARG:HA	14:J:2:ARG:HD2	1.90	0.42
16:L:65:ILE:O	16:L:65:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:225:PHE:O	2:2:228:ILE:HG22	2.19	0.42
10:F:143:ASP:OD1	10:F:144:GLN:N	2.52	0.42
1:1:65:ASP:OD1	1:1:65:ASP:C	2.62	0.42
21:1:616:LUT:H401	21:1:616:LUT:H35	1.80	0.42
2:2:205:LEU:HA	2:2:208:LYS:HD2	2.01	0.42
5:A:536:ILE:HG23	24:A:801:CL0:H70	2.01	0.42
18:A:828:CLA:HBB1	18:A:828:CLA:HMB1	2.01	0.42
18:A:825:CLA:HBA2	18:A:825:CLA:H3A	1.30	0.42
6:B:678:LEU:HD23	6:B:678:LEU:HA	1.87	0.42
18:B:825:CLA:H3A	18:B:825:CLA:HBA2	1.46	0.42
22:B:847:BCR:H11C	22:B:847:BCR:H341	1.88	0.42
18:B:834:CLA:HBA1	18:B:834:CLA:H3A	1.66	0.42
11:G:64:PRO:O	11:G:64:PRO:HD2	2.18	0.42
18:A:804:CLA:H62	18:A:804:CLA:H2	1.81	0.42
22:B:846:BCR:H351	22:B:846:BCR:H15C	1.82	0.42
20:1:615:LHG:H212	18:4:614:CLA:CMA	2.49	0.42
4:4:104:MET:SD	18:4:609:CLA:HAB	2.60	0.42
18:B:806:CLA:H151	18:B:828:CLA:HBB2	2.01	0.42
18:F:302:CLA:HAA2	14:J:22:LEU:HD11	2.02	0.42
18:3:601:CLA:H2	18:3:601:CLA:H62	1.81	0.42
4:4:245:THR:HG22	4:4:246:ILE:H	1.84	0.42
5:A:197:HIS:CG	18:A:814:CLA:HMC1	2.54	0.42
5:A:596:TRP:HH2	18:A:803:CLA:HAB	1.83	0.42
6:B:325:THR:OG1	6:B:403:ASN:OD1	2.26	0.42
6:B:574:ASP:OD1	6:B:706:ARG:NH1	2.52	0.42
3:3:239:TYR:CE1	21:3:613:LUT:H363	2.54	0.42
4:4:77:PHE:CE2	19:4:617:XAT:H382	2.46	0.42
24:A:801:CL0:H51	24:A:801:CL0:H42	1.71	0.42
22:A:852:BCR:H20C	22:A:852:BCR:H361	1.79	0.42
18:A:843:CLA:HMC2	18:B:839:CLA:H11	2.02	0.42
18:B:828:CLA:H161	18:B:828:CLA:H141	1.77	0.42
18:F:301:CLA:H41	18:F:301:CLA:H62	1.55	0.42
22:K:202:BCR:H15C	22:K:202:BCR:H351	1.80	0.42
21:1:616:LUT:H15	21:1:616:LUT:H201	1.90	0.42
2:2:103:LEU:HD12	2:2:103:LEU:HA	1.90	0.42
4:4:228:LYS:HB3	4:4:232:GLU:CD	2.45	0.42
5:A:571:PHE:CE1	5:A:585:SER:HB3	2.55	0.42
22:B:801:BCR:H312	18:B:832:CLA:HBB2	2.02	0.42
7:C:9:ASP:OD1	7:C:9:ASP:C	2.62	0.42
16:L:168:SER:O	16:L:168:SER:OG	2.34	0.42
3:3:119:ILE:HG22	3:3:120:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:206:LEU:HA	4:4:206:LEU:HD23	1.75	0.42
4:4:245:THR:HG22	4:4:246:ILE:N	2.35	0.42
6:B:432:HIS:HB2	22:B:849:BCR:H402	2.02	0.42
19:1:614:XAT:H31	19:1:614:XAT:H391	1.88	0.42
2:2:194:TRP:HB2	18:2:609:CLA:O2A	2.20	0.42
19:2:617:XAT:H12	18:2:603:CLA:HMC3	2.02	0.42
21:4:616:LUT:H35	21:4:616:LUT:H401	1.90	0.42
22:A:850:BCR:H331	22:A:850:BCR:HC7	1.77	0.42
6:B:280:ILE:HD13	6:B:280:ILE:HA	1.94	0.42
6:B:662:MET:HB2	18:B:803:CLA:C1C	2.50	0.42
18:B:805:CLA:H3A	18:B:805:CLA:HBA1	1.47	0.42
18:B:827:CLA:H72	18:B:827:CLA:H112	1.79	0.42
18:B:832:CLA:HHC	18:B:832:CLA:CBB	2.45	0.42
7:C:61:ASP:OD1	7:C:62:PHE:N	2.52	0.42
7:C:61:ASP:HB3	9:E:131:ASN:ND2	2.34	0.42
18:1:612:CLA:HED3	20:1:615:LHG:H322	2.02	0.41
5:A:175:TRP:HB2	18:A:812:CLA:HMC3	2.02	0.41
5:A:365:ALA:HB2	5:A:391:HIS:HB2	2.02	0.41
22:A:848:BCR:H23C	22:A:848:BCR:H392	2.02	0.41
22:B:848:BCR:H15C	22:B:848:BCR:H351	1.95	0.41
22:L:306:BCR:H351	22:L:306:BCR:H15C	1.83	0.41
1:1:92:ARG:HD3	18:1:607:CLA:OBD	2.21	0.41
1:1:202:PHE:CZ	19:1:614:XAT:H10	2.55	0.41
3:3:119:ILE:HD13	3:3:119:ILE:HA	1.87	0.41
5:A:61:SER:O	5:A:61:SER:OG	2.32	0.41
22:B:846:BCR:H343	18:B:822:CLA:HBB2	2.01	0.41
22:B:845:BCR:H19C	22:B:845:BCR:C37	2.50	0.41
19:1:614:XAT:H242	19:1:614:XAT:H362	2.02	0.41
20:1:615:LHG:HC62	20:1:615:LHG:H242	1.82	0.41
18:A:811:CLA:H2A	18:A:811:CLA:HED2	2.01	0.41
6:B:80:ASP:OD2	6:B:83:HIS:HB2	2.21	0.41
22:I:101:BCR:H11C	22:I:101:BCR:H341	1.93	0.41
2:2:145:LEU:HD12	2:2:145:LEU:HA	1.89	0.41
5:A:338:LEU:HD13	18:A:825:CLA:HMD3	2.02	0.41
18:A:833:CLA:HBB1	18:A:833:CLA:HMB3	2.03	0.41
1:1:161:ASP:OD2	1:1:164:LYS:HG2	2.20	0.41
20:1:615:LHG:H222	20:1:615:LHG:H372	2.02	0.41
3:3:108:MET:CE	18:3:608:CLA:HAB	2.49	0.41
18:A:841:CLA:H3A	18:A:841:CLA:HBA2	1.38	0.41
18:B:814:CLA:H162	18:B:814:CLA:H141	1.76	0.41
18:B:822:CLA:H112	18:B:822:CLA:H142	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:28:MET:HE3	7:C:28:MET:HB3	1.91	0.41
13:I:27:LEU:HD23	22:L:305:BCR:H323	2.02	0.41
3:3:120:LEU:HB3	3:3:125:LEU:HB2	2.01	0.41
24:A:801:CL0:H2	24:A:801:CL0:H15	2.02	0.41
18:A:807:CLA:H193	18:A:807:CLA:H161	1.73	0.41
18:B:825:CLA:H92	18:B:825:CLA:H61	1.80	0.41
22:K:202:BCR:H371	22:K:202:BCR:H24C	1.79	0.41
16:L:137:LEU:HD12	16:L:137:LEU:HA	1.91	0.41
18:L:303:CLA:H143	18:L:303:CLA:H111	1.82	0.41
18:1:609:CLA:CBB	18:1:609:CLA:HHC	2.51	0.41
19:2:617:XAT:H402	18:2:603:CLA:C2B	2.51	0.41
18:4:602:CLA:C9	19:4:617:XAT:H30	2.50	0.41
5:A:113:GLN:NE2	18:A:810:CLA:OBD	2.54	0.41
18:A:807:CLA:H143	18:A:807:CLA:H111	1.86	0.41
18:A:844:CLA:H43	6:B:441:ASP:HB3	2.03	0.41
26:A:855:PQN:H222	18:F:301:CLA:C1B	2.50	0.41
18:B:816:CLA:O1A	11:G:152:ASN:ND2	2.53	0.41
18:F:302:CLA:H52	18:F:302:CLA:H11	1.81	0.41
18:F:302:CLA:O1D	18:F:302:CLA:H2A	2.20	0.41
18:1:602:CLA:CBB	19:1:614:XAT:H32	2.50	0.41
21:2:619:LUT:H35	21:2:619:LUT:H401	1.83	0.41
18:A:821:CLA:HBA1	18:A:821:CLA:H3A	1.71	0.41
18:A:809:CLA:H62	18:A:809:CLA:H92	1.84	0.41
6:B:411:MET:HE1	18:B:830:CLA:CHD	2.51	0.41
6:B:521:HIS:CD2	22:B:849:BCR:H281	2.55	0.41
6:B:714:SER:HB2	27:B:850:DGD:HBN1	2.02	0.41
16:L:152:ILE:HD13	16:L:152:ILE:HA	1.86	0.41
2:2:98:CYS:HB3	2:2:213:GLY:HA3	2.03	0.41
3:3:171:LEU:HD21	18:3:612:CLA:HMC3	2.03	0.41
21:3:613:LUT:H401	21:3:613:LUT:C15	2.43	0.41
5:A:90:PHE:CG	18:A:808:CLA:HBC3	2.55	0.41
5:A:596:TRP:HE1	18:B:803:CLA:C1D	2.34	0.41
18:A:806:CLA:H12	18:A:807:CLA:HBB1	2.01	0.41
18:A:827:CLA:H71	18:A:838:CLA:H43	2.03	0.41
22:A:850:BCR:H11C	22:A:850:BCR:H341	1.84	0.41
18:B:814:CLA:H102	22:B:845:BCR:H363	2.03	0.41
22:B:843:BCR:H383	22:B:843:BCR:H23C	2.03	0.41
22:B:847:BCR:HC7	22:B:847:BCR:H331	1.81	0.41
18:G:201:CLA:CGA	18:G:201:CLA:H3A	2.50	0.41
14:J:26:LEU:HD23	14:J:26:LEU:HA	1.90	0.41
18:1:612:CLA:C3A	21:1:616:LUT:H383	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:73:ASP:OD1	3:3:73:ASP:C	2.64	0.41
4:4:246:ILE:HD13	18:4:612:CLA:HMD2	2.02	0.41
18:4:612:CLA:H3A	18:4:612:CLA:HBA2	1.82	0.41
18:A:818:CLA:H11	18:A:818:CLA:H52	1.86	0.41
18:A:811:CLA:H141	18:A:811:CLA:H162	1.78	0.41
18:L:303:CLA:H141	18:L:303:CLA:H161	1.71	0.41
2:2:168:ASP:HB3	2:2:171:PHE:O	2.21	0.40
17:2:601:CHL:HBA1	17:2:601:CHL:H3A	1.40	0.40
18:A:804:CLA:H12	26:A:855:PQN:H243	2.03	0.40
18:A:802:CLA:H3A	18:A:802:CLA:CGA	2.41	0.40
18:A:820:CLA:H3A	18:A:820:CLA:HBA2	1.26	0.40
18:B:814:CLA:H93	18:B:814:CLA:H111	1.90	0.40
22:L:301:BCR:H361	22:L:301:BCR:H21C	2.02	0.40
1:1:149:ILE:O	1:1:152:VAL:HG12	2.20	0.40
1:1:192:ILE:O	1:1:196:ARG:HG3	2.21	0.40
21:2:616:LUT:H401	21:2:616:LUT:C15	2.52	0.40
23:4:619:LMG:HC71	23:4:619:LMG:HC2	1.88	0.40
22:A:851:BCR:H321	22:A:851:BCR:HC7	1.85	0.40
18:B:823:CLA:HBB1	18:B:830:CLA:HBC2	2.01	0.40
27:B:850:DGD:HBH1	27:B:850:DGD:HBT2	1.80	0.40
18:4:609:CLA:CGA	18:4:609:CLA:C3A	2.99	0.40
6:B:294:ASN:OD1	6:B:294:ASN:N	2.54	0.40
18:B:824:CLA:H141	18:B:824:CLA:H193	2.03	0.40
22:G:204:BCR:H15C	22:G:204:BCR:H351	1.94	0.40
21:3:613:LUT:H181	21:3:613:LUT:H7	1.71	0.40
24:A:801:CL0:H35	24:A:801:CL0:H41	1.86	0.40
22:G:204:BCR:H20C	22:G:204:BCR:H361	1.91	0.40
22:K:202:BCR:H11C	22:K:202:BCR:H341	1.85	0.40
3:3:186:LEU:HD23	3:3:186:LEU:HA	1.83	0.40
22:4:618:BCR:H24C	22:4:618:BCR:H371	1.96	0.40
5:A:679:ALA:O	18:A:802:CLA:HAB	2.22	0.40
5:A:688:GLY:HA3	6:B:569:ASP:HB2	2.03	0.40
18:A:819:CLA:H3A	18:A:819:CLA:HBA2	1.69	0.40
18:B:823:CLA:HBA1	18:B:823:CLA:H3A	1.77	0.40
18:B:841:CLA:H161	18:B:841:CLA:H121	1.46	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	162/241 (67%)	157 (97%)	5 (3%)	0	100	100
2	2	199/257 (77%)	195 (98%)	4 (2%)	0	100	100
3	3	215/273 (79%)	210 (98%)	5 (2%)	0	100	100
4	4	194/251 (77%)	189 (97%)	5 (3%)	0	100	100
5	A	707/750 (94%)	690 (98%)	17 (2%)	0	100	100
6	B	730/734 (100%)	712 (98%)	18 (2%)	0	100	100
7	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
8	D	141/204 (69%)	135 (96%)	6 (4%)	0	100	100
9	E	62/143 (43%)	60 (97%)	2 (3%)	0	100	100
10	F	147/221 (66%)	146 (99%)	1 (1%)	0	100	100
11	G	89/160 (56%)	87 (98%)	2 (2%)	0	100	100
12	H	84/145 (58%)	84 (100%)	0	0	100	100
13	I	29/37 (78%)	28 (97%)	1 (3%)	0	100	100
14	J	39/44 (89%)	39 (100%)	0	0	100	100
15	K	52/130 (40%)	51 (98%)	1 (2%)	0	100	100
16	L	157/219 (72%)	153 (98%)	4 (2%)	0	100	100
All	All	3085/3890 (79%)	3009 (98%)	76 (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	134/190 (70%)	134 (100%)	0	100	100
2	2	163/205 (80%)	163 (100%)	0	100	100
3	3	167/211 (79%)	167 (100%)	0	100	100
4	4	163/210 (78%)	161 (99%)	2 (1%)	63	75
5	A	574/610 (94%)	573 (100%)	1 (0%)	87	87
6	B	599/600 (100%)	599 (100%)	0	100	100
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	122/185 (66%)	122 (100%)	0	100	100
11	G	77/133 (58%)	77 (100%)	0	100	100
12	H	72/113 (64%)	70 (97%)	2 (3%)	38	63
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	36/39 (92%)	36 (100%)	0	100	100
15	K	43/95 (45%)	43 (100%)	0	100	100
16	L	125/174 (72%)	125 (100%)	0	100	100
All	All	2550/3153 (81%)	2545 (100%)	5 (0%)	85	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	194	ASN
4	4	222	GLN
5	A	312	ASN
12	H	121	ASN
12	H	125	ASP

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

Mol	Chain	Res	Type
2	2	92	GLN
2	2	212	ASN
3	3	103	ASN
3	3	136	GLN
4	4	94	GLN
4	4	243	HIS

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Mol	Chain	Res	Type
4	4	244	ASN
5	A	107	HIS
5	A	307	HIS
5	A	703	HIS
5	A	704	ASN
6	B	178	HIS
6	B	210	ASN
6	B	275	HIS
6	B	289	HIS
6	B	375	HIS
11	G	85	ASN
11	G	99	GLN
11	G	122	ASN
13	I	30	HIS

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)

198 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	B	841	20	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
17	CHL	2	605	-	46,50,74	2.32	18 (39%)	52,85,114	3.08	21 (40%)
20	LHG	B	851	18	37,37,48	0.31	0	40,43,54	0.48	0
18	CLA	L	303	16	69,73,73	1.24	9 (13%)	83,113,113	1.34	5 (6%)
18	CLA	A	834	5	69,73,73	1.25	9 (13%)	83,113,113	1.32	5 (6%)
18	CLA	1	609	-	46,50,73	1.51	8 (17%)	55,85,113	1.54	4 (7%)
18	CLA	3	602	-	59,63,73	1.37	9 (15%)	71,101,113	1.34	5 (7%)
18	CLA	F	301	-	61,65,73	1.34	9 (14%)	73,103,113	1.35	6 (8%)
18	CLA	1	603	-	58,62,73	1.37	9 (15%)	69,99,113	1.38	6 (8%)
22	BCR	I	101	-	41,41,41	1.71	8 (19%)	56,56,56	1.50	8 (14%)
22	BCR	B	801	-	41,41,41	1.81	8 (19%)	56,56,56	1.83	12 (21%)
22	BCR	K	205	-	41,41,41	1.73	8 (19%)	56,56,56	1.90	16 (28%)
18	CLA	4	601	4	50,54,73	1.46	10 (20%)	60,90,113	1.46	6 (10%)
18	CLA	A	817	-	49,53,73	1.50	8 (16%)	59,89,113	1.46	5 (8%)
18	CLA	1	611	-	49,53,73	1.50	8 (16%)	59,89,113	1.46	5 (8%)
18	CLA	H	201	-	64,68,73	1.30	8 (12%)	77,107,113	1.31	6 (7%)
18	CLA	3	603	-	49,53,73	1.51	8 (16%)	59,89,113	1.46	7 (11%)
18	CLA	A	810	5	54,58,73	1.42	9 (16%)	65,95,113	1.48	9 (13%)
22	BCR	B	843	-	41,41,41	1.77	8 (19%)	56,56,56	1.92	13 (23%)
18	CLA	B	813	6	69,73,73	1.24	10 (14%)	83,113,113	1.39	9 (10%)
18	CLA	L	304	-	49,53,73	1.49	9 (18%)	59,89,113	1.47	5 (8%)
22	BCR	A	849	-	41,41,41	1.76	8 (19%)	56,56,56	2.00	13 (23%)
18	CLA	K	204	-	50,54,73	1.48	8 (16%)	60,90,113	1.43	6 (10%)
18	CLA	B	807	6	56,60,73	1.38	9 (16%)	67,97,113	1.42	7 (10%)
18	CLA	B	840	6	69,73,73	1.26	9 (13%)	83,113,113	1.30	5 (6%)
18	CLA	B	826	6	66,70,73	1.29	10 (15%)	79,109,113	1.32	7 (8%)
18	CLA	B	822	-	69,73,73	1.25	9 (13%)	83,113,113	1.34	8 (9%)
22	BCR	B	848	-	41,41,41	1.73	8 (19%)	56,56,56	1.55	10 (17%)
18	CLA	A	804	5	69,73,73	1.25	9 (13%)	83,113,113	1.45	8 (9%)
18	CLA	A	838	-	55,59,73	1.40	9 (16%)	66,96,113	1.40	6 (9%)
22	BCR	G	204	-	41,41,41	1.71	8 (19%)	56,56,56	1.67	12 (21%)
22	BCR	A	851	-	41,41,41	1.83	8 (19%)	56,56,56	2.47	20 (35%)
18	CLA	B	804	6	45,49,73	1.50	8 (17%)	54,84,113	1.56	7 (12%)
18	CLA	4	614	-	54,58,73	1.40	8 (14%)	65,95,113	1.47	6 (9%)
18	CLA	A	820	5	69,73,73	1.24	9 (13%)	83,113,113	1.33	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	B	814	6	69,73,73	1.24	9 (13%)	83,113,113	1.30	5 (6%)
18	CLA	A	826	-	69,73,73	1.25	9 (13%)	83,113,113	1.33	8 (9%)
17	CHL	3	606	-	49,53,74	2.31	18 (36%)	59,89,114	2.89	20 (33%)
18	CLA	A	835	-	69,73,73	1.24	8 (11%)	83,113,113	1.38	8 (9%)
18	CLA	4	613	4	49,53,73	1.48	9 (18%)	59,89,113	1.61	7 (11%)
20	LHG	A	846	-	48,48,48	0.28	0	51,54,54	0.33	0
18	CLA	B	809	6	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)
18	CLA	B	832	6	69,73,73	1.26	8 (11%)	83,113,113	1.26	5 (6%)
18	CLA	F	303	10	45,49,73	1.52	9 (20%)	54,84,113	1.50	6 (11%)
21	LUT	3	613	-	42,43,43	1.70	8 (19%)	51,60,60	1.99	14 (27%)
18	CLA	3	610	-	43,48,73	1.57	7 (16%)	51,83,113	1.52	6 (11%)
18	CLA	A	829	5	69,73,73	1.24	9 (13%)	83,113,113	1.31	6 (7%)
18	CLA	A	811	5	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
17	CHL	2	607	-	55,59,74	2.18	19 (34%)	62,96,114	2.90	22 (35%)
18	CLA	B	824	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	6 (7%)
18	CLA	3	609	-	57,62,73	1.39	9 (15%)	68,100,113	1.36	8 (11%)
18	CLA	3	612	3	43,48,73	1.53	8 (18%)	51,83,113	1.56	7 (13%)
18	CLA	2	602	-	69,73,73	1.25	10 (14%)	83,113,113	1.30	7 (8%)
18	CLA	A	832	-	54,58,73	1.40	8 (14%)	65,95,113	1.44	8 (12%)
18	CLA	3	607	-	49,53,73	1.50	9 (18%)	59,89,113	1.44	5 (8%)
27	DGD	B	850	-	67,67,67	0.84	2 (2%)	81,81,81	0.98	3 (3%)
18	CLA	3	605	-	45,49,73	1.59	10 (22%)	57,84,113	1.56	7 (12%)
18	CLA	A	828	5	69,73,73	1.25	10 (14%)	83,113,113	1.34	6 (7%)
18	CLA	L	302	16	49,53,73	1.48	9 (18%)	59,89,113	1.48	6 (10%)
22	BCR	A	850	-	41,41,41	1.79	8 (19%)	56,56,56	1.89	13 (23%)
18	CLA	G	202	-	46,50,73	1.51	9 (19%)	55,85,113	1.45	5 (9%)
25	SF4	A	854	-	0,12,12	-	-	-		
18	CLA	B	835	-	46,50,73	1.52	8 (17%)	55,85,113	1.45	6 (10%)
22	BCR	B	847	-	41,41,41	1.71	8 (19%)	56,56,56	1.56	9 (16%)
18	CLA	B	825	-	66,70,73	1.26	9 (13%)	79,109,113	1.38	9 (11%)
18	CLA	A	841	5	69,73,73	1.24	9 (13%)	83,113,113	1.30	7 (8%)
18	CLA	3	611	-	41,44,73	1.58	10 (24%)	49,77,113	1.49	6 (12%)
18	CLA	B	831	6	47,51,73	1.48	9 (19%)	56,86,113	1.48	6 (10%)
18	CLA	A	818	5	64,68,73	1.30	9 (14%)	77,107,113	4.90	9 (11%)
22	BCR	L	306	-	41,41,41	1.71	8 (19%)	56,56,56	2.03	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	CHL	4	615	4	44,49,74	2.29	17 (38%)	51,84,114	3.22	21 (41%)
18	CLA	B	830	-	47,51,73	1.47	9 (19%)	56,86,113	1.49	6 (10%)
18	CLA	B	817	-	63,67,73	1.31	10 (15%)	75,105,113	1.38	8 (10%)
17	CHL	2	615	2	47,51,74	2.34	18 (38%)	52,86,114	3.10	22 (42%)
18	CLA	A	830	-	69,73,73	1.24	9 (13%)	83,113,113	1.45	8 (9%)
18	CLA	B	833	6	49,53,73	1.48	10 (20%)	59,89,113	1.50	7 (11%)
24	CL0	A	801	5	64,67,73	2.05	19 (29%)	75,102,113	4.02	33 (44%)
18	CLA	A	812	-	69,73,73	1.26	8 (11%)	83,113,113	1.32	7 (8%)
22	BCR	F	304	-	41,41,41	1.87	8 (19%)	56,56,56	2.15	16 (28%)
17	CHL	4	606	-	45,49,74	2.48	18 (40%)	57,84,114	2.93	22 (38%)
21	LUT	2	619	-	42,43,43	1.68	8 (19%)	51,60,60	1.82	11 (21%)
18	CLA	A	807	-	69,73,73	1.27	10 (14%)	83,113,113	1.28	6 (7%)
18	CLA	B	816	6	59,63,73	1.34	8 (13%)	71,101,113	1.41	8 (11%)
17	CHL	2	606	-	47,51,74	2.36	18 (38%)	52,86,114	3.08	24 (46%)
18	CLA	A	809	5	69,73,73	1.25	9 (13%)	83,113,113	1.36	7 (8%)
22	BCR	B	846	-	41,41,41	1.74	8 (19%)	56,56,56	1.69	10 (17%)
22	BCR	K	202	-	41,41,41	1.80	7 (17%)	56,56,56	1.95	14 (25%)
18	CLA	4	608	4	49,53,73	1.50	9 (18%)	59,89,113	1.43	5 (8%)
18	CLA	G	201	-	49,53,73	1.50	9 (18%)	59,89,113	1.44	5 (8%)
22	BCR	A	853	-	41,41,41	1.82	8 (19%)	56,56,56	1.82	14 (25%)
18	CLA	2	608	2	49,53,73	1.47	9 (18%)	59,89,113	1.47	4 (6%)
18	CLA	B	808	-	69,73,73	1.23	10 (14%)	83,113,113	1.35	7 (8%)
22	BCR	B	849	-	41,41,41	1.77	8 (19%)	56,56,56	1.87	12 (21%)
20	LHG	2	618	18	36,36,48	0.31	0	39,42,54	0.48	0
18	CLA	1	602	1	58,62,73	1.36	9 (15%)	69,99,113	1.38	7 (10%)
18	CLA	4	611	-	44,49,73	1.55	9 (20%)	52,84,113	1.47	5 (9%)
18	CLA	K	203	-	49,53,73	1.48	7 (14%)	59,89,113	1.49	7 (11%)
23	LMG	4	619	-	39,39,55	0.23	0	47,47,63	0.23	0
18	CLA	B	838	6	51,55,73	1.44	9 (17%)	61,91,113	1.46	7 (11%)
18	CLA	2	611	-	48,52,73	1.53	8 (16%)	58,88,113	1.48	6 (10%)
18	CLA	B	805	6	69,73,73	1.25	9 (13%)	83,113,113	1.32	6 (7%)
18	CLA	A	821	5	49,53,73	1.48	9 (18%)	59,89,113	1.48	4 (6%)
18	CLA	3	608	-	45,49,73	1.52	10 (22%)	54,84,113	1.56	8 (14%)
18	CLA	1	604	-	53,57,73	1.42	8 (15%)	62,93,113	1.58	7 (11%)
17	CHL	1	606	-	44,49,74	2.54	20 (45%)	48,84,114	3.09	20 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
18	CLA	B	821	6	51,55,73	1.43	8 (15%)	61,91,113	1.55	7 (11%)
18	CLA	B	829	-	60,64,73	1.34	9 (15%)	72,102,113	1.39	6 (8%)
18	CLA	F	302	-	55,59,73	1.40	7 (12%)	66,96,113	1.50	5 (7%)
22	BCR	3	614	-	41,41,41	1.72	8 (19%)	56,56,56	1.63	13 (23%)
18	CLA	A	815	5	49,53,73	1.46	10 (20%)	59,89,113	1.56	9 (15%)
18	CLA	B	810	6	69,73,73	1.26	10 (14%)	83,113,113	1.30	7 (8%)
26	PQN	A	855	-	34,34,34	0.38	0	42,45,45	0.42	0
18	CLA	1	608	-	44,48,73	1.58	9 (20%)	56,83,113	1.58	7 (12%)
18	CLA	4	609	-	58,62,73	1.36	9 (15%)	69,99,113	1.40	7 (10%)
18	CLA	A	839	-	59,63,73	1.35	8 (13%)	71,101,113	1.41	7 (9%)
22	BCR	L	301	-	41,41,41	1.76	9 (21%)	56,56,56	2.22	12 (21%)
18	CLA	B	839	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
18	CLA	A	842	-	69,73,73	1.24	8 (11%)	83,113,113	1.40	8 (9%)
18	CLA	4	603	-	48,52,73	1.55	10 (20%)	61,88,113	1.53	7 (11%)
21	LUT	4	616	-	42,43,43	1.63	8 (19%)	51,60,60	1.60	10 (19%)
22	BCR	A	852	-	41,41,41	1.73	8 (19%)	56,56,56	2.02	15 (26%)
18	CLA	B	820	6	54,58,73	1.40	9 (16%)	65,95,113	1.47	10 (15%)
20	LHG	B	852	-	48,48,48	0.27	0	51,54,54	0.32	0
21	LUT	2	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.98	12 (23%)
17	CHL	1	601	1	55,60,74	2.19	19 (34%)	61,97,114	2.88	26 (42%)
18	CLA	B	837	6	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
18	CLA	A	840	5	56,60,73	1.39	9 (16%)	67,97,113	1.43	7 (10%)
18	CLA	A	808	5	54,58,73	1.39	9 (16%)	65,95,113	1.47	7 (10%)
22	BCR	B	844	-	41,41,41	1.76	8 (19%)	56,56,56	1.90	13 (23%)
18	CLA	A	831	5	69,73,73	1.24	9 (13%)	83,113,113	1.32	8 (9%)
18	CLA	A	837	5	49,53,73	1.50	8 (16%)	59,89,113	1.45	5 (8%)
18	CLA	A	813	5	58,62,73	1.36	8 (13%)	69,99,113	1.42	6 (8%)
19	XAT	4	617	-	39,47,47	6.04	29 (74%)	54,74,74	5.93	34 (62%)
18	CLA	B	811	6	58,62,73	1.41	10 (17%)	73,100,113	1.44	8 (10%)
19	XAT	2	617	-	39,47,47	1.81	7 (17%)	54,74,74	2.10	15 (27%)
18	CLA	A	805	5	56,60,73	1.38	9 (16%)	67,97,113	1.42	8 (11%)
20	LHG	1	615	18	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
25	SF4	C	101	-	0,12,12	-	-	-		
22	BCR	4	618	-	41,41,41	1.74	8 (19%)	56,56,56	1.66	9 (16%)
22	BCR	A	848	-	41,41,41	1.75	8 (19%)	56,56,56	1.66	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	A	806	5	69,73,73	1.25	10 (14%)	83,113,113	1.33	8 (9%)
18	CLA	A	833	5	60,64,73	1.33	8 (13%)	72,102,113	1.38	7 (9%)
18	CLA	A	814	5	69,73,73	1.26	10 (14%)	83,113,113	1.30	6 (7%)
18	CLA	A	822	-	69,73,73	1.24	9 (13%)	83,113,113	1.31	8 (9%)
18	CLA	A	803	-	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)
18	CLA	A	816	5	46,50,73	1.50	9 (19%)	55,85,113	1.48	5 (9%)
18	CLA	A	802	-	69,73,73	1.24	10 (14%)	83,113,113	1.37	7 (8%)
18	CLA	K	201	15	42,45,73	1.57	8 (19%)	50,78,113	1.50	5 (10%)
18	CLA	A	843	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	4 (4%)
18	CLA	A	844	-	69,73,73	1.25	10 (14%)	83,113,113	1.32	7 (8%)
18	CLA	B	823	6	49,53,73	1.48	10 (20%)	59,89,113	1.43	5 (8%)
18	CLA	4	610	-	46,50,73	1.49	9 (19%)	55,85,113	1.47	5 (9%)
18	CLA	A	819	-	63,67,73	1.30	10 (15%)	75,105,113	1.35	7 (9%)
18	CLA	2	610	20	41,45,73	2.58	11 (26%)	47,76,113	1.33	5 (10%)
18	CLA	B	819	-	59,63,73	1.36	10 (16%)	71,101,113	1.40	6 (8%)
18	CLA	A	836	5	49,53,73	1.50	8 (16%)	59,89,113	1.46	6 (10%)
18	CLA	4	612	-	61,65,73	1.32	8 (13%)	73,103,113	1.39	6 (8%)
18	CLA	B	836	6	54,58,73	1.41	10 (18%)	65,95,113	3.46	11 (16%)
19	XAT	1	614	-	39,47,47	0.85	1 (2%)	54,74,74	3.17	23 (42%)
18	CLA	B	828	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)
18	CLA	2	612	2	69,73,73	1.25	9 (13%)	83,113,113	1.31	5 (6%)
17	CHL	4	607	-	50,54,74	2.20	19 (38%)	56,90,114	3.09	23 (41%)
18	CLA	1	607	-	47,52,73	1.52	10 (21%)	56,88,113	1.45	5 (8%)
17	CHL	4	605	-	44,49,74	2.35	18 (40%)	49,84,114	3.06	21 (42%)
18	CLA	B	802	-	69,73,73	1.26	10 (14%)	83,113,113	1.30	7 (8%)
18	CLA	4	602	4	64,68,73	1.30	10 (15%)	77,107,113	1.33	7 (9%)
17	CHL	2	601	2	51,55,74	2.29	19 (37%)	57,91,114	2.98	22 (38%)
18	CLA	4	604	-	47,51,73	1.58	9 (19%)	60,87,113	1.52	7 (11%)
18	CLA	B	818	6	64,68,73	1.29	10 (15%)	77,107,113	1.42	10 (12%)
18	CLA	G	203	11	49,53,73	1.48	8 (16%)	59,89,113	1.46	5 (8%)
18	CLA	3	601	3	64,68,73	1.31	10 (15%)	77,107,113	1.35	7 (9%)
18	CLA	A	827	-	63,67,73	1.31	9 (14%)	75,105,113	1.34	6 (8%)
18	CLA	2	604	-	47,51,73	1.50	10 (21%)	55,86,113	1.52	6 (10%)
18	CLA	B	827	6	69,73,73	1.25	9 (13%)	83,113,113	1.34	6 (7%)
18	CLA	1	610	20	41,46,73	1.65	9 (21%)	52,81,113	1.60	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	B	806	6	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
22	BCR	J	102	-	41,41,41	1.75	8 (19%)	56,56,56	1.81	14 (25%)
22	BCR	L	305	-	41,41,41	1.76	8 (19%)	56,56,56	1.78	13 (23%)
18	CLA	1	612	-	50,54,73	1.46	8 (16%)	60,90,113	1.45	5 (8%)
18	CLA	3	604	-	44,49,73	1.54	9 (20%)	52,84,113	1.46	5 (9%)
18	CLA	A	824	-	45,49,73	1.54	7 (15%)	54,84,113	1.53	7 (12%)
22	BCR	B	845	-	41,41,41	1.83	8 (19%)	56,56,56	1.94	14 (25%)
18	CLA	2	603	-	47,52,73	1.51	9 (19%)	56,88,113	1.46	5 (8%)
23	LMG	4	620	-	33,33,55	0.24	0	41,41,63	0.26	0
18	CLA	1	605	-	50,54,73	1.47	6 (12%)	60,90,113	1.48	4 (6%)
26	PQN	B	842	-	34,34,34	0.40	0	42,45,45	0.41	0
18	CLA	1	613	-	41,46,73	1.68	10 (24%)	52,81,113	1.61	8 (15%)
18	CLA	2	609	-	51,55,73	1.43	9 (17%)	61,91,113	1.46	5 (8%)
18	CLA	B	815	-	47,51,73	1.48	10 (21%)	56,86,113	1.47	5 (8%)
18	CLA	B	803	-	69,73,73	1.23	9 (13%)	83,113,113	1.34	6 (7%)
18	CLA	A	823	5	46,50,73	1.50	7 (15%)	55,85,113	1.46	6 (10%)
18	CLA	A	825	-	59,63,73	1.34	8 (13%)	71,101,113	1.40	9 (12%)
25	SF4	C	102	-	0,12,12	-	-	-		
18	CLA	B	834	6	64,68,73	1.31	8 (12%)	77,107,113	1.33	7 (9%)
21	LUT	1	616	-	42,43,43	1.68	7 (16%)	51,60,60	2.10	14 (27%)
18	CLA	B	812	6	47,51,73	1.49	9 (19%)	56,86,113	1.46	5 (8%)
18	CLA	2	613	2	47,51,73	1.50	9 (19%)	56,86,113	1.49	5 (8%)
20	LHG	A	847	-	29,29,48	0.35	0	32,35,54	0.43	0

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	B	841	20	-	20/39/115/115	-
17	CHL	2	605	-	-	6/12/88/117	-
20	LHG	B	851	18	-	5/42/42/53	-
18	CLA	L	303	16	-	11/39/115/115	-
18	CLA	A	834	5	-	10/39/115/115	-
18	CLA	1	609	-	-	4/11/87/115	-
18	CLA	3	602	-	-	13/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	301	-	-	13/30/106/115	-
18	CLA	1	603	-	-	8/26/102/115	-
22	BCR	I	101	-	-	0/29/63/63	0/2/2/2
22	BCR	B	801	-	-	7/29/63/63	0/2/2/2
22	BCR	K	205	-	-	6/29/63/63	0/2/2/2
18	CLA	4	601	4	-	10/17/93/115	-
18	CLA	A	817	-	-	4/15/91/115	-
18	CLA	1	611	-	-	7/15/91/115	-
18	CLA	H	201	-	-	18/33/109/115	-
18	CLA	3	603	-	-	5/15/91/115	-
18	CLA	A	810	5	-	6/21/97/115	-
22	BCR	B	843	-	-	1/29/63/63	0/2/2/2
18	CLA	B	813	6	-	12/39/115/115	-
18	CLA	L	304	-	-	5/15/91/115	-
22	BCR	A	849	-	-	5/29/63/63	0/2/2/2
18	CLA	K	204	-	-	12/17/93/115	-
18	CLA	B	807	6	-	3/24/100/115	-
18	CLA	B	840	6	-	9/39/115/115	-
18	CLA	B	826	6	-	6/36/112/115	-
18	CLA	B	822	-	-	16/39/115/115	-
22	BCR	B	848	-	-	0/29/63/63	0/2/2/2
18	CLA	A	804	5	-	18/39/115/115	-
18	CLA	A	838	-	-	8/23/99/115	-
22	BCR	G	204	-	-	3/29/63/63	0/2/2/2
22	BCR	A	851	-	-	7/29/63/63	0/2/2/2
18	CLA	B	804	6	-	2/10/86/115	-
18	CLA	4	614	-	-	8/21/97/115	-
18	CLA	A	820	5	-	16/39/115/115	-
18	CLA	B	814	6	-	17/39/115/115	-
18	CLA	A	826	-	-	12/39/115/115	-
17	CHL	3	606	-	-	7/15/91/117	-
18	CLA	A	835	-	-	16/39/115/115	-
18	CLA	4	613	4	-	8/15/91/115	-
20	LHG	A	846	-	-	5/53/53/53	-
18	CLA	B	809	6	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	832	6	-	14/39/115/115	-
18	CLA	F	303	10	-	4/10/86/115	-
21	LUT	3	613	-	-	6/29/67/67	0/2/2/2
18	CLA	3	610	-	-	2/8/84/115	-
18	CLA	A	829	5	-	19/39/115/115	-
18	CLA	A	811	5	-	13/39/115/115	-
17	CHL	2	607	-	-	5/23/99/117	-
18	CLA	B	824	-	-	16/39/115/115	-
18	CLA	3	609	-	-	11/25/101/115	-
18	CLA	3	612	3	-	2/8/84/115	-
18	CLA	2	602	-	-	15/39/115/115	-
18	CLA	A	832	-	-	9/21/97/115	-
18	CLA	3	607	-	-	3/15/91/115	-
27	DGD	B	850	-	-	14/55/95/95	0/2/2/2
18	CLA	3	605	-	-	1/10/86/115	-
18	CLA	A	828	5	-	10/39/115/115	-
18	CLA	L	302	16	-	3/15/91/115	-
22	BCR	A	850	-	-	4/29/63/63	0/2/2/2
18	CLA	G	202	-	-	4/12/88/115	-
25	SF4	A	854	-	-	-	0/6/5/5
18	CLA	B	835	-	-	6/12/88/115	-
22	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	B	825	-	-	13/36/112/115	-
18	CLA	A	841	5	-	13/39/115/115	-
18	CLA	3	611	-	-	2/2/74/115	-
18	CLA	B	831	6	-	1/13/89/115	-
18	CLA	A	818	5	-	14/33/109/115	-
22	BCR	L	306	-	-	4/29/63/63	0/2/2/2
17	CHL	4	615	4	-	0/10/86/117	-
18	CLA	B	830	-	-	4/13/89/115	-
18	CLA	B	817	-	-	13/32/108/115	-
17	CHL	2	615	2	-	2/14/90/117	-
18	CLA	A	830	-	-	11/39/115/115	-
18	CLA	B	833	6	-	4/15/91/115	-
24	CL0	A	801	5	-	15/35/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	812	-	-	21/39/115/115	-
22	BCR	F	304	-	-	12/29/63/63	0/2/2/2
17	CHL	4	606	-	-	2/10/86/117	-
21	LUT	2	619	-	-	5/29/67/67	0/2/2/2
18	CLA	A	807	-	-	15/39/115/115	-
18	CLA	B	816	6	-	9/27/103/115	-
17	CHL	2	606	-	-	2/14/90/117	-
18	CLA	A	809	5	-	13/39/115/115	-
22	BCR	B	846	-	-	8/29/63/63	0/2/2/2
22	BCR	K	202	-	-	2/29/63/63	0/2/2/2
18	CLA	4	608	4	-	7/15/91/115	-
18	CLA	G	201	-	-	5/15/91/115	-
22	BCR	A	853	-	-	4/29/63/63	0/2/2/2
18	CLA	2	608	2	-	7/15/91/115	-
18	CLA	B	808	-	-	13/39/115/115	-
22	BCR	B	849	-	-	7/29/63/63	0/2/2/2
20	LHG	2	618	18	-	11/41/41/53	-
18	CLA	1	602	1	-	9/26/102/115	-
18	CLA	4	611	-	-	2/10/86/115	-
18	CLA	K	203	-	-	6/15/91/115	-
23	LMG	4	619	-	-	4/34/54/70	0/1/1/1
18	CLA	B	838	6	-	4/18/94/115	-
18	CLA	2	611	-	-	8/13/89/115	-
18	CLA	B	805	6	-	24/39/115/115	-
18	CLA	A	821	5	-	7/15/91/115	-
18	CLA	3	608	-	-	3/10/86/115	-
18	CLA	1	604	-	-	9/20/96/115	-
17	CHL	1	606	-	-	0/10/86/117	-
18	CLA	B	821	6	-	6/18/94/115	-
18	CLA	B	829	-	-	6/29/105/115	-
18	CLA	F	302	-	-	10/23/99/115	-
22	BCR	3	614	-	-	3/29/63/63	0/2/2/2
18	CLA	A	815	5	-	5/15/91/115	-
18	CLA	B	810	6	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PQN	A	855	-	-	1/23/43/43	0/2/2/2
18	CLA	1	608	-	-	3/8/84/115	-
18	CLA	4	609	-	-	4/26/102/115	-
18	CLA	A	839	-	-	7/27/103/115	-
22	BCR	L	301	-	-	3/29/63/63	0/2/2/2
18	CLA	B	839	-	-	9/39/115/115	-
18	CLA	A	842	-	-	11/39/115/115	-
18	CLA	4	603	-	-	4/13/89/115	-
21	LUT	4	616	-	-	2/29/67/67	0/2/2/2
22	BCR	A	852	-	-	14/29/63/63	0/2/2/2
18	CLA	B	820	6	-	5/21/97/115	-
20	LHG	B	852	-	-	11/53/53/53	-
21	LUT	2	616	-	-	6/29/67/67	0/2/2/2
17	CHL	1	601	1	-	8/24/100/117	-
18	CLA	B	837	6	-	13/39/115/115	-
18	CLA	A	840	5	-	5/24/100/115	-
18	CLA	A	808	5	-	0/21/97/115	-
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2
18	CLA	A	831	5	-	8/39/115/115	-
18	CLA	A	837	5	-	5/15/91/115	-
18	CLA	A	813	5	-	9/26/102/115	-
19	XAT	4	617	-	-	3/31/93/93	0/4/4/4
18	CLA	B	811	6	-	11/25/101/115	-
19	XAT	2	617	-	-	15/31/93/93	0/4/4/4
18	CLA	A	805	5	-	4/24/100/115	-
20	LHG	1	615	18	-	33/53/53/53	-
25	SF4	C	101	-	-	-	0/6/5/5
22	BCR	4	618	-	-	9/29/63/63	0/2/2/2
22	BCR	A	848	-	-	2/29/63/63	0/2/2/2
18	CLA	A	806	5	-	21/39/115/115	-
18	CLA	A	833	5	-	4/29/105/115	-
18	CLA	A	814	5	-	15/39/115/115	-
18	CLA	A	822	-	-	11/39/115/115	-
18	CLA	A	803	-	-	21/39/115/115	-
18	CLA	A	816	5	-	3/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	802	-	-	11/39/115/115	-
18	CLA	K	201	15	-	2/4/76/115	-
18	CLA	A	843	-	-	18/39/115/115	-
18	CLA	A	844	-	-	12/39/115/115	-
18	CLA	B	823	6	-	6/15/91/115	-
18	CLA	4	610	-	-	4/12/88/115	-
18	CLA	A	819	-	-	17/32/108/115	-
18	CLA	2	610	20	-	2/10/70/115	-
18	CLA	B	819	-	-	11/27/103/115	-
18	CLA	A	836	5	-	5/15/91/115	-
18	CLA	4	612	-	-	11/30/106/115	-
18	CLA	B	836	6	-	6/21/97/115	-
19	XAT	1	614	-	-	5/31/93/93	0/4/4/4
18	CLA	B	828	-	-	17/39/115/115	-
18	CLA	2	612	2	-	18/39/115/115	-
17	CHL	4	607	-	-	6/17/93/117	-
18	CLA	1	607	-	-	8/13/89/115	-
17	CHL	4	605	-	-	6/10/86/117	-
18	CLA	B	802	-	-	17/39/115/115	-
18	CLA	4	602	4	-	9/33/109/115	-
17	CHL	2	601	2	-	5/19/95/117	-
18	CLA	4	604	-	-	6/11/87/115	-
18	CLA	B	818	6	-	8/33/109/115	-
18	CLA	G	203	11	-	3/15/91/115	-
18	CLA	3	601	3	-	11/33/109/115	-
18	CLA	A	827	-	-	7/32/108/115	-
18	CLA	2	604	-	-	9/11/88/115	-
18	CLA	B	827	6	-	22/39/115/115	-
18	CLA	1	610	20	-	0/4/80/115	-
18	CLA	B	806	6	-	13/39/115/115	-
22	BCR	J	102	-	-	2/29/63/63	0/2/2/2
22	BCR	L	305	-	-	2/29/63/63	0/2/2/2
18	CLA	1	612	-	-	9/17/93/115	-
18	CLA	3	604	-	-	2/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	824	-	-	4/10/86/115	-
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
18	CLA	2	603	-	-	3/13/89/115	-
23	LMG	4	620	-	-	5/28/48/70	0/1/1/1
18	CLA	1	605	-	-	7/17/93/115	-
26	PQN	B	842	-	-	7/23/43/43	0/2/2/2
18	CLA	1	613	-	-	1/4/80/115	-
18	CLA	2	609	-	-	6/18/94/115	-
18	CLA	B	815	-	-	5/13/89/115	-
18	CLA	B	803	-	-	11/39/115/115	-
18	CLA	A	823	5	-	4/12/88/115	-
18	CLA	A	825	-	-	12/27/103/115	-
25	SF4	C	102	-	-	-	0/6/5/5
18	CLA	B	834	6	-	7/33/109/115	-
21	LUT	1	616	-	-	3/29/67/67	0/2/2/2
18	CLA	B	812	6	-	0/13/89/115	-
18	CLA	2	613	2	-	5/13/89/115	-
20	LHG	A	847	-	-	3/34/34/53	-

All (1753) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	617	XAT	O24-C25	-13.10	1.27	1.46
18	2	610	CLA	C1A-NA	12.61	1.40	1.29
19	4	617	XAT	C2-C3	-11.35	1.36	1.52
19	4	617	XAT	C2-C1	-10.99	1.37	1.54
19	4	617	XAT	O4-C5	-10.50	1.31	1.46
19	4	617	XAT	C24-C25	-10.18	1.37	1.52
19	4	617	XAT	C38-C25	-9.14	1.37	1.51
19	4	617	XAT	C4-C3	-8.48	1.40	1.52
19	4	617	XAT	C4-C5	-8.34	1.40	1.52
24	A	801	CL0	C1D-ND	8.20	1.47	1.37
19	4	617	XAT	C24-C23	-8.15	1.40	1.52
19	4	617	XAT	C22-C23	-7.74	1.41	1.52
19	4	617	XAT	C17-C1	-7.44	1.39	1.53
19	4	617	XAT	C20-C13	-7.29	1.35	1.50
19	4	617	XAT	C22-C21	-6.54	1.44	1.54
19	4	617	XAT	C19-C9	-6.48	1.37	1.50
24	A	801	CL0	C3D-C4D	-6.48	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	617	XAT	C37-C21	-5.55	1.43	1.53
19	4	617	XAT	C16-C1	-5.54	1.43	1.53
22	F	304	BCR	C21-C22	5.26	1.42	1.35
17	4	606	CHL	O2D-CGD	5.22	1.45	1.33
17	2	606	CHL	O2D-CGD	5.13	1.45	1.33
17	2	615	CHL	O2D-CGD	5.12	1.45	1.33
17	1	606	CHL	CHD-C1D	5.09	1.48	1.38
19	2	617	XAT	C34-C33	5.08	1.42	1.35
22	B	845	BCR	C21-C22	5.08	1.42	1.35
17	2	605	CHL	O2D-CGD	5.08	1.45	1.33
22	A	853	BCR	C10-C9	5.08	1.42	1.35
22	F	304	BCR	C17-C18	5.06	1.42	1.35
17	3	606	CHL	O2D-CGD	5.03	1.45	1.33
17	2	601	CHL	O2D-CGD	5.01	1.45	1.33
17	4	606	CHL	C3C-C2C	5.00	1.47	1.36
19	4	617	XAT	C39-C29	-5.00	1.40	1.50
17	1	606	CHL	CHC-C1C	4.98	1.48	1.38
17	2	607	CHL	O2D-CGD	4.98	1.45	1.33
17	1	606	CHL	C2C-C3C	4.97	1.47	1.36
17	4	606	CHL	CHD-C1D	4.95	1.48	1.38
19	4	617	XAT	C18-C5	-4.92	1.44	1.51
17	4	607	CHL	O2D-CGD	4.91	1.45	1.33
17	4	606	CHL	CHC-C1C	4.91	1.48	1.38
17	2	607	CHL	C3D-C4D	-4.86	1.33	1.44
17	2	606	CHL	CHC-C1C	4.80	1.48	1.38
17	2	601	CHL	C3D-C4D	-4.80	1.33	1.44
17	1	601	CHL	C3D-C4D	-4.79	1.33	1.44
22	B	801	BCR	C10-C9	4.76	1.42	1.35
17	4	607	CHL	C3D-C4D	-4.76	1.33	1.44
17	2	605	CHL	CHC-C1C	4.74	1.48	1.38
21	3	613	LUT	C10-C9	4.74	1.42	1.35
17	2	615	CHL	CHC-C1C	4.74	1.48	1.38
17	3	606	CHL	C3D-C4D	-4.72	1.33	1.44
17	2	606	CHL	C2C-C3C	4.72	1.46	1.36
17	4	606	CHL	C3D-C4D	-4.72	1.33	1.44
17	1	606	CHL	C3D-C4D	-4.72	1.33	1.44
17	2	615	CHL	C2C-C3C	4.69	1.46	1.36
22	A	850	BCR	C17-C18	4.69	1.42	1.35
17	2	605	CHL	C3D-C4D	-4.69	1.33	1.44
17	2	606	CHL	C3D-C4D	-4.68	1.33	1.44
17	4	605	CHL	C2C-C3C	4.68	1.46	1.37
17	2	615	CHL	C3D-C4D	-4.67	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	606	CHL	CHD-C1D	4.67	1.47	1.38
17	2	601	CHL	CHC-C1C	4.66	1.48	1.38
17	4	605	CHL	O2D-CGD	4.66	1.45	1.30
17	1	606	CHL	O2D-CGD	4.64	1.45	1.30
17	4	615	CHL	C3D-C4D	-4.64	1.33	1.44
17	2	615	CHL	CHD-C1D	4.64	1.47	1.38
19	4	617	XAT	C40-C33	-4.63	1.41	1.50
17	4	605	CHL	C3D-C4D	-4.63	1.33	1.44
17	4	615	CHL	O2D-CGD	4.63	1.45	1.30
22	A	850	BCR	C14-C13	4.62	1.41	1.35
19	4	617	XAT	C36-C21	-4.61	1.44	1.53
17	2	605	CHL	C2C-C3C	4.60	1.46	1.37
17	4	605	CHL	CHD-C1D	4.60	1.47	1.38
17	1	601	CHL	O2D-CGD	4.60	1.45	1.30
17	2	601	CHL	C2C-C3C	4.59	1.46	1.36
22	A	851	BCR	C21-C22	4.59	1.41	1.35
17	4	605	CHL	CHC-C1C	4.58	1.47	1.38
22	A	849	BCR	C21-C22	4.57	1.41	1.35
17	2	601	CHL	CHD-C1D	4.56	1.47	1.38
17	1	601	CHL	CHD-C1D	4.56	1.47	1.38
17	1	601	CHL	CHC-C1C	4.56	1.47	1.38
17	4	615	CHL	C2C-C3C	4.55	1.46	1.36
17	3	606	CHL	C3C-C2C	4.55	1.46	1.36
21	1	616	LUT	C30-C29	4.55	1.41	1.35
17	1	601	CHL	C2C-C3C	4.54	1.46	1.36
22	F	304	BCR	C10-C9	4.53	1.41	1.35
17	3	606	CHL	CHD-C1D	4.52	1.47	1.38
17	3	606	CHL	O2A-CGA	4.52	1.45	1.30
17	4	615	CHL	CHC-C1C	4.51	1.47	1.38
17	1	606	CHL	CHD-C4C	4.51	1.49	1.39
17	2	607	CHL	CHC-C1C	4.50	1.47	1.38
17	2	607	CHL	C2C-C3C	4.50	1.46	1.36
17	2	605	CHL	CHD-C1D	4.50	1.47	1.38
17	3	606	CHL	CHC-C1C	4.48	1.47	1.38
21	2	616	LUT	C34-C33	4.48	1.41	1.35
22	K	202	BCR	C10-C9	4.47	1.41	1.35
17	4	607	CHL	O2A-CGA	4.46	1.45	1.30
17	4	606	CHL	CHD-C4C	4.46	1.49	1.39
19	2	617	XAT	C14-C13	4.45	1.41	1.35
22	A	851	BCR	C14-C13	4.42	1.41	1.35
17	2	607	CHL	CHD-C1D	4.41	1.47	1.38
22	B	843	BCR	C14-C13	4.41	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	613	LUT	C34-C33	4.41	1.41	1.35
17	4	615	CHL	CHD-C1D	4.39	1.46	1.38
22	A	851	BCR	C17-C18	4.39	1.41	1.35
22	K	202	BCR	C17-C18	4.38	1.41	1.35
19	4	617	XAT	C10-C9	-4.37	1.30	1.35
22	B	844	BCR	C21-C22	4.37	1.41	1.35
22	K	202	BCR	C14-C13	4.37	1.41	1.35
19	2	617	XAT	C30-C29	4.36	1.41	1.35
22	B	849	BCR	C10-C9	4.35	1.41	1.35
22	K	202	BCR	C21-C22	4.35	1.41	1.35
22	B	849	BCR	C14-C13	4.31	1.41	1.35
22	B	845	BCR	C10-C9	4.31	1.41	1.35
22	A	851	BCR	C10-C9	4.28	1.41	1.35
19	2	617	XAT	C10-C9	4.27	1.41	1.35
24	A	801	CL0	C3D-C2D	4.27	1.45	1.37
22	A	849	BCR	C17-C18	4.27	1.41	1.35
22	A	853	BCR	C21-C22	4.26	1.41	1.35
22	B	845	BCR	C17-C18	4.26	1.41	1.35
17	4	607	CHL	C2C-C3C	4.26	1.45	1.36
20	1	615	LHG	O8-C23	4.26	1.45	1.33
22	A	853	BCR	C17-C18	4.25	1.41	1.35
17	2	607	CHL	O2A-CGA	4.25	1.45	1.33
21	1	616	LUT	C10-C9	4.23	1.41	1.35
27	B	850	DGD	O1G-C1A	4.23	1.45	1.33
17	4	607	CHL	CHD-C1D	4.22	1.46	1.38
22	K	205	BCR	C21-C22	4.21	1.41	1.35
22	A	853	BCR	C14-C13	4.21	1.41	1.35
22	L	301	BCR	C14-C13	4.20	1.41	1.35
21	1	616	LUT	C14-C13	4.20	1.41	1.35
22	B	849	BCR	C17-C18	4.20	1.41	1.35
22	J	102	BCR	C14-C13	4.20	1.41	1.35
22	B	843	BCR	C17-C18	4.19	1.41	1.35
17	2	606	CHL	CHD-C4C	4.19	1.48	1.39
22	B	843	BCR	C21-C22	4.18	1.41	1.35
17	1	601	CHL	O2A-CGA	4.18	1.45	1.33
22	B	801	BCR	C17-C18	4.17	1.41	1.35
22	L	301	BCR	C21-C22	4.17	1.41	1.35
22	F	304	BCR	C14-C13	4.17	1.41	1.35
21	2	619	LUT	C30-C29	4.16	1.41	1.35
22	J	102	BCR	C10-C9	4.15	1.41	1.35
22	B	845	BCR	C14-C13	4.15	1.41	1.35
17	4	605	CHL	CHD-C4C	4.14	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	607	CHL	CHC-C1C	4.14	1.46	1.38
22	A	852	BCR	C21-C22	4.14	1.41	1.35
22	A	848	BCR	C21-C22	4.14	1.41	1.35
24	A	801	CL0	C3C-C2C	4.13	1.45	1.36
21	2	619	LUT	C34-C33	4.13	1.41	1.35
22	4	618	BCR	C14-C13	4.13	1.41	1.35
22	A	849	BCR	C14-C13	4.13	1.41	1.35
22	J	102	BCR	C17-C18	4.12	1.41	1.35
22	A	848	BCR	C17-C18	4.12	1.41	1.35
17	1	601	CHL	CHD-C4C	4.11	1.48	1.39
22	L	301	BCR	C17-C18	4.11	1.41	1.35
21	2	619	LUT	C14-C13	4.11	1.41	1.35
22	B	844	BCR	C10-C9	4.10	1.41	1.35
22	4	618	BCR	C21-C22	4.10	1.41	1.35
17	2	615	CHL	CHD-C4C	4.10	1.48	1.39
22	B	843	BCR	C10-C9	4.10	1.41	1.35
22	B	849	BCR	C21-C22	4.10	1.41	1.35
22	B	801	BCR	C21-C22	4.09	1.41	1.35
22	J	102	BCR	C21-C22	4.09	1.41	1.35
22	L	305	BCR	C10-C9	4.09	1.41	1.35
21	2	619	LUT	C10-C9	4.09	1.41	1.35
22	L	306	BCR	C10-C9	4.09	1.41	1.35
22	B	801	BCR	C14-C13	4.08	1.41	1.35
17	2	601	CHL	CHD-C4C	4.08	1.48	1.39
17	3	606	CHL	CHD-C4C	4.07	1.48	1.39
27	B	850	DGD	O2G-C1B	4.07	1.45	1.34
21	3	613	LUT	C14-C13	4.06	1.41	1.35
22	L	305	BCR	C14-C13	4.06	1.41	1.35
22	4	618	BCR	C17-C18	4.05	1.41	1.35
22	A	848	BCR	C14-C13	4.04	1.41	1.35
17	2	607	CHL	CHD-C4C	4.04	1.48	1.39
21	1	616	LUT	C34-C33	4.04	1.41	1.35
24	A	801	CL0	O2A-CGA	4.04	1.45	1.33
17	2	605	CHL	CHD-C4C	4.04	1.48	1.39
20	1	615	LHG	O7-C7	4.03	1.45	1.34
22	A	849	BCR	C10-C9	4.03	1.41	1.35
22	B	848	BCR	C17-C18	4.03	1.41	1.35
22	B	846	BCR	C10-C9	4.03	1.41	1.35
22	L	305	BCR	C21-C22	4.03	1.41	1.35
22	B	846	BCR	C17-C18	4.03	1.41	1.35
22	B	846	BCR	C21-C22	4.02	1.41	1.35
22	A	852	BCR	C17-C18	4.02	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	844	BCR	C14-C13	4.01	1.41	1.35
22	K	205	BCR	C14-C13	4.00	1.41	1.35
17	1	606	CHL	CHC-C4B	4.00	1.48	1.39
18	3	603	CLA	C1D-ND	3.99	1.42	1.37
22	L	301	BCR	C10-C9	3.99	1.41	1.35
22	B	844	BCR	C17-C18	3.99	1.41	1.35
21	4	616	LUT	C30-C29	3.99	1.41	1.35
17	2	601	CHL	O2A-CGA	3.99	1.45	1.33
18	A	824	CLA	C1D-ND	3.99	1.42	1.37
18	1	605	CLA	C1D-ND	3.98	1.42	1.37
22	K	205	BCR	C17-C18	3.98	1.41	1.35
22	B	848	BCR	C14-C13	3.98	1.41	1.35
17	4	615	CHL	CHD-C4C	3.97	1.48	1.39
22	A	848	BCR	C10-C9	3.97	1.41	1.35
22	L	306	BCR	C14-C13	3.97	1.41	1.35
22	B	846	BCR	C14-C13	3.96	1.41	1.35
18	2	611	CLA	C1D-ND	3.96	1.42	1.37
22	I	101	BCR	C14-C13	3.96	1.41	1.35
22	G	204	BCR	C21-C22	3.95	1.41	1.35
22	L	305	BCR	C17-C18	3.95	1.41	1.35
18	B	835	CLA	C1D-ND	3.95	1.42	1.37
22	A	852	BCR	C10-C9	3.94	1.41	1.35
22	B	848	BCR	C10-C9	3.94	1.41	1.35
18	3	609	CLA	C1D-ND	3.94	1.42	1.37
21	4	616	LUT	C14-C13	3.93	1.41	1.35
22	A	850	BCR	C10-C9	3.93	1.41	1.35
18	K	201	CLA	C1D-ND	3.92	1.42	1.37
22	G	204	BCR	C17-C18	3.91	1.41	1.35
22	3	614	BCR	C21-C22	3.91	1.41	1.35
22	3	614	BCR	C17-C18	3.91	1.41	1.35
22	B	847	BCR	C14-C13	3.91	1.41	1.35
22	K	205	BCR	C10-C9	3.90	1.41	1.35
19	4	617	XAT	O3-C3	-3.90	1.31	1.43
22	3	614	BCR	C10-C9	3.89	1.40	1.35
22	I	101	BCR	C17-C18	3.89	1.40	1.35
22	4	618	BCR	C10-C9	3.89	1.40	1.35
22	G	204	BCR	C14-C13	3.89	1.40	1.35
22	L	306	BCR	C17-C18	3.89	1.40	1.35
21	4	616	LUT	C34-C33	3.88	1.40	1.35
18	A	817	CLA	C1D-ND	3.88	1.42	1.37
18	3	610	CLA	C1D-ND	3.87	1.42	1.37
22	A	852	BCR	C14-C13	3.87	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	605	CLA	C1D-ND	3.87	1.42	1.37
18	A	837	CLA	C1D-ND	3.87	1.42	1.37
18	2	604	CLA	C1D-ND	3.87	1.42	1.37
17	4	606	CHL	CHC-C4B	3.86	1.48	1.39
17	1	606	CHL	CHB-C1B	3.86	1.48	1.39
22	3	614	BCR	C14-C13	3.86	1.40	1.35
21	2	616	LUT	C10-C9	3.85	1.40	1.35
21	4	616	LUT	C10-C9	3.84	1.40	1.35
21	2	616	LUT	C14-C13	3.84	1.40	1.35
22	L	306	BCR	C21-C22	3.84	1.40	1.35
18	G	201	CLA	C1D-ND	3.84	1.42	1.37
18	A	808	CLA	C1D-ND	3.83	1.42	1.37
18	A	812	CLA	C1D-ND	3.83	1.42	1.37
18	2	613	CLA	C1D-ND	3.83	1.42	1.37
18	F	302	CLA	C1D-ND	3.83	1.42	1.37
18	F	301	CLA	C1D-ND	3.83	1.42	1.37
17	4	607	CHL	CHD-C4C	3.83	1.48	1.39
18	L	304	CLA	C1D-ND	3.83	1.42	1.37
18	A	826	CLA	C1D-ND	3.82	1.42	1.37
18	B	820	CLA	C1D-ND	3.82	1.42	1.37
17	4	606	CHL	CHB-C1B	3.82	1.48	1.39
18	1	604	CLA	C1D-ND	3.82	1.42	1.37
18	A	828	CLA	C1D-ND	3.81	1.42	1.37
18	3	602	CLA	C1D-ND	3.81	1.42	1.37
18	A	836	CLA	C1D-ND	3.81	1.42	1.37
22	I	101	BCR	C10-C9	3.81	1.40	1.35
18	B	827	CLA	C1D-ND	3.81	1.42	1.37
21	3	613	LUT	C30-C29	3.81	1.40	1.35
18	1	611	CLA	C1D-ND	3.80	1.42	1.37
18	4	608	CLA	C1D-ND	3.80	1.42	1.37
21	2	616	LUT	C30-C29	3.80	1.40	1.35
22	B	848	BCR	C21-C22	3.80	1.40	1.35
18	3	608	CLA	C1D-ND	3.80	1.42	1.37
18	F	303	CLA	C1D-ND	3.80	1.42	1.37
18	A	835	CLA	C1D-ND	3.80	1.42	1.37
18	B	810	CLA	C1D-ND	3.79	1.42	1.37
18	2	610	CLA	C1D-ND	3.79	1.42	1.37
18	A	839	CLA	C1D-ND	3.79	1.42	1.37
17	2	615	CHL	CHC-C4B	3.79	1.47	1.39
18	B	832	CLA	C1D-ND	3.79	1.42	1.37
18	1	612	CLA	C1D-ND	3.78	1.42	1.37
18	G	202	CLA	C1D-ND	3.78	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	203	CLA	C1D-ND	3.78	1.42	1.37
22	B	847	BCR	C17-C18	3.78	1.40	1.35
18	1	613	CLA	C1D-ND	3.77	1.42	1.37
17	2	606	CHL	CHC-C4B	3.77	1.47	1.39
18	A	804	CLA	C1D-ND	3.77	1.42	1.37
18	B	841	CLA	C1D-ND	3.77	1.42	1.37
18	K	204	CLA	C1D-ND	3.77	1.42	1.37
22	B	847	BCR	C21-C22	3.77	1.40	1.35
17	4	605	CHL	OBD-CAD	3.77	1.29	1.22
22	B	847	BCR	C10-C9	3.77	1.40	1.35
18	4	601	CLA	C1D-ND	3.77	1.42	1.37
17	2	605	CHL	CHC-C4B	3.76	1.47	1.39
18	B	834	CLA	C1D-ND	3.76	1.42	1.37
18	H	201	CLA	C1D-ND	3.75	1.42	1.37
18	A	823	CLA	C1D-ND	3.75	1.42	1.37
18	B	805	CLA	C1D-ND	3.75	1.42	1.37
18	G	203	CLA	C1D-ND	3.75	1.42	1.37
18	A	818	CLA	C1D-ND	3.75	1.42	1.37
17	4	615	CHL	OBD-CAD	3.75	1.28	1.22
18	A	809	CLA	C1D-ND	3.74	1.42	1.37
19	4	617	XAT	O23-C23	-3.74	1.32	1.43
18	1	610	CLA	C1D-ND	3.74	1.42	1.37
18	4	604	CLA	C1D-ND	3.74	1.42	1.37
18	A	820	CLA	C1D-ND	3.74	1.42	1.37
18	B	839	CLA	C1D-ND	3.74	1.42	1.37
18	1	602	CLA	C1D-ND	3.74	1.42	1.37
18	1	607	CLA	C1D-ND	3.74	1.42	1.37
18	B	818	CLA	C1D-ND	3.74	1.42	1.37
18	B	833	CLA	C1D-ND	3.74	1.42	1.37
18	A	807	CLA	C1D-ND	3.73	1.42	1.37
18	A	834	CLA	C1D-ND	3.73	1.42	1.37
18	2	602	CLA	C1D-ND	3.73	1.42	1.37
18	A	821	CLA	C1D-ND	3.73	1.42	1.37
18	A	816	CLA	C1D-ND	3.73	1.42	1.37
18	1	603	CLA	C1D-ND	3.73	1.42	1.37
18	4	611	CLA	C1D-ND	3.73	1.42	1.37
18	A	833	CLA	C1D-ND	3.73	1.42	1.37
18	B	840	CLA	C1D-ND	3.73	1.42	1.37
17	4	606	CHL	OBD-CAD	3.72	1.28	1.22
18	3	601	CLA	C1D-ND	3.72	1.42	1.37
18	B	824	CLA	C1D-ND	3.72	1.42	1.37
18	A	805	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	814	CLA	C1D-ND	3.72	1.42	1.37
17	2	606	CHL	OBD-CAD	3.72	1.28	1.22
18	B	807	CLA	C1D-ND	3.72	1.42	1.37
18	B	819	CLA	C1D-ND	3.72	1.42	1.37
18	3	607	CLA	C1D-ND	3.71	1.42	1.37
18	B	817	CLA	C1D-ND	3.71	1.42	1.37
18	L	302	CLA	C1D-ND	3.71	1.42	1.37
22	A	850	BCR	C21-C22	3.70	1.40	1.35
18	2	603	CLA	C1D-ND	3.70	1.42	1.37
18	3	611	CLA	C1D-ND	3.70	1.42	1.37
18	A	832	CLA	C1D-ND	3.70	1.42	1.37
18	B	814	CLA	C1D-ND	3.70	1.42	1.37
18	B	815	CLA	C1D-ND	3.70	1.42	1.37
18	B	804	CLA	C1D-ND	3.70	1.42	1.37
18	4	613	CLA	C1D-ND	3.70	1.42	1.37
18	A	806	CLA	C1D-ND	3.70	1.42	1.37
22	I	101	BCR	C21-C22	3.70	1.40	1.35
18	A	827	CLA	C1D-ND	3.69	1.42	1.37
18	A	840	CLA	C1D-ND	3.69	1.42	1.37
18	4	602	CLA	C1D-ND	3.69	1.42	1.37
18	2	612	CLA	C1D-ND	3.69	1.42	1.37
18	A	813	CLA	C1D-ND	3.68	1.42	1.37
18	4	614	CLA	C1D-ND	3.68	1.42	1.37
18	L	303	CLA	C1D-ND	3.68	1.42	1.37
17	4	607	CHL	OBD-CAD	3.68	1.28	1.22
18	B	822	CLA	C1D-ND	3.68	1.42	1.37
18	B	837	CLA	C1D-ND	3.67	1.42	1.37
17	4	605	CHL	CHC-C4B	3.67	1.47	1.39
18	B	809	CLA	C1D-ND	3.67	1.42	1.37
18	B	816	CLA	C1D-ND	3.67	1.42	1.37
18	A	811	CLA	C1D-ND	3.67	1.42	1.37
18	A	838	CLA	C1D-ND	3.66	1.42	1.37
18	B	806	CLA	C1D-ND	3.66	1.42	1.37
18	B	838	CLA	C1D-ND	3.66	1.42	1.37
18	B	811	CLA	C1D-ND	3.65	1.42	1.37
18	B	821	CLA	C1D-ND	3.65	1.42	1.37
18	B	825	CLA	C1D-ND	3.65	1.42	1.37
18	3	612	CLA	C1D-ND	3.65	1.42	1.37
17	1	606	CHL	OBD-CAD	3.65	1.28	1.22
17	2	615	CHL	OBD-CAD	3.65	1.28	1.22
18	A	842	CLA	C1D-ND	3.65	1.42	1.37
17	1	601	CHL	OBD-CAD	3.64	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	843	CLA	C1D-ND	3.64	1.42	1.37
18	B	812	CLA	C1D-ND	3.64	1.42	1.37
18	A	829	CLA	C1D-ND	3.64	1.42	1.37
18	B	836	CLA	C1D-ND	3.63	1.42	1.37
18	4	609	CLA	C1D-ND	3.63	1.42	1.37
18	B	823	CLA	C1D-ND	3.63	1.42	1.37
17	2	601	CHL	OBD-CAD	3.63	1.28	1.22
22	G	204	BCR	C10-C9	3.63	1.40	1.35
18	B	826	CLA	C1D-ND	3.63	1.42	1.37
18	1	608	CLA	C1D-ND	3.63	1.42	1.37
18	B	831	CLA	C1D-ND	3.63	1.42	1.37
18	A	825	CLA	C1D-ND	3.63	1.42	1.37
18	A	831	CLA	C1D-ND	3.62	1.42	1.37
18	B	813	CLA	C1D-ND	3.62	1.42	1.37
18	A	844	CLA	C1D-ND	3.62	1.42	1.37
18	A	841	CLA	C1D-ND	3.62	1.42	1.37
17	1	601	CHL	CHC-C4B	3.62	1.47	1.39
18	4	603	CLA	C1D-ND	3.61	1.42	1.37
17	2	601	CHL	CHC-C4B	3.61	1.47	1.39
18	4	612	CLA	C1D-ND	3.61	1.42	1.37
18	A	810	CLA	C1D-ND	3.61	1.42	1.37
18	A	815	CLA	C1D-ND	3.60	1.42	1.37
18	A	802	CLA	C1D-ND	3.60	1.42	1.37
17	2	605	CHL	OBD-CAD	3.59	1.28	1.22
18	B	829	CLA	C1D-ND	3.59	1.42	1.37
18	3	604	CLA	C1D-ND	3.59	1.42	1.37
18	A	803	CLA	C1D-ND	3.59	1.42	1.37
18	4	610	CLA	C1D-ND	3.58	1.42	1.37
18	2	609	CLA	C1D-ND	3.58	1.42	1.37
17	2	607	CHL	CHC-C4B	3.58	1.47	1.39
17	2	601	CHL	CHB-C1B	3.58	1.47	1.39
17	3	606	CHL	OBD-CAD	3.57	1.28	1.22
18	A	822	CLA	C1D-ND	3.57	1.42	1.37
18	A	819	CLA	C1D-ND	3.56	1.42	1.37
17	3	606	CHL	CHC-C4B	3.56	1.47	1.39
18	2	608	CLA	C1D-ND	3.56	1.42	1.37
18	A	836	CLA	C4B-NB	3.54	1.42	1.37
18	B	828	CLA	C1D-ND	3.54	1.42	1.37
18	A	830	CLA	C1D-ND	3.53	1.42	1.37
18	B	808	CLA	C1D-ND	3.53	1.42	1.37
18	B	803	CLA	C1D-ND	3.51	1.42	1.37
17	4	615	CHL	CHC-C4B	3.50	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	607	CHL	OBD-CAD	3.50	1.28	1.22
18	A	807	CLA	C4B-NB	3.48	1.42	1.37
17	2	606	CHL	CHB-C1B	3.46	1.47	1.39
18	A	837	CLA	C4B-NB	3.46	1.42	1.37
18	1	607	CLA	C4B-NB	3.44	1.42	1.37
17	2	607	CHL	CHB-C1B	3.43	1.47	1.39
18	B	802	CLA	C1D-ND	3.43	1.42	1.37
18	B	832	CLA	C4B-NB	3.43	1.42	1.37
17	2	615	CHL	CHB-C1B	3.43	1.47	1.39
18	1	609	CLA	C1D-ND	3.43	1.42	1.37
17	4	605	CHL	CHB-C1B	3.43	1.47	1.39
17	2	605	CHL	CHB-C1B	3.43	1.47	1.39
17	1	601	CHL	CHB-C1B	3.42	1.47	1.39
18	2	611	CLA	C4B-NB	3.42	1.42	1.37
18	G	201	CLA	C4B-NB	3.42	1.42	1.37
17	3	606	CHL	CHB-C1B	3.42	1.47	1.39
18	2	613	CLA	C4B-NB	3.41	1.42	1.37
18	4	611	CLA	C4B-NB	3.41	1.42	1.37
18	1	605	CLA	C4B-NB	3.41	1.42	1.37
18	A	817	CLA	C4B-NB	3.41	1.42	1.37
18	B	830	CLA	C1D-ND	3.40	1.42	1.37
18	B	834	CLA	C4B-NB	3.40	1.42	1.37
18	B	828	CLA	C4B-NB	3.40	1.42	1.37
18	K	204	CLA	C4B-NB	3.38	1.41	1.37
18	1	611	CLA	C4B-NB	3.37	1.41	1.37
18	4	608	CLA	C4B-NB	3.37	1.41	1.37
18	A	813	CLA	C4B-NB	3.37	1.41	1.37
18	G	202	CLA	C4B-NB	3.37	1.41	1.37
18	B	805	CLA	C4B-NB	3.36	1.41	1.37
18	B	835	CLA	C4B-NB	3.36	1.41	1.37
18	A	824	CLA	C4B-NB	3.36	1.41	1.37
17	4	607	CHL	CHC-C4B	3.35	1.46	1.39
18	3	604	CLA	C4B-NB	3.35	1.41	1.37
18	3	610	CLA	C4B-NB	3.35	1.41	1.37
18	B	812	CLA	C4B-NB	3.35	1.41	1.37
18	A	810	CLA	C4B-NB	3.35	1.41	1.37
18	F	302	CLA	C4B-NB	3.34	1.41	1.37
18	4	601	CLA	C4B-NB	3.34	1.41	1.37
18	1	609	CLA	C4B-NB	3.34	1.41	1.37
18	B	838	CLA	C4B-NB	3.33	1.41	1.37
17	4	606	CHL	C3D-C2D	3.33	1.48	1.39
18	3	603	CLA	C4B-NB	3.32	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	606	CHL	C3D-C2D	3.31	1.48	1.39
18	K	201	CLA	C4B-NB	3.31	1.41	1.37
18	A	823	CLA	C4B-NB	3.31	1.41	1.37
18	F	303	CLA	C4B-NB	3.31	1.41	1.37
18	3	607	CLA	C4B-NB	3.31	1.41	1.37
18	B	802	CLA	C4B-NB	3.31	1.41	1.37
18	1	613	CLA	C4B-NB	3.31	1.41	1.37
19	4	617	XAT	C11-C10	3.29	1.53	1.43
18	4	604	CLA	C4B-NB	3.29	1.41	1.37
18	4	614	CLA	C4B-NB	3.29	1.41	1.37
18	L	302	CLA	C4B-NB	3.29	1.41	1.37
18	A	812	CLA	C4B-NB	3.29	1.41	1.37
18	B	841	CLA	C4B-NB	3.29	1.41	1.37
18	3	611	CLA	C4B-NB	3.28	1.41	1.37
17	1	606	CHL	C1D-C2D	3.28	1.51	1.45
18	A	840	CLA	C4B-NB	3.28	1.41	1.37
18	3	609	CLA	C4B-NB	3.27	1.41	1.37
17	4	615	CHL	CHB-C1B	3.27	1.46	1.39
18	K	203	CLA	C4B-NB	3.27	1.41	1.37
18	3	602	CLA	C4B-NB	3.26	1.41	1.37
18	A	838	CLA	C4B-NB	3.26	1.41	1.37
18	3	605	CLA	C4B-NB	3.25	1.41	1.37
18	L	304	CLA	C4B-NB	3.24	1.41	1.37
18	H	201	CLA	C4B-NB	3.24	1.41	1.37
18	F	301	CLA	C4B-NB	3.24	1.41	1.37
18	B	840	CLA	C4B-NB	3.24	1.41	1.37
18	A	814	CLA	C4B-NB	3.23	1.41	1.37
18	A	816	CLA	C4B-NB	3.23	1.41	1.37
18	B	826	CLA	C4D-ND	-3.23	1.33	1.37
18	A	814	CLA	C3B-C4B	3.23	1.50	1.42
18	1	604	CLA	C4B-NB	3.23	1.41	1.37
18	A	821	CLA	C4B-NB	3.23	1.41	1.37
17	4	606	CHL	C1D-C2D	3.23	1.51	1.45
18	B	822	CLA	C4B-NB	3.23	1.41	1.37
18	B	823	CLA	C4B-NB	3.22	1.41	1.37
18	B	815	CLA	C4B-NB	3.22	1.41	1.37
18	B	811	CLA	C4B-NB	3.22	1.41	1.37
18	2	610	CLA	C4B-NB	3.22	1.41	1.37
18	A	834	CLA	C4B-NB	3.22	1.41	1.37
18	B	839	CLA	C4B-NB	3.21	1.41	1.37
18	1	603	CLA	C4B-NB	3.21	1.41	1.37
18	B	817	CLA	C4B-NB	3.21	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	810	CLA	C4B-NB	3.21	1.41	1.37
18	4	602	CLA	C4B-NB	3.21	1.41	1.37
17	4	607	CHL	CHB-C1B	3.21	1.46	1.39
18	B	831	CLA	C4B-NB	3.21	1.41	1.37
18	3	601	CLA	C4B-NB	3.21	1.41	1.37
18	B	819	CLA	C4B-NB	3.20	1.41	1.37
18	B	804	CLA	C4B-NB	3.20	1.41	1.37
18	B	837	CLA	C4B-NB	3.20	1.41	1.37
18	B	830	CLA	C4B-NB	3.20	1.41	1.37
18	1	610	CLA	C4B-NB	3.19	1.41	1.37
18	A	804	CLA	C4B-NB	3.19	1.41	1.37
18	A	844	CLA	C4B-NB	3.19	1.41	1.37
18	B	829	CLA	C4B-NB	3.19	1.41	1.37
18	1	612	CLA	C4B-NB	3.19	1.41	1.37
18	2	603	CLA	C4B-NB	3.19	1.41	1.37
18	A	832	CLA	C4B-NB	3.19	1.41	1.37
18	G	203	CLA	C4B-NB	3.19	1.41	1.37
18	A	819	CLA	C4B-NB	3.18	1.41	1.37
17	2	606	CHL	C3D-C2D	3.18	1.47	1.39
18	4	604	CLA	CAB-C3B	-3.18	1.44	1.50
18	A	806	CLA	C4B-NB	3.18	1.41	1.37
18	A	818	CLA	C4B-NB	3.17	1.41	1.37
18	4	613	CLA	C4B-NB	3.16	1.41	1.37
18	B	802	CLA	C3B-C4B	3.16	1.50	1.42
18	A	805	CLA	C4B-NB	3.16	1.41	1.37
18	4	610	CLA	C4B-NB	3.16	1.41	1.37
18	L	303	CLA	C4B-NB	3.16	1.41	1.37
18	B	836	CLA	C4B-NB	3.16	1.41	1.37
18	A	827	CLA	C4B-NB	3.16	1.41	1.37
18	B	820	CLA	C4B-NB	3.15	1.41	1.37
18	A	809	CLA	C4B-NB	3.15	1.41	1.37
18	B	824	CLA	C4B-NB	3.15	1.41	1.37
18	1	608	CLA	CAB-C3B	-3.15	1.44	1.50
18	A	828	CLA	C4B-NB	3.14	1.41	1.37
18	4	612	CLA	C4B-NB	3.14	1.41	1.37
18	B	826	CLA	C4B-NB	3.14	1.41	1.37
18	B	827	CLA	C4B-NB	3.13	1.41	1.37
18	B	814	CLA	C4B-NB	3.13	1.41	1.37
18	B	809	CLA	C4B-NB	3.13	1.41	1.37
18	A	822	CLA	C4B-NB	3.13	1.41	1.37
18	B	825	CLA	C4B-NB	3.12	1.41	1.37
18	1	609	CLA	C4D-ND	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	608	CLA	C4B-NB	3.12	1.41	1.37
18	A	803	CLA	C4D-ND	-3.12	1.33	1.37
18	2	610	CLA	CAB-C3B	-3.11	1.44	1.50
18	A	831	CLA	C4B-NB	3.11	1.41	1.37
18	1	610	CLA	CAB-C3B	-3.11	1.44	1.50
18	A	808	CLA	C4B-NB	3.11	1.41	1.37
18	2	608	CLA	C4B-NB	3.11	1.41	1.37
18	4	603	CLA	C4B-NB	3.11	1.41	1.37
18	2	612	CLA	C4B-NB	3.10	1.41	1.37
18	B	832	CLA	C3B-C4B	3.10	1.50	1.42
18	A	835	CLA	C4B-NB	3.10	1.41	1.37
17	2	615	CHL	C3D-C2D	3.10	1.47	1.39
18	B	811	CLA	CAB-C3B	-3.09	1.44	1.50
18	A	811	CLA	C4B-NB	3.09	1.41	1.37
18	2	611	CLA	C3B-C4B	3.09	1.50	1.42
18	1	608	CLA	C4B-NB	3.09	1.41	1.37
18	2	609	CLA	C4B-NB	3.09	1.41	1.37
18	B	832	CLA	C4D-ND	-3.09	1.33	1.37
18	4	603	CLA	CAB-C3B	-3.09	1.44	1.50
18	A	820	CLA	C4B-NB	3.09	1.41	1.37
18	A	825	CLA	C4B-NB	3.08	1.41	1.37
18	B	828	CLA	C3B-C4B	3.08	1.50	1.42
18	4	609	CLA	C4B-NB	3.08	1.41	1.37
18	K	204	CLA	C4D-ND	-3.08	1.33	1.37
18	B	803	CLA	C4B-NB	3.08	1.41	1.37
18	1	613	CLA	CAB-C3B	-3.08	1.44	1.50
18	A	839	CLA	C4B-NB	3.08	1.41	1.37
17	2	606	CHL	C1D-C2D	3.08	1.51	1.45
18	B	806	CLA	C4B-NB	3.07	1.41	1.37
18	3	605	CLA	CAB-C3B	-3.07	1.44	1.50
18	1	602	CLA	C4B-NB	3.07	1.41	1.37
18	A	806	CLA	C4D-ND	-3.07	1.33	1.37
17	1	606	CHL	MG-NA	-3.07	1.99	2.06
18	3	612	CLA	C4B-NB	3.06	1.41	1.37
18	B	807	CLA	C4B-NB	3.06	1.41	1.37
18	A	841	CLA	C4B-NB	3.06	1.41	1.37
18	B	821	CLA	C4B-NB	3.06	1.41	1.37
18	A	802	CLA	C4B-NB	3.06	1.41	1.37
18	B	813	CLA	C4D-ND	-3.06	1.33	1.37
18	A	833	CLA	C4B-NB	3.06	1.41	1.37
18	A	842	CLA	C4B-NB	3.06	1.41	1.37
18	A	815	CLA	C4B-NB	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	833	CLA	C4B-NB	3.05	1.41	1.37
18	A	830	CLA	C4B-NB	3.05	1.41	1.37
18	A	829	CLA	C4B-NB	3.05	1.41	1.37
18	B	836	CLA	C4D-ND	-3.05	1.33	1.37
18	A	826	CLA	C4B-NB	3.05	1.41	1.37
18	A	843	CLA	C4B-NB	3.05	1.41	1.37
18	B	838	CLA	C4D-ND	-3.05	1.33	1.37
22	B	845	BCR	C23-C22	-3.05	1.39	1.45
18	2	602	CLA	C4B-NB	3.04	1.41	1.37
22	B	849	BCR	C23-C22	-3.04	1.39	1.45
18	1	612	CLA	C4D-ND	-3.03	1.33	1.37
18	B	816	CLA	C4D-ND	-3.03	1.33	1.37
18	3	603	CLA	C4D-ND	-3.03	1.33	1.37
18	B	813	CLA	C4B-NB	3.03	1.41	1.37
18	3	607	CLA	C3B-C4B	3.03	1.49	1.42
18	B	824	CLA	C4D-ND	-3.02	1.33	1.37
18	B	807	CLA	C4D-ND	-3.02	1.33	1.37
18	A	827	CLA	C4D-ND	-3.02	1.33	1.37
18	A	840	CLA	C3B-C4B	3.02	1.49	1.42
18	A	842	CLA	C4D-ND	-3.02	1.33	1.37
18	1	613	CLA	C4D-ND	-3.02	1.33	1.37
18	3	601	CLA	C4D-ND	-3.02	1.33	1.37
18	A	814	CLA	C4D-ND	-3.02	1.33	1.37
18	B	840	CLA	C4D-ND	-3.01	1.33	1.37
18	A	839	CLA	C4D-ND	-3.01	1.33	1.37
18	2	609	CLA	C4D-ND	-3.01	1.33	1.37
18	B	834	CLA	C3B-C4B	3.01	1.49	1.42
18	A	816	CLA	C4D-ND	-3.01	1.33	1.37
17	4	605	CHL	C3D-C2D	3.01	1.47	1.39
17	2	615	CHL	C1D-C2D	3.01	1.51	1.45
18	B	831	CLA	C4D-ND	-3.01	1.33	1.37
18	4	613	CLA	C4D-ND	-3.01	1.33	1.37
17	4	606	CHL	MG-NA	-3.01	1.99	2.06
24	A	801	CL0	CHB-C4A	-3.01	1.30	1.37
18	B	805	CLA	C3B-C4B	3.00	1.49	1.42
18	1	602	CLA	C4D-ND	-3.00	1.33	1.37
18	2	612	CLA	C4D-ND	-3.00	1.33	1.37
18	A	841	CLA	C4D-ND	-3.00	1.33	1.37
18	A	813	CLA	C3B-C4B	3.00	1.49	1.42
18	B	810	CLA	C3B-C4B	3.00	1.49	1.42
18	B	818	CLA	C4B-NB	3.00	1.41	1.37
18	2	604	CLA	C4D-ND	-3.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	812	CLA	C3B-C4B	3.00	1.49	1.42
18	A	836	CLA	C3B-C4B	3.00	1.49	1.42
18	A	828	CLA	C4D-ND	-2.99	1.33	1.37
18	B	818	CLA	C4D-ND	-2.99	1.33	1.37
18	A	810	CLA	C4D-ND	-2.99	1.33	1.37
18	A	830	CLA	C4D-ND	-2.99	1.33	1.37
17	1	601	CHL	C1D-C2D	2.99	1.51	1.45
18	B	816	CLA	C4B-NB	2.99	1.41	1.37
18	A	840	CLA	C4D-ND	-2.99	1.33	1.37
18	A	807	CLA	C3B-C4B	2.98	1.49	1.42
18	2	602	CLA	C4D-ND	-2.98	1.33	1.37
18	2	608	CLA	C4D-ND	-2.98	1.33	1.37
18	1	607	CLA	C3B-C4B	2.98	1.49	1.42
18	A	819	CLA	C4D-ND	-2.98	1.33	1.37
18	B	808	CLA	C4B-NB	2.98	1.41	1.37
18	B	821	CLA	C4D-ND	-2.98	1.33	1.37
18	B	806	CLA	C4D-ND	-2.98	1.33	1.37
18	3	607	CLA	C4D-ND	-2.98	1.33	1.37
17	2	601	CHL	C3D-C2D	2.97	1.47	1.39
18	B	829	CLA	C4D-ND	-2.97	1.33	1.37
18	A	807	CLA	C4D-ND	-2.97	1.33	1.37
17	2	605	CHL	C3D-C2D	2.97	1.47	1.39
18	4	603	CLA	C4D-ND	-2.97	1.33	1.37
18	B	802	CLA	C4D-ND	-2.97	1.33	1.37
17	2	601	CHL	C1D-C2D	2.96	1.51	1.45
18	1	603	CLA	C4D-ND	-2.96	1.33	1.37
18	A	817	CLA	C3B-C4B	2.96	1.49	1.42
18	4	611	CLA	C4D-ND	-2.96	1.33	1.37
18	A	838	CLA	C3B-C4B	2.96	1.49	1.42
18	2	610	CLA	C4D-ND	-2.96	1.33	1.37
24	A	801	CL0	CHC-C1C	2.96	1.44	1.38
18	A	831	CLA	C4D-ND	-2.96	1.33	1.37
18	G	203	CLA	C4D-ND	-2.96	1.33	1.37
18	A	837	CLA	C3B-C4B	2.96	1.49	1.42
18	4	602	CLA	C4D-ND	-2.96	1.33	1.37
18	A	829	CLA	C4D-ND	-2.96	1.33	1.37
18	L	303	CLA	C4D-ND	-2.96	1.33	1.37
18	B	815	CLA	C4D-ND	-2.96	1.33	1.37
22	I	101	BCR	C23-C22	-2.96	1.39	1.45
18	B	833	CLA	C4D-ND	-2.96	1.33	1.37
19	4	617	XAT	C15-C14	2.96	1.52	1.43
18	1	611	CLA	C3B-C4B	2.95	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	614	CLA	C3B-C4B	2.95	1.49	1.42
22	4	618	BCR	C8-C9	-2.95	1.39	1.45
18	B	823	CLA	C4D-ND	-2.95	1.33	1.37
17	1	601	CHL	C3D-C2D	2.95	1.47	1.39
17	4	615	CHL	C3D-C2D	2.95	1.47	1.39
18	3	605	CLA	C4D-ND	-2.95	1.33	1.37
18	A	810	CLA	C3B-C4B	2.95	1.49	1.42
18	B	827	CLA	C4D-ND	-2.95	1.33	1.37
18	A	826	CLA	C4D-ND	-2.95	1.33	1.37
18	G	202	CLA	C4D-ND	-2.95	1.33	1.37
18	F	303	CLA	C3B-C4B	2.95	1.49	1.42
18	B	840	CLA	C3B-C4B	2.95	1.49	1.42
18	B	839	CLA	C4D-ND	-2.95	1.33	1.37
18	F	301	CLA	C4D-ND	-2.95	1.33	1.37
18	3	608	CLA	C4D-ND	-2.94	1.33	1.37
18	4	608	CLA	C4D-ND	-2.94	1.33	1.37
18	B	830	CLA	C4D-ND	-2.94	1.33	1.37
18	B	809	CLA	C4D-ND	-2.94	1.33	1.37
18	3	604	CLA	C4D-ND	-2.94	1.33	1.37
18	B	810	CLA	C4D-ND	-2.94	1.33	1.37
18	2	603	CLA	C4D-ND	-2.94	1.33	1.37
18	4	601	CLA	C4D-ND	-2.94	1.33	1.37
18	1	604	CLA	C4D-ND	-2.94	1.33	1.37
18	B	812	CLA	C4D-ND	-2.94	1.33	1.37
18	4	611	CLA	C3B-C4B	2.94	1.49	1.42
18	B	808	CLA	C4D-ND	-2.94	1.33	1.37
18	B	841	CLA	C4D-ND	-2.94	1.33	1.37
18	A	818	CLA	C4D-ND	-2.94	1.33	1.37
18	B	828	CLA	C4D-ND	-2.94	1.33	1.37
18	1	611	CLA	C4D-ND	-2.94	1.33	1.37
18	A	833	CLA	C4D-ND	-2.94	1.33	1.37
18	B	838	CLA	C3B-C4B	2.94	1.49	1.42
18	2	609	CLA	C3B-C4B	2.93	1.49	1.42
18	A	811	CLA	C4D-ND	-2.93	1.33	1.37
18	B	814	CLA	C4D-ND	-2.93	1.33	1.37
18	A	821	CLA	C4D-ND	-2.93	1.33	1.37
18	G	201	CLA	C3B-C4B	2.93	1.49	1.42
22	A	850	BCR	C23-C22	-2.93	1.39	1.45
18	4	604	CLA	C4D-ND	-2.93	1.33	1.37
18	3	609	CLA	C4D-ND	-2.93	1.33	1.37
18	A	820	CLA	C4D-ND	-2.93	1.33	1.37
22	A	852	BCR	C8-C9	-2.93	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	812	CLA	C3B-C4B	2.93	1.49	1.42
18	B	805	CLA	C4D-ND	-2.93	1.33	1.37
18	A	844	CLA	C4D-ND	-2.92	1.33	1.37
22	B	847	BCR	C23-C22	-2.92	1.39	1.45
18	B	817	CLA	C4D-ND	-2.92	1.33	1.37
18	A	802	CLA	C3B-C4B	2.92	1.49	1.42
18	A	843	CLA	C4D-ND	-2.92	1.33	1.37
18	3	603	CLA	C3B-C4B	2.92	1.49	1.42
18	3	610	CLA	C3B-C4B	2.92	1.49	1.42
18	A	825	CLA	C4D-ND	-2.92	1.33	1.37
18	B	820	CLA	C4D-ND	-2.92	1.33	1.37
18	B	825	CLA	C3B-C4B	2.92	1.49	1.42
18	4	610	CLA	C4D-ND	-2.92	1.33	1.37
18	A	805	CLA	C4D-ND	-2.91	1.33	1.37
18	A	815	CLA	C4D-ND	-2.91	1.33	1.37
18	A	832	CLA	C4D-ND	-2.91	1.33	1.37
18	B	841	CLA	C3B-C4B	2.91	1.49	1.42
18	2	613	CLA	C4D-ND	-2.91	1.33	1.37
18	2	602	CLA	C3B-C4B	2.91	1.49	1.42
18	4	609	CLA	C4D-ND	-2.91	1.33	1.37
18	B	804	CLA	C4D-ND	-2.91	1.33	1.37
18	L	304	CLA	C4D-ND	-2.91	1.33	1.37
22	B	848	BCR	C23-C22	-2.91	1.39	1.45
17	2	607	CHL	C1D-C2D	2.91	1.51	1.45
18	1	608	CLA	C4D-ND	-2.91	1.33	1.37
17	4	615	CHL	C1D-C2D	2.91	1.51	1.45
18	1	610	CLA	C4D-ND	-2.90	1.33	1.37
18	A	834	CLA	C4D-ND	-2.90	1.33	1.37
18	4	601	CLA	C3B-C4B	2.90	1.49	1.42
17	4	605	CHL	C1D-C2D	2.90	1.51	1.45
18	A	806	CLA	C3B-C4B	2.90	1.49	1.42
18	A	805	CLA	C3B-C4B	2.90	1.49	1.42
18	B	835	CLA	C3B-C4B	2.90	1.49	1.42
18	B	837	CLA	C4D-ND	-2.90	1.33	1.37
18	B	811	CLA	C4D-ND	-2.90	1.33	1.37
18	A	812	CLA	C4D-ND	-2.90	1.33	1.37
18	A	804	CLA	C4D-ND	-2.90	1.33	1.37
17	3	606	CHL	C3D-C2D	2.90	1.47	1.39
18	K	203	CLA	C4D-ND	-2.90	1.33	1.37
18	B	820	CLA	C3B-C4B	2.89	1.49	1.42
18	L	302	CLA	C4D-ND	-2.89	1.33	1.37
18	A	819	CLA	C3B-C4B	2.89	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	609	CLA	C3B-C4B	2.89	1.49	1.42
18	1	605	CLA	C3B-C4B	2.89	1.49	1.42
18	A	823	CLA	C3B-C4B	2.89	1.49	1.42
18	4	613	CLA	C3B-C4B	2.89	1.49	1.42
18	1	607	CLA	C4D-ND	-2.89	1.33	1.37
18	2	604	CLA	C4B-NB	2.89	1.41	1.37
17	2	607	CHL	C3D-C2D	2.89	1.47	1.39
18	2	613	CLA	C3B-C4B	2.89	1.49	1.42
18	B	804	CLA	C3B-C4B	2.89	1.49	1.42
18	G	202	CLA	C3B-C4B	2.89	1.49	1.42
18	1	612	CLA	C3B-C4B	2.89	1.49	1.42
18	F	301	CLA	C3B-C4B	2.89	1.49	1.42
18	4	609	CLA	C3B-C4B	2.89	1.49	1.42
18	4	610	CLA	C3B-C4B	2.88	1.49	1.42
18	B	839	CLA	C3B-C4B	2.88	1.49	1.42
18	F	303	CLA	C4D-ND	-2.88	1.33	1.37
22	G	204	BCR	C8-C9	-2.88	1.39	1.45
18	A	808	CLA	C4D-ND	-2.88	1.33	1.37
18	A	822	CLA	C4D-ND	-2.88	1.33	1.37
18	3	609	CLA	C3B-C4B	2.88	1.49	1.42
18	A	815	CLA	C3B-C4B	2.88	1.49	1.42
18	3	608	CLA	C3B-C4B	2.88	1.49	1.42
18	A	824	CLA	C3B-C4B	2.88	1.49	1.42
18	B	836	CLA	C3B-C4B	2.88	1.49	1.42
18	K	201	CLA	C4D-ND	-2.88	1.33	1.37
18	A	831	CLA	C3B-C4B	2.88	1.49	1.42
18	3	602	CLA	C3B-C4B	2.88	1.49	1.42
18	A	809	CLA	C4D-ND	-2.87	1.33	1.37
18	B	819	CLA	C4D-ND	-2.87	1.33	1.37
18	B	834	CLA	C4D-ND	-2.87	1.33	1.37
18	A	811	CLA	C3B-C4B	2.87	1.49	1.42
22	3	614	BCR	C23-C22	-2.87	1.39	1.45
17	2	605	CHL	C1D-C2D	2.87	1.51	1.45
18	K	203	CLA	C3B-C4B	2.87	1.49	1.42
18	A	832	CLA	C3B-C4B	2.87	1.49	1.42
18	3	611	CLA	C3B-C4B	2.87	1.49	1.42
18	4	612	CLA	C4D-ND	-2.87	1.33	1.37
18	A	835	CLA	C4D-ND	-2.87	1.33	1.37
18	3	604	CLA	C3B-C4B	2.87	1.49	1.42
18	B	822	CLA	C4D-ND	-2.87	1.33	1.37
18	B	817	CLA	C3B-C4B	2.87	1.49	1.42
22	B	847	BCR	C8-C9	-2.87	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	201	CLA	C3B-C4B	2.86	1.49	1.42
18	B	837	CLA	C3B-C4B	2.86	1.49	1.42
18	4	602	CLA	C3B-C4B	2.86	1.49	1.42
18	A	833	CLA	C3B-C4B	2.86	1.49	1.42
18	A	827	CLA	C3B-C4B	2.86	1.49	1.42
18	L	302	CLA	C3B-C4B	2.86	1.49	1.42
18	B	818	CLA	C3B-C4B	2.86	1.49	1.42
18	4	608	CLA	C3B-C4B	2.86	1.49	1.42
18	3	610	CLA	C4D-ND	-2.86	1.33	1.37
18	A	826	CLA	C3B-C4B	2.86	1.49	1.42
18	4	614	CLA	C4D-ND	-2.85	1.33	1.37
18	B	822	CLA	C3B-C4B	2.85	1.49	1.42
18	B	823	CLA	C3B-C4B	2.85	1.49	1.42
18	A	821	CLA	C3B-C4B	2.85	1.49	1.42
18	B	816	CLA	C3B-C4B	2.85	1.49	1.42
18	A	817	CLA	C4D-ND	-2.85	1.33	1.37
18	2	611	CLA	C4D-ND	-2.85	1.33	1.37
22	B	846	BCR	C23-C22	-2.85	1.39	1.45
18	K	204	CLA	C3B-C4B	2.85	1.49	1.42
18	A	809	CLA	C3B-C4B	2.85	1.49	1.42
18	B	814	CLA	C3B-C4B	2.85	1.49	1.42
18	B	821	CLA	C3B-C4B	2.84	1.49	1.42
18	3	602	CLA	C4D-ND	-2.84	1.33	1.37
18	A	803	CLA	C4B-NB	2.84	1.41	1.37
18	H	201	CLA	C4D-ND	-2.84	1.33	1.37
18	B	826	CLA	C3B-C4B	2.84	1.49	1.42
18	B	819	CLA	C3B-C4B	2.84	1.49	1.42
18	G	203	CLA	C3B-C4B	2.83	1.49	1.42
17	3	606	CHL	C1D-C2D	2.83	1.50	1.45
18	B	829	CLA	C3B-C4B	2.83	1.49	1.42
18	A	834	CLA	C3B-C4B	2.83	1.49	1.42
22	3	614	BCR	C8-C9	-2.83	1.39	1.45
18	L	304	CLA	C3B-C4B	2.83	1.49	1.42
18	L	303	CLA	C3B-C4B	2.83	1.49	1.42
18	A	816	CLA	C3B-C4B	2.83	1.49	1.42
18	A	818	CLA	C3B-C4B	2.83	1.49	1.42
22	L	305	BCR	C8-C9	-2.82	1.39	1.45
18	3	611	CLA	C4D-ND	-2.82	1.33	1.37
22	B	801	BCR	C8-C9	-2.82	1.39	1.45
18	A	802	CLA	C4D-ND	-2.82	1.33	1.37
22	B	848	BCR	C8-C9	-2.82	1.39	1.45
18	H	201	CLA	C3B-C4B	2.82	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	820	CLA	C3B-C4B	2.82	1.49	1.42
18	A	841	CLA	C3B-C4B	2.82	1.49	1.42
18	A	828	CLA	C3B-C4B	2.82	1.49	1.42
18	B	831	CLA	C3B-C4B	2.81	1.49	1.42
18	A	824	CLA	C4D-ND	-2.81	1.33	1.37
18	A	836	CLA	C4D-ND	-2.81	1.33	1.37
18	1	604	CLA	C3B-C4B	2.81	1.49	1.42
22	G	204	BCR	C23-C22	-2.81	1.39	1.45
18	3	612	CLA	C4D-ND	-2.80	1.33	1.37
18	A	838	CLA	C4D-ND	-2.80	1.33	1.37
18	B	809	CLA	C3B-C4B	2.80	1.49	1.42
18	3	601	CLA	C3B-C4B	2.80	1.49	1.42
22	I	101	BCR	C8-C9	-2.80	1.39	1.45
18	A	822	CLA	C3B-C4B	2.80	1.49	1.42
18	B	803	CLA	C4D-ND	-2.80	1.33	1.37
22	L	301	BCR	C8-C9	-2.80	1.39	1.45
18	F	302	CLA	C3B-C4B	2.79	1.49	1.42
18	B	803	CLA	C3B-C4B	2.79	1.49	1.42
18	A	844	CLA	C3B-C4B	2.79	1.49	1.42
22	B	844	BCR	C8-C9	-2.79	1.39	1.45
18	B	835	CLA	C4D-ND	-2.79	1.33	1.37
18	2	612	CLA	C3B-C4B	2.79	1.49	1.42
18	A	803	CLA	C3B-C4B	2.78	1.49	1.42
18	B	815	CLA	C3B-C4B	2.78	1.49	1.42
18	B	813	CLA	C3B-C4B	2.78	1.49	1.42
18	2	603	CLA	C3B-C4B	2.78	1.49	1.42
18	B	825	CLA	C4D-ND	-2.78	1.33	1.37
21	3	613	LUT	C8-C9	-2.78	1.40	1.45
18	A	808	CLA	C3B-C4B	2.77	1.49	1.42
18	1	603	CLA	C3B-C4B	2.77	1.49	1.42
18	G	201	CLA	C4D-ND	-2.77	1.33	1.37
18	B	824	CLA	C3B-C4B	2.77	1.49	1.42
22	A	852	BCR	C23-C22	-2.77	1.40	1.45
22	A	849	BCR	C23-C22	-2.77	1.40	1.45
18	B	827	CLA	C3B-C4B	2.77	1.49	1.42
17	4	607	CHL	C3D-C2D	2.77	1.46	1.39
24	A	801	CL0	OBD-CAD	2.77	1.28	1.22
18	B	807	CLA	C3B-C4B	2.77	1.49	1.42
18	A	823	CLA	C4D-ND	-2.77	1.33	1.37
22	L	305	BCR	C23-C22	-2.76	1.40	1.45
17	4	607	CHL	C1D-C2D	2.76	1.50	1.45
18	A	843	CLA	C3B-C4B	2.76	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	605	CLA	C1B-C2B	2.76	1.49	1.43
18	B	808	CLA	C3B-C4B	2.76	1.49	1.42
22	K	205	BCR	C8-C9	-2.76	1.40	1.45
18	A	835	CLA	C3B-C4B	2.76	1.49	1.42
18	3	612	CLA	C3B-C4B	2.76	1.49	1.42
18	F	302	CLA	C4D-ND	-2.75	1.33	1.37
21	4	616	LUT	C8-C9	-2.75	1.40	1.45
18	A	804	CLA	C3B-C4B	2.75	1.49	1.42
18	2	608	CLA	C3B-C4B	2.75	1.49	1.42
18	A	839	CLA	C3B-C4B	2.75	1.49	1.42
22	A	850	BCR	C8-C9	-2.75	1.40	1.45
18	A	842	CLA	C3B-C4B	2.74	1.49	1.42
18	B	833	CLA	C3B-C4B	2.74	1.49	1.42
22	K	205	BCR	C23-C22	-2.74	1.40	1.45
18	B	830	CLA	C3B-C4B	2.74	1.49	1.42
22	A	848	BCR	C23-C22	-2.73	1.40	1.45
18	A	837	CLA	C4D-ND	-2.73	1.33	1.37
18	1	602	CLA	C3B-C4B	2.73	1.49	1.42
18	4	612	CLA	C3B-C4B	2.73	1.49	1.42
22	4	618	BCR	C23-C22	-2.72	1.40	1.45
18	A	830	CLA	C3B-C4B	2.72	1.49	1.42
18	1	613	CLA	C1B-C2B	2.72	1.49	1.43
18	A	829	CLA	C3B-C4B	2.72	1.49	1.42
22	B	845	BCR	C8-C9	-2.72	1.40	1.45
18	A	813	CLA	C4D-ND	-2.72	1.34	1.37
22	B	846	BCR	C8-C9	-2.72	1.40	1.45
17	1	606	CHL	C3B-C4B	2.72	1.49	1.42
22	B	844	BCR	C23-C22	-2.72	1.40	1.45
18	4	614	CLA	C1B-C2B	2.71	1.49	1.43
18	A	825	CLA	C3B-C4B	2.71	1.49	1.42
22	B	801	BCR	C23-C22	-2.71	1.40	1.45
22	L	306	BCR	C23-C22	-2.71	1.40	1.45
22	A	849	BCR	C8-C9	-2.71	1.40	1.45
22	A	848	BCR	C8-C9	-2.70	1.40	1.45
22	L	306	BCR	C8-C9	-2.70	1.40	1.45
18	3	610	CLA	C1B-C2B	2.70	1.49	1.43
22	A	853	BCR	C8-C9	-2.70	1.40	1.45
17	4	606	CHL	C1B-C2B	2.70	1.49	1.43
18	1	605	CLA	C4D-ND	-2.70	1.34	1.37
18	B	806	CLA	C1B-C2B	2.69	1.49	1.43
22	B	843	BCR	C8-C9	-2.69	1.40	1.45
18	3	605	CLA	C4B-C3B	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	605	CLA	C1B-C2B	2.68	1.49	1.43
18	K	204	CLA	C1B-C2B	2.68	1.49	1.43
18	A	804	CLA	C1B-C2B	2.68	1.49	1.43
18	K	201	CLA	C1B-C2B	2.68	1.49	1.43
24	A	801	CL0	CHD-C1D	2.68	1.43	1.38
18	2	610	CLA	C1B-C2B	2.67	1.49	1.43
21	2	619	LUT	C8-C9	-2.67	1.40	1.45
18	A	824	CLA	C1B-C2B	2.67	1.49	1.43
18	1	610	CLA	C1B-C2B	2.66	1.49	1.43
22	J	102	BCR	C8-C9	-2.66	1.40	1.45
18	1	610	CLA	C4B-C3B	2.66	1.49	1.43
18	3	611	CLA	C1B-C2B	2.66	1.49	1.43
18	B	806	CLA	C3B-C4B	2.66	1.49	1.42
17	2	615	CHL	C3B-C4B	2.66	1.49	1.42
18	A	811	CLA	C1B-C2B	2.66	1.49	1.43
18	B	823	CLA	C1B-C2B	2.66	1.49	1.43
22	A	853	BCR	C23-C22	-2.66	1.40	1.45
17	2	615	CHL	MG-NA	-2.66	2.00	2.06
18	4	604	CLA	C4B-C3B	2.66	1.49	1.43
18	A	837	CLA	C1B-C2B	2.66	1.49	1.43
18	H	201	CLA	C1B-C2B	2.66	1.49	1.43
18	B	811	CLA	C4B-C3B	2.66	1.49	1.43
21	1	616	LUT	C8-C9	-2.65	1.40	1.45
18	3	602	CLA	C1B-C2B	2.65	1.49	1.43
18	A	839	CLA	C1B-C2B	2.65	1.49	1.43
18	A	823	CLA	C1B-C2B	2.65	1.49	1.43
22	J	102	BCR	C23-C22	-2.65	1.40	1.45
22	B	843	BCR	C23-C22	-2.64	1.40	1.45
17	2	605	CHL	C3B-C4B	2.64	1.48	1.42
18	F	303	CLA	C1B-C2B	2.63	1.49	1.43
22	A	851	BCR	C8-C9	-2.63	1.40	1.45
18	2	604	CLA	C3B-C4B	2.63	1.48	1.42
18	1	608	CLA	C1B-C2B	2.63	1.49	1.43
18	K	203	CLA	C1B-C2B	2.63	1.49	1.43
22	L	301	BCR	C23-C22	-2.63	1.40	1.45
18	2	613	CLA	C1B-C2B	2.63	1.49	1.43
18	G	202	CLA	C1B-C2B	2.63	1.49	1.43
18	G	201	CLA	C1B-C2B	2.62	1.49	1.43
18	2	611	CLA	C1B-C2B	2.62	1.49	1.43
18	B	811	CLA	C1B-C2B	2.62	1.49	1.43
17	2	606	CHL	C3B-C4B	2.62	1.48	1.42
18	A	834	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	606	CHL	C4C-C3C	2.62	1.49	1.45
18	1	612	CLA	C1B-C2B	2.61	1.49	1.43
18	3	601	CLA	C1B-C2B	2.61	1.49	1.43
18	4	612	CLA	C1B-C2B	2.61	1.49	1.43
17	1	601	CHL	C3B-C4B	2.61	1.48	1.42
18	A	817	CLA	C1B-C2B	2.61	1.49	1.43
18	A	812	CLA	C1B-C2B	2.60	1.49	1.43
18	1	609	CLA	C1B-C2B	2.60	1.49	1.43
18	1	611	CLA	C1B-C2B	2.60	1.49	1.43
18	3	608	CLA	C1B-C2B	2.60	1.49	1.43
18	A	843	CLA	C1B-C2B	2.60	1.49	1.43
18	F	301	CLA	C1B-C2B	2.60	1.49	1.43
18	B	833	CLA	C1B-C2B	2.60	1.49	1.43
18	1	607	CLA	C1B-C2B	2.59	1.49	1.43
17	4	605	CHL	C3B-C4B	2.59	1.48	1.42
18	2	609	CLA	C1B-C2B	2.59	1.49	1.43
22	F	304	BCR	C8-C9	-2.59	1.40	1.45
18	B	835	CLA	C1B-C2B	2.59	1.49	1.43
17	4	606	CHL	C4C-C3C	2.59	1.49	1.45
18	B	821	CLA	C1B-C2B	2.59	1.49	1.43
18	A	828	CLA	C1B-C2B	2.58	1.49	1.43
18	1	604	CLA	C1B-C2B	2.58	1.49	1.43
18	3	604	CLA	C1B-C2B	2.58	1.49	1.43
22	A	851	BCR	C23-C22	-2.58	1.40	1.45
18	4	611	CLA	C1B-C2B	2.58	1.49	1.43
18	1	613	CLA	C4B-C3B	2.58	1.49	1.43
18	B	837	CLA	C1B-C2B	2.58	1.49	1.43
18	A	827	CLA	C1B-C2B	2.58	1.49	1.43
18	2	608	CLA	C1B-C2B	2.58	1.49	1.43
18	G	203	CLA	C1B-C2B	2.57	1.49	1.43
17	1	606	CHL	C1B-C2B	2.57	1.49	1.43
18	2	603	CLA	C1B-C2B	2.57	1.49	1.43
18	A	821	CLA	C1B-C2B	2.57	1.49	1.43
18	2	610	CLA	C4B-C3B	2.57	1.49	1.43
18	B	824	CLA	C1B-C2B	2.57	1.49	1.43
18	B	826	CLA	C1B-C2B	2.57	1.49	1.43
18	L	304	CLA	C1B-C2B	2.57	1.49	1.43
18	4	604	CLA	C1B-C2B	2.56	1.49	1.43
18	B	841	CLA	C1B-C2B	2.56	1.49	1.43
18	B	810	CLA	C1B-C2B	2.56	1.49	1.43
18	B	804	CLA	C1B-C2B	2.56	1.49	1.43
18	B	805	CLA	C1B-C2B	2.56	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	606	CHL	MG-NA	-2.56	2.00	2.06
18	4	603	CLA	C1B-C2B	2.56	1.49	1.43
18	4	610	CLA	C1B-C2B	2.55	1.49	1.43
18	L	303	CLA	C1B-C2B	2.55	1.49	1.43
17	4	605	CHL	MG-NA	-2.55	2.00	2.06
18	B	840	CLA	C1B-C2B	2.55	1.49	1.43
22	B	849	BCR	C8-C9	-2.55	1.40	1.45
18	3	609	CLA	C1B-C2B	2.55	1.49	1.43
18	A	809	CLA	C1B-C2B	2.55	1.49	1.43
24	A	801	CL0	CHD-C4C	2.55	1.45	1.39
18	A	841	CLA	C1B-C2B	2.55	1.49	1.43
17	2	601	CHL	C3B-C4B	2.55	1.48	1.42
17	4	605	CHL	C1B-C2B	2.55	1.49	1.43
18	A	816	CLA	C1B-C2B	2.55	1.49	1.43
18	B	814	CLA	C1B-C2B	2.55	1.49	1.43
18	L	302	CLA	C1B-C2B	2.55	1.49	1.43
18	B	820	CLA	C1B-C2B	2.55	1.49	1.43
17	3	606	CHL	C3B-C4B	2.55	1.48	1.42
18	A	833	CLA	C1B-C2B	2.55	1.49	1.43
18	4	602	CLA	C1B-C2B	2.55	1.49	1.43
18	B	831	CLA	C1B-C2B	2.54	1.49	1.43
18	B	807	CLA	C1B-C2B	2.54	1.49	1.43
18	4	608	CLA	C1B-C2B	2.54	1.49	1.43
18	B	815	CLA	C1B-C2B	2.54	1.49	1.43
18	B	812	CLA	C1B-C2B	2.54	1.49	1.43
18	B	834	CLA	C1B-C2B	2.54	1.49	1.43
21	2	616	LUT	C8-C9	-2.54	1.40	1.45
22	K	202	BCR	C8-C9	-2.54	1.40	1.45
18	1	603	CLA	C1B-C2B	2.54	1.49	1.43
18	4	601	CLA	C1B-C2B	2.54	1.49	1.43
18	A	830	CLA	C1B-C2B	2.54	1.49	1.43
17	1	601	CHL	MG-NA	-2.53	2.00	2.06
18	1	602	CLA	C1B-C2B	2.53	1.49	1.43
18	A	836	CLA	C1B-C2B	2.53	1.49	1.43
18	A	808	CLA	C1B-C2B	2.53	1.49	1.43
18	B	830	CLA	C1B-C2B	2.53	1.49	1.43
18	1	608	CLA	C4B-C3B	2.53	1.49	1.43
18	3	603	CLA	C1B-C2B	2.53	1.49	1.43
18	2	612	CLA	C1B-C2B	2.53	1.49	1.43
17	2	606	CHL	C1B-C2B	2.52	1.49	1.43
18	A	818	CLA	C1B-C2B	2.52	1.49	1.43
18	F	302	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	807	CLA	C1B-C2B	2.51	1.49	1.43
18	3	612	CLA	C1B-C2B	2.51	1.49	1.43
18	B	822	CLA	C1B-C2B	2.51	1.49	1.43
22	B	847	BCR	C12-C13	-2.51	1.40	1.45
18	4	603	CLA	C4B-C3B	2.51	1.49	1.43
18	A	825	CLA	C1B-C2B	2.50	1.49	1.43
18	B	839	CLA	C1B-C2B	2.50	1.49	1.43
18	B	832	CLA	C1B-C2B	2.50	1.49	1.43
22	K	202	BCR	C23-C22	-2.50	1.40	1.45
17	4	606	CHL	C4B-NB	-2.50	1.34	1.37
18	B	829	CLA	C1B-C2B	2.50	1.49	1.43
18	A	810	CLA	C1B-C2B	2.50	1.49	1.43
18	A	813	CLA	C1B-C2B	2.50	1.49	1.43
18	1	609	CLA	CMD-C2D	-2.49	1.45	1.50
18	A	838	CLA	C1B-C2B	2.49	1.49	1.43
17	2	601	CHL	C1B-C2B	2.49	1.49	1.43
18	4	609	CLA	C1B-C2B	2.48	1.49	1.43
18	A	832	CLA	C1B-C2B	2.48	1.49	1.43
18	B	803	CLA	C1B-C2B	2.48	1.49	1.43
18	4	613	CLA	C1B-C2B	2.48	1.49	1.43
18	B	808	CLA	C1B-C2B	2.48	1.49	1.43
18	B	809	CLA	C1B-C2B	2.48	1.49	1.43
18	B	836	CLA	C1B-C2B	2.48	1.49	1.43
18	B	825	CLA	C1B-C2B	2.47	1.49	1.43
18	A	831	CLA	C1B-C2B	2.47	1.49	1.43
18	A	819	CLA	C1B-C2B	2.47	1.49	1.43
18	A	835	CLA	C1B-C2B	2.47	1.49	1.43
22	A	850	BCR	C19-C18	-2.47	1.40	1.45
18	A	820	CLA	C1B-C2B	2.47	1.49	1.43
18	A	806	CLA	C1B-C2B	2.46	1.49	1.43
18	A	829	CLA	C1B-C2B	2.46	1.49	1.43
18	B	827	CLA	C1B-C2B	2.46	1.49	1.43
17	3	606	CHL	C1B-C2B	2.46	1.49	1.43
18	B	838	CLA	C1B-C2B	2.46	1.49	1.43
17	1	606	CHL	C3A-C2A	-2.46	1.52	1.54
18	B	819	CLA	C1B-C2B	2.46	1.49	1.43
18	A	805	CLA	C1B-C2B	2.45	1.49	1.43
18	B	817	CLA	C1B-C2B	2.45	1.49	1.43
18	A	826	CLA	C1B-C2B	2.45	1.49	1.43
18	A	842	CLA	C1B-C2B	2.45	1.49	1.43
18	3	607	CLA	C1B-C2B	2.45	1.49	1.43
17	2	615	CHL	C1B-C2B	2.44	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	813	CLA	C1B-C2B	2.44	1.49	1.43
18	2	602	CLA	C1B-C2B	2.43	1.49	1.43
17	2	605	CHL	C1B-C2B	2.43	1.49	1.43
18	B	818	CLA	C1B-C2B	2.42	1.49	1.43
17	1	606	CHL	C4B-NB	-2.42	1.34	1.37
18	B	816	CLA	C1B-C2B	2.42	1.48	1.43
17	2	607	CHL	C3B-C4B	2.41	1.48	1.42
18	2	604	CLA	C1B-C2B	2.41	1.48	1.43
22	B	848	BCR	C19-C18	-2.41	1.40	1.45
18	A	840	CLA	C1B-C2B	2.41	1.48	1.43
21	2	616	LUT	C12-C13	-2.40	1.40	1.45
17	4	607	CHL	C3B-C4B	2.40	1.48	1.42
17	2	606	CHL	C4C-C3C	2.40	1.49	1.45
17	2	601	CHL	MG-NA	-2.39	2.00	2.06
17	4	615	CHL	C1B-C2B	2.39	1.48	1.43
18	A	822	CLA	C1B-C2B	2.39	1.48	1.43
18	B	802	CLA	C1B-C2B	2.39	1.48	1.43
17	2	601	CHL	C4C-C3C	2.39	1.49	1.45
22	4	618	BCR	C12-C13	-2.39	1.40	1.45
21	4	616	LUT	C12-C13	-2.38	1.40	1.45
17	2	605	CHL	MG-NA	-2.38	2.00	2.06
18	A	815	CLA	C1B-C2B	2.38	1.48	1.43
22	L	301	BCR	C12-C13	-2.38	1.40	1.45
17	1	601	CHL	C1B-C2B	2.38	1.48	1.43
22	B	847	BCR	C19-C18	-2.38	1.40	1.45
22	G	204	BCR	C19-C18	-2.38	1.40	1.45
18	B	828	CLA	C1B-C2B	2.37	1.48	1.43
24	A	801	CL0	C3B-C4B	2.36	1.48	1.42
17	1	606	CHL	C1B-NB	-2.36	1.34	1.37
24	A	801	CL0	CHA-C1A	2.36	1.45	1.39
22	3	614	BCR	C19-C18	-2.36	1.40	1.45
18	A	823	CLA	CHC-C1C	2.35	1.43	1.38
22	I	101	BCR	C12-C13	-2.35	1.40	1.45
22	F	304	BCR	C23-C22	-2.35	1.40	1.45
22	G	204	BCR	C12-C13	-2.35	1.40	1.45
17	4	607	CHL	C1B-C2B	2.35	1.48	1.43
18	A	844	CLA	C1B-C2B	2.35	1.48	1.43
22	I	101	BCR	C19-C18	-2.35	1.40	1.45
17	4	605	CHL	C4C-C3C	2.34	1.49	1.44
17	3	606	CHL	C4C-C3C	2.34	1.49	1.45
17	4	606	CHL	C1B-NB	-2.34	1.34	1.37
17	2	605	CHL	C4C-C3C	2.33	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	613	LUT	C32-C33	-2.33	1.40	1.45
17	1	601	CHL	C1B-NB	-2.33	1.34	1.37
22	3	614	BCR	C12-C13	-2.33	1.40	1.45
17	2	607	CHL	C1B-C2B	2.33	1.48	1.43
18	2	604	CLA	MG-NB	-2.32	2.01	2.05
18	A	803	CLA	MG-NB	-2.32	2.01	2.05
17	3	606	CHL	MG-NA	-2.32	2.00	2.06
22	B	846	BCR	C19-C18	-2.32	1.41	1.45
21	4	616	LUT	C32-C33	-2.31	1.41	1.45
22	4	618	BCR	C19-C18	-2.31	1.41	1.45
18	A	802	CLA	C1B-C2B	2.31	1.48	1.43
22	A	848	BCR	C19-C18	-2.31	1.41	1.45
22	L	305	BCR	C12-C13	-2.31	1.41	1.45
17	2	607	CHL	C4C-C3C	2.31	1.49	1.45
21	2	616	LUT	C28-C29	-2.31	1.41	1.45
24	A	801	CL0	CHC-C4B	2.31	1.44	1.39
18	A	842	CLA	CMB-C2B	-2.30	1.45	1.50
24	A	801	CL0	C1B-C2B	2.30	1.48	1.43
22	B	844	BCR	C12-C13	-2.30	1.41	1.45
18	1	604	CLA	CHC-C1C	2.29	1.43	1.38
17	2	615	CHL	C4B-NB	-2.29	1.35	1.37
22	B	845	BCR	C19-C18	-2.29	1.41	1.45
22	B	848	BCR	C12-C13	-2.29	1.41	1.45
18	A	818	CLA	CHC-C1C	2.29	1.43	1.38
24	A	801	CL0	CHB-C1B	2.29	1.44	1.39
17	2	615	CHL	C1B-NB	-2.28	1.35	1.37
18	B	841	CLA	CHC-C1C	2.28	1.43	1.38
21	2	616	LUT	C32-C33	-2.28	1.41	1.45
18	A	814	CLA	C1B-C2B	2.28	1.48	1.43
21	3	613	LUT	C28-C29	-2.28	1.41	1.45
18	A	807	CLA	CHC-C1C	2.28	1.43	1.38
18	A	844	CLA	CHC-C1C	2.28	1.43	1.38
17	4	615	CHL	MG-NA	-2.28	2.00	2.06
18	A	805	CLA	CHC-C1C	2.28	1.43	1.38
21	3	613	LUT	C12-C13	-2.27	1.41	1.45
18	4	603	CLA	CMD-C2D	-2.27	1.46	1.50
22	L	305	BCR	C19-C18	-2.27	1.41	1.45
18	B	837	CLA	CHC-C1C	2.27	1.43	1.38
24	A	801	CL0	C1D-C2D	2.27	1.49	1.45
22	A	850	BCR	C12-C13	-2.27	1.41	1.45
18	A	803	CLA	CHC-C1C	2.26	1.43	1.38
18	B	822	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	812	CLA	CHC-C1C	2.26	1.43	1.38
18	B	834	CLA	CHC-C1C	2.26	1.43	1.38
18	1	613	CLA	CMD-C2D	-2.26	1.46	1.50
18	1	611	CLA	CHC-C1C	2.26	1.43	1.38
18	3	603	CLA	MG-NB	-2.26	2.01	2.05
18	A	802	CLA	CHC-C1C	2.26	1.43	1.38
17	4	606	CHL	C4B-C3B	2.26	1.48	1.43
22	A	848	BCR	C12-C13	-2.25	1.41	1.45
18	B	828	CLA	CMD-C2D	-2.25	1.46	1.50
22	B	801	BCR	C19-C18	-2.25	1.41	1.45
18	1	603	CLA	MG-NB	-2.25	2.01	2.05
18	A	832	CLA	CHC-C1C	2.25	1.43	1.38
18	B	802	CLA	CHC-C1C	2.25	1.43	1.38
21	2	619	LUT	C12-C13	-2.25	1.41	1.45
18	B	819	CLA	CMB-C2B	-2.25	1.46	1.50
18	B	828	CLA	CMB-C2B	-2.25	1.46	1.50
18	A	806	CLA	CHC-C1C	2.25	1.43	1.38
17	2	615	CHL	C4C-C3C	2.24	1.48	1.45
19	2	617	XAT	C28-C29	-2.24	1.41	1.45
21	2	619	LUT	C32-C33	-2.24	1.41	1.45
19	1	614	XAT	O24-C25	-2.24	1.43	1.46
18	A	819	CLA	CHC-C1C	2.24	1.43	1.38
18	4	611	CLA	CHC-C1C	2.24	1.43	1.38
18	A	836	CLA	CHC-C1C	2.24	1.43	1.38
18	B	831	CLA	CHC-C1C	2.24	1.43	1.38
18	4	608	CLA	CHC-C1C	2.24	1.43	1.38
18	B	829	CLA	CMB-C2B	-2.24	1.46	1.50
18	K	203	CLA	CHC-C1C	2.24	1.43	1.38
22	B	846	BCR	C12-C13	-2.23	1.41	1.45
22	B	845	BCR	C12-C13	-2.23	1.41	1.45
18	A	810	CLA	CMD-C2D	-2.23	1.46	1.50
18	4	603	CLA	MG-NB	-2.23	2.01	2.05
18	4	609	CLA	CHC-C1C	2.23	1.43	1.38
18	B	804	CLA	CHC-C1C	2.23	1.43	1.38
18	1	610	CLA	CHC-C1C	2.23	1.43	1.38
18	K	201	CLA	CHC-C1C	2.23	1.43	1.38
17	4	607	CHL	C1B-NB	-2.23	1.35	1.37
18	A	803	CLA	C1B-C2B	2.23	1.48	1.43
18	A	828	CLA	CHC-C1C	2.23	1.43	1.38
22	B	801	BCR	C12-C13	-2.23	1.41	1.45
18	2	602	CLA	CHC-C1C	2.23	1.43	1.38
18	A	843	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	619	LUT	C28-C29	-2.23	1.41	1.45
18	B	816	CLA	MG-NB	-2.23	2.01	2.05
18	B	808	CLA	MG-NB	-2.23	2.01	2.05
18	B	817	CLA	CHC-C1C	2.22	1.43	1.38
18	1	603	CLA	CHC-C1C	2.22	1.43	1.38
18	A	837	CLA	CHC-C1C	2.22	1.43	1.38
18	4	610	CLA	CHC-C1C	2.22	1.43	1.38
18	B	828	CLA	CHC-C1C	2.22	1.43	1.38
18	A	814	CLA	CHC-C1C	2.22	1.43	1.38
17	2	606	CHL	C1B-NB	-2.22	1.35	1.37
18	1	603	CLA	CMD-C2D	-2.22	1.46	1.50
17	2	607	CHL	C1B-NB	-2.22	1.35	1.37
18	2	609	CLA	CMC-C2C	-2.22	1.46	1.50
18	A	838	CLA	CHC-C1C	2.21	1.43	1.38
18	3	605	CLA	CHC-C1C	2.21	1.43	1.38
18	A	810	CLA	CHC-C1C	2.21	1.43	1.38
17	2	607	CHL	MG-NA	-2.21	2.01	2.06
18	B	829	CLA	CHC-C1C	2.21	1.43	1.38
18	B	838	CLA	CHC-C1C	2.21	1.43	1.38
18	G	202	CLA	CHC-C1C	2.21	1.43	1.38
18	A	824	CLA	CHC-C1C	2.21	1.43	1.38
18	B	809	CLA	MG-NB	-2.21	2.01	2.05
18	3	609	CLA	CHC-C1C	2.21	1.43	1.38
22	B	849	BCR	C19-C18	-2.21	1.41	1.45
18	A	809	CLA	CHC-C1C	2.21	1.43	1.38
18	A	806	CLA	CMC-C2C	-2.21	1.46	1.50
18	4	602	CLA	CHC-C1C	2.21	1.43	1.38
18	4	611	CLA	CMD-C2D	-2.20	1.46	1.50
18	A	844	CLA	MG-NB	-2.20	2.01	2.05
18	B	814	CLA	CHC-C1C	2.20	1.43	1.38
18	B	835	CLA	CHC-C1C	2.20	1.43	1.38
18	B	821	CLA	CHC-C1C	2.20	1.43	1.38
17	2	606	CHL	C4B-NB	-2.20	1.35	1.37
18	A	833	CLA	CHC-C1C	2.20	1.43	1.38
18	B	826	CLA	CHC-C1C	2.20	1.43	1.38
22	J	102	BCR	C19-C18	-2.20	1.41	1.45
18	3	612	CLA	MG-NB	-2.20	2.01	2.05
18	3	607	CLA	CHC-C1C	2.20	1.43	1.38
17	2	601	CHL	C4B-NB	-2.20	1.35	1.37
18	B	839	CLA	CHC-C1C	2.20	1.43	1.38
18	B	836	CLA	CHC-C1C	2.20	1.43	1.38
18	B	809	CLA	CMB-C2B	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	615	CHL	C4C-C3C	2.20	1.48	1.45
21	4	616	LUT	C28-C29	-2.19	1.41	1.45
18	B	825	CLA	CHC-C1C	2.19	1.43	1.38
18	G	201	CLA	CHC-C1C	2.19	1.43	1.38
18	B	811	CLA	CHC-C1C	2.19	1.43	1.38
18	G	203	CLA	CHC-C1C	2.19	1.43	1.38
18	B	818	CLA	MG-NB	-2.19	2.01	2.05
18	1	613	CLA	CHC-C1C	2.19	1.43	1.38
22	K	205	BCR	C19-C18	-2.19	1.41	1.45
18	4	601	CLA	CHC-C1C	2.19	1.43	1.38
18	F	302	CLA	CHC-C1C	2.19	1.43	1.38
18	A	840	CLA	CHC-C1C	2.19	1.43	1.38
22	A	849	BCR	C19-C18	-2.19	1.41	1.45
18	A	831	CLA	CHC-C1C	2.19	1.43	1.38
18	1	608	CLA	MG-NB	-2.19	2.01	2.05
18	A	815	CLA	CHC-C1C	2.19	1.43	1.38
18	A	822	CLA	CMB-C2B	-2.19	1.46	1.50
17	4	615	CHL	C4B-NB	-2.19	1.35	1.37
18	A	822	CLA	MG-NB	-2.19	2.01	2.05
18	B	816	CLA	CHC-C1C	2.18	1.43	1.38
18	A	825	CLA	MG-NB	-2.18	2.01	2.05
18	4	613	CLA	CHC-C1C	2.18	1.43	1.38
18	K	204	CLA	CHC-C1C	2.18	1.43	1.38
17	4	606	CHL	C1D-ND	-2.18	1.35	1.37
18	B	820	CLA	CHC-C1C	2.18	1.43	1.38
18	3	608	CLA	CHC-C1C	2.18	1.43	1.38
17	1	601	CHL	C4C-C3C	2.18	1.48	1.45
22	A	852	BCR	C19-C18	-2.18	1.41	1.45
18	B	815	CLA	CHC-C1C	2.18	1.43	1.38
17	3	606	CHL	C1B-NB	-2.18	1.35	1.37
18	F	301	CLA	CHC-C1C	2.18	1.42	1.38
18	B	802	CLA	CMD-C2D	-2.18	1.46	1.50
18	B	833	CLA	MG-NB	-2.17	2.01	2.05
17	2	601	CHL	C1B-NB	-2.17	1.35	1.37
18	A	842	CLA	MG-NB	-2.17	2.01	2.05
18	L	302	CLA	CHC-C1C	2.17	1.42	1.38
18	B	826	CLA	MG-NB	-2.17	2.01	2.05
18	B	803	CLA	CHC-C1C	2.17	1.42	1.38
18	2	610	CLA	CHC-C1C	2.17	1.42	1.38
18	B	808	CLA	CMD-C2D	-2.17	1.46	1.50
18	B	813	CLA	MG-NB	-2.17	2.01	2.05
22	B	844	BCR	C20-C19	2.17	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	301	BCR	C20-C19	2.17	1.40	1.34
18	B	824	CLA	MG-NB	-2.17	2.01	2.05
18	A	816	CLA	MG-NB	-2.17	2.01	2.05
18	B	807	CLA	CHC-C1C	2.17	1.42	1.38
19	4	617	XAT	C12-C13	-2.17	1.41	1.45
22	L	306	BCR	C19-C18	-2.17	1.41	1.45
18	A	826	CLA	CMD-C2D	-2.16	1.46	1.50
18	B	819	CLA	CHC-C1C	2.16	1.42	1.38
18	B	823	CLA	CHC-C1C	2.16	1.42	1.38
18	4	603	CLA	CMB-C2B	-2.16	1.46	1.50
18	4	609	CLA	MG-NB	-2.16	2.01	2.05
18	2	608	CLA	CHC-C1C	2.16	1.42	1.38
18	A	822	CLA	CHC-C1C	2.16	1.42	1.38
18	3	602	CLA	CHC-C1C	2.16	1.42	1.38
18	3	611	CLA	CHC-C1C	2.16	1.42	1.38
18	B	827	CLA	CHC-C1C	2.16	1.42	1.38
22	A	849	BCR	C12-C13	-2.16	1.41	1.45
21	1	616	LUT	C32-C33	-2.16	1.41	1.45
18	1	602	CLA	CHC-C1C	2.16	1.42	1.38
18	A	826	CLA	CHC-C1C	2.16	1.42	1.38
18	4	613	CLA	MG-NB	-2.16	2.01	2.05
24	A	801	CL0	MG-NC	2.16	2.11	2.06
18	A	844	CLA	CMB-C2B	-2.16	1.46	1.50
18	3	601	CLA	CHC-C1C	2.16	1.42	1.38
18	L	303	CLA	CHC-C1C	2.16	1.42	1.38
18	B	819	CLA	MG-NB	-2.16	2.01	2.05
22	B	843	BCR	C12-C13	-2.16	1.41	1.45
18	1	612	CLA	CHC-C1C	2.16	1.42	1.38
18	2	611	CLA	CHC-C1C	2.16	1.42	1.38
17	1	601	CHL	C4B-NB	-2.16	1.35	1.37
18	B	836	CLA	CMB-C2B	-2.16	1.46	1.50
18	F	303	CLA	CHC-C1C	2.16	1.42	1.38
18	1	605	CLA	CHC-C1C	2.16	1.42	1.38
18	B	810	CLA	CHC-C1C	2.16	1.42	1.38
18	H	201	CLA	MG-NB	-2.16	2.01	2.05
18	A	829	CLA	CHC-C1C	2.16	1.42	1.38
18	A	829	CLA	MG-NB	-2.15	2.01	2.05
18	B	833	CLA	CHC-C1C	2.15	1.42	1.38
18	3	610	CLA	CHC-C1C	2.15	1.42	1.38
18	A	817	CLA	CHC-C1C	2.15	1.42	1.38
18	A	816	CLA	CHC-C1C	2.15	1.42	1.38
18	2	613	CLA	CHC-C1C	2.15	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	609	CLA	CHC-C1C	2.15	1.42	1.38
17	4	615	CHL	C1B-NB	-2.15	1.35	1.37
18	A	830	CLA	CMD-C2D	-2.15	1.46	1.50
18	1	602	CLA	MG-NB	-2.15	2.01	2.05
18	A	835	CLA	CHC-C1C	2.15	1.42	1.38
18	B	823	CLA	CMD-C2D	-2.15	1.46	1.50
18	A	841	CLA	MG-NB	-2.15	2.01	2.05
18	L	303	CLA	MG-NB	-2.15	2.01	2.05
17	2	607	CHL	C4B-NB	-2.15	1.35	1.37
18	B	818	CLA	CHC-C1C	2.15	1.42	1.38
18	2	602	CLA	MG-NB	-2.15	2.01	2.05
18	3	609	CLA	MG-NB	-2.15	2.01	2.05
18	B	840	CLA	CMB-C2B	-2.15	1.46	1.50
22	B	843	BCR	C19-C18	-2.15	1.41	1.45
17	2	605	CHL	C1B-NB	-2.15	1.35	1.37
18	1	612	CLA	MG-NB	-2.15	2.01	2.05
18	A	820	CLA	MG-NB	-2.15	2.01	2.05
18	4	602	CLA	MG-NB	-2.15	2.01	2.05
18	A	843	CLA	MG-NB	-2.15	2.01	2.05
18	A	804	CLA	CMD-C2D	-2.15	1.46	1.50
18	A	821	CLA	CHC-C1C	2.14	1.42	1.38
18	B	811	CLA	CMB-C2B	-2.14	1.46	1.50
18	2	603	CLA	MG-NB	-2.14	2.01	2.05
18	A	831	CLA	MG-NB	-2.14	2.01	2.05
18	A	826	CLA	MG-NB	-2.14	2.01	2.05
18	A	814	CLA	CMC-C2C	-2.14	1.46	1.50
17	4	615	CHL	C4B-C3B	2.14	1.48	1.43
18	1	609	CLA	MG-NB	-2.14	2.01	2.05
18	2	603	CLA	CHC-C1C	2.14	1.42	1.38
18	2	608	CLA	MG-NB	-2.14	2.01	2.05
18	B	805	CLA	CHC-C1C	2.14	1.42	1.38
18	1	607	CLA	CHC-C1C	2.14	1.42	1.38
22	L	306	BCR	C12-C13	-2.14	1.41	1.45
18	B	813	CLA	CMB-C2B	-2.14	1.46	1.50
17	2	615	CHL	C1D-ND	-2.14	1.35	1.37
18	4	614	CLA	CHC-C1C	2.14	1.42	1.38
18	A	808	CLA	CHC-C1C	2.14	1.42	1.38
18	4	604	CLA	CHC-C1C	2.14	1.42	1.38
18	B	830	CLA	MG-NB	-2.14	2.01	2.05
18	B	825	CLA	MG-NB	-2.13	2.01	2.05
18	3	602	CLA	MG-NB	-2.13	2.01	2.05
18	A	827	CLA	MG-NB	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	606	CHL	C1D-ND	-2.13	1.35	1.37
24	A	801	CL0	CHA-C4D	2.13	1.42	1.38
18	A	803	CLA	CMB-C2B	-2.13	1.46	1.50
18	3	601	CLA	MG-NB	-2.13	2.01	2.05
18	A	836	CLA	CMB-C2B	-2.13	1.46	1.50
19	4	617	XAT	C14-C13	-2.13	1.33	1.35
18	3	607	CLA	MG-NB	-2.13	2.01	2.05
18	A	834	CLA	CMD-C2D	-2.13	1.46	1.50
18	A	804	CLA	MG-NB	-2.13	2.01	2.05
18	B	821	CLA	CMD-C2D	-2.13	1.46	1.50
18	B	818	CLA	CMB-C2B	-2.13	1.46	1.50
18	A	841	CLA	CHC-C1C	2.13	1.42	1.38
22	A	853	BCR	C12-C13	-2.13	1.41	1.45
18	3	604	CLA	CMB-C2B	-2.13	1.46	1.50
18	B	831	CLA	MG-NB	-2.13	2.01	2.05
18	G	203	CLA	MG-NB	-2.13	2.01	2.05
18	B	824	CLA	CHC-C1C	2.13	1.42	1.38
18	B	805	CLA	CMD-C2D	-2.13	1.46	1.50
18	B	823	CLA	CMC-C2C	-2.13	1.46	1.50
18	A	831	CLA	CMB-C2B	-2.13	1.46	1.50
18	A	811	CLA	MG-NB	-2.12	2.01	2.05
17	2	607	CHL	C1D-ND	-2.12	1.35	1.37
18	1	608	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	806	CLA	CMD-C2D	-2.12	1.46	1.50
18	B	803	CLA	MG-NB	-2.12	2.01	2.05
18	2	610	CLA	MG-NB	-2.12	2.01	2.05
18	A	820	CLA	CMB-C2B	-2.12	1.46	1.50
18	A	814	CLA	CMD-C2D	-2.12	1.46	1.50
18	B	830	CLA	CMD-C2D	-2.12	1.46	1.50
18	B	810	CLA	CMD-C2D	-2.12	1.46	1.50
18	B	822	CLA	MG-NB	-2.12	2.01	2.05
18	A	803	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	816	CLA	CMD-C2D	-2.12	1.46	1.50
18	3	604	CLA	MG-NB	-2.12	2.01	2.05
18	A	828	CLA	MG-NB	-2.12	2.01	2.05
18	B	827	CLA	MG-NB	-2.12	2.01	2.05
18	A	820	CLA	CMD-C2D	-2.12	1.46	1.50
18	3	603	CLA	CHC-C1C	2.12	1.42	1.38
18	A	832	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	821	CLA	MG-NB	-2.12	2.01	2.05
17	4	605	CHL	C4B-NB	-2.12	1.35	1.37
18	3	604	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	802	CLA	MG-NB	-2.12	2.01	2.05
18	3	607	CLA	CMB-C2B	-2.12	1.46	1.50
18	A	807	CLA	CMD-C2D	-2.12	1.46	1.50
18	2	612	CLA	CHC-C1C	2.12	1.42	1.38
18	B	836	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	810	CLA	MG-NB	-2.12	2.01	2.05
18	B	815	CLA	CMB-C2B	-2.12	1.46	1.50
18	2	608	CLA	CMD-C2D	-2.12	1.46	1.50
18	3	601	CLA	CMD-C2D	-2.12	1.46	1.50
18	A	820	CLA	CHC-C1C	2.11	1.42	1.38
18	B	814	CLA	MG-NB	-2.11	2.01	2.05
18	2	603	CLA	CMD-C2D	-2.11	1.46	1.50
18	A	835	CLA	MG-NB	-2.11	2.01	2.05
18	B	806	CLA	MG-NB	-2.11	2.01	2.05
18	3	602	CLA	CMD-C2D	-2.11	1.46	1.50
18	4	611	CLA	MG-NB	-2.11	2.01	2.05
18	B	839	CLA	MG-NB	-2.11	2.01	2.05
18	B	835	CLA	CMB-C2B	-2.11	1.46	1.50
18	4	610	CLA	MG-NB	-2.11	2.01	2.05
18	2	604	CLA	CHC-C1C	2.11	1.42	1.38
18	B	830	CLA	CHC-C1C	2.11	1.42	1.38
17	2	601	CHL	C1D-ND	-2.11	1.35	1.37
18	A	839	CLA	MG-NB	-2.11	2.01	2.05
18	A	815	CLA	MG-NB	-2.11	2.01	2.05
18	B	817	CLA	CMB-C2B	-2.11	1.46	1.50
18	2	612	CLA	MG-NB	-2.11	2.01	2.05
18	B	823	CLA	MG-NB	-2.11	2.01	2.05
22	A	851	BCR	C12-C13	-2.11	1.41	1.45
18	3	612	CLA	CMD-C2D	-2.11	1.46	1.50
18	B	829	CLA	CMD-C2D	-2.11	1.46	1.50
18	3	611	CLA	MG-NB	-2.11	2.01	2.05
18	A	811	CLA	CHC-C1C	2.11	1.42	1.38
18	L	302	CLA	CMD-C2D	-2.11	1.46	1.50
18	3	605	CLA	MG-NB	-2.11	2.01	2.05
18	A	819	CLA	CMD-C2D	-2.10	1.46	1.50
18	A	825	CLA	CMB-C2B	-2.10	1.46	1.50
18	L	304	CLA	CMB-C2B	-2.10	1.46	1.50
18	B	821	CLA	MG-NB	-2.10	2.01	2.05
18	B	820	CLA	CMD-C2D	-2.10	1.46	1.50
18	4	603	CLA	CHC-C1C	2.10	1.42	1.38
21	1	616	LUT	C12-C13	-2.10	1.41	1.45
18	K	201	CLA	CBD-CAD	2.10	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	838	CLA	CMB-C2B	-2.10	1.46	1.50
18	3	608	CLA	MG-NB	-2.10	2.01	2.05
18	2	613	CLA	CMD-C2D	-2.10	1.46	1.50
18	B	812	CLA	CHC-C1C	2.10	1.42	1.38
18	A	838	CLA	CMD-C2D	-2.10	1.46	1.50
18	L	302	CLA	CMB-C2B	-2.10	1.46	1.50
18	A	813	CLA	CMB-C2B	-2.10	1.46	1.50
18	4	608	CLA	CMD-C2D	-2.10	1.46	1.50
18	4	608	CLA	MG-NB	-2.10	2.01	2.05
18	B	840	CLA	MG-NB	-2.10	2.01	2.05
18	B	804	CLA	CMD-C2D	-2.10	1.46	1.50
18	A	808	CLA	MG-NB	-2.10	2.01	2.05
18	A	827	CLA	CHC-C1C	2.10	1.42	1.38
18	4	609	CLA	CMB-C2B	-2.10	1.46	1.50
18	4	604	CLA	MG-NB	-2.10	2.01	2.05
18	A	821	CLA	CMD-C2D	-2.10	1.46	1.50
18	B	812	CLA	CMB-C2B	-2.10	1.46	1.50
18	1	613	CLA	MG-NB	-2.10	2.01	2.05
18	4	608	CLA	CMB-C2B	-2.10	1.46	1.50
22	K	202	BCR	C19-C18	-2.10	1.41	1.45
18	4	612	CLA	CHC-C1C	2.10	1.42	1.38
18	A	806	CLA	MG-NB	-2.10	2.01	2.05
17	2	605	CHL	C4B-NB	-2.10	1.35	1.37
18	B	836	CLA	MG-NB	-2.10	2.01	2.05
18	G	201	CLA	MG-NB	-2.10	2.01	2.05
18	4	609	CLA	CMD-C2D	-2.10	1.46	1.50
18	A	802	CLA	CMD-C2D	-2.10	1.46	1.50
18	A	843	CLA	CHC-C1C	2.10	1.42	1.38
18	1	604	CLA	MG-NB	-2.10	2.01	2.05
22	A	853	BCR	C19-C18	-2.09	1.41	1.45
18	4	612	CLA	MG-NB	-2.09	2.01	2.05
18	3	608	CLA	CMD-C2D	-2.09	1.46	1.50
22	F	304	BCR	C19-C18	-2.09	1.41	1.45
18	B	808	CLA	CHC-C1C	2.09	1.42	1.38
18	1	610	CLA	CMD-C2D	-2.09	1.46	1.50
18	4	613	CLA	CMD-C2D	-2.09	1.46	1.50
18	A	832	CLA	CMB-C2B	-2.09	1.46	1.50
18	B	817	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	840	CLA	CMD-C2D	-2.09	1.46	1.50
22	J	102	BCR	C12-C13	-2.09	1.41	1.45
18	2	604	CLA	CMD-C2D	-2.09	1.46	1.50
22	A	851	BCR	C19-C18	-2.09	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	304	CLA	CHC-C1C	2.09	1.42	1.38
18	B	829	CLA	MG-NB	-2.09	2.01	2.05
17	2	606	CHL	C1D-ND	-2.09	1.35	1.37
18	A	819	CLA	CMB-C2B	-2.09	1.46	1.50
18	B	822	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	807	CLA	MG-NB	-2.09	2.01	2.05
18	A	813	CLA	CHC-C1C	2.09	1.42	1.38
18	B	833	CLA	CMD-C2D	-2.09	1.46	1.50
17	2	605	CHL	C1D-ND	-2.09	1.35	1.37
18	1	611	CLA	MG-NB	-2.09	2.01	2.05
18	B	803	CLA	CMD-C2D	-2.09	1.46	1.50
18	1	607	CLA	MG-NB	-2.09	2.01	2.05
18	B	817	CLA	MG-NB	-2.09	2.01	2.05
18	B	832	CLA	CHC-C1C	2.09	1.42	1.38
18	B	839	CLA	CMB-C2B	-2.09	1.46	1.50
18	F	301	CLA	CMD-C2D	-2.09	1.46	1.50
24	A	801	CL0	C1C-C2C	2.09	1.48	1.44
18	A	834	CLA	CMB-C2B	-2.09	1.46	1.50
18	A	841	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	818	CLA	CMD-C2D	-2.09	1.46	1.50
18	B	826	CLA	CMD-C2D	-2.09	1.46	1.50
18	2	602	CLA	CMD-C2D	-2.09	1.46	1.50
17	1	601	CHL	C1D-ND	-2.08	1.35	1.37
18	2	604	CLA	CMB-C2B	-2.08	1.46	1.50
18	B	833	CLA	CMB-C2B	-2.08	1.46	1.50
18	A	825	CLA	CHC-C1C	2.08	1.42	1.38
18	B	804	CLA	MG-NB	-2.08	2.01	2.05
18	2	609	CLA	MG-NB	-2.08	2.01	2.05
18	B	837	CLA	MG-NB	-2.08	2.01	2.05
18	A	817	CLA	CMB-C2B	-2.08	1.46	1.50
18	3	602	CLA	CMB-C2B	-2.08	1.46	1.50
18	A	840	CLA	CMD-C2D	-2.08	1.46	1.50
18	B	834	CLA	CMB-C2B	-2.08	1.46	1.50
18	B	813	CLA	CMD-C2D	-2.08	1.46	1.50
18	K	203	CLA	MG-NB	-2.08	2.01	2.05
18	L	302	CLA	MG-NB	-2.08	2.01	2.05
18	A	833	CLA	CMD-C2D	-2.08	1.46	1.50
18	G	202	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	830	CLA	CHC-C1C	2.08	1.42	1.38
18	B	820	CLA	MG-NB	-2.08	2.01	2.05
18	A	838	CLA	CMB-C2B	-2.08	1.46	1.50
18	B	815	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	840	CLA	CMB-C2B	-2.08	1.46	1.50
17	4	607	CHL	C4C-C3C	2.08	1.48	1.45
18	B	808	CLA	CMC-C2C	-2.08	1.46	1.50
18	B	810	CLA	MG-NB	-2.08	2.01	2.05
18	L	303	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	835	CLA	CMB-C2B	-2.07	1.46	1.50
18	A	839	CLA	CMD-C2D	-2.07	1.46	1.50
18	2	609	CLA	CMD-C2D	-2.07	1.46	1.50
18	B	838	CLA	CMD-C2D	-2.07	1.46	1.50
18	H	201	CLA	CMD-C2D	-2.07	1.46	1.50
18	2	613	CLA	MG-NB	-2.07	2.01	2.05
19	2	617	XAT	C12-C13	-2.07	1.41	1.45
18	B	817	CLA	CMC-C2C	-2.07	1.46	1.50
18	A	834	CLA	MG-NB	-2.07	2.01	2.05
18	A	807	CLA	CMB-C2B	-2.07	1.46	1.50
18	A	830	CLA	MG-NB	-2.07	2.01	2.05
22	B	849	BCR	C12-C13	-2.07	1.41	1.45
18	A	818	CLA	MG-NB	-2.07	2.01	2.05
18	B	841	CLA	MG-NB	-2.07	2.01	2.05
18	3	604	CLA	CMD-C2D	-2.07	1.46	1.50
18	1	608	CLA	CHC-C1C	2.07	1.42	1.38
18	A	828	CLA	CMD-C2D	-2.07	1.46	1.50
18	1	610	CLA	MG-NB	-2.07	2.01	2.05
18	L	304	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	818	CLA	CMD-C2D	-2.07	1.46	1.50
18	B	822	CLA	CMB-C2B	-2.07	1.46	1.50
18	1	607	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	811	CLA	CMD-C2D	-2.07	1.46	1.50
18	3	610	CLA	MG-NB	-2.07	2.01	2.05
18	4	614	CLA	CMD-C2D	-2.07	1.46	1.50
18	B	816	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	819	CLA	MG-NB	-2.07	2.01	2.05
18	3	611	CLA	CBD-CAD	2.07	1.56	1.51
18	B	812	CLA	MG-NB	-2.07	2.01	2.05
18	A	826	CLA	CMB-C2B	-2.07	1.46	1.50
18	B	837	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	840	CLA	MG-NB	-2.07	2.01	2.05
18	B	838	CLA	MG-NB	-2.07	2.01	2.05
18	G	202	CLA	MG-NB	-2.07	2.01	2.05
18	A	817	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	838	CLA	MG-NB	-2.07	2.01	2.05
18	L	304	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	833	CLA	MG-NB	-2.07	2.01	2.05
18	4	612	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	816	CLA	CMB-C2B	-2.07	1.46	1.50
18	B	809	CLA	CHC-C1C	2.07	1.42	1.38
22	A	852	BCR	C11-C12	2.06	1.39	1.34
18	2	610	CLA	CMD-C2D	-2.06	1.46	1.50
18	K	204	CLA	MG-NB	-2.06	2.01	2.05
18	A	828	CLA	CMC-C2C	-2.06	1.46	1.50
18	B	805	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	806	CLA	CMD-C2D	-2.06	1.46	1.50
18	3	607	CLA	CMD-C2D	-2.06	1.46	1.50
18	1	607	CLA	CMB-C2B	-2.06	1.46	1.50
18	A	802	CLA	CMB-C2B	-2.06	1.46	1.50
18	A	843	CLA	CMC-C2C	-2.06	1.46	1.50
18	B	808	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	807	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	804	CLA	CHC-C1C	2.06	1.42	1.38
18	1	602	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	802	CLA	CMC-C2C	-2.06	1.46	1.50
18	H	201	CLA	CHC-C1C	2.06	1.42	1.38
17	4	607	CHL	MG-NA	-2.06	2.01	2.06
18	A	810	CLA	CMB-C2B	-2.06	1.46	1.50
18	A	834	CLA	CHC-C1C	2.06	1.42	1.38
18	B	827	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	831	CLA	CMB-C2B	-2.06	1.46	1.50
18	2	608	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	824	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	834	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	815	CLA	MG-NB	-2.06	2.01	2.05
18	B	825	CLA	CMD-C2D	-2.06	1.46	1.50
18	4	610	CLA	CMB-C2B	-2.06	1.46	1.50
18	A	831	CLA	CMD-C2D	-2.06	1.46	1.50
22	F	304	BCR	C11-C12	2.06	1.39	1.34
18	B	831	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	807	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	827	CLA	CMB-C2B	-2.06	1.46	1.50
18	B	839	CLA	CMD-C2D	-2.06	1.46	1.50
18	4	601	CLA	MG-NB	-2.06	2.01	2.05
18	A	813	CLA	CMD-C2D	-2.05	1.46	1.50
18	4	613	CLA	CMB-C2B	-2.05	1.46	1.50
19	2	617	XAT	C32-C33	-2.05	1.41	1.45
18	A	809	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	813	CLA	CHC-C1C	2.05	1.42	1.38
18	A	842	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	813	CLA	CMC-C2C	-2.05	1.46	1.50
18	2	612	CLA	CMB-C2B	-2.05	1.46	1.50
18	A	827	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	809	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	829	CLA	CMD-C2D	-2.05	1.46	1.50
18	3	609	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	815	CLA	CMC-C2C	-2.05	1.46	1.50
18	B	811	CLA	MG-NB	-2.05	2.01	2.05
18	A	814	CLA	CMB-C2B	-2.05	1.46	1.50
18	F	303	CLA	MG-NB	-2.05	2.01	2.05
18	4	602	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	806	CLA	CMB-C2B	-2.05	1.46	1.50
18	A	815	CLA	CMB-C2B	-2.05	1.46	1.50
18	A	808	CLA	CMD-C2D	-2.05	1.46	1.50
18	F	301	CLA	CMB-C2B	-2.05	1.46	1.50
18	B	814	CLA	CMD-C2D	-2.04	1.46	1.50
18	2	602	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	812	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	819	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	826	CLA	CMC-C2C	-2.04	1.46	1.50
17	4	605	CHL	C1D-ND	-2.04	1.35	1.37
18	A	823	CLA	MG-NB	-2.04	2.01	2.05
18	B	802	CLA	CMC-C2C	-2.04	1.46	1.50
18	A	839	CLA	CHC-C1C	2.04	1.42	1.38
18	B	840	CLA	CHC-C1C	2.04	1.42	1.38
17	3	606	CHL	C4B-NB	-2.04	1.35	1.37
18	3	611	CLA	CMB-C2B	-2.04	1.46	1.50
18	3	605	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	805	CLA	MG-NB	-2.04	2.01	2.05
18	B	814	CLA	CMB-C2B	-2.04	1.46	1.50
18	F	301	CLA	MG-NB	-2.04	2.01	2.05
18	B	810	CLA	CMB-C2B	-2.04	1.46	1.50
18	A	821	CLA	CMB-C2B	-2.04	1.46	1.50
17	4	605	CHL	C1B-NB	-2.04	1.35	1.37
18	B	832	CLA	CMD-C2D	-2.04	1.46	1.50
18	K	201	CLA	MG-NB	-2.04	2.01	2.05
18	B	830	CLA	CMB-C2B	-2.04	1.46	1.50
18	B	836	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	828	CLA	MG-NB	-2.04	2.01	2.05
18	4	601	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	815	CLA	CMC-C2C	-2.04	1.46	1.50
18	4	611	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	804	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	809	CLA	CMB-C2B	-2.03	1.46	1.50
18	4	614	CLA	MG-NB	-2.03	2.01	2.05
18	A	836	CLA	MG-NB	-2.03	2.01	2.05
18	1	602	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	807	CLA	CMC-C2C	-2.03	1.46	1.50
18	A	805	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	837	CLA	CMC-C2C	-2.03	1.46	1.50
18	A	837	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	814	CLA	MG-NB	-2.03	2.01	2.05
18	3	605	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	837	CLA	MG-NB	-2.03	2.01	2.05
18	4	602	CLA	CMB-C2B	-2.03	1.46	1.50
18	3	611	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	844	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	815	CLA	CMD-C2D	-2.03	1.46	1.50
18	F	302	CLA	MG-NB	-2.03	2.01	2.05
18	3	609	CLA	CMB-C2B	-2.03	1.46	1.50
18	A	811	CLA	CMB-C2B	-2.03	1.46	1.50
18	B	802	CLA	CMB-C2B	-2.03	1.46	1.50
18	2	611	CLA	MG-NB	-2.03	2.01	2.05
18	3	601	CLA	CMB-C2B	-2.02	1.46	1.50
18	4	604	CLA	CMB-C2B	-2.02	1.46	1.50
18	G	202	CLA	CMB-C2B	-2.02	1.46	1.50
18	1	603	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	819	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	806	CLA	CHC-C1C	2.02	1.42	1.38
18	B	819	CLA	CMC-C2C	-2.02	1.46	1.50
18	K	204	CLA	CMD-C2D	-2.02	1.46	1.50
18	2	612	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	824	CLA	MG-NB	-2.02	2.01	2.05
18	B	809	CLA	CMD-C2D	-2.02	1.46	1.50
18	3	603	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	807	CLA	MG-NB	-2.02	2.01	2.05
18	1	607	CLA	CMC-C2C	-2.02	1.46	1.50
18	A	827	CLA	CMC-C2C	-2.02	1.46	1.50
18	B	803	CLA	CMC-C2C	-2.02	1.46	1.50
18	B	841	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	844	CLA	CMC-C2C	-2.02	1.46	1.50
18	1	611	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	602	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	824	CLA	CMB-C2B	-2.02	1.46	1.50
18	G	201	CLA	CMB-C2B	-2.02	1.46	1.50
18	4	601	CLA	CMB-C2B	-2.02	1.46	1.50
18	1	613	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	822	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	812	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	825	CLA	CMB-C2B	-2.02	1.46	1.50
18	1	612	CLA	CMB-C2B	-2.02	1.46	1.50
18	A	829	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	820	CLA	CMB-C2B	-2.02	1.46	1.50
18	L	303	CLA	CMB-C2B	-2.02	1.46	1.50
18	1	609	CLA	CHC-C1C	2.02	1.42	1.38
18	3	608	CLA	CMB-C2B	-2.01	1.46	1.50
18	4	610	CLA	CMD-C2D	-2.01	1.46	1.50
18	A	830	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	812	CLA	CMD-C2D	-2.01	1.46	1.50
17	4	607	CHL	C1D-ND	-2.01	1.35	1.37
18	4	602	CLA	CMC-C2C	-2.01	1.46	1.50
18	A	805	CLA	CMB-C2B	-2.01	1.46	1.50
18	A	828	CLA	CMB-C2B	-2.01	1.46	1.50
18	B	810	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	818	CLA	CMC-C2C	-2.01	1.46	1.50
19	4	617	XAT	C8-C9	-2.01	1.41	1.45
18	G	201	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	809	CLA	CMC-C2C	-2.01	1.46	1.50
18	2	613	CLA	CMB-C2B	-2.01	1.46	1.50
18	B	835	CLA	MG-NB	-2.01	2.01	2.05
18	3	612	CLA	CMB-C2B	-2.01	1.46	1.50
18	3	608	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	826	CLA	CMB-C2B	-2.01	1.46	1.50
18	G	203	CLA	CMD-C2D	-2.01	1.46	1.50
18	F	303	CLA	CMD-C2D	-2.01	1.46	1.50
17	1	606	CHL	C3B-C2B	2.01	1.48	1.41
18	4	601	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	823	CLA	CMB-C2B	-2.01	1.46	1.50
18	F	303	CLA	CMB-C2B	-2.01	1.46	1.50
18	2	611	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	805	CLA	CMC-C2C	-2.01	1.46	1.50
18	B	811	CLA	CMD-C2D	-2.01	1.46	1.50
19	4	617	XAT	C31-C32	-2.01	1.29	1.34
18	2	603	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	604	CLA	CMC-C2C	-2.01	1.46	1.50
22	L	301	BCR	C19-C18	-2.00	1.41	1.45
18	2	610	CLA	CMB-C2B	-2.00	1.46	1.50
18	A	818	CLA	CMB-C2B	-2.00	1.46	1.50
18	A	841	CLA	CMC-C2C	-2.00	1.46	1.50
17	4	607	CHL	CHB-C4A	-2.00	1.32	1.37
22	K	205	BCR	C11-C12	2.00	1.39	1.34
18	B	802	CLA	MG-NB	-2.00	2.01	2.05
18	B	832	CLA	CMB-C2B	-2.00	1.46	1.50
18	B	837	CLA	CMB-C2B	-2.00	1.46	1.50
18	1	604	CLA	CMD-C2D	-2.00	1.46	1.50
18	3	601	CLA	CMC-C2C	-2.00	1.46	1.50
18	B	833	CLA	CMC-C2C	-2.00	1.46	1.50
18	A	808	CLA	CMB-C2B	-2.00	1.46	1.50

All (1651) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	818	CLA	O2D-CGD-CBD	26.07	157.59	111.27
18	A	818	CLA	O2D-CGD-O1D	-25.32	74.34	123.84
18	A	818	CLA	O1D-CGD-CBD	-20.15	83.25	124.48
19	4	617	XAT	C4-C3-C2	-19.33	73.45	110.77
18	B	836	CLA	C5-C3-C4	-16.75	77.61	114.60
19	4	617	XAT	C38-C25-C26	-15.95	95.53	122.26
24	A	801	CL0	C2B-C1B-NB	14.55	119.98	110.23
18	B	836	CLA	C4-C3-C2	-13.80	82.76	122.65
19	4	617	XAT	C18-C5-C6	-13.43	99.75	122.26
18	B	836	CLA	C5-C3-C2	13.05	160.37	122.65
24	A	801	CL0	C2C-C1C-NC	10.50	119.81	109.97
19	4	617	XAT	C28-C29-C30	10.20	134.59	118.94
24	A	801	CL0	C4A-NA-C1A	-9.99	102.21	106.71
17	4	607	CHL	C2B-C1B-NB	9.71	116.74	110.23
17	4	615	CHL	C2B-C1B-NB	9.69	116.73	110.23
24	A	801	CL0	CHA-C4D-C3D	-9.54	108.95	125.26
17	3	606	CHL	C2B-C1B-NB	9.44	116.56	110.23
17	4	605	CHL	C2B-C1B-NB	9.21	116.41	110.23
17	1	601	CHL	C2B-C1B-NB	9.07	116.31	110.23
17	2	605	CHL	C2B-C1B-NB	9.05	116.30	110.23
17	2	615	CHL	C2B-C1B-NB	8.95	116.23	110.23
17	2	606	CHL	C2B-C1B-NB	8.92	116.21	110.23
17	2	601	CHL	C2B-C1B-NB	8.91	116.20	110.23
17	2	607	CHL	C2B-C1B-NB	8.75	116.10	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	801	CL0	C3D-C2D-C1D	-8.57	98.89	107.08
19	1	614	XAT	O4-C5-C4	8.50	119.77	113.38
19	4	617	XAT	C18-C5-C4	8.40	123.73	114.28
17	2	607	CHL	CMD-C2D-C1D	8.37	139.47	124.71
19	4	617	XAT	O3-C3-C2	-8.31	93.29	109.80
17	4	607	CHL	CMD-C2D-C1D	8.27	139.29	124.71
19	4	617	XAT	C25-C24-C23	-8.25	96.42	112.75
17	3	606	CHL	CMD-C2D-C1D	8.24	139.23	124.71
17	4	605	CHL	CMD-C2D-C1D	8.20	139.17	124.71
17	1	601	CHL	CMD-C2D-C1D	8.18	139.13	124.71
17	2	601	CHL	CMD-C2D-C1D	8.16	139.10	124.71
19	1	614	XAT	C38-C25-C26	-8.16	108.59	122.26
17	2	615	CHL	CMD-C2D-C1D	8.15	139.08	124.71
17	2	605	CHL	CMD-C2D-C1D	8.13	139.04	124.71
17	4	615	CHL	CMD-C2D-C1D	8.12	139.03	124.71
24	A	801	CL0	C3C-C4C-NC	8.12	119.67	110.57
24	A	801	CL0	CMD-C2D-C1D	8.02	138.84	124.71
17	4	606	CHL	CMD-C2D-C1D	8.00	138.82	124.71
17	1	606	CHL	CMD-C2D-C1D	7.97	138.77	124.71
17	1	606	CHL	CHD-C1D-ND	-7.91	117.19	124.45
22	B	843	BCR	C16-C15-C14	7.91	139.67	123.47
17	2	606	CHL	CMD-C2D-C1D	7.88	138.61	124.71
19	4	617	XAT	C39-C29-C28	-7.86	105.69	118.08
19	4	617	XAT	C26-C27-C28	-7.77	109.56	125.99
17	1	606	CHL	C2B-C1B-NB	7.75	115.43	110.23
17	4	606	CHL	C2B-C1B-NB	7.74	115.42	110.23
19	1	614	XAT	O24-C25-C24	7.74	119.19	113.38
22	A	849	BCR	C15-C16-C17	7.73	139.31	123.47
17	4	606	CHL	CHD-C1D-ND	-7.70	117.38	124.45
22	L	301	BCR	C15-C16-C17	7.67	139.19	123.47
22	L	301	BCR	C16-C15-C14	7.65	139.13	123.47
19	1	614	XAT	C18-C5-C6	-7.64	109.45	122.26
19	4	617	XAT	O24-C25-C38	7.58	124.14	115.06
17	2	601	CHL	C2C-C3C-C4C	-7.37	101.24	106.49
18	F	302	CLA	C4A-NA-C1A	7.36	110.02	106.71
19	4	617	XAT	C5-C4-C3	-7.34	98.23	112.75
17	4	615	CHL	C2C-C3C-C4C	-7.33	101.26	106.49
18	1	609	CLA	C4A-NA-C1A	7.30	109.99	106.71
17	2	605	CHL	C2C-C3C-C4C	-7.29	101.08	106.49
17	2	607	CHL	C2C-C3C-C4C	-7.25	101.32	106.49
17	2	606	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
22	A	851	BCR	C16-C15-C14	7.19	138.20	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	614	CLA	C4A-NA-C1A	7.19	109.94	106.71
17	2	615	CHL	C2C-C3C-C4C	-7.15	101.39	106.49
17	2	606	CHL	CHD-C1D-ND	-7.14	117.90	124.45
17	4	607	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
18	A	839	CLA	C4A-NA-C1A	7.10	109.90	106.71
18	B	805	CLA	C4A-NA-C1A	7.05	109.88	106.71
18	A	830	CLA	C4A-NA-C1A	7.05	109.87	106.71
19	4	617	XAT	C11-C10-C9	7.05	137.37	127.31
22	A	851	BCR	C8-C9-C10	7.03	129.73	118.94
18	1	605	CLA	C4A-NA-C1A	7.02	109.86	106.71
18	A	813	CLA	C4A-NA-C1A	7.01	109.86	106.71
24	A	801	CL0	C2D-C1D-ND	7.01	115.27	110.10
18	A	804	CLA	C4A-NA-C1A	6.98	109.84	106.71
19	4	617	XAT	O4-C5-C18	6.97	123.40	115.06
21	2	616	LUT	C15-C35-C34	6.95	137.71	123.47
18	2	609	CLA	C4A-NA-C1A	6.95	109.83	106.71
24	A	801	CL0	C3B-C4B-NB	6.94	116.95	110.52
17	1	606	CHL	C2C-C3C-C4C	-6.91	101.56	106.49
18	4	612	CLA	C4A-NA-C1A	6.91	109.81	106.71
18	2	613	CLA	C4A-NA-C1A	6.90	109.81	106.71
18	A	828	CLA	C4A-NA-C1A	6.89	109.81	106.71
17	1	601	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
18	B	840	CLA	C4A-NA-C1A	6.87	109.79	106.71
17	4	615	CHL	C1B-C2B-C3B	-6.86	100.52	107.03
21	3	613	LUT	C15-C35-C34	6.85	137.51	123.47
17	2	615	CHL	CHD-C1D-ND	-6.85	118.16	124.45
18	B	811	CLA	C4A-NA-C1A	6.83	109.78	106.71
18	L	304	CLA	C4A-NA-C1A	6.83	109.78	106.71
18	A	842	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	B	824	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	B	814	CLA	C4A-NA-C1A	6.80	109.76	106.71
18	A	809	CLA	C4A-NA-C1A	6.80	109.76	106.71
18	A	834	CLA	C4A-NA-C1A	6.80	109.76	106.71
18	A	821	CLA	C4A-NA-C1A	6.79	109.76	106.71
17	2	601	CHL	CHD-C1D-ND	-6.79	118.21	124.45
18	A	808	CLA	C4A-NA-C1A	6.78	109.76	106.71
18	A	835	CLA	C4A-NA-C1A	6.78	109.76	106.71
18	1	604	CLA	C4A-NA-C1A	6.78	109.75	106.71
18	1	612	CLA	C4A-NA-C1A	6.77	109.75	106.71
18	1	607	CLA	C4A-NA-C1A	6.76	109.74	106.71
18	B	812	CLA	C4A-NA-C1A	6.76	109.74	106.71
24	A	801	CL0	CHA-C4D-ND	6.75	130.66	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	827	CLA	C4A-NA-C1A	6.74	109.74	106.71
18	B	829	CLA	C4A-NA-C1A	6.74	109.74	106.71
17	4	606	CHL	C1B-C2B-C3B	-6.73	100.64	107.03
18	1	611	CLA	C4A-NA-C1A	6.73	109.73	106.71
18	A	840	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	A	807	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	B	821	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	4	601	CLA	C4A-NA-C1A	6.71	109.72	106.71
17	4	605	CHL	C2C-C3C-C4C	-6.71	101.51	106.49
18	A	831	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	K	204	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	4	603	CLA	C4A-NA-C1A	6.69	109.72	106.71
18	B	803	CLA	C4A-NA-C1A	6.69	109.71	106.71
17	1	601	CHL	CHD-C1D-ND	-6.68	118.31	124.45
17	2	607	CHL	CHD-C1D-ND	-6.67	118.32	124.45
18	2	608	CLA	C4A-NA-C1A	6.67	109.71	106.71
18	B	831	CLA	C4A-NA-C1A	6.67	109.70	106.71
17	4	605	CHL	CHD-C1D-ND	-6.67	118.33	124.45
18	3	601	CLA	C4A-NA-C1A	6.67	109.70	106.71
18	B	834	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	B	825	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	A	817	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	4	604	CLA	C4A-NA-C1A	6.65	109.70	106.71
18	B	837	CLA	C4A-NA-C1A	6.65	109.69	106.71
18	B	830	CLA	C4A-NA-C1A	6.65	109.69	106.71
19	4	617	XAT	O24-C25-C26	-6.64	53.46	58.96
19	4	617	XAT	O23-C23-C24	-6.64	96.61	109.80
18	A	812	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	B	817	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	3	612	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	A	826	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	G	202	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	B	804	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	1	613	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	B	808	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	B	806	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	B	832	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	3	609	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	A	818	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	H	201	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	A	850	BCR	C16-C15-C14	6.60	137.00	123.47
18	B	819	CLA	C4A-NA-C1A	6.60	109.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	807	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	B	820	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	A	837	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	B	809	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	2	611	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	B	813	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	B	815	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	K	203	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	B	828	CLA	C4A-NA-C1A	6.57	109.66	106.71
18	3	602	CLA	C4A-NA-C1A	6.56	109.66	106.71
18	3	605	CLA	C4A-NA-C1A	6.56	109.66	106.71
18	A	843	CLA	C4A-NA-C1A	6.55	109.65	106.71
18	A	824	CLA	C4A-NA-C1A	6.55	109.65	106.71
18	B	838	CLA	C4A-NA-C1A	6.55	109.65	106.71
18	A	816	CLA	C4A-NA-C1A	6.53	109.64	106.71
18	K	201	CLA	C4A-NA-C1A	6.53	109.64	106.71
18	B	818	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	A	820	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	F	301	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	G	201	CLA	C4A-NA-C1A	6.52	109.64	106.71
18	3	604	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	A	805	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	A	811	CLA	C4A-NA-C1A	6.51	109.63	106.71
18	A	827	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	2	603	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	A	833	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	2	612	CLA	C4A-NA-C1A	6.50	109.63	106.71
18	G	203	CLA	C4A-NA-C1A	6.49	109.63	106.71
18	1	608	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	F	303	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	4	611	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	A	806	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	L	303	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	B	826	CLA	C4A-NA-C1A	6.47	109.62	106.71
18	A	822	CLA	C4A-NA-C1A	6.47	109.61	106.71
18	4	610	CLA	C4A-NA-C1A	6.46	109.61	106.71
18	A	819	CLA	C4A-NA-C1A	6.46	109.61	106.71
17	2	605	CHL	CHD-C1D-ND	-6.45	118.53	124.45
18	A	815	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	1	603	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	L	302	CLA	C4A-NA-C1A	6.43	109.60	106.71
18	B	833	CLA	C4A-NA-C1A	6.43	109.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	835	CLA	C4A-NA-C1A	6.42	109.59	106.71
17	4	615	CHL	CHD-C1D-ND	-6.41	118.56	124.45
18	A	836	CLA	C4A-NA-C1A	6.41	109.59	106.71
17	3	606	CHL	CHD-C1D-ND	-6.41	118.56	124.45
18	4	609	CLA	C4A-NA-C1A	6.40	109.58	106.71
18	A	823	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	2	602	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	B	810	CLA	C4A-NA-C1A	6.38	109.58	106.71
18	1	610	CLA	C4A-NA-C1A	6.38	109.58	106.71
18	A	841	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	2	604	CLA	C4A-NA-C1A	6.36	109.56	106.71
18	3	611	CLA	C4A-NA-C1A	6.36	109.56	106.71
18	A	838	CLA	C4A-NA-C1A	6.35	109.56	106.71
18	3	610	CLA	C4A-NA-C1A	6.34	109.56	106.71
18	A	832	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	4	617	XAT	C15-C14-C13	6.34	136.36	127.31
18	B	836	CLA	C4A-NA-C1A	6.33	109.55	106.71
18	4	602	CLA	C4A-NA-C1A	6.32	109.55	106.71
19	2	617	XAT	C35-C15-C14	6.32	136.41	123.47
18	A	829	CLA	C4A-NA-C1A	6.32	109.55	106.71
18	A	802	CLA	C4A-NA-C1A	6.29	109.53	106.71
18	A	825	CLA	C4A-NA-C1A	6.28	109.53	106.71
18	4	613	CLA	C4A-NA-C1A	6.27	109.53	106.71
18	B	822	CLA	C4A-NA-C1A	6.27	109.52	106.71
18	B	841	CLA	C4A-NA-C1A	6.27	109.52	106.71
18	B	816	CLA	C4A-NA-C1A	6.26	109.52	106.71
19	4	617	XAT	C37-C21-C36	-6.26	98.14	107.37
18	4	608	CLA	C4A-NA-C1A	6.26	109.52	106.71
18	B	839	CLA	C4A-NA-C1A	6.25	109.51	106.71
18	3	607	CLA	C4A-NA-C1A	6.24	109.51	106.71
24	A	801	CL0	C3B-C2B-C1B	-6.20	99.67	107.16
18	B	823	CLA	C4A-NA-C1A	6.20	109.49	106.71
17	4	607	CHL	CHD-C1D-ND	-6.18	118.77	124.45
18	A	810	CLA	C4A-NA-C1A	6.17	109.48	106.71
22	A	850	BCR	C15-C16-C17	6.15	136.07	123.47
19	1	614	XAT	O4-C5-C18	6.15	122.42	115.06
22	F	304	BCR	C24-C23-C22	6.14	135.52	126.23
18	A	814	CLA	C4A-NA-C1A	6.13	109.46	106.71
18	A	844	CLA	C4A-NA-C1A	6.13	109.46	106.71
24	A	801	CL0	CHD-C4C-C3C	-6.06	115.93	124.84
19	4	617	XAT	O23-C23-C22	-6.05	97.77	109.80
18	1	602	CLA	C4A-NA-C1A	6.05	109.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	608	CLA	C4A-NA-C1A	6.03	109.42	106.71
17	4	606	CHL	CHB-C1B-NB	-6.02	117.88	124.26
18	3	603	CLA	C4A-NA-C1A	6.02	109.41	106.71
19	4	617	XAT	O3-C3-C4	-5.95	97.97	109.80
17	1	606	CHL	CHB-C1B-NB	-5.94	117.97	124.26
18	B	802	CLA	C4A-NA-C1A	5.87	109.35	106.71
22	F	304	BCR	C15-C16-C17	5.87	135.50	123.47
19	2	617	XAT	C15-C35-C34	5.83	135.42	123.47
19	1	614	XAT	C35-C34-C33	-5.76	119.09	127.31
21	2	619	LUT	C15-C35-C34	5.74	135.24	123.47
24	A	801	CL0	CHD-C1D-ND	-5.64	119.27	124.45
17	4	605	CHL	C3B-C2B-C1B	-5.53	100.49	107.16
17	4	615	CHL	C3B-C4B-NB	5.50	113.92	110.23
22	B	845	BCR	C19-C18-C17	5.49	127.36	118.94
17	2	606	CHL	C3B-C2B-C1B	-5.45	100.58	107.16
19	4	617	XAT	C40-C33-C34	-5.44	115.31	122.92
17	2	605	CHL	C3B-C2B-C1B	-5.38	100.66	107.16
17	2	615	CHL	C3B-C2B-C1B	-5.38	100.67	107.16
22	K	202	BCR	C16-C15-C14	5.38	134.49	123.47
22	A	851	BCR	C34-C9-C10	-5.37	115.40	122.92
17	2	615	CHL	CHB-C1B-NB	-5.34	118.61	124.26
17	3	606	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
17	2	601	CHL	C3B-C2B-C1B	-5.31	100.76	107.16
17	1	606	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
17	1	601	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
17	2	606	CHL	O2D-CGD-CBD	5.26	120.62	111.27
17	4	607	CHL	C3B-C2B-C1B	-5.18	100.91	107.16
21	1	616	LUT	C15-C35-C34	5.18	134.07	123.47
17	2	607	CHL	C3B-C2B-C1B	-5.16	100.93	107.16
18	A	803	CLA	C4A-NA-C1A	5.14	109.02	106.71
22	J	102	BCR	C16-C15-C14	5.14	134.00	123.47
22	A	851	BCR	C7-C8-C9	-5.10	118.53	126.23
19	1	614	XAT	O24-C25-C38	5.09	121.15	115.06
17	2	601	CHL	O2D-CGD-CBD	5.09	120.30	111.27
22	K	205	BCR	C15-C16-C17	5.07	133.85	123.47
17	2	606	CHL	CHB-C1B-NB	-5.06	118.91	124.26
17	2	605	CHL	O2D-CGD-CBD	5.04	120.23	111.27
22	B	849	BCR	C30-C25-C26	-5.01	115.56	122.61
17	4	605	CHL	CHB-C1B-NB	-5.00	118.97	124.26
24	A	801	CL0	C1C-C2C-C3C	-4.99	101.71	106.96
24	A	801	CL0	C4D-CHA-C1A	-4.97	114.64	126.62
17	2	615	CHL	O2D-CGD-CBD	4.97	120.10	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	853	BCR	C16-C15-C14	4.94	133.59	123.47
17	4	607	CHL	C3C-C4C-NC	4.92	116.09	110.57
22	A	851	BCR	C23-C22-C21	4.92	126.49	118.94
22	B	846	BCR	C16-C15-C14	4.91	133.53	123.47
17	3	606	CHL	O2D-CGD-CBD	4.91	119.99	111.27
19	1	614	XAT	C26-C27-C28	-4.89	115.66	125.99
24	A	801	CL0	C1D-CHD-C4C	-4.88	115.53	126.06
17	4	615	CHL	C3C-C4C-NC	4.85	116.01	110.57
17	2	605	CHL	C3C-C4C-NC	4.84	115.86	110.57
17	1	606	CHL	C4A-NA-C1A	4.80	108.86	106.71
22	L	306	BCR	C8-C9-C10	4.78	126.27	118.94
22	B	847	BCR	C16-C15-C14	4.77	133.24	123.47
21	1	616	LUT	C30-C31-C32	4.77	138.09	123.22
22	4	618	BCR	C16-C15-C14	4.76	133.22	123.47
17	2	607	CHL	C3C-C4C-NC	4.75	115.89	110.57
17	4	606	CHL	O2D-CGD-CBD	4.74	119.69	111.27
19	1	614	XAT	C6-C7-C8	-4.70	116.05	125.99
17	2	605	CHL	CHB-C1B-NB	-4.69	119.29	124.26
22	L	306	BCR	C34-C9-C10	-4.67	116.38	122.92
19	4	617	XAT	C38-C25-C24	4.67	119.53	114.28
22	K	202	BCR	C15-C16-C17	4.67	133.04	123.47
17	3	606	CHL	C3C-C4C-NC	4.66	115.79	110.57
17	4	607	CHL	C3D-C2D-C1D	-4.66	99.48	105.83
22	L	306	BCR	C37-C22-C21	-4.65	116.41	122.92
22	B	845	BCR	C36-C18-C17	-4.65	116.42	122.92
22	A	851	BCR	C37-C22-C21	-4.64	116.42	122.92
21	3	613	LUT	C39-C29-C30	-4.63	116.44	122.92
19	4	617	XAT	C32-C33-C34	4.62	126.03	118.94
17	2	601	CHL	C3C-C4C-NC	4.62	115.75	110.57
17	2	607	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
22	A	851	BCR	C11-C10-C9	4.60	133.87	127.31
17	2	601	CHL	CHB-C1B-NB	-4.58	119.40	124.26
17	2	607	CHL	O2D-CGD-CBD	4.55	119.36	111.27
21	2	616	LUT	C7-C8-C9	4.55	133.12	126.23
22	A	852	BCR	C23-C22-C21	4.53	125.89	118.94
21	2	616	LUT	C39-C29-C30	-4.53	116.58	122.92
22	A	852	BCR	C37-C22-C21	-4.53	116.58	122.92
22	B	801	BCR	C16-C15-C14	4.53	132.75	123.47
19	4	617	XAT	C35-C34-C33	4.52	133.77	127.31
17	4	605	CHL	C3C-C4C-NC	4.51	115.50	110.57
18	A	804	CLA	CAA-C2A-C3A	-4.51	100.42	112.78
17	4	606	CHL	C4A-NA-C1A	4.51	108.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	605	CHL	C3D-C2D-C1D	-4.50	99.68	105.83
18	4	613	CLA	CAA-C2A-C3A	-4.49	100.49	112.78
17	4	615	CHL	C3D-C2D-C1D	-4.48	99.72	105.83
17	4	607	CHL	O2D-CGD-CBD	4.48	119.22	111.27
21	2	619	LUT	C19-C9-C10	-4.46	116.67	122.92
17	2	601	CHL	C3D-C2D-C1D	-4.45	99.76	105.83
22	J	102	BCR	C34-C9-C10	-4.45	116.69	122.92
22	A	852	BCR	C16-C15-C14	4.45	132.59	123.47
22	L	301	BCR	C37-C22-C21	-4.44	116.70	122.92
17	3	606	CHL	CHB-C1B-NB	-4.42	119.57	124.26
17	3	606	CHL	C2C-C1C-NC	4.42	114.11	109.97
22	K	202	BCR	C37-C22-C21	-4.40	116.76	122.92
17	3	606	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
17	1	601	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
17	2	615	CHL	C3C-C4C-NC	4.38	115.49	110.57
22	B	844	BCR	C37-C22-C21	-4.38	116.79	122.92
21	2	616	LUT	C19-C9-C10	-4.37	116.80	122.92
22	B	843	BCR	C34-C9-C10	-4.37	116.81	122.92
17	2	615	CHL	C3D-C2D-C1D	-4.36	99.87	105.83
17	4	605	CHL	C3D-C2D-C1D	-4.36	99.88	105.83
17	2	606	CHL	C3C-C4C-NC	4.34	115.44	110.57
22	K	205	BCR	C37-C22-C21	-4.33	116.85	122.92
17	1	601	CHL	C3C-C4C-NC	4.33	115.43	110.57
22	B	844	BCR	C21-C20-C19	4.33	136.72	123.22
22	B	801	BCR	C8-C9-C10	4.32	125.57	118.94
19	2	617	XAT	C39-C29-C30	-4.32	116.87	122.92
22	B	846	BCR	C34-C9-C10	-4.32	116.88	122.92
22	G	204	BCR	C15-C16-C17	4.32	132.31	123.47
17	2	606	CHL	C3D-C2D-C1D	-4.31	99.95	105.83
22	K	205	BCR	C34-C9-C10	-4.30	116.90	122.92
21	1	616	LUT	C19-C9-C10	-4.30	116.90	122.92
22	A	849	BCR	C30-C25-C26	-4.28	116.58	122.61
22	L	306	BCR	C23-C22-C21	4.26	125.48	118.94
22	B	844	BCR	C15-C16-C17	4.26	132.20	123.47
19	4	617	XAT	O4-C5-C6	-4.26	55.43	58.96
22	F	304	BCR	C34-C9-C10	-4.26	116.96	122.92
27	B	850	DGD	O2G-C1B-C2B	4.24	120.64	111.50
21	1	616	LUT	C32-C33-C34	4.24	125.45	118.94
22	A	850	BCR	C34-C9-C10	-4.24	116.99	122.92
21	1	616	LUT	C39-C29-C28	4.23	124.75	118.08
17	4	606	CHL	C3D-C2D-C1D	-4.21	100.08	105.83
19	2	617	XAT	C28-C29-C30	4.21	125.40	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L	305	BCR	C37-C22-C21	-4.21	117.03	122.92
22	B	844	BCR	C23-C22-C21	4.21	125.40	118.94
17	1	606	CHL	C3D-C2D-C1D	-4.21	100.09	105.83
22	A	848	BCR	C15-C16-C17	4.21	132.09	123.47
17	4	607	CHL	CHD-C4C-C3C	-4.21	118.66	124.84
22	B	844	BCR	C34-C9-C10	-4.20	117.03	122.92
22	G	204	BCR	C37-C22-C21	-4.19	117.06	122.92
22	3	614	BCR	C34-C9-C10	-4.18	117.07	122.92
21	3	613	LUT	C28-C29-C30	4.17	125.35	118.94
22	K	202	BCR	C34-C9-C10	-4.17	117.08	122.92
17	4	615	CHL	CHB-C1B-NB	-4.17	119.85	124.26
22	L	301	BCR	C12-C13-C14	4.16	125.32	118.94
21	2	619	LUT	C39-C29-C30	-4.15	117.10	122.92
22	L	305	BCR	C16-C15-C14	4.13	131.94	123.47
22	G	204	BCR	C34-C9-C10	-4.13	117.14	122.92
19	2	617	XAT	C19-C9-C10	-4.12	117.15	122.92
22	J	102	BCR	C37-C22-C21	-4.12	117.15	122.92
22	L	301	BCR	C36-C18-C17	-4.12	117.15	122.92
22	4	618	BCR	C37-C22-C21	-4.11	117.17	122.92
17	1	601	CHL	CHB-C1B-NB	-4.10	119.91	124.26
22	L	306	BCR	C16-C15-C14	4.10	131.87	123.47
22	B	845	BCR	C1-C6-C5	-4.09	116.85	122.61
22	A	848	BCR	C37-C22-C21	-4.08	117.20	122.92
22	L	301	BCR	C34-C9-C10	-4.08	117.20	122.92
17	4	607	CHL	C2D-C1D-ND	4.08	113.11	110.10
22	A	848	BCR	C34-C9-C10	-4.08	117.21	122.92
22	B	847	BCR	C34-C9-C10	-4.08	117.21	122.92
22	K	205	BCR	C19-C18-C17	4.07	125.19	118.94
22	B	849	BCR	C1-C6-C5	-4.06	116.89	122.61
22	B	844	BCR	C16-C15-C14	4.06	131.80	123.47
22	A	853	BCR	C37-C22-C21	-4.06	117.23	122.92
22	I	101	BCR	C34-C9-C10	-4.06	117.24	122.92
22	I	101	BCR	C15-C16-C17	4.05	131.77	123.47
22	F	304	BCR	C16-C15-C14	4.04	131.75	123.47
22	B	845	BCR	C34-C9-C10	-4.04	117.26	122.92
22	B	801	BCR	C37-C22-C21	-4.03	117.28	122.92
22	K	202	BCR	C12-C13-C14	4.02	125.12	118.94
21	1	616	LUT	C40-C33-C34	-4.02	117.29	122.92
22	F	304	BCR	C12-C13-C14	4.01	125.09	118.94
22	A	849	BCR	C21-C20-C19	4.00	135.72	123.22
19	1	614	XAT	C38-C25-C24	3.99	118.77	114.28
22	L	301	BCR	C35-C13-C14	-3.98	117.34	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	616	LUT	C15-C35-C34	3.98	131.63	123.47
22	B	848	BCR	C15-C16-C17	3.98	131.63	123.47
21	2	616	LUT	C28-C29-C30	3.98	125.05	118.94
22	A	849	BCR	C34-C9-C10	-3.98	117.35	122.92
22	K	205	BCR	C36-C18-C17	-3.97	117.36	122.92
22	I	101	BCR	C37-C22-C21	-3.97	117.36	122.92
22	L	305	BCR	C34-C9-C10	-3.97	117.36	122.92
22	B	843	BCR	C37-C22-C21	-3.96	117.38	122.92
22	A	852	BCR	C19-C18-C17	3.95	125.00	118.94
22	B	844	BCR	C36-C18-C17	-3.94	117.40	122.92
22	B	849	BCR	C34-C9-C10	-3.94	117.40	122.92
22	A	850	BCR	C37-C22-C21	-3.93	117.42	122.92
22	A	851	BCR	C12-C13-C14	3.93	124.97	118.94
21	1	616	LUT	C31-C30-C29	3.93	132.91	127.31
17	4	607	CHL	CAC-C3C-C4C	3.93	129.90	124.81
17	4	607	CHL	C3B-C4B-NB	3.93	114.16	110.52
22	B	849	BCR	C16-C15-C14	3.92	131.51	123.47
21	4	616	LUT	C19-C9-C10	-3.92	117.43	122.92
22	B	847	BCR	C37-C22-C21	-3.92	117.43	122.92
22	A	852	BCR	C35-C13-C14	-3.92	117.44	122.92
21	1	616	LUT	C1-C6-C5	-3.91	117.10	122.61
22	B	845	BCR	C20-C21-C22	3.91	132.89	127.31
22	4	618	BCR	C34-C9-C10	-3.90	117.45	122.92
22	K	202	BCR	C35-C13-C14	-3.90	117.45	122.92
22	B	848	BCR	C34-C9-C10	-3.90	117.46	122.92
17	2	607	CHL	CHB-C1B-NB	-3.90	120.13	124.26
22	3	614	BCR	C37-C22-C21	-3.89	117.47	122.92
22	B	848	BCR	C37-C22-C21	-3.89	117.48	122.92
18	A	830	CLA	CAA-C2A-C3A	-3.88	102.16	112.78
17	3	606	CHL	C4C-C3C-C2C	-3.87	101.25	106.90
21	2	619	LUT	C32-C33-C34	3.87	124.88	118.94
22	B	846	BCR	C37-C22-C21	-3.87	117.50	122.92
20	1	615	LHG	O7-C7-C8	3.87	119.84	111.50
17	4	615	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
21	4	616	LUT	C39-C29-C30	-3.87	117.51	122.92
22	J	102	BCR	C8-C9-C10	3.86	124.86	118.94
22	B	843	BCR	C8-C9-C10	3.85	124.85	118.94
22	F	304	BCR	C35-C13-C14	-3.85	117.53	122.92
22	L	306	BCR	C12-C13-C14	3.85	124.85	118.94
17	4	606	CHL	C4C-C3C-C2C	-3.85	101.29	106.90
21	2	619	LUT	C40-C33-C34	-3.84	117.54	122.92
22	L	306	BCR	C35-C13-C14	-3.84	117.55	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	852	BCR	C36-C18-C17	-3.84	117.55	122.92
22	A	852	BCR	C34-C9-C10	-3.83	117.55	122.92
22	L	306	BCR	C15-C16-C17	3.83	131.32	123.47
17	4	607	CHL	C1D-ND-C4D	-3.83	103.61	106.33
22	A	852	BCR	C10-C11-C12	3.81	135.09	123.22
19	4	617	XAT	C12-C13-C14	3.80	124.77	118.94
22	J	102	BCR	C35-C13-C14	-3.79	117.61	122.92
22	F	304	BCR	C20-C21-C22	3.79	132.72	127.31
22	J	102	BCR	C12-C13-C14	3.78	124.75	118.94
17	4	606	CHL	C3B-C4B-NB	3.78	112.77	110.23
22	B	849	BCR	C37-C22-C21	-3.78	117.62	122.92
22	B	845	BCR	C12-C13-C14	3.77	124.72	118.94
22	B	849	BCR	C15-C16-C17	3.77	131.19	123.47
22	L	301	BCR	C21-C20-C19	3.76	134.97	123.22
17	4	606	CHL	C3C-C4C-NC	3.75	114.77	110.57
22	A	853	BCR	C35-C13-C14	-3.74	117.68	122.92
17	2	607	CHL	CHD-C4C-C3C	-3.74	119.35	124.84
22	A	853	BCR	C12-C13-C14	3.72	124.65	118.94
22	B	844	BCR	C30-C25-C26	-3.71	117.38	122.61
17	1	606	CHL	CAC-C3C-C4C	3.71	129.62	124.81
22	B	801	BCR	C7-C8-C9	-3.70	120.64	126.23
22	4	618	BCR	C30-C25-C26	-3.69	117.41	122.61
22	3	614	BCR	C16-C15-C14	3.69	131.04	123.47
22	K	202	BCR	C19-C18-C17	3.69	124.61	118.94
22	B	801	BCR	C10-C11-C12	3.69	134.74	123.22
22	L	305	BCR	C36-C18-C17	-3.69	117.76	122.92
22	K	202	BCR	C36-C18-C17	-3.68	117.77	122.92
17	2	601	CHL	CAC-C3C-C4C	3.67	129.58	124.81
17	4	606	CHL	CAC-C3C-C4C	3.67	129.57	124.81
22	L	305	BCR	C15-C16-C17	3.66	130.98	123.47
18	B	813	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
18	L	303	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
22	B	845	BCR	C35-C13-C14	-3.66	117.80	122.92
22	B	846	BCR	C35-C13-C14	-3.66	117.80	122.92
22	F	304	BCR	C10-C11-C12	3.64	134.57	123.22
17	3	606	CHL	CAC-C3C-C4C	3.63	129.53	124.81
24	A	801	CL0	C4C-C3C-C2C	-3.63	101.61	106.90
22	A	853	BCR	C11-C10-C9	3.62	132.48	127.31
22	A	853	BCR	C10-C11-C12	3.61	134.48	123.22
22	L	306	BCR	C7-C8-C9	3.61	131.68	126.23
17	4	615	CHL	C2D-C1D-ND	3.61	112.76	110.10
17	1	606	CHL	C3C-C4C-NC	3.61	114.61	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	304	BCR	C21-C20-C19	3.60	134.46	123.22
22	B	846	BCR	C12-C13-C14	3.58	124.43	118.94
21	1	616	LUT	C20-C13-C14	-3.57	117.92	122.92
22	B	801	BCR	C35-C13-C14	-3.57	117.93	122.92
18	A	803	CLA	C3B-C4B-NB	-3.56	107.21	110.52
22	L	301	BCR	C19-C18-C17	3.56	124.40	118.94
17	3	606	CHL	CHD-C4C-C3C	-3.55	119.61	124.84
18	4	604	CLA	C3B-C4B-NB	-3.55	107.85	110.23
22	L	305	BCR	C19-C18-C17	3.55	124.38	118.94
18	1	613	CLA	C3B-C4B-NB	-3.54	107.86	110.23
17	1	601	CHL	C1-C2-C3	-3.54	119.93	126.04
22	L	306	BCR	C36-C18-C17	-3.53	117.97	122.92
17	2	606	CHL	CAC-C3C-C4C	3.53	129.39	124.81
17	3	606	CHL	C3B-C4B-NB	3.52	113.78	110.52
17	2	607	CHL	CAC-C3C-C4C	3.52	129.38	124.81
18	1	604	CLA	CAA-C2A-C3A	-3.52	103.15	112.78
24	A	801	CL0	CHB-C1B-NB	-3.52	120.53	124.26
21	2	619	LUT	C8-C9-C10	3.52	124.33	118.94
19	2	617	XAT	C32-C33-C34	3.51	124.33	118.94
19	1	614	XAT	C31-C30-C29	-3.51	122.30	127.31
17	1	601	CHL	CAC-C3C-C4C	3.51	129.37	124.81
22	L	305	BCR	C35-C13-C14	-3.51	118.01	122.92
17	2	605	CHL	CHD-C4C-C3C	-3.51	119.50	124.98
17	1	606	CHL	CHC-C4B-NB	-3.51	120.55	124.26
22	L	301	BCR	C23-C22-C21	3.51	124.32	118.94
21	1	616	LUT	C39-C29-C30	-3.50	118.02	122.92
18	B	836	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
18	1	610	CLA	C3B-C4B-NB	-3.49	107.89	110.23
18	A	813	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
21	1	616	LUT	C12-C13-C14	3.48	124.29	118.94
22	B	847	BCR	C35-C13-C14	-3.48	118.04	122.92
18	B	811	CLA	C3B-C4B-NB	-3.47	107.90	110.23
17	2	601	CHL	CHD-C4C-C3C	-3.46	119.75	124.84
21	3	613	LUT	C19-C9-C10	-3.46	118.08	122.92
19	4	617	XAT	O24-C25-C24	3.46	115.98	113.38
18	B	805	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
18	2	610	CLA	C3B-C4B-NB	-3.45	107.92	110.23
18	A	835	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
22	G	204	BCR	C30-C25-C26	-3.45	117.75	122.61
24	A	801	CL0	CHC-C1C-C2C	-3.45	117.15	126.73
22	4	618	BCR	C35-C13-C14	-3.44	118.10	122.92
22	B	849	BCR	C36-C18-C17	-3.44	118.11	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	606	CHL	C2C-C1C-NC	3.42	113.18	109.97
17	4	607	CHL	C3D-C4D-ND	3.42	115.76	110.24
22	A	848	BCR	C36-C18-C17	-3.41	118.14	122.92
18	A	804	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
17	1	601	CHL	CHD-C4C-C3C	-3.41	119.82	124.84
22	B	849	BCR	C35-C13-C14	-3.41	118.15	122.92
22	K	205	BCR	C10-C11-C12	3.41	133.85	123.22
22	A	849	BCR	C20-C21-C22	3.41	132.17	127.31
18	B	837	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
17	1	601	CHL	C6-C5-C3	-3.40	109.06	114.62
22	L	306	BCR	C10-C11-C12	3.40	133.82	123.22
22	B	801	BCR	C12-C13-C14	3.40	124.15	118.94
19	1	614	XAT	C35-C15-C14	-3.39	116.53	123.47
22	K	205	BCR	C35-C13-C14	-3.39	118.17	122.92
22	G	204	BCR	C36-C18-C17	-3.39	118.18	122.92
22	B	846	BCR	C8-C9-C10	3.39	124.14	118.94
22	B	844	BCR	C35-C13-C14	-3.37	118.20	122.92
22	B	845	BCR	C16-C17-C18	3.36	132.10	127.31
22	L	306	BCR	C19-C18-C17	3.36	124.10	118.94
17	2	607	CHL	C2D-C1D-ND	3.36	112.58	110.10
18	B	825	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
17	1	601	CHL	C3D-C4D-ND	3.35	115.66	110.24
18	A	809	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
18	A	828	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
17	2	605	CHL	C2D-C1D-ND	3.34	112.57	110.10
18	4	614	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
18	1	608	CLA	C3B-C4B-NB	-3.33	108.00	110.23
17	2	615	CHL	CAC-C3C-C4C	3.33	129.13	124.81
17	4	615	CHL	C3D-C4D-ND	3.33	115.63	110.24
18	3	605	CLA	C3B-C4B-NB	-3.33	108.00	110.23
18	A	844	CLA	C3B-C4B-NB	-3.33	107.43	110.52
18	L	302	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
17	4	605	CHL	CHD-C4C-C3C	-3.32	119.79	124.98
22	3	614	BCR	C35-C13-C14	-3.32	118.27	122.92
22	3	614	BCR	C15-C16-C17	3.32	130.28	123.47
18	A	815	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
22	L	305	BCR	C12-C13-C14	3.32	124.03	118.94
18	B	818	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
18	2	604	CLA	C3B-C4B-NB	-3.32	107.44	110.52
22	B	847	BCR	C12-C13-C14	3.31	124.03	118.94
18	A	819	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
18	B	820	CLA	O2D-CGD-O1D	-3.31	117.36	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	838	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
22	F	304	BCR	C8-C9-C10	3.30	124.01	118.94
22	K	202	BCR	C23-C22-C21	3.30	124.01	118.94
17	2	601	CHL	C3D-C4D-ND	3.30	115.58	110.24
22	B	801	BCR	C34-C9-C10	-3.30	118.30	122.92
22	A	853	BCR	C36-C18-C17	-3.29	118.32	122.92
18	A	831	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
18	A	840	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
17	3	606	CHL	C2D-C1D-ND	3.28	112.52	110.10
22	A	851	BCR	C36-C18-C17	-3.28	118.33	122.92
22	A	851	BCR	C35-C13-C14	-3.27	118.34	122.92
18	3	605	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
21	4	616	LUT	C40-C33-C34	-3.27	118.34	122.92
22	A	852	BCR	C21-C20-C19	3.26	133.40	123.22
17	2	607	CHL	C1-C2-C3	-3.26	121.47	126.75
22	4	618	BCR	C12-C13-C14	3.26	123.94	118.94
18	4	603	CLA	C3B-C4B-NB	-3.26	108.05	110.23
22	I	101	BCR	C36-C18-C17	-3.26	118.36	122.92
18	A	832	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
22	B	849	BCR	C19-C18-C17	3.25	123.93	118.94
22	F	304	BCR	C37-C22-C21	-3.25	118.37	122.92
22	K	205	BCR	C23-C22-C21	3.25	123.93	118.94
22	A	852	BCR	C1-C6-C5	-3.25	118.04	122.61
22	3	614	BCR	C36-C18-C17	-3.25	118.37	122.92
21	2	616	LUT	C35-C34-C33	3.25	131.94	127.31
18	B	833	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
18	A	820	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
17	4	615	CHL	C1D-ND-C4D	-3.24	104.03	106.33
18	B	807	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
18	B	827	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
18	4	601	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
18	B	821	CLA	CAA-C2A-C3A	-3.23	103.95	112.78
17	2	607	CHL	C3D-C4D-ND	3.23	115.45	110.24
18	B	808	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
18	B	841	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
17	4	605	CHL	C2D-C1D-ND	3.22	112.48	110.10
21	2	616	LUT	C20-C13-C14	-3.22	118.42	122.92
17	2	606	CHL	C3D-C4D-ND	3.21	115.44	110.24
22	A	852	BCR	C15-C16-C17	3.21	130.05	123.47
22	A	851	BCR	C15-C16-C17	3.21	130.05	123.47
22	B	843	BCR	C15-C14-C13	3.21	131.89	127.31
22	B	844	BCR	C8-C9-C10	3.21	123.86	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	801	CL0	C1-C2-C3	-3.20	120.50	126.04
22	B	848	BCR	C36-C18-C17	-3.20	118.44	122.92
18	4	602	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
18	B	802	CLA	C3B-C4B-NB	-3.19	107.55	110.52
21	1	616	LUT	C8-C9-C10	3.19	123.84	118.94
17	2	615	CHL	CHD-C4C-C3C	-3.19	120.16	124.84
22	A	850	BCR	C15-C14-C13	3.18	131.85	127.31
22	A	848	BCR	C35-C13-C14	-3.18	118.47	122.92
22	B	801	BCR	C36-C18-C17	-3.18	118.47	122.92
17	4	615	CHL	CAC-C3C-C4C	3.18	128.93	124.81
18	1	612	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
18	B	819	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
21	1	616	LUT	C35-C15-C14	3.17	129.97	123.47
21	2	616	LUT	C30-C31-C32	3.17	133.11	123.22
18	A	806	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
18	4	613	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
22	K	202	BCR	C8-C9-C10	3.17	123.80	118.94
17	2	601	CHL	C3B-C4B-NB	3.16	113.45	110.52
17	4	605	CHL	C3D-C4D-ND	3.16	115.36	110.24
18	B	818	CLA	C1-C2-C3	-3.16	120.58	126.04
21	2	616	LUT	C19-C9-C8	3.16	123.06	118.08
22	A	848	BCR	C19-C18-C17	3.16	123.79	118.94
22	A	849	BCR	C37-C22-C21	-3.16	118.50	122.92
17	3	606	CHL	C3D-C4D-ND	3.15	115.33	110.24
18	B	838	CLA	C3B-C4B-NB	-3.15	107.59	110.52
18	B	822	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
18	B	832	CLA	C3B-C4B-NB	-3.15	107.59	110.52
18	A	814	CLA	C3B-C4B-NB	-3.14	107.60	110.52
22	A	848	BCR	C16-C15-C14	3.14	129.91	123.47
22	4	618	BCR	C36-C18-C17	-3.14	118.53	122.92
22	G	204	BCR	C19-C18-C17	3.14	123.75	118.94
18	A	826	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
18	A	814	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
22	B	849	BCR	C12-C13-C14	3.13	123.75	118.94
18	2	613	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
18	3	607	CLA	C3B-C4B-NB	-3.12	107.62	110.52
18	B	816	CLA	C3B-C4B-NB	-3.12	107.62	110.52
17	1	601	CHL	C2D-C1D-ND	3.12	112.41	110.10
22	A	850	BCR	C16-C17-C18	3.12	131.77	127.31
18	A	837	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
17	2	601	CHL	C2D-C1D-ND	3.12	112.40	110.10
18	B	829	CLA	O2D-CGD-O1D	-3.12	117.75	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	812	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
18	B	808	CLA	C3B-C4B-NB	-3.10	107.64	110.52
18	A	811	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
19	1	614	XAT	C15-C14-C13	-3.10	122.89	127.31
18	B	840	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
18	A	842	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
18	4	612	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
18	A	833	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
18	A	817	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
18	B	816	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
22	J	102	BCR	C36-C18-C17	-3.09	118.60	122.92
18	B	810	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
24	A	801	CL0	O2A-CGA-CBA	3.08	121.58	111.91
21	3	613	LUT	C20-C13-C14	-3.08	118.61	122.92
18	A	805	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
17	4	606	CHL	C3D-C4D-ND	3.08	115.22	110.24
19	2	617	XAT	C40-C33-C34	-3.08	118.61	122.92
18	B	817	CLA	C3B-C4B-NB	-3.08	107.66	110.52
18	B	811	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
18	A	829	CLA	C3B-C4B-NB	-3.08	107.66	110.52
17	2	605	CHL	C3D-C4D-ND	3.07	115.20	110.24
22	G	204	BCR	C35-C13-C14	-3.07	118.62	122.92
18	A	808	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
18	3	608	CLA	CAA-C2A-C3A	-3.06	108.95	116.10
18	B	839	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
18	A	819	CLA	C3B-C4B-NB	-3.06	107.67	110.52
21	3	613	LUT	C8-C9-C10	3.06	123.64	118.94
18	A	802	CLA	C3B-C4B-NB	-3.06	107.67	110.52
18	A	834	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
17	2	607	CHL	C3B-C4B-NB	3.05	113.34	110.52
17	2	606	CHL	CHD-C4C-C3C	-3.05	120.36	124.84
17	2	615	CHL	C3D-C4D-ND	3.05	115.17	110.24
19	2	617	XAT	C20-C13-C14	-3.05	118.65	122.92
18	A	821	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
22	B	844	BCR	C12-C13-C14	3.05	123.62	118.94
17	2	615	CHL	CHC-C4B-NB	-3.04	121.03	124.26
22	B	846	BCR	C36-C18-C17	-3.04	118.66	122.92
18	A	802	CLA	CHB-C4A-NA	3.04	128.72	124.51
17	4	605	CHL	C3B-C4B-NB	3.04	113.34	110.52
22	I	101	BCR	C35-C13-C14	-3.04	118.67	122.92
18	A	804	CLA	CHB-C4A-NA	3.04	128.72	124.51
22	A	852	BCR	C12-C13-C14	3.04	123.60	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	815	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
18	B	802	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
18	B	814	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
18	B	828	CLA	C3B-C4B-NB	-3.03	107.71	110.52
24	A	801	CL0	CAC-C3C-C4C	3.03	128.74	124.81
18	B	836	CLA	C3B-C4B-NB	-3.03	107.71	110.52
18	B	821	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
18	A	825	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	A	849	BCR	C16-C17-C18	3.02	131.62	127.31
18	B	803	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
17	1	601	CHL	C3B-C4B-NB	3.01	113.31	110.52
18	B	803	CLA	C3B-C4B-NB	-3.01	107.72	110.52
18	B	830	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	A	810	CLA	C3B-C4B-NB	-3.01	107.72	110.52
18	A	838	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
18	B	813	CLA	O2D-CGD-CBD	3.01	116.61	111.27
18	B	826	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
18	4	610	CLA	C3B-C4B-NB	-3.01	107.73	110.52
17	2	615	CHL	CMB-C2B-C1B	3.01	129.95	125.37
18	B	804	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
18	A	830	CLA	CHB-C4A-NA	3.00	128.66	124.51
18	A	832	CLA	C3B-C4B-NB	-3.00	107.73	110.52
17	4	605	CHL	CMB-C2B-C1B	3.00	129.94	125.37
21	3	613	LUT	C30-C31-C32	2.99	132.56	123.22
18	1	602	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
21	4	616	LUT	C20-C13-C14	-2.99	118.73	122.92
22	A	849	BCR	C35-C13-C14	-2.99	118.74	122.92
18	B	832	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
18	4	613	CLA	C3B-C4B-NB	-2.99	107.75	110.52
18	G	203	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
18	1	604	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
17	3	606	CHL	CMB-C2B-C1B	2.98	129.91	125.37
22	B	848	BCR	C35-C13-C14	-2.98	118.75	122.92
18	2	612	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
22	B	844	BCR	C19-C18-C17	2.98	123.51	118.94
18	A	818	CLA	C3B-C4B-NB	-2.98	107.75	110.52
18	1	605	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
22	A	853	BCR	C19-C18-C17	2.97	123.50	118.94
18	4	611	CLA	C3B-C4B-NB	-2.97	107.76	110.52
18	2	602	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
18	A	840	CLA	C3B-C4B-NB	-2.97	107.76	110.52
18	K	203	CLA	O2D-CGD-O1D	-2.97	118.04	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	847	BCR	C36-C18-C17	-2.97	118.77	122.92
18	B	809	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
17	1	606	CHL	C3D-C4D-ND	2.96	115.03	110.24
18	A	823	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
18	1	611	CLA	C3B-C4B-NB	-2.96	107.77	110.52
18	B	824	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
22	A	853	BCR	C34-C9-C10	-2.96	118.78	122.92
18	A	830	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
18	A	841	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
21	4	616	LUT	C35-C15-C14	2.95	129.53	123.47
17	4	607	CHL	CMB-C2B-C1B	2.95	129.87	125.37
18	A	810	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
18	A	835	CLA	C3B-C4B-NB	-2.95	107.78	110.52
18	B	834	CLA	C3B-C4B-NB	-2.95	107.78	110.52
18	4	608	CLA	C3B-C4B-NB	-2.94	107.78	110.52
18	A	816	CLA	C3B-C4B-NB	-2.94	107.78	110.52
18	A	827	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
27	B	850	DGD	C2G-O2G-C1B	-2.94	110.55	117.79
18	1	609	CLA	CHB-C4A-NA	2.94	128.58	124.51
18	1	609	CLA	C3B-C4B-NB	-2.94	107.79	110.52
22	F	304	BCR	C16-C17-C18	2.93	131.50	127.31
17	2	601	CHL	CMB-C2B-C1B	2.93	129.83	125.37
18	B	812	CLA	C3B-C4B-NB	-2.93	107.80	110.52
17	2	607	CHL	O2A-CGA-CBA	2.93	121.10	111.91
17	2	605	CHL	CAC-C3C-C4C	2.93	129.50	125.04
18	B	804	CLA	CAA-C2A-C3A	-2.93	109.27	116.10
18	A	807	CLA	C3B-C4B-NB	-2.93	107.80	110.52
17	2	605	CHL	CMB-C2B-C1B	2.92	129.82	125.37
18	A	836	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
22	B	801	BCR	C15-C16-C17	2.92	129.46	123.47
18	2	603	CLA	C3B-C4B-NB	-2.92	107.81	110.52
18	F	302	CLA	CHB-C4A-NA	2.92	128.55	124.51
22	A	853	BCR	C15-C16-C17	2.92	129.46	123.47
18	B	807	CLA	C3B-C4B-NB	-2.92	107.81	110.52
18	B	823	CLA	C3B-C4B-NB	-2.92	107.81	110.52
18	2	602	CLA	C3B-C4B-NB	-2.91	107.81	110.52
17	4	607	CHL	CHB-C1B-NB	-2.91	121.17	124.26
18	A	836	CLA	C3B-C4B-NB	-2.91	107.81	110.52
18	L	304	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
18	3	601	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
18	4	609	CLA	C3B-C4B-NB	-2.91	107.82	110.52
18	B	829	CLA	C3B-C4B-NB	-2.91	107.82	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	601	CHL	O2A-CGA-CBA	2.91	121.03	111.91
18	A	816	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	3	614	BCR	C12-C13-C14	2.90	123.40	118.94
18	B	819	CLA	C3B-C4B-NB	-2.90	107.82	110.52
17	3	606	CHL	CMD-C2D-C3D	-2.90	120.94	127.61
18	G	201	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	A	801	CL0	C4-C3-C5	2.90	120.15	115.27
18	3	612	CLA	C3B-C4B-NB	-2.90	107.83	110.52
18	F	301	CLA	C3B-C4B-NB	-2.90	107.83	110.52
17	4	605	CHL	CMD-C2D-C3D	-2.90	120.94	127.61
18	A	802	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
18	A	807	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
18	A	815	CLA	C3B-C4B-NB	-2.90	107.83	110.52
18	A	838	CLA	C3B-C4B-NB	-2.90	107.83	110.52
18	B	839	CLA	C3B-C4B-NB	-2.89	107.83	110.52
18	B	803	CLA	CHB-C4A-NA	2.89	128.51	124.51
18	A	806	CLA	C3B-C4B-NB	-2.89	107.83	110.52
22	K	205	BCR	C16-C15-C14	2.89	129.40	123.47
18	3	608	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
17	4	606	CHL	CMB-C2B-C1B	2.89	129.77	125.37
18	1	607	CLA	C3B-C4B-NB	-2.88	107.84	110.52
17	2	607	CHL	CMB-C2B-C1B	2.88	129.76	125.37
18	B	830	CLA	C3B-C4B-NB	-2.88	107.84	110.52
22	A	852	BCR	C24-C23-C22	2.88	130.59	126.23
21	3	613	LUT	C35-C15-C14	2.88	129.38	123.47
18	4	601	CLA	C3B-C4B-NB	-2.88	107.84	110.52
18	B	841	CLA	C3B-C4B-NB	-2.88	107.84	110.52
18	K	201	CLA	C3B-C4B-NB	-2.88	107.84	110.52
18	3	601	CLA	C3B-C4B-NB	-2.88	107.84	110.52
17	2	606	CHL	CMB-C2B-C1B	2.88	129.75	125.37
22	B	843	BCR	C36-C18-C17	-2.88	118.89	122.92
18	3	603	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
17	2	607	CHL	CMD-C2D-C3D	-2.88	121.00	127.61
18	4	610	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
21	3	613	LUT	C32-C33-C34	2.87	123.35	118.94
17	2	607	CHL	C1D-ND-C4D	-2.87	104.30	106.33
17	3	606	CHL	C1D-ND-C4D	-2.87	104.30	106.33
18	B	828	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
18	A	824	CLA	C3B-C4B-NB	-2.87	107.86	110.52
18	A	812	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	B	831	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	L	302	CLA	C3B-C4B-NB	-2.86	107.86	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	601	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
21	2	616	LUT	C12-C13-C14	2.86	123.33	118.94
18	2	604	CLA	CHB-C4A-NA	2.86	128.47	124.51
18	H	201	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	2	615	CHL	CMD-C2D-C3D	-2.86	121.05	127.61
18	A	822	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
18	F	303	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
18	A	843	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
18	A	837	CLA	C3B-C4B-NB	-2.85	107.87	110.52
18	B	834	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
18	3	602	CLA	C3B-C4B-NB	-2.85	107.87	110.52
17	1	601	CHL	C1D-ND-C4D	-2.85	104.31	106.33
17	2	615	CHL	C2D-C1D-ND	2.85	112.20	110.10
17	4	615	CHL	CMB-C2B-C1B	2.85	129.71	125.37
18	2	604	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	2	610	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
17	4	606	CHL	CHC-C4B-NB	-2.84	121.25	124.26
18	L	303	CLA	O2D-CGD-CBD	2.84	116.31	111.27
18	K	204	CLA	C3B-C4B-NB	-2.84	107.88	110.52
22	B	801	BCR	C11-C10-C9	2.84	131.36	127.31
18	A	813	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	K	205	BCR	C21-C20-C19	2.84	132.07	123.22
22	F	304	BCR	C1-C6-C5	-2.84	118.62	122.61
18	1	608	CLA	CAA-C2A-C3A	-2.84	109.48	116.10
18	B	835	CLA	C3B-C4B-NB	-2.83	107.89	110.52
18	A	829	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
18	G	202	CLA	C3B-C4B-NB	-2.83	107.89	110.52
17	4	606	CHL	CMD-C2D-C3D	-2.83	121.10	127.61
22	J	102	BCR	C10-C11-C12	2.83	132.06	123.22
24	A	801	CL0	C2A-C1A-CHA	-2.83	117.34	123.39
22	A	849	BCR	C36-C18-C17	-2.83	118.96	122.92
18	3	603	CLA	C3B-C4B-NB	-2.83	107.89	110.52
18	B	814	CLA	C3B-C4B-NB	-2.83	107.89	110.52
18	A	844	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
18	A	839	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
18	3	604	CLA	C3B-C4B-NB	-2.83	107.89	110.52
22	A	851	BCR	C19-C18-C17	2.82	123.28	118.94
18	B	810	CLA	C3B-C4B-NB	-2.82	107.89	110.52
18	3	611	CLA	C3B-C4B-NB	-2.82	107.90	110.52
18	3	608	CLA	CMA-C3A-C2A	-2.82	109.52	116.10
18	B	805	CLA	C3B-C4B-NB	-2.82	107.90	110.52
19	4	617	XAT	C20-C13-C14	-2.82	118.97	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	801	CL0	CMC-C2C-C1C	2.82	129.33	125.04
18	4	614	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	3	610	CLA	C3B-C4B-NB	-2.82	107.90	110.52
18	A	821	CLA	C3B-C4B-NB	-2.81	107.90	110.52
17	1	606	CHL	CMD-C2D-C3D	-2.81	121.14	127.61
18	B	817	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
18	4	614	CLA	C3B-C4B-NB	-2.81	107.91	110.52
18	G	201	CLA	C3B-C4B-NB	-2.81	107.91	110.52
18	2	608	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
17	2	601	CHL	CMD-C2D-C3D	-2.81	121.15	127.61
18	L	303	CLA	C3B-C4B-NB	-2.81	107.91	110.52
18	1	608	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
18	A	834	CLA	C3B-C4B-NB	-2.81	107.91	110.52
18	2	610	CLA	C1A-CHA-C4D	-2.80	121.79	125.72
18	B	835	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
18	1	602	CLA	C3B-C4B-NB	-2.80	107.91	110.52
18	K	204	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
17	2	615	CHL	C3B-C4B-NB	2.80	113.11	110.52
18	B	826	CLA	C3B-C4B-NB	-2.80	107.92	110.52
17	2	606	CHL	C3B-C4B-NB	2.80	113.11	110.52
21	4	616	LUT	C32-C33-C34	2.80	123.24	118.94
18	F	302	CLA	C3B-C4B-NB	-2.80	107.92	110.52
18	4	604	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
18	B	836	CLA	C1-C2-C3	-2.80	122.23	126.75
18	B	823	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	I	101	BCR	C19-C18-C17	2.79	123.23	118.94
17	2	605	CHL	C3B-C4B-NB	2.79	113.11	110.52
18	3	609	CLA	C3B-C4B-NB	-2.79	107.92	110.52
18	A	813	CLA	C3B-C4B-NB	-2.79	107.92	110.52
18	2	611	CLA	CHB-C4A-NA	2.79	128.37	124.51
18	1	603	CLA	C3B-C4B-NB	-2.79	107.93	110.52
18	2	613	CLA	C3B-C4B-NB	-2.79	107.93	110.52
18	K	203	CLA	C3B-C4B-NB	-2.79	107.93	110.52
18	A	803	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
17	1	606	CHL	CHD-C1D-C2D	2.78	131.32	125.48
18	A	802	CLA	O2A-CGA-O1A	-2.78	116.57	123.59
18	F	303	CLA	C3B-C4B-NB	-2.78	107.94	110.52
22	B	848	BCR	C19-C18-C17	2.78	123.21	118.94
18	A	824	CLA	CAA-C2A-C3A	-2.78	109.61	116.10
18	B	822	CLA	C3B-C4B-NB	-2.78	107.94	110.52
18	F	301	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
18	1	604	CLA	CBA-CAA-C2A	2.78	122.06	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	607	CHL	CMD-C2D-C3D	-2.78	121.23	127.61
19	1	614	XAT	O24-C25-C26	-2.78	56.66	58.96
17	2	606	CHL	C2D-C1D-ND	2.77	112.15	110.10
18	4	613	CLA	CHB-C4A-NA	2.77	128.34	124.51
17	4	615	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
18	B	805	CLA	CHB-C4A-NA	2.76	128.33	124.51
22	3	614	BCR	C19-C18-C17	2.76	123.18	118.94
18	1	604	CLA	CHB-C4A-NA	2.76	128.33	124.51
18	2	608	CLA	C3B-C4B-NB	-2.76	107.95	110.52
18	A	822	CLA	C3B-C4B-NB	-2.76	107.95	110.52
18	1	603	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	A	851	BCR	C20-C21-C22	2.76	131.25	127.31
18	A	813	CLA	O2D-CGD-CBD	2.76	116.17	111.27
21	2	619	LUT	C20-C13-C14	-2.76	119.06	122.92
18	A	841	CLA	C3B-C4B-NB	-2.76	107.96	110.52
21	3	613	LUT	C35-C34-C33	2.76	131.25	127.31
17	2	605	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
18	G	202	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
18	B	827	CLA	CHB-C4A-NA	2.75	128.32	124.51
18	3	608	CLA	C3B-C4B-NB	-2.75	107.96	110.52
18	B	806	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
18	L	304	CLA	C3B-C4B-NB	-2.75	107.97	110.52
24	A	801	CL0	CHB-C1B-C2B	-2.75	119.48	127.24
18	1	612	CLA	C3B-C4B-NB	-2.75	107.97	110.52
18	B	821	CLA	C3B-C4B-NB	-2.75	107.97	110.52
22	I	101	BCR	C16-C15-C14	2.75	129.10	123.47
22	A	848	BCR	C12-C13-C14	2.74	123.15	118.94
22	B	845	BCR	C21-C20-C19	2.74	131.78	123.22
18	B	840	CLA	C3B-C4B-NB	-2.74	107.97	110.52
22	A	850	BCR	C8-C9-C10	2.74	123.15	118.94
18	4	603	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
17	2	606	CHL	CHC-C4B-NB	-2.74	121.36	124.26
19	2	617	XAT	C35-C34-C33	2.74	131.22	127.31
18	B	827	CLA	C3B-C4B-NB	-2.74	107.97	110.52
21	3	613	LUT	C40-C33-C34	-2.74	119.09	122.92
18	2	611	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
21	2	619	LUT	C28-C29-C30	2.74	123.14	118.94
18	A	843	CLA	C3B-C4B-NB	-2.73	107.98	110.52
18	1	611	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
18	B	818	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	G	203	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	B	845	BCR	C16-C15-C14	2.73	129.07	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	609	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	A	812	CLA	C3B-C4B-NB	-2.73	107.98	110.52
18	4	609	CLA	CHB-C4A-NA	2.73	128.29	124.51
17	1	606	CHL	CMB-C2B-C1B	2.73	129.52	125.37
18	A	842	CLA	CMB-C2B-C1B	-2.73	121.21	125.37
18	B	831	CLA	C3B-C4B-NB	-2.73	107.99	110.52
18	1	604	CLA	C3B-C4B-NB	-2.72	107.99	110.52
18	A	817	CLA	C3B-C4B-NB	-2.72	107.99	110.52
18	3	602	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
18	3	612	CLA	CAA-C2A-C3A	-2.72	109.74	116.10
18	3	610	CLA	CAA-C2A-C3A	-2.72	109.74	116.10
22	B	801	BCR	C19-C18-C17	2.72	123.12	118.94
18	3	611	CLA	CAA-C2A-C3A	-2.72	109.75	116.10
18	A	844	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	B	843	BCR	C35-C13-C14	-2.72	119.11	122.92
18	B	817	CLA	CHB-C4A-NA	2.72	128.27	124.51
17	2	601	CHL	C1D-ND-C4D	-2.72	104.40	106.33
18	A	831	CLA	C3B-C4B-NB	-2.72	107.99	110.52
19	4	617	XAT	C30-C31-C32	-2.72	114.74	123.22
18	A	809	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	2	617	XAT	C30-C31-C32	2.71	131.68	123.22
22	A	849	BCR	C19-C18-C17	2.71	123.10	118.94
18	2	609	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	L	305	BCR	C23-C22-C21	2.71	123.09	118.94
17	4	607	CHL	CHB-C4A-NA	2.70	128.25	124.51
18	A	834	CLA	CHB-C4A-NA	2.70	128.25	124.51
18	A	810	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
18	B	828	CLA	CHB-C4A-NA	2.70	128.25	124.51
18	3	612	CLA	O2D-CGD-O1D	-2.70	117.97	124.09
18	A	827	CLA	C3B-C4B-NB	-2.69	108.02	110.52
19	1	614	XAT	C5-C4-C3	-2.69	107.42	112.75
18	A	824	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
17	4	605	CHL	C1D-ND-C4D	-2.68	104.43	106.33
18	B	815	CLA	C3B-C4B-NB	-2.68	108.03	110.52
17	2	606	CHL	CMD-C2D-C3D	-2.68	121.44	127.61
18	A	809	CLA	C3B-C4B-NB	-2.68	108.03	110.52
18	A	828	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	2	617	XAT	C12-C13-C14	2.68	123.05	118.94
18	A	832	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	A	835	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	A	808	CLA	C3B-C4B-NB	-2.68	108.03	110.52
18	4	608	CLA	O2D-CGD-O1D	-2.68	118.60	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	613	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	B	834	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	A	807	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	A	809	CLA	O2D-CGD-CBD	2.67	116.02	111.27
18	A	842	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	L	306	BCR	C21-C20-C19	2.67	131.55	123.22
18	B	804	CLA	CHB-C4A-NA	2.67	128.20	124.51
18	3	612	CLA	CHB-C4A-NA	2.66	128.20	124.51
18	B	814	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	B	848	BCR	C16-C15-C14	2.66	128.93	123.47
22	4	618	BCR	C19-C18-C17	2.66	123.02	118.94
24	A	801	CL0	CMB-C2B-C1B	2.66	129.42	125.37
18	B	825	CLA	C3B-C4B-NB	-2.66	108.05	110.52
18	1	605	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	4	602	CLA	C3B-C4B-NB	-2.65	108.05	110.52
17	2	605	CHL	C1D-ND-C4D	-2.65	104.45	106.33
18	A	821	CLA	CHB-C4A-NA	2.65	128.18	124.51
18	B	825	CLA	CHB-C4A-NA	2.65	128.18	124.51
18	4	612	CLA	C3B-C4B-NB	-2.65	108.05	110.52
18	2	602	CLA	CHB-C4A-NA	2.65	128.18	124.51
18	B	840	CLA	CHB-C4A-NA	2.65	128.18	124.51
18	A	805	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	2	612	CLA	C3B-C4B-NB	-2.65	108.06	110.52
22	F	304	BCR	C36-C18-C17	-2.64	119.22	122.92
17	4	605	CHL	CAC-C3C-C4C	2.64	129.07	125.04
17	1	601	CHL	CMB-C2B-C1B	2.64	129.40	125.37
18	A	824	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	4	601	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	A	805	CLA	C3B-C4B-NB	-2.64	108.06	110.52
17	1	601	CHL	CHC-C4B-NB	-2.64	121.47	124.26
17	2	601	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
18	2	608	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	B	824	CLA	C3B-C4B-NB	-2.63	108.07	110.52
18	A	836	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	A	835	CLA	O2D-CGD-CBD	2.63	115.94	111.27
18	B	820	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	B	810	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	A	826	CLA	C3B-C4B-NB	-2.63	108.08	110.52
18	B	833	CLA	C3B-C4B-NB	-2.63	108.08	110.52
17	4	606	CHL	CHD-C1D-C2D	2.63	130.99	125.48
18	A	840	CLA	CHB-C4A-NA	2.63	128.15	124.51
18	B	808	CLA	O2A-CGA-O1A	-2.63	116.96	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	F	303	CLA	CAA-C2A-C3A	-2.62	109.97	116.10
18	B	809	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	A	829	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	1	605	CLA	C3B-C4B-NB	-2.62	108.08	110.52
18	F	302	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
18	A	823	CLA	C3B-C4B-NB	-2.62	108.08	110.52
18	B	819	CLA	CHB-C4A-NA	2.62	128.13	124.51
18	B	821	CLA	CHB-C4A-NA	2.62	128.13	124.51
18	K	201	CLA	CAA-C2A-C3A	-2.61	110.00	116.10
18	B	818	CLA	C3B-C4B-NB	-2.61	108.09	110.52
22	3	614	BCR	C1-C6-C5	-2.61	118.94	122.61
18	1	613	CLA	CAA-C2A-C3A	-2.61	110.01	116.10
18	A	814	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	A	801	CL0	C4D-C3D-C2D	2.61	108.89	106.75
18	B	802	CLA	CGD-CBD-CAD	2.61	119.17	110.73
19	2	617	XAT	C15-C14-C13	2.60	131.03	127.31
18	A	818	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	3	607	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
18	2	611	CLA	C3B-C4B-NB	-2.60	108.10	110.52
18	A	815	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	4	612	CLA	CHB-C4A-NA	2.60	128.10	124.51
18	1	611	CLA	CHB-C4A-NA	2.60	128.10	124.51
18	B	825	CLA	O2D-CGD-CBD	2.59	115.88	111.27
18	A	825	CLA	C3B-C4B-NB	-2.59	108.11	110.52
18	A	833	CLA	CHB-C4A-NA	2.59	128.10	124.51
18	A	812	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	A	848	BCR	C23-C22-C21	2.59	122.92	118.94
18	A	804	CLA	C3B-C4B-NB	-2.59	108.11	110.52
18	2	610	CLA	CAB-C3B-C2B	2.59	130.30	123.59
18	3	609	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	A	811	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	2	603	CLA	O2D-CGD-O1D	-2.59	118.22	124.09
18	A	833	CLA	C3B-C4B-NB	-2.58	108.12	110.52
18	B	804	CLA	C3B-C4B-NB	-2.58	108.12	110.52
18	B	837	CLA	C3B-C4B-NB	-2.58	108.12	110.52
17	1	601	CHL	C4-C3-C5	2.58	119.62	115.27
18	B	811	CLA	CHB-C4A-NA	2.58	128.08	124.51
19	1	614	XAT	C25-C24-C23	-2.58	107.65	112.75
18	1	613	CLA	CAB-C3B-C2B	2.58	130.27	123.59
18	B	837	CLA	CHB-C4A-NA	2.58	128.07	124.51
18	3	607	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	K	203	CLA	CHB-C4A-NA	2.57	128.07	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	820	CLA	CMB-C2B-C1B	-2.57	121.45	125.37
19	1	614	XAT	O4-C5-C6	-2.57	56.83	58.96
18	A	822	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	1	608	CLA	CAB-C3B-C2B	2.57	130.25	123.59
18	4	603	CLA	CAB-C3B-C2B	2.57	130.24	123.59
18	3	604	CLA	O2D-CGD-O1D	-2.57	118.26	124.09
18	A	838	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	B	831	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	4	617	XAT	C16-C1-C6	-2.56	103.12	110.05
22	G	204	BCR	C16-C15-C14	2.56	128.72	123.47
18	B	820	CLA	C3B-C4B-NB	-2.56	108.14	110.52
18	3	601	CLA	C1-C2-C3	-2.56	121.61	126.04
18	A	839	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	A	808	CLA	CHB-C4A-NA	2.56	128.05	124.51
18	B	830	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	L	301	BCR	C8-C9-C10	2.56	122.87	118.94
18	A	843	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	3	613	LUT	C12-C13-C14	2.56	122.86	118.94
22	J	102	BCR	C15-C16-C17	2.55	128.71	123.47
18	1	607	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	F	303	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	3	602	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	A	816	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	B	816	CLA	C1-C2-C3	-2.55	121.63	126.04
22	B	846	BCR	C15-C16-C17	2.55	128.70	123.47
22	F	304	BCR	C37-C22-C23	2.55	122.10	118.08
18	3	610	CLA	O2D-CGD-O1D	-2.55	118.30	124.09
18	H	201	CLA	C3B-C4B-NB	-2.55	108.15	110.52
17	4	607	CHL	C2A-C1A-CHA	-2.55	119.40	123.86
18	4	604	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	F	301	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	G	203	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	B	838	CLA	CHB-C4A-NA	2.55	128.03	124.51
18	B	806	CLA	C3B-C4B-NB	-2.55	108.15	110.52
18	4	611	CLA	CHB-C4A-NA	2.55	128.03	124.51
21	3	613	LUT	C10-C11-C12	2.54	131.16	123.22
18	4	611	CLA	O2D-CGD-O1D	-2.54	118.32	124.09
18	1	610	CLA	CHB-C4A-NA	2.54	128.03	124.51
18	L	304	CLA	CHB-C4A-NA	2.54	128.03	124.51
21	4	616	LUT	C19-C9-C8	2.54	122.08	118.08
22	J	102	BCR	C19-C18-C17	2.54	122.84	118.94
18	B	802	CLA	CHB-C4A-NA	2.54	128.02	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	812	CLA	CHB-C4A-NA	2.53	128.02	124.51
18	A	817	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	4	607	CHL	C1C-C2C-C3C	-2.53	105.10	107.11
18	4	602	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	L	303	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	B	822	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	3	605	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	1	610	CLA	CAA-C2A-C3A	-2.53	110.19	116.10
18	A	823	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	2	606	CHL	C4A-NA-C1A	2.53	107.84	106.71
18	2	609	CLA	C3B-C4B-NB	-2.53	108.17	110.52
18	A	806	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	1	607	CLA	O2D-CGD-O1D	-2.53	118.35	124.09
18	A	826	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
18	3	601	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	A	811	CLA	C3B-C4B-NB	-2.52	108.18	110.52
18	3	610	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	4	609	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
22	J	102	BCR	C7-C8-C9	2.52	130.04	126.23
19	2	617	XAT	C27-C28-C29	-2.52	121.62	125.53
18	A	814	CLA	CHB-C1B-NB	2.52	126.92	124.26
18	1	608	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	L	306	BCR	C24-C23-C22	2.52	130.04	126.23
18	B	808	CLA	CHB-C4A-NA	2.52	127.99	124.51
18	B	816	CLA	CHB-C4A-NA	2.52	127.99	124.51
17	2	615	CHL	C4A-NA-C1A	2.52	107.84	106.71
18	B	813	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	K	201	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	A	810	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	B	835	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	3	609	CLA	O2D-CGD-O1D	-2.51	118.39	124.09
18	2	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	A	831	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	4	610	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	B	806	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	B	829	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	B	836	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	A	820	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	G	202	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	2	612	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	A	825	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	B	807	CLA	CHB-C4A-NA	2.50	127.97	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	608	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	A	837	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	3	611	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	B	824	CLA	CHB-C4A-NA	2.49	127.96	124.51
20	1	615	LHG	O8-C23-C24	2.49	119.73	111.91
17	2	605	CHL	CHC-C4B-NB	-2.49	121.62	124.26
22	G	204	BCR	C23-C22-C21	2.49	122.76	118.94
18	B	830	CLA	CHD-C1D-ND	-2.49	122.17	124.45
18	B	815	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	4	603	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	G	201	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	A	851	BCR	C15-C14-C13	2.49	130.86	127.31
18	A	826	CLA	CHB-C4A-NA	2.48	127.95	124.51
17	4	607	CHL	CBC-CAC-C3C	-2.48	105.58	112.43
18	A	820	CLA	C3B-C4B-NB	-2.48	108.21	110.52
22	K	205	BCR	C8-C9-C10	2.48	122.75	118.94
19	1	614	XAT	C27-C28-C29	-2.48	121.68	125.53
18	L	302	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	L	306	BCR	C1-C6-C5	-2.48	119.13	122.61
18	A	819	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	K	202	BCR	C30-C25-C24	2.47	122.78	115.78
22	K	202	BCR	C10-C11-C12	2.47	130.94	123.22
18	A	828	CLA	C3B-C4B-NB	-2.47	108.22	110.52
17	4	605	CHL	C1C-C2C-C3C	-2.47	105.15	107.11
18	A	803	CLA	CHB-C1B-NB	2.47	126.87	124.26
24	A	801	CL0	CMD-C2D-C3D	-2.47	122.26	128.30
22	F	304	BCR	C19-C18-C17	2.47	122.73	118.94
18	A	841	CLA	CHB-C4A-NA	2.47	127.92	124.51
18	1	610	CLA	O2D-CGD-O1D	-2.46	118.49	124.09
19	4	617	XAT	C15-C35-C34	2.46	128.52	123.47
18	1	603	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	B	843	BCR	C12-C13-C14	2.46	122.71	118.94
18	4	608	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	1	615	LHG	C5-O7-C7	-2.46	111.74	117.79
17	1	601	CHL	O2D-CGD-O1D	-2.46	118.51	124.09
17	2	607	CHL	C5-C3-C4	2.45	120.02	114.60
22	A	849	BCR	C1-C6-C5	-2.45	119.16	122.61
22	B	849	BCR	C30-C25-C24	2.45	122.72	115.78
22	I	101	BCR	C12-C13-C14	2.45	122.70	118.94
18	B	809	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
22	B	845	BCR	C37-C22-C21	-2.45	119.49	122.92
18	1	609	CLA	O2D-CGD-O1D	-2.45	119.05	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	204	BCR	C12-C13-C14	2.45	122.70	118.94
18	B	813	CLA	C3B-C4B-NB	-2.45	108.24	110.52
18	3	603	CLA	CHB-C4A-NA	2.45	127.90	124.51
17	1	601	CHL	C1C-C2C-C3C	-2.44	105.17	107.11
18	B	832	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	B	826	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	B	809	CLA	C3B-C4B-NB	-2.44	108.25	110.52
18	1	610	CLA	CAB-C3B-C2B	2.44	129.92	123.59
18	A	815	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
18	3	604	CLA	CHB-C4A-NA	2.44	127.88	124.51
18	A	803	CLA	CHB-C4A-NA	2.44	127.88	124.51
18	4	614	CLA	O2D-CGD-CBD	2.44	115.60	111.27
18	B	839	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	B	846	BCR	C19-C18-C17	2.43	122.67	118.94
21	4	616	LUT	C39-C29-C28	2.43	121.90	118.08
22	A	850	BCR	C35-C13-C14	-2.43	119.52	122.92
18	1	610	CLA	CMB-C2B-C3B	2.43	129.88	123.59
22	3	614	BCR	C8-C9-C10	2.43	122.66	118.94
18	3	605	CLA	CAB-C3B-C2B	2.43	129.87	123.59
17	2	601	CHL	CHC-C4B-NB	-2.42	121.69	124.26
18	3	605	CLA	CMB-C2B-C3B	2.42	129.86	123.59
22	J	102	BCR	C23-C22-C21	2.42	122.65	118.94
18	B	841	CLA	CHB-C4A-NA	2.42	127.85	124.51
18	H	201	CLA	CHB-C4A-NA	2.41	127.85	124.51
18	3	607	CLA	CHB-C1B-NB	2.41	126.81	124.26
18	A	830	CLA	C3B-C4B-NB	-2.41	108.28	110.52
18	B	820	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
18	B	816	CLA	CHB-C1B-NB	2.41	126.81	124.26
18	B	818	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
19	1	614	XAT	C10-C11-C12	-2.41	115.70	123.22
18	1	602	CLA	CHB-C4A-NA	2.41	127.84	124.51
18	A	839	CLA	C3B-C4B-NB	-2.40	108.28	110.52
18	4	603	CLA	CMB-C2B-C3B	2.40	129.82	123.59
19	1	614	XAT	C11-C10-C9	-2.40	123.88	127.31
18	1	608	CLA	CMB-C2B-C3B	2.40	129.82	123.59
17	2	606	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
18	B	833	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	K	204	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	B	822	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
22	K	205	BCR	C12-C13-C14	2.40	122.62	118.94
18	1	613	CLA	CMB-C2B-C3B	2.39	129.79	123.59
17	4	615	CHL	CMB-C2B-C3B	2.39	129.78	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	3	603	CLA	CHB-C1B-NB	2.38	126.78	124.26
27	B	850	DGD	O1G-C1A-C2A	2.38	119.38	111.91
18	B	821	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
18	A	832	CLA	C1-C2-C3	-2.37	122.91	126.75
18	B	811	CLA	CMB-C2B-C3B	2.37	129.73	123.59
18	A	804	CLA	O2D-CGD-CBD	2.37	115.48	111.27
18	A	827	CLA	CHB-C4A-NA	2.37	127.79	124.51
18	4	604	CLA	CMB-C2B-C3B	2.36	129.71	123.59
18	1	612	CLA	CHB-C4A-NA	2.36	127.78	124.51
17	4	615	CHL	C1C-C2C-C3C	-2.36	105.24	107.11
17	2	605	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
18	A	844	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
18	B	813	CLA	CMB-C2B-C1B	-2.35	121.78	125.37
22	A	849	BCR	C12-C13-C14	2.35	122.55	118.94
22	4	618	BCR	C15-C16-C17	2.35	128.29	123.47
18	B	811	CLA	CAB-C3B-C2B	2.35	129.68	123.59
21	3	613	LUT	C11-C10-C9	2.35	130.66	127.31
21	2	616	LUT	C35-C15-C14	2.35	128.28	123.47
18	A	810	CLA	C1-C2-C3	-2.35	122.95	126.75
17	4	605	CHL	CHC-C4B-NB	-2.35	121.77	124.26
18	2	610	CLA	CMB-C2B-C3B	2.34	129.66	123.59
18	4	604	CLA	CAB-C3B-C2B	2.34	129.66	123.59
18	A	842	CLA	C3B-C4B-NB	-2.34	108.34	110.52
18	B	841	CLA	O2D-CGD-CBD	2.34	115.43	111.27
22	A	851	BCR	C30-C25-C26	-2.34	119.32	122.61
22	B	843	BCR	C1-C6-C7	2.33	122.38	115.78
19	4	617	XAT	C37-C21-C26	2.33	116.34	110.05
22	B	847	BCR	C19-C18-C17	2.33	122.51	118.94
18	A	822	CLA	CHB-C1B-NB	2.33	126.72	124.26
18	B	823	CLA	CHB-C4A-NA	2.32	127.72	124.51
17	2	607	CHL	C1C-C2C-C3C	-2.32	105.27	107.11
17	4	606	CHL	CMB-C2B-C3B	2.32	129.60	123.59
18	A	815	CLA	CHB-C1B-NB	2.32	126.71	124.26
21	2	616	LUT	C40-C33-C34	-2.31	119.68	122.92
18	B	813	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
18	1	613	CLA	CHB-C4A-NA	2.31	127.71	124.51
21	4	616	LUT	C12-C13-C14	2.31	122.49	118.94
18	A	829	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
18	B	803	CLA	C1-C2-C3	-2.31	122.05	126.04
17	3	606	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
18	B	828	CLA	CHB-C1B-NB	2.31	126.70	124.26
18	A	841	CLA	O2A-CGA-O1A	-2.31	117.77	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	835	CLA	C1-C2-C3	-2.31	122.05	126.04
22	B	846	BCR	C10-C11-C12	2.31	130.42	123.22
22	K	202	BCR	C30-C25-C26	-2.30	119.37	122.61
18	A	805	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
17	2	615	CHL	O2D-CGD-O1D	-2.30	119.35	123.84
19	4	617	XAT	C7-C8-C9	2.30	129.09	125.53
18	A	828	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
21	1	616	LUT	C10-C11-C12	2.29	130.37	123.22
19	4	617	XAT	C39-C29-C30	-2.29	119.71	122.92
22	K	202	BCR	C21-C20-C19	2.29	130.37	123.22
18	A	810	CLA	CHB-C1B-NB	2.29	126.68	124.26
17	3	606	CHL	CHC-C4B-NB	-2.29	121.84	124.26
22	B	848	BCR	C12-C13-C14	2.29	122.45	118.94
22	K	205	BCR	C1-C6-C5	-2.29	119.39	122.61
18	B	839	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
18	3	609	CLA	C1-C2-C3	-2.28	122.10	126.04
18	2	604	CLA	CHB-C1B-NB	2.28	126.67	124.26
22	A	848	BCR	C30-C25-C24	2.28	122.23	115.78
18	B	838	CLA	CHB-C1B-NB	2.27	126.67	124.26
18	B	836	CLA	CHB-C1B-NB	2.27	126.66	124.26
18	4	614	CLA	C1-C2-C3	-2.27	123.07	126.75
18	B	819	CLA	CHB-C1B-NB	2.27	126.66	124.26
22	3	614	BCR	C37-C22-C23	2.27	121.65	118.08
19	2	617	XAT	C8-C9-C10	2.27	122.42	118.94
18	3	603	CLA	CHD-C1D-ND	-2.26	122.37	124.45
18	A	804	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
18	B	803	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
18	A	825	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
18	B	817	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
17	2	607	CHL	O2D-CGD-O1D	-2.26	119.43	123.84
22	A	850	BCR	C36-C18-C17	-2.26	119.76	122.92
18	3	608	CLA	CHD-C1D-ND	-2.26	122.38	124.45
18	A	820	CLA	CHB-C1B-NB	2.26	126.64	124.26
18	B	825	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
17	2	605	CHL	OMC-CMC-C2C	-2.25	120.59	125.69
22	B	849	BCR	C24-C23-C22	2.25	129.64	126.23
18	4	609	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
18	F	301	CLA	CHD-C1D-ND	-2.25	122.38	124.45
18	4	612	CLA	C1-C2-C3	-2.25	122.15	126.04
22	K	205	BCR	C30-C25-C24	2.25	122.15	115.78
18	A	844	CLA	CHB-C1B-NB	2.25	126.64	124.26
18	A	840	CLA	O2D-CGD-CBD	2.25	115.27	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	601	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
18	A	818	CLA	CHB-C1B-NB	2.25	126.64	124.26
22	A	848	BCR	C30-C25-C26	-2.25	119.45	122.61
19	1	614	XAT	C18-C5-C4	2.25	116.81	114.28
22	A	851	BCR	C30-C25-C24	2.25	122.13	115.78
18	A	802	CLA	CHB-C1B-NB	2.24	126.63	124.26
17	4	605	CHL	OMC-CMC-C2C	-2.24	120.61	125.69
17	1	606	CHL	O2D-CGD-O1D	-2.24	119.00	124.09
18	A	825	CLA	CHB-C1B-NB	2.24	126.63	124.26
18	A	819	CLA	O2D-CGD-CBD	2.24	115.25	111.27
18	A	831	CLA	CHB-C1B-NB	2.24	126.62	124.26
19	1	614	XAT	C30-C31-C32	-2.24	116.24	123.22
22	A	853	BCR	C23-C22-C21	2.23	122.37	118.94
18	A	835	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
22	B	845	BCR	C30-C25-C26	-2.23	119.47	122.61
18	L	302	CLA	O2D-CGD-CBD	2.23	115.23	111.27
17	2	615	CHL	C1C-C2C-C3C	-2.23	105.34	107.11
18	2	613	CLA	O2D-CGD-CBD	2.23	115.23	111.27
18	B	804	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
18	A	828	CLA	O2D-CGD-CBD	2.22	115.22	111.27
18	A	831	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
18	A	830	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
18	B	837	CLA	O2D-CGD-CBD	2.22	115.21	111.27
17	4	607	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
18	B	828	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
22	L	305	BCR	C1-C6-C7	2.22	122.05	115.78
18	B	833	CLA	O2D-CGD-CBD	2.22	115.21	111.27
18	A	840	CLA	CHB-C1B-NB	2.22	126.60	124.26
18	B	832	CLA	CHB-C1B-NB	2.22	126.60	124.26
18	B	817	CLA	C1-C2-C3	-2.22	122.21	126.04
18	A	827	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
18	A	832	CLA	O2D-CGD-CBD	2.21	115.20	111.27
18	A	815	CLA	CHD-C1D-ND	-2.21	122.42	124.45
18	B	838	CLA	O2D-CGD-CBD	2.21	115.20	111.27
22	A	851	BCR	C11-C12-C13	2.21	132.63	126.42
17	2	605	CHL	CAA-C2A-C3A	-2.21	108.73	114.26
18	B	810	CLA	C1-C2-C3	-2.21	122.22	126.04
22	B	843	BCR	C10-C11-C12	2.21	130.11	123.22
22	B	843	BCR	C19-C18-C17	2.21	122.33	118.94
21	2	619	LUT	C15-C14-C13	2.21	130.46	127.31
17	2	606	CHL	C1D-ND-C4D	-2.20	104.77	106.33
18	B	826	CLA	CMB-C2B-C1B	-2.20	122.02	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	805	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
22	A	850	BCR	C12-C13-C14	2.20	122.32	118.94
18	A	839	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
22	J	102	BCR	C1-C6-C7	2.20	121.99	115.78
17	4	615	CHL	O2D-CGD-O1D	-2.19	119.11	124.09
18	A	819	CLA	CHB-C1B-NB	2.19	126.58	124.26
22	K	205	BCR	C30-C25-C26	-2.19	119.53	122.61
22	A	851	BCR	C24-C23-C22	-2.19	122.92	126.23
18	B	820	CLA	O2D-CGD-CBD	2.19	115.16	111.27
22	A	853	BCR	C30-C25-C24	2.19	121.97	115.78
24	A	801	CL0	CHB-C4A-NA	2.19	127.54	124.51
18	B	834	CLA	CHB-C1B-NB	2.19	126.57	124.26
18	A	808	CLA	C1-C2-C3	-2.19	123.21	126.75
18	A	815	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
18	B	836	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
22	B	843	BCR	C16-C17-C18	2.19	130.43	127.31
22	B	845	BCR	C24-C23-C22	-2.18	122.93	126.23
18	B	816	CLA	CHD-C1D-ND	-2.18	122.45	124.45
18	3	602	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
22	L	305	BCR	C30-C25-C24	2.18	121.95	115.78
22	L	306	BCR	C1-C6-C7	2.18	121.95	115.78
18	B	829	CLA	CHB-C1B-NB	2.18	126.57	124.26
18	A	802	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
18	A	838	CLA	CHB-C1B-NB	2.18	126.56	124.26
22	K	205	BCR	C1-C6-C7	2.18	121.94	115.78
18	B	822	CLA	CHB-C1B-NB	2.18	126.56	124.26
18	B	807	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
18	A	807	CLA	CHD-C1D-ND	-2.18	122.45	124.45
17	1	601	CHL	C4D-CHA-C1A	-2.17	118.60	121.25
18	4	610	CLA	CHB-C1B-NB	2.17	126.56	124.26
18	4	611	CLA	CHB-C1B-NB	2.17	126.56	124.26
18	B	834	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	J	102	BCR	C1-C6-C5	-2.17	119.56	122.61
18	3	612	CLA	CHB-C1B-NB	2.17	126.56	124.26
18	A	839	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
22	B	845	BCR	C8-C9-C10	2.17	122.27	118.94
18	1	612	CLA	CHB-C1B-NB	2.16	126.55	124.26
18	A	810	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
18	A	825	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	A	850	BCR	C19-C18-C17	2.16	122.26	118.94
18	B	818	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
18	A	811	CLA	CMB-C2B-C1B	-2.16	122.08	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	843	BCR	C1-C6-C5	-2.16	119.58	122.61
18	L	302	CLA	CHB-C1B-NB	2.16	126.54	124.26
22	B	848	BCR	C30-C25-C24	2.16	121.88	115.78
18	B	816	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
19	4	617	XAT	C35-C15-C14	2.15	127.89	123.47
18	1	602	CLA	CHD-C1D-ND	-2.15	122.47	124.45
18	2	602	CLA	CHB-C1B-NB	2.15	126.54	124.26
19	1	614	XAT	C20-C13-C12	2.15	121.47	118.08
18	F	301	CLA	CHB-C1B-NB	2.15	126.53	124.26
18	A	842	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
18	A	808	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
18	A	812	CLA	C1-C2-C3	-2.15	122.33	126.04
18	B	813	CLA	C1-C2-C3	-2.15	122.33	126.04
18	2	611	CLA	O2A-CGA-O1A	-2.14	117.95	123.30
18	K	203	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
18	A	832	CLA	CHB-C1B-NB	2.14	126.53	124.26
18	B	836	CLA	O2D-CGD-CBD	2.14	115.07	111.27
18	B	822	CLA	C1-C2-C3	-2.14	122.34	126.04
17	2	615	CHL	CAA-C2A-C3A	-2.14	108.91	114.26
18	B	825	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
18	A	826	CLA	CHB-C1B-NB	2.14	126.52	124.26
18	B	818	CLA	CHB-C1B-NB	2.14	126.52	124.26
17	4	606	CHL	CHD-C4C-C3C	-2.14	121.70	124.84
18	A	831	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
18	B	839	CLA	CHB-C1B-NB	2.14	126.52	124.26
17	4	606	CHL	O2D-CGD-O1D	-2.13	119.66	123.84
18	A	812	CLA	CHB-C1B-NB	2.13	126.52	124.26
18	A	840	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
22	A	853	BCR	C30-C25-C26	-2.13	119.61	122.61
22	A	852	BCR	C30-C25-C24	2.13	121.81	115.78
18	A	816	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	B	827	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	A	806	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
17	2	606	CHL	CHD-C1D-C2D	2.13	129.95	125.48
18	A	835	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	A	832	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	A	801	CL0	O2A-CGA-O1A	-2.13	118.22	123.59
18	B	810	CLA	CHB-C1B-NB	2.13	126.51	124.26
22	B	848	BCR	C37-C22-C23	2.12	121.42	118.08
17	2	615	CHL	C1D-ND-C4D	-2.12	104.83	106.33
22	B	847	BCR	C8-C9-C10	2.12	122.20	118.94
22	A	849	BCR	C15-C14-C13	2.12	130.34	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	825	CLA	C1-C2-C3	-2.12	122.37	126.04
18	A	844	CLA	C1-C2-C3	-2.12	122.37	126.04
18	B	827	CLA	O2D-CGD-CBD	2.12	115.04	111.27
22	A	850	BCR	C37-C22-C23	2.12	121.42	118.08
18	A	839	CLA	C1-C2-C3	-2.12	122.37	126.04
18	B	810	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
18	K	204	CLA	CHD-C1D-ND	-2.12	122.50	124.45
18	A	842	CLA	CMB-C2B-C3B	2.12	131.72	126.59
18	1	613	CLA	O2D-CGD-O1D	-2.12	119.27	124.09
22	G	204	BCR	C8-C9-C10	2.12	122.19	118.94
22	A	852	BCR	C34-C9-C8	2.12	121.42	118.08
18	4	613	CLA	O2A-CGA-O1A	-2.12	118.02	123.30
18	A	806	CLA	CHB-C1B-NB	2.12	126.50	124.26
18	A	834	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
18	A	815	CLA	O2D-CGD-CBD	2.12	115.03	111.27
18	A	829	CLA	CHB-C1B-NB	2.12	126.50	124.26
18	K	201	CLA	CHB-C1B-NB	2.12	126.50	124.26
18	A	812	CLA	CHD-C1D-ND	-2.12	122.51	124.45
18	B	829	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
18	2	612	CLA	CHB-C1B-NB	2.11	126.50	124.26
18	A	842	CLA	CHB-C1B-NB	2.11	126.50	124.26
17	2	606	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
18	B	802	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	B	835	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	A	831	CLA	CHD-C1D-ND	-2.11	122.52	124.45
18	4	601	CLA	O2D-CGD-CBD	2.11	115.02	111.27
21	2	619	LUT	C11-C10-C9	2.11	130.32	127.31
18	B	839	CLA	CHD-C1D-ND	-2.11	122.52	124.45
18	B	808	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	B	818	CLA	O2D-CGD-CBD	2.11	115.01	111.27
18	B	820	CLA	C1-C2-C3	-2.11	123.34	126.75
18	4	613	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	B	841	CLA	CHB-C1B-NB	2.11	126.49	124.26
22	B	847	BCR	C15-C16-C17	2.11	127.79	123.47
18	B	831	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	A	806	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	B	808	CLA	C1-C2-C3	-2.10	122.41	126.04
18	3	609	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	A	822	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	4	609	CLA	CHD-C1D-ND	-2.10	122.52	124.45
17	4	607	CHL	OMC-CMC-C2C	-2.10	120.94	125.69
18	4	609	CLA	CHB-C1B-NB	2.10	126.48	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	841	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	B	825	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	1	602	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	K	203	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	4	603	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	1	603	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	H	201	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
18	4	602	CLA	CMB-C2B-C1B	-2.10	122.18	125.37
17	1	606	CHL	C3B-C4B-NB	2.10	112.46	110.52
18	2	604	CLA	CHC-C4B-NB	2.10	126.47	124.26
18	3	610	CLA	CHB-C1B-NB	2.09	126.47	124.26
18	A	818	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
18	B	807	CLA	CHB-C1B-NB	2.09	126.47	124.26
18	4	612	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
18	3	604	CLA	CHB-C1B-NB	2.09	126.47	124.26
18	3	605	CLA	CHD-C1D-ND	-2.09	122.54	124.45
18	B	826	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
18	A	830	CLA	C2A-C1A-CHA	2.09	127.51	123.86
18	2	611	CLA	CHD-C1D-ND	-2.08	122.54	124.45
18	3	601	CLA	CHB-C1B-NB	2.08	126.46	124.26
21	2	619	LUT	C30-C31-C32	2.08	129.72	123.22
22	3	614	BCR	C30-C25-C24	2.08	121.67	115.78
17	4	615	CHL	C4B-C3B-C2B	-2.08	105.05	107.03
18	B	817	CLA	CHD-C1D-ND	-2.08	122.54	124.45
18	3	601	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
17	4	605	CHL	O2D-CGD-O1D	-2.08	119.36	124.09
18	B	813	CLA	CHB-C1B-NB	2.08	126.46	124.26
18	A	827	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	B	815	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	B	835	CLA	CHD-C1D-ND	-2.08	122.55	124.45
18	4	602	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
18	1	602	CLA	CHB-C1B-NB	2.08	126.45	124.26
18	B	826	CLA	CHB-C1B-NB	2.08	126.45	124.26
18	A	826	CLA	CMB-C2B-C3B	2.08	131.61	126.59
17	1	601	CHL	OMC-CMC-C2C	-2.08	121.00	125.69
17	2	606	CHL	O1D-CGD-CBD	-2.07	120.24	124.48
18	A	824	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	H	201	CLA	C1-C2-C3	-2.07	122.46	126.04
18	1	613	CLA	CHB-C1B-NB	2.07	126.45	124.26
18	L	304	CLA	CHB-C1B-NB	2.07	126.45	124.26
18	B	824	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
18	A	810	CLA	CHD-C1D-ND	-2.07	122.55	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	819	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	A	850	BCR	C1-C6-C7	2.07	121.64	115.78
18	B	825	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	2	602	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
18	B	809	CLA	CHB-C1B-NB	2.06	126.44	124.26
18	A	833	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	A	825	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	A	820	CLA	CMB-C2B-C3B	2.06	131.58	126.59
18	B	837	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
18	B	837	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
17	4	606	CHL	C2D-C1D-ND	2.06	111.62	110.10
18	B	831	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	1	604	CLA	CHB-C1B-NB	2.06	126.44	124.26
18	B	833	CLA	CHB-C1B-NB	2.06	126.44	124.26
18	K	203	CLA	CHB-C1B-NB	2.06	126.44	124.26
18	3	611	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	A	805	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	A	824	CLA	CHB-C1B-NB	2.06	126.43	124.26
18	K	204	CLA	CHB-C1B-NB	2.06	126.43	124.26
18	B	824	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
18	2	602	CLA	CMB-C2B-C1B	-2.05	122.24	125.37
18	2	609	CLA	CMB-C2B-C1B	-2.05	122.24	125.37
18	A	809	CLA	CMB-C2B-C1B	-2.05	122.24	125.37
24	A	801	CL0	C4B-CHC-C1C	-2.05	121.47	126.34
18	B	838	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	A	814	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
22	L	305	BCR	C30-C25-C26	-2.05	119.72	122.61
17	1	606	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
18	3	608	CLA	CHB-C1B-NB	2.05	126.43	124.26
18	A	833	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
22	A	851	BCR	C10-C11-C12	-2.05	116.82	123.22
18	3	609	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	A	836	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	A	833	CLA	CHB-C1B-NB	2.05	126.42	124.26
18	A	805	CLA	CHB-C1B-NB	2.05	126.42	124.26
18	B	806	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
18	B	807	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	B	840	CLA	CHB-C1B-NB	2.05	126.42	124.26
18	B	820	CLA	CMB-C2B-C3B	2.05	131.54	126.59
18	4	602	CLA	O2D-CGD-CBD	2.05	114.90	111.27
18	B	822	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
18	A	837	CLA	O2D-CGD-CBD	2.04	114.90	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	814	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
18	A	811	CLA	O2D-CGD-CBD	2.04	114.90	111.27
22	G	204	BCR	C1-C6-C7	2.04	121.56	115.78
18	3	612	CLA	CHC-C4B-NB	2.04	126.42	124.26
18	B	809	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
17	2	606	CHL	OMC-CMC-C2C	-2.04	121.07	125.69
18	2	603	CLA	CHB-C1B-NB	2.04	126.42	124.26
18	A	809	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
18	B	811	CLA	O2D-CGD-CBD	2.04	114.89	111.27
18	A	807	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	A	851	BCR	C34-C9-C8	-2.04	114.87	118.08
18	3	603	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
18	B	817	CLA	CHB-C1B-NB	2.03	126.41	124.26
18	A	808	CLA	CHB-C1B-NB	2.03	126.41	124.26
18	B	821	CLA	CHB-C1B-NB	2.03	126.41	124.26
18	3	609	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	B	811	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
18	A	819	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	L	305	BCR	C21-C20-C19	2.03	129.55	123.22
18	A	826	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
18	1	611	CLA	CHB-C1B-NB	2.03	126.40	124.26
18	B	812	CLA	CHB-C1B-NB	2.03	126.40	124.26
18	B	841	CLA	CHD-C1D-ND	-2.03	122.59	124.45
18	4	608	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
19	2	617	XAT	C17-C1-C2	-2.03	105.46	108.98
22	A	853	BCR	C1-C6-C7	2.03	121.51	115.78
17	1	606	CHL	C1C-C2C-C3C	-2.03	105.51	107.11
18	B	805	CLA	CHB-C1B-NB	2.02	126.40	124.26
17	2	601	CHL	OMC-CMC-C2C	-2.02	121.11	125.69
22	L	301	BCR	C10-C11-C12	2.02	129.53	123.22
18	1	603	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	F	302	CLA	CHB-C1B-NB	2.02	126.40	124.26
18	B	809	CLA	C1-C2-C3	-2.02	122.55	126.04
18	A	836	CLA	CHB-C1B-NB	2.02	126.40	124.26
18	A	838	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
17	4	605	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
18	B	823	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
18	A	822	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
18	B	834	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
18	3	611	CLA	CHB-C1B-NB	2.02	126.39	124.26
18	B	830	CLA	CHB-C1B-NB	2.02	126.39	124.26
18	A	841	CLA	C1-C2-C3	-2.02	122.55	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	823	CLA	CHD-C1D-ND	-2.02	122.60	124.45
18	A	804	CLA	C2A-C1A-CHA	2.02	127.38	123.86
18	A	806	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
18	B	820	CLA	CHB-C1B-NB	2.01	126.39	124.26
18	B	818	CLA	CMB-C2B-C3B	2.01	131.47	126.59
18	B	804	CLA	O2D-CGD-CBD	2.01	114.85	111.27
17	1	606	CHL	CHD-C4C-C3C	-2.01	121.88	124.84
18	G	203	CLA	CHB-C1B-NB	2.01	126.39	124.26
22	3	614	BCR	C30-C25-C26	-2.01	119.78	122.61
18	A	805	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	A	817	CLA	CHB-C1B-NB	2.01	126.39	124.26
18	G	202	CLA	CHD-C1D-ND	-2.01	122.61	124.45
18	A	830	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	B	844	BCR	C20-C19-C18	2.01	132.06	126.42
18	G	201	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
18	1	607	CLA	CHB-C1B-NB	2.01	126.38	124.26
18	B	820	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	A	803	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
17	2	601	CHL	O2A-CGA-CBA	2.01	120.17	112.23
17	1	601	CHL	O2A-CGA-O1A	-2.01	118.53	123.59
17	4	615	CHL	C2A-C1A-CHA	-2.01	120.35	123.86
18	4	604	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	813	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
18	F	303	CLA	CHB-C1B-NB	2.00	126.38	124.26
18	A	823	CLA	CHB-C1B-NB	2.00	126.38	124.26
18	B	833	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
18	A	818	CLA	CHD-C1D-ND	-2.00	122.61	124.45
24	A	801	CL0	C2A-C3A-C4A	-2.00	98.64	101.87
18	4	601	CLA	CHB-C1B-NB	2.00	126.38	124.26
18	B	802	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

There are no chirality outliers.

All (1558) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	601	CHL	CAD-CBD-CGD-O1D
17	1	601	CHL	CAD-CBD-CGD-O2D
17	2	601	CHL	C1A-C2A-CAA-CBA
17	2	601	CHL	C3A-C2A-CAA-CBA
17	3	606	CHL	C2A-CAA-CBA-CGA
17	3	606	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	3	606	CHL	CHA-CBD-CGD-O2D
17	4	605	CHL	C1A-C2A-CAA-CBA
17	4	605	CHL	C3C-C2C-CMC-OMC
17	4	607	CHL	CBD-CGD-O2D-CED
18	1	602	CLA	CBD-CGD-O2D-CED
18	1	604	CLA	C1A-C2A-CAA-CBA
18	1	607	CLA	C1A-C2A-CAA-CBA
18	1	607	CLA	C3A-C2A-CAA-CBA
18	1	609	CLA	CBD-CGD-O2D-CED
18	1	611	CLA	CBD-CGD-O2D-CED
18	1	612	CLA	CHA-CBD-CGD-O2D
18	2	604	CLA	C1A-C2A-CAA-CBA
18	2	604	CLA	C3A-C2A-CAA-CBA
18	2	604	CLA	C4B-C3B-CAB-CBB
18	2	612	CLA	CHA-CBD-CGD-O1D
18	2	612	CLA	CHA-CBD-CGD-O2D
18	2	612	CLA	CBD-CGD-O2D-CED
18	2	613	CLA	CHA-CBD-CGD-O1D
18	2	613	CLA	CHA-CBD-CGD-O2D
18	2	610	CLA	CMA-C3A-C4A-CHB
18	2	611	CLA	CBD-CGD-O2D-CED
18	2	609	CLA	CBD-CGD-O2D-CED
18	2	608	CLA	C1A-C2A-CAA-CBA
18	2	608	CLA	C3A-C2A-CAA-CBA
18	3	603	CLA	C1A-C2A-CAA-CBA
18	3	603	CLA	C3A-C2A-CAA-CBA
18	3	611	CLA	C2B-C3B-CAB-CBB
18	3	611	CLA	C4B-C3B-CAB-CBB
18	4	604	CLA	CBD-CGD-O2D-CED
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
18	4	610	CLA	CHA-CBD-CGD-O1D
18	4	610	CLA	CHA-CBD-CGD-O2D
18	4	614	CLA	CBD-CGD-O2D-CED
18	4	613	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	CAD-CBD-CGD-O1D
18	A	804	CLA	CAD-CBD-CGD-O2D
18	A	802	CLA	C1A-C2A-CAA-CBA
18	A	802	CLA	C3A-C2A-CAA-CBA
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	819	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	A	833	CLA	C4-C3-C5-C6
18	A	828	CLA	CHA-CBD-CGD-O1D
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	835	CLA	C2B-C3B-CAB-CBB
18	A	835	CLA	C4B-C3B-CAB-CBB
18	A	830	CLA	C1A-C2A-CAA-CBA
18	A	830	CLA	C3A-C2A-CAA-CBA
18	A	830	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	O1A-CGA-O2A-C1
18	A	830	CLA	O2A-C1-C2-C3
18	A	830	CLA	C2-C3-C5-C6
18	A	830	CLA	C4-C3-C5-C6
18	A	842	CLA	C1A-C2A-CAA-CBA
18	A	842	CLA	C3A-C2A-CAA-CBA
18	A	827	CLA	C1A-C2A-CAA-CBA
18	A	827	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	809	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	837	CLA	CHA-CBD-CGD-O1D
18	A	837	CLA	CHA-CBD-CGD-O2D
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	839	CLA	C2-C3-C5-C6
18	A	839	CLA	C4-C3-C5-C6
18	A	816	CLA	C3A-C2A-CAA-CBA
18	A	816	CLA	CHA-CBD-CGD-O1D
18	A	816	CLA	CHA-CBD-CGD-O2D
18	A	820	CLA	C3A-C2A-CAA-CBA
18	A	818	CLA	CBD-CGD-O2D-CED
18	A	843	CLA	C1A-C2A-CAA-CBA
18	A	843	CLA	C3A-C2A-CAA-CBA
18	A	843	CLA	C2-C1-O2A-CGA
18	A	829	CLA	CHA-CBD-CGD-O1D
18	A	829	CLA	CHA-CBD-CGD-O2D
18	A	829	CLA	CBD-CGD-O2D-CED
18	A	832	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	A	832	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	C1A-C2A-CAA-CBA
18	A	841	CLA	C3A-C2A-CAA-CBA
18	A	841	CLA	CHA-CBD-CGD-O1D
18	A	841	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	CBD-CGD-O2D-CED
18	A	813	CLA	CHA-CBD-CGD-O2D
18	A	824	CLA	C2B-C3B-CAB-CBB
18	A	824	CLA	C4B-C3B-CAB-CBB
18	B	802	CLA	C3A-C2A-CAA-CBA
18	B	808	CLA	C6-C7-C8-C9
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	803	CLA	CHA-CBD-CGD-O1D
18	B	803	CLA	CHA-CBD-CGD-O2D
18	B	803	CLA	CBD-CGD-O2D-CED
18	B	819	CLA	C2B-C3B-CAB-CBB
18	B	819	CLA	C4B-C3B-CAB-CBB
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C3A-C2A-CAA-CBA
18	B	824	CLA	C2-C3-C5-C6
18	B	824	CLA	C4-C3-C5-C6
18	B	805	CLA	C3A-C2A-CAA-CBA
18	B	805	CLA	C11-C10-C8-C9
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	817	CLA	C4B-C3B-CAB-CBB
18	B	838	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C3A-C2A-CAA-CBA
18	B	836	CLA	CHA-CBD-CGD-O2D
18	B	833	CLA	CHA-CBD-CGD-O1D
18	B	833	CLA	CHA-CBD-CGD-O2D
18	B	823	CLA	C1A-C2A-CAA-CBA
18	B	823	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	CBD-CGD-O2D-CED
18	B	809	CLA	C1A-C2A-CAA-CBA
18	B	809	CLA	C2-C3-C5-C6
18	B	809	CLA	C4-C3-C5-C6
18	B	810	CLA	C6-C7-C8-C10
18	B	818	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	818	CLA	C2-C3-C5-C6
18	B	818	CLA	C4-C3-C5-C6
18	B	828	CLA	C1A-C2A-CAA-CBA
18	B	828	CLA	C3A-C2A-CAA-CBA
18	B	828	CLA	CHA-CBD-CGD-O1D
18	B	828	CLA	CHA-CBD-CGD-O2D
18	F	302	CLA	CBD-CGD-O2D-CED
18	F	301	CLA	C2-C3-C5-C6
18	F	301	CLA	C4-C3-C5-C6
18	G	202	CLA	C1A-C2A-CAA-CBA
18	G	202	CLA	C3A-C2A-CAA-CBA
18	G	201	CLA	CBD-CGD-O2D-CED
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	C3A-C2A-CAA-CBA
18	L	304	CLA	C1A-C2A-CAA-CBA
18	L	304	CLA	C3A-C2A-CAA-CBA
18	L	303	CLA	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	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	C30-C31-C32-C33
19	2	617	XAT	C31-C32-C33-C34
19	2	617	XAT	C31-C32-C33-C40
19	2	617	XAT	C33-C34-C35-C15
19	4	617	XAT	O4-C6-C7-C8
19	4	617	XAT	C11-C12-C13-C14
19	4	617	XAT	C11-C12-C13-C20
20	1	615	LHG	O1-C1-C2-O2
20	1	615	LHG	C2-C3-O3-P
20	1	615	LHG	C4-O6-P-O5
20	1	615	LHG	O10-C23-O8-C6
20	1	615	LHG	C24-C23-O8-C6
20	2	618	LHG	C3-O3-P-O5
20	2	618	LHG	C3-O3-P-O6
20	2	618	LHG	C8-C7-O7-C5
20	2	618	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
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	852	LHG	C2-C3-O3-P
20	B	852	LHG	C3-O3-P-O5
20	B	852	LHG	C4-O6-P-O3
21	2	616	LUT	C21-C26-C27-C28
21	2	616	LUT	C25-C26-C27-C28
21	2	619	LUT	C1-C6-C7-C8
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	A	848	BCR	C5-C6-C7-C8
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	849	BCR	C23-C24-C25-C26
22	A	849	BCR	C23-C24-C25-C30
22	A	851	BCR	C11-C12-C13-C14
22	A	851	BCR	C11-C12-C13-C35
22	B	801	BCR	C1-C6-C7-C8
22	B	801	BCR	C5-C6-C7-C8
22	B	801	BCR	C7-C8-C9-C34
22	B	846	BCR	C37-C22-C23-C24
22	B	846	BCR	C23-C24-C25-C26
22	B	846	BCR	C23-C24-C25-C30
22	B	849	BCR	C20-C21-C22-C23
22	B	849	BCR	C20-C21-C22-C37
22	B	844	BCR	C12-C13-C14-C15
22	B	844	BCR	C35-C13-C14-C15
22	F	304	BCR	C15-C16-C17-C18
22	J	102	BCR	C7-C8-C9-C10
22	J	102	BCR	C7-C8-C9-C34
22	K	205	BCR	C10-C11-C12-C13
27	B	850	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
18	1	608	CLA	O1D-CGD-O2D-CED
18	2	609	CLA	O1D-CGD-O2D-CED
18	4	604	CLA	O1D-CGD-O2D-CED
18	B	802	CLA	O1D-CGD-O2D-CED
18	B	822	CLA	O1D-CGD-O2D-CED
18	B	835	CLA	O1D-CGD-O2D-CED
18	H	201	CLA	O1D-CGD-O2D-CED
18	3	607	CLA	O1D-CGD-O2D-CED
18	4	609	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	O1D-CGD-O2D-CED
18	A	841	CLA	O1D-CGD-O2D-CED
18	B	803	CLA	O1D-CGD-O2D-CED
18	F	301	CLA	O1D-CGD-O2D-CED
18	K	204	CLA	O1D-CGD-O2D-CED
17	2	607	CHL	CBD-CGD-O2D-CED
17	3	606	CHL	CBD-CGD-O2D-CED
17	4	606	CHL	CBD-CGD-O2D-CED
18	1	605	CLA	CBD-CGD-O2D-CED
18	1	608	CLA	CBD-CGD-O2D-CED
18	2	608	CLA	CBD-CGD-O2D-CED
18	3	607	CLA	CBD-CGD-O2D-CED
18	3	608	CLA	CBD-CGD-O2D-CED
18	4	609	CLA	CBD-CGD-O2D-CED
18	4	612	CLA	CBD-CGD-O2D-CED
18	A	802	CLA	CBD-CGD-O2D-CED
18	A	824	CLA	CBD-CGD-O2D-CED
18	B	802	CLA	CBD-CGD-O2D-CED
18	B	830	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	CBD-CGD-O2D-CED
18	B	835	CLA	CBD-CGD-O2D-CED
18	F	301	CLA	CBD-CGD-O2D-CED
18	3	602	CLA	O1A-CGA-O2A-C1
18	A	803	CLA	O1A-CGA-O2A-C1
18	1	602	CLA	O1D-CGD-O2D-CED
18	1	605	CLA	O1D-CGD-O2D-CED
18	2	611	CLA	O1D-CGD-O2D-CED
18	3	608	CLA	O1D-CGD-O2D-CED
18	A	824	CLA	O1D-CGD-O2D-CED
18	F	302	CLA	O1D-CGD-O2D-CED
18	1	611	CLA	O1D-CGD-O2D-CED
18	2	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	4	614	CLA	O1D-CGD-O2D-CED
18	A	829	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
17	2	615	CHL	CBD-CGD-O2D-CED
18	2	604	CLA	CBD-CGD-O2D-CED
18	A	832	CLA	CBD-CGD-O2D-CED
18	A	814	CLA	CBD-CGD-O2D-CED
18	A	811	CLA	CBD-CGD-O2D-CED
18	B	816	CLA	CBD-CGD-O2D-CED
18	A	839	CLA	O1A-CGA-O2A-C1
18	A	820	CLA	O1A-CGA-O2A-C1
18	B	802	CLA	O1A-CGA-O2A-C1
18	1	609	CLA	O1D-CGD-O2D-CED
17	4	607	CHL	O1D-CGD-O2D-CED
18	B	814	CLA	CBD-CGD-O2D-CED
20	2	618	LHG	O9-C7-O7-C5
18	4	602	CLA	C3-C5-C6-C7
18	A	828	CLA	C3-C5-C6-C7
18	A	830	CLA	C3-C5-C6-C7
18	A	807	CLA	C3-C5-C6-C7
18	A	803	CLA	C3-C5-C6-C7
18	A	844	CLA	C3-C5-C6-C7
18	A	843	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7
18	A	814	CLA	C3-C5-C6-C7
18	B	808	CLA	C3-C5-C6-C7
18	B	814	CLA	C3-C5-C6-C7
18	B	840	CLA	C3-C5-C6-C7
18	B	822	CLA	C3-C5-C6-C7
18	H	201	CLA	C3-C5-C6-C7
18	A	839	CLA	CBA-CGA-O2A-C1
18	B	802	CLA	CBA-CGA-O2A-C1
20	B	851	LHG	C8-C7-O7-C5
17	3	606	CHL	O1D-CGD-O2D-CED
18	A	813	CLA	CBD-CGD-O2D-CED
18	B	836	CLA	O1A-CGA-O2A-C1
17	1	601	CHL	C4-C3-C5-C6
18	2	602	CLA	C4-C3-C5-C6
18	A	833	CLA	C2-C3-C5-C6
18	B	815	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	2	607	CHL	C2A-CAA-CBA-CGA
17	2	601	CHL	C2A-CAA-CBA-CGA
18	2	603	CLA	C2A-CAA-CBA-CGA
18	A	830	CLA	C2A-CAA-CBA-CGA
18	A	838	CLA	C2A-CAA-CBA-CGA
18	B	802	CLA	C2A-CAA-CBA-CGA
18	B	813	CLA	C2A-CAA-CBA-CGA
18	B	817	CLA	C2A-CAA-CBA-CGA
18	B	839	CLA	C2A-CAA-CBA-CGA
18	H	201	CLA	C2A-CAA-CBA-CGA
24	A	801	CL0	C2A-CAA-CBA-CGA
18	2	609	CLA	O1A-CGA-O2A-C1
18	L	303	CLA	O1A-CGA-O2A-C1
18	B	827	CLA	C3-C5-C6-C7
18	2	609	CLA	CBA-CGA-O2A-C1
18	A	820	CLA	CBA-CGA-O2A-C1
18	B	827	CLA	CBA-CGA-O2A-C1
18	L	303	CLA	CBA-CGA-O2A-C1
18	1	604	CLA	CBD-CGD-O2D-CED
18	K	203	CLA	CBD-CGD-O2D-CED
18	2	608	CLA	O1D-CGD-O2D-CED
20	B	851	LHG	O9-C7-O7-C5
18	A	818	CLA	O1A-CGA-O2A-C1
18	A	843	CLA	O1A-CGA-O2A-C1
18	A	811	CLA	O1A-CGA-O2A-C1
18	B	827	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	850	BCR	C13-C14-C15-C16
22	A	850	BCR	C15-C16-C17-C18
22	A	853	BCR	C9-C10-C11-C12
22	A	849	BCR	C15-C16-C17-C18
22	A	849	BCR	C19-C20-C21-C22
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
17	2	601	CHL	CBD-CGD-O2D-CED
18	A	803	CLA	CBD-CGD-O2D-CED
18	B	823	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	818	CLA	C3-C5-C6-C7
18	1	603	CLA	CBA-CGA-O2A-C1
18	A	818	CLA	CBA-CGA-O2A-C1
18	B	836	CLA	CBA-CGA-O2A-C1
18	4	612	CLA	O1D-CGD-O2D-CED
18	B	827	CLA	CBD-CGD-O2D-CED
17	4	606	CHL	O1D-CGD-O2D-CED
18	B	830	CLA	O1D-CGD-O2D-CED
18	B	810	CLA	O1D-CGD-O2D-CED
18	A	819	CLA	C3-C5-C6-C7
18	B	806	CLA	C3-C5-C6-C7
18	1	604	CLA	CBA-CGA-O2A-C1
18	A	843	CLA	CBA-CGA-O2A-C1
18	A	811	CLA	CBA-CGA-O2A-C1
17	2	607	CHL	O1D-CGD-O2D-CED
20	1	615	LHG	C5-C4-O6-P
18	A	819	CLA	C4-C3-C5-C6
26	B	842	PQN	C14-C13-C15-C16
18	2	602	CLA	C2-C3-C5-C6
18	A	819	CLA	C2-C3-C5-C6
26	B	842	PQN	C12-C13-C15-C16
18	A	838	CLA	CBD-CGD-O2D-CED
18	A	809	CLA	C2A-CAA-CBA-CGA
18	A	843	CLA	C2A-CAA-CBA-CGA
18	1	603	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	CBA-CGA-O2A-C1
18	A	814	CLA	O1D-CGD-O2D-CED
18	1	604	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C1-C2-C3-O3
18	2	612	CLA	C3-C5-C6-C7
18	A	841	CLA	C3-C5-C6-C7
18	L	303	CLA	C3-C5-C6-C7
18	A	832	CLA	O1D-CGD-O2D-CED
18	1	602	CLA	CBA-CGA-O2A-C1
18	A	802	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	CBA-CGA-O2A-C1
18	A	842	CLA	CBA-CGA-O2A-C1
18	A	825	CLA	CBA-CGA-O2A-C1
18	A	814	CLA	CBA-CGA-O2A-C1
18	B	814	CLA	CBA-CGA-O2A-C1
18	B	840	CLA	CBA-CGA-O2A-C1
18	B	811	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	F	301	CLA	CBA-CGA-O2A-C1
18	A	835	CLA	C8-C10-C11-C12
18	A	822	CLA	C15-C16-C17-C18
18	B	802	CLA	C15-C16-C17-C18
18	B	814	CLA	O1A-CGA-O2A-C1
18	B	811	CLA	O1A-CGA-O2A-C1
18	F	301	CLA	O1A-CGA-O2A-C1
17	1	601	CHL	C2-C3-C5-C6
18	3	601	CLA	C11-C10-C8-C9
18	4	612	CLA	C6-C7-C8-C9
18	A	826	CLA	C11-C10-C8-C9
18	A	835	CLA	C11-C10-C8-C9
18	A	807	CLA	C11-C10-C8-C9
18	A	803	CLA	C6-C7-C8-C9
18	A	812	CLA	C6-C7-C8-C9
18	A	820	CLA	C11-C10-C8-C9
18	A	841	CLA	C14-C13-C15-C16
18	B	802	CLA	C11-C12-C13-C14
18	B	808	CLA	C14-C13-C15-C16
18	B	825	CLA	C11-C10-C8-C9
18	B	825	CLA	C11-C12-C13-C14
18	B	805	CLA	C6-C7-C8-C9
18	B	805	CLA	C14-C13-C15-C16
18	B	840	CLA	C6-C7-C8-C9
18	B	809	CLA	C6-C7-C8-C9
18	H	201	CLA	C6-C7-C8-C9
18	A	812	CLA	CBD-CGD-O2D-CED
18	4	602	CLA	C5-C6-C7-C8
18	A	802	CLA	C13-C15-C16-C17
18	A	812	CLA	C10-C11-C12-C13
18	A	839	CLA	C2A-CAA-CBA-CGA
18	A	829	CLA	C2A-CAA-CBA-CGA
18	A	814	CLA	C2A-CAA-CBA-CGA
18	B	820	CLA	C2A-CAA-CBA-CGA
19	1	614	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	C7-C8-C9-C34
22	B	845	BCR	C36-C18-C19-C20
22	B	845	BCR	C37-C22-C23-C24
22	F	304	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
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	B	846	BCR	C7-C8-C9-C10
22	B	845	BCR	C17-C18-C19-C20
22	B	845	BCR	C21-C22-C23-C24
22	F	304	BCR	C11-C12-C13-C14
22	L	306	BCR	C7-C8-C9-C10
22	L	306	BCR	C21-C22-C23-C24
18	B	840	CLA	O1A-CGA-O2A-C1
18	B	808	CLA	C13-C15-C16-C17
18	B	837	CLA	C15-C16-C17-C18
18	B	841	CLA	C8-C10-C11-C12
18	4	601	CLA	CBA-CGA-O2A-C1
18	B	841	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	CBA-CGA-O2A-C1
18	A	822	CLA	CBA-CGA-O2A-C1
18	B	813	CLA	CBA-CGA-O2A-C1
18	A	820	CLA	C5-C6-C7-C8
18	B	822	CLA	C13-C15-C16-C17
18	B	826	CLA	C5-C6-C7-C8
18	B	809	CLA	C5-C6-C7-C8
18	A	825	CLA	O1A-CGA-O2A-C1
18	A	826	CLA	C8-C10-C11-C12
18	A	828	CLA	C5-C6-C7-C8
18	A	806	CLA	C10-C11-C12-C13
18	A	806	CLA	C13-C15-C16-C17
18	B	805	CLA	C5-C6-C7-C8
18	B	837	CLA	C5-C6-C7-C8
18	L	303	CLA	C10-C11-C12-C13
17	2	615	CHL	O1D-CGD-O2D-CED
20	1	615	LHG	C7-C8-C9-C10
20	B	851	LHG	C23-C24-C25-C26
18	2	612	CLA	C8-C10-C11-C12
18	A	807	CLA	C5-C6-C7-C8
18	B	824	CLA	C8-C10-C11-C12
18	B	826	CLA	C8-C10-C11-C12
18	A	832	CLA	CBA-CGA-O2A-C1
18	A	811	CLA	O1D-CGD-O2D-CED
17	2	606	CHL	CBD-CGD-O2D-CED
18	2	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	B	809	CLA	CBD-CGD-O2D-CED
18	B	831	CLA	C2A-CAA-CBA-CGA
20	1	615	LHG	C11-C10-C9-C8
18	A	803	CLA	C8-C10-C11-C12
18	B	832	CLA	C15-C16-C17-C18
18	2	604	CLA	O1D-CGD-O2D-CED
18	2	602	CLA	C6-C7-C8-C10
18	A	804	CLA	C6-C7-C8-C10
18	B	802	CLA	C11-C10-C8-C7
18	B	827	CLA	C11-C12-C13-C15
18	1	602	CLA	O1A-CGA-O2A-C1
18	A	835	CLA	O1A-CGA-O2A-C1
18	A	814	CLA	O1A-CGA-O2A-C1
17	1	601	CHL	C2A-CAA-CBA-CGA
18	A	818	CLA	C2A-CAA-CBA-CGA
18	B	832	CLA	C2A-CAA-CBA-CGA
18	B	816	CLA	O1D-CGD-O2D-CED
18	2	602	CLA	C15-C16-C17-C18
18	A	812	CLA	C5-C6-C7-C8
18	B	813	CLA	C13-C15-C16-C17
18	B	827	CLA	C8-C10-C11-C12
18	B	828	CLA	C5-C6-C7-C8
18	B	828	CLA	C10-C11-C12-C13
18	B	828	CLA	C13-C15-C16-C17
18	H	201	CLA	C8-C10-C11-C12
18	A	823	CLA	CBD-CGD-O2D-CED
19	2	617	XAT	C10-C11-C12-C13
18	B	814	CLA	O1D-CGD-O2D-CED
20	1	615	LHG	O2-C2-C3-O3
18	1	602	CLA	C3-C5-C6-C7
18	A	828	CLA	C8-C10-C11-C12
18	A	841	CLA	C5-C6-C7-C8
18	B	814	CLA	C8-C10-C11-C12
18	A	842	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	O1A-CGA-O2A-C1
18	A	819	CLA	C5-C6-C7-C8
18	A	835	CLA	C10-C11-C12-C13
18	A	812	CLA	C8-C10-C11-C12
18	A	829	CLA	C15-C16-C17-C18
18	B	814	CLA	C5-C6-C7-C8
18	B	805	CLA	C13-C15-C16-C17
18	B	840	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	B	811	CLA	C5-C6-C7-C8
18	A	802	CLA	O1A-CGA-O2A-C1
18	A	819	CLA	O1A-CGA-O2A-C1
18	A	822	CLA	O1A-CGA-O2A-C1
18	B	813	CLA	O1A-CGA-O2A-C1
18	A	806	CLA	C15-C16-C17-C18
18	A	842	CLA	C8-C10-C11-C12
18	B	813	CLA	C15-C16-C17-C18
18	B	841	CLA	C13-C15-C16-C17
20	1	615	LHG	C3-O3-P-O6
18	B	837	CLA	C3-C5-C6-C7
17	1	601	CHL	CBA-CGA-O2A-C1
18	B	805	CLA	C8-C10-C11-C12
18	A	813	CLA	O1D-CGD-O2D-CED
18	1	603	CLA	C4-C3-C5-C6
18	B	822	CLA	C10-C11-C12-C13
18	3	609	CLA	C2A-CAA-CBA-CGA
18	A	819	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C2A-CAA-CBA-CGA
18	B	828	CLA	C2A-CAA-CBA-CGA
18	G	203	CLA	C2A-CAA-CBA-CGA
18	G	201	CLA	C2A-CAA-CBA-CGA
18	A	838	CLA	CBA-CGA-O2A-C1
24	A	801	CL0	C10-C11-C12-C13
20	1	615	LHG	C33-C34-C35-C36
18	4	608	CLA	CBD-CGD-O2D-CED
18	B	839	CLA	C5-C6-C7-C8
19	2	617	XAT	C11-C10-C9-C19
19	2	617	XAT	C20-C13-C14-C15
21	3	613	LUT	C11-C10-C9-C19
22	A	852	BCR	C35-C13-C14-C15
22	B	844	BCR	C16-C17-C18-C36
22	F	304	BCR	C11-C10-C9-C34
22	F	304	BCR	C35-C13-C14-C15
18	B	802	CLA	C3-C5-C6-C7
18	B	815	CLA	O1D-CGD-O2D-CED
18	A	839	CLA	C6-C7-C8-C10
18	B	824	CLA	C16-C17-C18-C20
18	B	840	CLA	C16-C17-C18-C20
18	B	841	CLA	CBA-CGA-O2A-C1
18	1	604	CLA	O1D-CGD-O2D-CED
26	A	855	PQN	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
20	1	615	LHG	C28-C29-C30-C31
18	K	203	CLA	O1D-CGD-O2D-CED
18	A	832	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C24-C25-C26-C27
19	2	617	XAT	C11-C10-C9-C8
19	2	617	XAT	C12-C13-C14-C15
21	3	613	LUT	C11-C10-C9-C8
22	A	852	BCR	C12-C13-C14-C15
22	B	844	BCR	C16-C17-C18-C19
22	F	304	BCR	C11-C10-C9-C8
22	F	304	BCR	C12-C13-C14-C15
23	4	620	LMG	C2-C1-O1-C7
18	L	303	CLA	C8-C10-C11-C12
18	A	822	CLA	C2-C3-C5-C6
18	A	809	CLA	C11-C12-C13-C14
18	A	820	CLA	C11-C12-C13-C14
18	B	806	CLA	C6-C7-C8-C9
18	B	810	CLA	C14-C13-C15-C16
18	B	803	CLA	C13-C15-C16-C17
18	4	603	CLA	C2A-CAA-CBA-CGA
18	B	841	CLA	C2A-CAA-CBA-CGA
17	1	601	CHL	O1A-CGA-O2A-C1
20	1	615	LHG	O1-C1-C2-C3
19	1	614	XAT	C11-C12-C13-C14
18	2	602	CLA	C3-C5-C6-C7
18	A	834	CLA	C3-C5-C6-C7
18	A	814	CLA	C13-C15-C16-C17
18	B	805	CLA	C10-C11-C12-C13
27	B	850	DGD	C2B-C1B-O2G-C2G
20	1	615	LHG	C11-C12-C13-C14
18	4	610	CLA	C4B-C3B-CAB-CBB
18	4	611	CLA	C4B-C3B-CAB-CBB
18	A	803	CLA	C4B-C3B-CAB-CBB
18	A	832	CLA	C4B-C3B-CAB-CBB
18	B	839	CLA	C4B-C3B-CAB-CBB
18	B	823	CLA	C4B-C3B-CAB-CBB
18	B	835	CLA	C4B-C3B-CAB-CBB
18	K	201	CLA	C4B-C3B-CAB-CBB
18	L	302	CLA	C4B-C3B-CAB-CBB
18	2	612	CLA	C16-C17-C18-C19
18	A	839	CLA	C6-C7-C8-C9
18	B	824	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	B	840	CLA	C16-C17-C18-C19
18	A	820	CLA	C13-C15-C16-C17
20	1	615	LHG	C27-C28-C29-C30
27	B	850	DGD	C9A-CAA-CBA-CCA
18	A	804	CLA	C10-C11-C12-C13
18	A	838	CLA	O1A-CGA-O2A-C1
18	B	819	CLA	CBD-CGD-O2D-CED
18	1	604	CLA	C3A-C2A-CAA-CBA
18	1	605	CLA	C3A-C2A-CAA-CBA
18	1	612	CLA	C3A-C2A-CAA-CBA
18	2	611	CLA	C3A-C2A-CAA-CBA
18	A	815	CLA	C3A-C2A-CAA-CBA
18	A	810	CLA	C3A-C2A-CAA-CBA
18	B	821	CLA	C3A-C2A-CAA-CBA
18	B	825	CLA	C3A-C2A-CAA-CBA
18	B	824	CLA	C3A-C2A-CAA-CBA
18	B	838	CLA	C3A-C2A-CAA-CBA
18	B	815	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	C3A-C2A-CAA-CBA
18	B	809	CLA	C3A-C2A-CAA-CBA
18	B	810	CLA	C3A-C2A-CAA-CBA
18	A	843	CLA	C5-C6-C7-C8
17	2	601	CHL	O1D-CGD-O2D-CED
18	2	612	CLA	C16-C17-C18-C20
18	A	812	CLA	C16-C17-C18-C20
20	1	615	LHG	C25-C26-C27-C28
18	B	823	CLA	O1D-CGD-O2D-CED
27	B	850	DGD	O1B-C1B-O2G-C2G
18	3	602	CLA	CBD-CGD-O2D-CED
18	A	820	CLA	CBD-CGD-O2D-CED
22	B	844	BCR	C14-C15-C16-C17
18	3	602	CLA	C4-C3-C5-C6
18	3	601	CLA	C4-C3-C5-C6
18	A	804	CLA	C4-C3-C5-C6
18	A	822	CLA	C4-C3-C5-C6
18	3	601	CLA	C2-C3-C5-C6
18	A	804	CLA	C2-C3-C5-C6
18	A	803	CLA	O1D-CGD-O2D-CED
18	1	611	CLA	C2A-CAA-CBA-CGA
18	B	841	CLA	C16-C17-C18-C20
18	1	611	CLA	C2B-C3B-CAB-CBB
18	2	604	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	3	609	CLA	C2B-C3B-CAB-CBB
18	4	610	CLA	C2B-C3B-CAB-CBB
18	4	611	CLA	C2B-C3B-CAB-CBB
18	4	614	CLA	C2B-C3B-CAB-CBB
18	A	803	CLA	C2B-C3B-CAB-CBB
18	A	832	CLA	C2B-C3B-CAB-CBB
18	B	817	CLA	C2B-C3B-CAB-CBB
18	B	839	CLA	C2B-C3B-CAB-CBB
18	B	823	CLA	C2B-C3B-CAB-CBB
18	B	835	CLA	C2B-C3B-CAB-CBB
18	K	201	CLA	C2B-C3B-CAB-CBB
18	L	302	CLA	C2B-C3B-CAB-CBB
18	B	805	CLA	C3-C5-C6-C7
18	B	841	CLA	O1A-CGA-O2A-C1
20	1	615	LHG	C14-C15-C16-C17
18	A	812	CLA	C2-C1-O2A-CGA
18	L	303	CLA	C15-C16-C17-C18
18	B	832	CLA	C3-C5-C6-C7
21	1	616	LUT	C5-C6-C7-C8
21	4	616	LUT	C5-C6-C7-C8
22	4	618	BCR	C1-C6-C7-C8
22	4	618	BCR	C5-C6-C7-C8
22	4	618	BCR	C23-C24-C25-C26
22	A	848	BCR	C1-C6-C7-C8
22	A	852	BCR	C5-C6-C7-C8
22	B	849	BCR	C23-C24-C25-C26
22	B	845	BCR	C5-C6-C7-C8
22	B	844	BCR	C23-C24-C25-C26
22	B	844	BCR	C23-C24-C25-C30
22	G	204	BCR	C23-C24-C25-C26
22	G	204	BCR	C23-C24-C25-C30
18	B	806	CLA	C5-C6-C7-C8
20	1	615	LHG	C26-C27-C28-C29
18	3	601	CLA	C11-C10-C8-C7
18	A	826	CLA	C11-C10-C8-C7
18	A	807	CLA	C11-C10-C8-C7
18	A	809	CLA	C11-C12-C13-C15
18	A	803	CLA	C6-C7-C8-C10
18	A	829	CLA	C11-C10-C8-C7
18	A	831	CLA	C11-C10-C8-C7
18	A	831	CLA	C12-C13-C15-C16
18	B	805	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	B	806	CLA	C6-C7-C8-C10
18	B	806	CLA	C11-C12-C13-C15
18	B	827	CLA	C12-C13-C15-C16
18	B	810	CLA	C12-C13-C15-C16
18	4	601	CLA	O1A-CGA-O2A-C1
18	A	834	CLA	CBA-CGA-O2A-C1
18	A	813	CLA	CBA-CGA-O2A-C1
18	B	829	CLA	CBA-CGA-O2A-C1
18	1	602	CLA	C2A-CAA-CBA-CGA
18	A	802	CLA	C2A-CAA-CBA-CGA
18	A	806	CLA	C2A-CAA-CBA-CGA
18	A	832	CLA	C2A-CAA-CBA-CGA
18	B	811	CLA	C2A-CAA-CBA-CGA
18	H	201	CLA	C5-C6-C7-C8
18	A	806	CLA	C8-C10-C11-C12
18	1	603	CLA	C5-C6-C7-C8
22	B	801	BCR	C6-C7-C8-C9
17	2	605	CHL	CBD-CGD-O2D-CED
18	A	811	CLA	C16-C17-C18-C19
18	A	838	CLA	O1D-CGD-O2D-CED
22	L	301	BCR	C18-C19-C20-C21
18	A	812	CLA	C13-C15-C16-C17
18	B	827	CLA	O1D-CGD-O2D-CED
23	4	619	LMG	C2-C1-O1-C7
18	B	828	CLA	C15-C16-C17-C18
23	4	619	LMG	O6-C5-C6-O5
18	B	811	CLA	C4-C3-C5-C6
18	1	603	CLA	C2-C3-C5-C6
18	B	827	CLA	C2-C3-C5-C6
18	2	602	CLA	C6-C7-C8-C9
18	A	806	CLA	C11-C10-C8-C9
18	A	831	CLA	C14-C13-C15-C16
18	B	802	CLA	C11-C10-C8-C9
18	B	814	CLA	C11-C12-C13-C14
18	B	805	CLA	C11-C12-C13-C14
18	B	806	CLA	C11-C12-C13-C14
18	A	826	CLA	C3-C5-C6-C7
18	B	803	CLA	C3-C5-C6-C7
18	B	816	CLA	C3-C5-C6-C7
18	4	604	CLA	C2A-CAA-CBA-CGA
18	A	813	CLA	C2A-CAA-CBA-CGA
18	B	818	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	1	615	LHG	C13-C14-C15-C16
18	B	841	CLA	C10-C11-C12-C13
20	1	615	LHG	C16-C17-C18-C19
17	4	607	CHL	C1A-C2A-CAA-CBA
18	1	605	CLA	C1A-C2A-CAA-CBA
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	609	CLA	C1A-C2A-CAA-CBA
18	4	604	CLA	C1A-C2A-CAA-CBA
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	812	CLA	C1A-C2A-CAA-CBA
18	A	815	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C1A-C2A-CAA-CBA
18	B	802	CLA	C1A-C2A-CAA-CBA
18	B	821	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C1A-C2A-CAA-CBA
18	B	824	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	815	CLA	C1A-C2A-CAA-CBA
18	B	822	CLA	C1A-C2A-CAA-CBA
18	B	810	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C1A-C2A-CAA-CBA
18	F	302	CLA	C1A-C2A-CAA-CBA
18	H	201	CLA	C1A-C2A-CAA-CBA
18	K	203	CLA	C1A-C2A-CAA-CBA
18	B	816	CLA	C6-C7-C8-C10
18	B	841	CLA	C16-C17-C18-C19
20	1	615	LHG	C29-C30-C31-C32
18	3	601	CLA	C8-C10-C11-C12
18	A	818	CLA	C5-C6-C7-C8
18	A	814	CLA	C10-C11-C12-C13
24	A	801	CL0	C3-C5-C6-C7
18	A	813	CLA	O1A-CGA-O2A-C1
18	B	825	CLA	CBA-CGA-O2A-C1
18	B	827	CLA	C10-C11-C12-C13
18	B	827	CLA	C4-C3-C5-C6
18	A	835	CLA	C2-C3-C5-C6
18	B	835	CLA	C3A-C2A-CAA-CBA
18	A	830	CLA	C8-C10-C11-C12
18	A	834	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	B	816	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	C16-C17-C18-C20
18	H	201	CLA	C11-C12-C13-C14
18	3	601	CLA	C3-C5-C6-C7
20	B	852	LHG	C4-C5-C6-O8
18	A	809	CLA	CBA-CGA-O2A-C1
18	B	810	CLA	C5-C6-C7-C8
18	B	829	CLA	O1A-CGA-O2A-C1
27	B	850	DGD	CCA-CDA-CEA-CFA
18	B	825	CLA	C10-C11-C12-C13
18	B	829	CLA	C11-C10-C8-C9
27	B	850	DGD	O6D-C1D-O3G-C3G
20	1	615	LHG	C35-C36-C37-C38
18	B	817	CLA	CBA-CGA-O2A-C1
24	A	801	CL0	CAA-CBA-CGA-O2A
18	A	807	CLA	C8-C10-C11-C12
18	B	817	CLA	C5-C6-C7-C8
18	A	835	CLA	C4-C3-C5-C6
18	A	803	CLA	C4-C3-C5-C6
18	B	813	CLA	C4-C3-C5-C6
18	A	803	CLA	C2-C3-C5-C6
18	B	813	CLA	C2-C3-C5-C6
18	B	816	CLA	C6-C7-C8-C9
18	B	827	CLA	C16-C17-C18-C20
18	A	812	CLA	CBA-CGA-O2A-C1
20	B	851	LHG	C26-C27-C28-C29
20	2	618	LHG	C6-C5-O7-C7
18	2	612	CLA	C13-C15-C16-C17
18	A	807	CLA	C2-C1-O2A-CGA
18	A	820	CLA	C2-C1-O2A-CGA
18	A	814	CLA	C2-C1-O2A-CGA
18	B	827	CLA	C2-C1-O2A-CGA
18	B	809	CLA	O1D-CGD-O2D-CED
18	A	819	CLA	C11-C12-C13-C14
18	2	602	CLA	O1D-CGD-O2D-CED
18	A	812	CLA	O1D-CGD-O2D-CED
18	B	824	CLA	CBA-CGA-O2A-C1
18	B	805	CLA	CBA-CGA-O2A-C1
24	A	801	CL0	CBA-CGA-O2A-C1
18	1	609	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C15-C16-C17-C18
17	2	606	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	B	825	CLA	O1A-CGA-O2A-C1
18	3	602	CLA	C3-C5-C6-C7
18	A	835	CLA	C15-C16-C17-C18
18	A	844	CLA	C5-C6-C7-C8
17	1	601	CHL	C3-C5-C6-C7
18	A	840	CLA	C3-C5-C6-C7
18	4	601	CLA	CAA-CBA-CGA-O2A
18	B	827	CLA	C15-C16-C17-C18
23	4	619	LMG	C30-C31-C32-C33
18	2	602	CLA	C12-C13-C15-C16
18	A	804	CLA	C12-C13-C15-C16
18	A	835	CLA	C11-C10-C8-C7
18	A	835	CLA	C11-C12-C13-C15
18	A	842	CLA	C11-C10-C8-C7
18	A	803	CLA	C11-C12-C13-C15
18	A	812	CLA	C6-C7-C8-C10
18	A	844	CLA	C12-C13-C15-C16
18	B	802	CLA	C11-C12-C13-C15
18	B	808	CLA	C12-C13-C15-C16
18	B	814	CLA	C11-C10-C8-C7
18	B	814	CLA	C11-C12-C13-C15
18	B	824	CLA	C12-C13-C15-C16
18	B	817	CLA	C6-C7-C8-C10
18	B	841	CLA	C6-C7-C8-C10
18	B	841	CLA	C12-C13-C15-C16
18	B	809	CLA	C12-C13-C15-C16
18	H	201	CLA	C6-C7-C8-C10
18	L	303	CLA	C11-C12-C13-C15
24	A	801	CL0	C11-C12-C13-C15
23	4	620	LMG	O7-C10-C11-C12
18	A	804	CLA	C14-C13-C15-C16
18	A	806	CLA	C14-C13-C15-C16
18	A	835	CLA	C11-C12-C13-C14
18	A	842	CLA	C11-C10-C8-C9
18	A	803	CLA	C11-C12-C13-C14
18	A	803	CLA	C14-C13-C15-C16
18	A	812	CLA	C14-C13-C15-C16
18	A	844	CLA	C14-C13-C15-C16
18	A	818	CLA	C6-C7-C8-C9
18	A	818	CLA	C11-C10-C8-C9
18	A	814	CLA	C14-C13-C15-C16
18	A	831	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
18	B	808	CLA	C11-C12-C13-C14
18	B	824	CLA	C14-C13-C15-C16
18	B	827	CLA	C14-C13-C15-C16
18	B	841	CLA	C6-C7-C8-C9
18	B	841	CLA	C11-C12-C13-C14
18	B	809	CLA	C14-C13-C15-C16
18	B	834	CLA	C6-C7-C8-C9
18	2	611	CLA	C2A-CAA-CBA-CGA
18	A	823	CLA	O1D-CGD-O2D-CED
18	B	841	CLA	O1D-CGD-O2D-CED
22	K	205	BCR	C7-C8-C9-C34
18	B	827	CLA	C16-C17-C18-C19
22	B	846	BCR	C21-C22-C23-C24
18	A	811	CLA	C8-C10-C11-C12
18	B	817	CLA	O1A-CGA-O2A-C1
18	1	611	CLA	C4B-C3B-CAB-CBB
18	3	610	CLA	C4B-C3B-CAB-CBB
18	3	609	CLA	C4B-C3B-CAB-CBB
18	3	602	CLA	C4B-C3B-CAB-CBB
18	3	603	CLA	C4B-C3B-CAB-CBB
18	4	614	CLA	C4B-C3B-CAB-CBB
18	A	819	CLA	C4B-C3B-CAB-CBB
18	A	834	CLA	C4B-C3B-CAB-CBB
18	A	818	CLA	C4B-C3B-CAB-CBB
18	A	829	CLA	C4B-C3B-CAB-CBB
18	B	807	CLA	C4B-C3B-CAB-CBB
18	G	202	CLA	C4B-C3B-CAB-CBB
18	G	201	CLA	C4B-C3B-CAB-CBB
18	K	204	CLA	C4B-C3B-CAB-CBB
18	A	829	CLA	C5-C6-C7-C8
20	1	615	LHG	O6-C4-C5-C6
18	B	816	CLA	C5-C6-C7-C8
18	B	821	CLA	CAA-CBA-CGA-O2A
18	A	844	CLA	C4-C3-C5-C6
18	3	602	CLA	C2-C3-C5-C6
20	1	615	LHG	C18-C19-C20-C21
20	A	846	LHG	C27-C28-C29-C30
18	B	802	CLA	C8-C10-C11-C12
18	A	809	CLA	O1A-CGA-O2A-C1
18	1	605	CLA	CBA-CGA-O2A-C1
18	4	612	CLA	CBA-CGA-O2A-C1
18	A	806	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	B	826	CLA	CBA-CGA-O2A-C1
27	B	850	DGD	C5B-C6B-C7B-C8B
20	2	618	LHG	C5-C4-O6-P
20	B	852	LHG	C5-C4-O6-P
18	A	813	CLA	C3A-C2A-CAA-CBA
18	B	819	CLA	C3A-C2A-CAA-CBA
18	H	201	CLA	C3A-C2A-CAA-CBA
18	K	204	CLA	C3A-C2A-CAA-CBA
18	4	608	CLA	O1D-CGD-O2D-CED
18	A	804	CLA	C8-C10-C11-C12
18	A	809	CLA	C16-C17-C18-C19
18	H	201	CLA	C11-C12-C13-C15
18	A	826	CLA	CBA-CGA-O2A-C1
18	A	814	CLA	C15-C16-C17-C18
18	2	604	CLA	C2A-CAA-CBA-CGA
27	B	850	DGD	C1G-C2G-C3G-O3G
24	A	801	CL0	O1A-CGA-O2A-C1
18	A	828	CLA	C15-C16-C17-C18
18	B	817	CLA	CAA-CBA-CGA-O2A
17	2	605	CHL	C3C-C2C-CMC-OMC
18	B	805	CLA	O1A-CGA-O2A-C1
18	A	833	CLA	C3-C5-C6-C7
18	1	612	CLA	C2A-CAA-CBA-CGA
18	2	612	CLA	C5-C6-C7-C8
18	2	602	CLA	CBA-CGA-O2A-C1
18	A	812	CLA	O1A-CGA-O2A-C1
18	B	824	CLA	O1A-CGA-O2A-C1
18	A	812	CLA	C16-C17-C18-C19
18	3	610	CLA	C2B-C3B-CAB-CBB
18	3	602	CLA	C2B-C3B-CAB-CBB
18	3	603	CLA	C2B-C3B-CAB-CBB
18	A	834	CLA	C2B-C3B-CAB-CBB
18	A	829	CLA	C2B-C3B-CAB-CBB
18	G	202	CLA	C2B-C3B-CAB-CBB
18	G	201	CLA	C2B-C3B-CAB-CBB
18	A	819	CLA	C8-C10-C11-C12
18	L	303	CLA	C13-C15-C16-C17
17	2	605	CHL	O1D-CGD-O2D-CED
18	1	603	CLA	C6-C7-C8-C9
18	A	811	CLA	C16-C17-C18-C20
18	4	612	CLA	C5-C6-C7-C8
18	A	804	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	A	806	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	C11-C10-C8-C9
18	A	826	CLA	C11-C12-C13-C14
18	A	828	CLA	C11-C10-C8-C9
18	A	809	CLA	C11-C10-C8-C9
18	A	843	CLA	C6-C7-C8-C9
18	B	806	CLA	C14-C13-C15-C16
24	A	801	CL0	C6-C7-C8-C9
20	2	618	LHG	C2-C3-O3-P
18	3	602	CLA	C2A-CAA-CBA-CGA
18	4	612	CLA	C2A-CAA-CBA-CGA
18	A	820	CLA	O1D-CGD-O2D-CED
21	1	616	LUT	C1-C6-C7-C8
21	4	616	LUT	C1-C6-C7-C8
22	4	618	BCR	C23-C24-C25-C30
22	A	852	BCR	C1-C6-C7-C8
22	F	304	BCR	C1-C6-C7-C8
22	F	304	BCR	C5-C6-C7-C8
18	3	602	CLA	O1D-CGD-O2D-CED
19	1	614	XAT	C31-C32-C33-C34
22	4	618	BCR	C7-C8-C9-C10
22	B	801	BCR	C7-C8-C9-C10
18	B	819	CLA	O1D-CGD-O2D-CED
22	F	304	BCR	C14-C15-C16-C17
18	A	819	CLA	C6-C7-C8-C10
18	A	806	CLA	C12-C13-C15-C16
18	A	809	CLA	C11-C10-C8-C7
18	A	812	CLA	C12-C13-C15-C16
18	A	820	CLA	C11-C12-C13-C15
18	A	843	CLA	C6-C7-C8-C10
18	A	829	CLA	C6-C7-C8-C10
18	A	814	CLA	C12-C13-C15-C16
18	A	841	CLA	C12-C13-C15-C16
18	B	808	CLA	C6-C7-C8-C10
18	B	808	CLA	C11-C12-C13-C15
18	B	825	CLA	C11-C10-C8-C7
18	B	825	CLA	C11-C12-C13-C15
18	B	805	CLA	C6-C7-C8-C10
18	B	805	CLA	C11-C10-C8-C7
18	B	840	CLA	C6-C7-C8-C10
18	B	828	CLA	C6-C7-C8-C10
18	B	834	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	H	201	CLA	C11-C10-C8-C7
18	1	607	CLA	C2A-CAA-CBA-CGA
22	4	618	BCR	C11-C10-C9-C34
22	A	849	BCR	C20-C21-C22-C37
22	K	205	BCR	C20-C21-C22-C37
18	A	843	CLA	CBD-CGD-O2D-CED
18	B	839	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	CBA-CGA-O2A-C1
18	B	806	CLA	C8-C10-C11-C12
18	1	608	CLA	CAD-CBD-CGD-O2D
18	4	603	CLA	CAD-CBD-CGD-O2D
18	4	609	CLA	CAD-CBD-CGD-O2D
18	4	614	CLA	CAD-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O2D
18	A	803	CLA	CAD-CBD-CGD-O2D
18	A	810	CLA	CAD-CBD-CGD-O2D
18	A	836	CLA	CAD-CBD-CGD-O2D
18	B	815	CLA	CAD-CBD-CGD-O2D
18	B	839	CLA	CAD-CBD-CGD-O2D
18	B	841	CLA	CAD-CBD-CGD-O2D
18	B	810	CLA	CAD-CBD-CGD-O2D
18	B	835	CLA	CAD-CBD-CGD-O2D
18	B	834	CLA	CAD-CBD-CGD-O2D
18	F	301	CLA	CAD-CBD-CGD-O2D
18	L	304	CLA	CAD-CBD-CGD-O2D
18	L	302	CLA	CAD-CBD-CGD-O2D
18	B	828	CLA	CBA-CGA-O2A-C1
18	F	302	CLA	CBA-CGA-O2A-C1
18	B	805	CLA	C4-C3-C5-C6
20	1	615	LHG	O6-C4-C5-O7
18	A	825	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C2A-CAA-CBA-CGA
18	A	820	CLA	C2A-CAA-CBA-CGA
18	K	204	CLA	C2A-CAA-CBA-CGA
18	1	602	CLA	CHA-CBD-CGD-O1D
18	1	602	CLA	CHA-CBD-CGD-O2D
18	1	604	CLA	CHA-CBD-CGD-O1D
18	1	604	CLA	CHA-CBD-CGD-O2D
18	1	612	CLA	CHA-CBD-CGD-O1D
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	A	828	CLA	CHA-CBD-CGD-O2D
18	A	835	CLA	CHA-CBD-CGD-O1D
18	A	835	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	CHA-CBD-CGD-O1D
18	A	825	CLA	CHA-CBD-CGD-O2D
18	A	840	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O2D
18	A	823	CLA	CHA-CBD-CGD-O1D
18	A	823	CLA	CHA-CBD-CGD-O2D
18	A	813	CLA	CHA-CBD-CGD-O1D
18	B	821	CLA	CHA-CBD-CGD-O1D
18	B	821	CLA	CHA-CBD-CGD-O2D
18	B	819	CLA	CHA-CBD-CGD-O1D
18	B	819	CLA	CHA-CBD-CGD-O2D
18	B	813	CLA	CHA-CBD-CGD-O1D
18	B	836	CLA	CHA-CBD-CGD-O1D
18	B	822	CLA	CHA-CBD-CGD-O1D
18	B	822	CLA	CHA-CBD-CGD-O2D
18	B	811	CLA	CHA-CBD-CGD-O1D
18	B	811	CLA	CHA-CBD-CGD-O2D
18	F	303	CLA	CHA-CBD-CGD-O1D
18	F	303	CLA	CHA-CBD-CGD-O2D
18	H	201	CLA	CHA-CBD-CGD-O1D
18	H	201	CLA	CHA-CBD-CGD-O2D
18	4	612	CLA	O1A-CGA-O2A-C1
18	2	602	CLA	O1A-CGA-O2A-C1
18	A	826	CLA	O1A-CGA-O2A-C1
18	A	806	CLA	O1A-CGA-O2A-C1
18	B	805	CLA	CAA-CBA-CGA-O2A
18	A	843	CLA	C16-C17-C18-C20
18	B	824	CLA	C3-C5-C6-C7
18	B	809	CLA	C3-C5-C6-C7
18	B	841	CLA	C4-C3-C5-C6
18	A	830	CLA	C2C-C3C-CAC-CBC
18	B	826	CLA	O1A-CGA-O2A-C1
18	B	841	CLA	C2-C3-C5-C6
18	B	810	CLA	C6-C7-C8-C9
18	B	828	CLA	C6-C7-C8-C9
18	H	201	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
18	F	302	CLA	O1A-CGA-O2A-C1
18	K	204	CLA	C2C-C3C-CAC-CBC
18	F	301	CLA	C3-C5-C6-C7
17	4	605	CHL	CHA-CBD-CGD-O2D
18	A	813	CLA	C1A-C2A-CAA-CBA
18	4	602	CLA	CBD-CGD-O2D-CED
18	A	819	CLA	CAA-CBA-CGA-O2A
18	B	811	CLA	C2-C3-C5-C6
18	B	839	CLA	O1A-CGA-O2A-C1
18	B	837	CLA	O1A-CGA-O2A-C1
18	1	612	CLA	C4B-C3B-CAB-CBB
18	2	613	CLA	C4B-C3B-CAB-CBB
18	3	612	CLA	C4B-C3B-CAB-CBB
18	3	604	CLA	C4B-C3B-CAB-CBB
18	4	608	CLA	C4B-C3B-CAB-CBB
18	4	601	CLA	C4B-C3B-CAB-CBB
18	A	821	CLA	C4B-C3B-CAB-CBB
18	A	837	CLA	C4B-C3B-CAB-CBB
18	A	838	CLA	C4B-C3B-CAB-CBB
18	A	810	CLA	C4B-C3B-CAB-CBB
18	A	836	CLA	C4B-C3B-CAB-CBB
18	B	808	CLA	C4B-C3B-CAB-CBB
18	B	836	CLA	C4B-C3B-CAB-CBB
18	B	834	CLA	C4B-C3B-CAB-CBB
18	F	303	CLA	C4B-C3B-CAB-CBB
18	F	301	CLA	C4B-C3B-CAB-CBB
18	H	201	CLA	C4B-C3B-CAB-CBB
18	L	304	CLA	C4B-C3B-CAB-CBB
20	1	615	LHG	C3-O3-P-O4
20	B	852	LHG	C4-O6-P-O4
18	B	826	CLA	C13-C15-C16-C17
18	A	829	CLA	C16-C17-C18-C20
18	1	602	CLA	CAD-CBD-CGD-O1D
18	1	605	CLA	CAD-CBD-CGD-O1D
18	4	613	CLA	CAD-CBD-CGD-O1D
18	A	841	CLA	CAD-CBD-CGD-O1D
18	B	822	CLA	CAD-CBD-CGD-O1D
18	F	302	CLA	CAD-CBD-CGD-O1D
18	F	302	CLA	C2-C3-C5-C6
18	2	613	CLA	C2A-CAA-CBA-CGA
18	A	828	CLA	C11-C12-C13-C15
18	A	820	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
18	A	811	CLA	C11-C12-C13-C15
18	A	836	CLA	C3A-C2A-CAA-CBA
18	B	814	CLA	C6-C7-C8-C10
18	B	805	CLA	C12-C13-C15-C16
18	B	809	CLA	C6-C7-C8-C10
26	B	842	PQN	C16-C17-C18-C20
26	B	842	PQN	C22-C23-C25-C26
18	B	817	CLA	C11-C12-C13-C14
18	B	828	CLA	O1A-CGA-O2A-C1
27	B	850	DGD	C3B-C4B-C5B-C6B
18	3	601	CLA	C2A-CAA-CBA-CGA
18	A	822	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	C2A-CAA-CBA-CGA
18	B	828	CLA	C16-C17-C18-C20
23	4	619	LMG	C28-C29-C30-C31
27	B	850	DGD	C1B-C2B-C3B-C4B
17	2	605	CHL	C1C-C2C-CMC-OMC
17	4	605	CHL	C1C-C2C-CMC-OMC
18	3	609	CLA	CAD-CBD-CGD-O1D
18	A	844	CLA	C8-C10-C11-C12
18	B	805	CLA	C2-C3-C5-C6
18	2	602	CLA	C14-C13-C15-C16
18	A	804	CLA	C6-C7-C8-C9
18	A	829	CLA	C6-C7-C8-C9
18	B	827	CLA	C11-C12-C13-C14
18	B	832	CLA	C11-C10-C8-C9
21	2	616	LUT	C6-C7-C8-C9
18	A	812	CLA	C3-C5-C6-C7
20	1	615	LHG	C32-C33-C34-C35
22	A	852	BCR	C10-C11-C12-C13
22	B	844	BCR	C18-C19-C20-C21
22	F	304	BCR	C10-C11-C12-C13
18	B	839	CLA	C16-C17-C18-C19
18	4	613	CLA	C2B-C3B-CAB-CBB
18	A	821	CLA	C2B-C3B-CAB-CBB
18	A	819	CLA	C2B-C3B-CAB-CBB
18	A	844	CLA	C2B-C3B-CAB-CBB
18	A	818	CLA	C2B-C3B-CAB-CBB
18	A	843	CLA	C2B-C3B-CAB-CBB
18	B	808	CLA	C2B-C3B-CAB-CBB
18	B	807	CLA	C2B-C3B-CAB-CBB
18	F	301	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	K	204	CLA	C2B-C3B-CAB-CBB
22	3	614	BCR	C20-C21-C22-C37
18	A	814	CLA	C16-C17-C18-C20
18	B	840	CLA	C15-C16-C17-C18
18	1	604	CLA	C1-C2-C3-C4
18	A	804	CLA	CAA-CBA-CGA-O2A
18	A	841	CLA	CAA-CBA-CGA-O2A
18	4	602	CLA	C2A-CAA-CBA-CGA
18	A	815	CLA	C2A-CAA-CBA-CGA
18	B	807	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	C2-C1-O2A-CGA
18	A	829	CLA	C16-C17-C18-C19
18	A	802	CLA	C5-C6-C7-C8
27	B	850	DGD	C6B-C7B-C8B-C9B
18	A	806	CLA	O1D-CGD-O2D-CED
18	L	303	CLA	C16-C17-C18-C20
22	B	845	BCR	C1-C6-C7-C8
18	B	828	CLA	C16-C17-C18-C19
21	2	619	LUT	C11-C10-C9-C8
22	A	851	BCR	C11-C10-C9-C8
20	B	852	LHG	O7-C5-C6-O8
20	2	618	LHG	C4-O6-P-O3
20	A	847	LHG	C4-O6-P-O3
20	A	846	LHG	C3-O3-P-O6
20	B	852	LHG	C3-O3-P-O6
18	A	804	CLA	C16-C17-C18-C20
18	A	843	CLA	O1D-CGD-O2D-CED
23	4	620	LMG	C7-C8-C9-O8
18	A	825	CLA	O1D-CGD-O2D-CED
18	A	818	CLA	C11-C10-C8-C7
18	B	806	CLA	C12-C13-C15-C16
18	A	834	CLA	C11-C10-C8-C9
18	B	817	CLA	C6-C7-C8-C9
18	B	802	CLA	C10-C11-C12-C13
18	B	822	CLA	C8-C10-C11-C12
22	A	852	BCR	C13-C14-C15-C16
18	A	806	CLA	C16-C17-C18-C20
22	B	849	BCR	C36-C18-C19-C20
18	A	820	CLA	C8-C10-C11-C12
18	B	829	CLA	C11-C10-C8-C7
18	A	844	CLA	C2-C3-C5-C6
18	A	802	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
18	4	602	CLA	O1D-CGD-O2D-CED
18	1	607	CLA	CAA-CBA-CGA-O1A
18	A	825	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	CBD-CGD-O2D-CED
18	4	613	CLA	C4B-C3B-CAB-CBB
18	A	807	CLA	C4B-C3B-CAB-CBB
18	A	825	CLA	C4B-C3B-CAB-CBB
18	A	844	CLA	C4B-C3B-CAB-CBB
18	A	843	CLA	C4B-C3B-CAB-CBB
18	B	803	CLA	C4B-C3B-CAB-CBB
18	B	830	CLA	C4B-C3B-CAB-CBB
18	2	612	CLA	C2A-CAA-CBA-CGA
18	B	825	CLA	C5-C6-C7-C8
22	B	844	BCR	C15-C16-C17-C18
18	B	819	CLA	C3-C5-C6-C7
18	B	816	CLA	C4-C3-C5-C6
18	1	612	CLA	CBA-CGA-O2A-C1
18	B	816	CLA	C2-C3-C5-C6
18	G	203	CLA	CAA-CBA-CGA-O2A
18	B	841	CLA	C2-C1-O2A-CGA
18	2	602	CLA	C2A-CAA-CBA-CGA
18	2	608	CLA	C2A-CAA-CBA-CGA
18	4	614	CLA	C2A-CAA-CBA-CGA
20	A	847	LHG	O7-C7-C8-C9
18	4	613	CLA	C3A-C2A-CAA-CBA
18	A	803	CLA	C3A-C2A-CAA-CBA
18	B	834	CLA	C3A-C2A-CAA-CBA
24	A	801	CL0	C3A-C2A-CAA-CBA
18	A	826	CLA	C6-C7-C8-C9
18	B	803	CLA	C11-C10-C8-C9
18	B	825	CLA	C14-C13-C15-C16
18	B	818	CLA	C6-C7-C8-C9
18	B	828	CLA	C14-C13-C15-C16
18	A	806	CLA	C16-C17-C18-C19
18	L	303	CLA	C16-C17-C18-C19
21	2	619	LUT	C11-C10-C9-C19
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	K	202	BCR	C16-C17-C18-C36
22	L	305	BCR	C16-C17-C18-C36
18	1	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	1	607	CLA	CAA-CBA-CGA-O2A
18	A	826	CLA	C5-C6-C7-C8
18	B	826	CLA	C10-C11-C12-C13
24	A	801	CL0	CAA-CBA-CGA-O1A
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	803	CLA	C1A-C2A-CAA-CBA
18	A	836	CLA	C1A-C2A-CAA-CBA
18	B	819	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	C1A-C2A-CAA-CBA
18	A	844	CLA	CBA-CGA-O2A-C1
18	A	806	CLA	C11-C10-C8-C7
18	A	807	CLA	C6-C7-C8-C10
18	A	811	CLA	C11-C10-C8-C7
18	B	806	CLA	C11-C10-C8-C7
18	B	837	CLA	C11-C12-C13-C15
18	4	603	CLA	CAA-CBA-CGA-O1A
18	4	601	CLA	CAA-CBA-CGA-O1A
18	2	609	CLA	C2A-CAA-CBA-CGA
18	B	805	CLA	C16-C17-C18-C20
18	B	822	CLA	C5-C6-C7-C8
18	B	806	CLA	C4-C3-C5-C6
18	A	807	CLA	C15-C16-C17-C18
18	1	612	CLA	C2B-C3B-CAB-CBB
18	2	613	CLA	C2B-C3B-CAB-CBB
18	3	612	CLA	C2B-C3B-CAB-CBB
18	3	604	CLA	C2B-C3B-CAB-CBB
18	4	608	CLA	C2B-C3B-CAB-CBB
18	4	601	CLA	C2B-C3B-CAB-CBB
18	A	837	CLA	C2B-C3B-CAB-CBB
18	A	825	CLA	C2B-C3B-CAB-CBB
18	A	838	CLA	C2B-C3B-CAB-CBB
18	A	810	CLA	C2B-C3B-CAB-CBB
18	A	836	CLA	C2B-C3B-CAB-CBB
18	B	827	CLA	C2B-C3B-CAB-CBB
18	B	836	CLA	C2B-C3B-CAB-CBB
18	B	830	CLA	C2B-C3B-CAB-CBB
18	B	834	CLA	C2B-C3B-CAB-CBB
18	F	303	CLA	C2B-C3B-CAB-CBB
18	H	201	CLA	C2B-C3B-CAB-CBB
18	L	304	CLA	C2B-C3B-CAB-CBB
18	A	834	CLA	C13-C15-C16-C17
22	A	852	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	A	851	BCR	C20-C21-C22-C23
22	B	845	BCR	C16-C17-C18-C19
22	K	205	BCR	C20-C21-C22-C23
22	K	202	BCR	C16-C17-C18-C19
22	L	305	BCR	C16-C17-C18-C19
18	A	807	CLA	CBA-CGA-O2A-C1
18	A	834	CLA	O1D-CGD-O2D-CED
22	B	849	BCR	C22-C23-C24-C25
18	B	809	CLA	C16-C17-C18-C20
18	A	807	CLA	O1A-CGA-O2A-C1
18	B	808	CLA	C4-C3-C5-C6
18	A	809	CLA	C2-C1-O2A-CGA
18	B	817	CLA	C2-C1-O2A-CGA
18	G	203	CLA	CAA-CBA-CGA-O1A
18	2	612	CLA	C6-C7-C8-C9
18	B	818	CLA	C11-C10-C8-C9
18	A	844	CLA	O1A-CGA-O2A-C1
18	F	302	CLA	C4-C3-C5-C6
18	A	826	CLA	C15-C16-C17-C18
22	B	801	BCR	C23-C24-C25-C26
22	B	849	BCR	C23-C24-C25-C30
22	G	204	BCR	C5-C6-C7-C8
18	B	822	CLA	CAA-CBA-CGA-O2A
18	4	603	CLA	CAA-CBA-CGA-O2A
18	2	602	CLA	C5-C6-C7-C8
22	A	852	BCR	C15-C16-C17-C18
22	K	205	BCR	C7-C8-C9-C10
18	A	807	CLA	C16-C17-C18-C19
18	B	802	CLA	C5-C6-C7-C8
18	2	603	CLA	CAA-CBA-CGA-O2A
17	4	607	CHL	C2A-CAA-CBA-CGA
18	2	612	CLA	C15-C16-C17-C18
18	A	829	CLA	C13-C15-C16-C17
18	2	608	CLA	CAA-CBA-CGA-O2A
18	4	601	CLA	O1D-CGD-O2D-CED
18	A	804	CLA	C4B-C3B-CAB-CBB
18	B	827	CLA	C4B-C3B-CAB-CBB
18	B	814	CLA	C10-C11-C12-C13
18	A	825	CLA	C4-C3-C5-C6
18	B	821	CLA	CAA-CBA-CGA-O1A
18	3	609	CLA	C2-C3-C5-C6
18	A	828	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
18	A	831	CLA	C11-C12-C13-C15
18	B	813	CLA	C11-C12-C13-C15
24	A	801	CL0	C11-C10-C8-C7
18	A	817	CLA	CAA-CBA-CGA-O2A
18	K	203	CLA	CAA-CBA-CGA-O1A
19	2	617	XAT	C29-C30-C31-C32
22	4	618	BCR	C15-C16-C17-C18
18	A	835	CLA	C16-C17-C18-C20
18	K	203	CLA	CAA-CBA-CGA-O2A
23	4	620	LMG	O7-C8-C9-O8
18	A	805	CLA	CBA-CGA-O2A-C1
22	B	845	BCR	C16-C17-C18-C36
22	B	844	BCR	C11-C10-C9-C34
22	L	301	BCR	C11-C10-C9-C34
18	A	807	CLA	C4-C3-C5-C6
18	B	829	CLA	C4-C3-C5-C6
18	B	810	CLA	C4-C3-C5-C6
18	B	808	CLA	C2-C3-C5-C6
18	B	819	CLA	CBA-CGA-O2A-C1
18	4	602	CLA	C6-C7-C8-C9
18	A	802	CLA	C6-C7-C8-C9
18	A	811	CLA	C11-C10-C8-C9
18	A	811	CLA	C11-C12-C13-C14
18	B	814	CLA	C6-C7-C8-C9
18	B	813	CLA	C11-C12-C13-C14
18	B	837	CLA	C11-C12-C13-C14
26	B	842	PQN	C24-C23-C25-C26
18	A	805	CLA	O1A-CGA-O2A-C1
18	2	608	CLA	CAA-CBA-CGA-O1A
27	B	850	DGD	CEB-CFB-CGB-CHB
18	3	609	CLA	C3A-C2A-CAA-CBA
18	A	821	CLA	C3A-C2A-CAA-CBA
18	A	833	CLA	C3A-C2A-CAA-CBA
18	A	822	CLA	C3A-C2A-CAA-CBA
18	A	829	CLA	C3A-C2A-CAA-CBA
18	B	837	CLA	C3A-C2A-CAA-CBA
18	F	302	CLA	C3A-C2A-CAA-CBA
18	1	611	CLA	CAA-CBA-CGA-O2A
18	A	815	CLA	CAA-CBA-CGA-O2A
18	2	611	CLA	CAD-CBD-CGD-O2D
18	3	608	CLA	CAD-CBD-CGD-O2D
18	3	605	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	A	817	CLA	CAD-CBD-CGD-O2D
18	A	821	CLA	CAD-CBD-CGD-O2D
18	A	826	CLA	CAD-CBD-CGD-O2D
18	A	827	CLA	CAD-CBD-CGD-O2D
18	A	838	CLA	CAD-CBD-CGD-O2D
18	A	812	CLA	CAD-CBD-CGD-O2D
18	A	814	CLA	CAD-CBD-CGD-O2D
18	A	831	CLA	CAD-CBD-CGD-O2D
18	B	802	CLA	CAD-CBD-CGD-O2D
18	B	808	CLA	CAD-CBD-CGD-O2D
18	B	813	CLA	CAD-CBD-CGD-O2D
18	B	805	CLA	CAD-CBD-CGD-O2D
18	B	838	CLA	CAD-CBD-CGD-O2D
18	B	832	CLA	CAD-CBD-CGD-O2D
18	B	837	CLA	CAD-CBD-CGD-O2D
18	A	818	CLA	C8-C10-C11-C12
18	F	302	CLA	C2-C1-O2A-CGA
17	4	607	CHL	CAA-CBA-CGA-O2A
18	A	840	CLA	CAA-CBA-CGA-O2A
18	B	832	CLA	CAA-CBA-CGA-O2A
23	4	620	LMG	O9-C10-C11-C12
18	A	843	CLA	C16-C17-C18-C19
18	B	809	CLA	CAA-CBA-CGA-O2A
18	A	827	CLA	O1A-CGA-O2A-C1
18	4	613	CLA	CAA-CBA-CGA-O2A
18	A	827	CLA	CBA-CGA-O2A-C1
18	B	820	CLA	CAA-CBA-CGA-O2A
20	1	615	LHG	O7-C7-C8-C9
18	B	817	CLA	CAA-CBA-CGA-O1A
18	A	817	CLA	CAA-CBA-CGA-O1A
18	3	602	CLA	O2A-C1-C2-C3
18	4	614	CLA	O2A-C1-C2-C3
18	B	829	CLA	O2A-C1-C2-C3
18	F	301	CLA	O2A-C1-C2-C3
18	4	613	CLA	C2A-CAA-CBA-CGA
18	B	824	CLA	C2A-CAA-CBA-CGA
18	2	612	CLA	C10-C11-C12-C13
17	4	607	CHL	CAA-CBA-CGA-O1A
18	2	603	CLA	CAA-CBA-CGA-O1A
18	B	805	CLA	C16-C17-C18-C19
18	2	602	CLA	CHA-CBD-CGD-O1D
18	2	610	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	3	603	CLA	CHA-CBD-CGD-O2D
18	3	601	CLA	CHA-CBD-CGD-O1D
18	3	601	CLA	CHA-CBD-CGD-O2D
18	4	602	CLA	CHA-CBD-CGD-O1D
18	4	602	CLA	CHA-CBD-CGD-O2D
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	CHA-CBD-CGD-O2D
18	A	818	CLA	CHA-CBD-CGD-O2D
18	A	843	CLA	CHA-CBD-CGD-O1D
18	A	843	CLA	CHA-CBD-CGD-O2D
18	A	811	CLA	CHA-CBD-CGD-O1D
18	A	811	CLA	CHA-CBD-CGD-O2D
18	B	825	CLA	CHA-CBD-CGD-O1D
18	B	825	CLA	CHA-CBD-CGD-O2D
18	B	804	CLA	CHA-CBD-CGD-O1D
18	B	804	CLA	CHA-CBD-CGD-O2D
18	B	813	CLA	CHA-CBD-CGD-O2D
18	B	824	CLA	CHA-CBD-CGD-O1D
18	B	824	CLA	CHA-CBD-CGD-O2D
18	B	837	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O2D
18	1	611	CLA	CAA-CBA-CGA-O1A
18	4	604	CLA	CAA-CBA-CGA-O2A
18	A	815	CLA	CAA-CBA-CGA-O1A
18	3	609	CLA	CAA-CBA-CGA-O2A
18	A	820	CLA	C10-C11-C12-C13
22	4	618	BCR	C11-C10-C9-C8
22	B	844	BCR	C11-C10-C9-C8
22	L	301	BCR	C11-C10-C9-C8
18	B	819	CLA	O1A-CGA-O2A-C1
18	1	603	CLA	CAA-CBA-CGA-O2A
18	F	301	CLA	CAA-CBA-CGA-O2A
20	B	852	LHG	O7-C7-C8-C9
17	3	606	CHL	CAA-CBA-CGA-O2A
18	A	827	CLA	C11-C12-C13-C14
18	A	831	CLA	C3-C5-C6-C7
18	A	826	CLA	C11-C12-C13-C15
18	A	807	CLA	C2-C3-C5-C6
18	B	803	CLA	C11-C12-C13-C15
18	K	204	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	A	807	CLA	C6-C7-C8-C9
18	A	831	CLA	C11-C12-C13-C14
18	B	832	CLA	C6-C7-C8-C9
26	B	842	PQN	C16-C17-C18-C19
20	A	847	LHG	C5-C6-O8-C23
17	2	605	CHL	C2B-C3B-CAB-CBB
18	A	828	CLA	C2B-C3B-CAB-CBB
27	B	850	DGD	CAA-CBA-CCA-CDA
18	B	832	CLA	CBA-CGA-O2A-C1
18	B	841	CLA	CAA-CBA-CGA-O2A
18	B	832	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	C2A-CAA-CBA-CGA
18	A	821	CLA	CAA-CBA-CGA-O2A
18	B	832	CLA	CAA-CBA-CGA-O1A
18	B	810	CLA	C2-C3-C5-C6
18	A	840	CLA	CAA-CBA-CGA-O1A
18	B	809	CLA	CAA-CBA-CGA-O1A
18	1	607	CLA	CHA-CBD-CGD-O2D
18	3	609	CLA	C1A-C2A-CAA-CBA
18	A	821	CLA	C1A-C2A-CAA-CBA
18	A	822	CLA	C1A-C2A-CAA-CBA
18	B	803	CLA	C1A-C2A-CAA-CBA
18	B	817	CLA	C1A-C2A-CAA-CBA
18	B	837	CLA	C1A-C2A-CAA-CBA
18	B	834	CLA	C1A-C2A-CAA-CBA
24	A	801	CL0	C1A-C2A-CAA-CBA
18	A	842	CLA	C4C-C3C-CAC-CBC
20	1	615	LHG	O9-C7-C8-C9
18	4	613	CLA	CAA-CBA-CGA-O1A
18	A	844	CLA	C2A-CAA-CBA-CGA
18	B	837	CLA	C2A-CAA-CBA-CGA
20	1	615	LHG	C4-O6-P-O3
17	3	606	CHL	CAA-CBA-CGA-O1A
18	3	609	CLA	C4-C3-C5-C6
18	1	612	CLA	O1A-CGA-O2A-C1
17	2	607	CHL	C4B-C3B-CAB-CBB
17	2	605	CHL	C4B-C3B-CAB-CBB
17	4	605	CHL	C4B-C3B-CAB-CBB
18	1	607	CLA	C4B-C3B-CAB-CBB
18	3	607	CLA	C4B-C3B-CAB-CBB
18	A	817	CLA	C4B-C3B-CAB-CBB
18	B	838	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	1	615	LHG	C4-O6-P-O4
20	A	846	LHG	C3-O3-P-O5
18	K	204	CLA	CAA-CBA-CGA-O1A
17	2	607	CHL	CAA-CBA-CGA-O2A
22	A	853	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
18	3	609	CLA	CAA-CBA-CGA-O1A
20	B	852	LHG	O9-C7-C8-C9
18	4	612	CLA	C8-C10-C11-C12
20	2	618	LHG	O7-C7-C8-C9
18	2	611	CLA	CAA-CBA-CGA-O2A
22	K	205	BCR	C18-C19-C20-C21
18	B	820	CLA	CAA-CBA-CGA-O1A
18	2	612	CLA	O1A-CGA-O2A-C1
18	4	604	CLA	CAA-CBA-CGA-O1A
18	B	811	CLA	CAA-CBA-CGA-O2A
18	A	841	CLA	C4-C3-C5-C6
18	4	614	CLA	CAD-CBD-CGD-O1D
18	A	822	CLA	CAD-CBD-CGD-O1D
18	A	842	CLA	CAD-CBD-CGD-O1D
18	A	834	CLA	CAD-CBD-CGD-O1D
18	B	827	CLA	CAD-CBD-CGD-O1D
20	B	851	LHG	C4-C5-O7-C7
18	4	601	CLA	CBD-CGD-O2D-CED
18	1	603	CLA	CAA-CBA-CGA-O1A
18	F	301	CLA	CAA-CBA-CGA-O1A
18	B	806	CLA	CAA-CBA-CGA-O2A
18	A	829	CLA	C11-C10-C8-C9
18	B	839	CLA	C6-C7-C8-C9
18	B	841	CLA	C14-C13-C15-C16
18	B	822	CLA	C11-C10-C8-C9
18	B	828	CLA	C11-C12-C13-C14
24	A	801	CL0	C14-C13-C15-C16
18	A	804	CLA	C13-C15-C16-C17
18	2	612	CLA	CAA-CBA-CGA-O2A
18	A	842	CLA	CAA-CBA-CGA-O2A
18	A	821	CLA	CAA-CBA-CGA-O1A
20	B	852	LHG	C30-C31-C32-C33
18	4	602	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	A	803	CLA	C10-C11-C12-C13
24	A	801	CL0	C4-C3-C5-C6
17	4	605	CHL	CHA-CBD-CGD-O1D
18	1	607	CLA	CHA-CBD-CGD-O1D
18	1	613	CLA	CHA-CBD-CGD-O1D
18	3	609	CLA	CAD-CBD-CGD-O2D
18	4	612	CLA	C6-C7-C8-C10
18	A	827	CLA	C6-C7-C8-C10
18	A	829	CLA	C12-C13-C15-C16
18	B	803	CLA	C3A-C2A-CAA-CBA
18	B	806	CLA	C2-C3-C5-C6
18	B	832	CLA	C6-C7-C8-C10
18	B	832	CLA	C11-C12-C13-C15
18	B	837	CLA	C12-C13-C15-C16
18	B	818	CLA	C11-C10-C8-C7
21	2	619	LUT	C25-C26-C27-C28
24	A	801	CL0	C12-C13-C15-C16
18	2	612	CLA	CAA-CBA-CGA-O1A
18	3	602	CLA	CAA-CBA-CGA-O1A
18	2	611	CLA	CAA-CBA-CGA-O1A
18	3	602	CLA	CAA-CBA-CGA-O2A
18	3	601	CLA	CAA-CBA-CGA-O2A
18	A	812	CLA	CAA-CBA-CGA-O2A
22	B	849	BCR	C17-C18-C19-C20
18	A	837	CLA	CAA-CBA-CGA-O2A
27	B	850	DGD	CDA-CEA-CFA-CGA
18	3	601	CLA	CAA-CBA-CGA-O1A
18	B	805	CLA	CAA-CBA-CGA-O1A
18	4	608	CLA	CAA-CBA-CGA-O2A
18	B	833	CLA	CAA-CBA-CGA-O2A
26	B	842	PQN	C15-C16-C17-C18
18	A	842	CLA	C2C-C3C-CAC-CBC
18	A	810	CLA	CAA-CBA-CGA-O2A
18	B	811	CLA	CAA-CBA-CGA-O1A
18	B	833	CLA	CAA-CBA-CGA-O1A
18	A	809	CLA	C4C-C3C-CAC-CBC
18	B	824	CLA	C13-C15-C16-C17
18	2	612	CLA	CBA-CGA-O2A-C1
18	4	609	CLA	C4-C3-C5-C6
18	A	814	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

156 monomers are involved in 471 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	841	CLA	2	0
17	2	605	CHL	2	0
18	L	303	CLA	4	0
18	A	834	CLA	2	0
18	1	609	CLA	6	0
18	F	301	CLA	2	0
18	1	603	CLA	2	0
22	I	101	BCR	2	0
22	B	801	BCR	9	0
22	K	205	BCR	4	0
18	H	201	CLA	1	0
18	3	603	CLA	2	0
18	A	810	CLA	1	0
22	B	843	BCR	4	0
18	B	813	CLA	3	0
18	L	304	CLA	1	0
22	A	849	BCR	3	0
18	B	840	CLA	1	0
18	B	826	CLA	3	0
18	B	822	CLA	7	0
22	B	848	BCR	3	0
18	A	804	CLA	8	0
18	A	838	CLA	1	0
22	G	204	BCR	3	0
22	A	851	BCR	7	0
18	4	614	CLA	3	0
18	A	820	CLA	4	0
18	B	814	CLA	5	0
18	A	826	CLA	2	0
18	A	835	CLA	1	0
18	4	613	CLA	3	0
20	A	846	LHG	3	0
18	B	809	CLA	2	0
18	B	832	CLA	6	0
21	3	613	LUT	7	0
18	A	829	CLA	6	0
18	A	811	CLA	2	0
17	2	607	CHL	1	0
18	B	824	CLA	2	0
18	3	609	CLA	3	0
18	3	612	CLA	2	0
18	2	602	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	832	CLA	1	0
18	3	607	CLA	1	0
27	B	850	DGD	8	0
18	A	828	CLA	2	0
18	L	302	CLA	1	0
22	A	850	BCR	6	0
22	B	847	BCR	6	0
18	B	825	CLA	5	0
18	A	841	CLA	5	0
18	B	831	CLA	1	0
18	A	818	CLA	3	0
22	L	306	BCR	2	0
18	B	830	CLA	3	0
18	B	817	CLA	1	0
17	2	615	CHL	1	0
18	A	830	CLA	6	0
18	B	833	CLA	1	0
24	A	801	CL0	7	0
18	A	812	CLA	6	0
22	F	304	BCR	1	0
17	4	606	CHL	2	0
21	2	619	LUT	4	0
18	A	807	CLA	3	0
18	B	816	CLA	1	0
18	A	809	CLA	9	0
22	B	846	BCR	7	0
22	K	202	BCR	6	0
18	4	608	CLA	2	0
18	G	201	CLA	1	0
22	A	853	BCR	4	0
18	2	608	CLA	2	0
18	B	808	CLA	4	0
22	B	849	BCR	9	0
18	1	602	CLA	2	0
18	K	203	CLA	1	0
23	4	619	LMG	1	0
18	B	838	CLA	2	0
18	2	611	CLA	2	0
18	B	805	CLA	4	0
18	A	821	CLA	2	0
18	3	608	CLA	2	0
18	1	604	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	829	CLA	2	0
18	F	302	CLA	6	0
22	3	614	BCR	2	0
18	A	815	CLA	1	0
26	A	855	PQN	5	0
18	1	608	CLA	2	0
18	4	609	CLA	3	0
18	A	839	CLA	1	0
22	L	301	BCR	4	0
18	B	839	CLA	1	0
18	A	842	CLA	6	0
18	4	603	CLA	1	0
21	4	616	LUT	3	0
22	A	852	BCR	4	0
20	B	852	LHG	1	0
21	2	616	LUT	8	0
17	1	601	CHL	7	0
18	B	837	CLA	2	0
18	A	808	CLA	1	0
22	B	844	BCR	6	0
18	A	831	CLA	1	0
18	A	813	CLA	2	0
19	4	617	XAT	18	0
18	B	811	CLA	1	0
19	2	617	XAT	6	0
18	A	805	CLA	1	0
20	1	615	LHG	20	0
22	4	618	BCR	8	0
22	A	848	BCR	7	0
18	A	806	CLA	7	0
18	A	833	CLA	2	0
18	A	814	CLA	2	0
18	A	822	CLA	3	0
18	A	803	CLA	6	0
18	A	802	CLA	7	0
18	A	843	CLA	3	0
18	A	844	CLA	7	0
18	B	823	CLA	2	0
18	4	610	CLA	1	0
18	A	819	CLA	4	0
18	B	819	CLA	1	0
18	A	836	CLA	1	0

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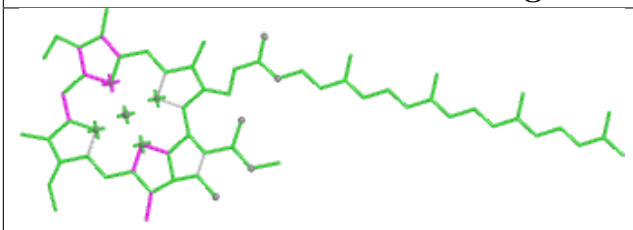
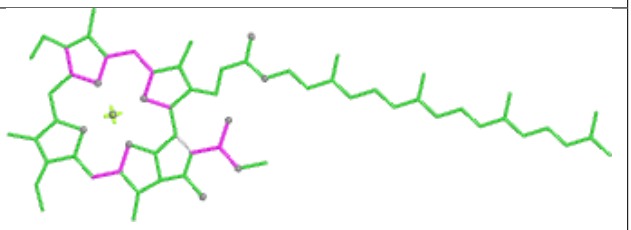
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	4	612	CLA	2	0
18	B	836	CLA	2	0
19	1	614	XAT	9	0
18	B	828	CLA	7	0
18	2	612	CLA	2	0
17	4	607	CHL	1	0
18	1	607	CLA	5	0
17	4	605	CHL	1	0
18	B	802	CLA	4	0
18	4	602	CLA	5	0
17	2	601	CHL	1	0
18	4	604	CLA	2	0
18	3	601	CLA	1	0
18	A	827	CLA	2	0
18	2	604	CLA	4	0
18	B	827	CLA	3	0
18	B	806	CLA	5	0
22	J	102	BCR	4	0
22	L	305	BCR	8	0
18	1	612	CLA	5	0
22	B	845	BCR	6	0
18	2	603	CLA	2	0
18	1	605	CLA	1	0
26	B	842	PQN	1	0
18	2	609	CLA	3	0
18	B	803	CLA	4	0
18	A	825	CLA	4	0
18	B	834	CLA	1	0
21	1	616	LUT	9	0
20	A	847	LHG	3	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.

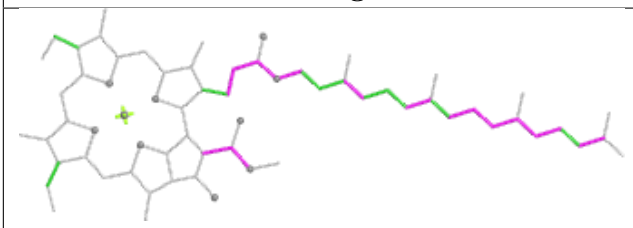
Ligand CLA B 841



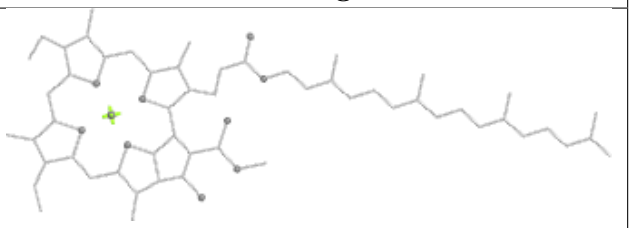
Bond lengths



Bond angles

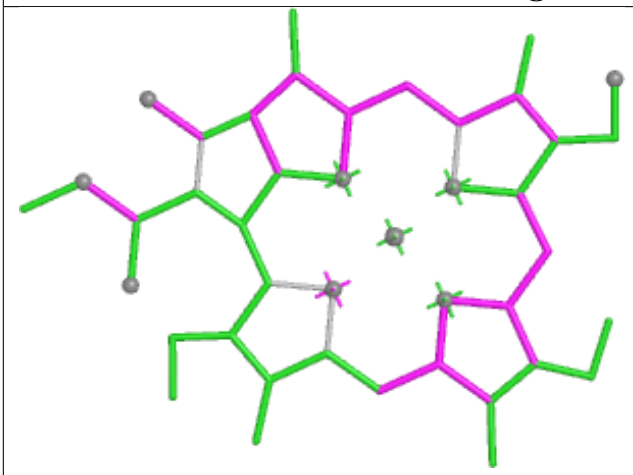


Torsions

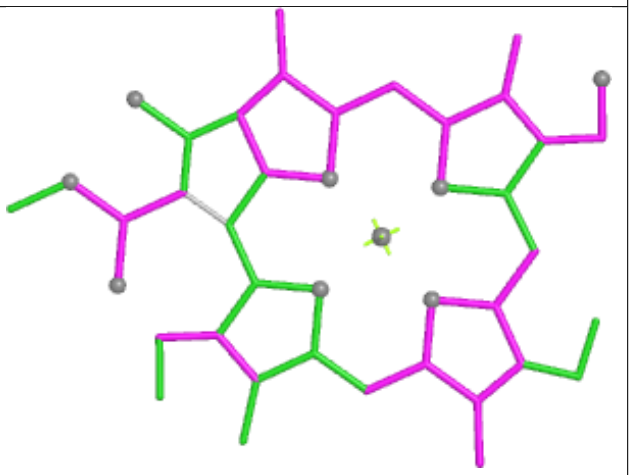


Rings

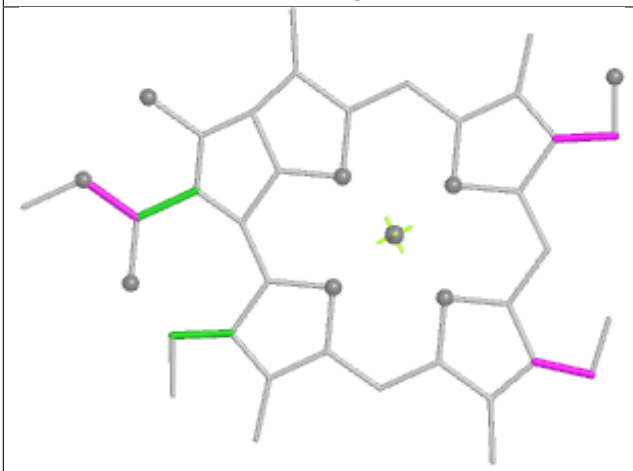
Ligand CHL 2 605



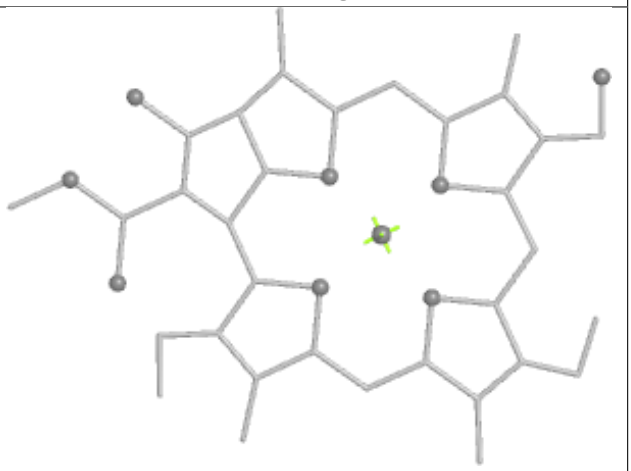
Bond lengths



Bond angles

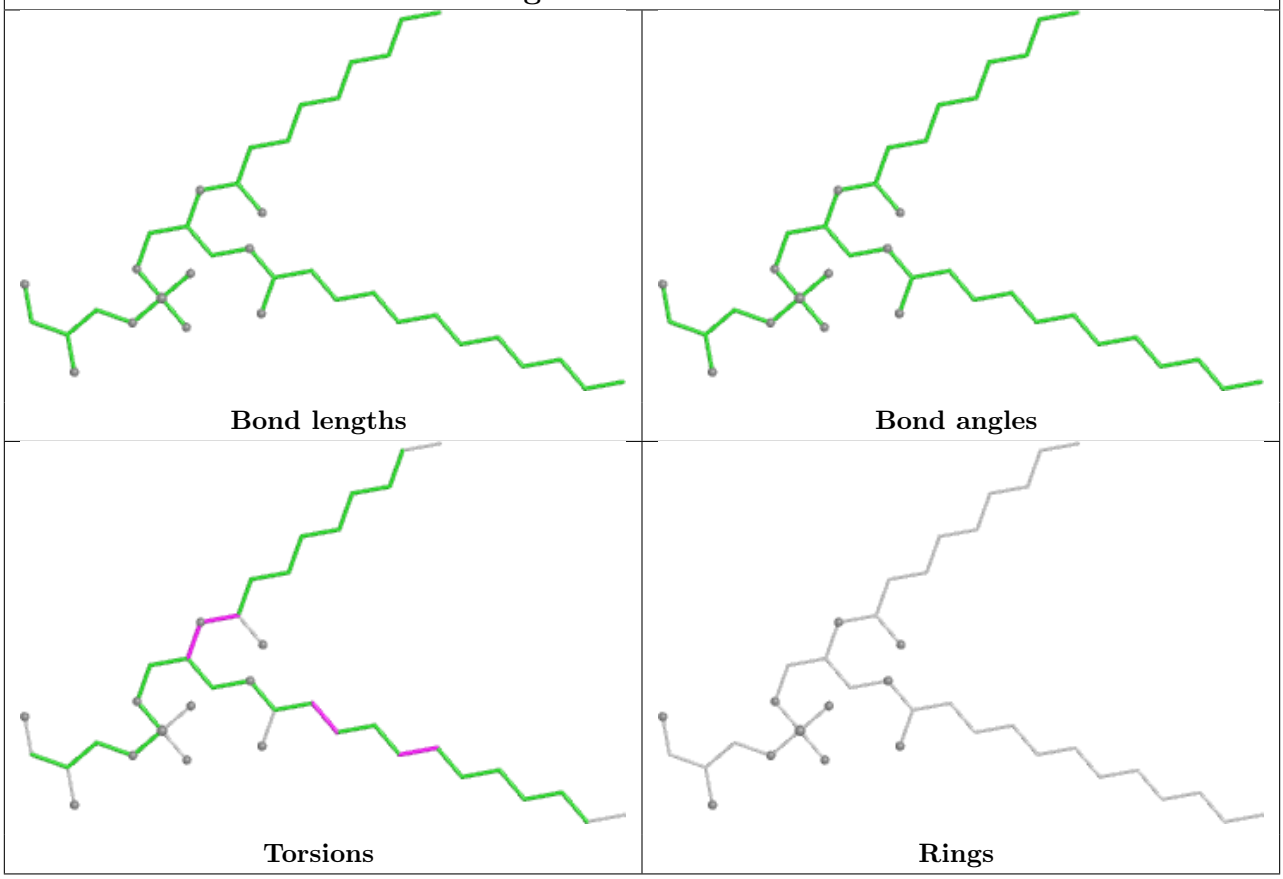


Torsions

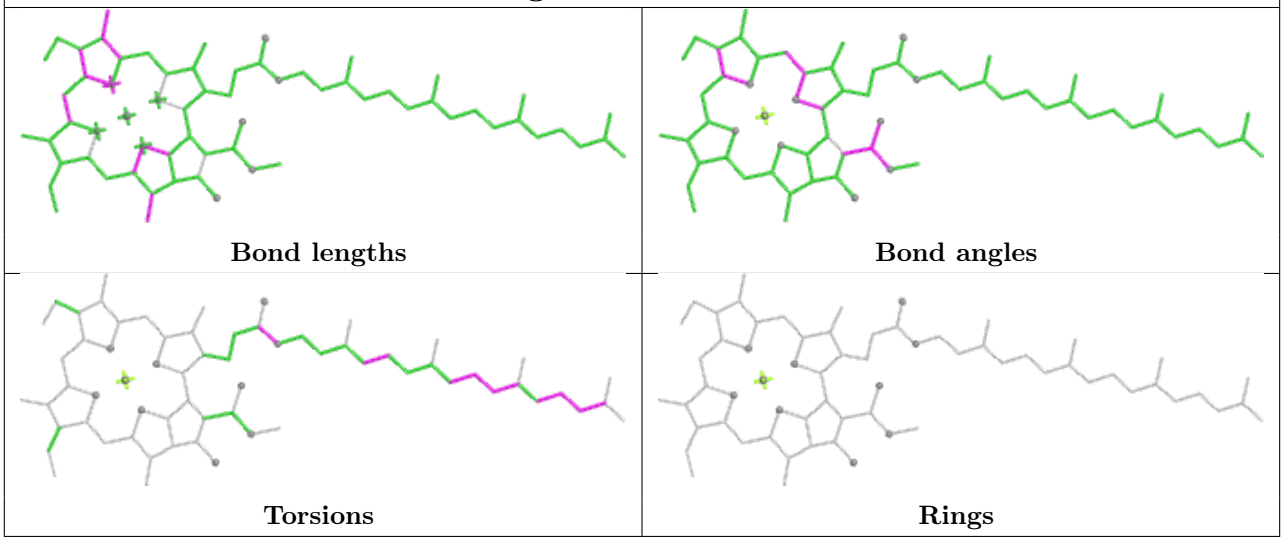


Rings

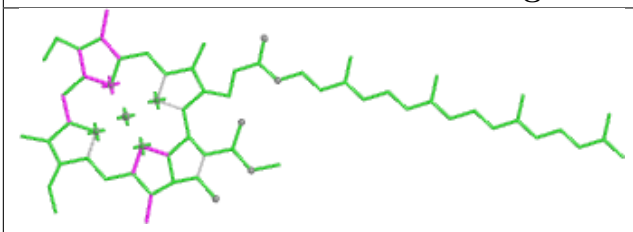
Ligand LHG B 851



Ligand CLA L 303



Ligand CLA A 834



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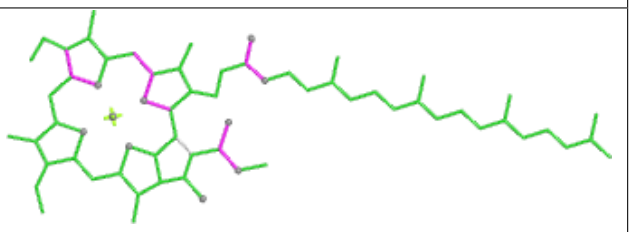
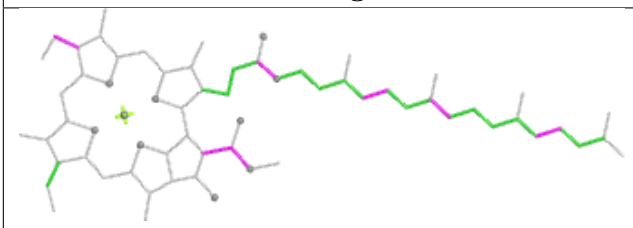
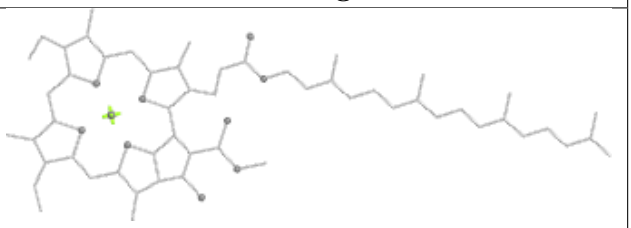


Bond angles

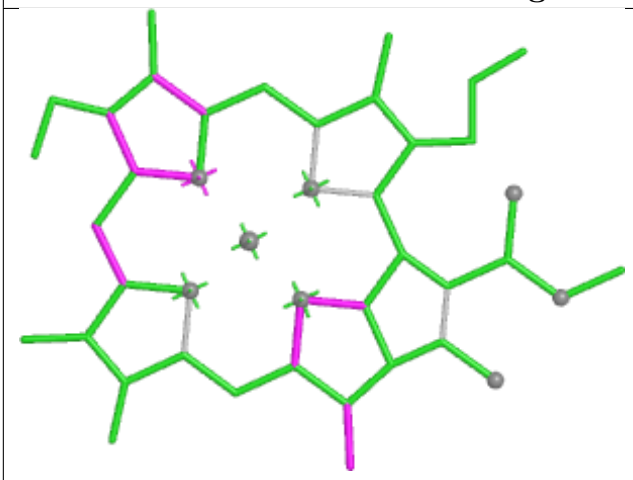


Torsions



Rings

Ligand CLA 1 609



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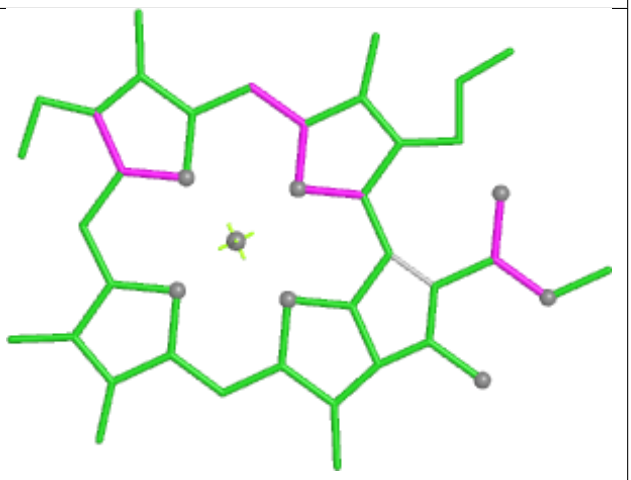

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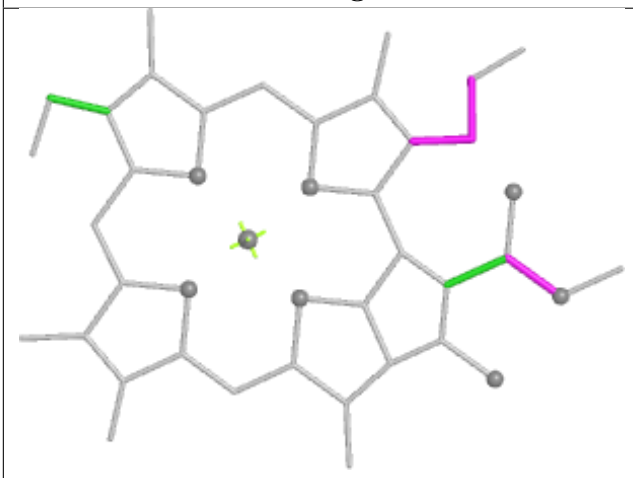
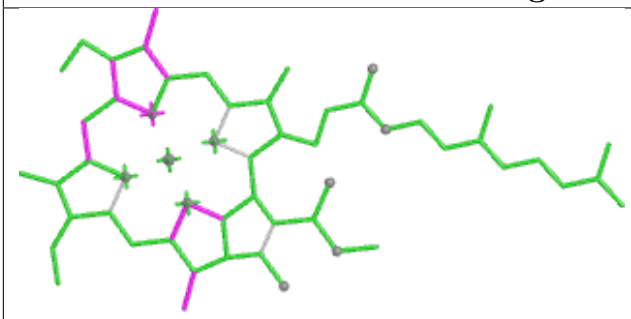


Torsions

Rings

Ligand CLA 3 602



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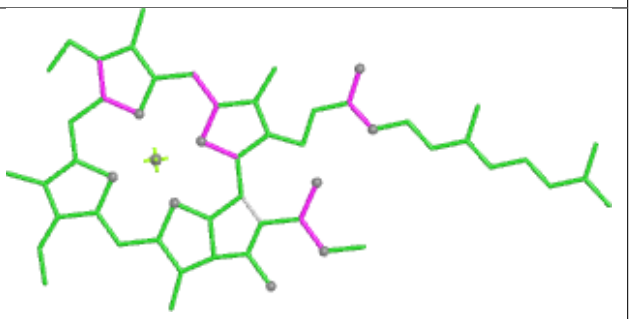

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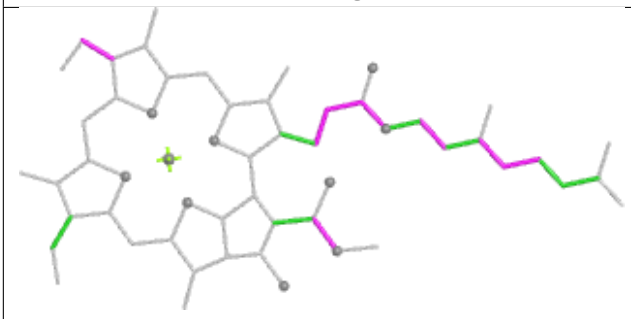

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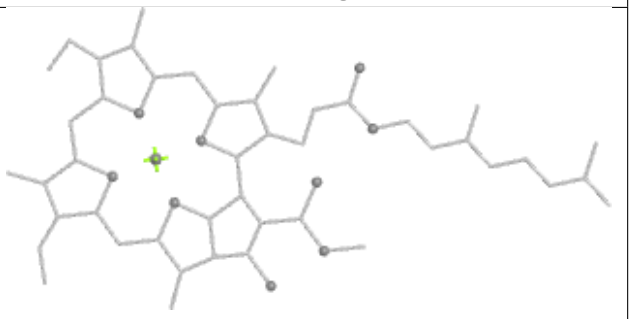
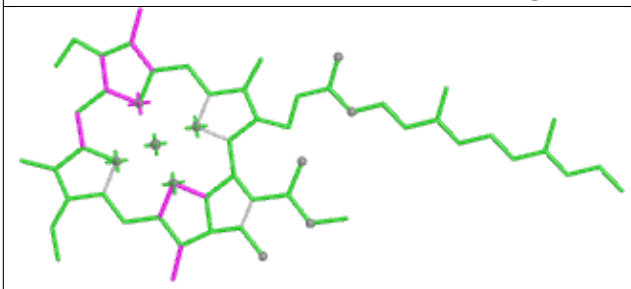


Rings

Ligand CLA F 301



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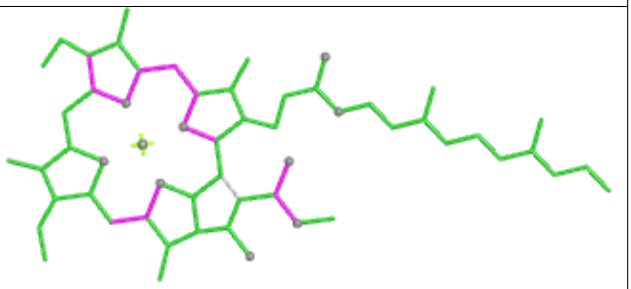

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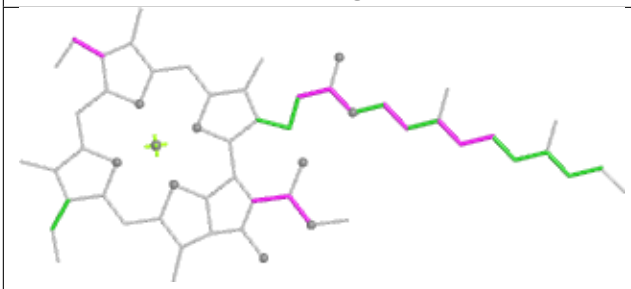

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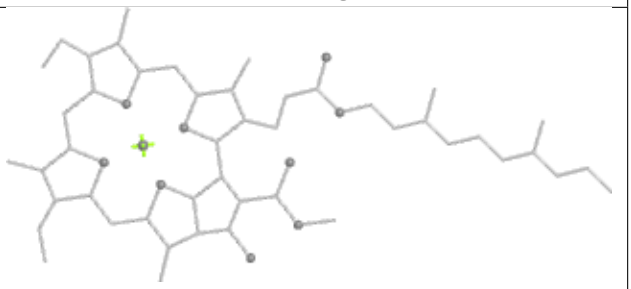
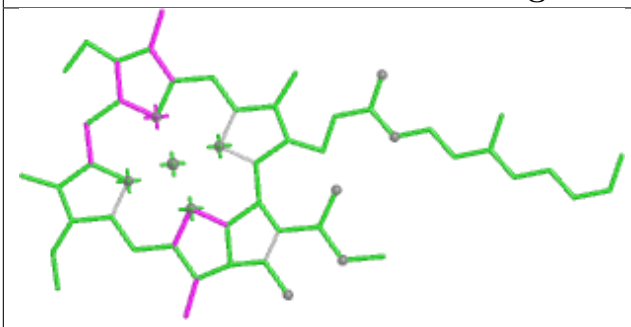
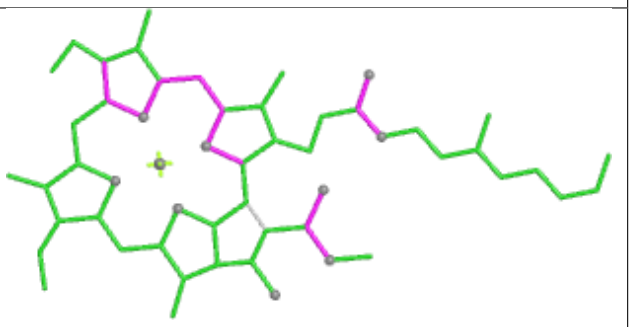
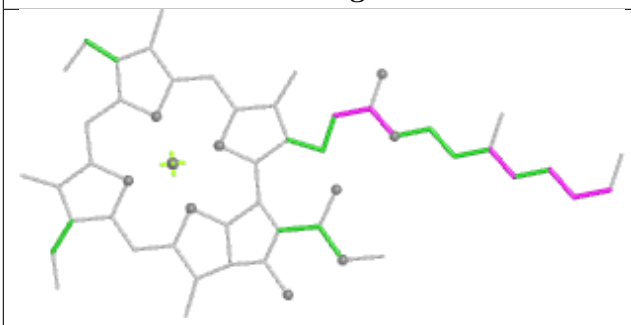
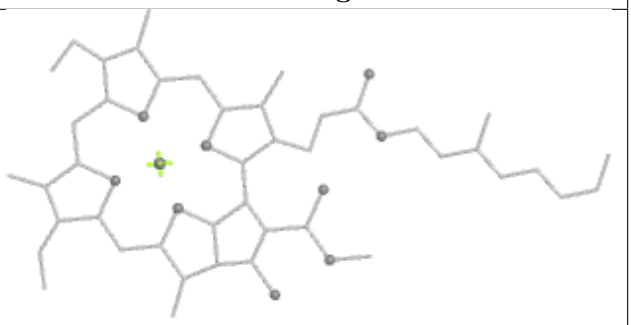


Rings

Ligand CLA 1 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

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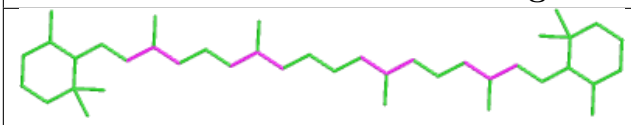
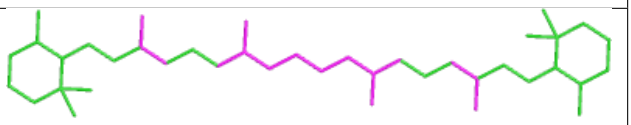
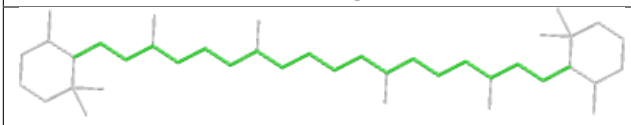
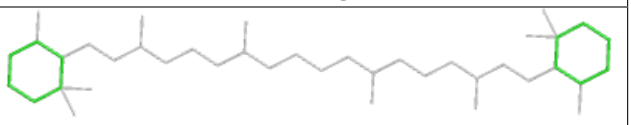
 Bond lengths	 Bond angles
 Torsions	 Rings

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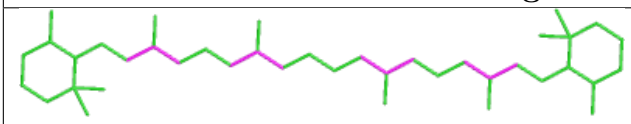
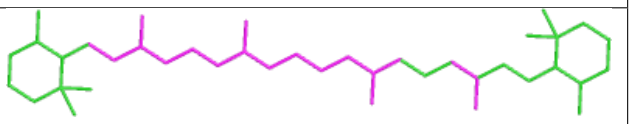
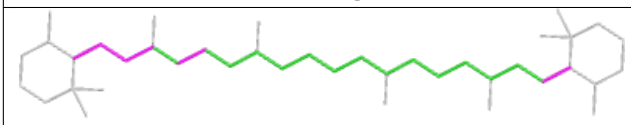
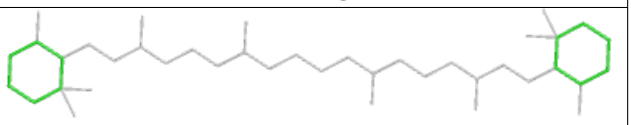
 Bond lengths	 Bond angles
 Torsions	 Rings

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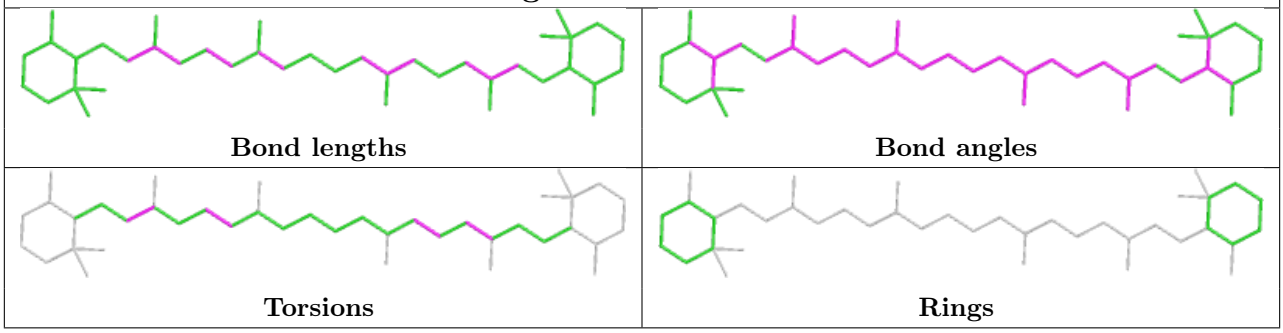
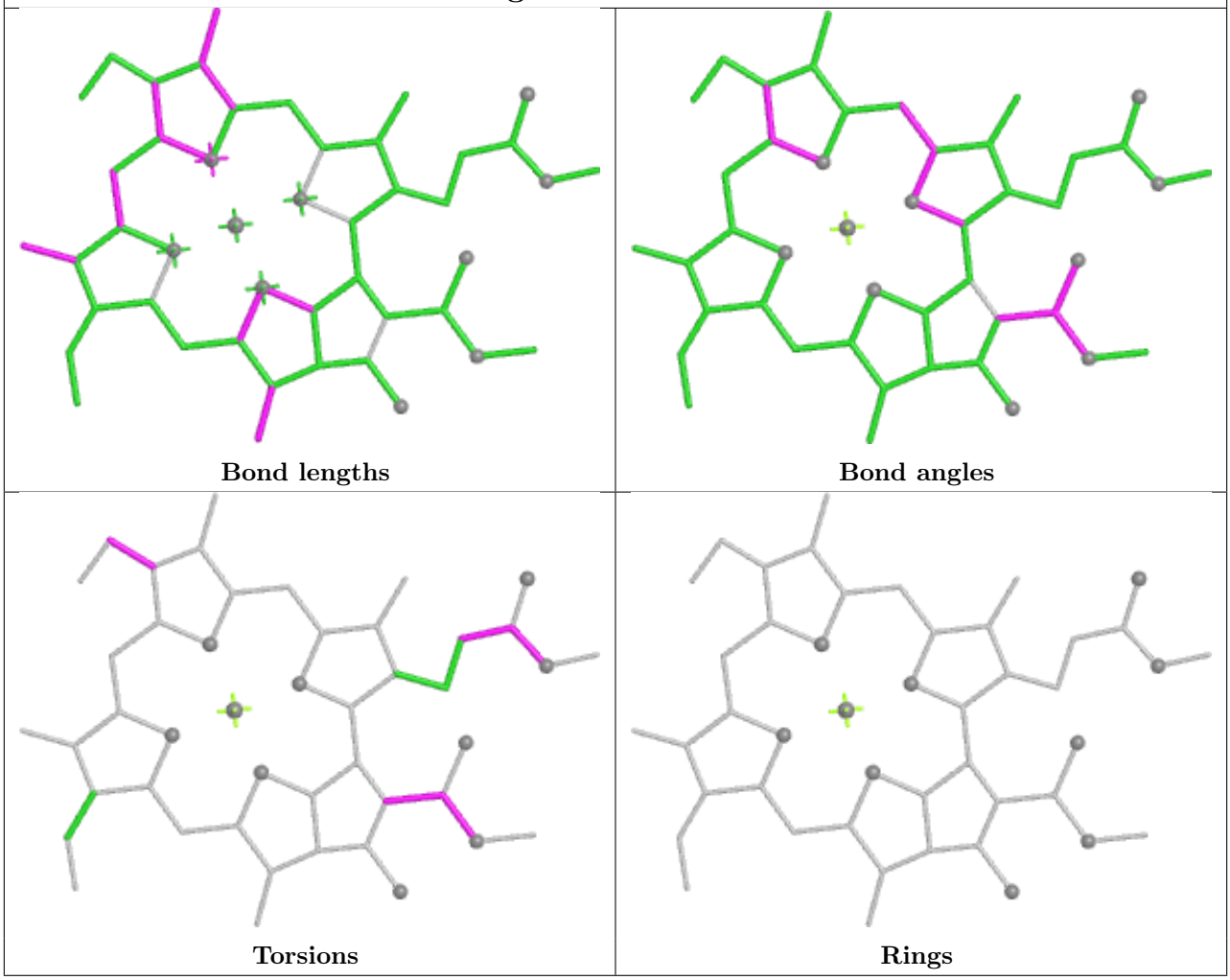
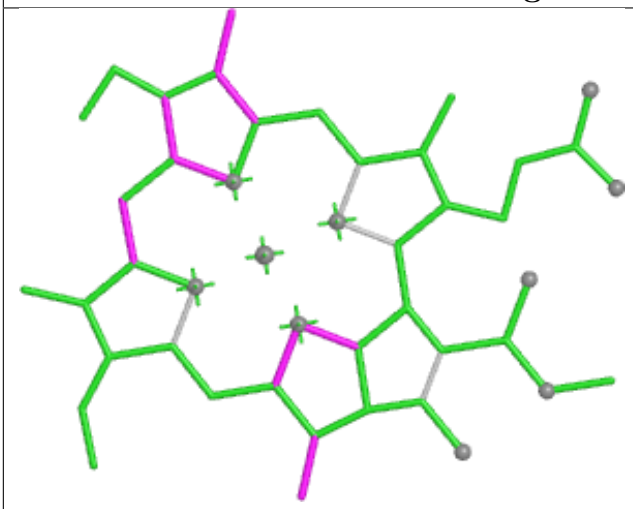


Ligand CLA 4 601



Ligand CLA A 817



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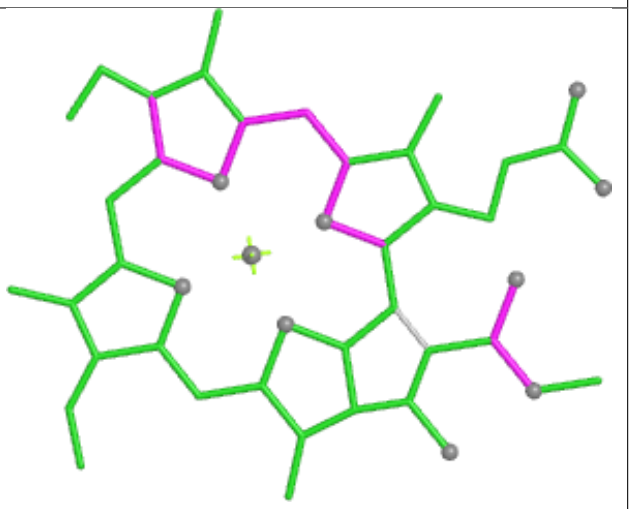
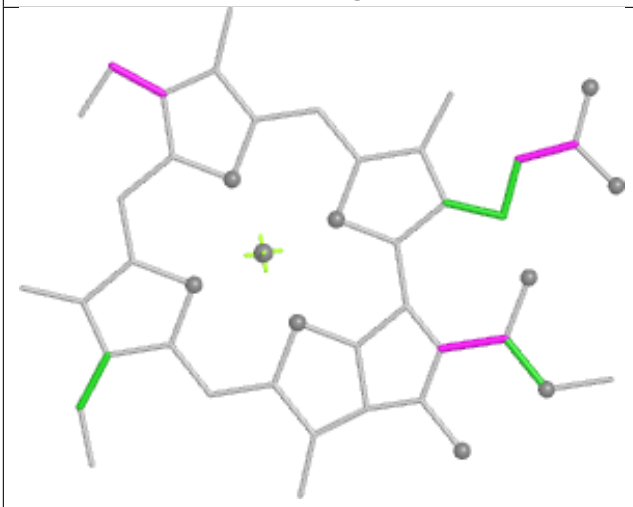


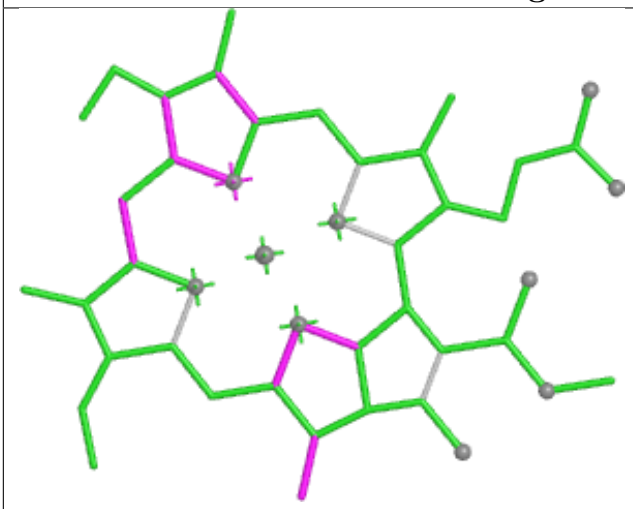
Bond angles



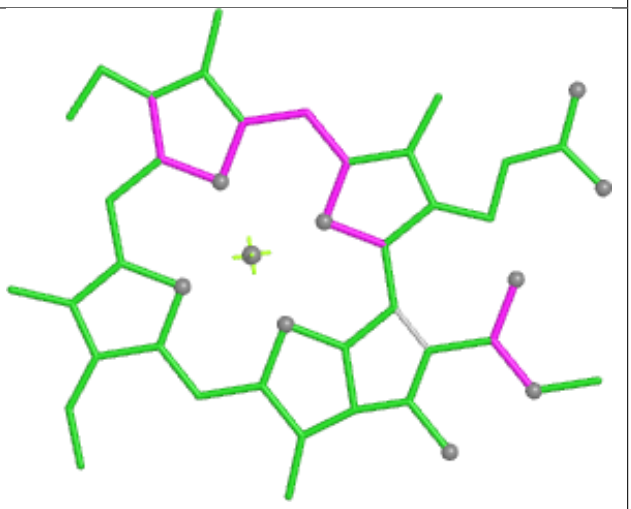
Torsions

Rings

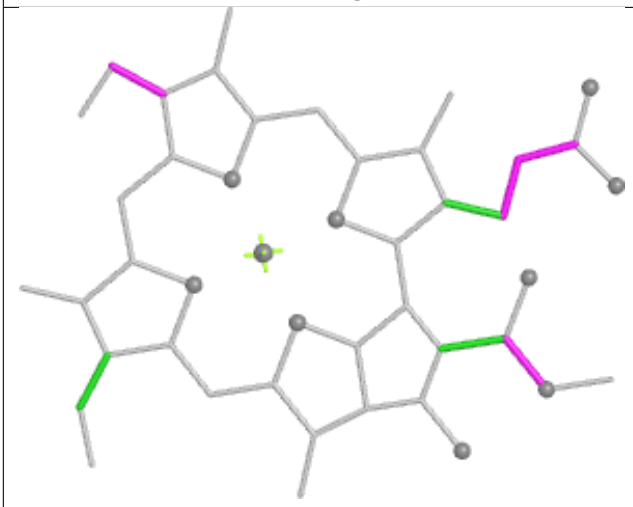
Ligand CLA 1 611



Bond lengths



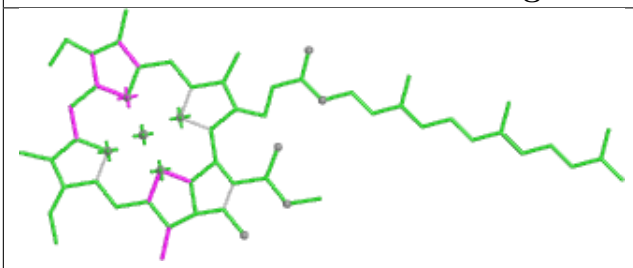
Bond angles



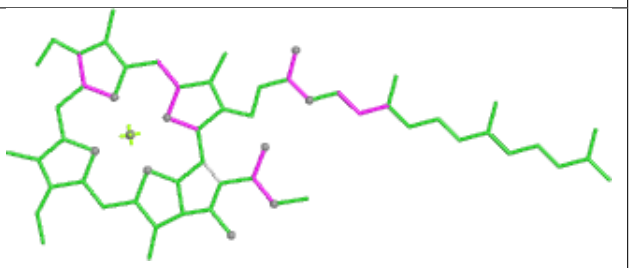
Torsions

Rings

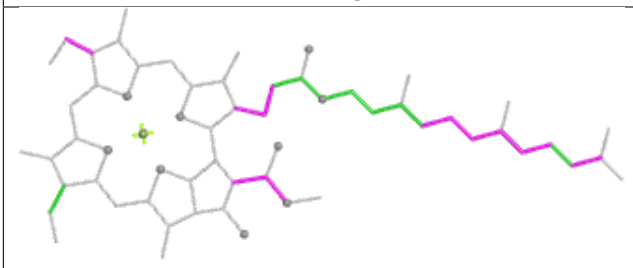
Ligand CLA H 201



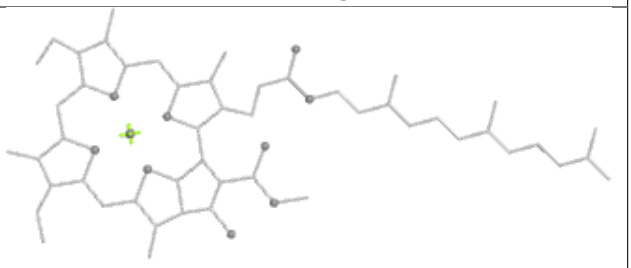
Bond lengths



Bond angles

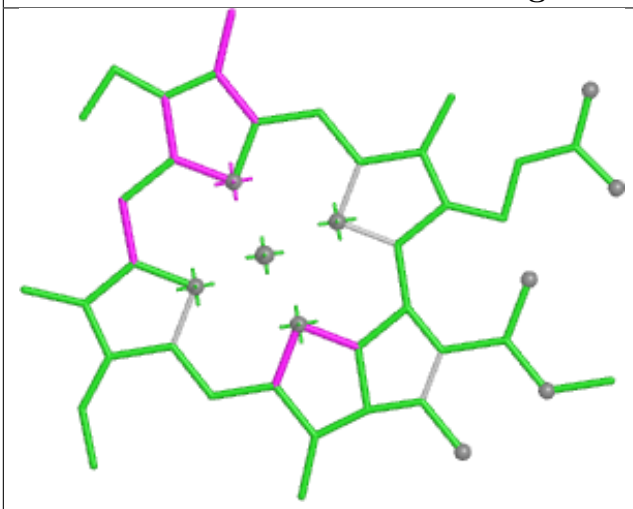


Torsions



Rings

Ligand CLA 3 603



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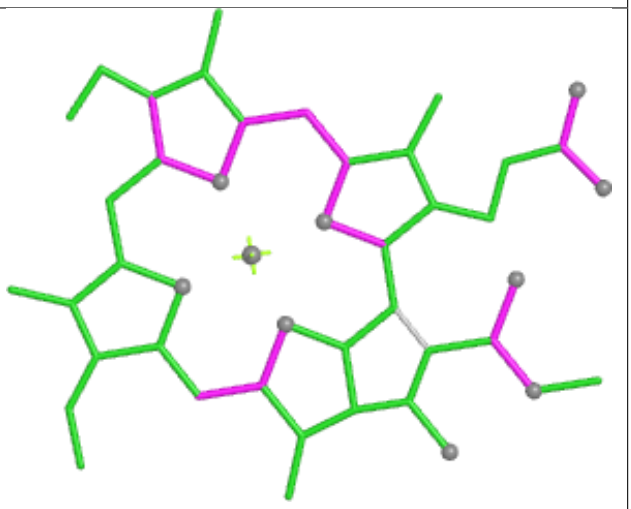
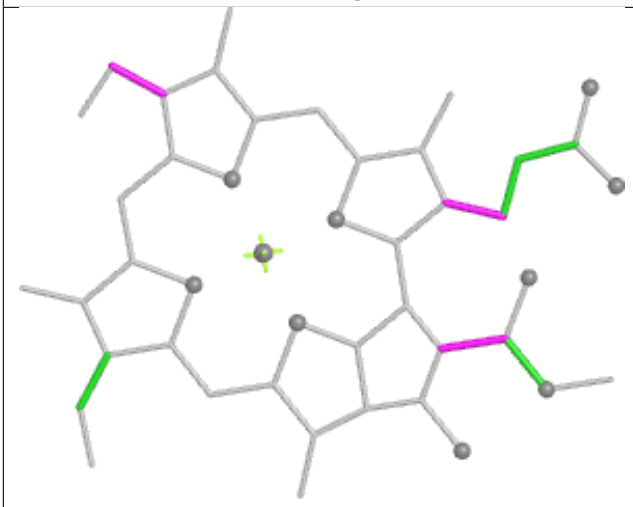
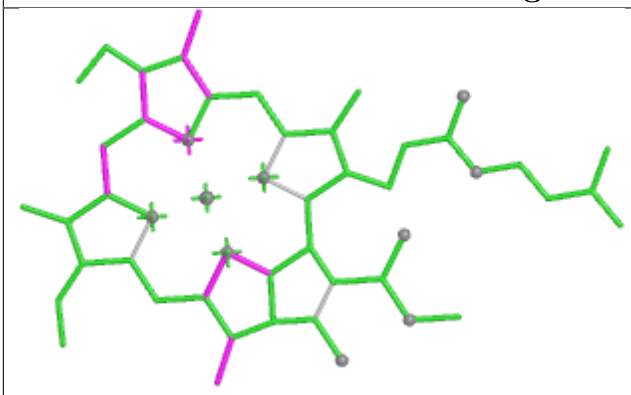
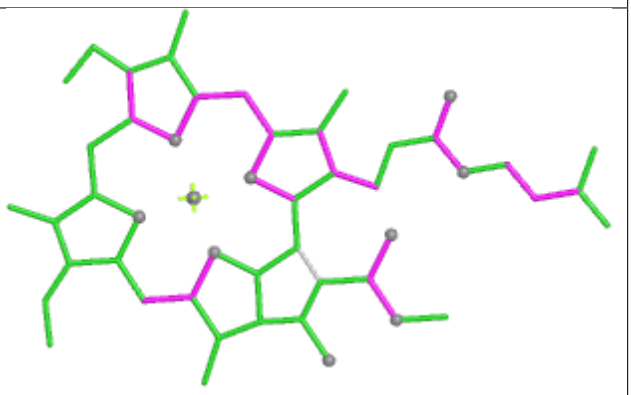
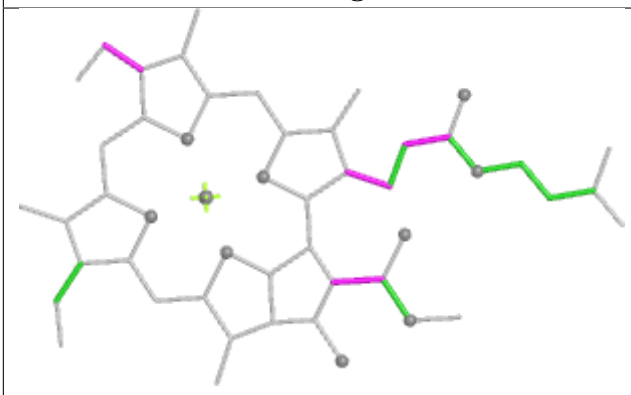
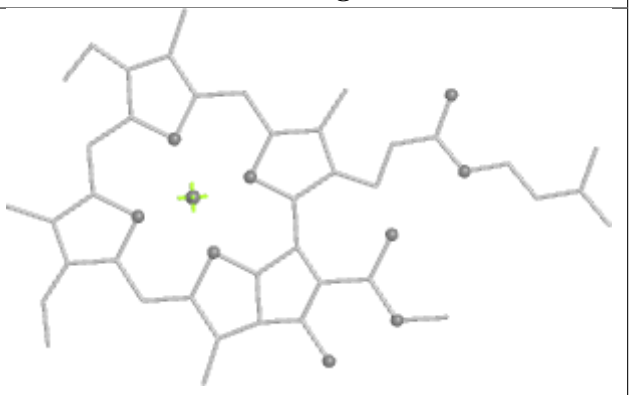


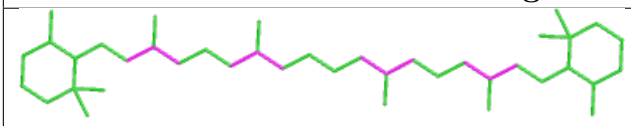
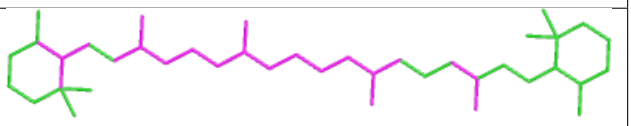
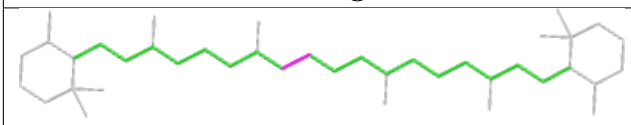
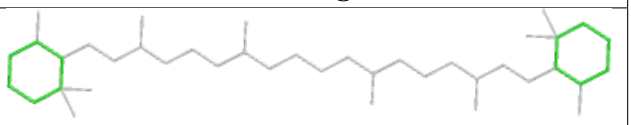
Bond angles



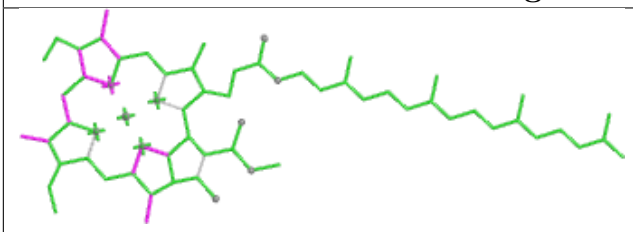
Torsions

Rings

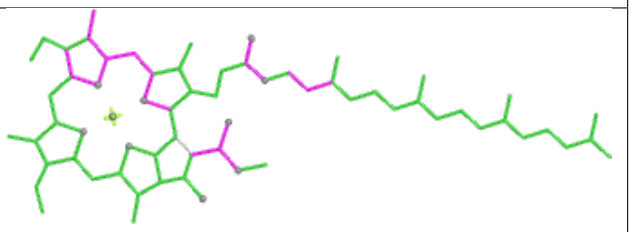
Ligand CLA A 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

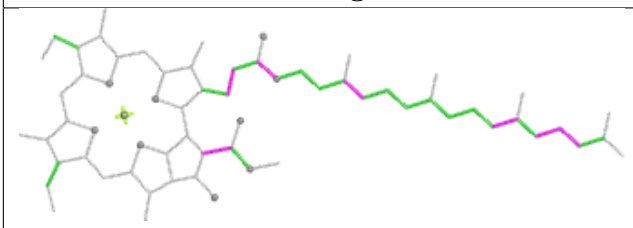
Ligand CLA B 813



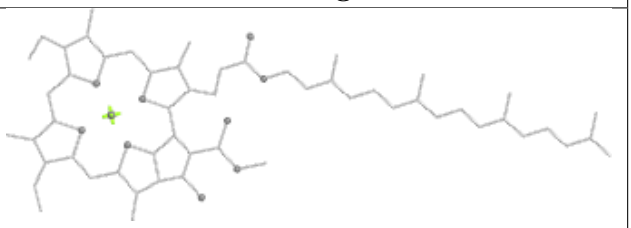
Bond lengths



Bond angles

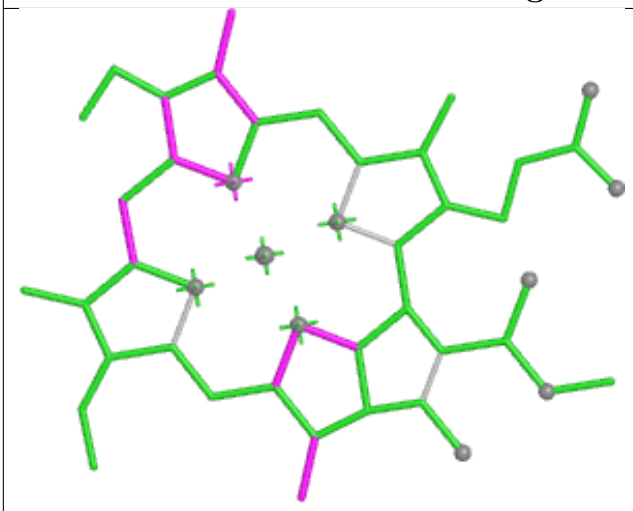


Torsions

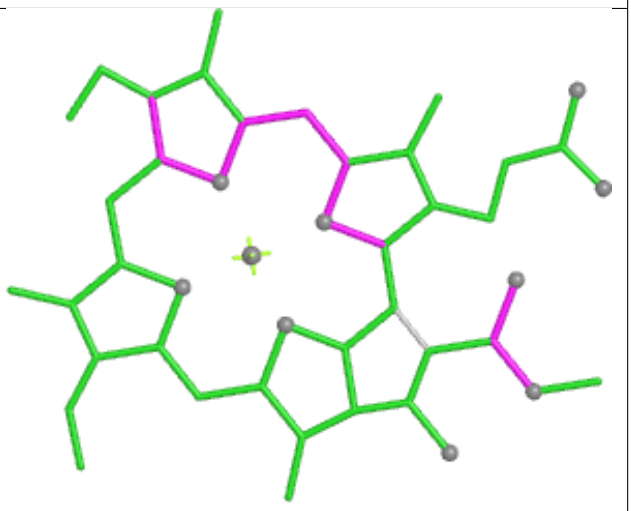


Rings

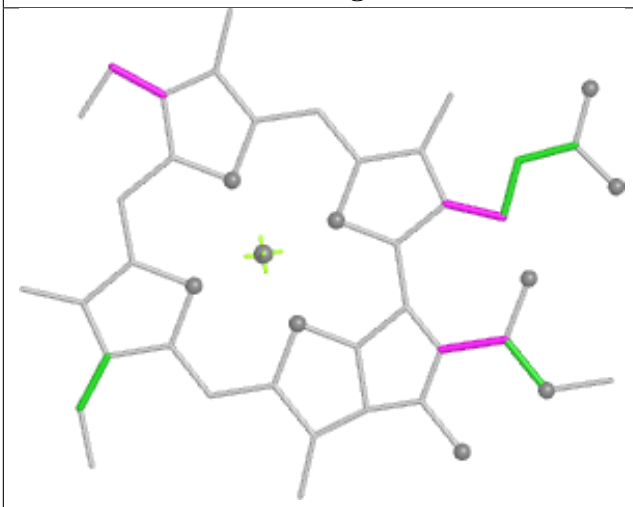
Ligand CLA L 304



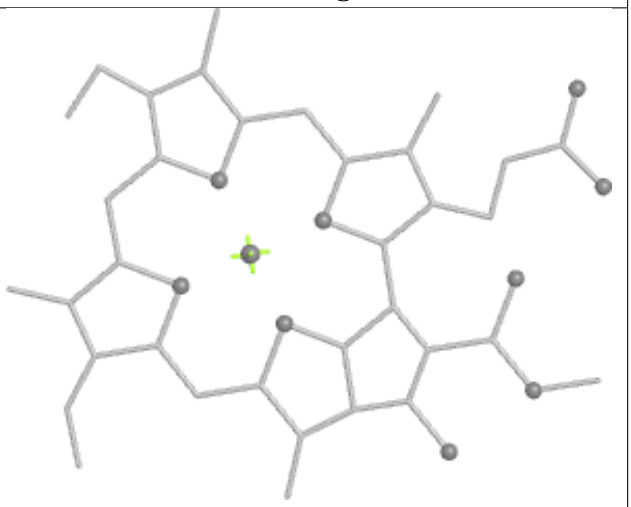
Bond lengths



Bond angles

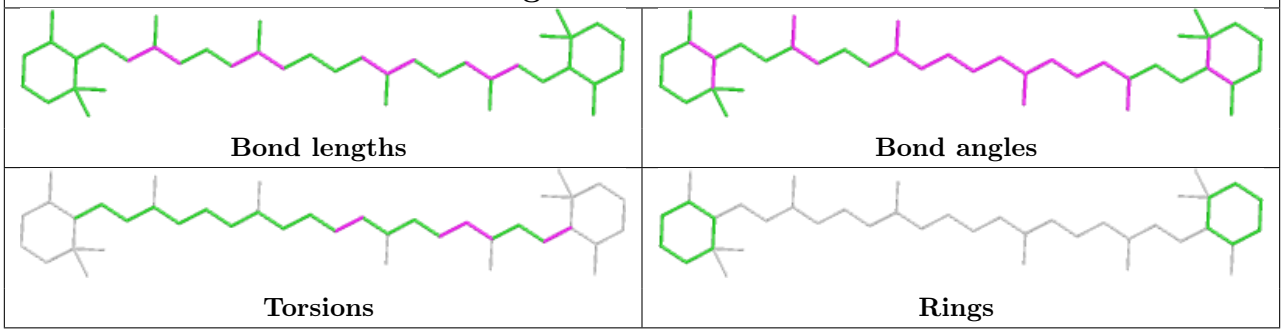


Torsions

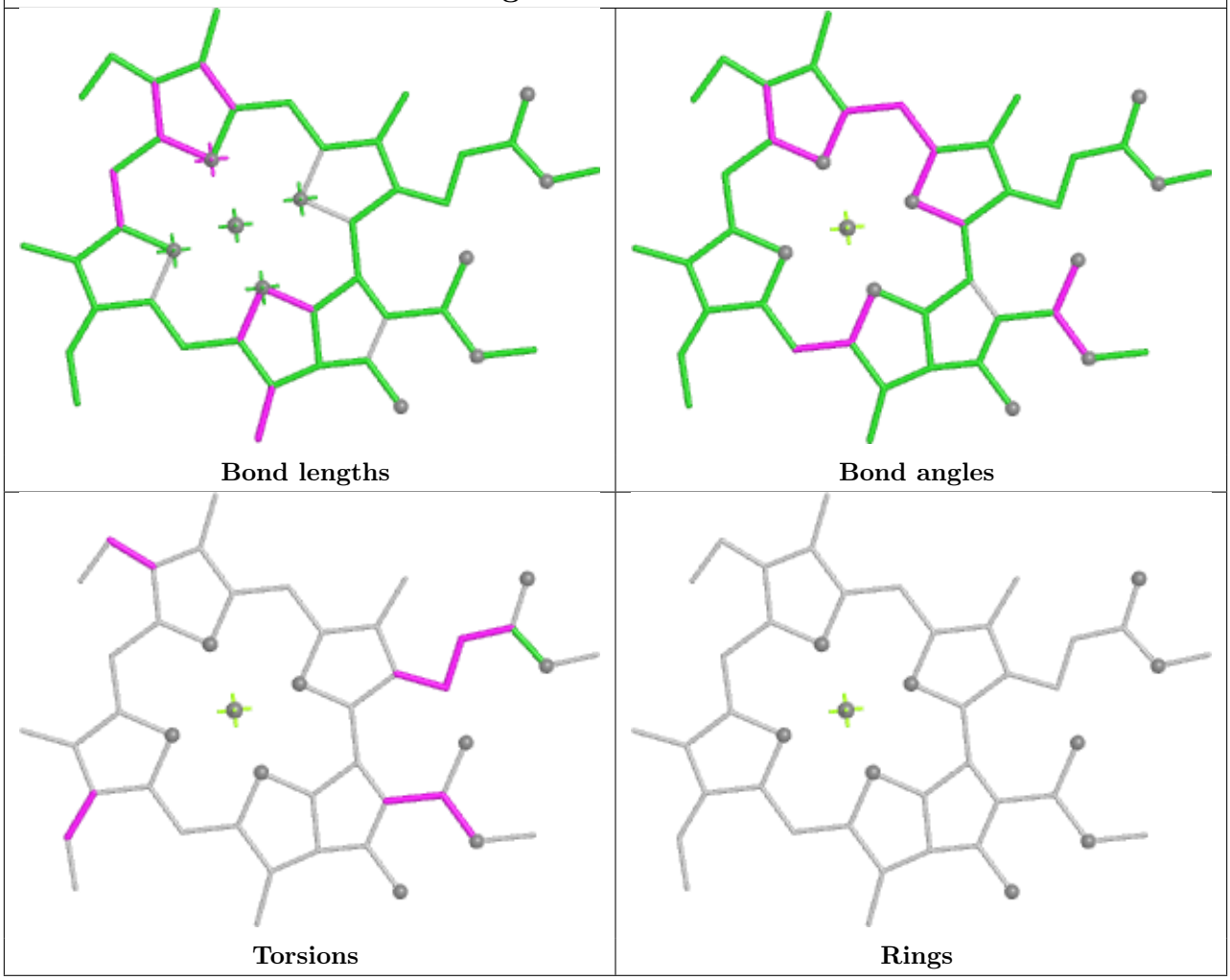


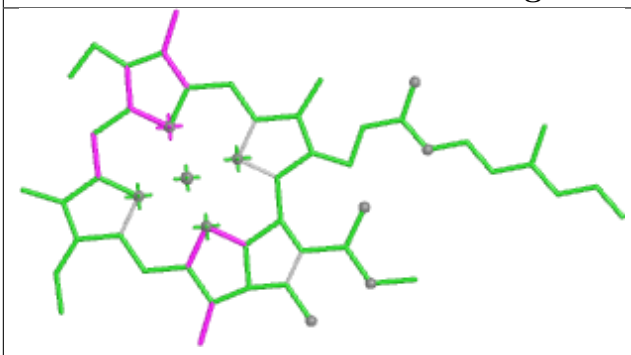
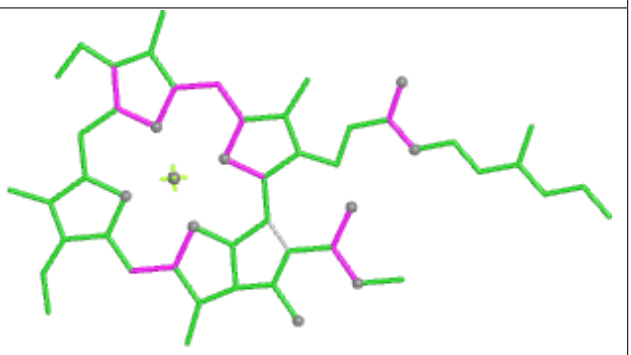
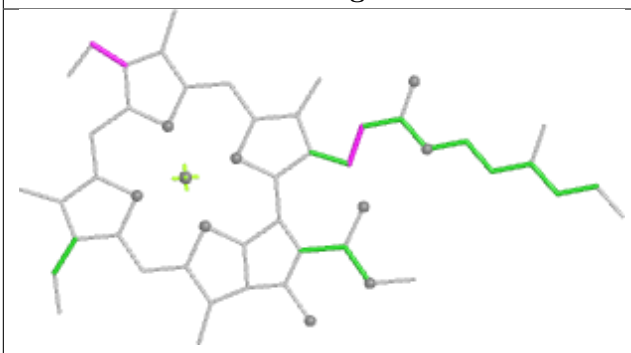
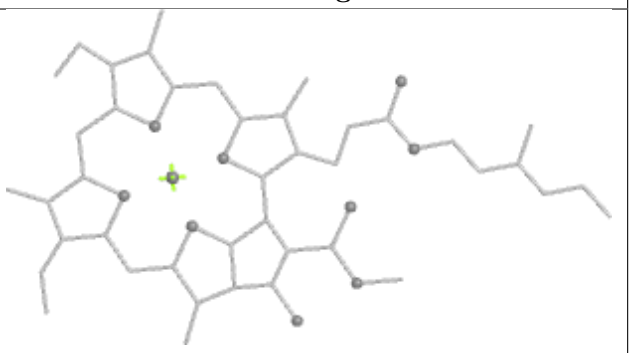
Rings

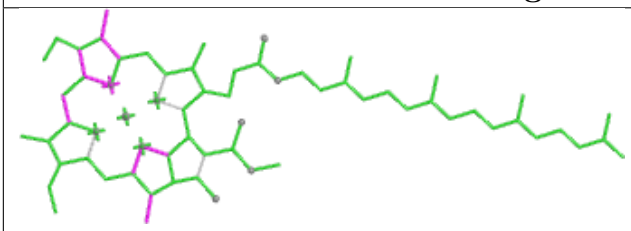
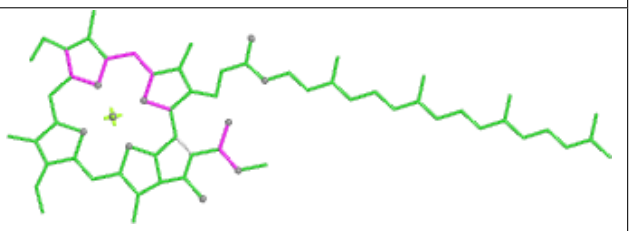
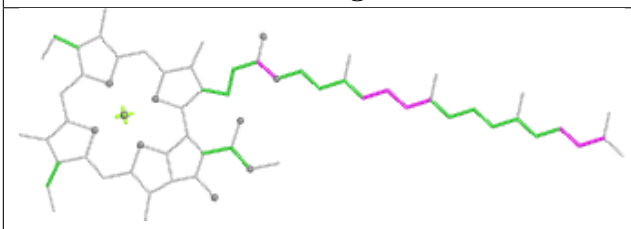
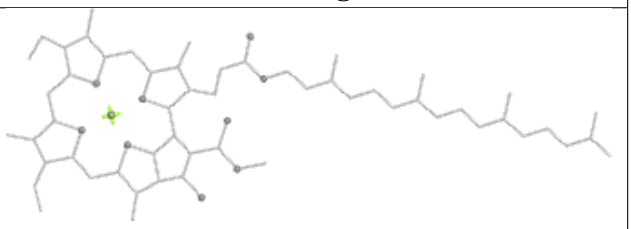
Ligand BCR A 849



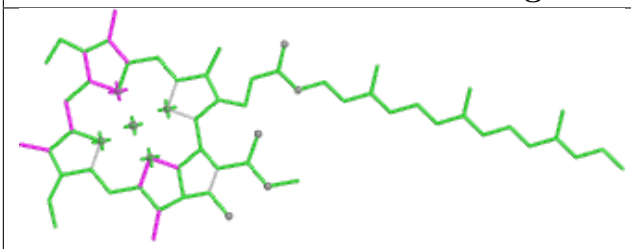
Ligand CLA K 204



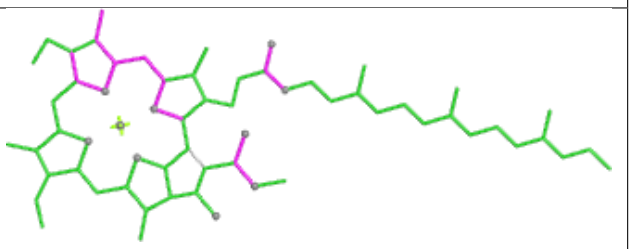
Ligand CLA B 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

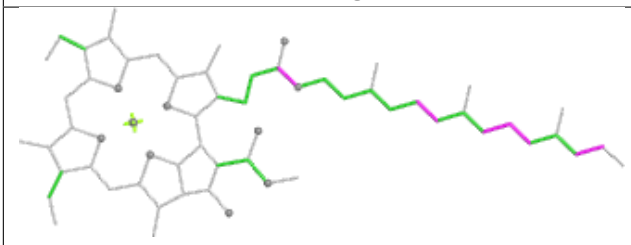
Ligand CLA B 826



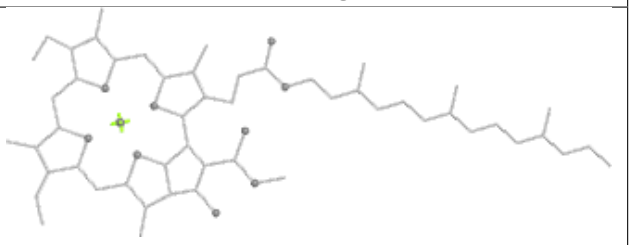
Bond lengths



Bond angles

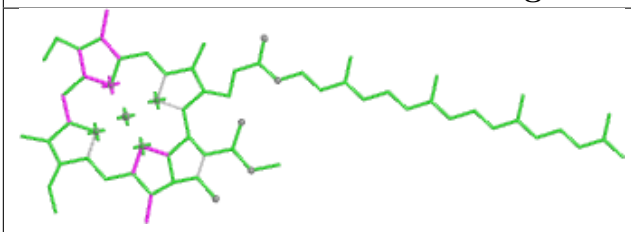


Torsions

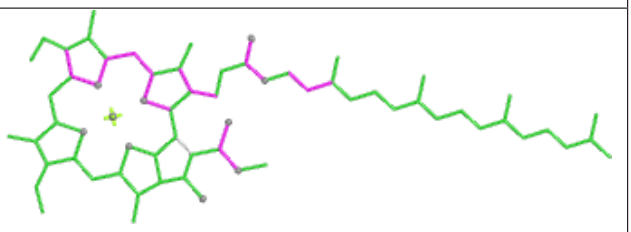


Rings

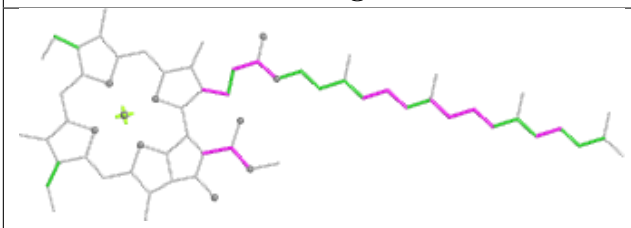
Ligand CLA B 822



Bond lengths



Bond angles



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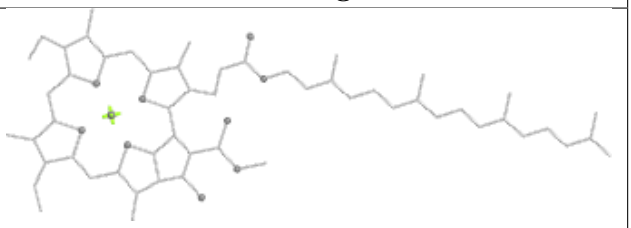
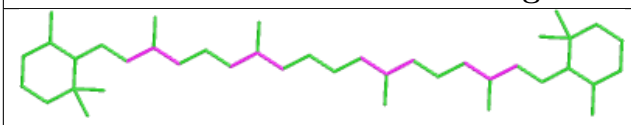


Rings

Ligand BCR B 848



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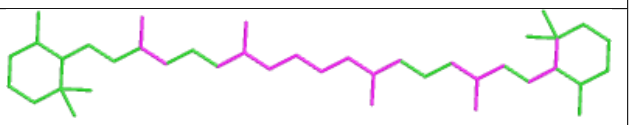
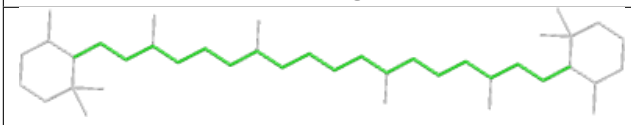
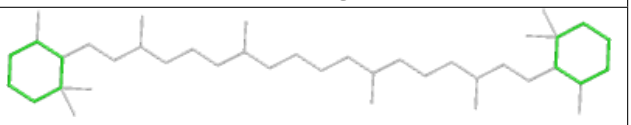


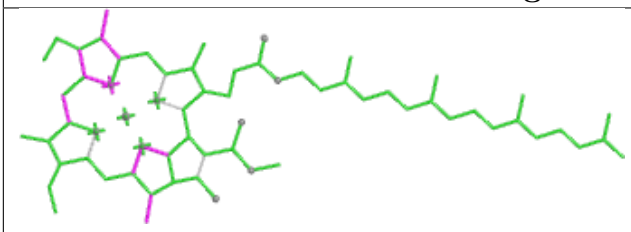
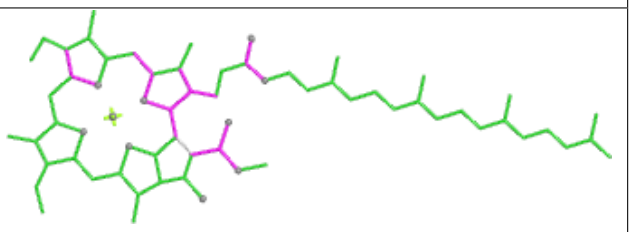
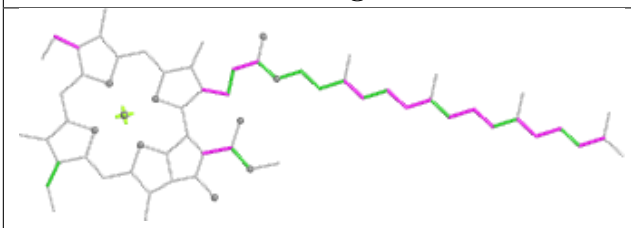
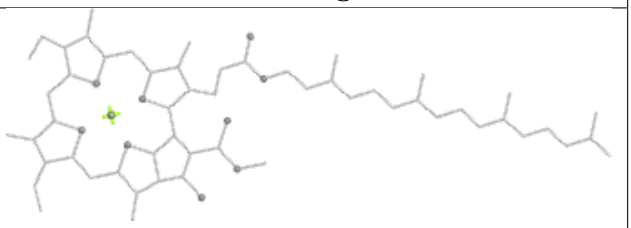
Bond angles

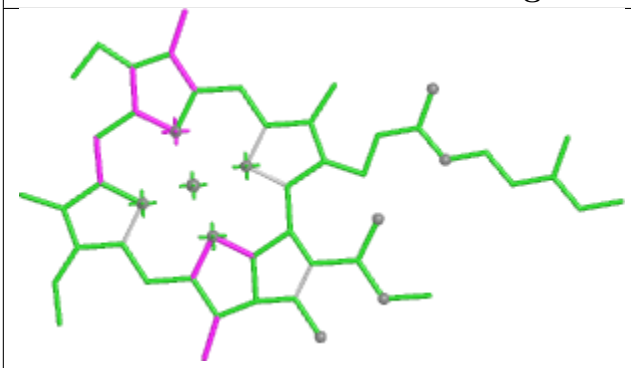
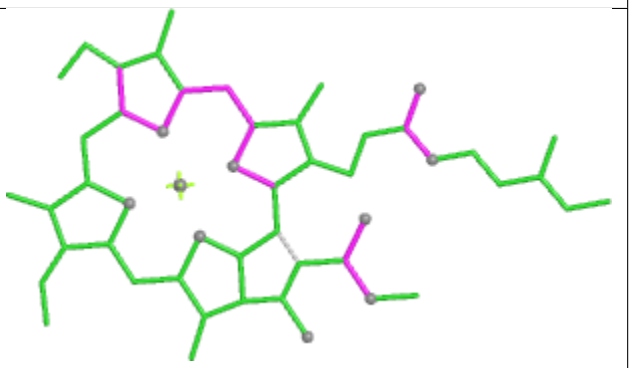
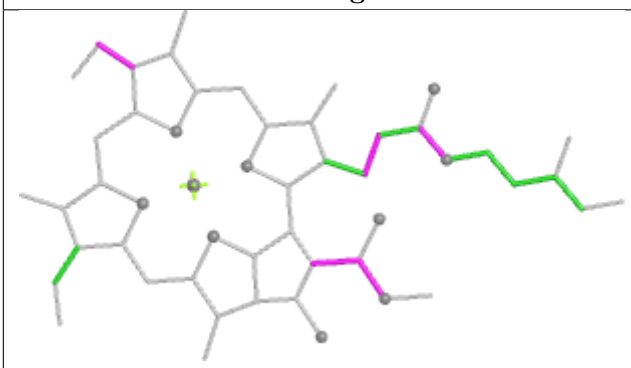
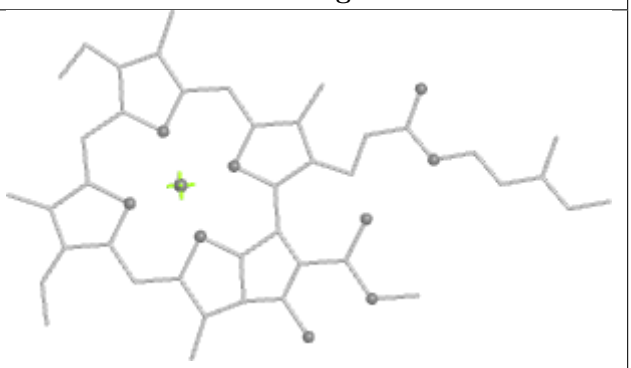


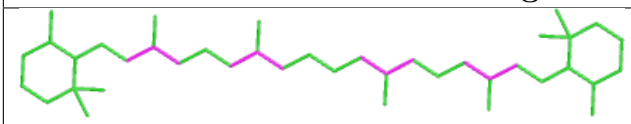
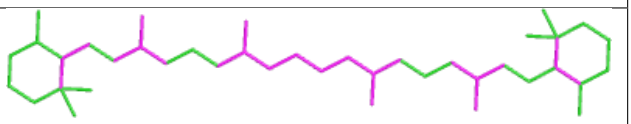
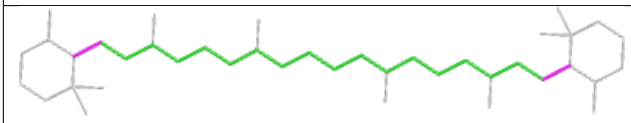
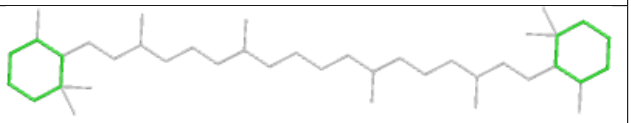
Torsions

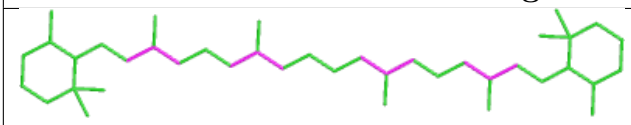
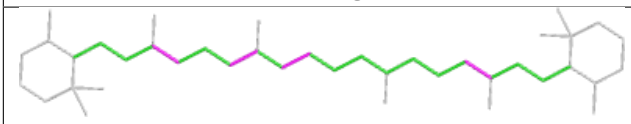
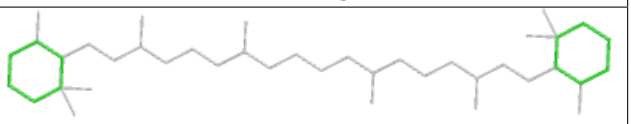


Rings

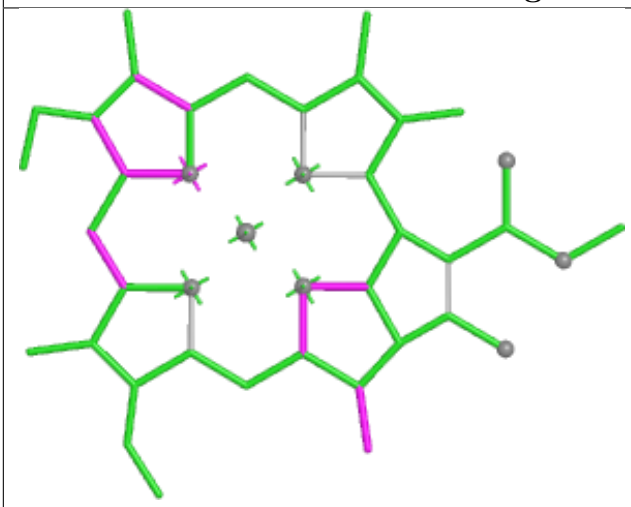
Ligand CLA A 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

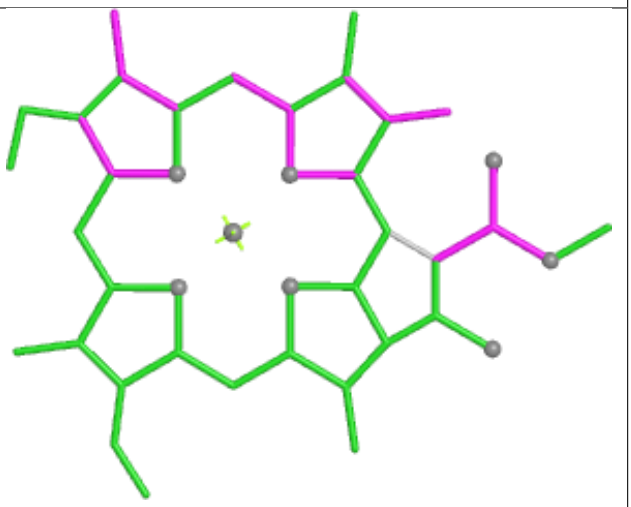
Ligand BCR G 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 851	
 Bond lengths	Bond angles
 Torsions	 Rings

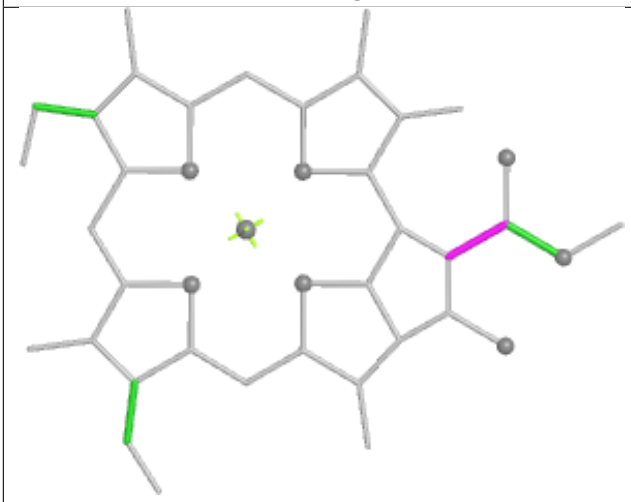
Ligand CLA B 804



Bond lengths



Bond angles



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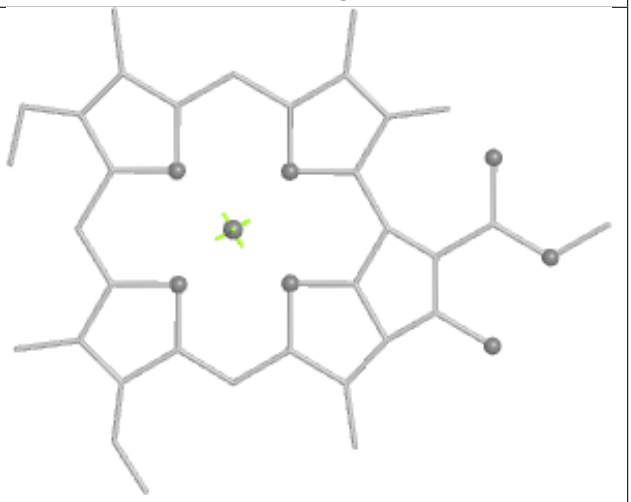
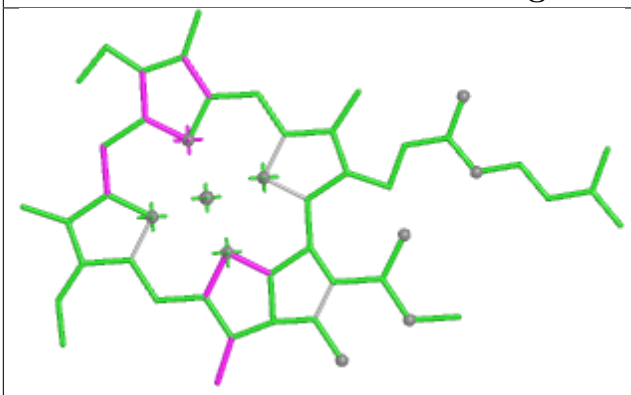


Rings

Ligand CLA 4 614



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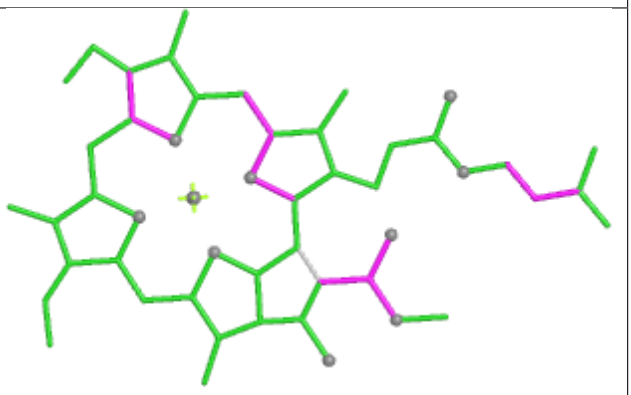
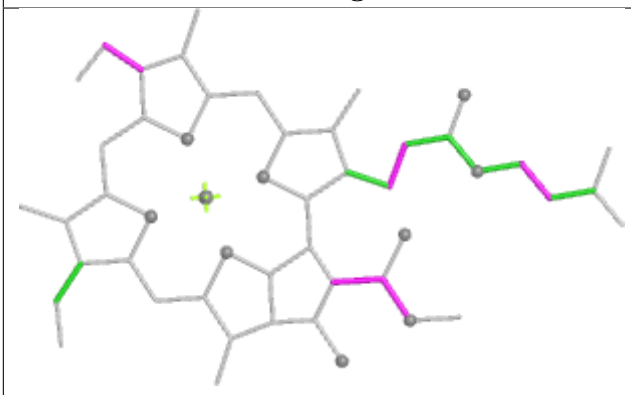


Bond angles



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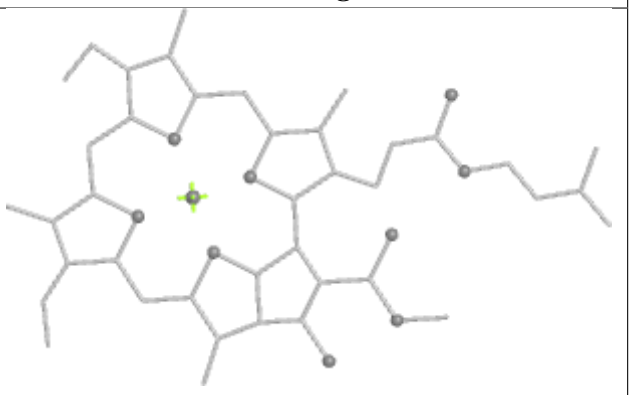
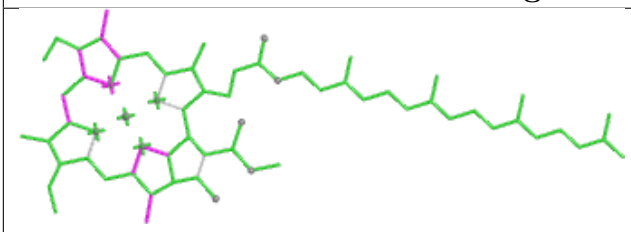


Rings

Ligand CLA A 820



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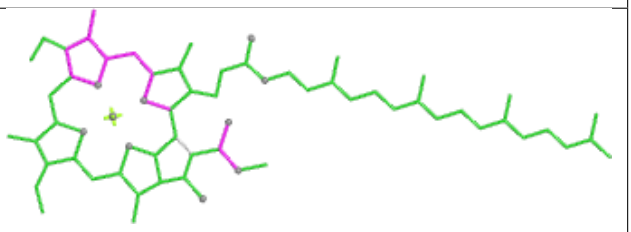
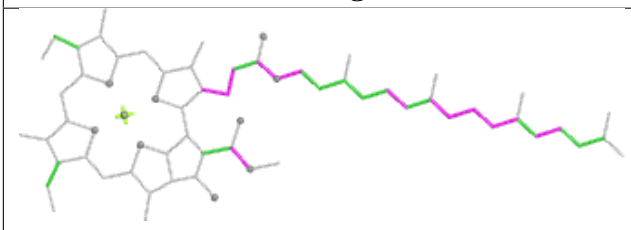


Bond angles



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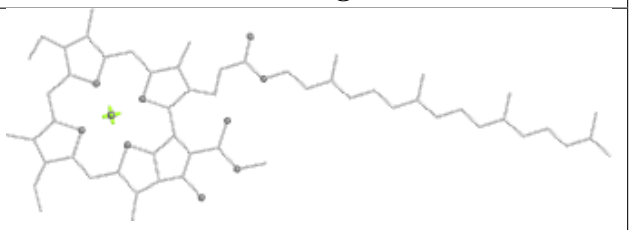
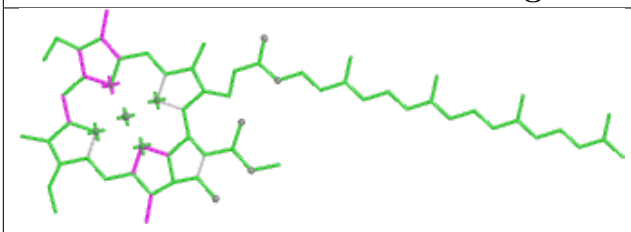
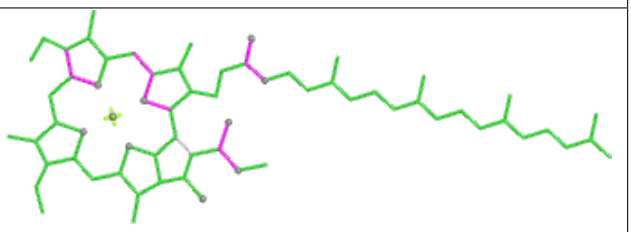
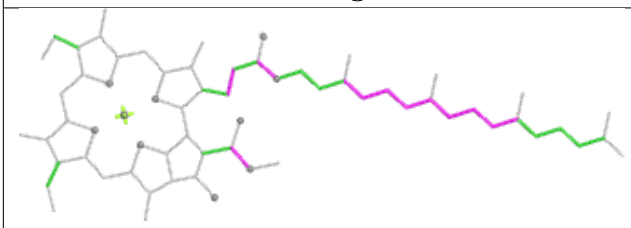
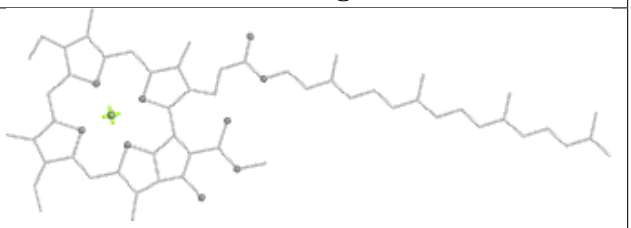


Rings

Ligand CLA B 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

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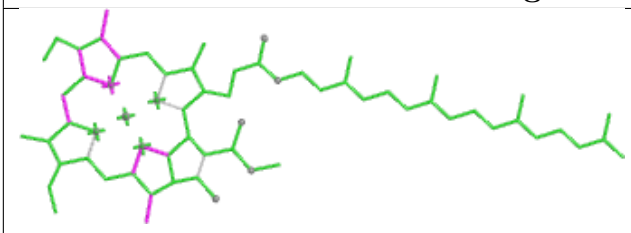
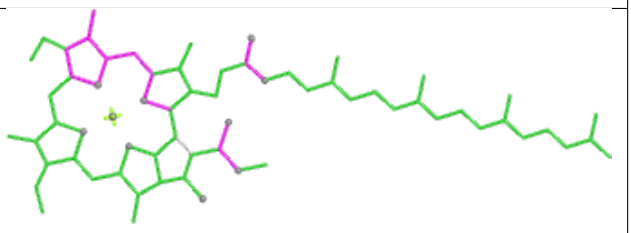
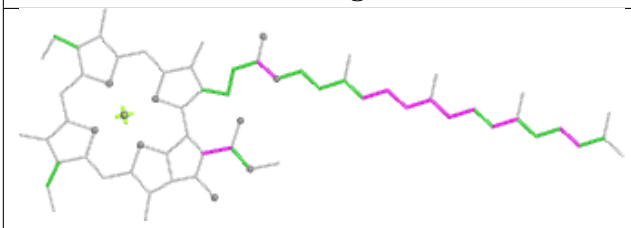
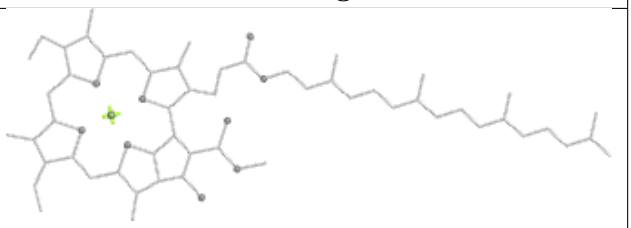
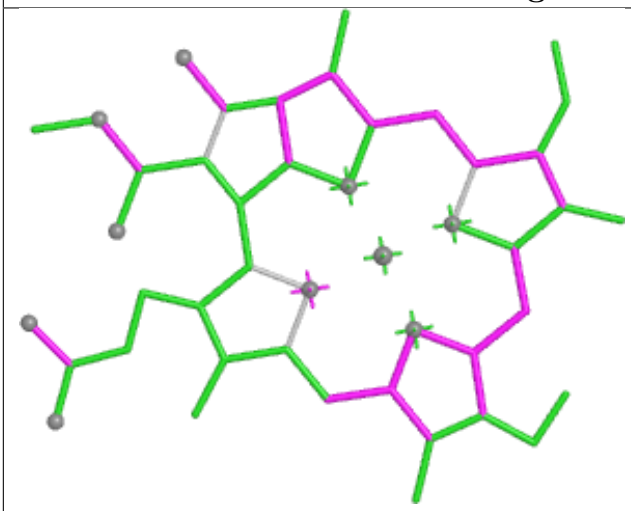
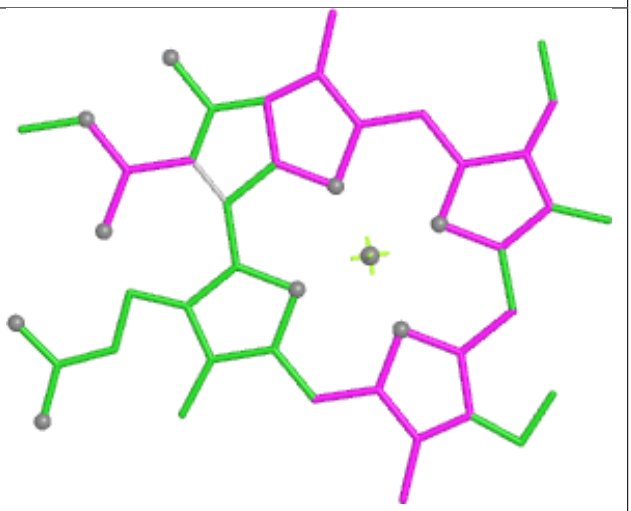
 Bond lengths	 Bond angles
 Torsions	 Rings

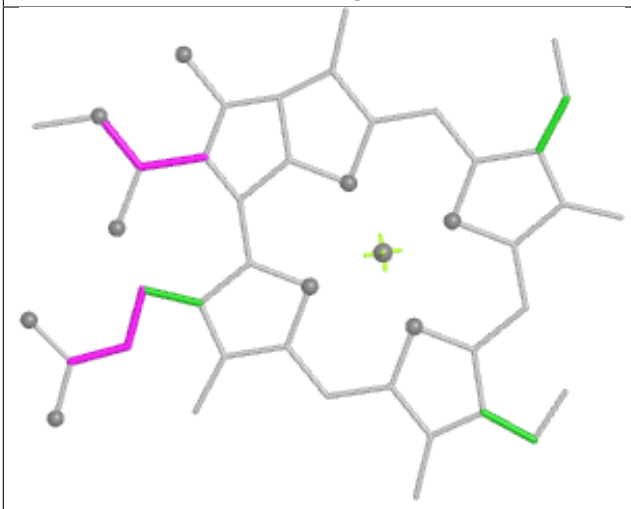
Ligand CHL 3 606



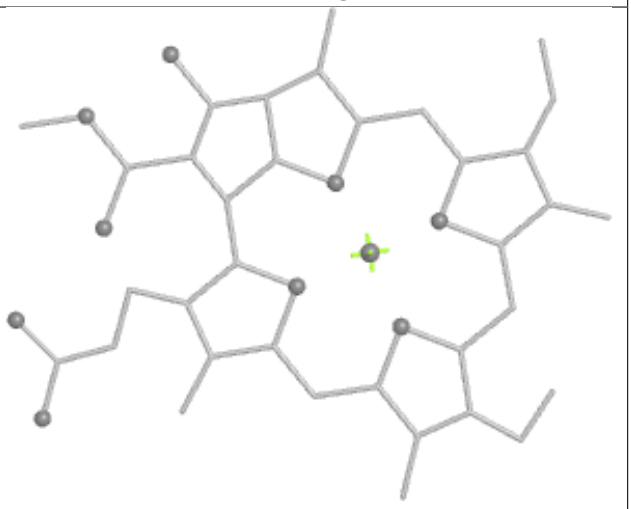
Bond lengths



Bond angles

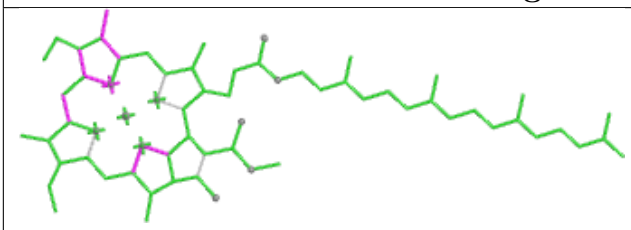


Torsions



Rings

Ligand CLA A 835



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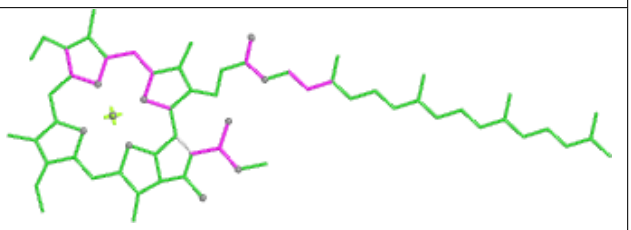
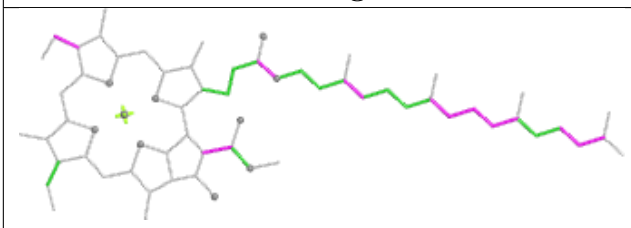


Bond angles



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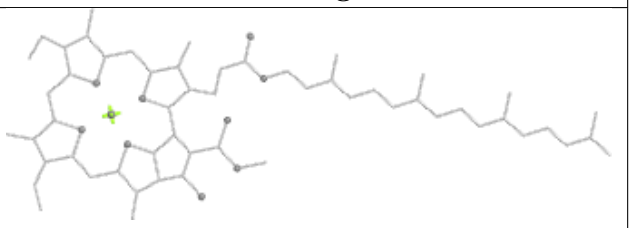
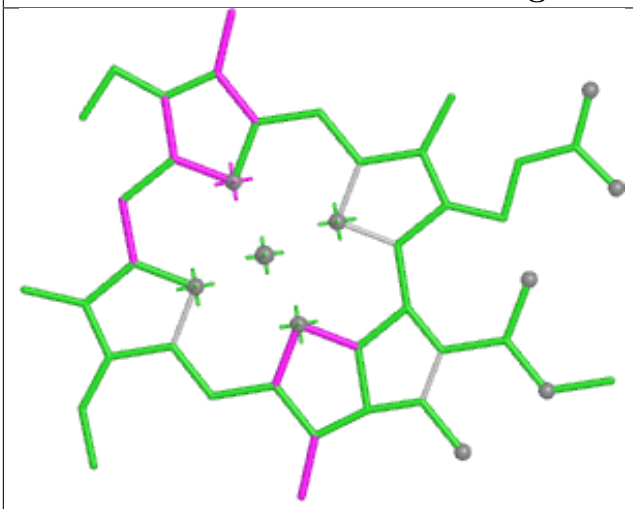


Rings

Ligand CLA 4 613



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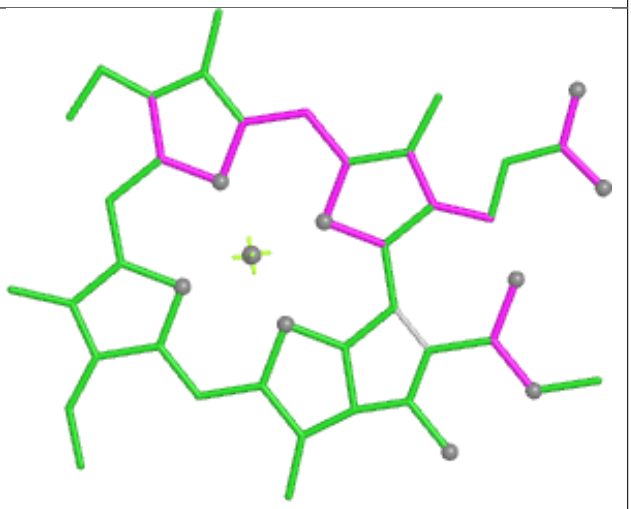
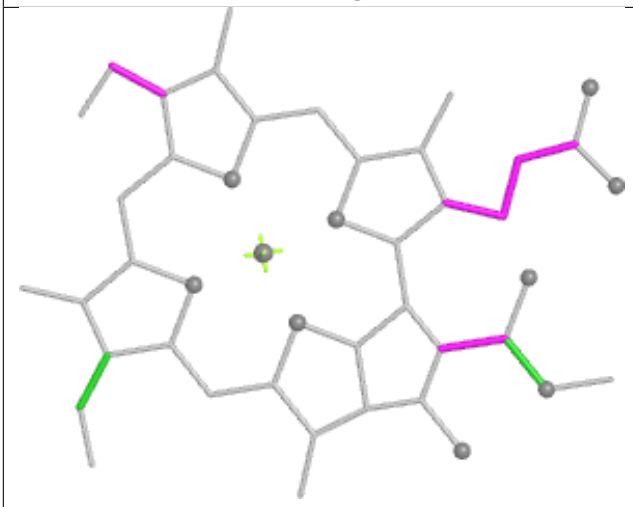


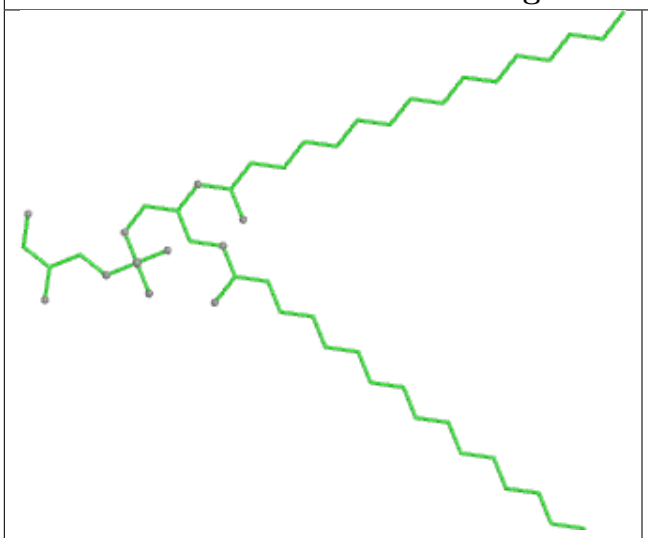
Bond angles



Torsions

Rings

Ligand LHG A 846



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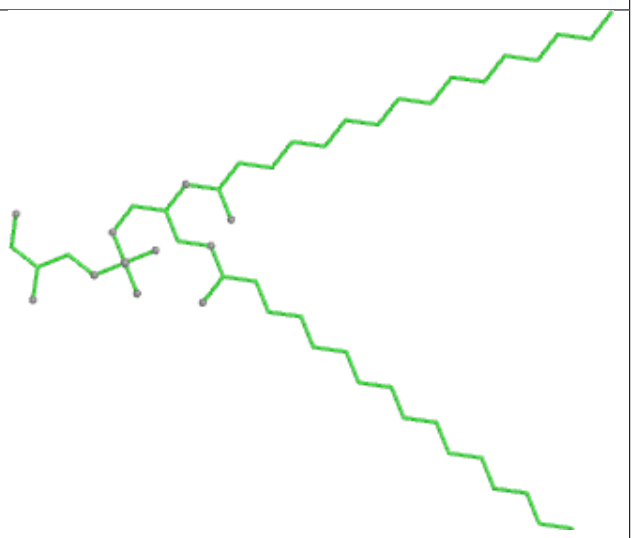
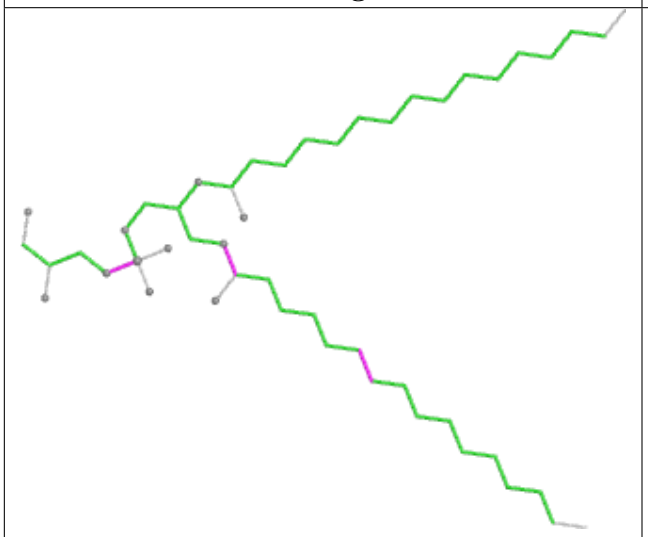
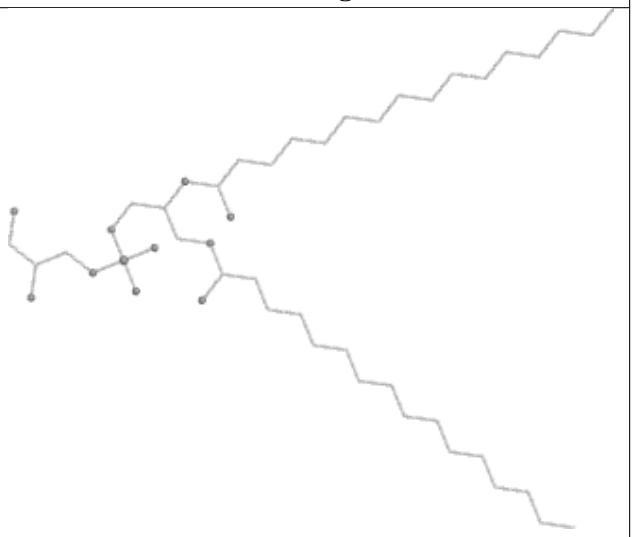


Bond angles

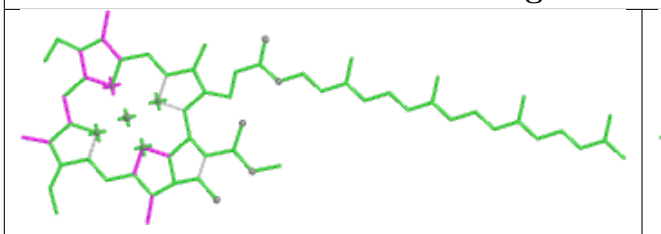


Torsions



Rings

Ligand CLA B 809



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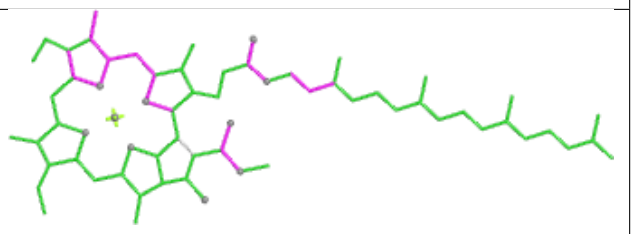
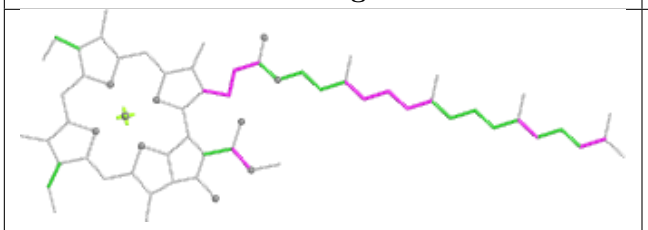


Bond angles



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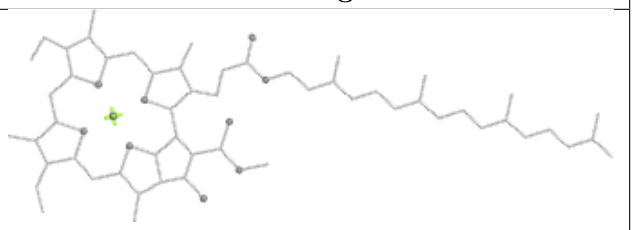
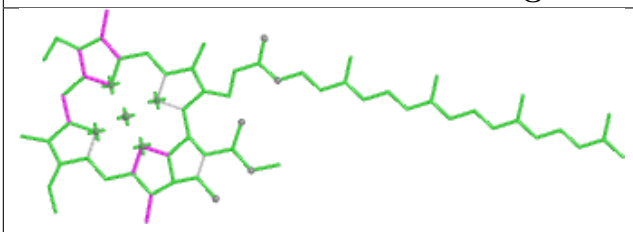
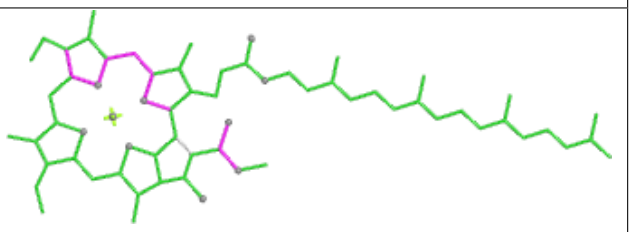


Rings

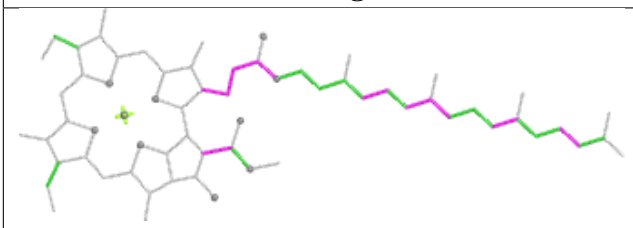
Ligand CLA B 832



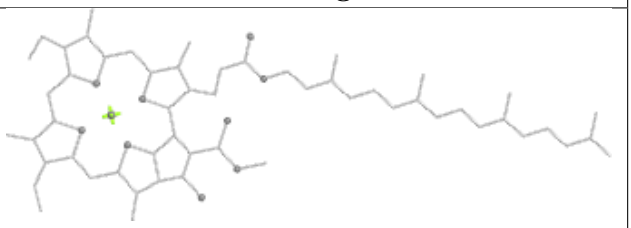
Bond lengths



Bond angles

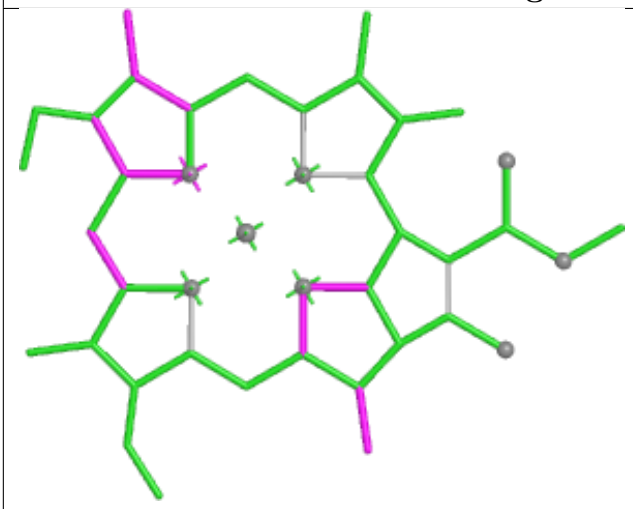


Torsions



Rings

Ligand CLA F 303



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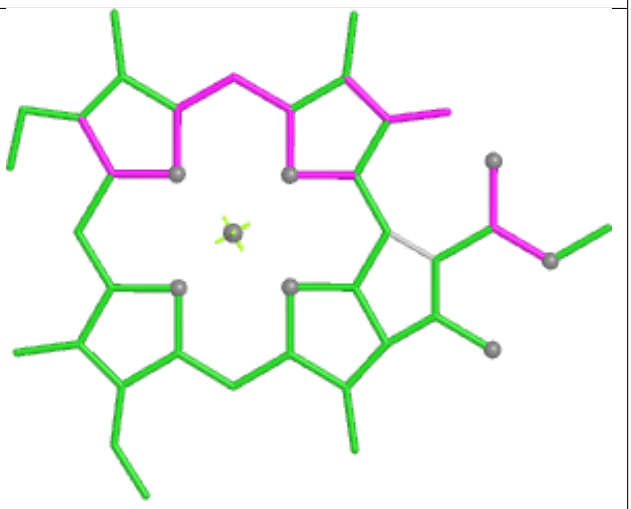
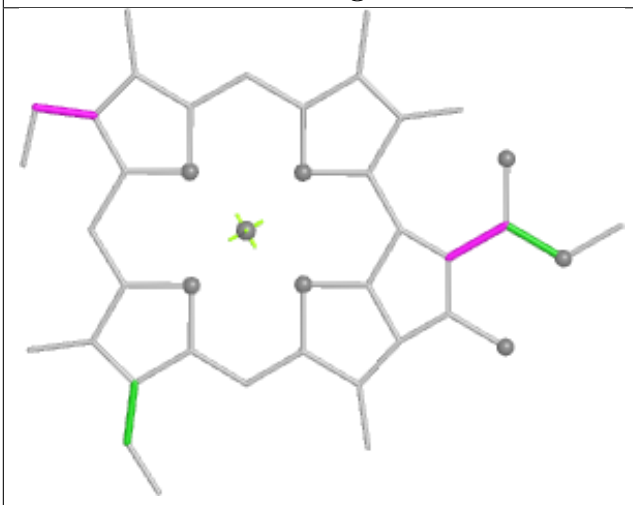
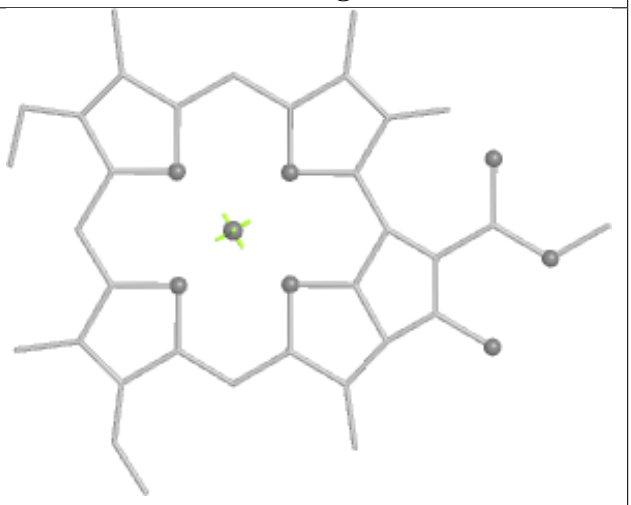


Bond angles

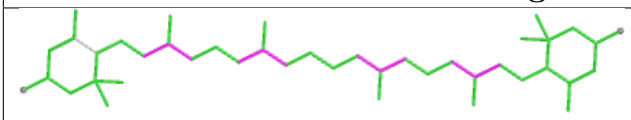


Torsions

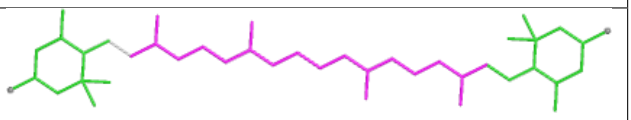


Rings

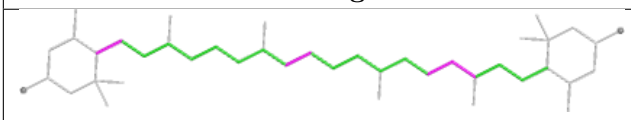
Ligand LUT 3 613



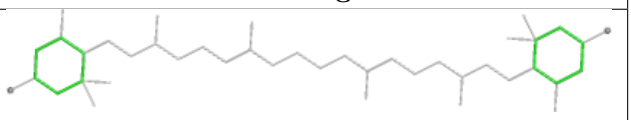
Bond lengths



Bond angles

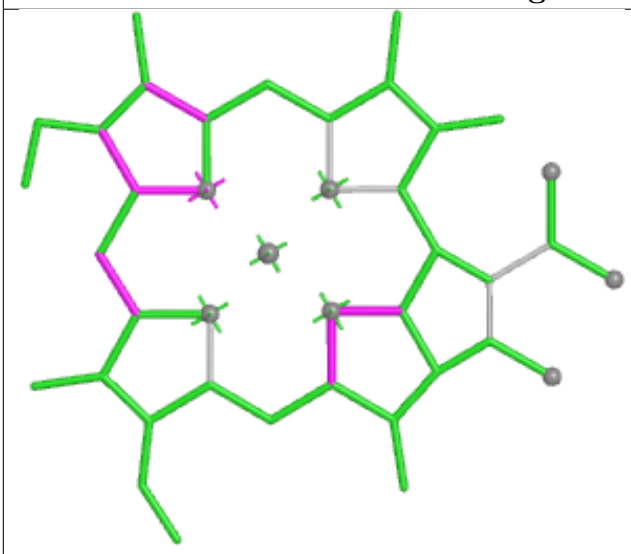


Torsions



Rings

Ligand CLA 3 610



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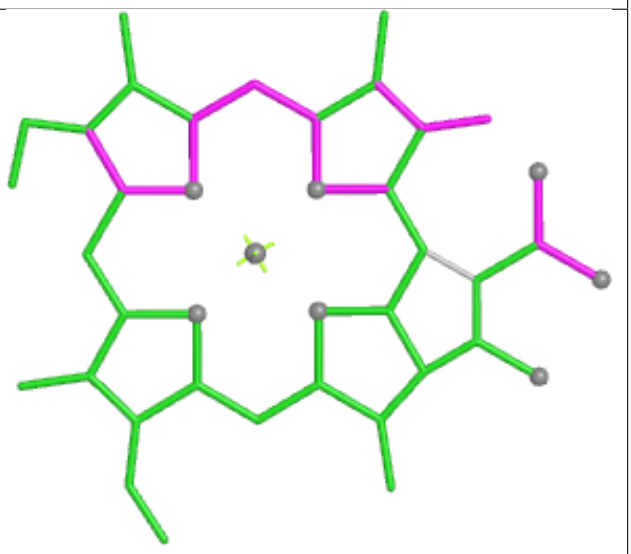
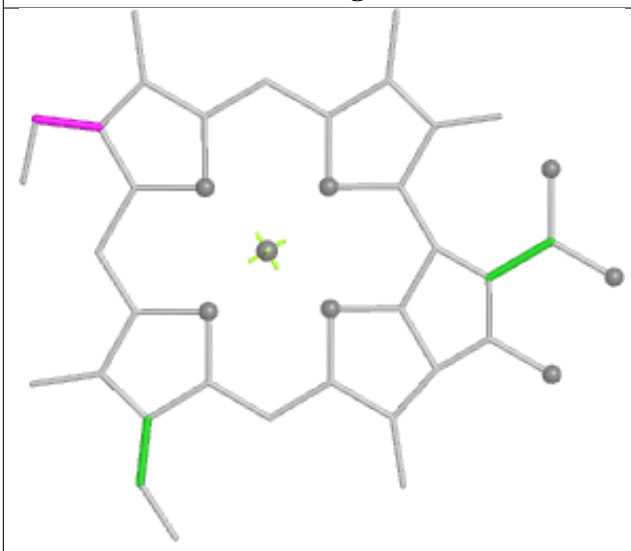


Bond angles



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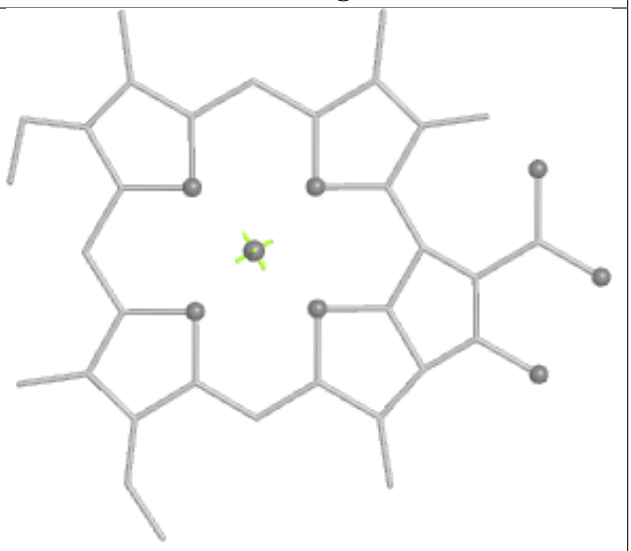
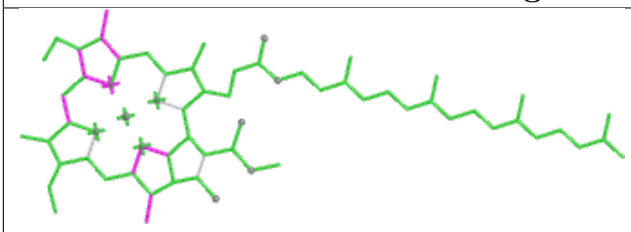
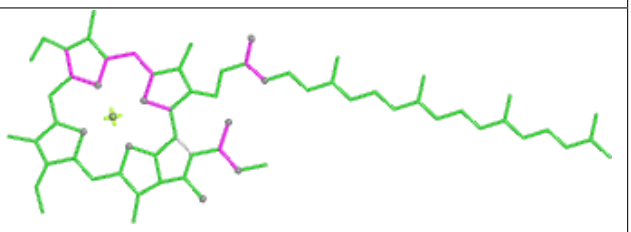
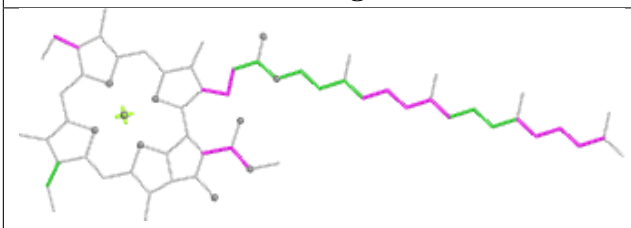
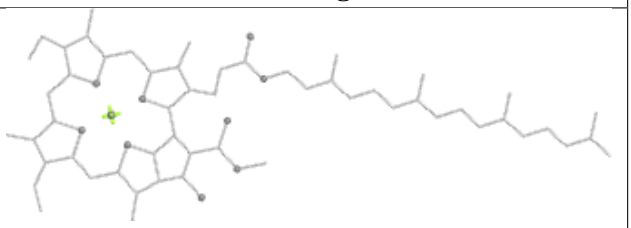
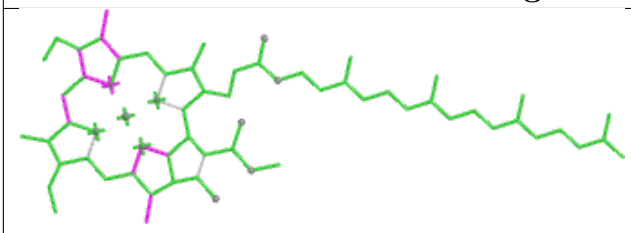
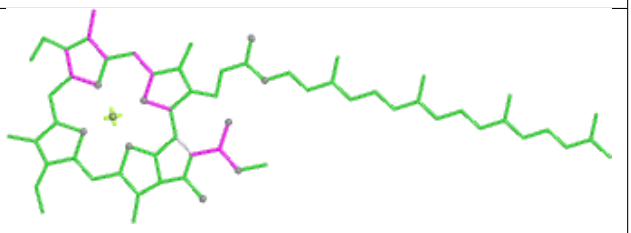
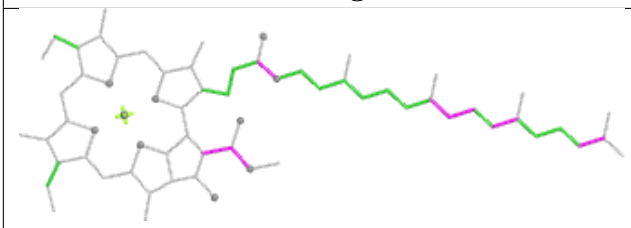
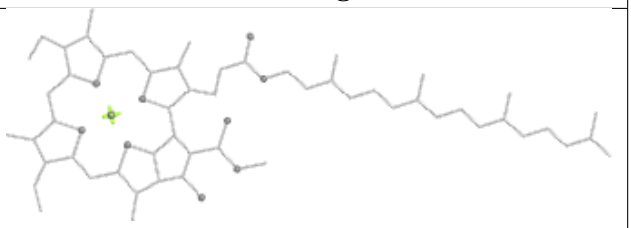
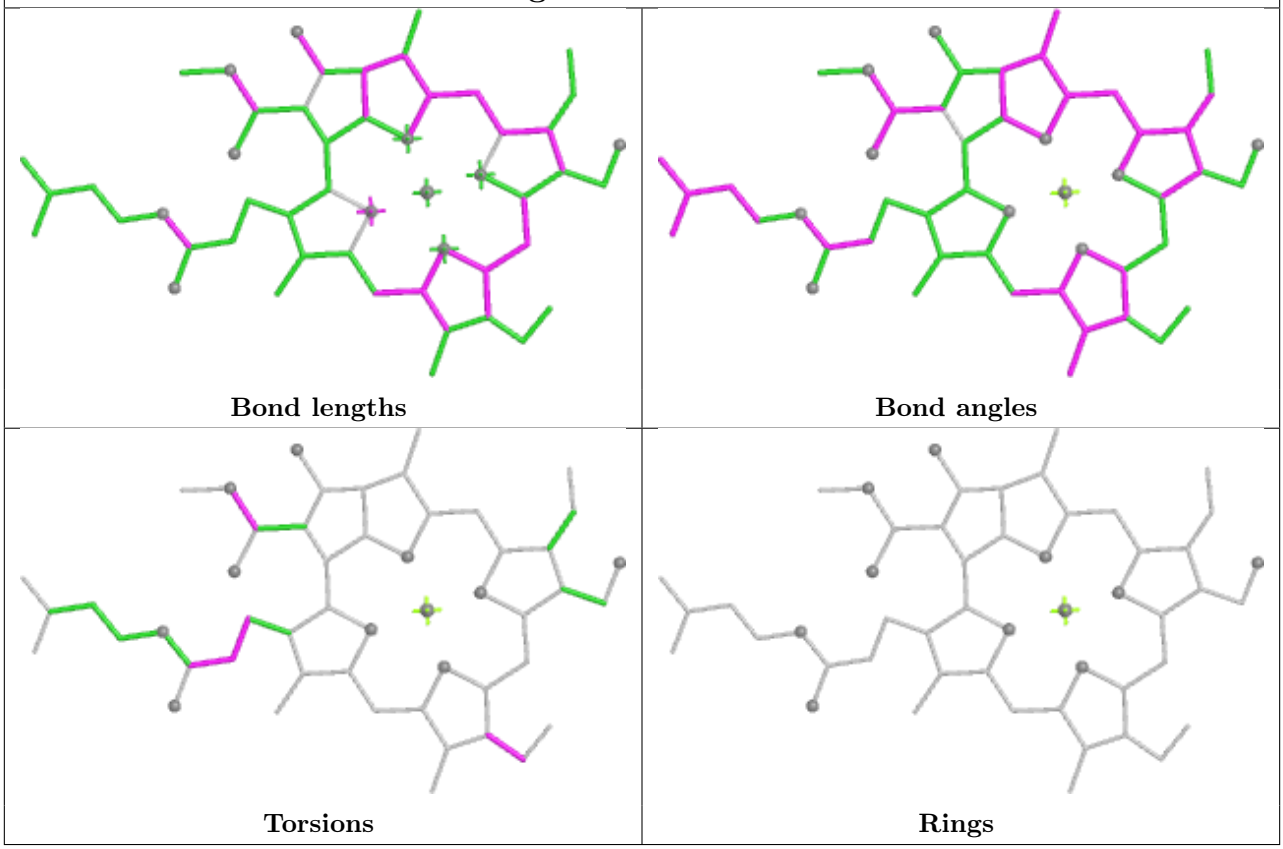


Rings

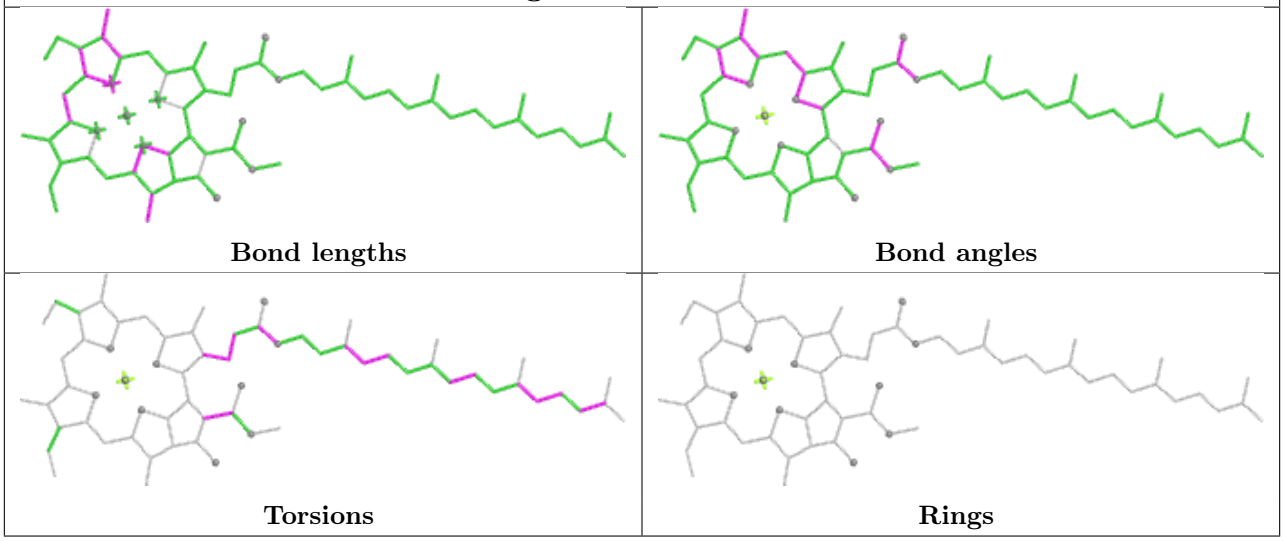
Ligand CLA A 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

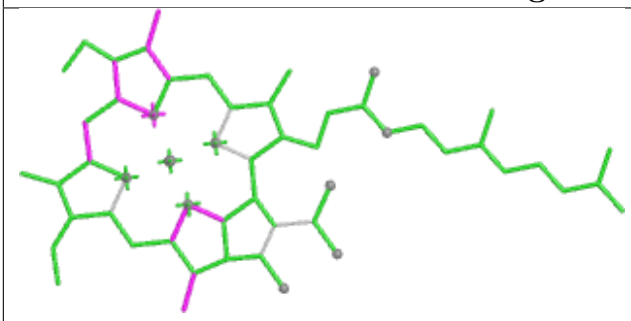
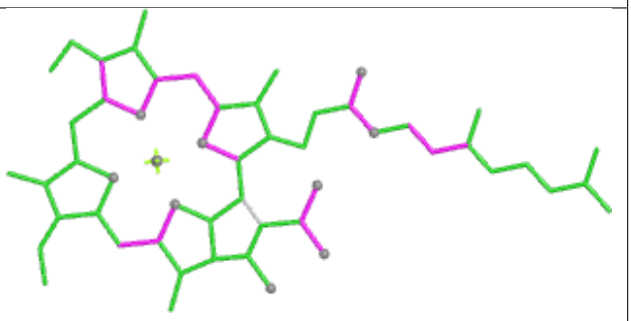
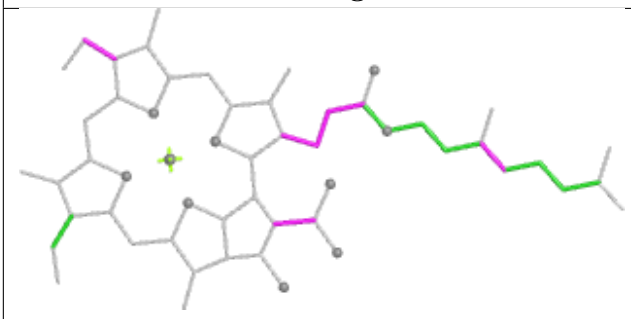
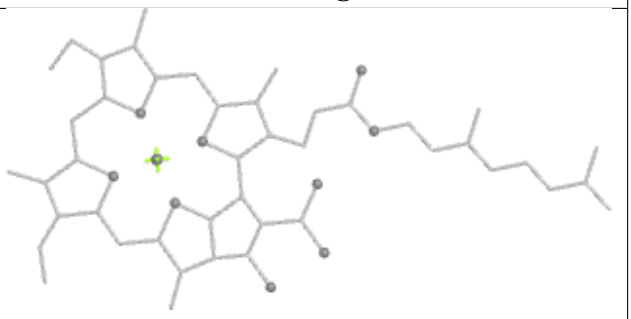
Ligand CLA A 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 2 607

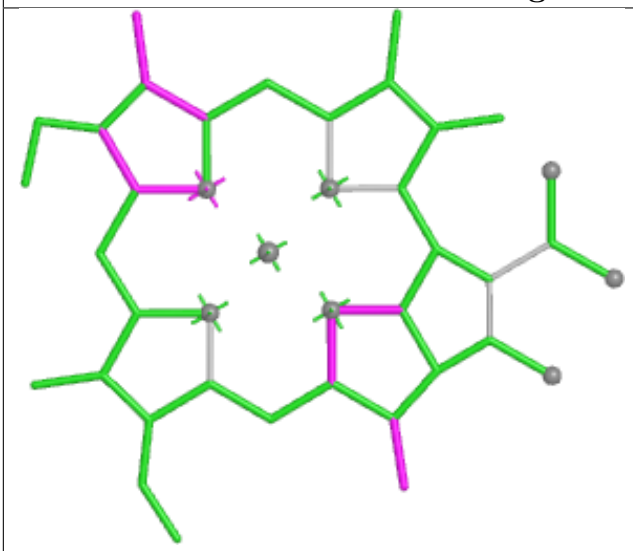


Ligand CLA B 824

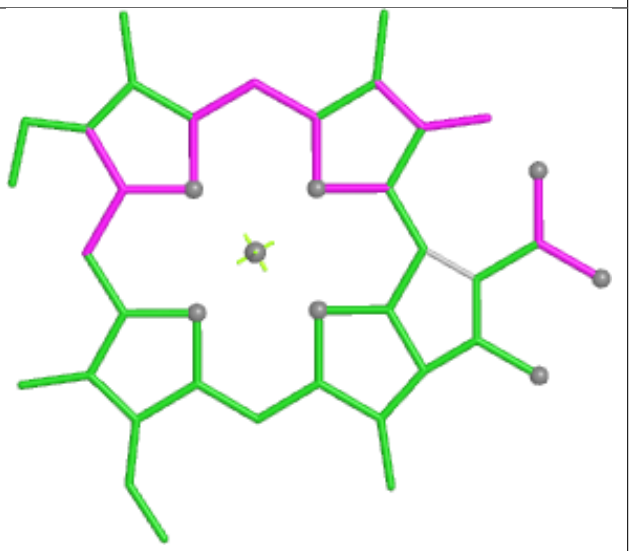


Ligand CLA 3 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

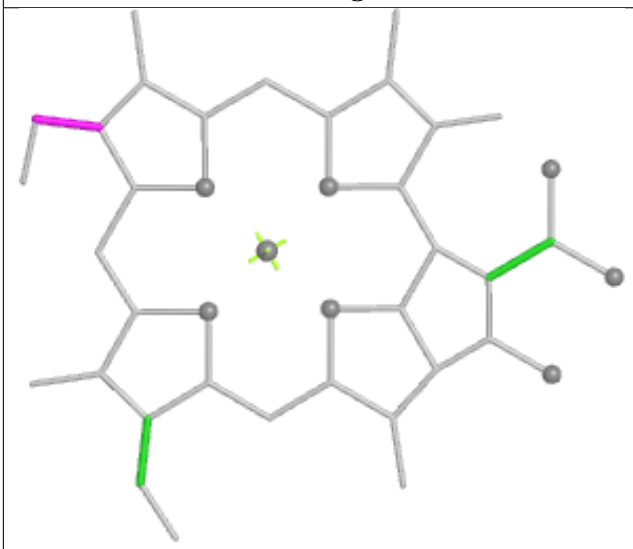
Ligand CLA 3 612



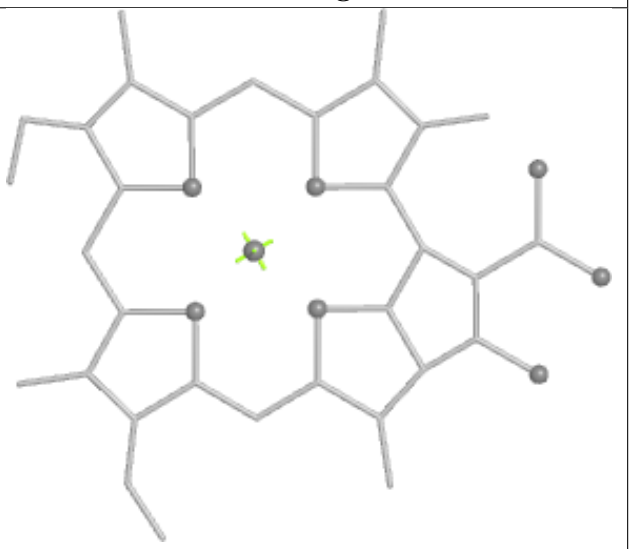
Bond lengths



Bond angles

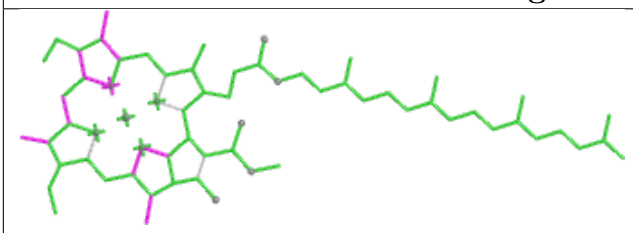


Torsions

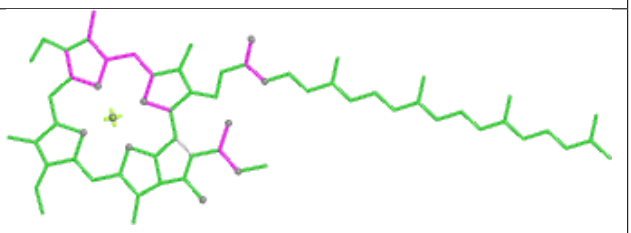


Rings

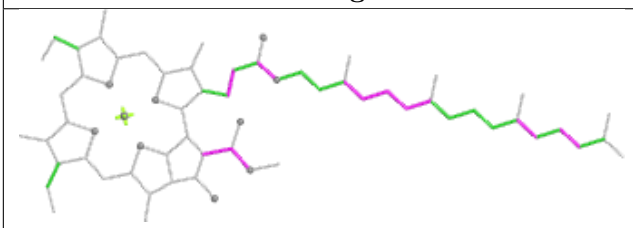
Ligand CLA 2 602



Bond lengths



Bond angles



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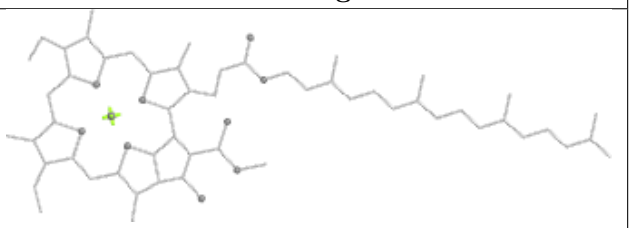
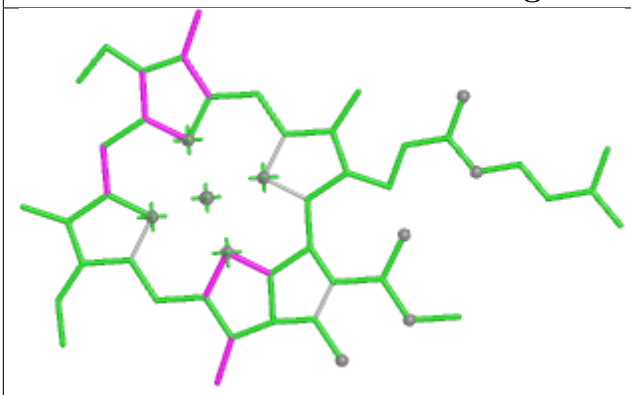
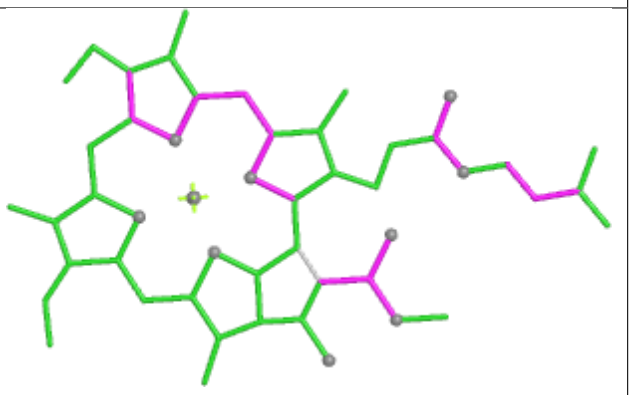
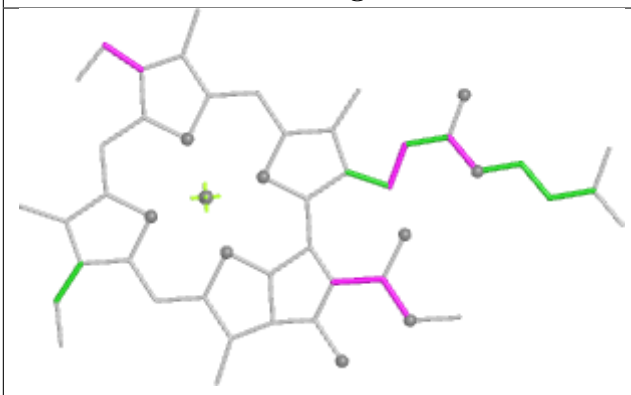
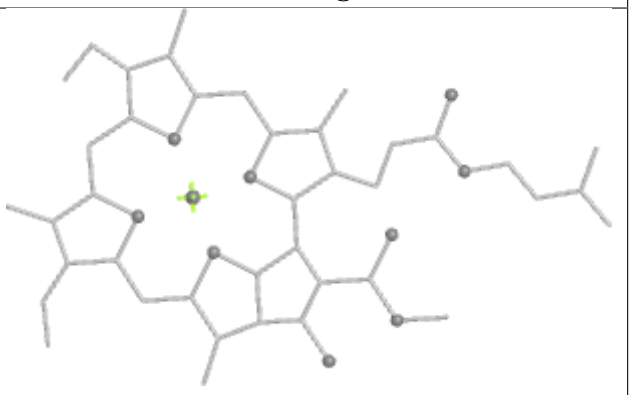
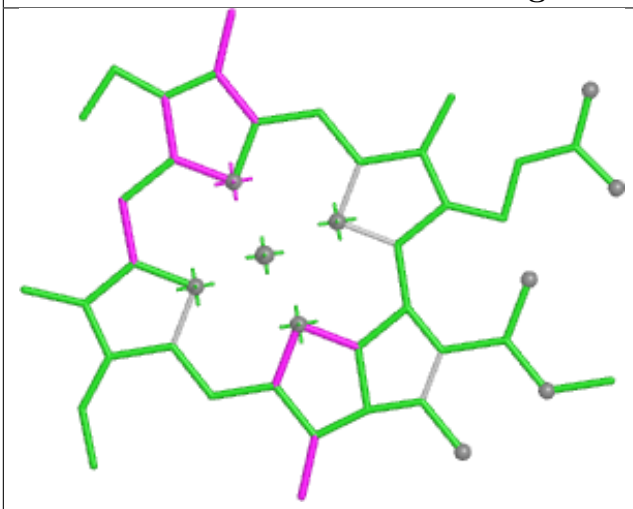


Rings

Ligand CLA A 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 607



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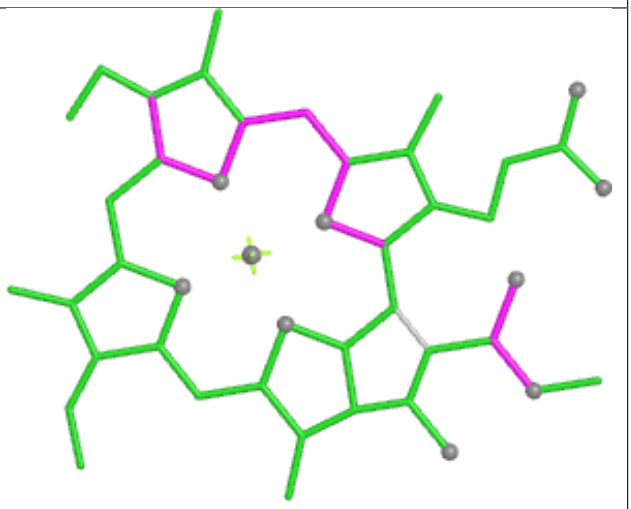
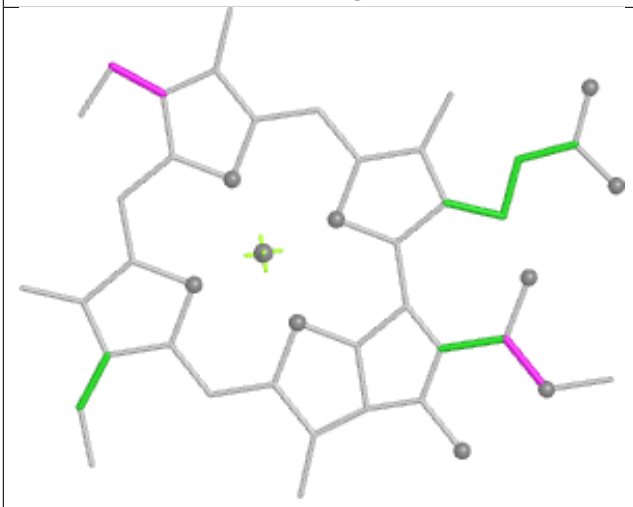


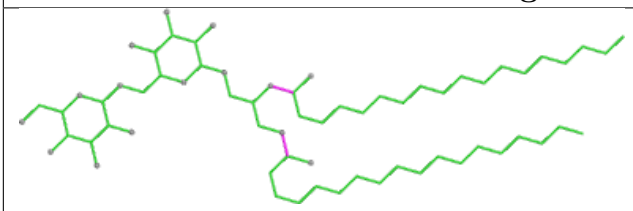
Bond angles



Torsions

Rings

Ligand DGD B 850



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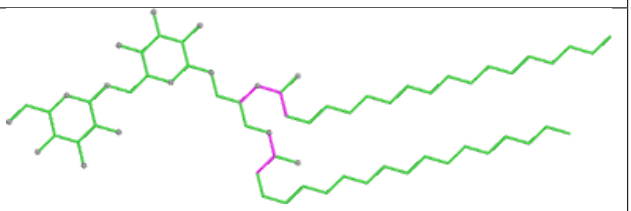

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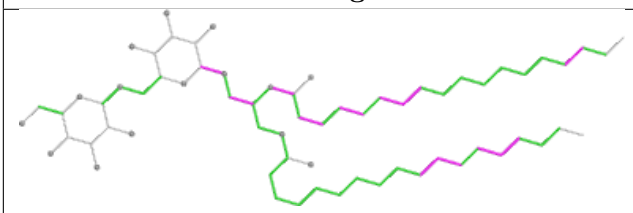
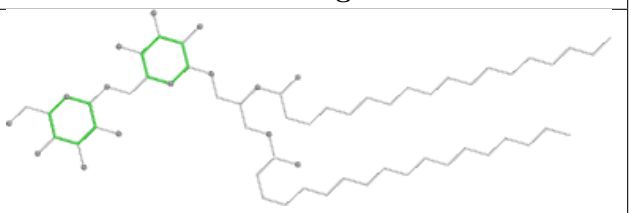
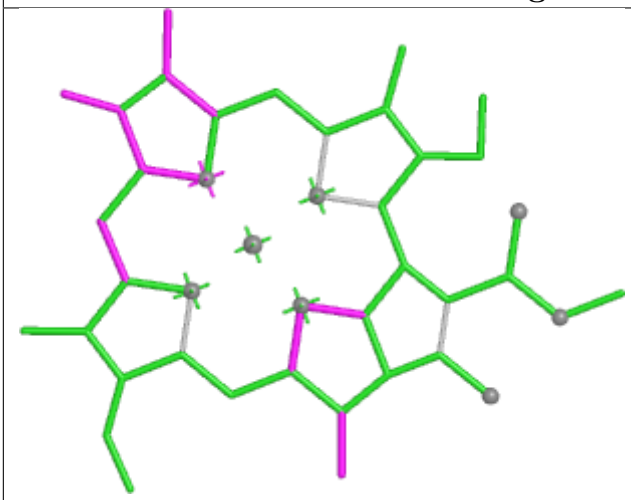


Torsions



Rings

Ligand CLA 3 605



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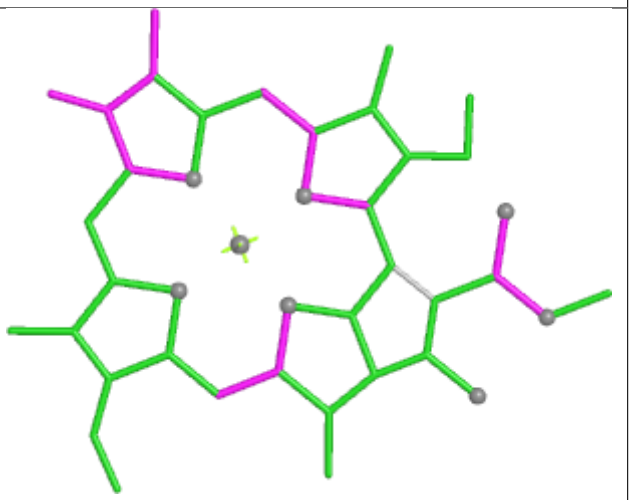
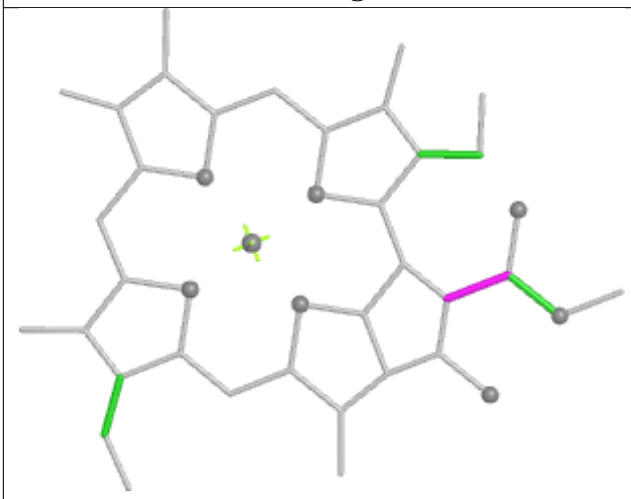


Bond angles



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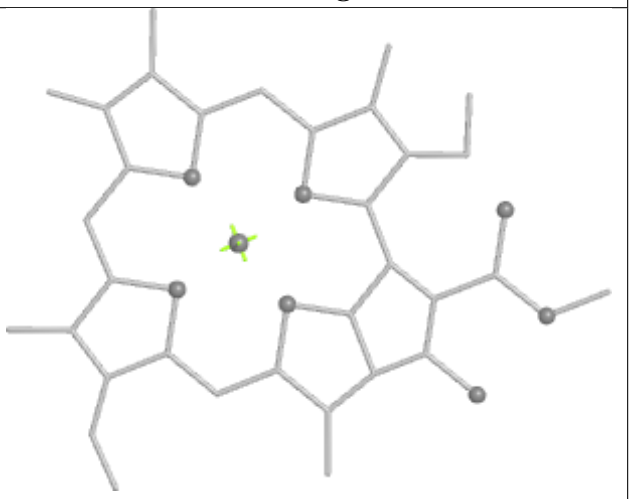
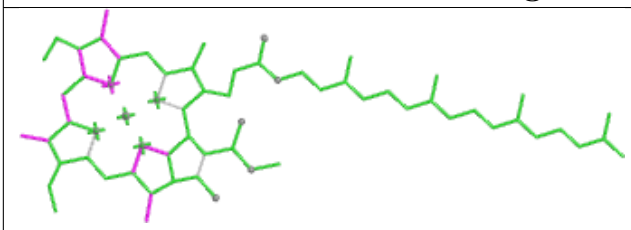


Rings

Ligand CLA A 828



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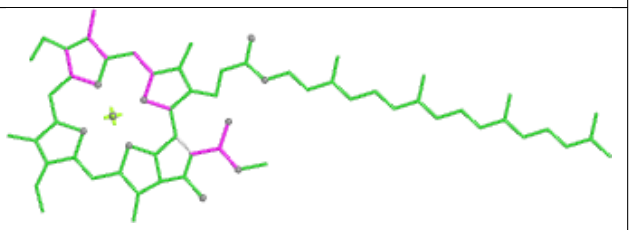
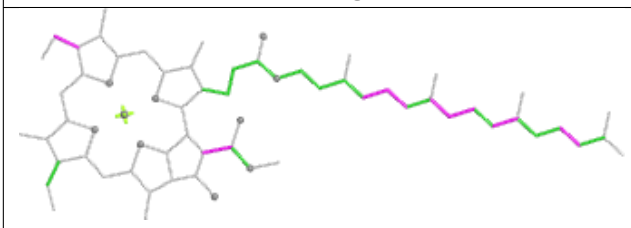


Bond angles



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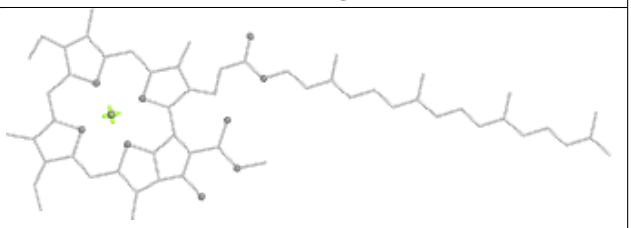
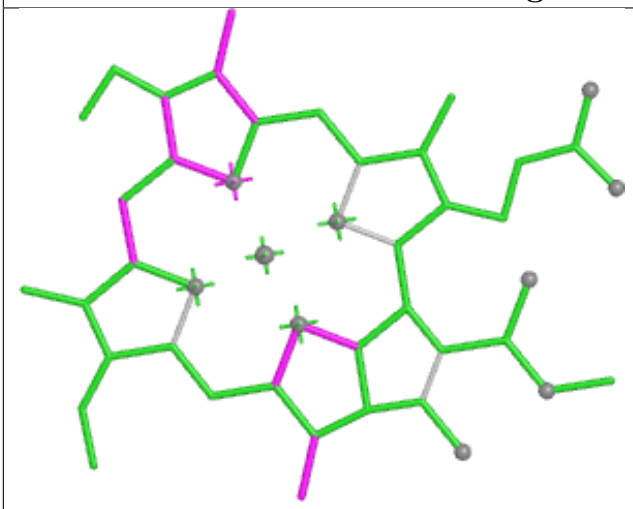


Rings

Ligand CLA L 302



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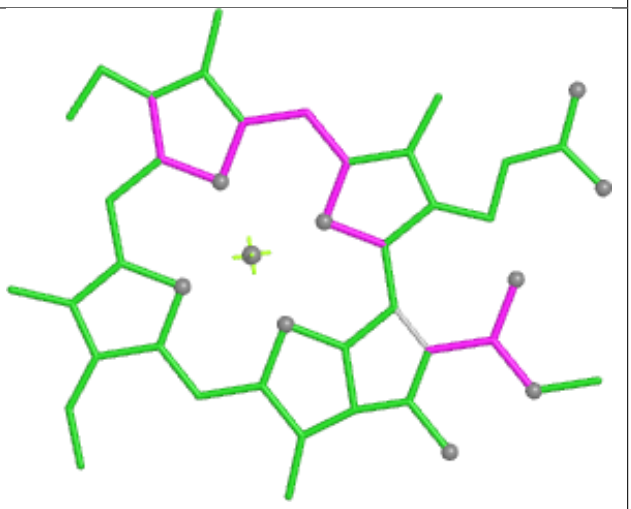
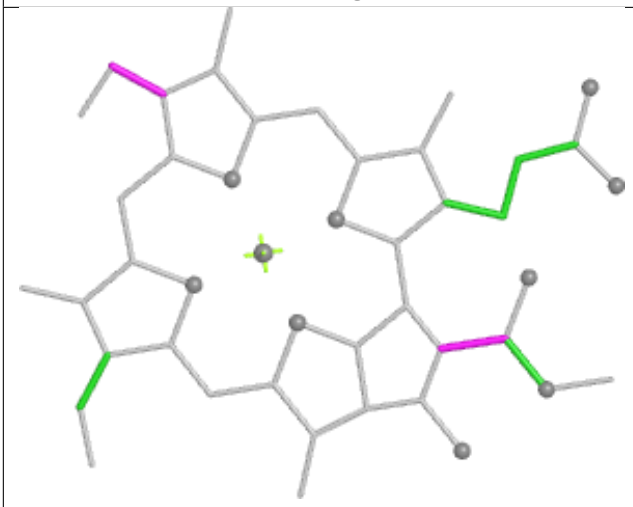


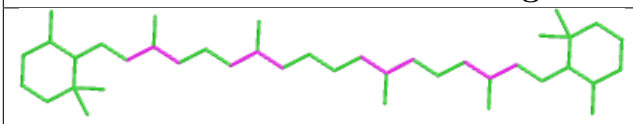
Bond angles



Torsions

Rings

Ligand BCR A 850



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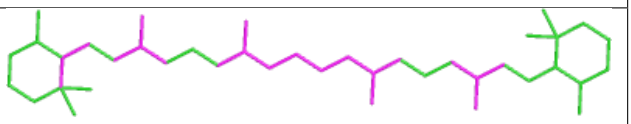
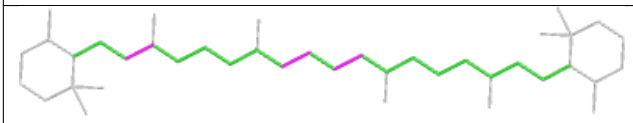
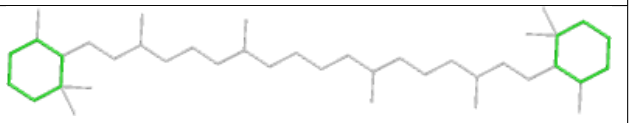


Bond angles

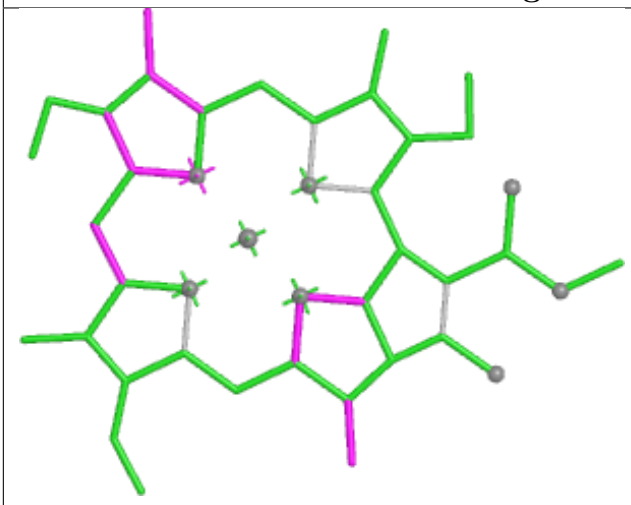


Torsions

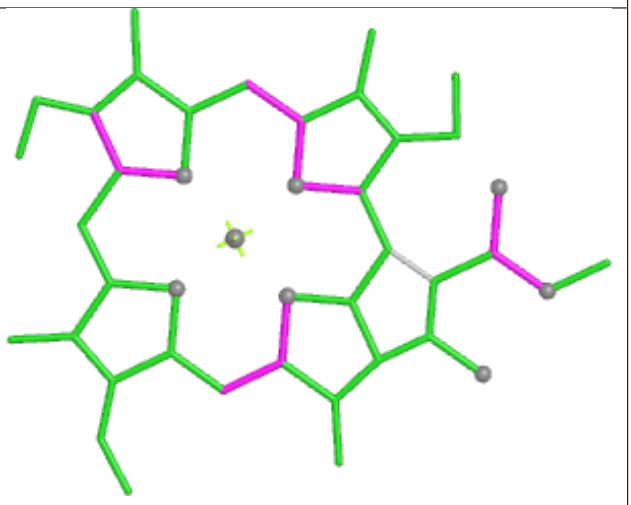


Rings

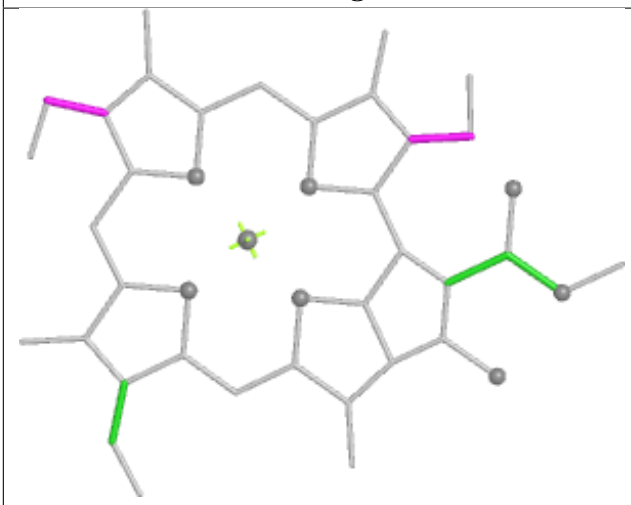
Ligand CLA G 202



Bond lengths



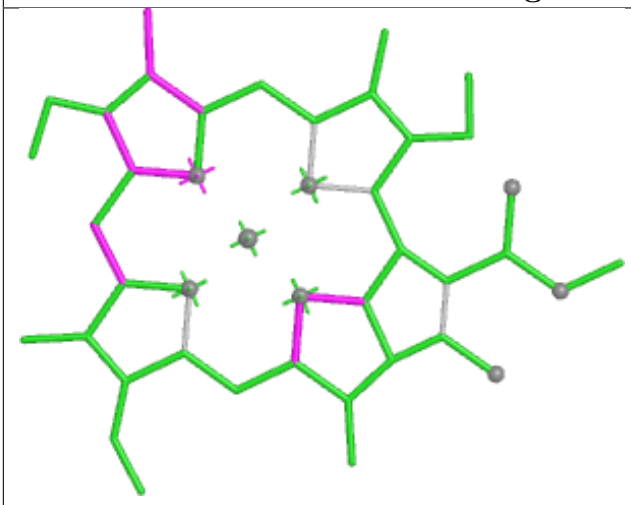
Bond angles



Torsions

Rings

Ligand CLA B 835



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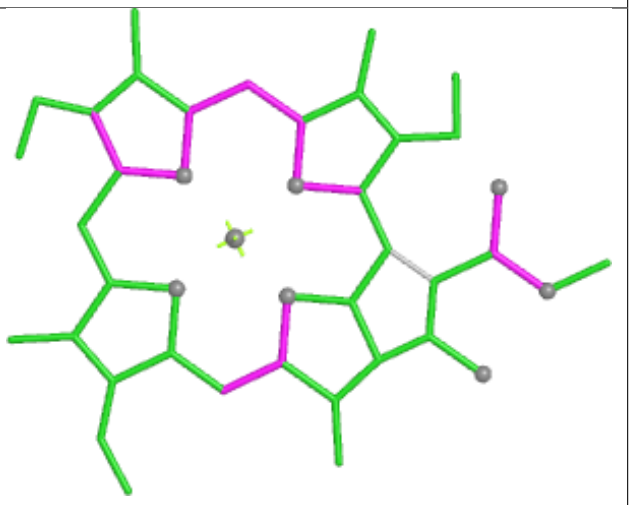

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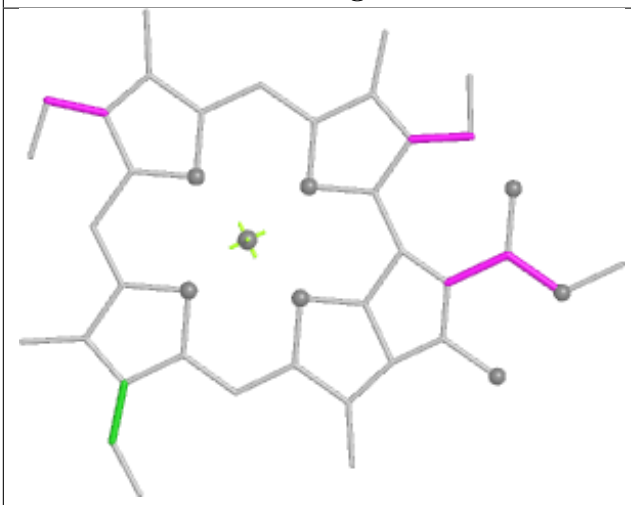
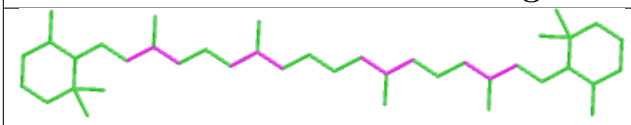


Torsions

Rings

Ligand BCR B 847



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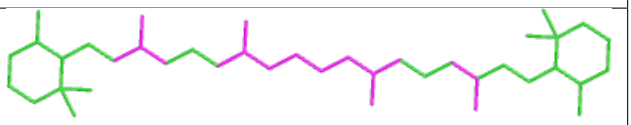

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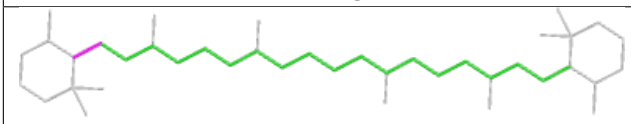

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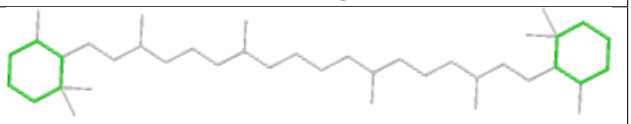
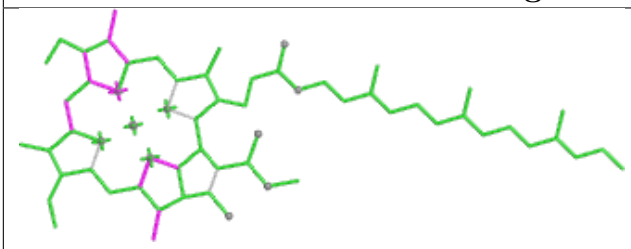
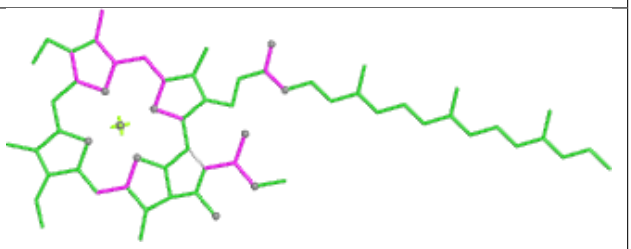
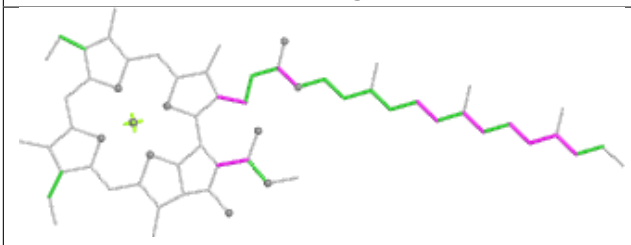
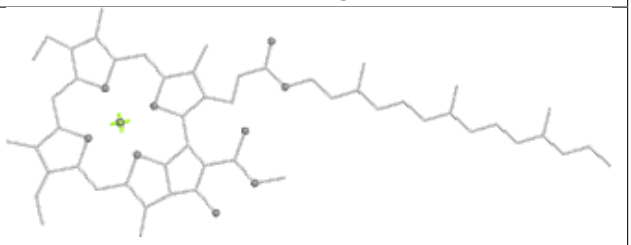
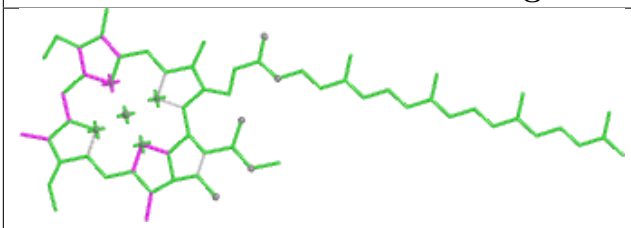
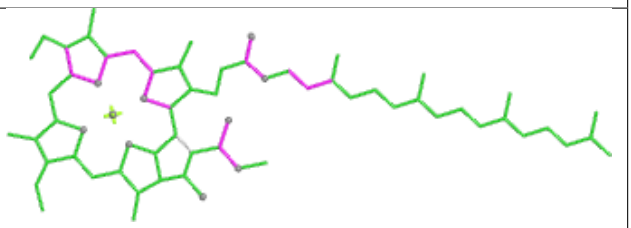
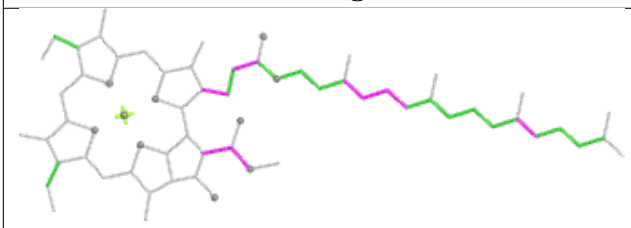
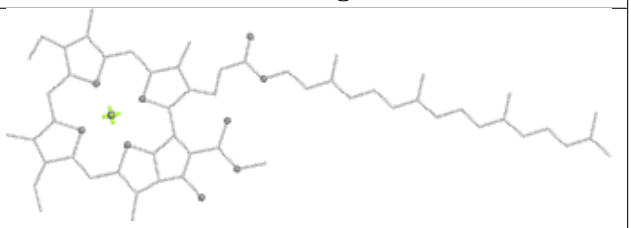
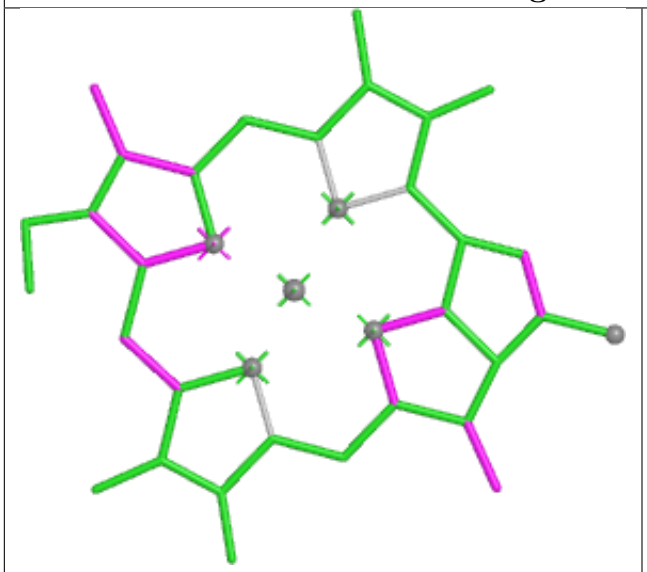


Rings

Ligand CLA B 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 611



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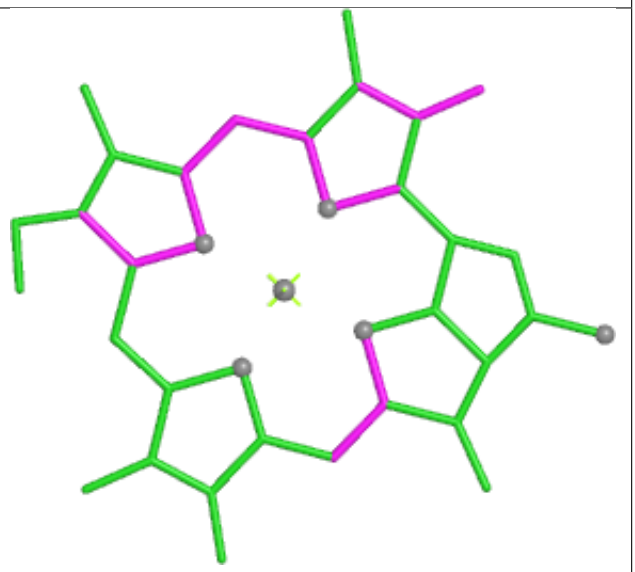
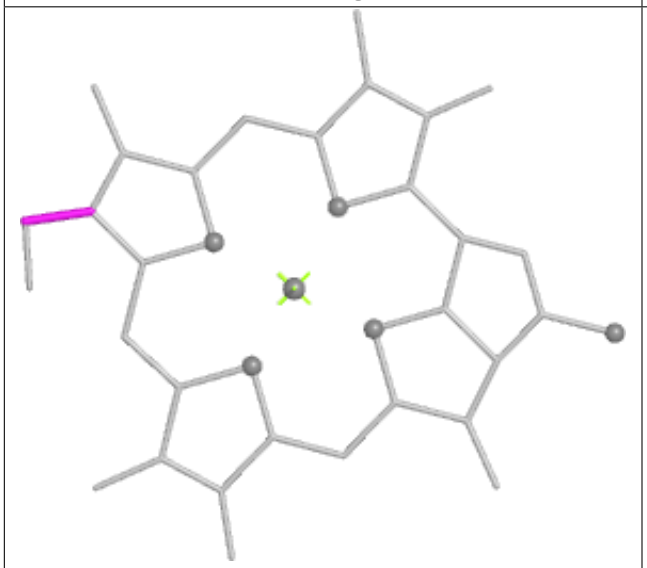


Bond angles



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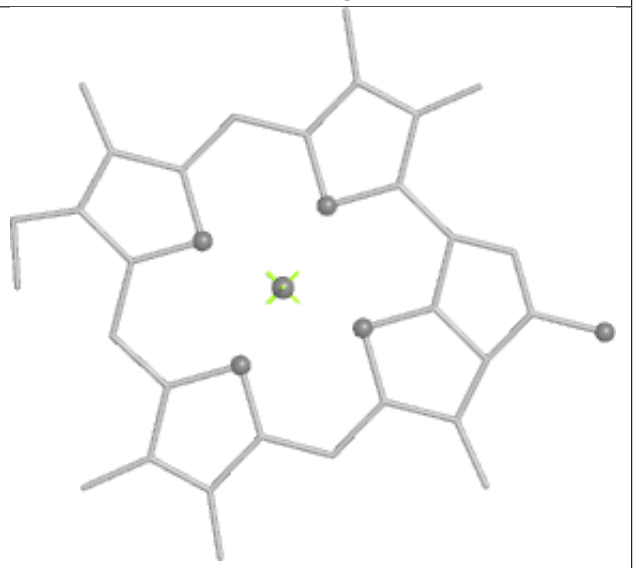
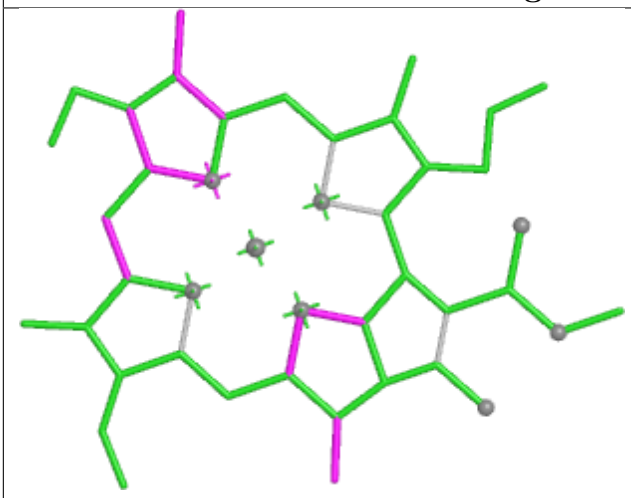


Rings

Ligand CLA B 831



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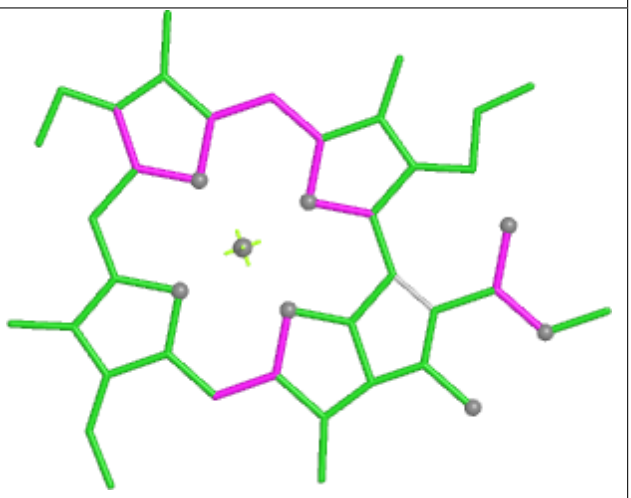
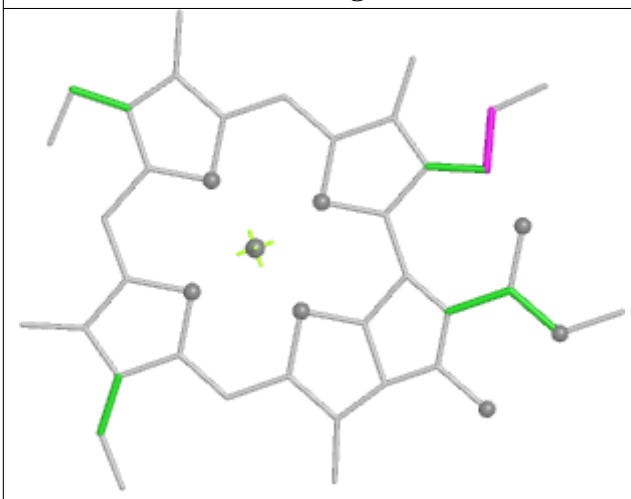


Bond angles



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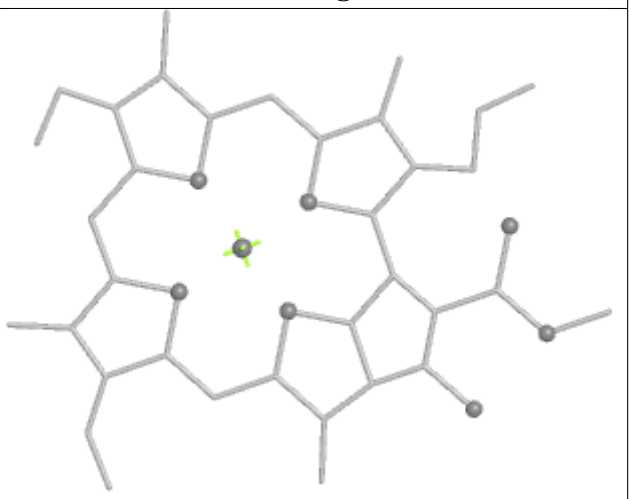
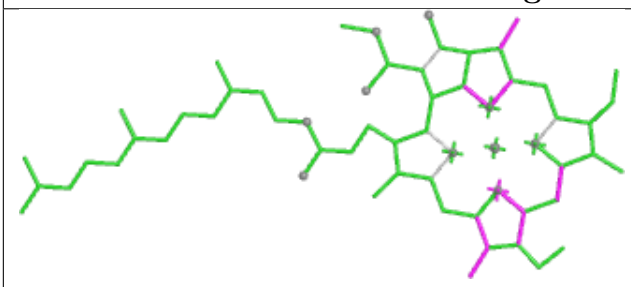


Rings

Ligand CLA A 818



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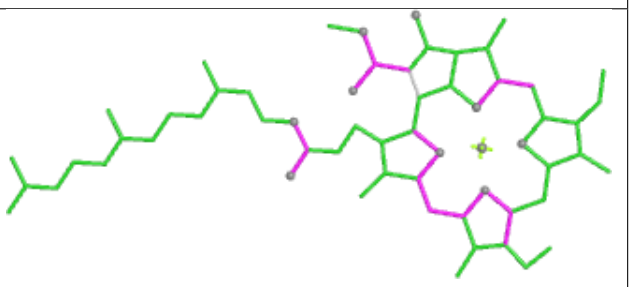

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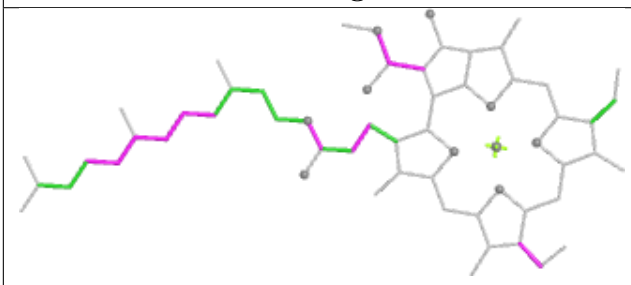

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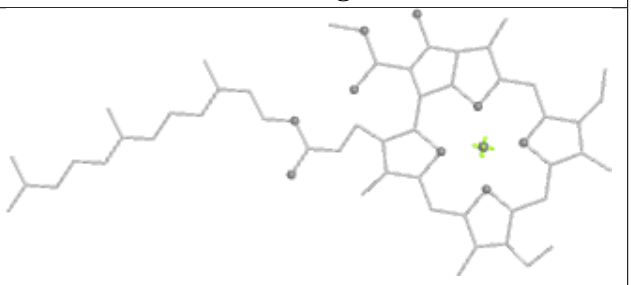
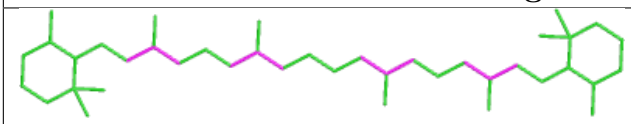


Rings

Ligand BCR L 306



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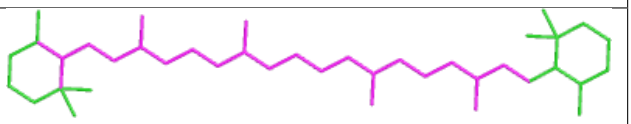
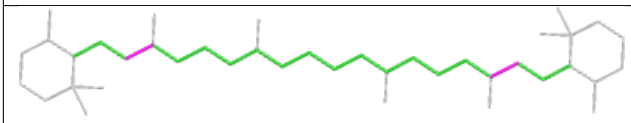


Bond angles



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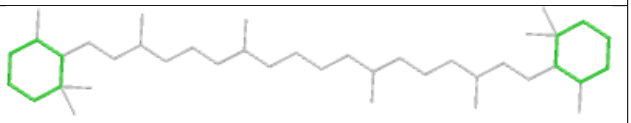
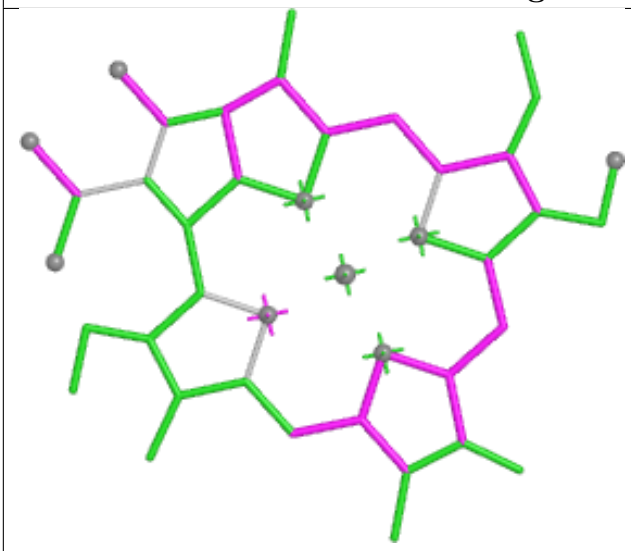


Rings

Ligand CHL 4 615



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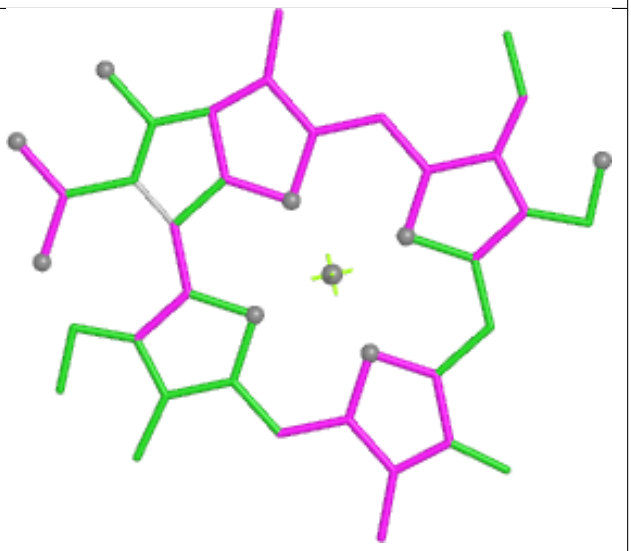
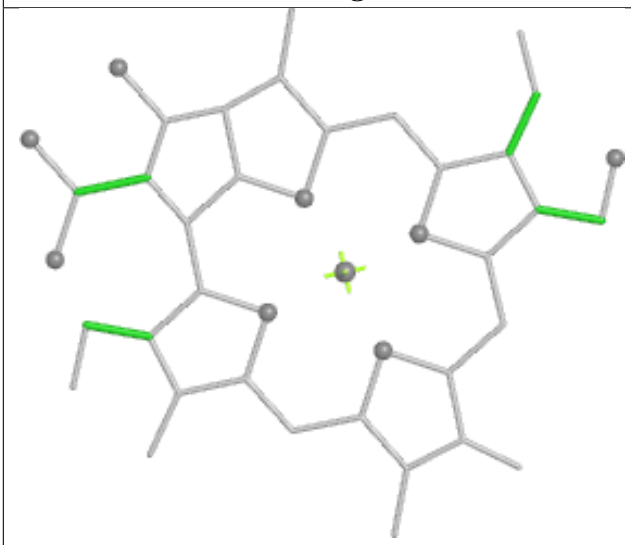


Bond angles



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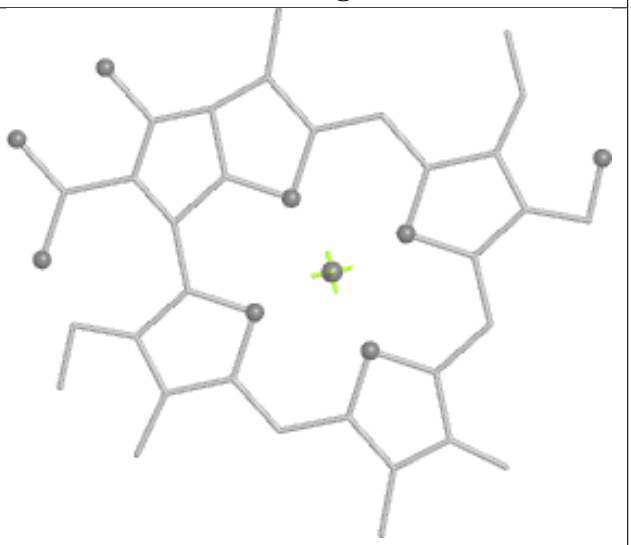
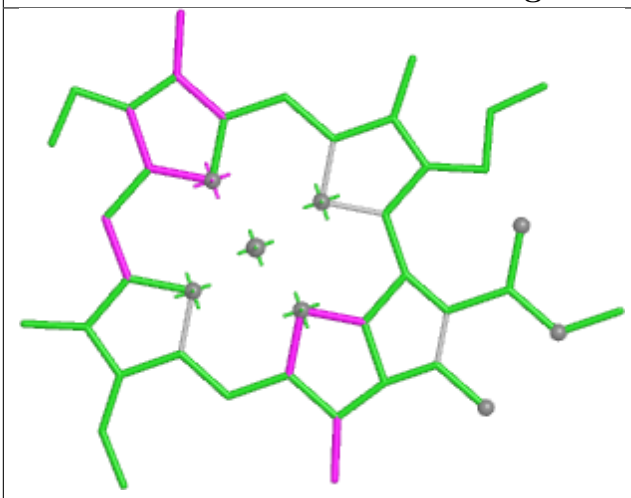


Rings

Ligand CLA B 830



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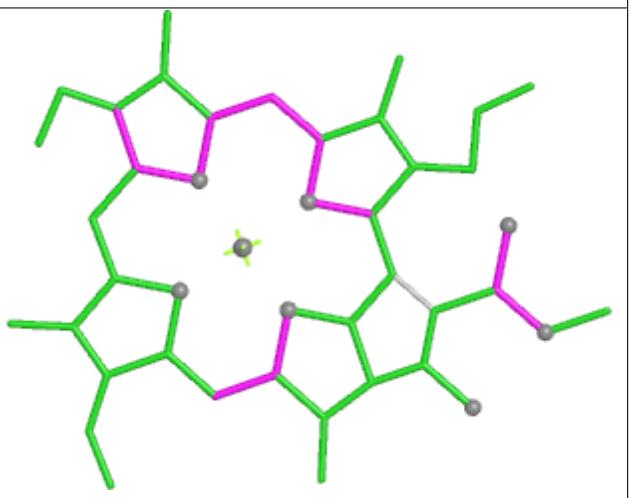
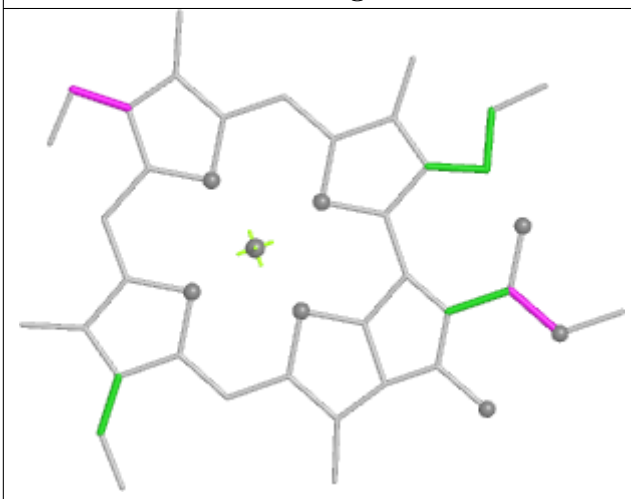


Bond angles



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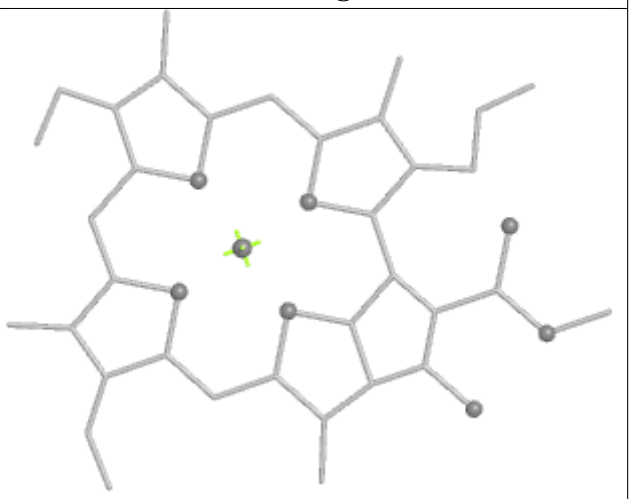
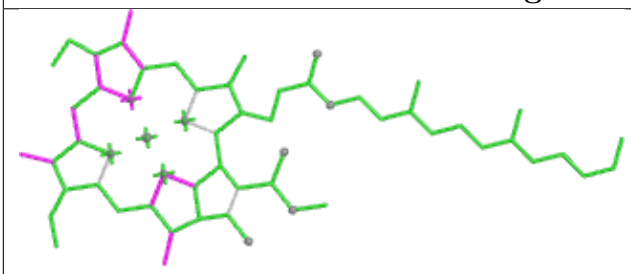


Rings

Ligand CLA B 817



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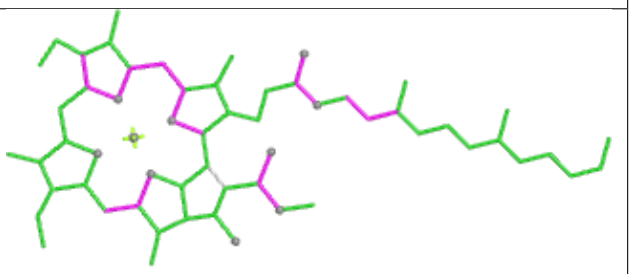
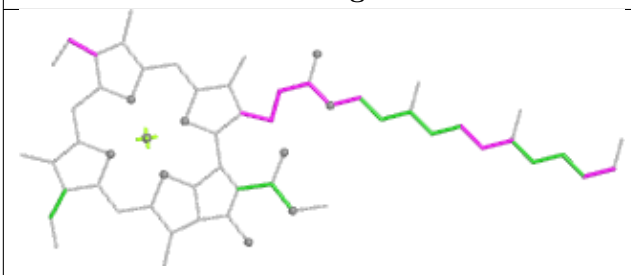


Bond angles



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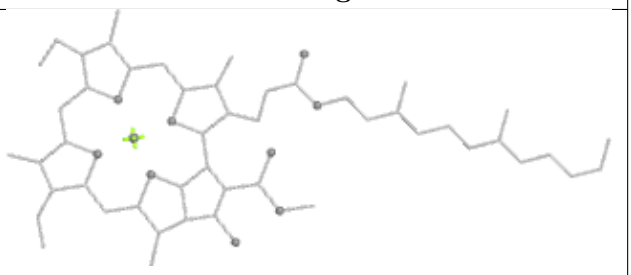
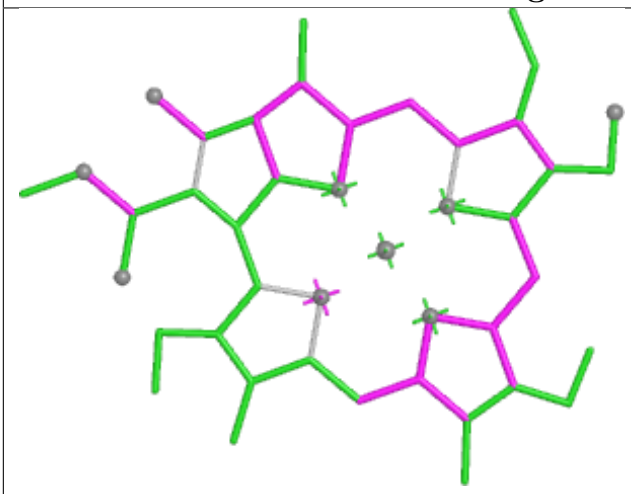


Rings

Ligand CHL 2 615



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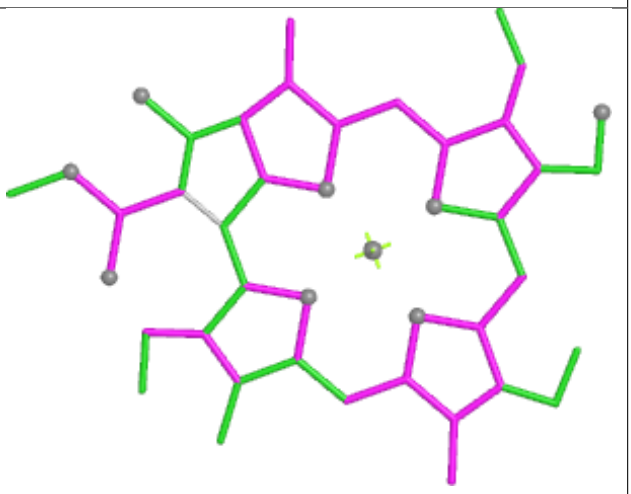
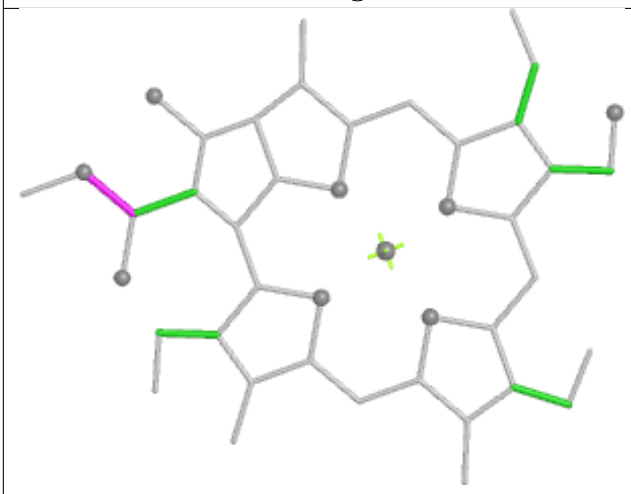


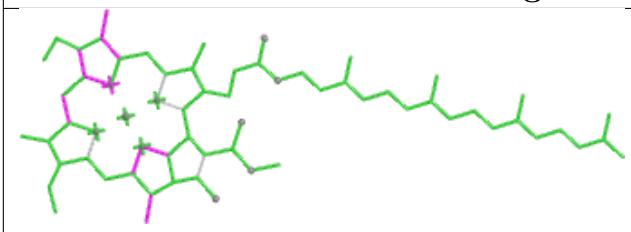
Bond angles



Torsions

Rings

Ligand CLA A 830



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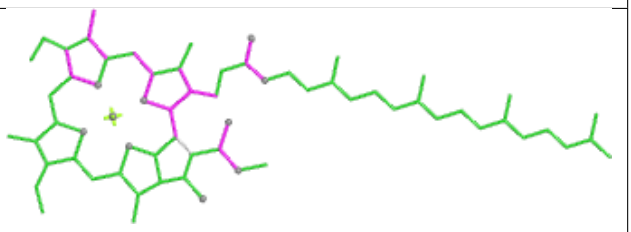
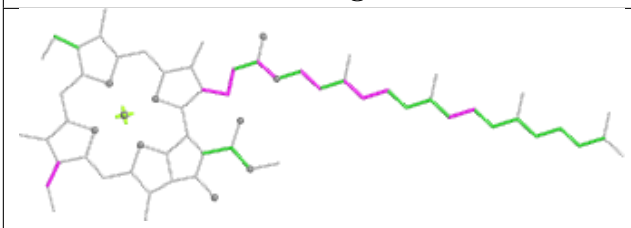
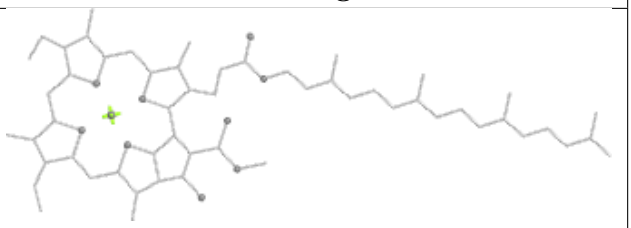


Bond angles

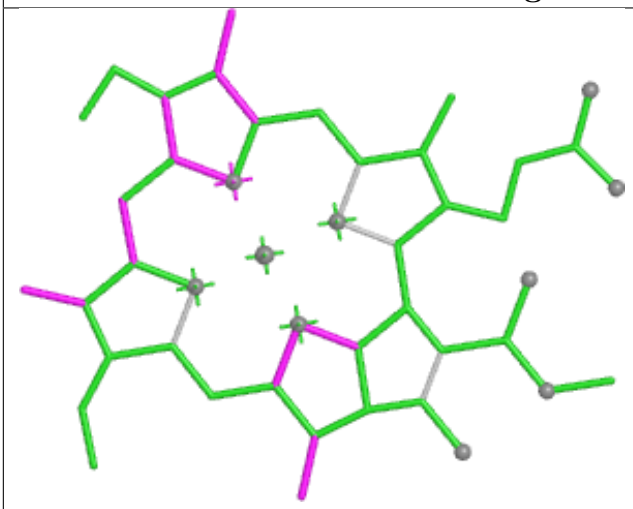


Torsions

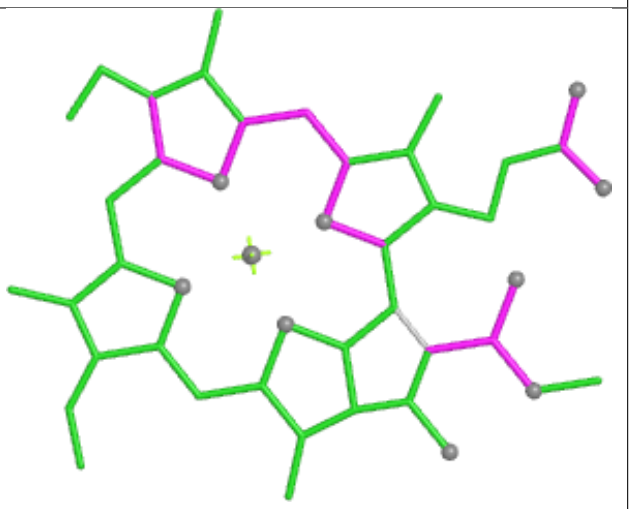


Rings

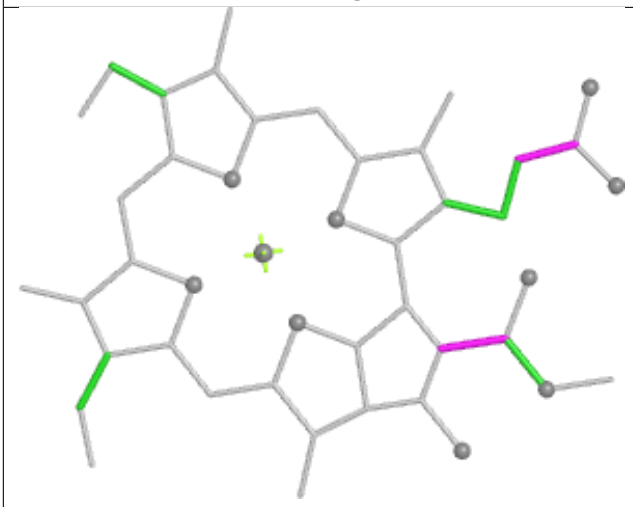
Ligand CLA B 833



Bond lengths



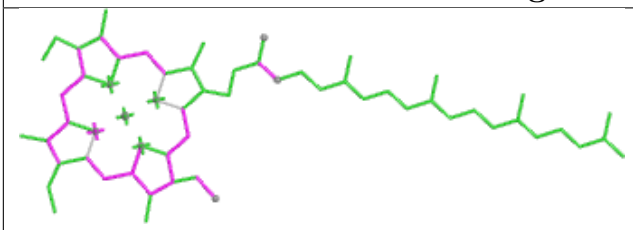
Bond angles



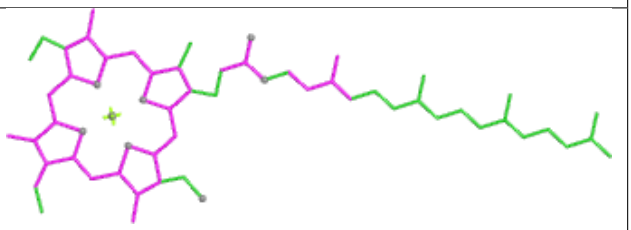
Torsions

Rings

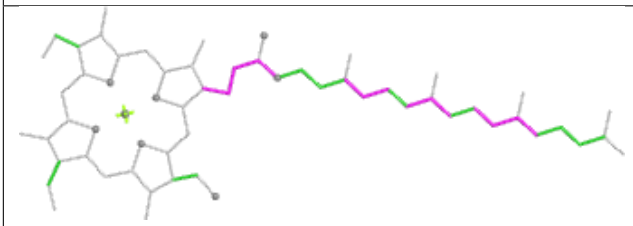
Ligand CL0 A 801



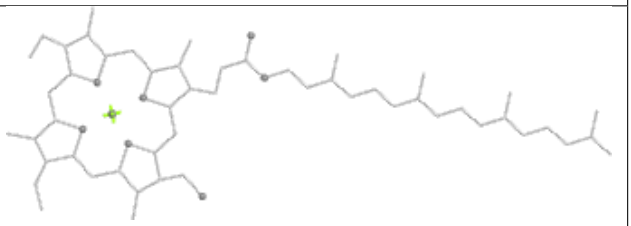
Bond lengths



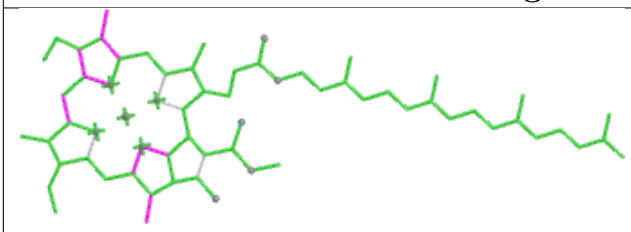
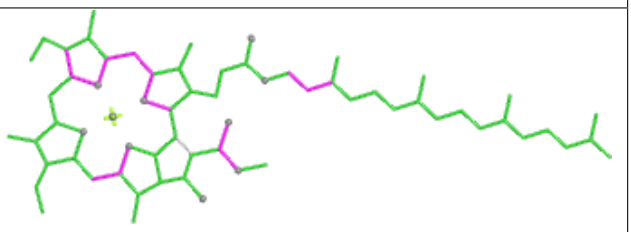
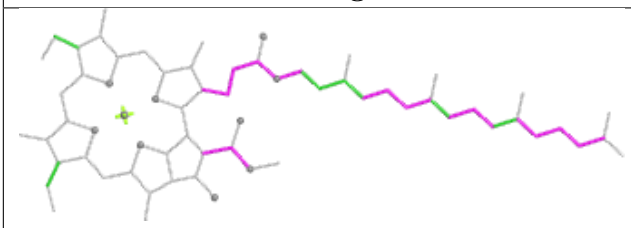
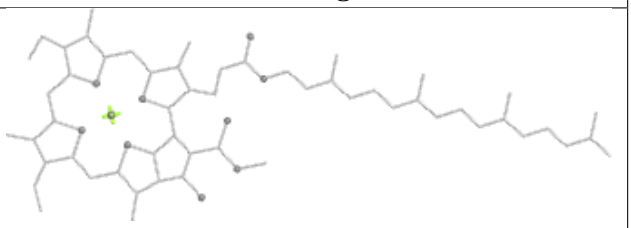
Bond angles

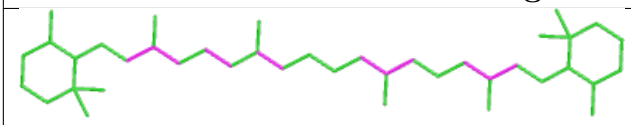
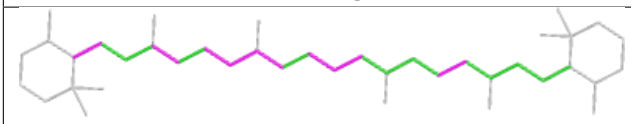
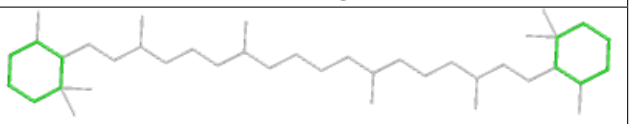


Torsions

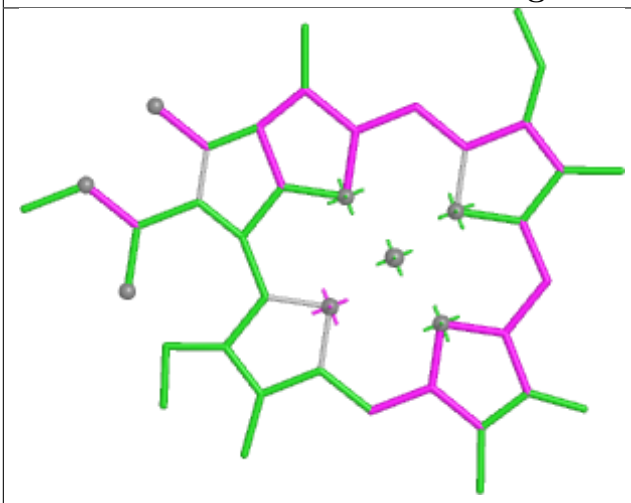


Rings

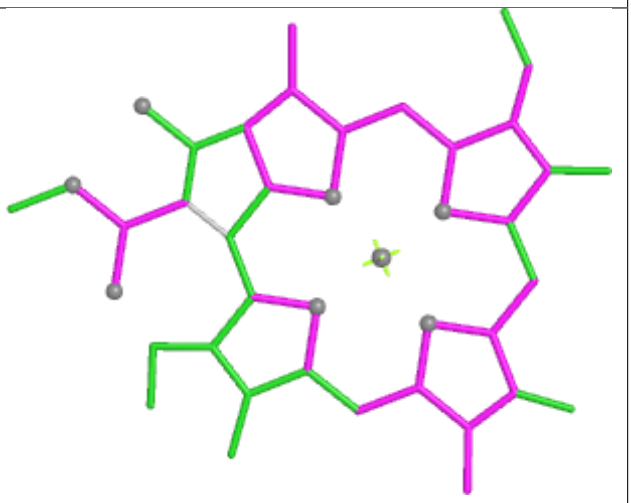
Ligand CLA A 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR F 304	
 Bond lengths	Bond angles
 Torsions	 Rings

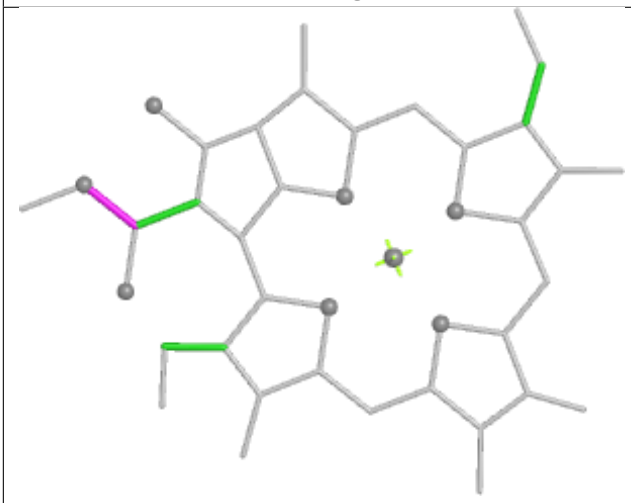
Ligand CHL 4 606



Bond lengths



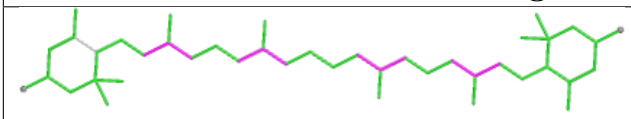
Bond angles



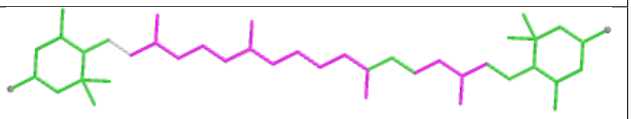
Torsions

Rings

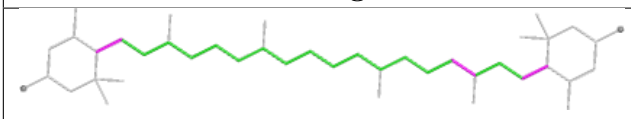
Ligand LUT 2 619



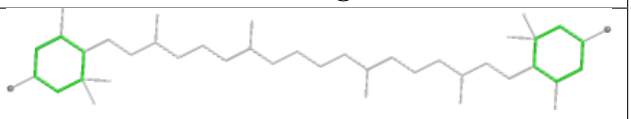
Bond lengths



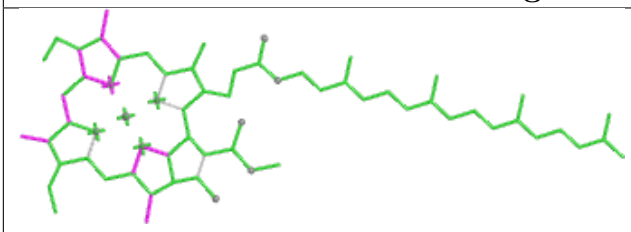
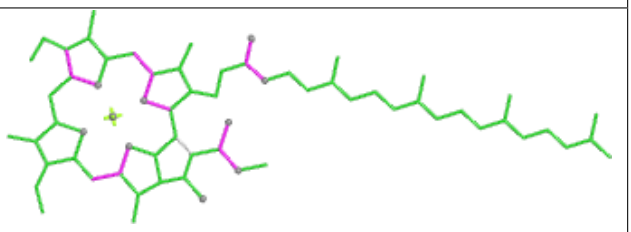
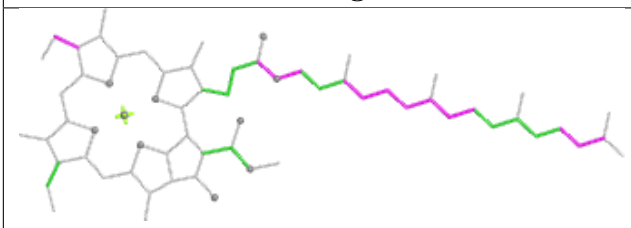
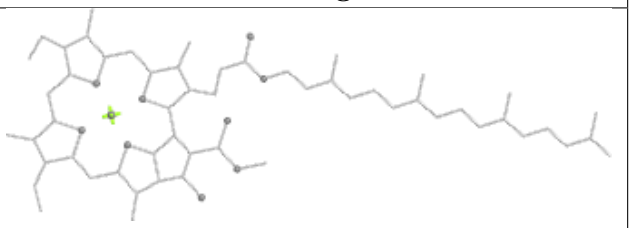
Bond angles

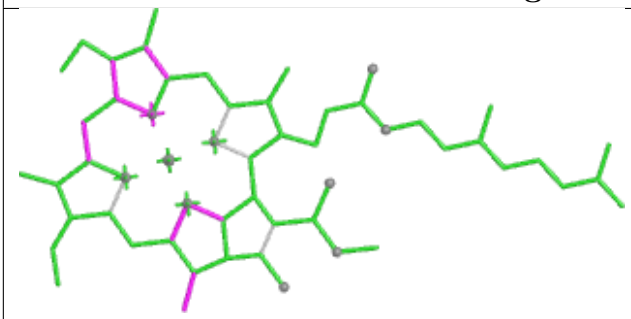
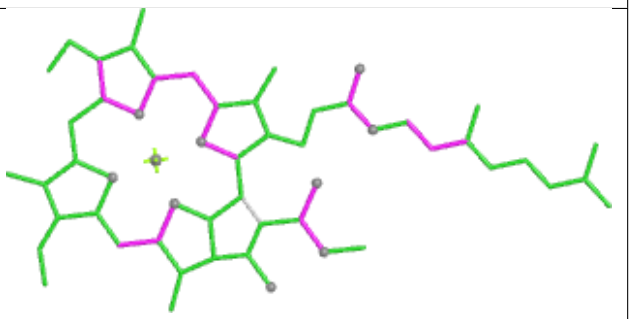
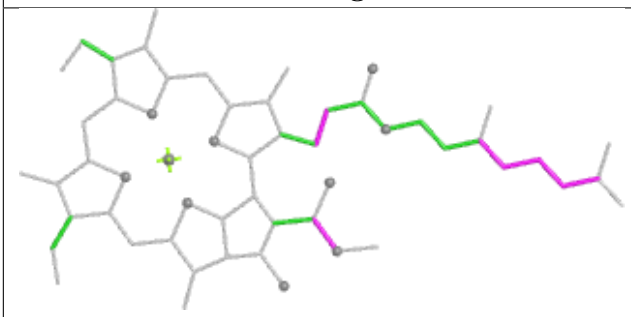
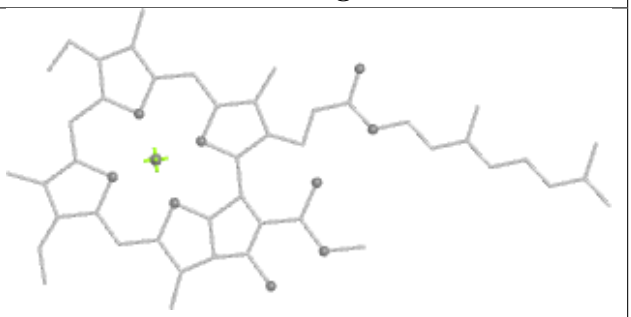


Torsions

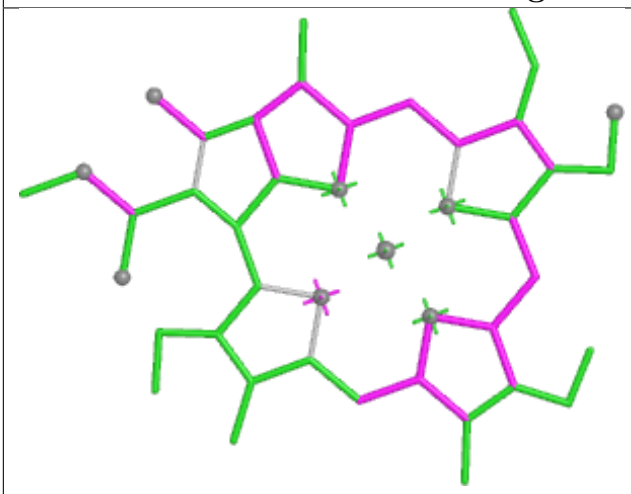


Rings

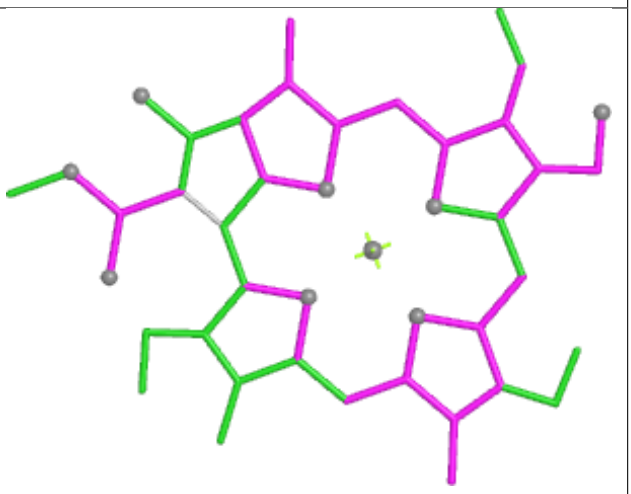
Ligand CLA A 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

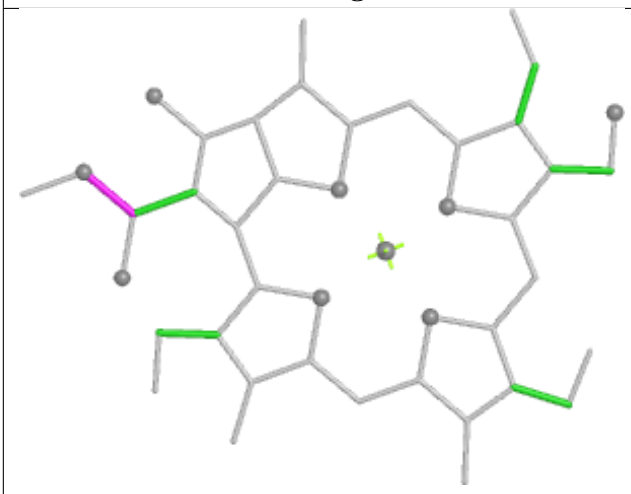
Ligand CHL 2 606



Bond lengths



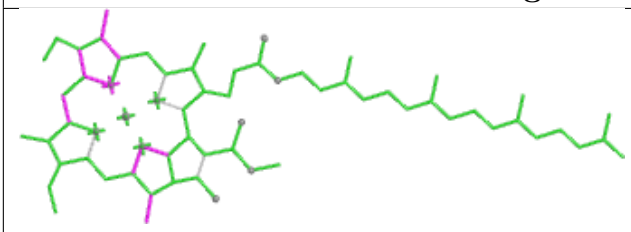
Bond angles



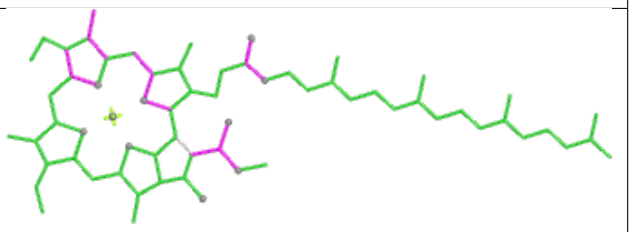
Torsions

Rings

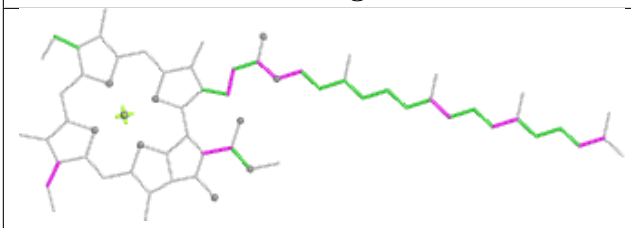
Ligand CLA A 809



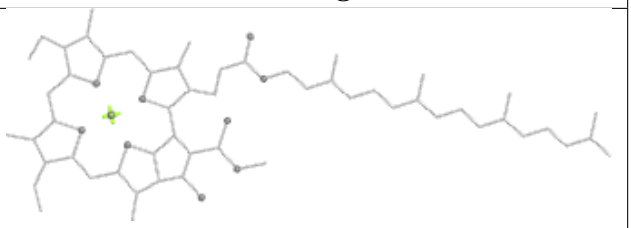
Bond lengths



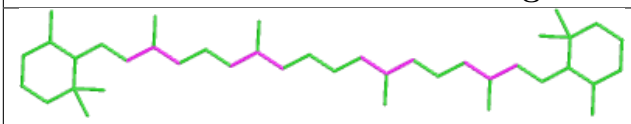
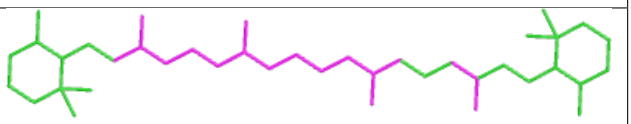
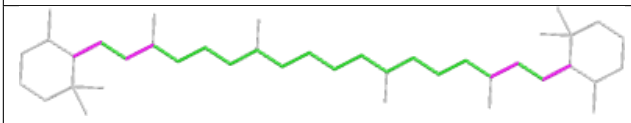
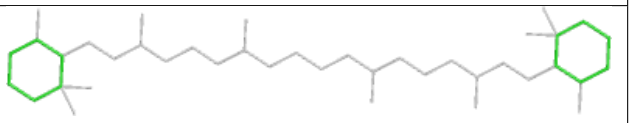
Bond angles

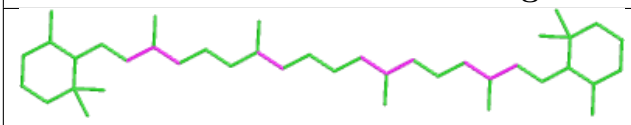
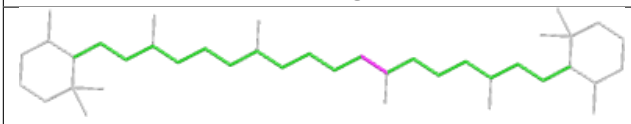
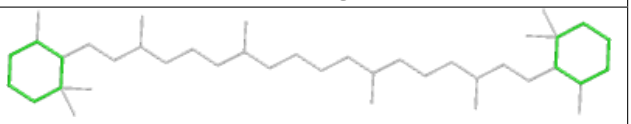


Torsions

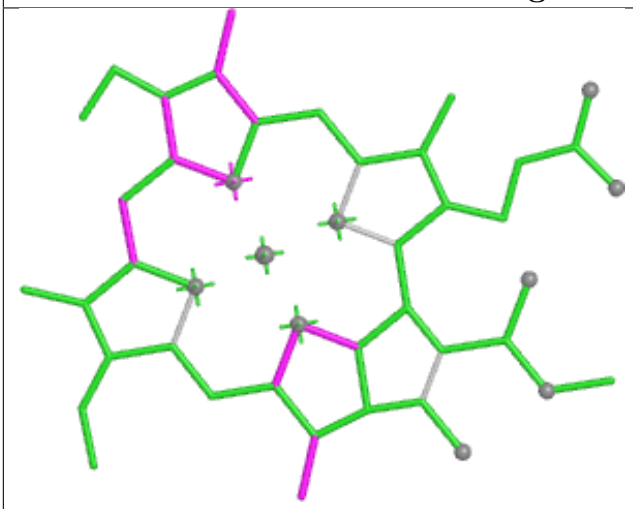


Rings

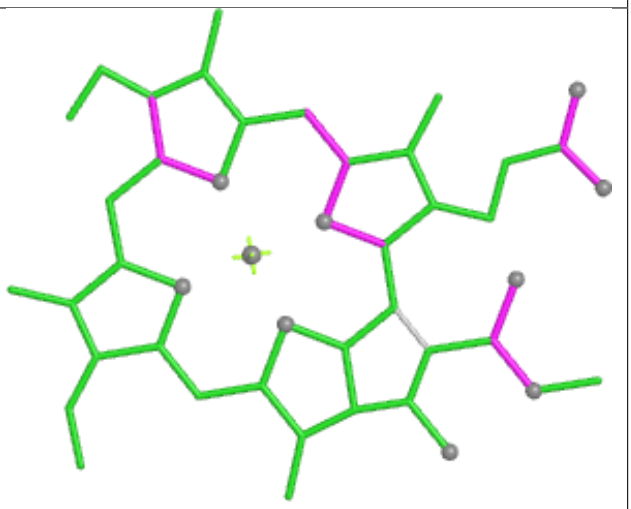
Ligand BCR B 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR K 202	
 Bond lengths	Bond angles
 Torsions	 Rings

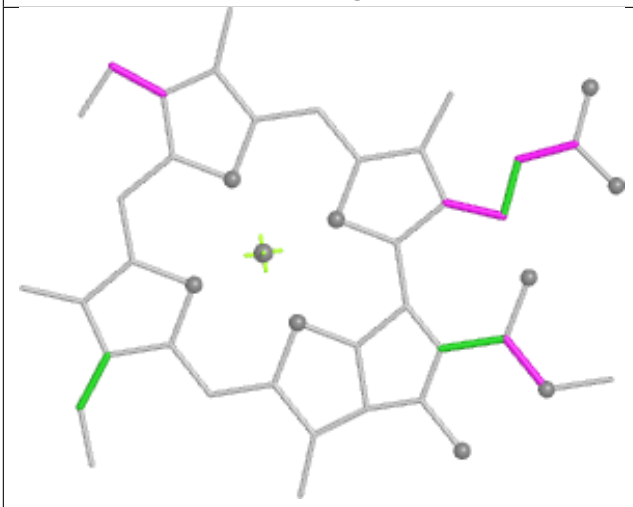
Ligand CLA 4 608



Bond lengths



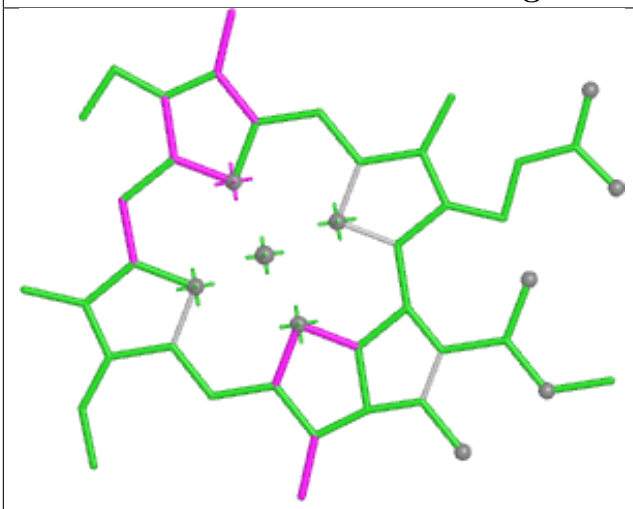
Bond angles



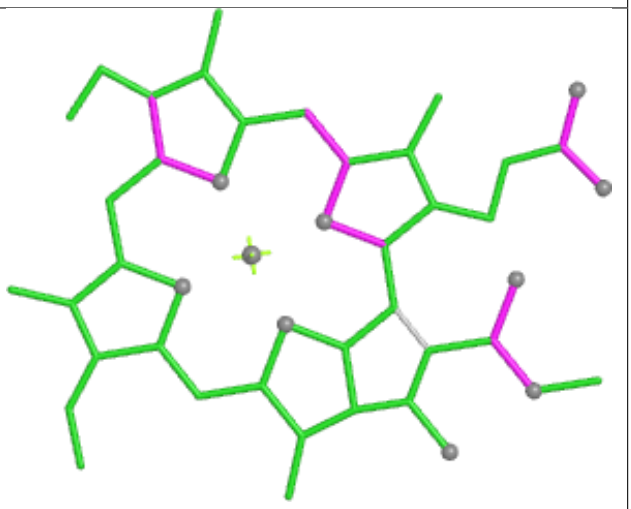
Torsions

Rings

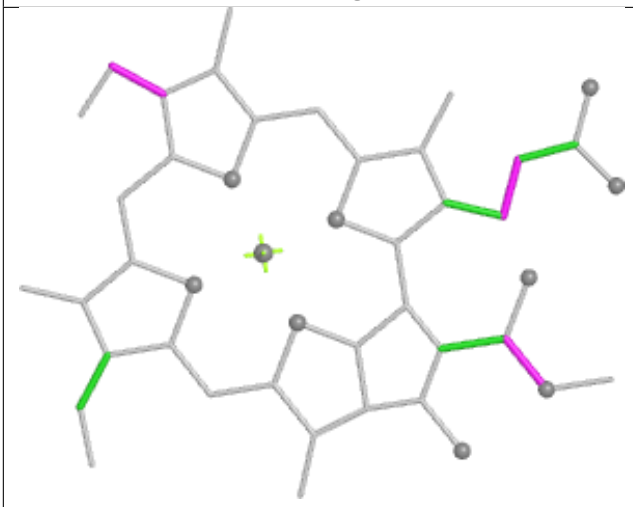
Ligand CLA G 201



Bond lengths



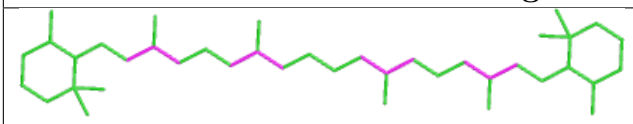
Bond angles



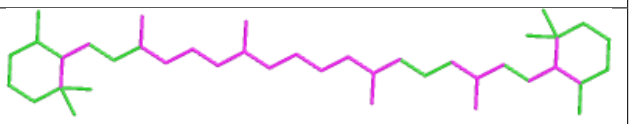
Torsions

Rings

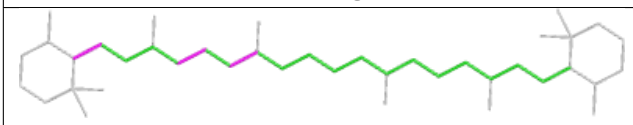
Ligand BCR A 853



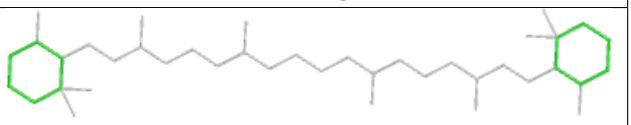
Bond lengths



Bond angles

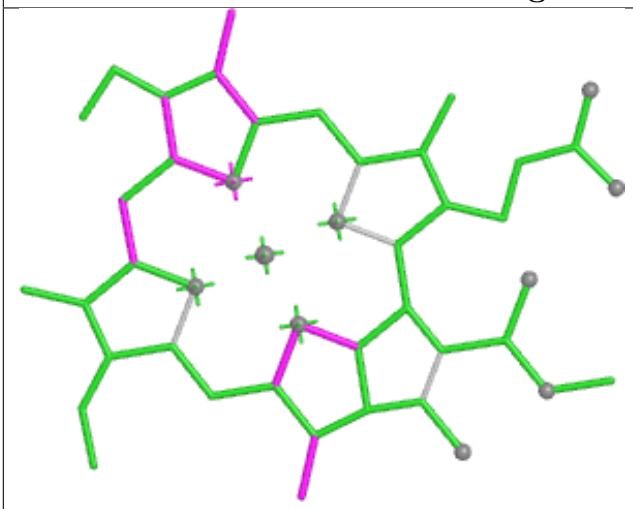


Torsions

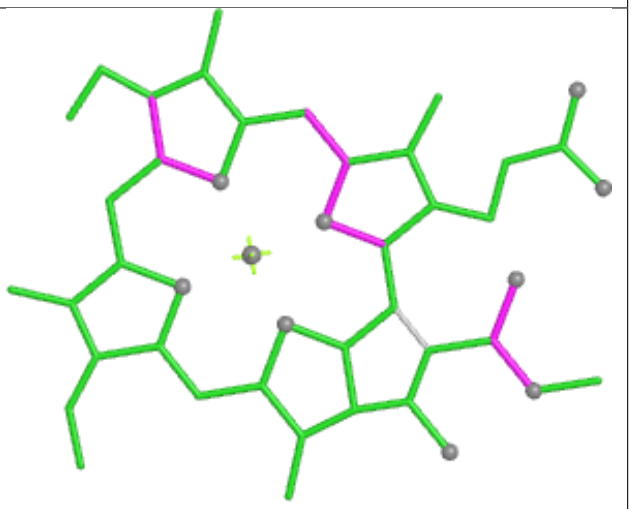


Rings

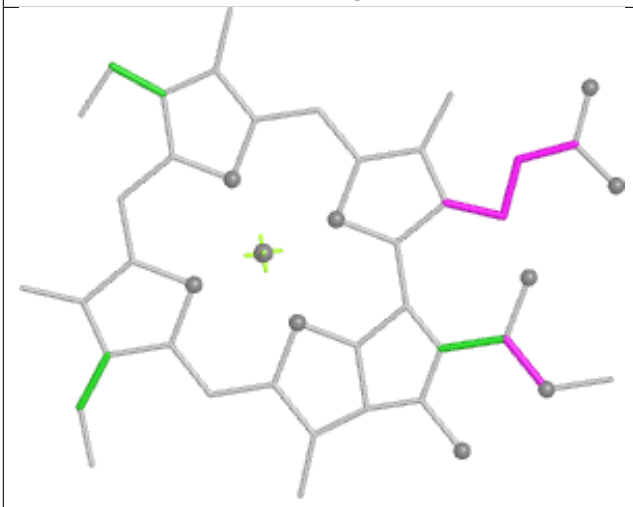
Ligand CLA 2 608



Bond lengths



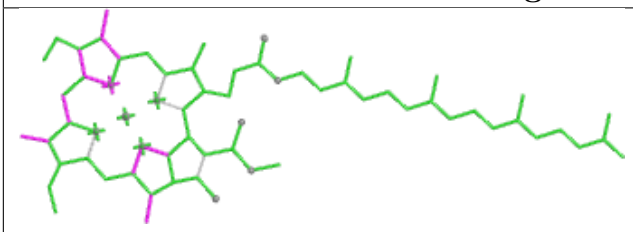
Bond angles



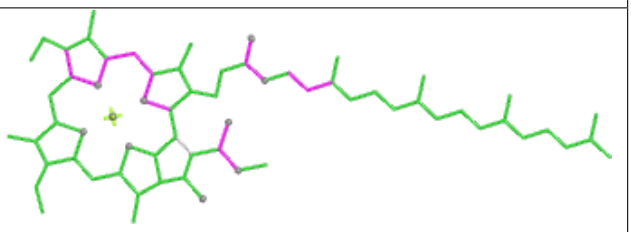
Torsions

Rings

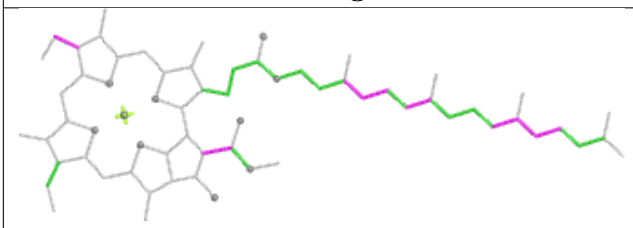
Ligand CLA B 808



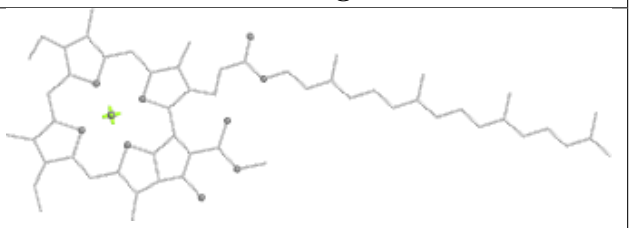
Bond lengths



Bond angles

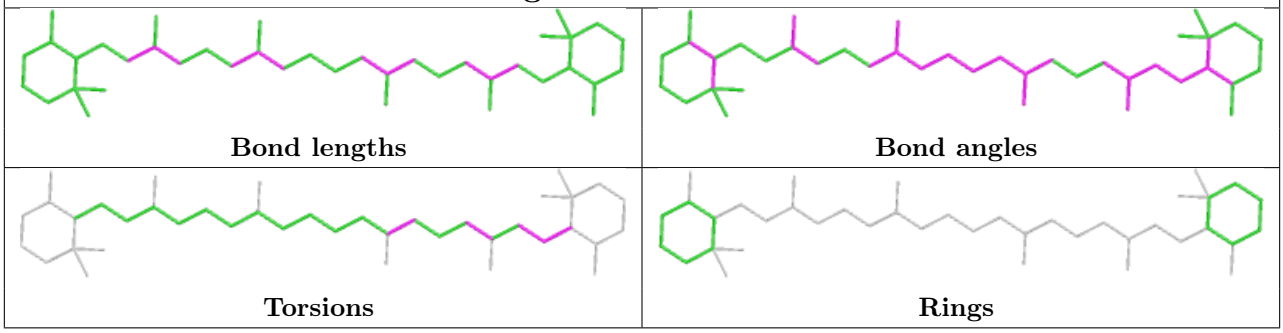


Torsions

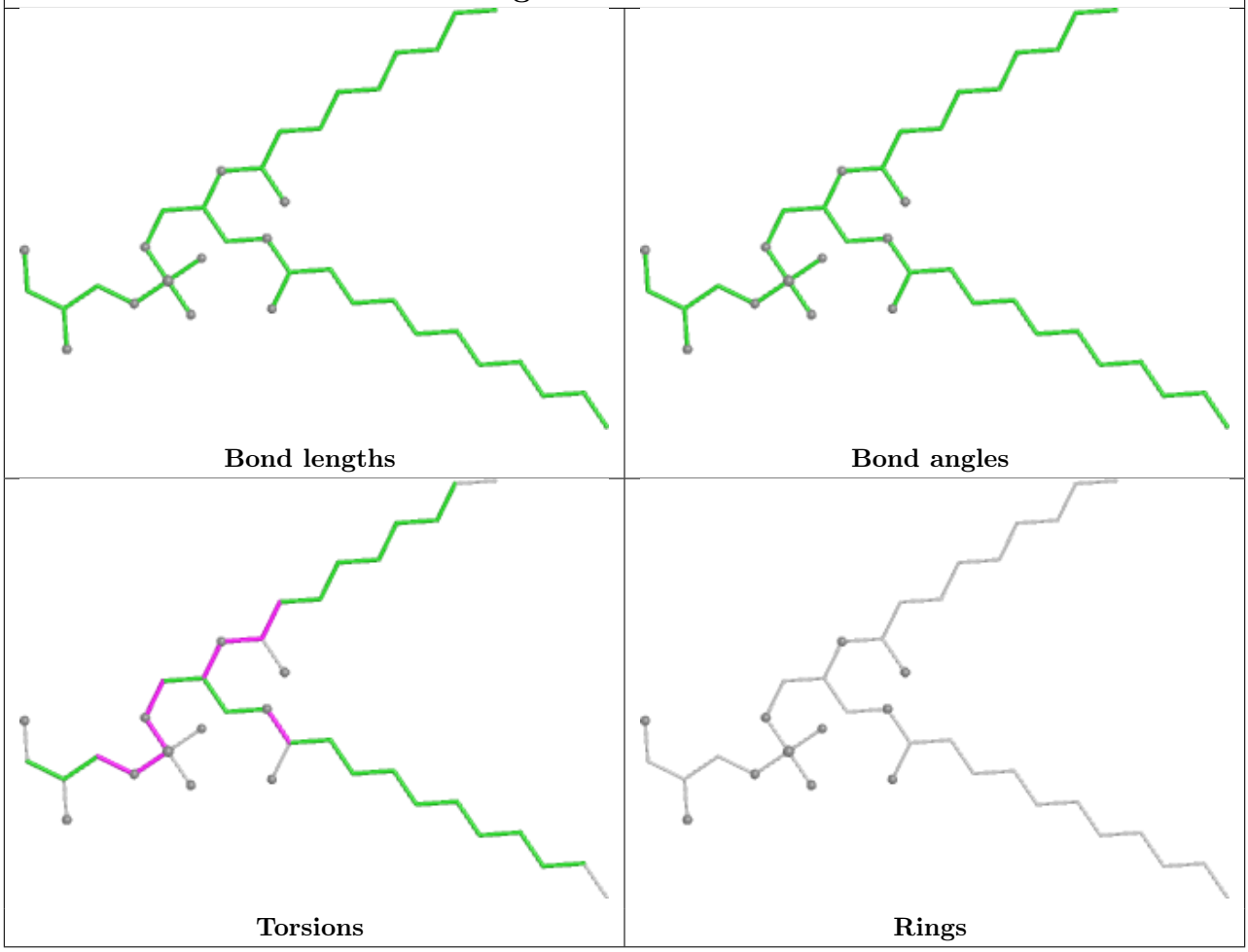


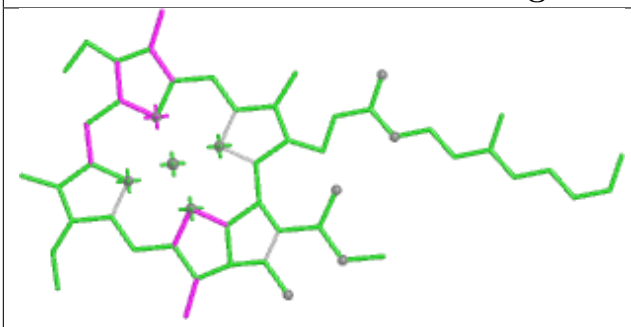
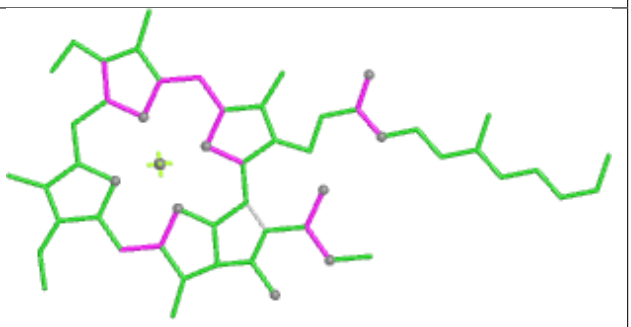
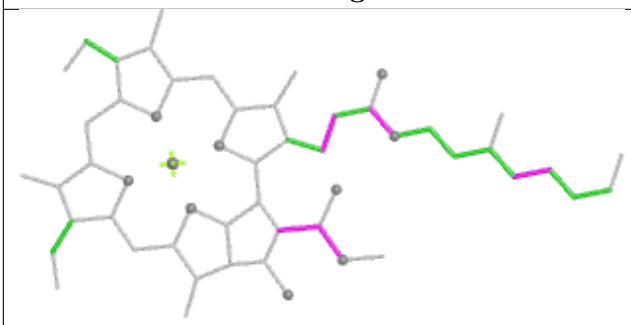
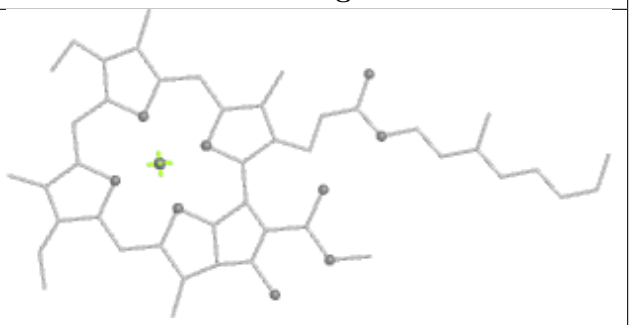
Rings

Ligand BCR B 849

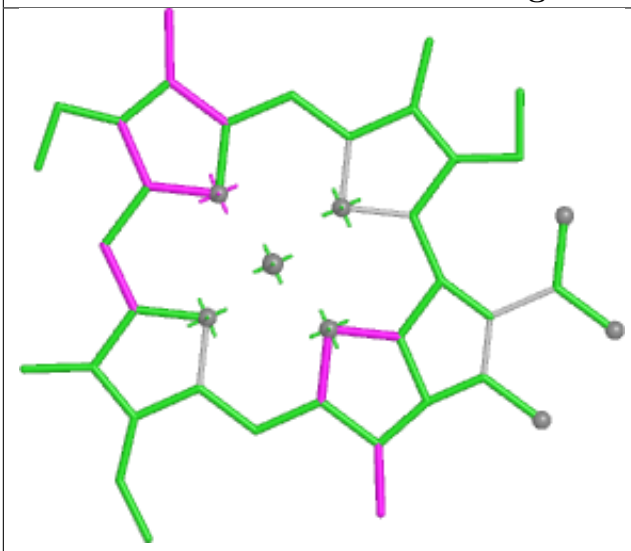


Ligand LHG 2 618

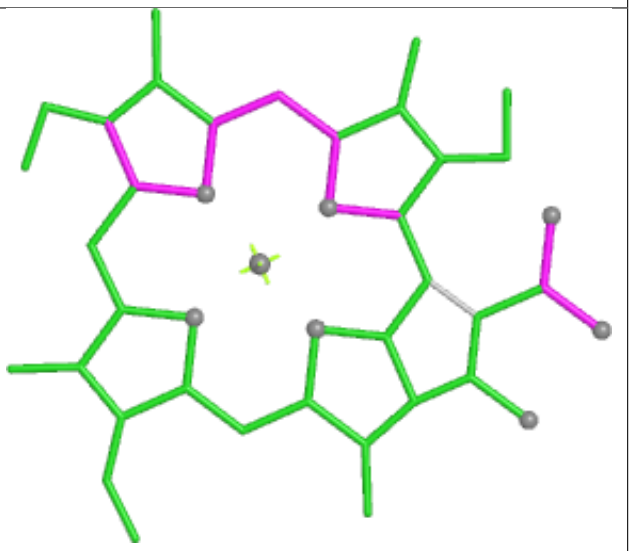


Ligand CLA 1 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

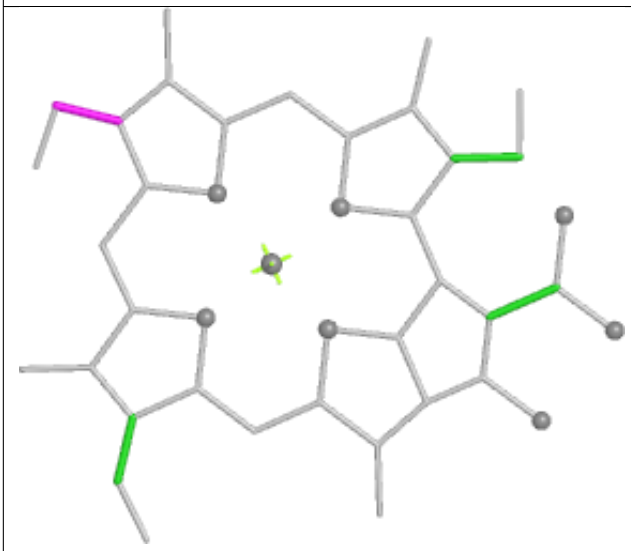
Ligand CLA 4 611



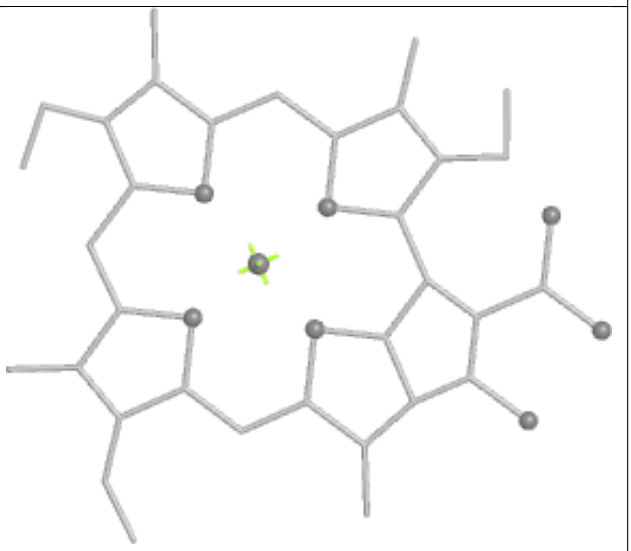
Bond lengths



Bond angles

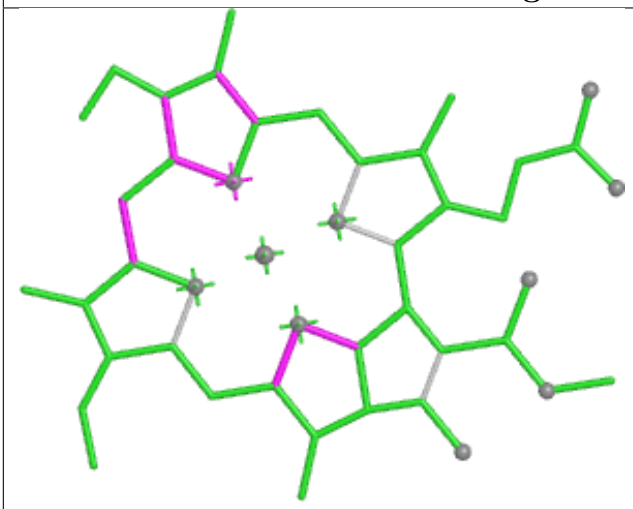


Torsions



Rings

Ligand CLA K 203



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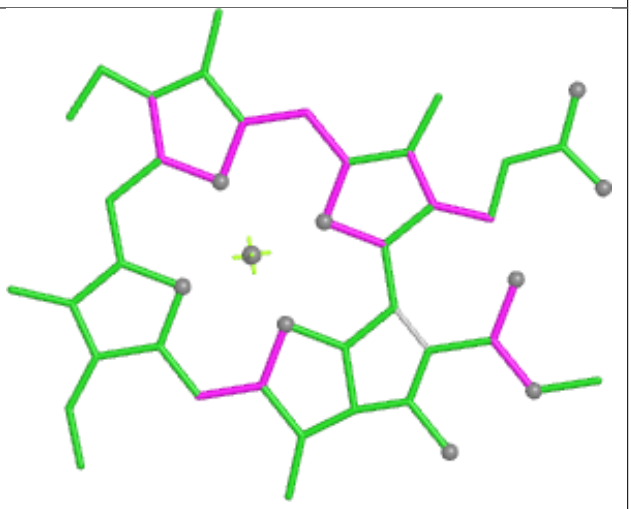
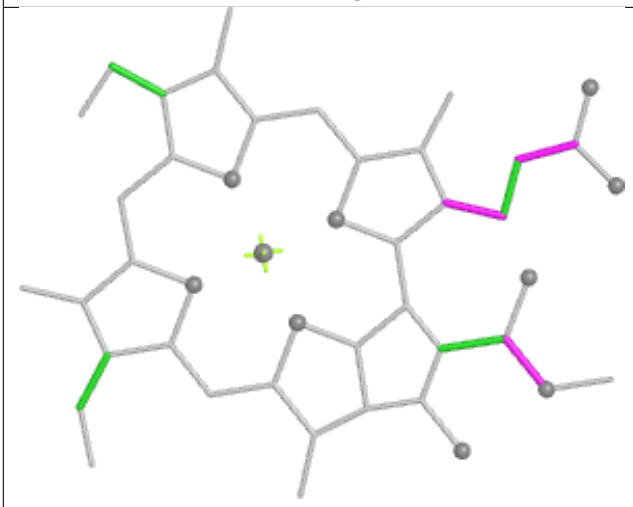


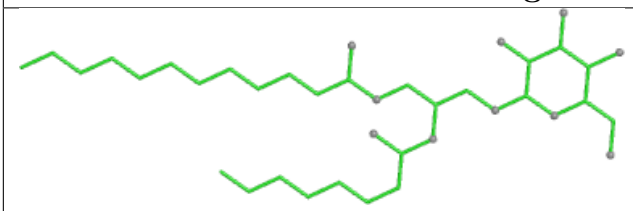
Bond angles



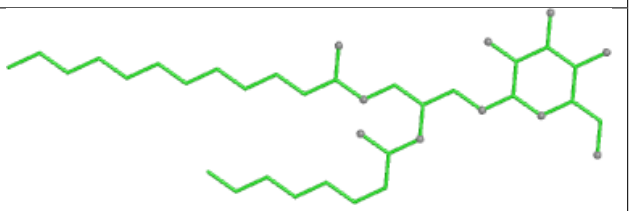
Torsions

Rings

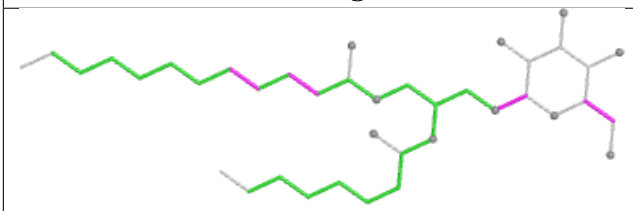
Ligand LMG 4 619



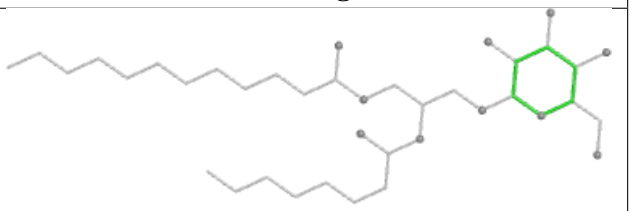
Bond lengths



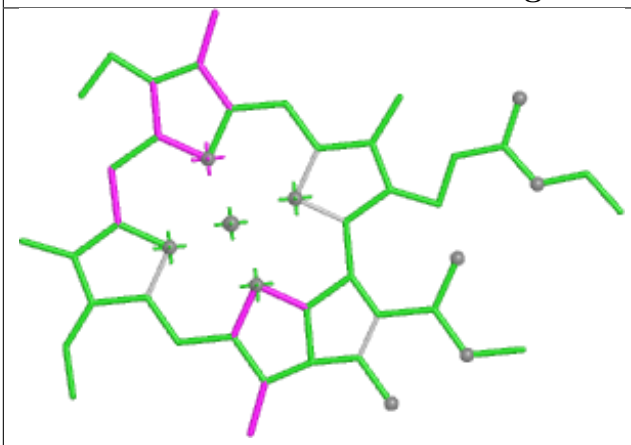
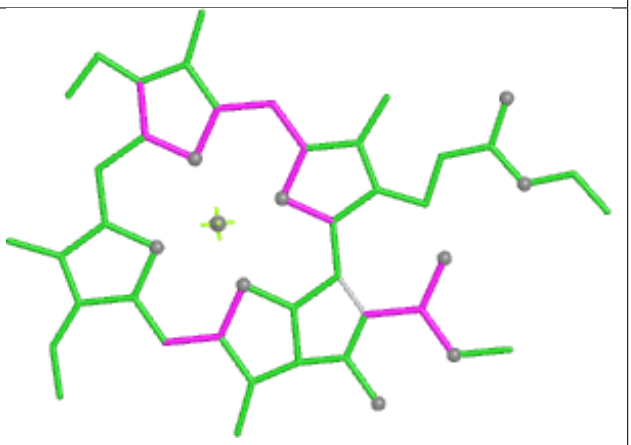
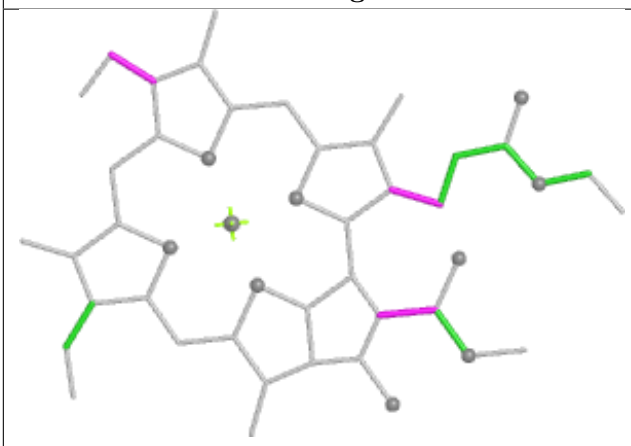
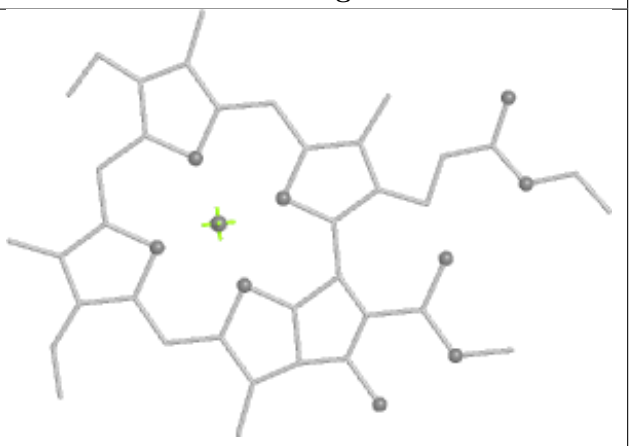
Bond angles



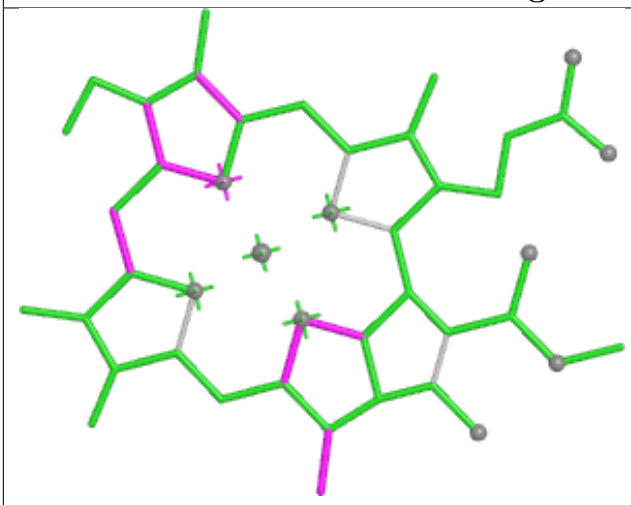
Torsions



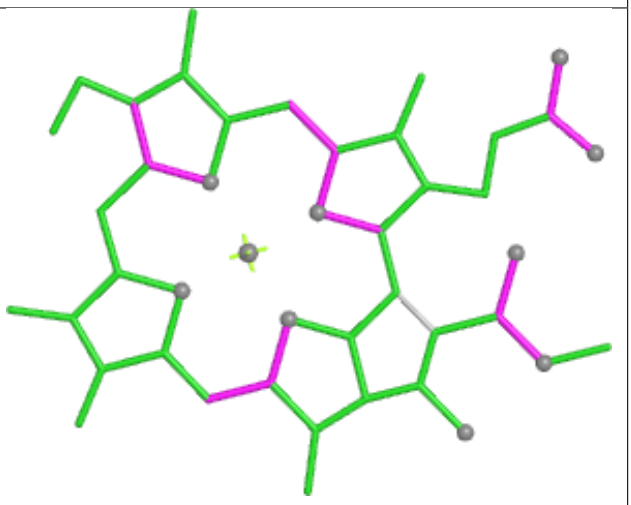
Rings

Ligand CLA B 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

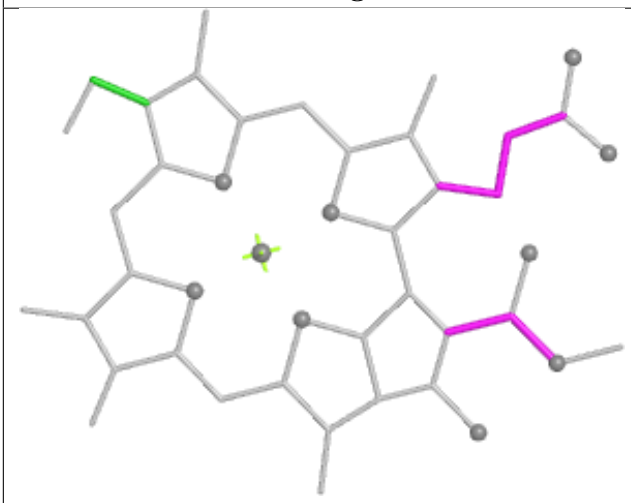
Ligand CLA 2 611



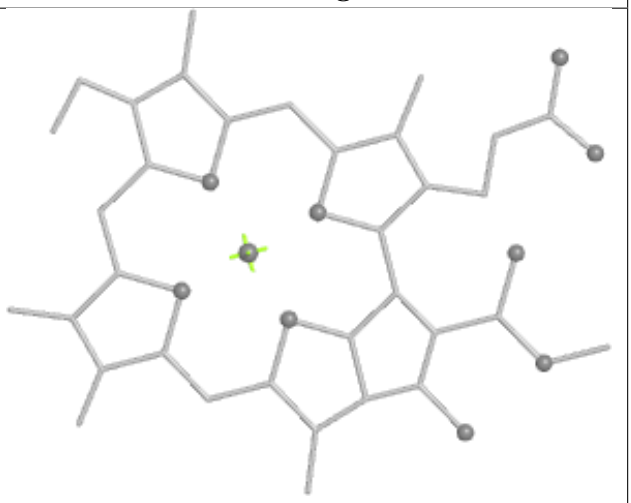
Bond lengths



Bond angles

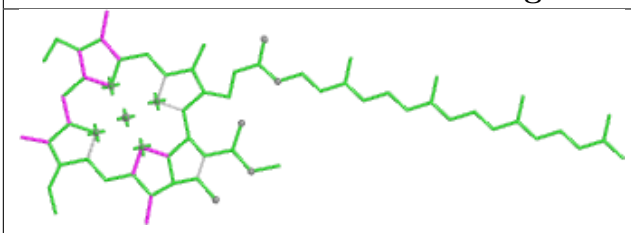


Torsions

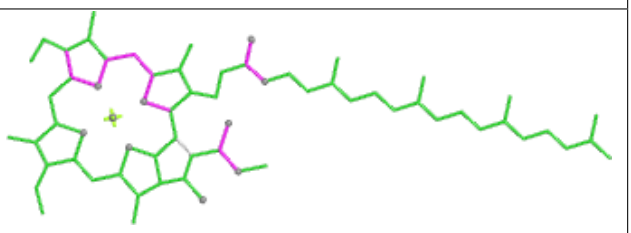


Rings

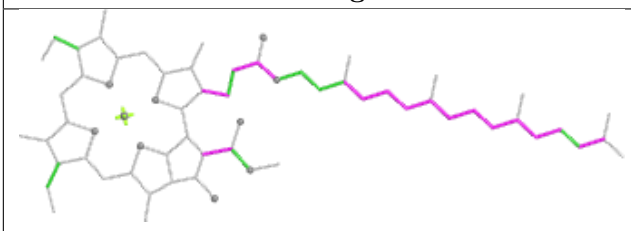
Ligand CLA B 805



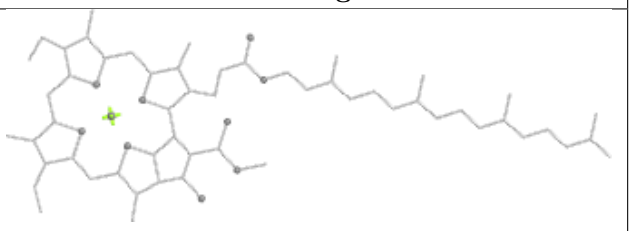
Bond lengths



Bond angles

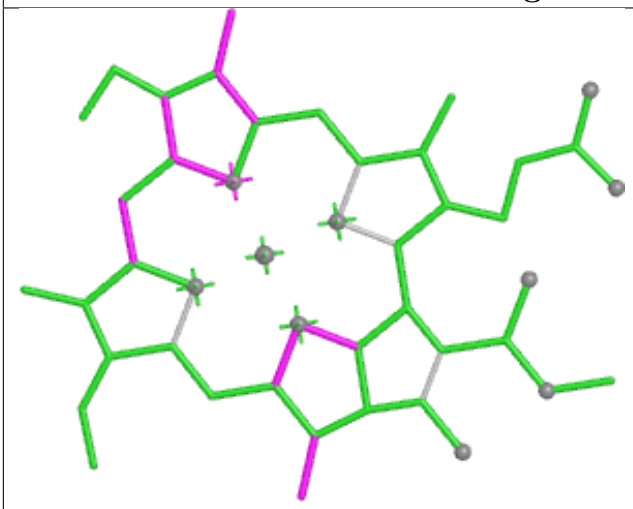


Torsions



Rings

Ligand CLA A 821



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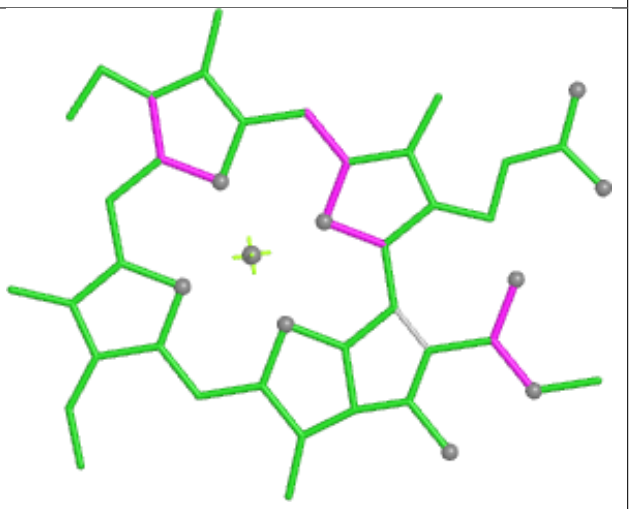
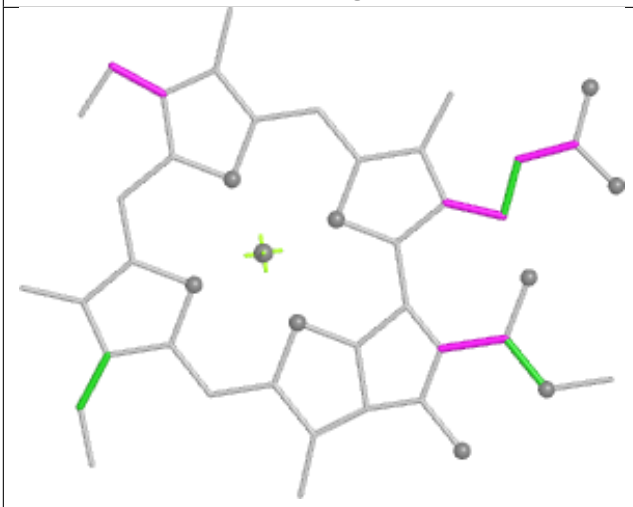


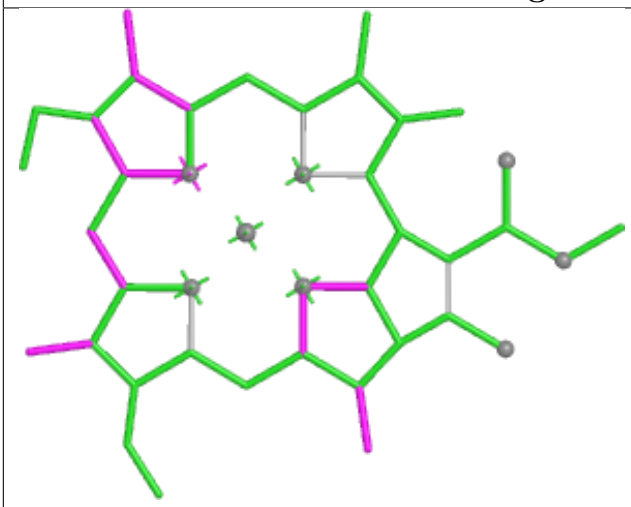
Bond angles



Torsions

Rings

Ligand CLA 3 608



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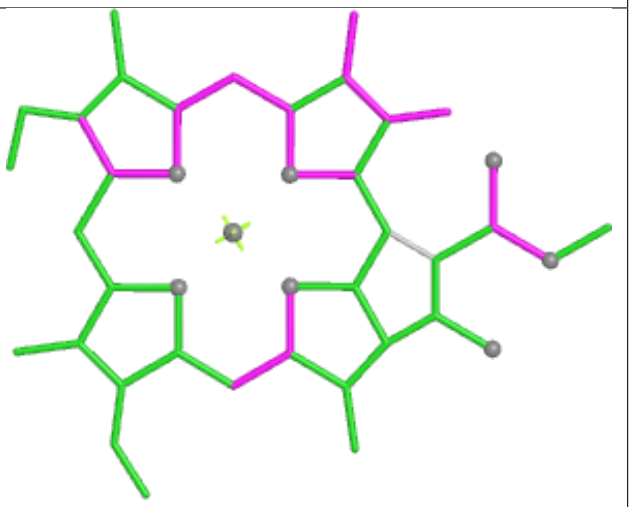
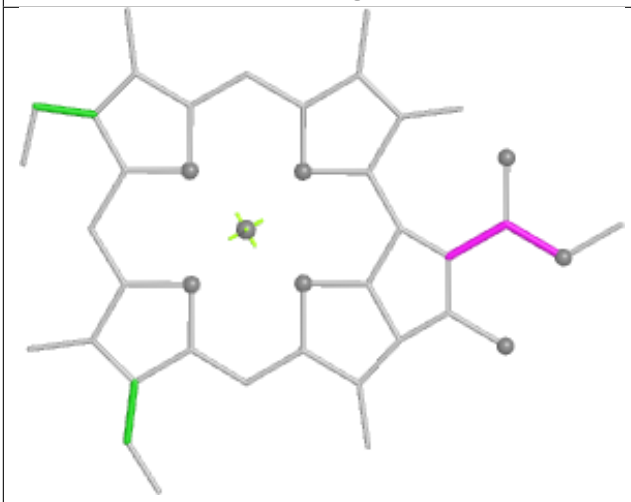
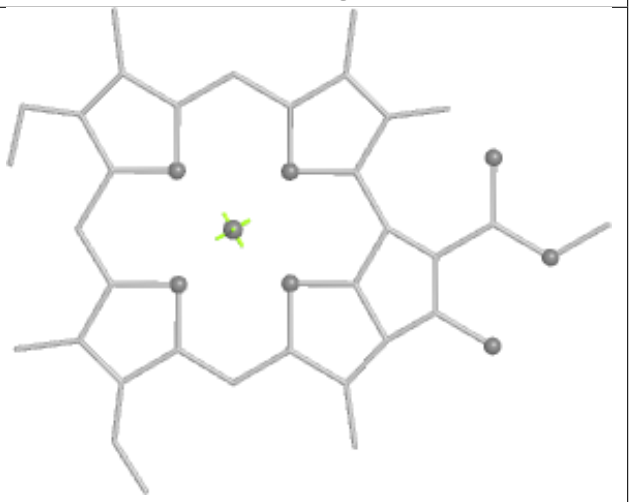


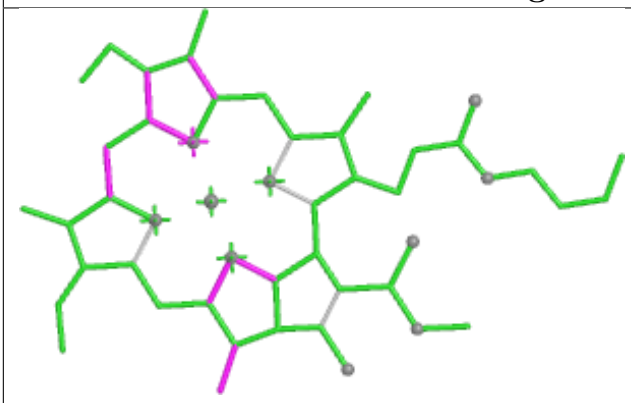
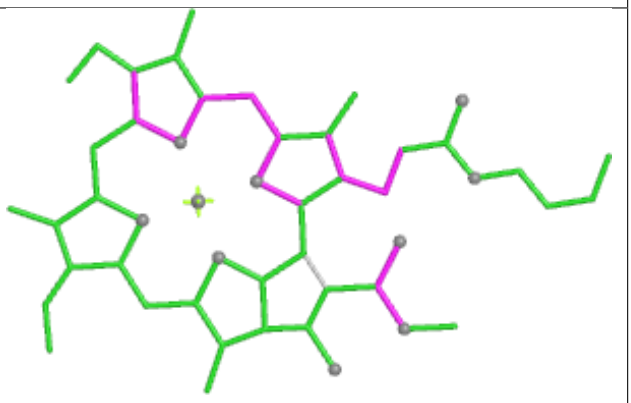
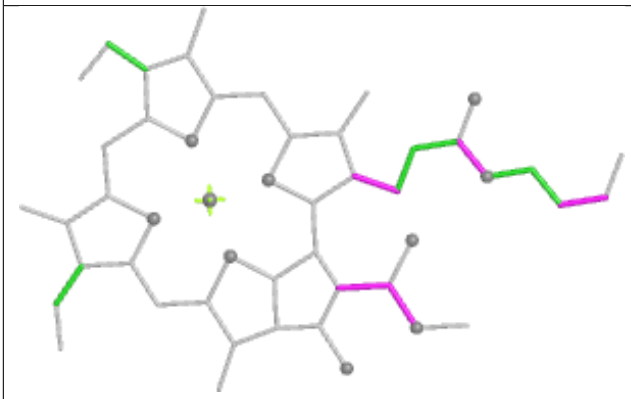
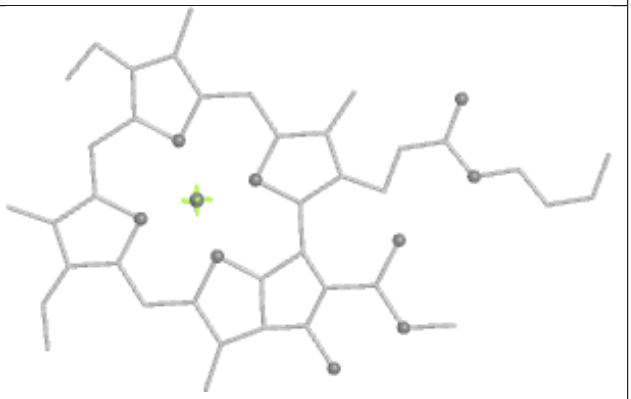
Bond angles



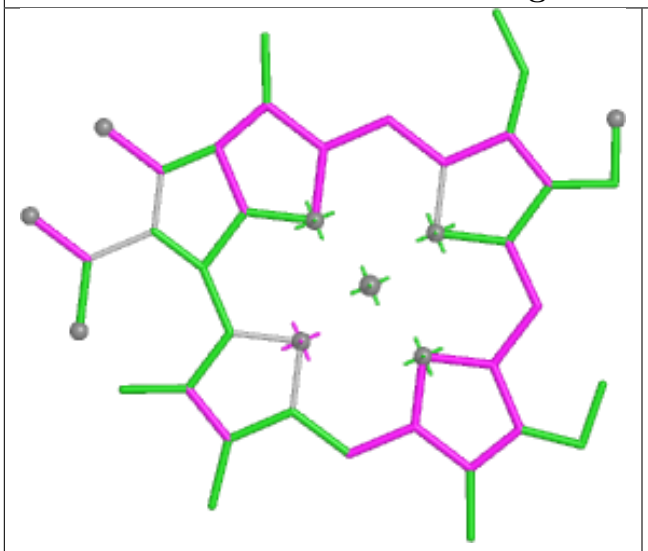
Torsions



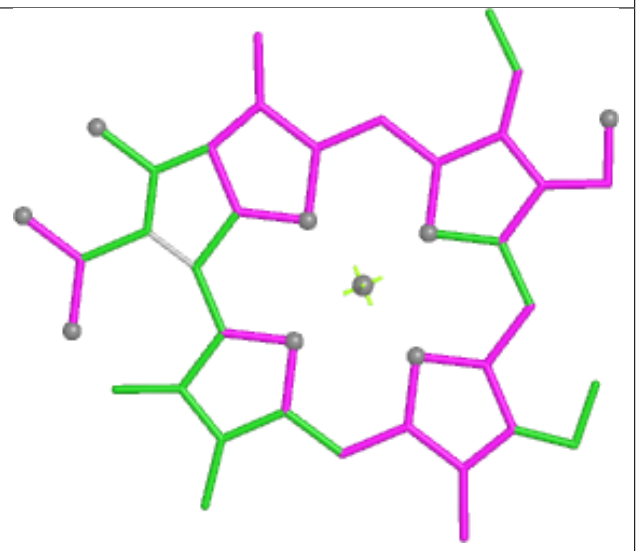
Rings

Ligand CLA 1 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

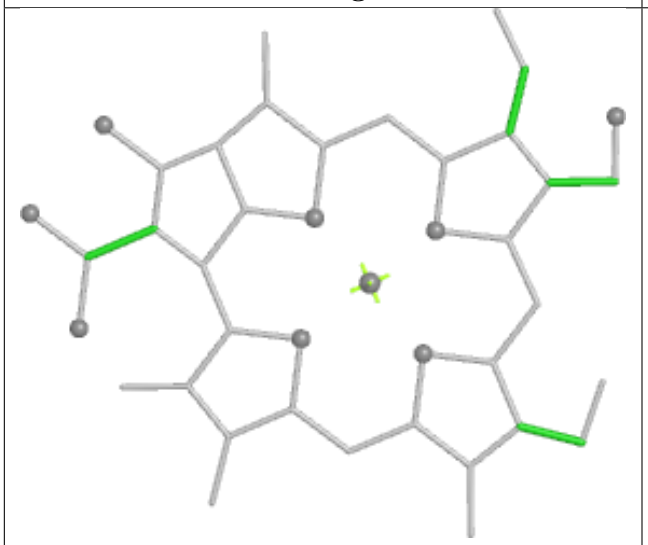
Ligand CHL 1 606



Bond lengths



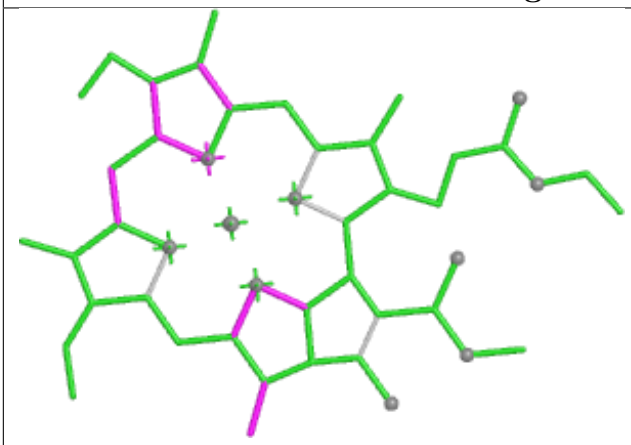
Bond angles



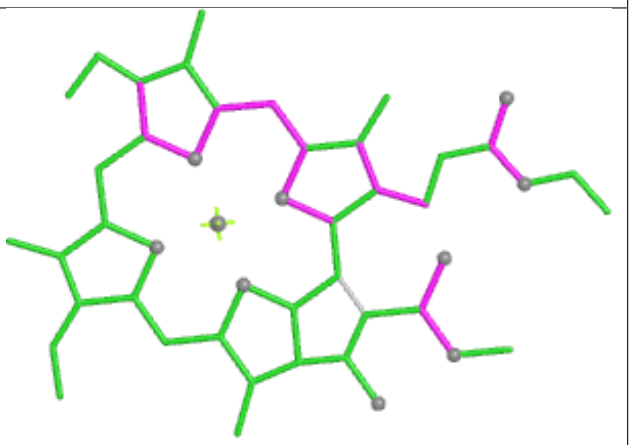
Torsions

Rings

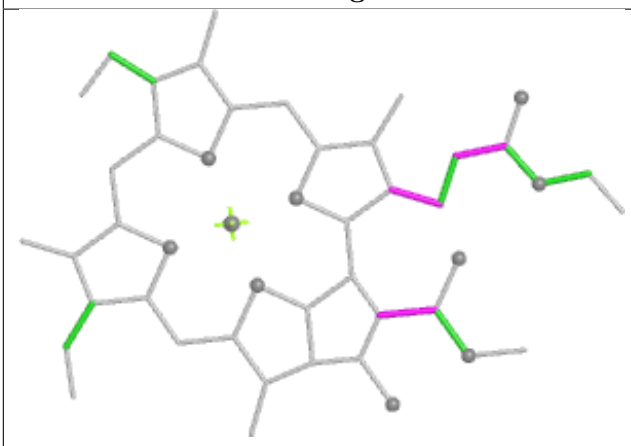
Ligand CLA B 821



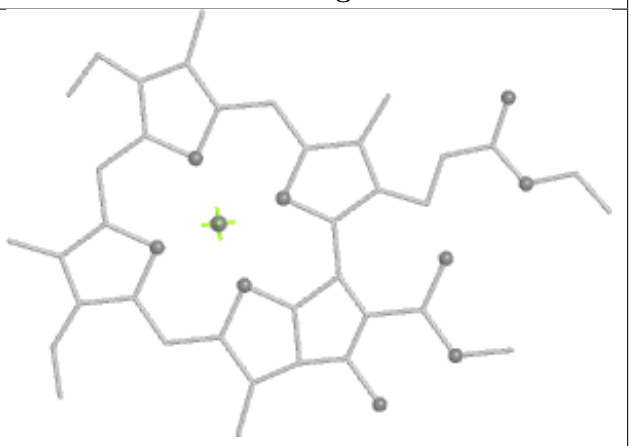
Bond lengths



Bond angles

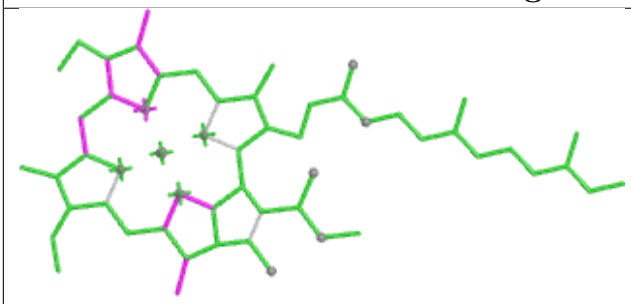


Torsions

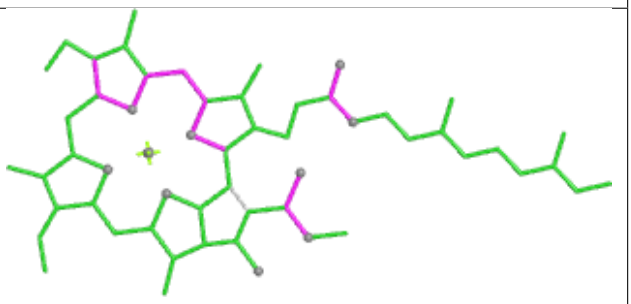


Rings

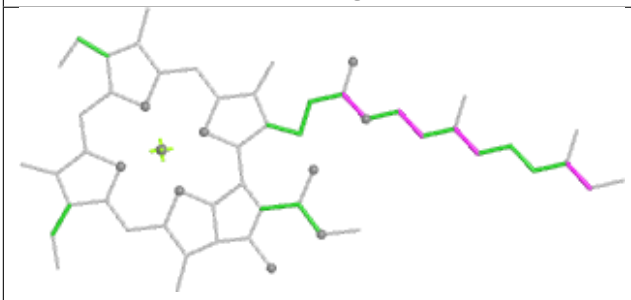
Ligand CLA B 829



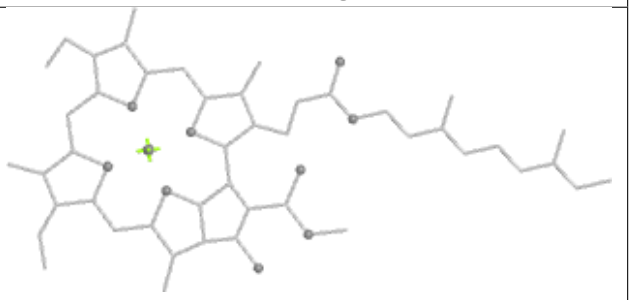
Bond lengths



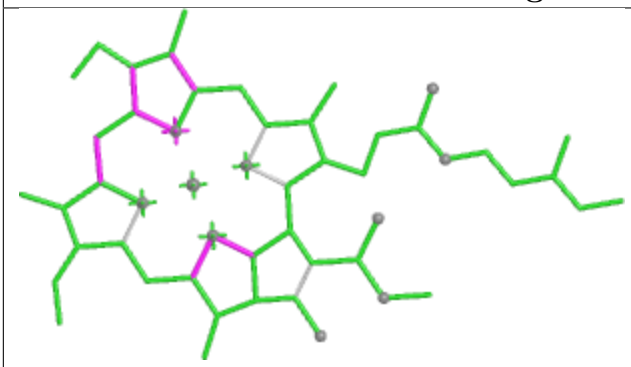
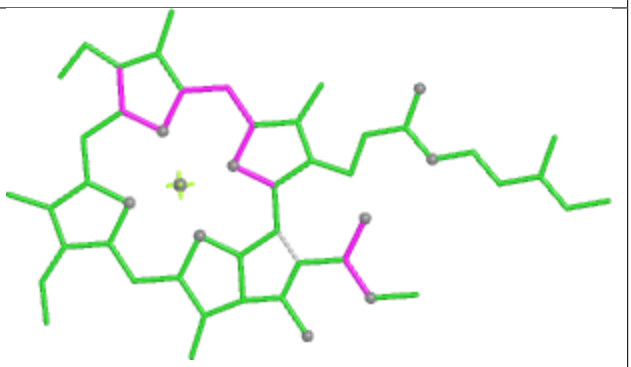
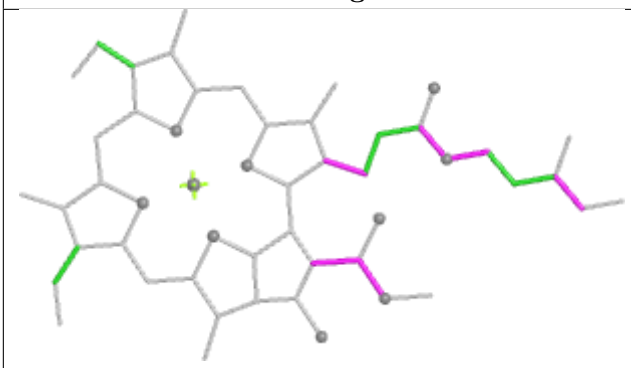
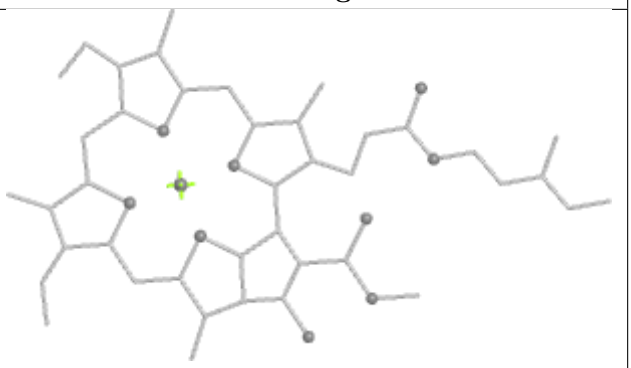
Bond angles

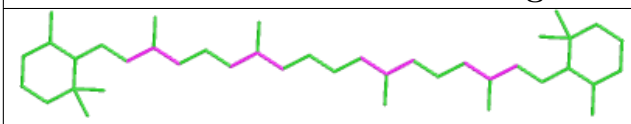
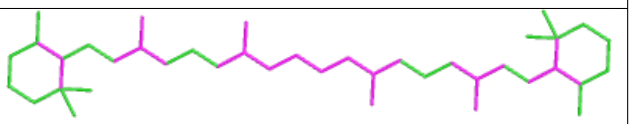
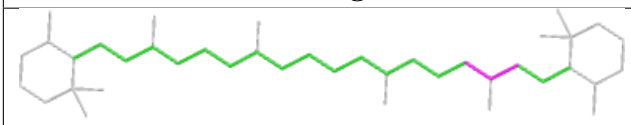
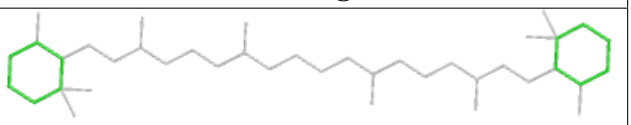


Torsions

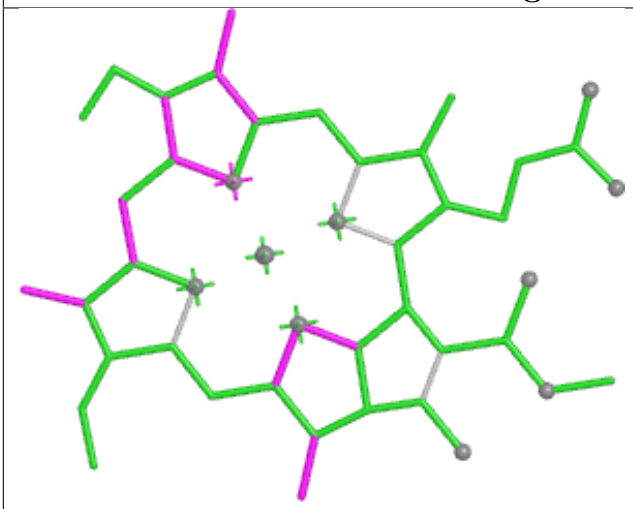


Rings

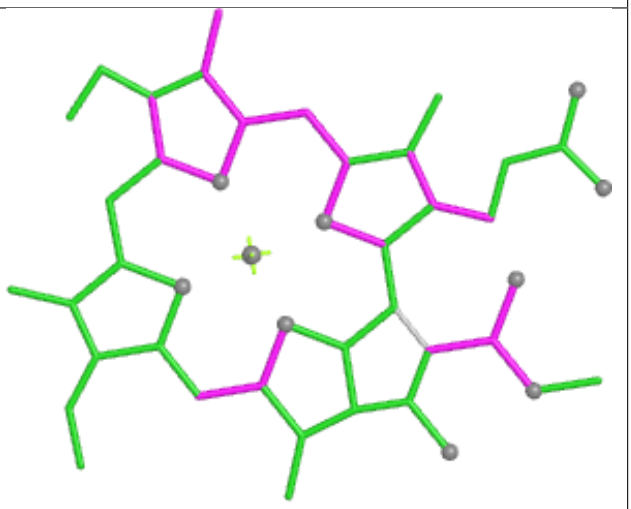
Ligand CLA F 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR 3 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

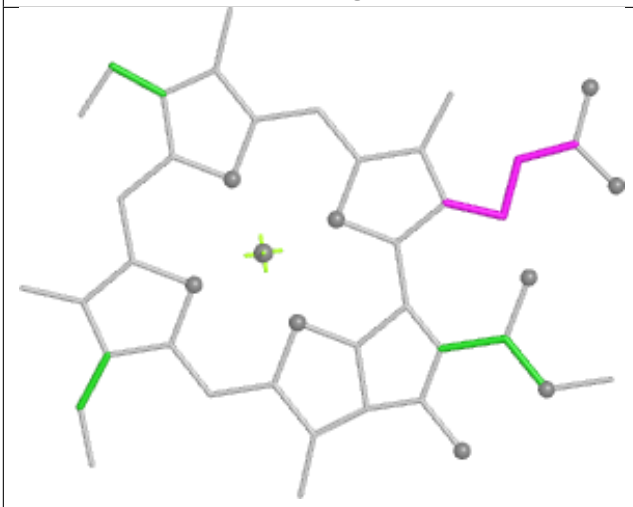
Ligand CLA A 815



Bond lengths



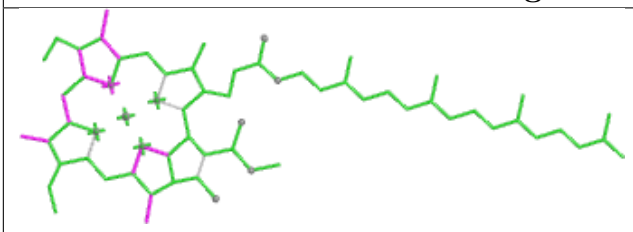
Bond angles



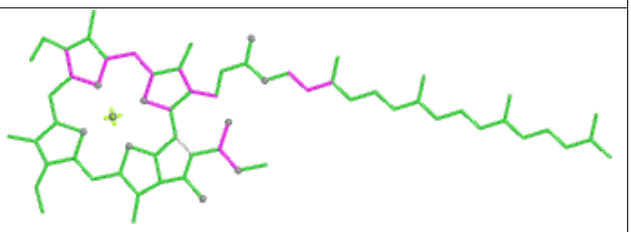
Torsions

Rings

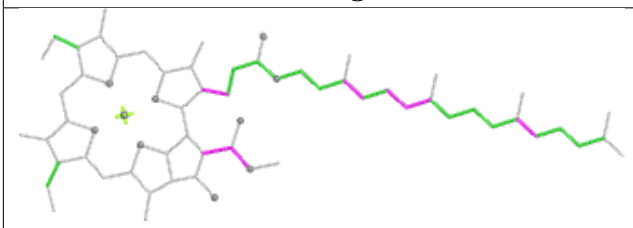
Ligand CLA B 810



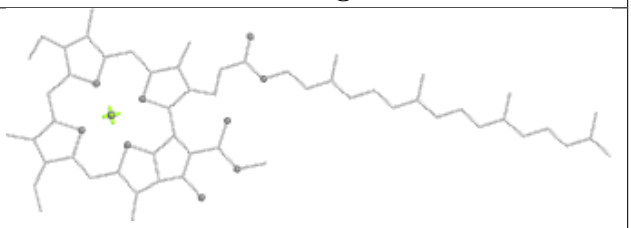
Bond lengths



Bond angles

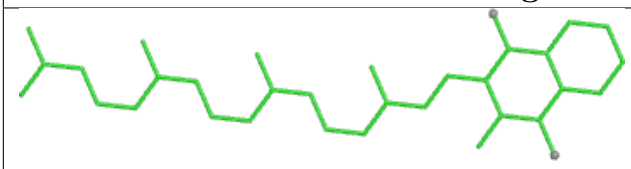


Torsions



Rings

Ligand PQN A 855



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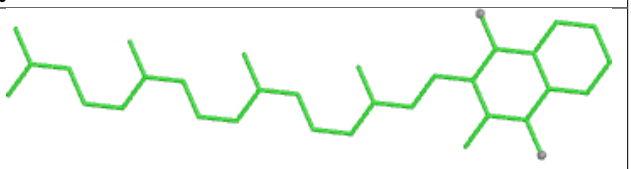
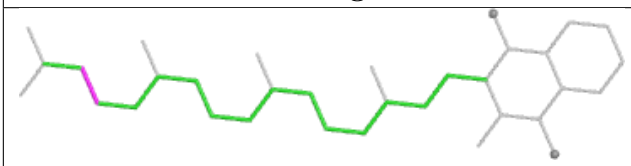


Bond angles



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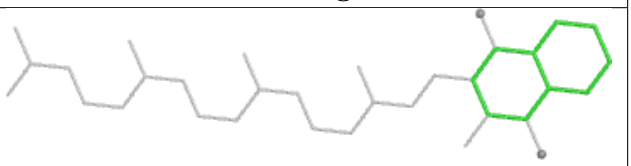
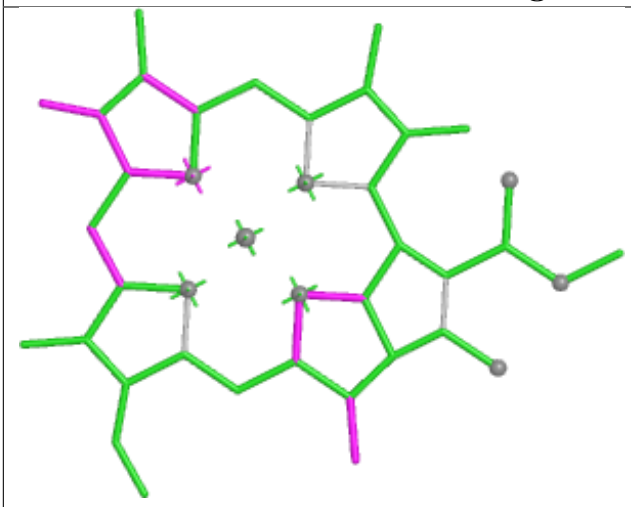
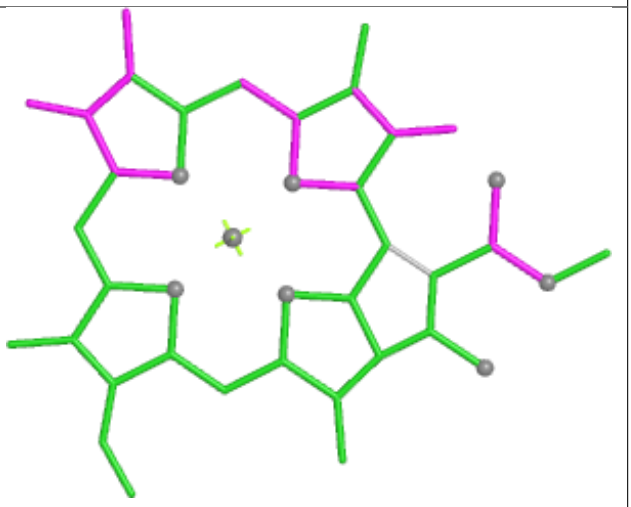


Rings

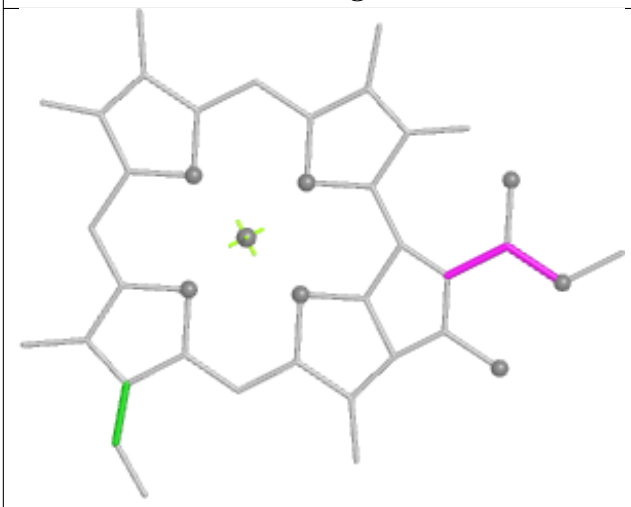
Ligand CLA 1 608



Bond lengths



Bond angles



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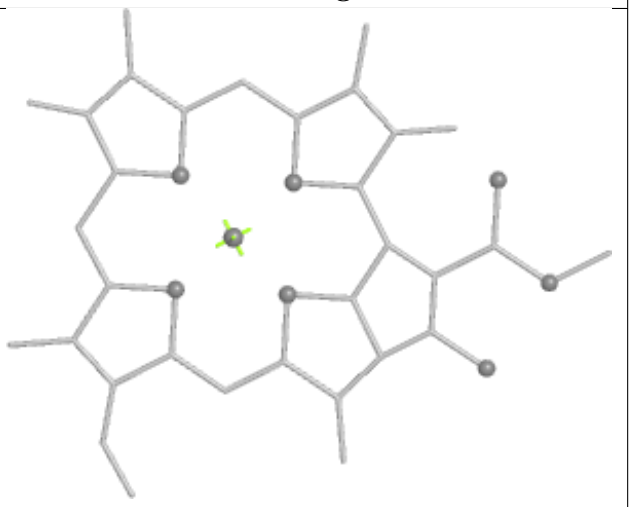
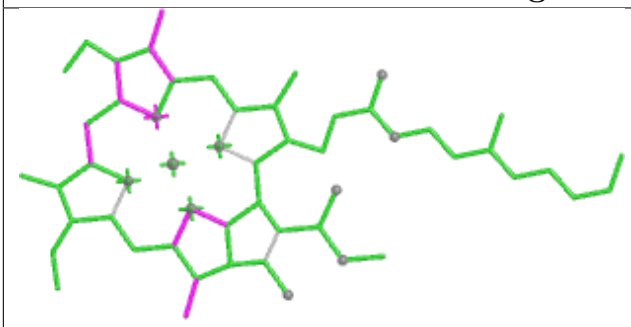
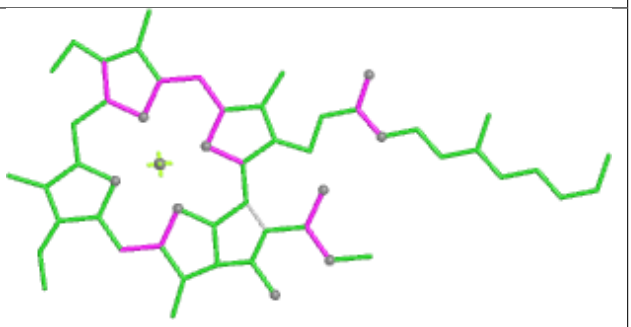
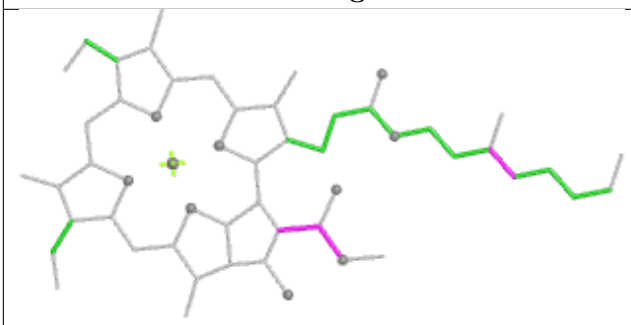
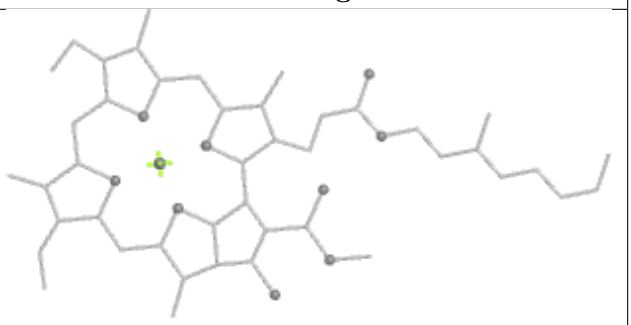
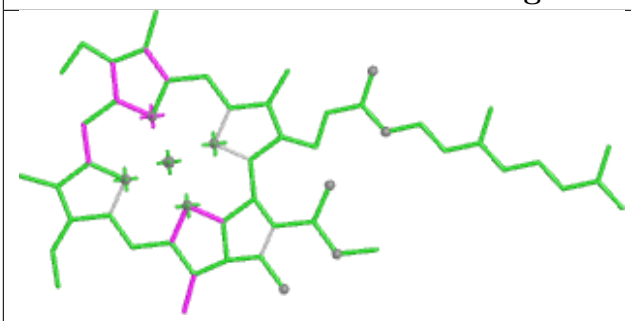
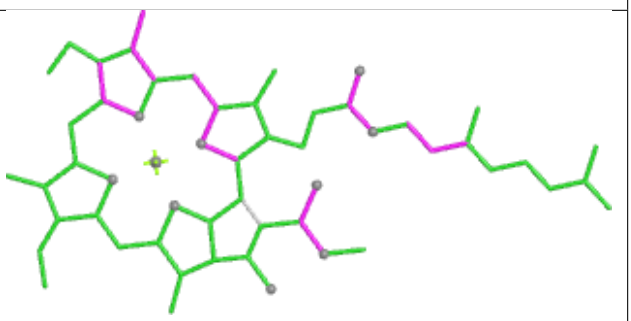
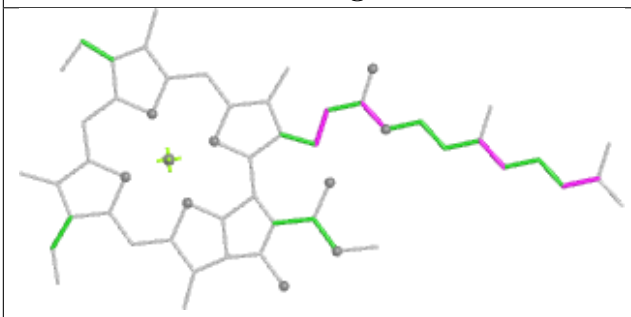
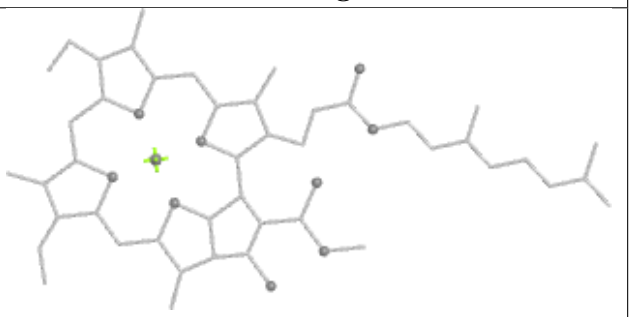
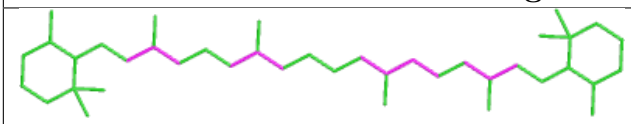


Rings

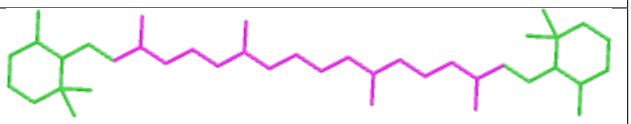
Ligand CLA 4 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

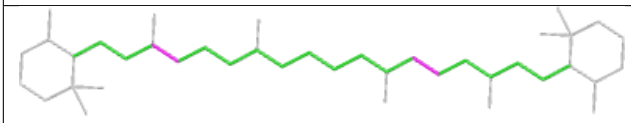
Ligand BCR L 301



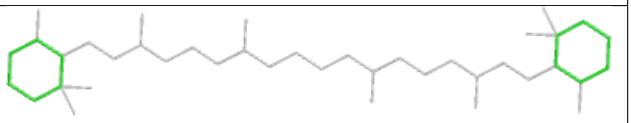
Bond lengths



Bond angles

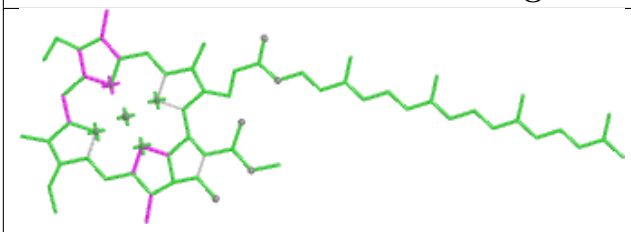


Torsions



Rings

Ligand CLA B 839



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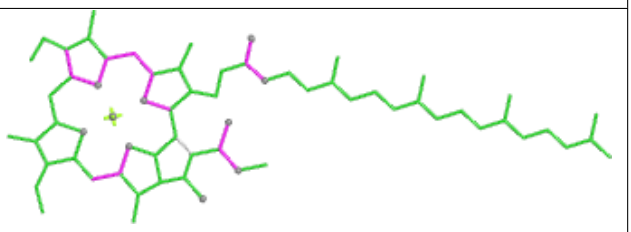
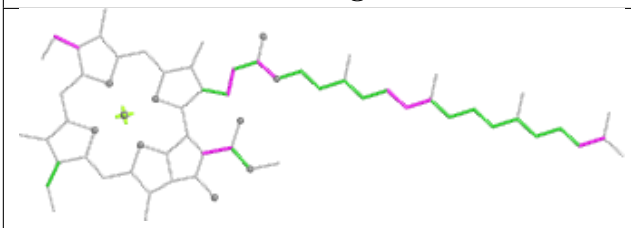
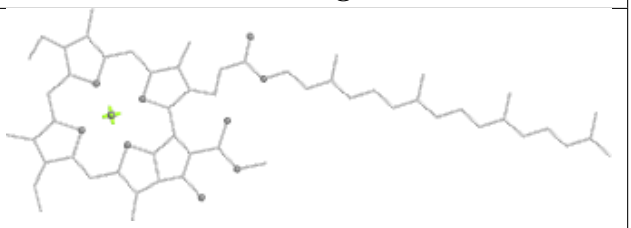


Bond angles

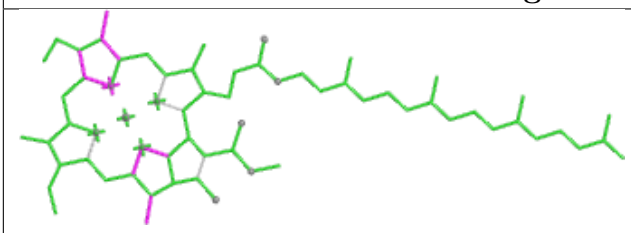


Torsions



Rings

Ligand CLA A 842



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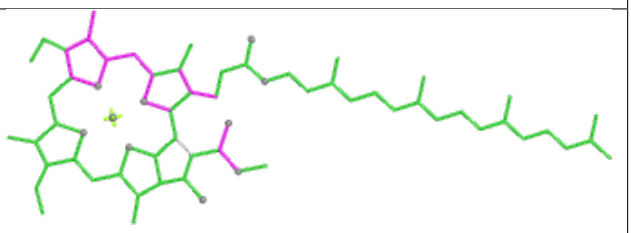
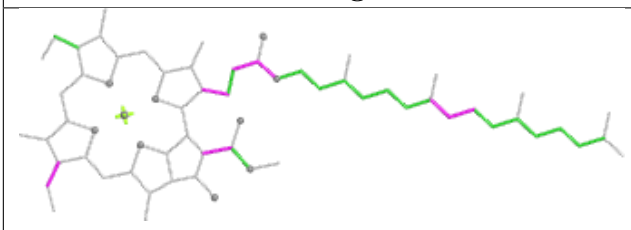
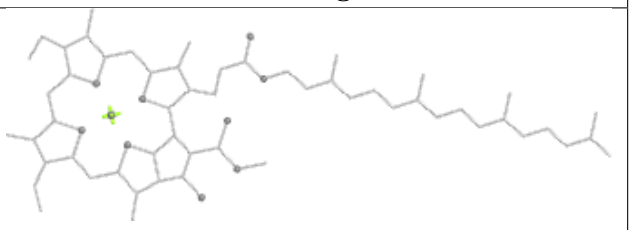


Bond angles

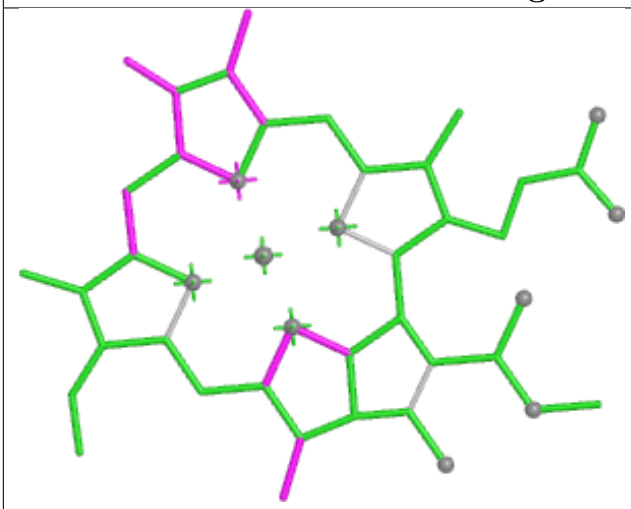


Torsions

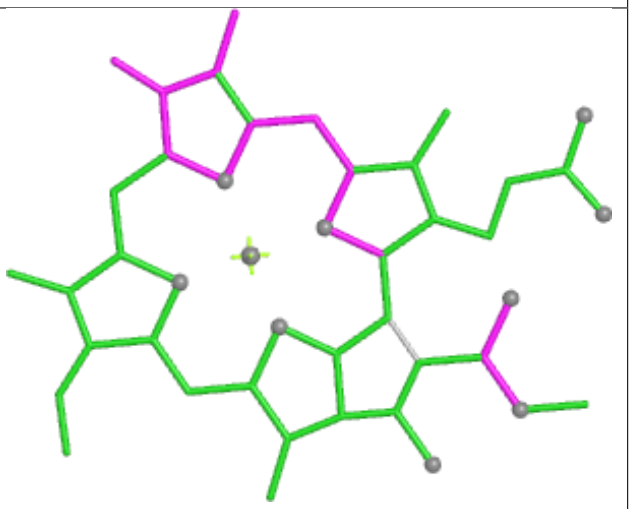


Rings

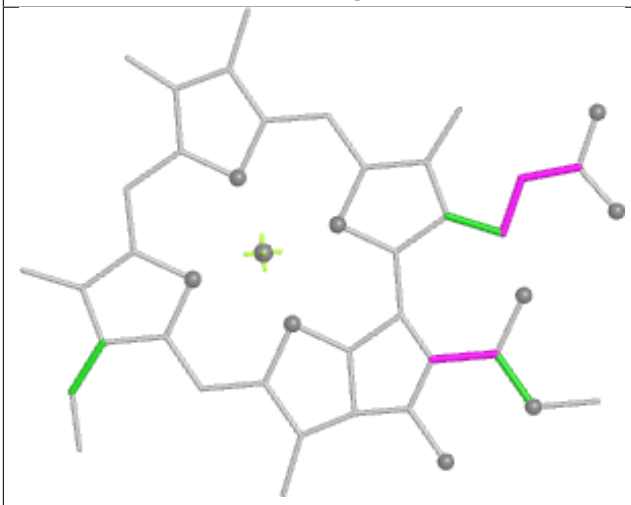
Ligand CLA 4 603



Bond lengths



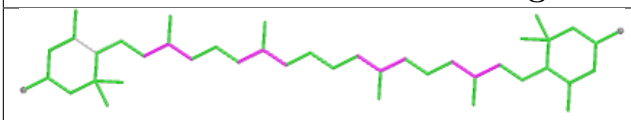
Bond angles



Torsions

Rings

Ligand LUT 4 616



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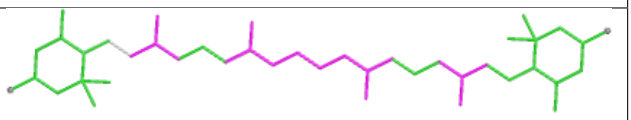
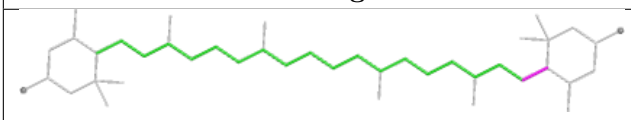
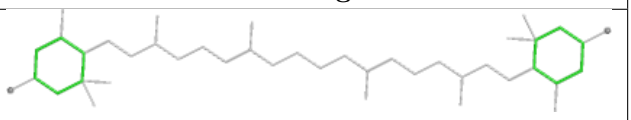


Bond angles

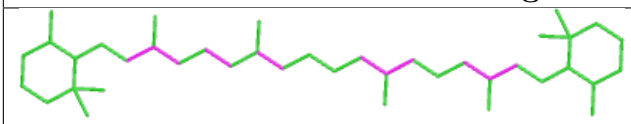


Torsions

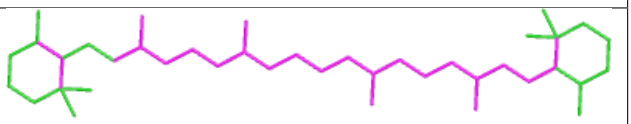


Rings

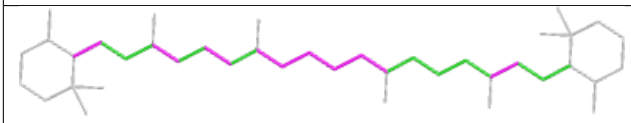
Ligand BCR A 852



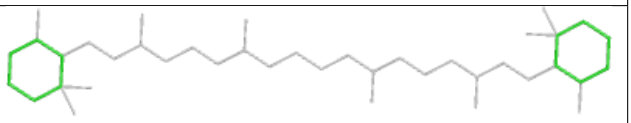
Bond lengths



Bond angles

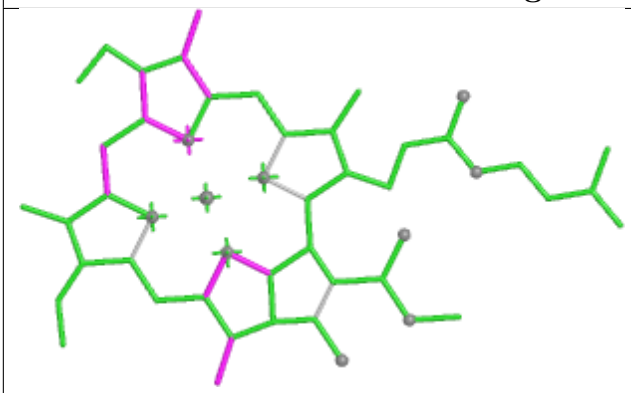


Torsions

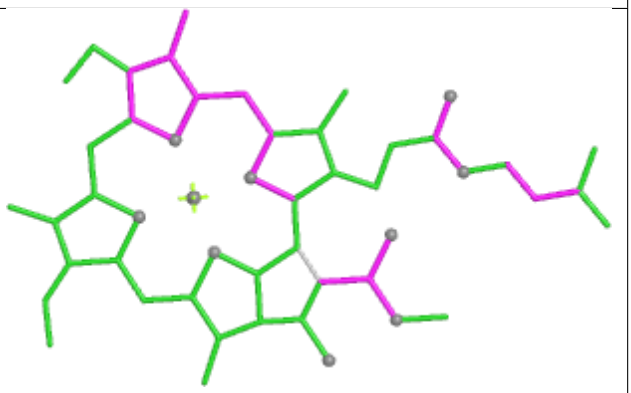


Rings

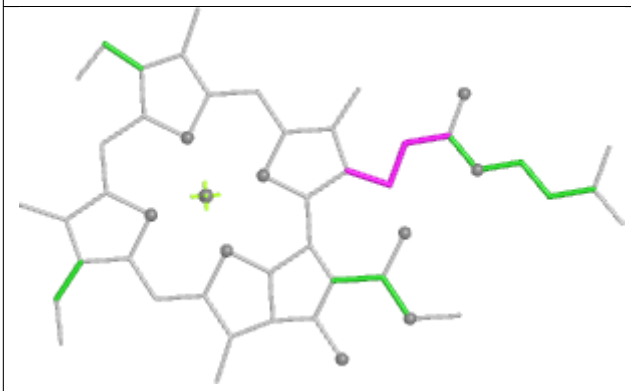
Ligand CLA B 820



Bond lengths



Bond angles



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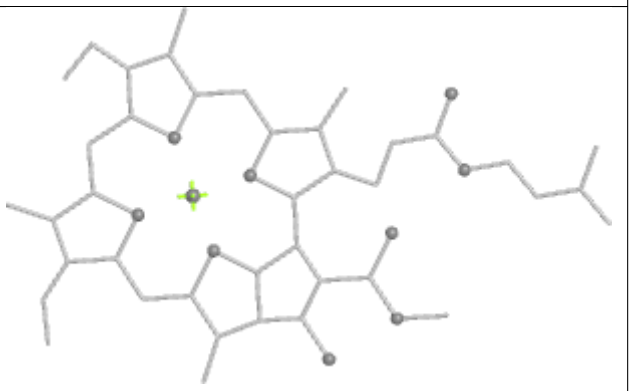
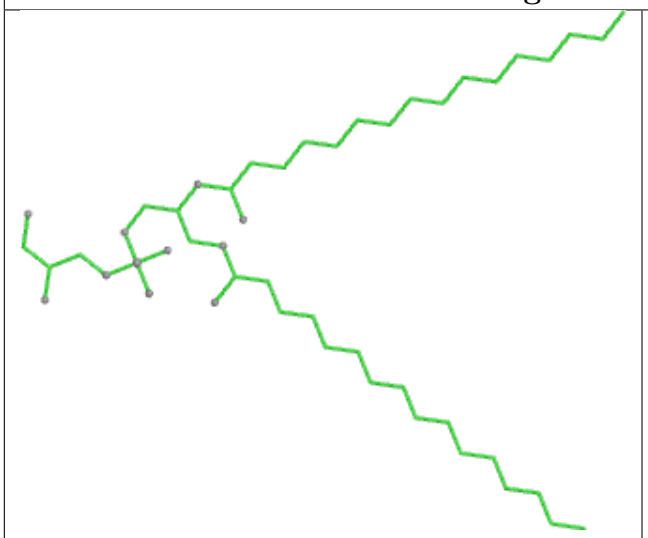


Rings

Ligand LHG B 852



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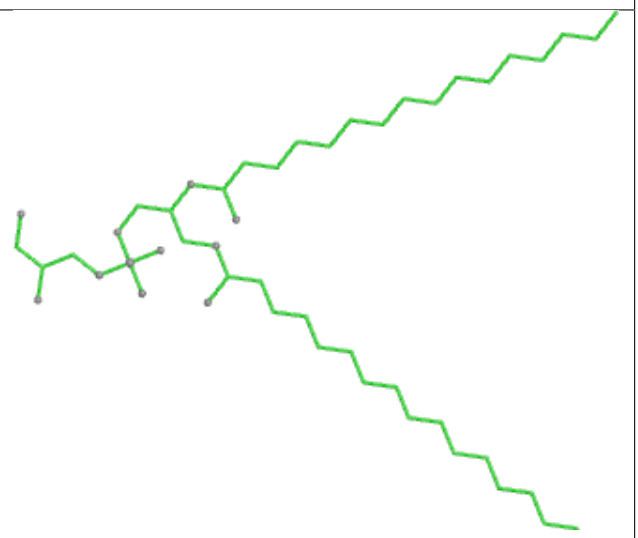
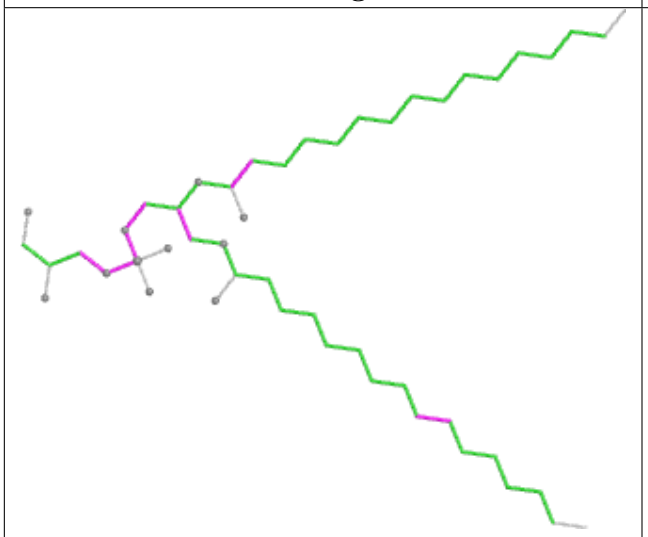
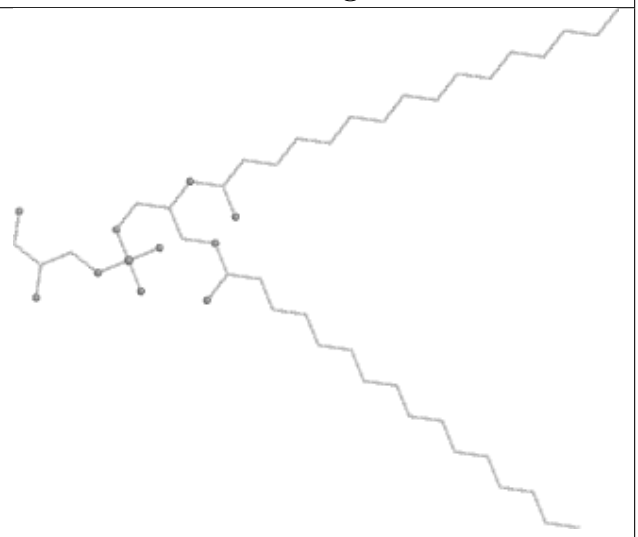


Bond angles



Torsions

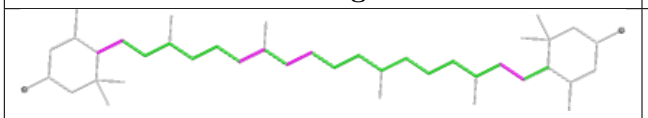


Rings

Ligand LUT 2 616

Bond lengths

Bond angles



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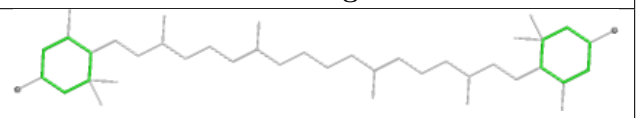
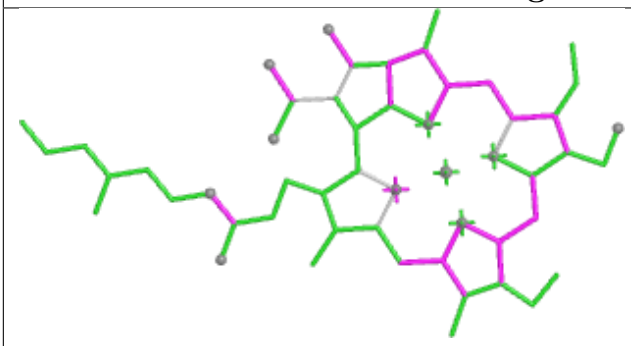
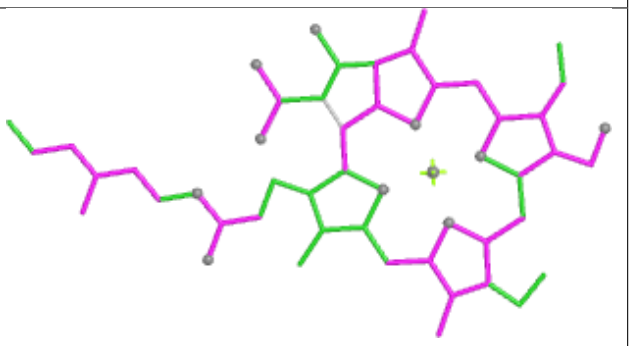


Rings

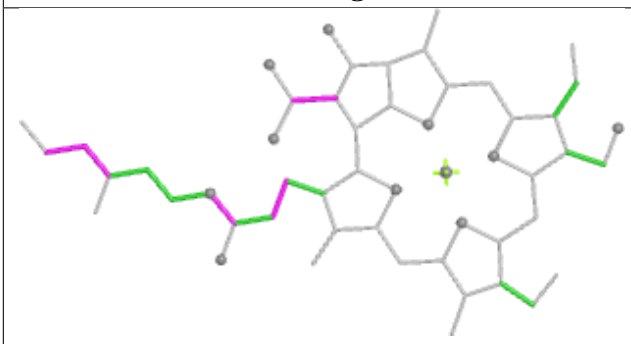
Ligand CHL 1 601



Bond lengths



Bond angles



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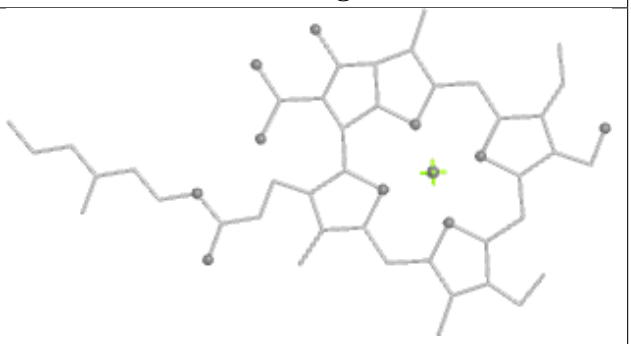
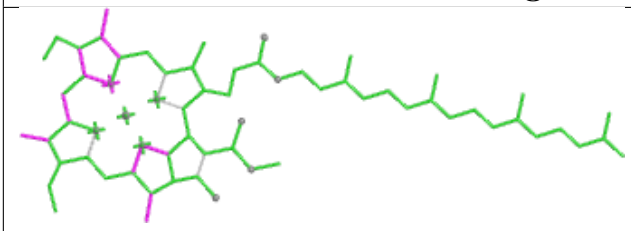


Rings

Ligand CLA B 837



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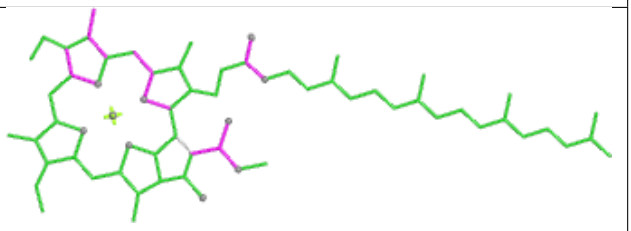

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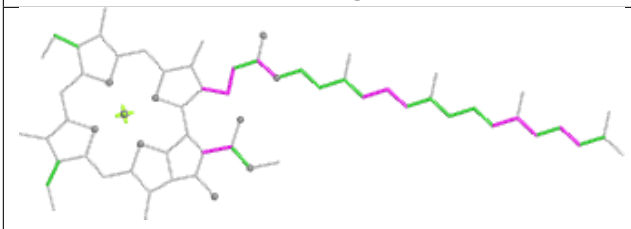

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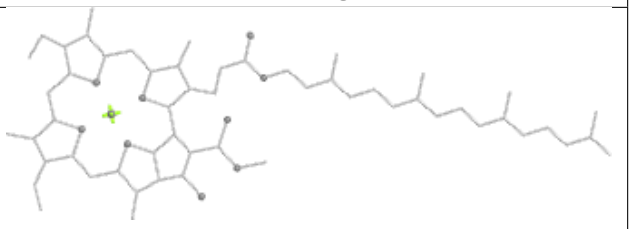
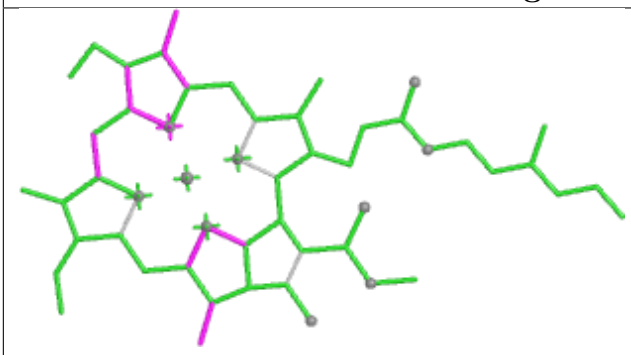
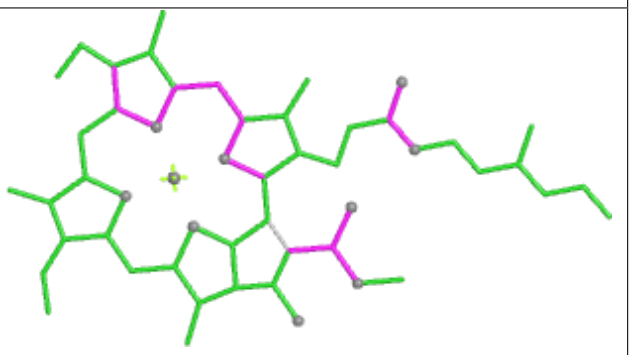
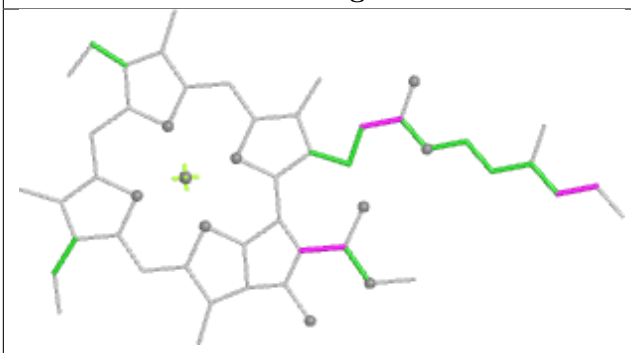
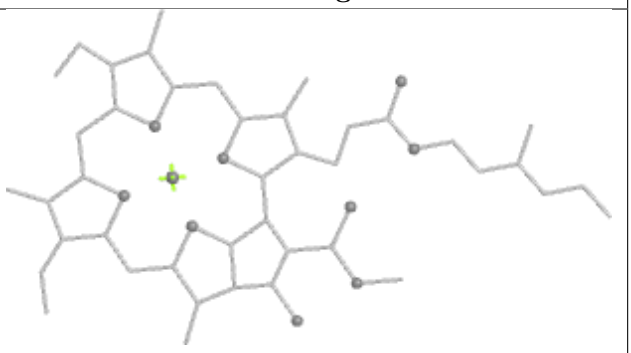
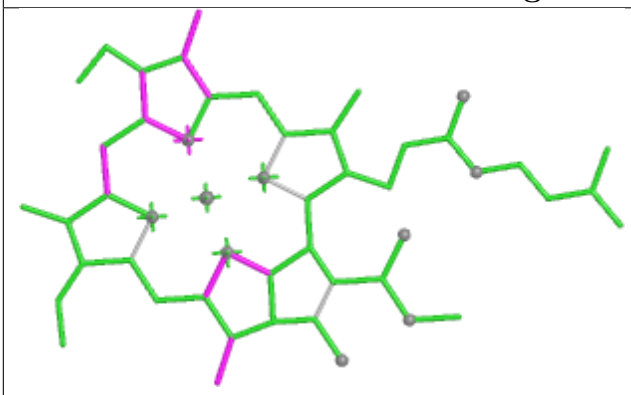
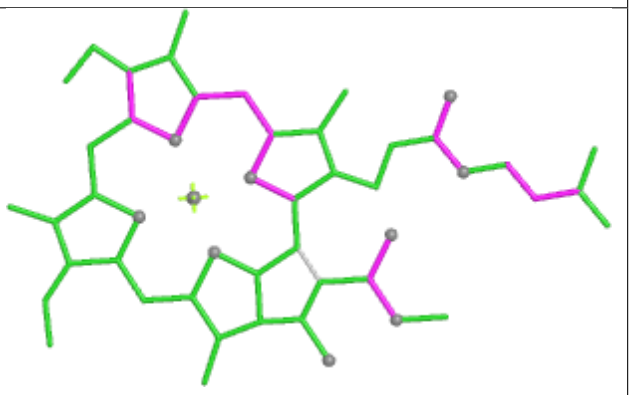
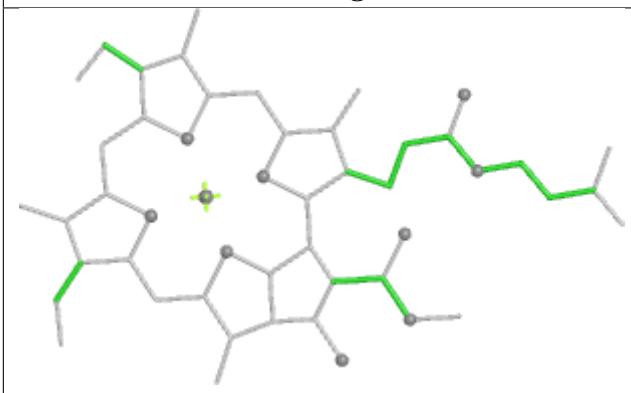
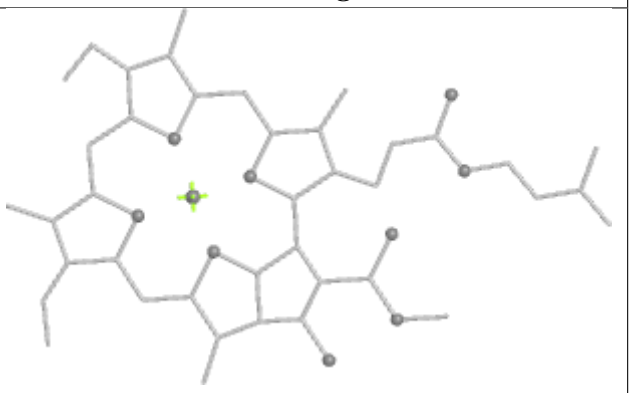


Rings

Ligand CLA A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

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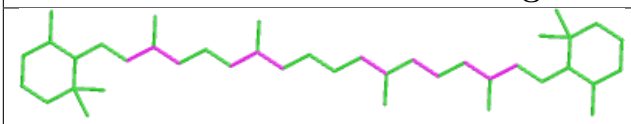
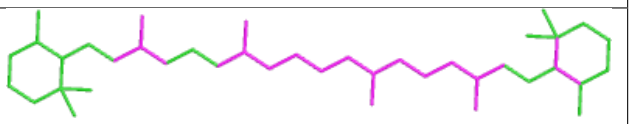
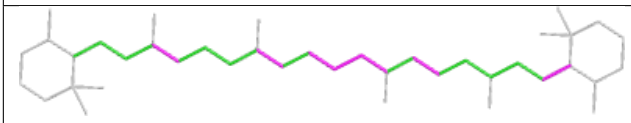
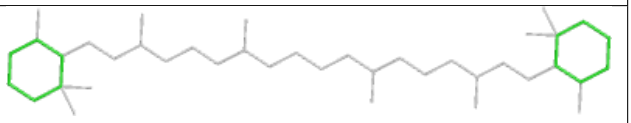
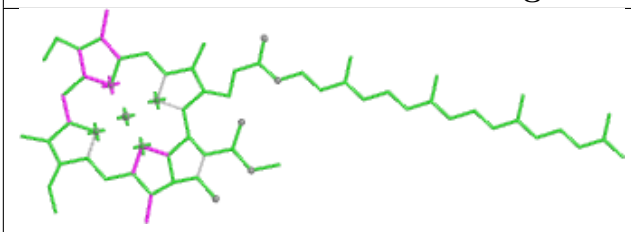
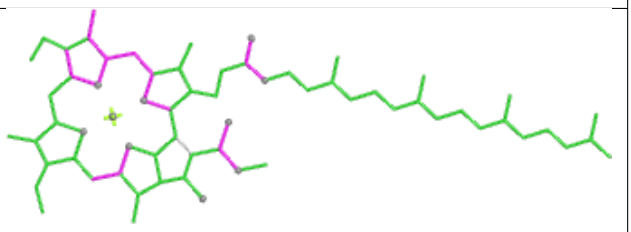
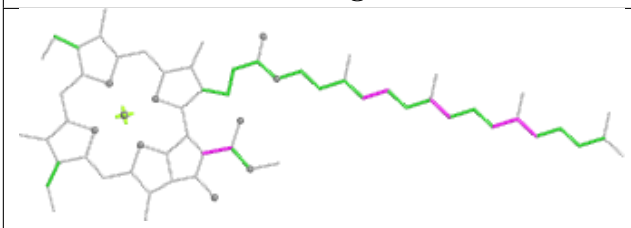
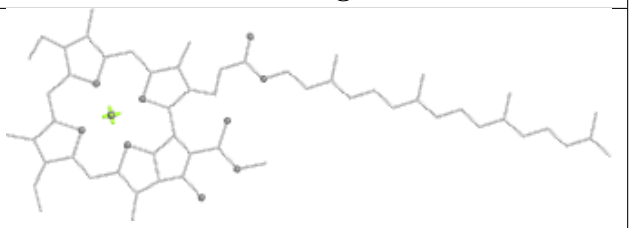
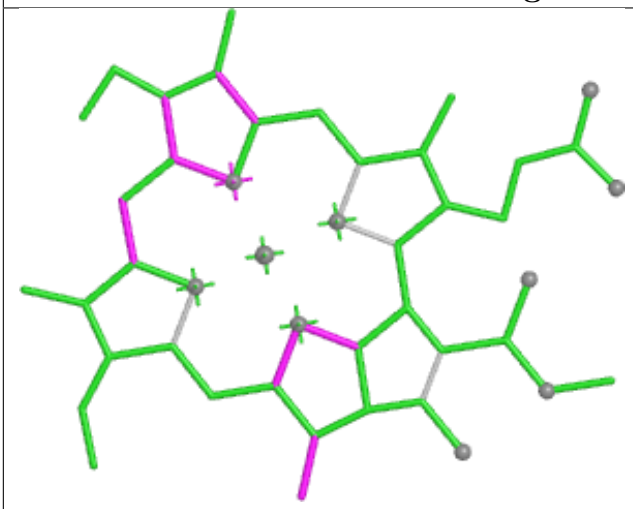
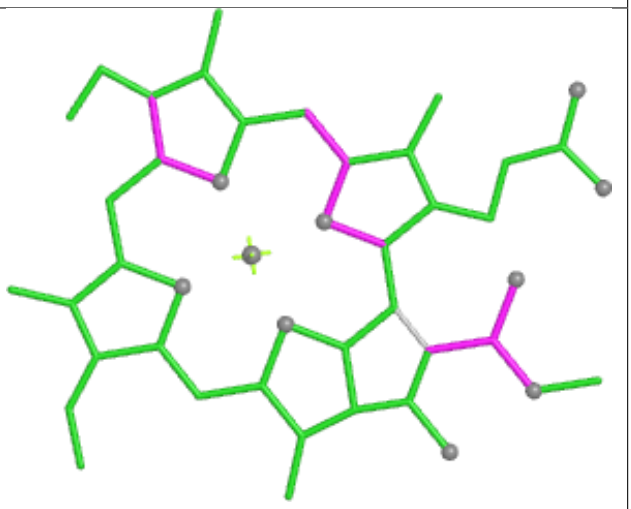
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

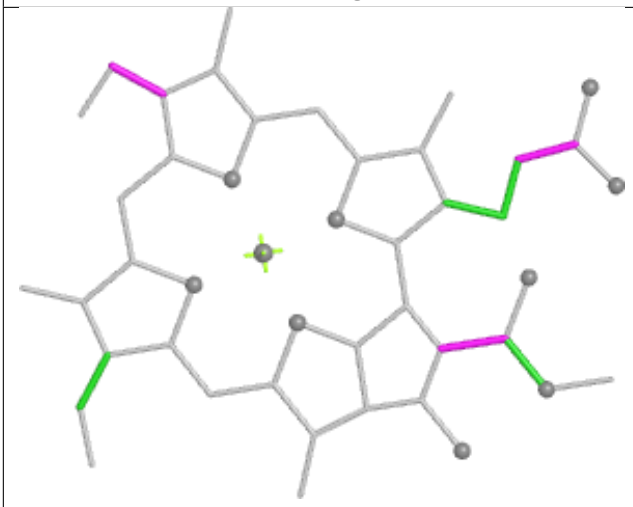
Ligand CLA A 837



Bond lengths

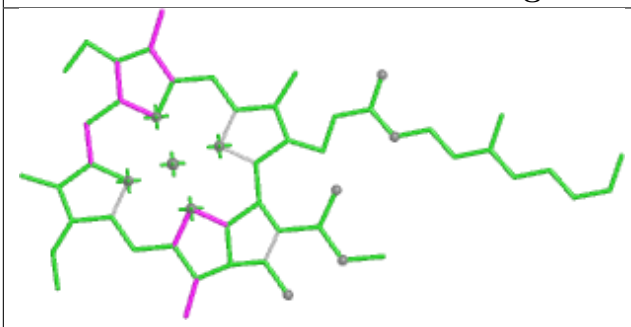
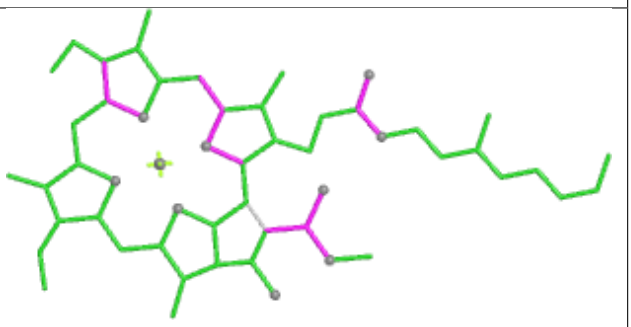
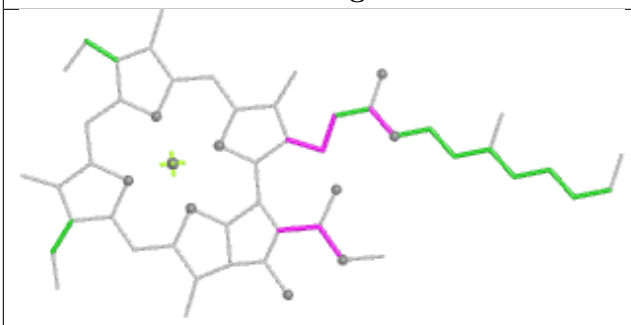
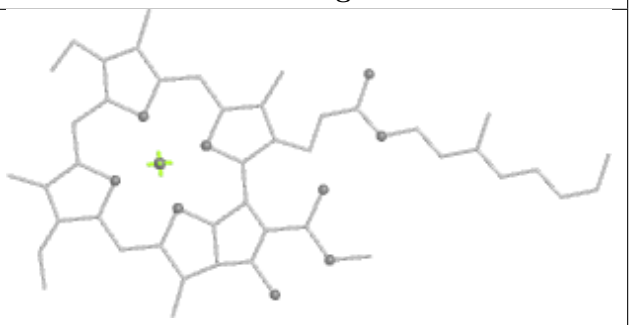


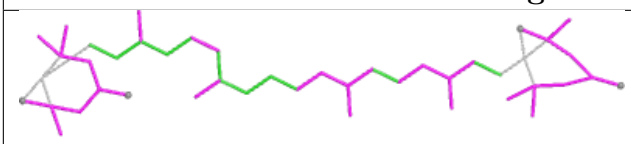
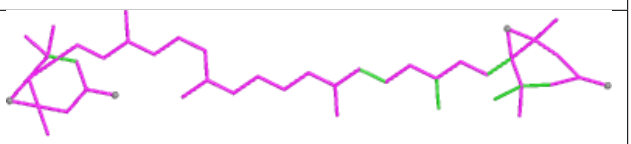
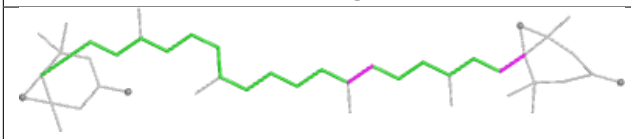
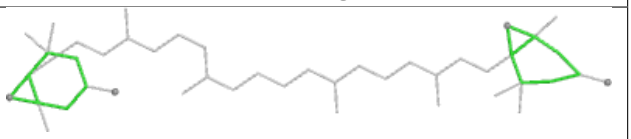
Bond angles

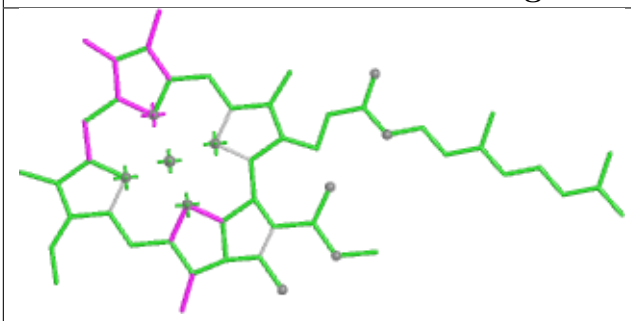
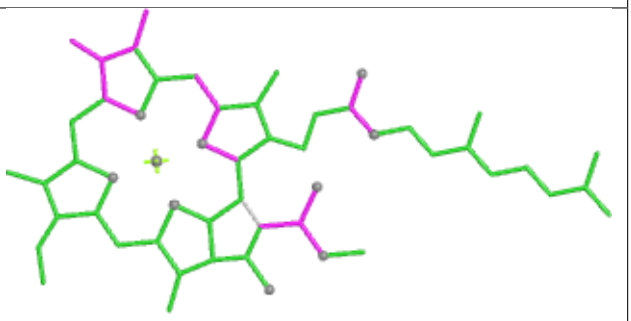
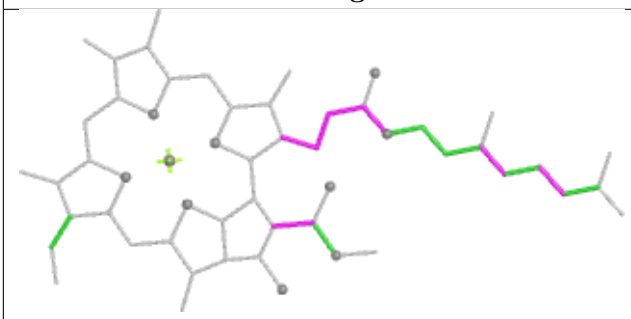
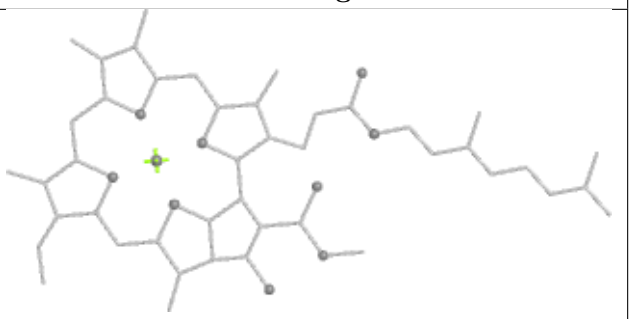


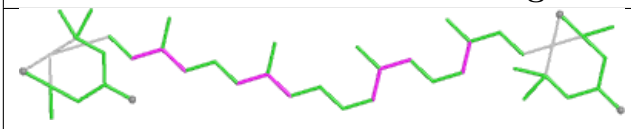
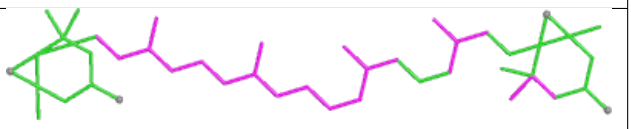
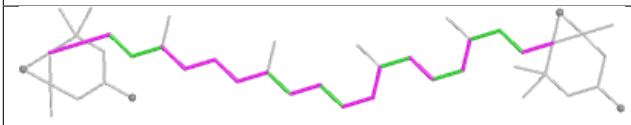
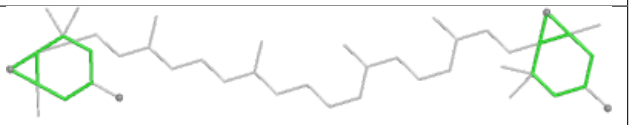
Torsions

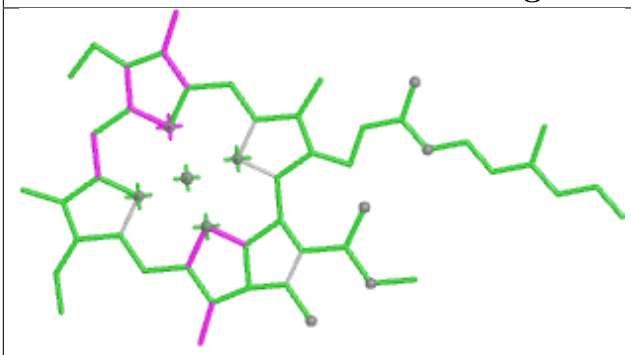
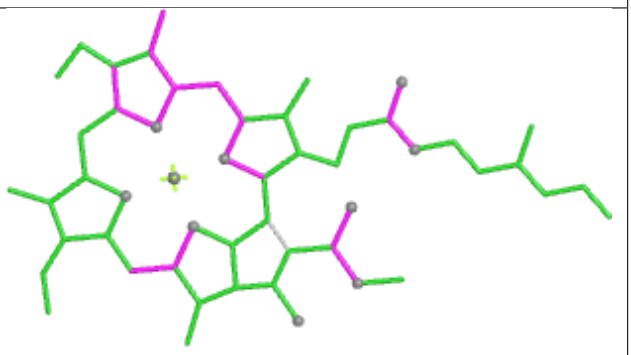
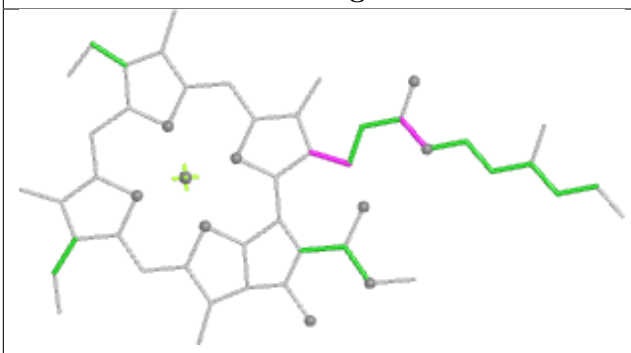
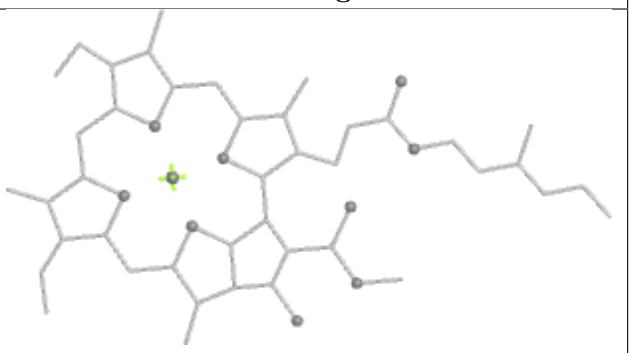
Rings

Ligand CLA A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

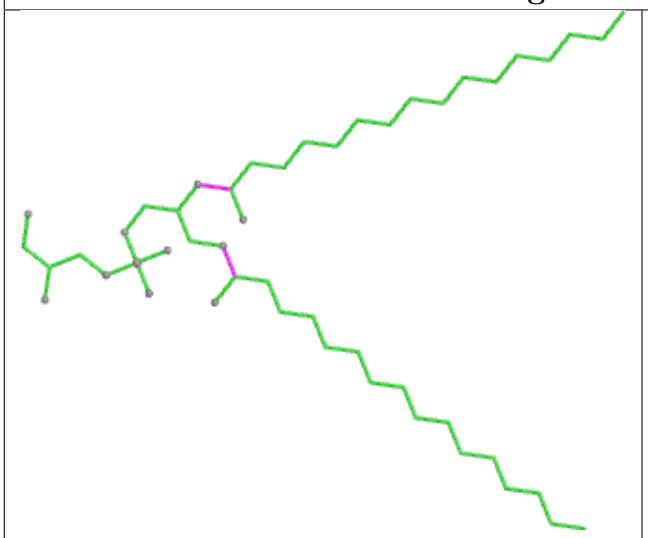
Ligand XAT 4 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

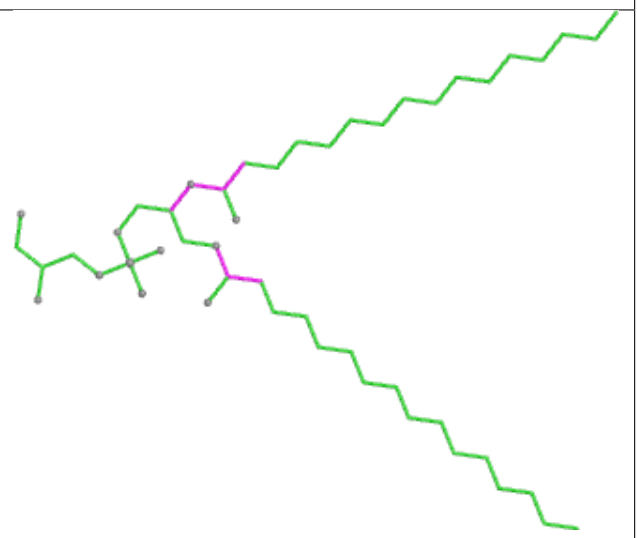
Ligand XAT 2 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

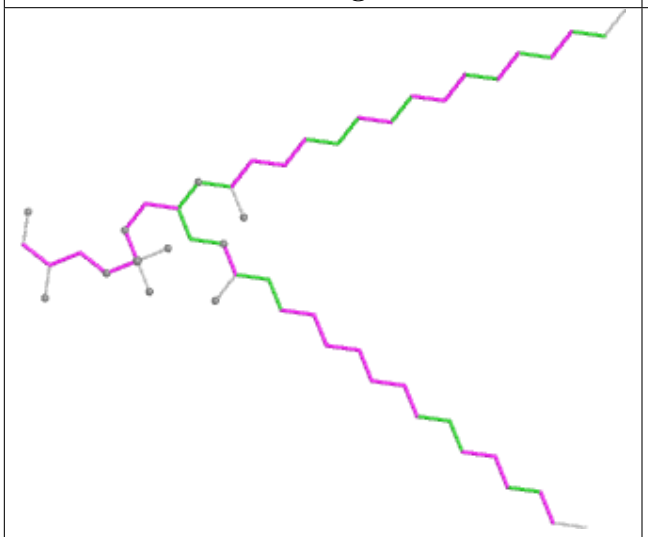
Ligand LHG 1 615



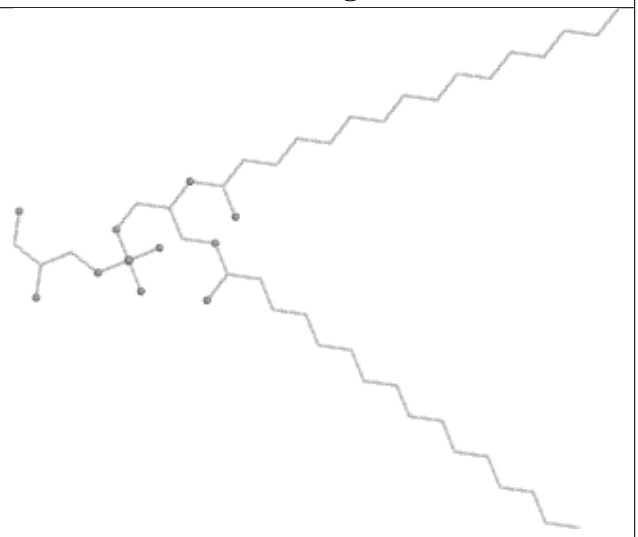
Bond lengths



Bond angles

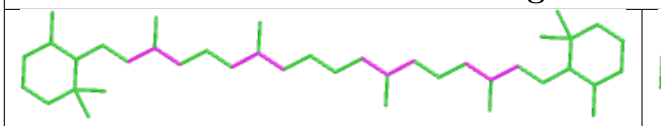


Torsions



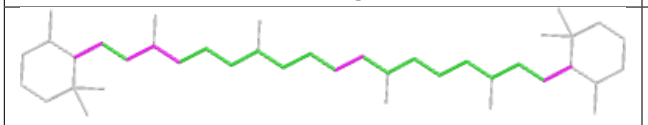
Rings

Ligand BCR 4 618



Bond lengths

Bond angles



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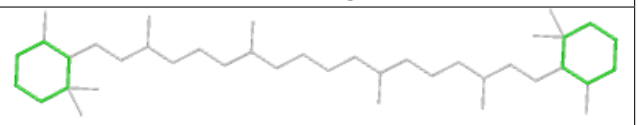
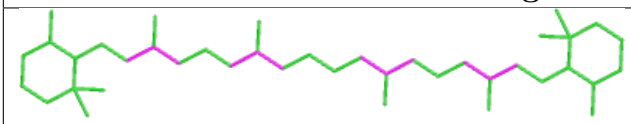


Rings

Ligand BCR A 848



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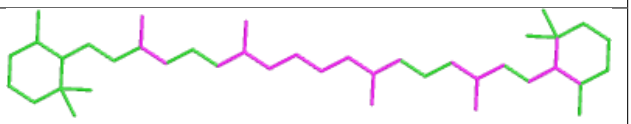
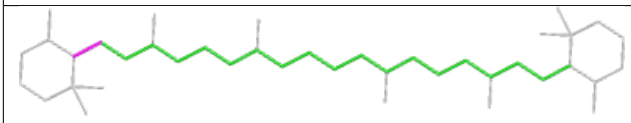


Bond angles



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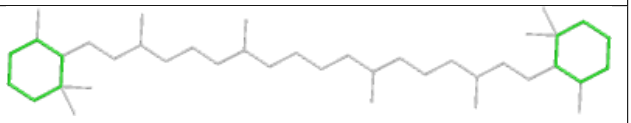
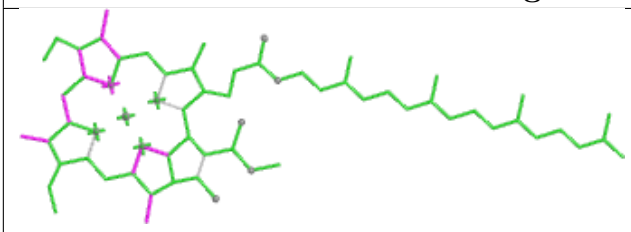


Rings

Ligand CLA A 806



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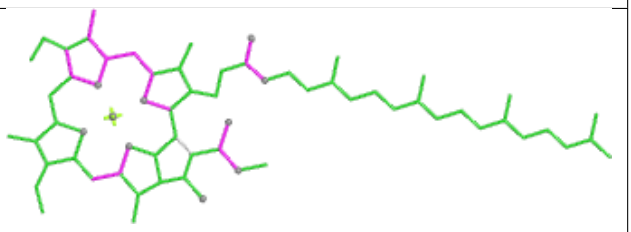

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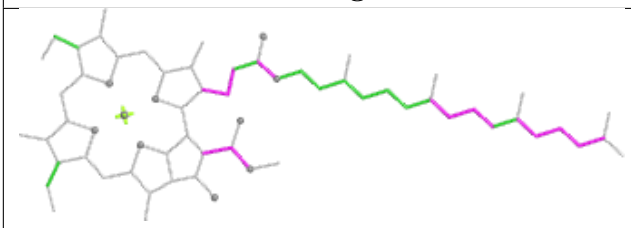

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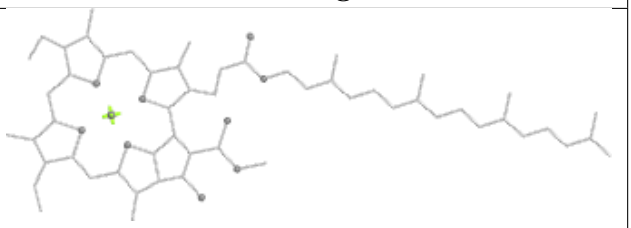
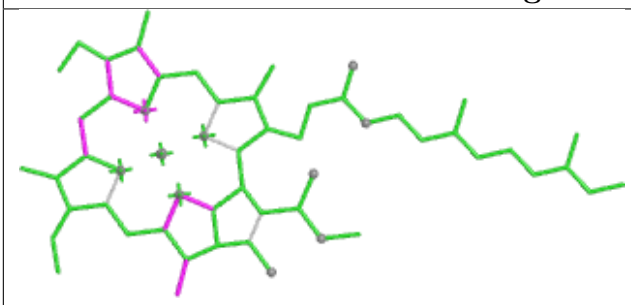


Rings

Ligand CLA A 833



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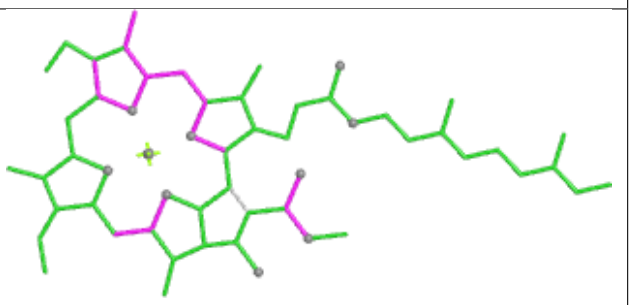
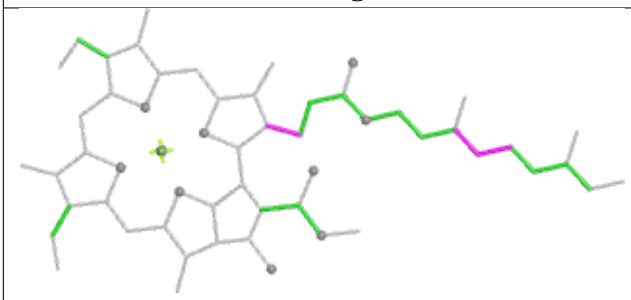


Bond angles



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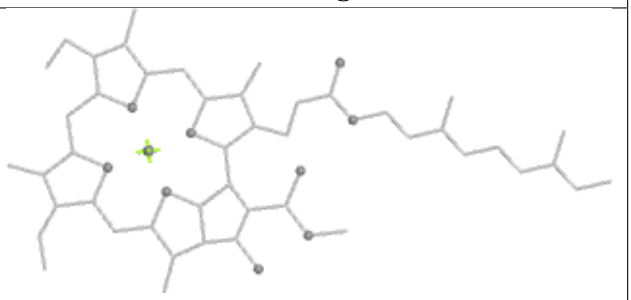
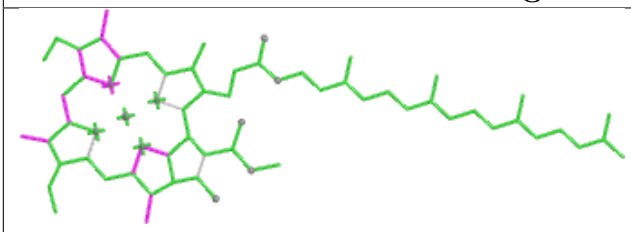
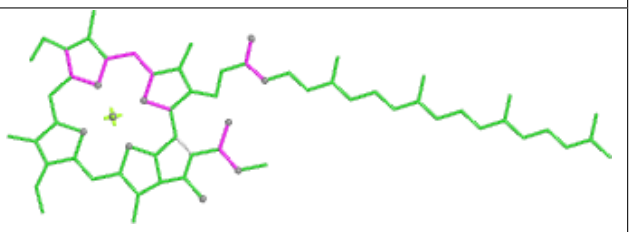
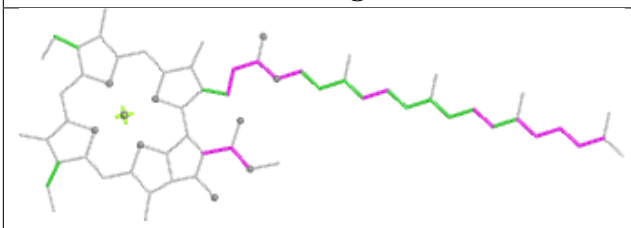
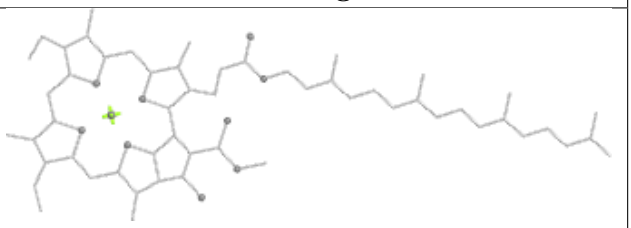


Rings

Ligand CLA A 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

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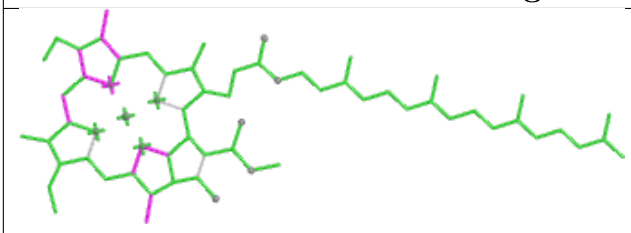
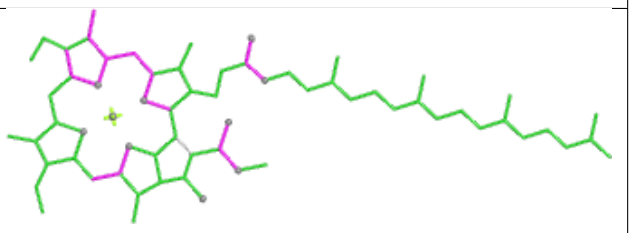
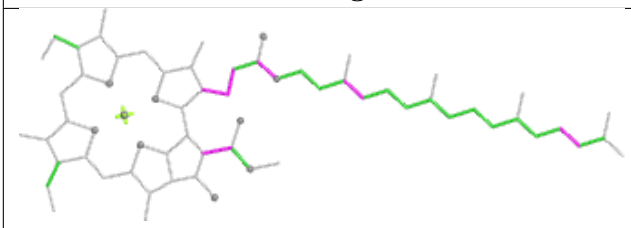
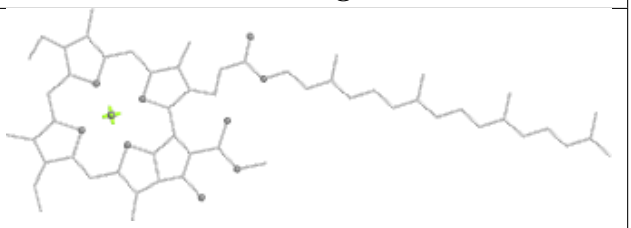
 Bond lengths	 Bond angles
 Torsions	 Rings

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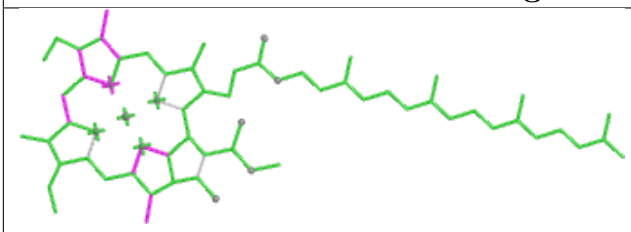
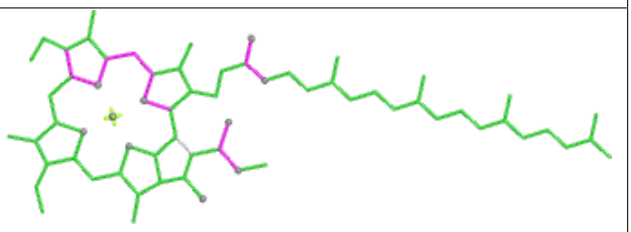
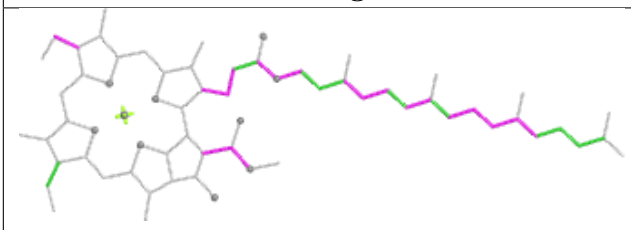
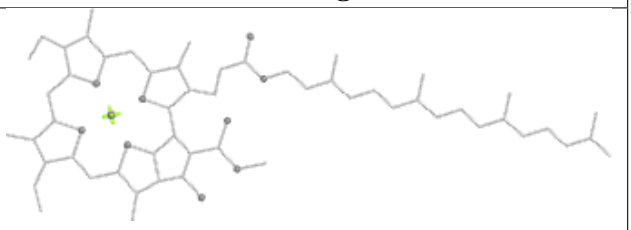
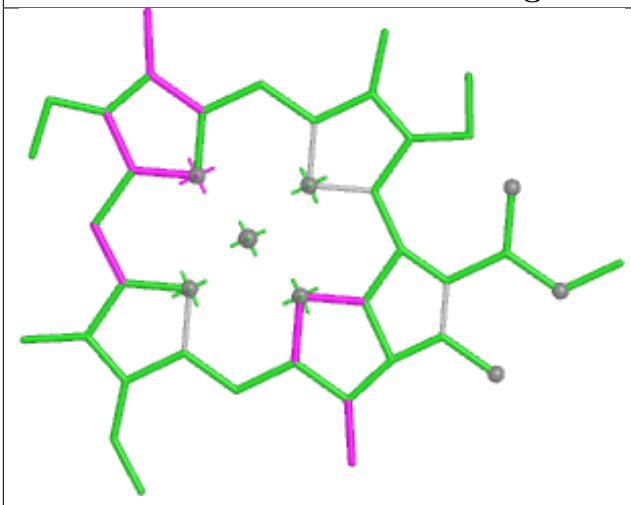
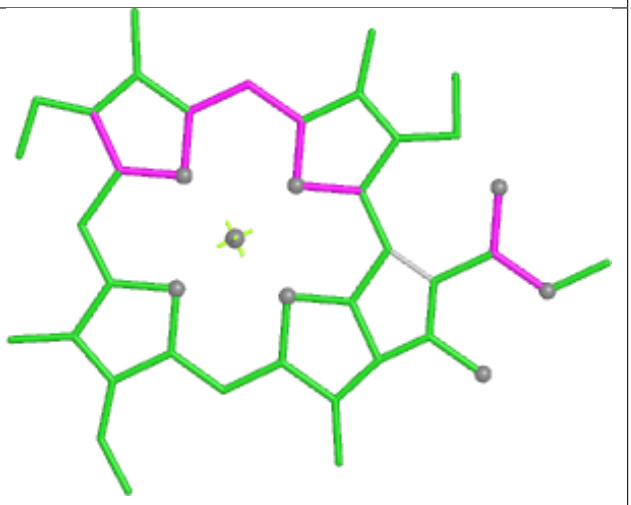
 Bond lengths	 Bond angles
 Torsions	 Rings

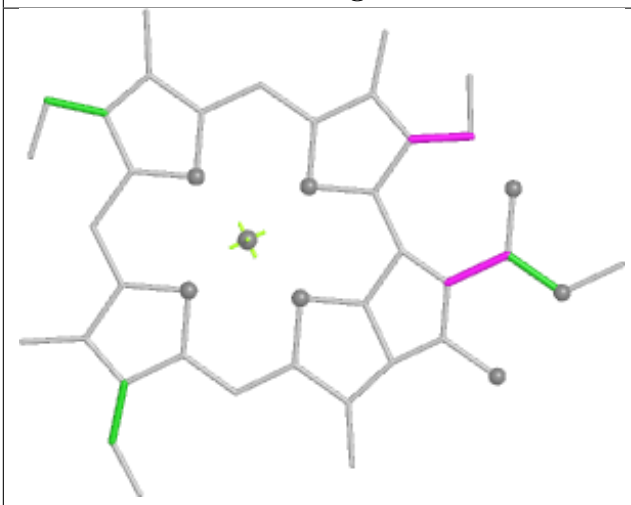
Ligand CLA A 816



Bond lengths



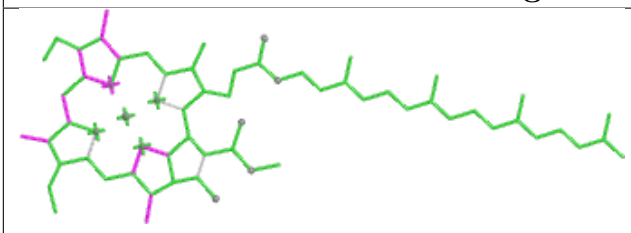
Bond angles



Torsions

Rings

Ligand CLA A 802



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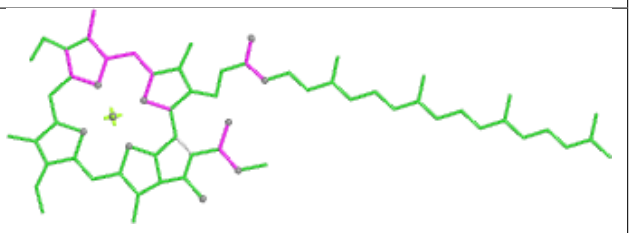
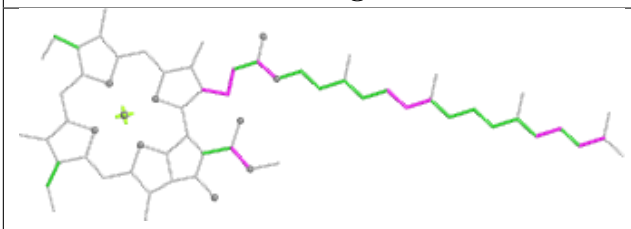


Bond angles



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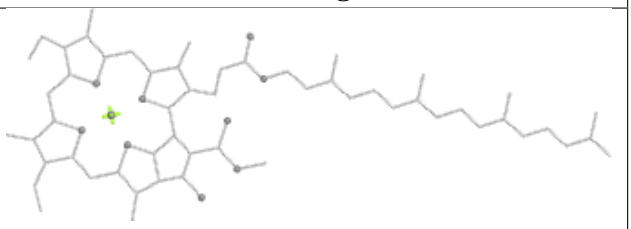
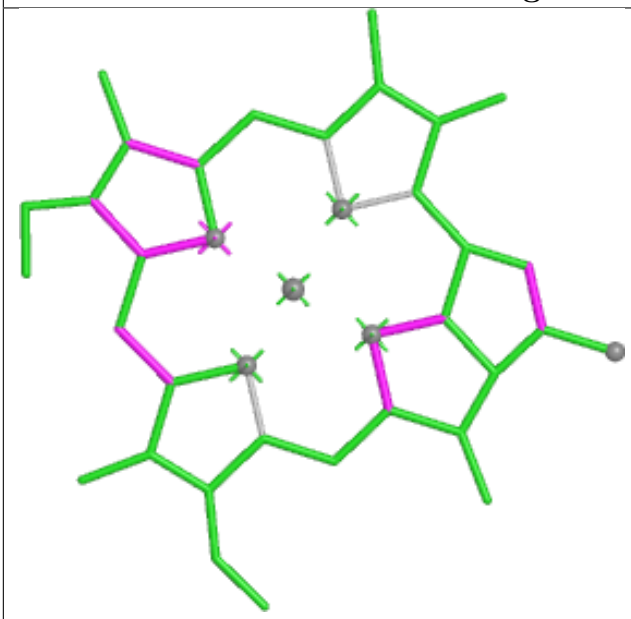


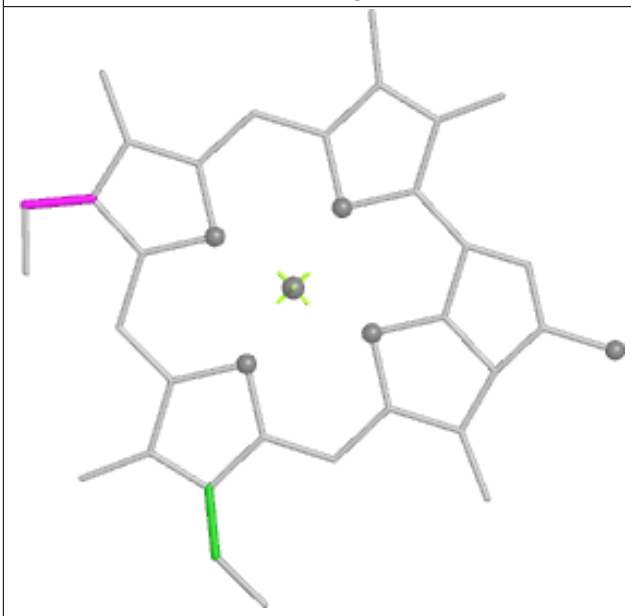
Rings

Ligand CLA K 201

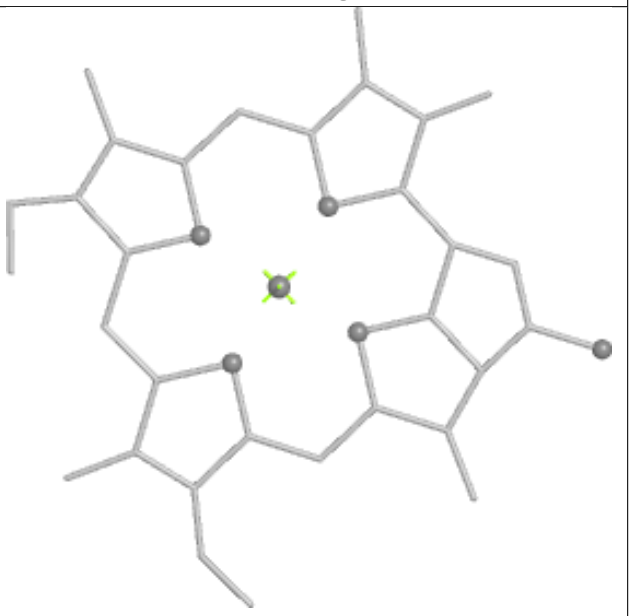


Bond lengths

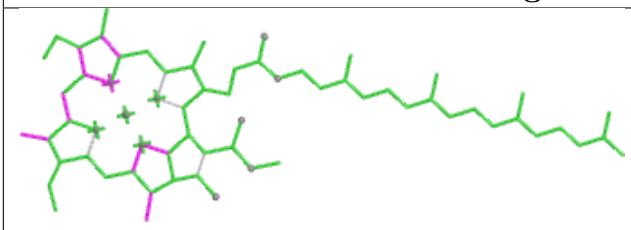
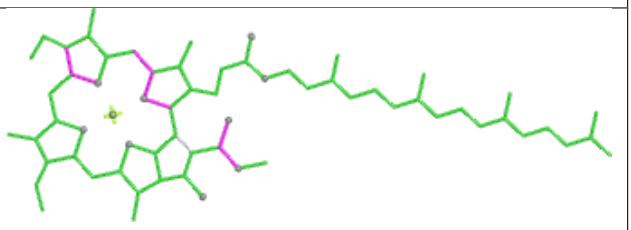
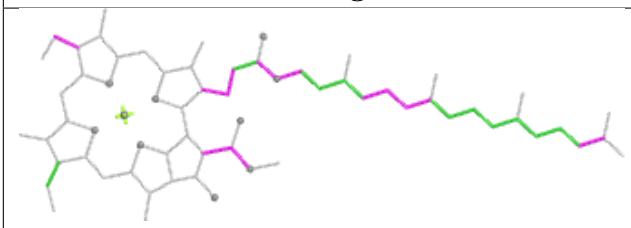
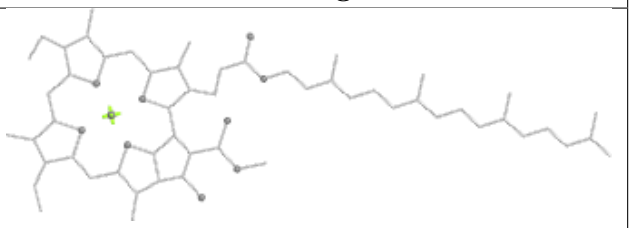
Bond angles

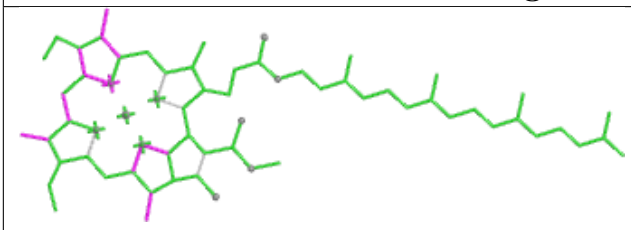
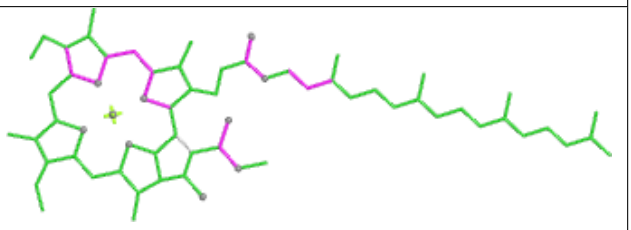
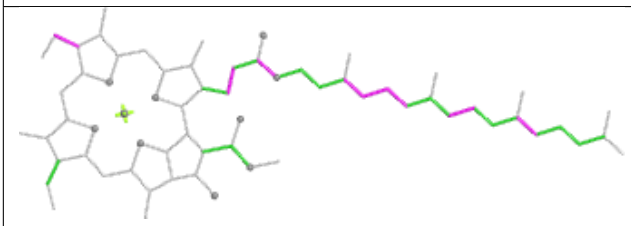
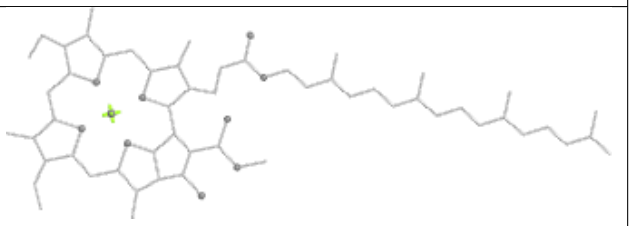


Torsions

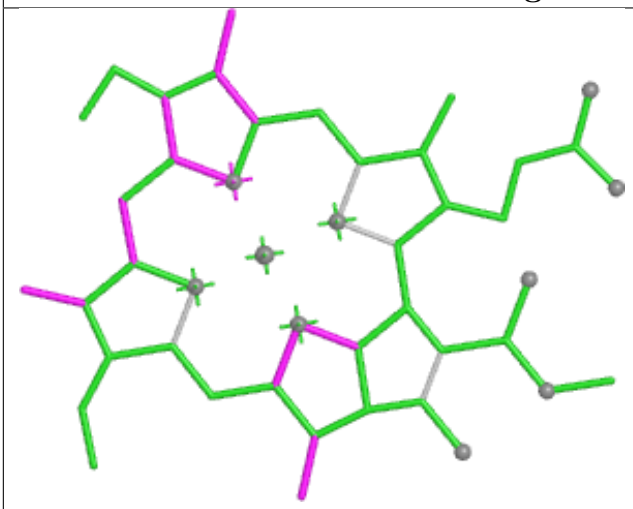


Rings

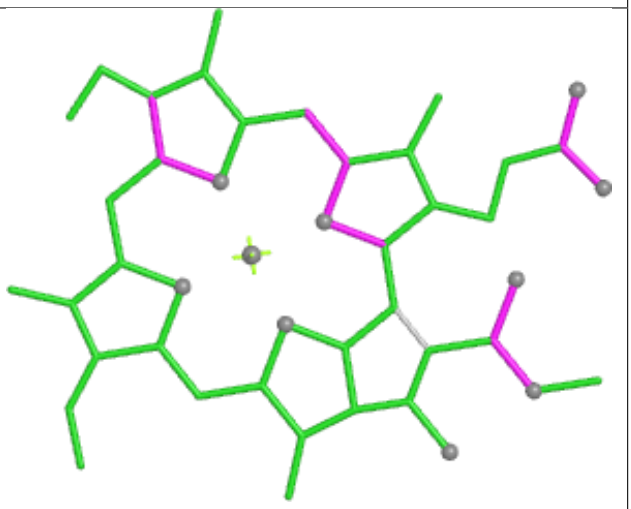
Ligand CLA A 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

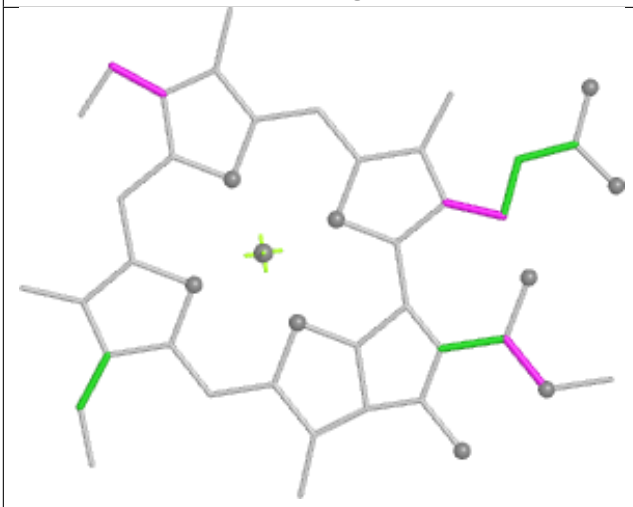
Ligand CLA B 823



Bond lengths



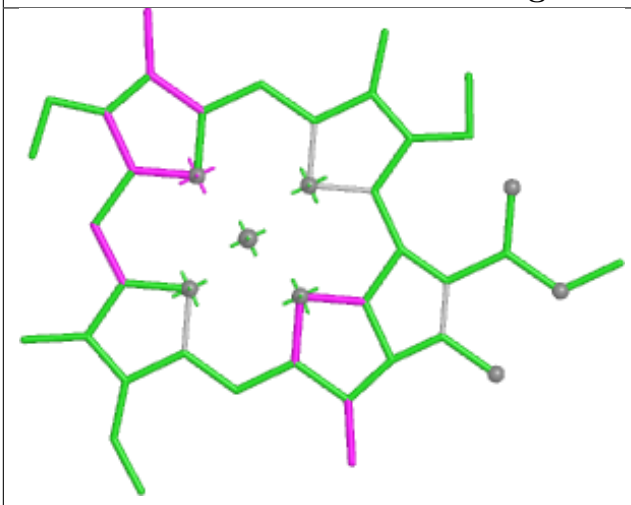
Bond angles



Torsions

Rings

Ligand CLA 4 610



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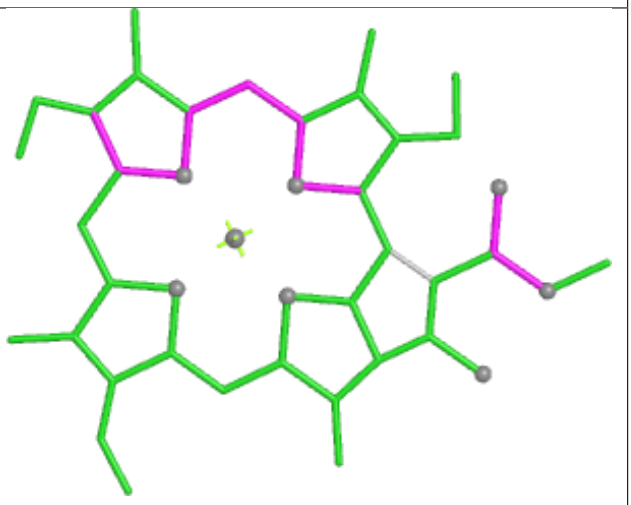
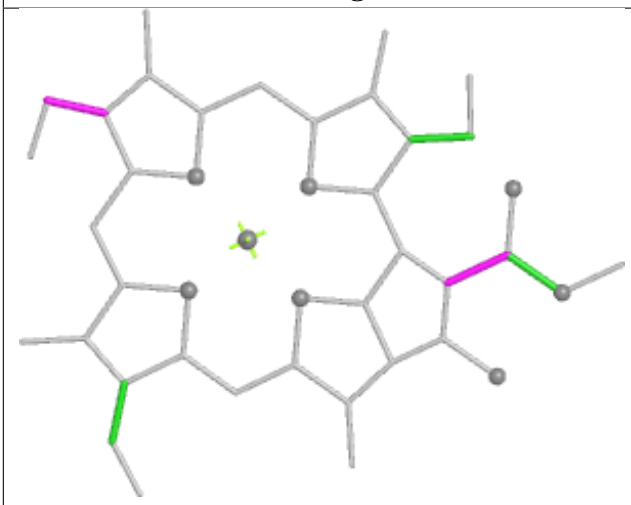


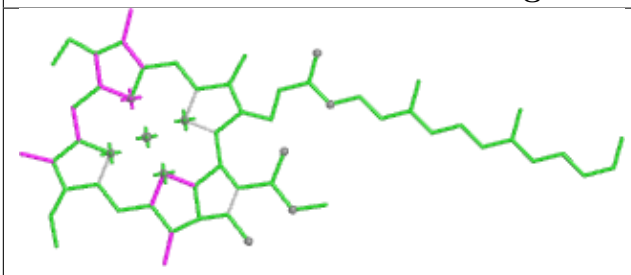
Bond angles



Torsions

Rings

Ligand CLA A 819



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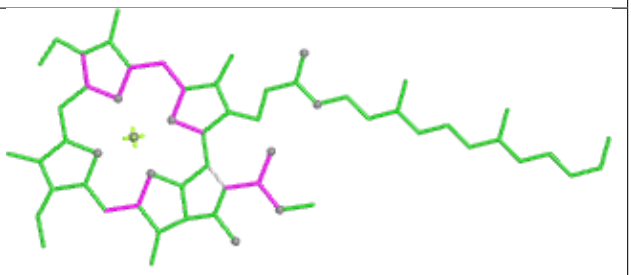
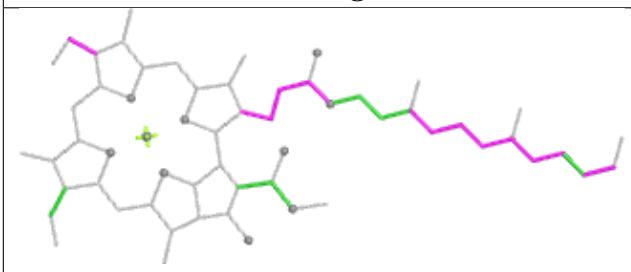
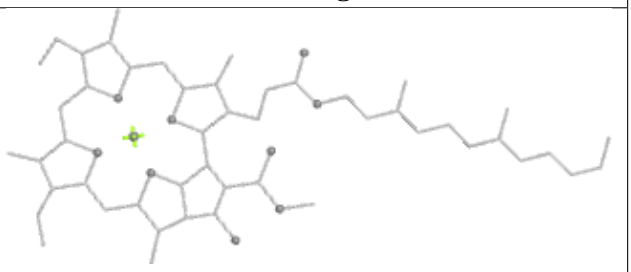


Bond angles

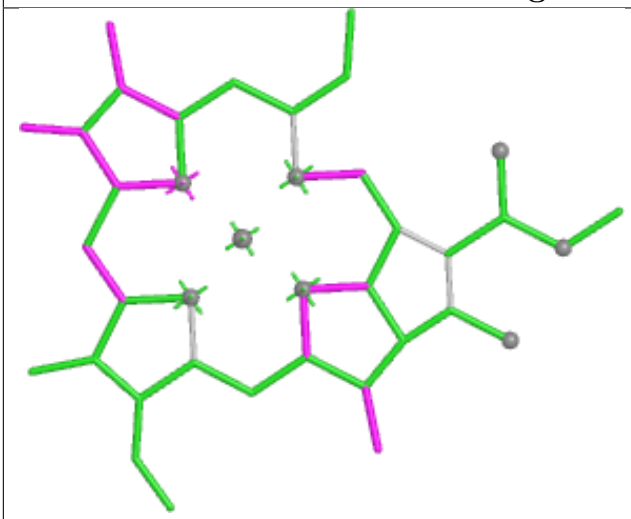


Torsions

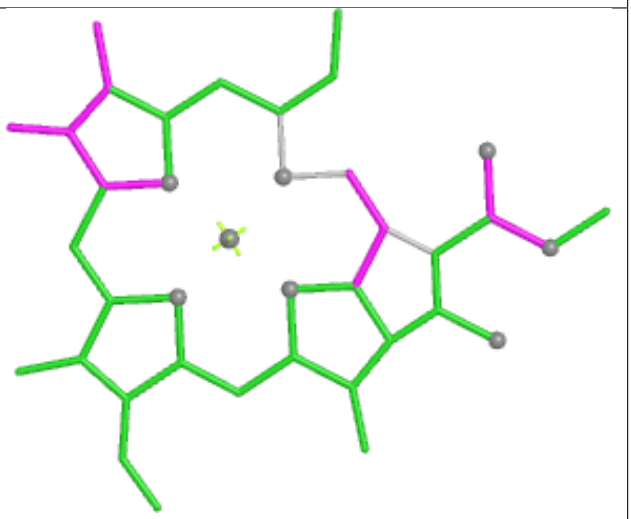


Rings

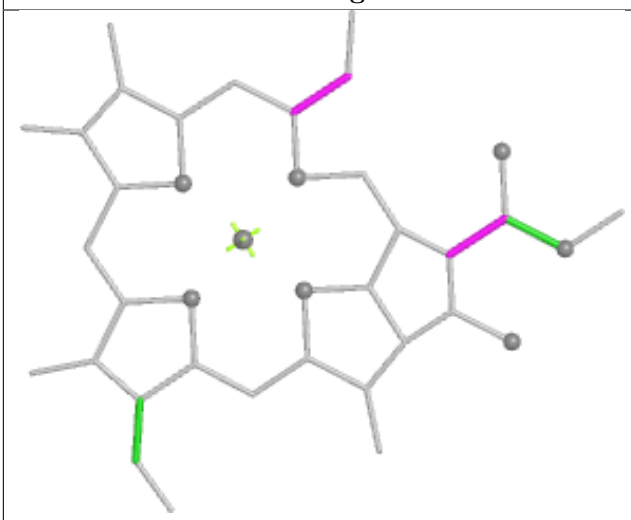
Ligand CLA 2 610



Bond lengths



Bond angles



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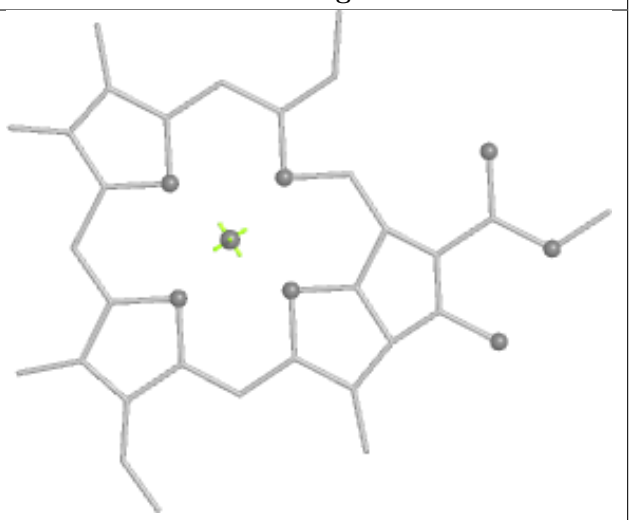
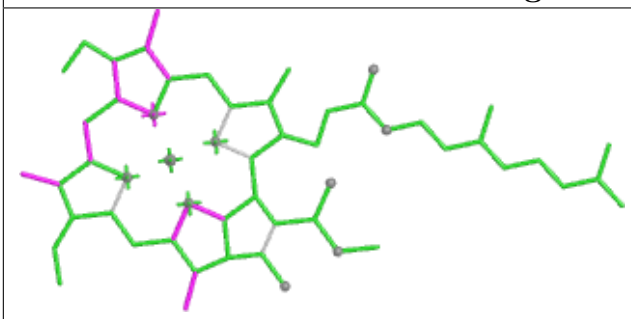
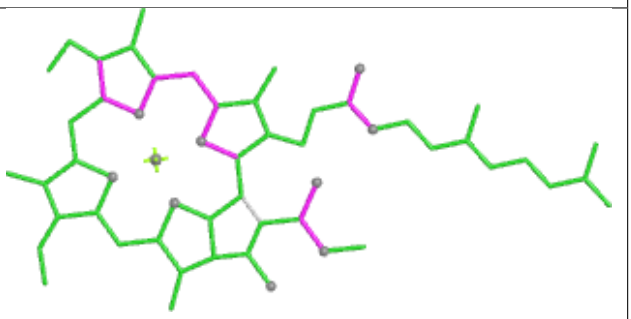
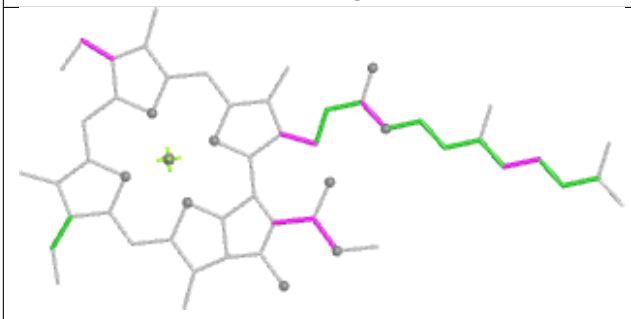
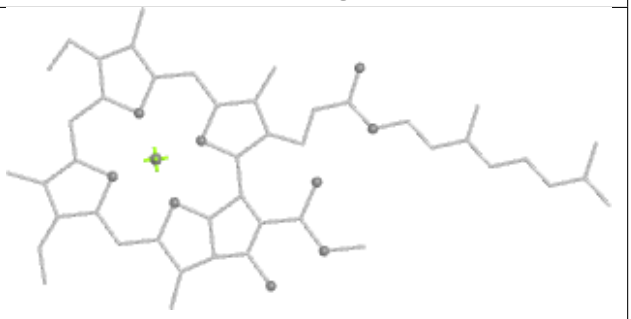
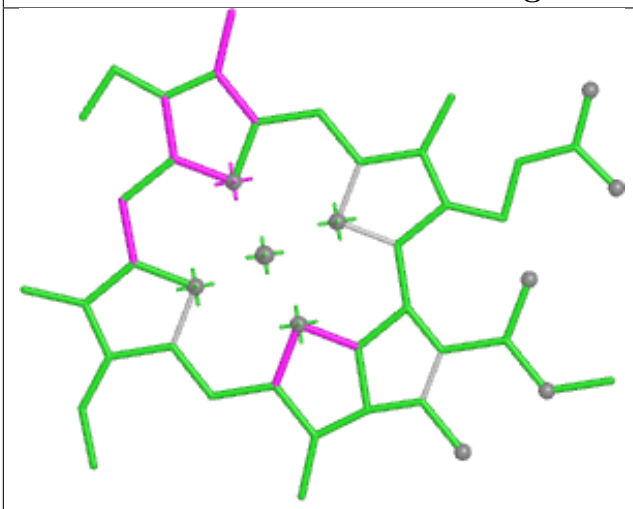


Rings

Ligand CLA B 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 836



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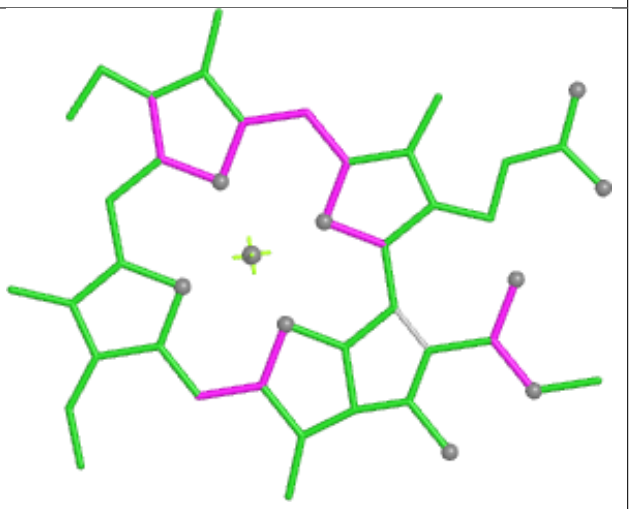
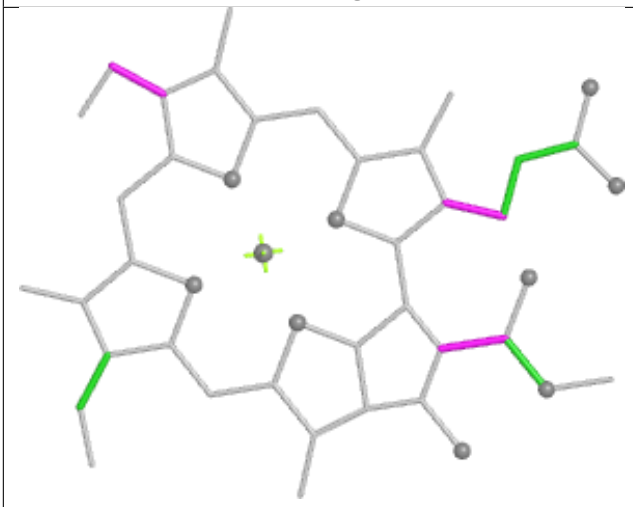
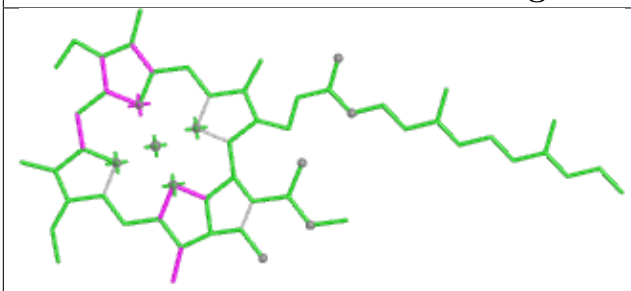
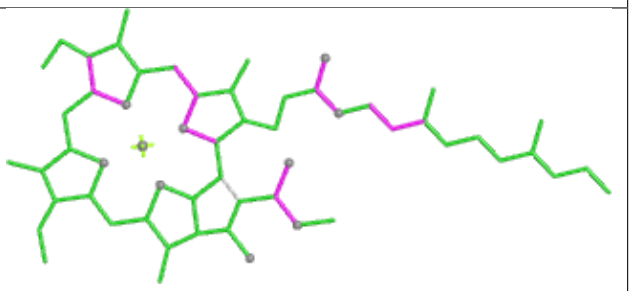
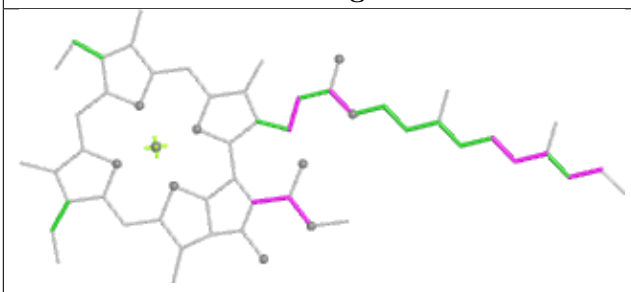
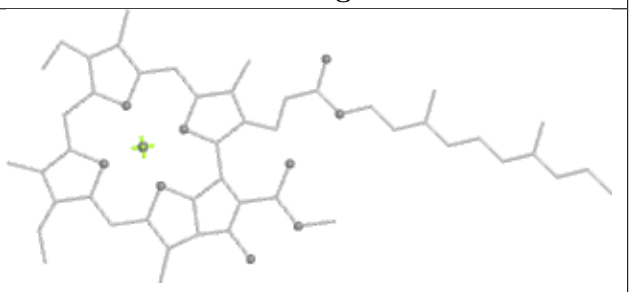


Bond angles



Torsions

Rings

Ligand CLA 4 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

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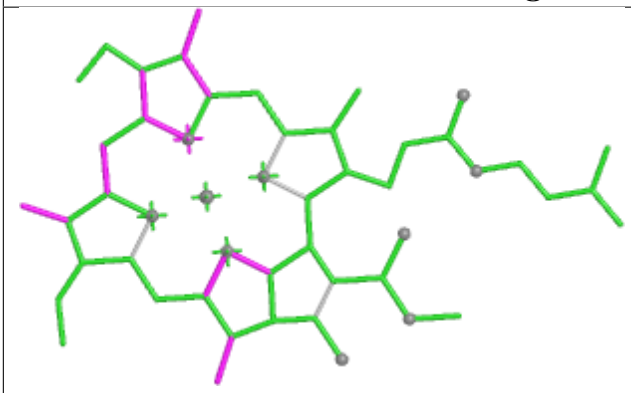
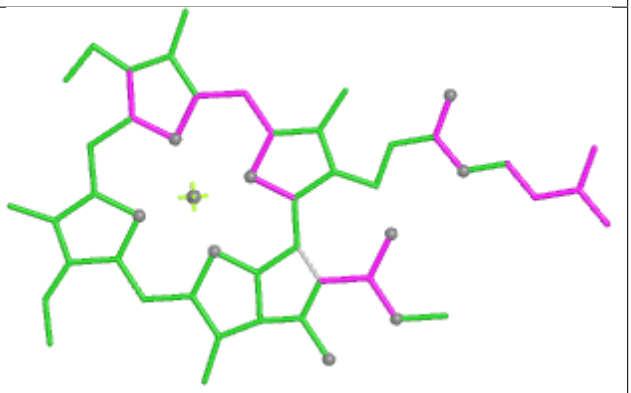
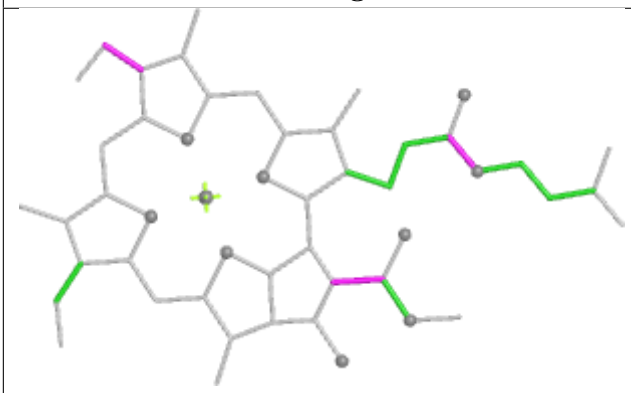
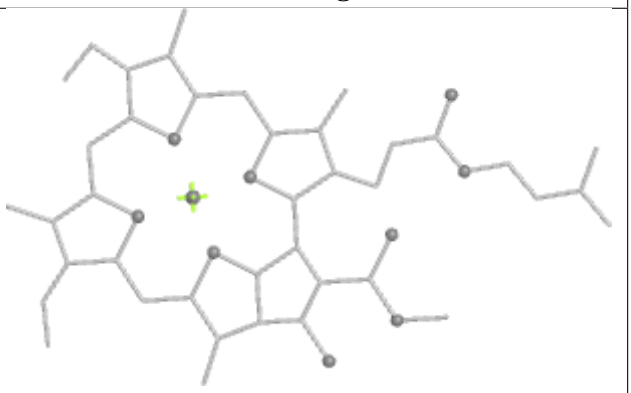
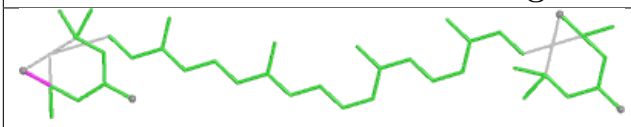
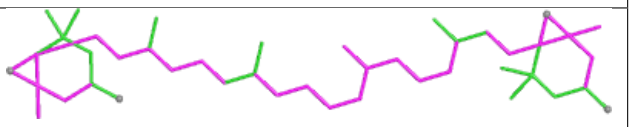
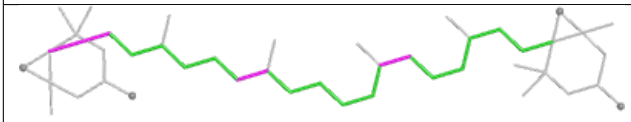
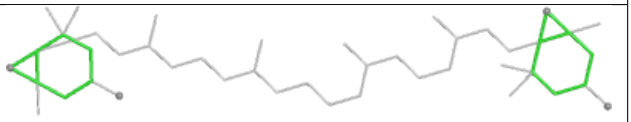
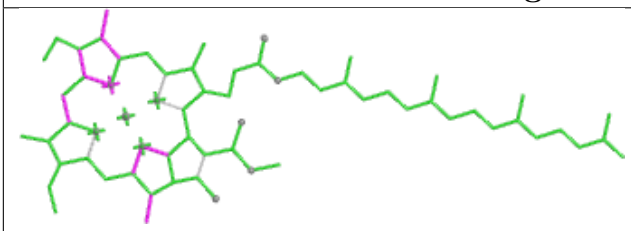
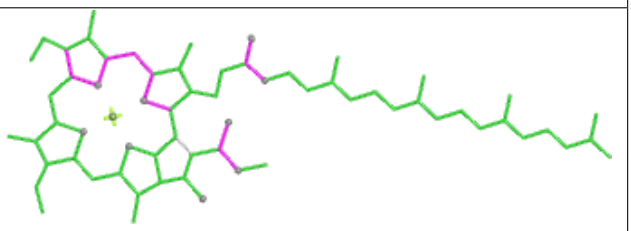
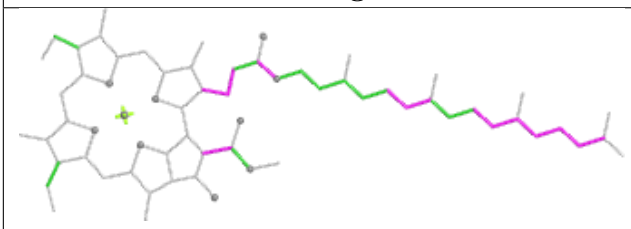
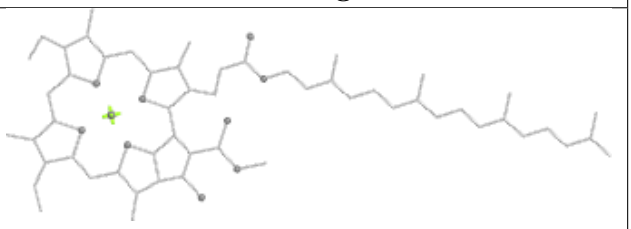
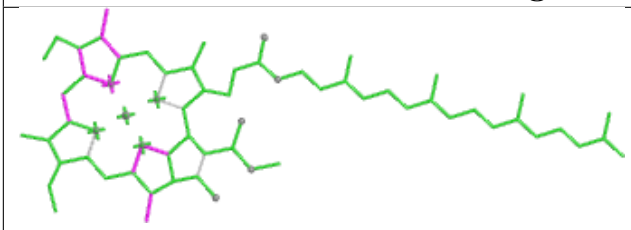
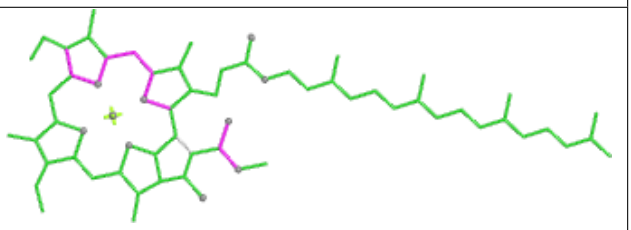
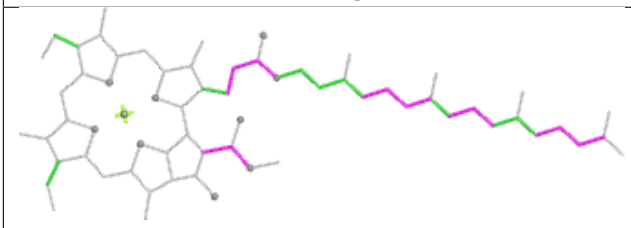
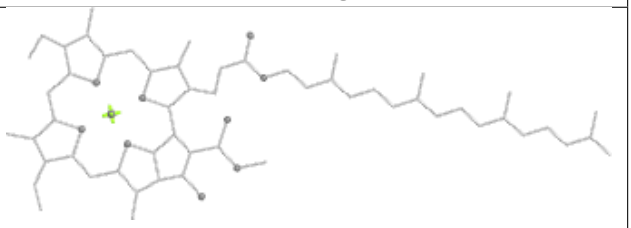
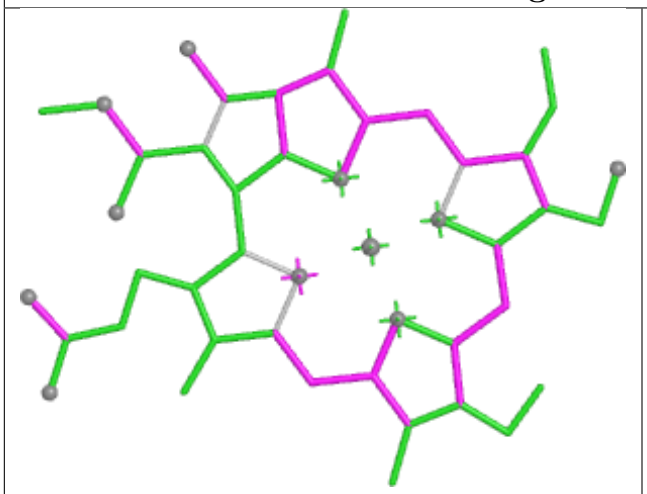
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT 1 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

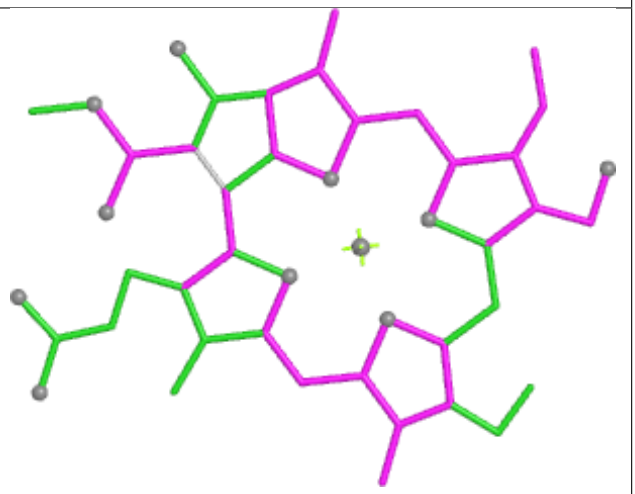
Ligand CLA B 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

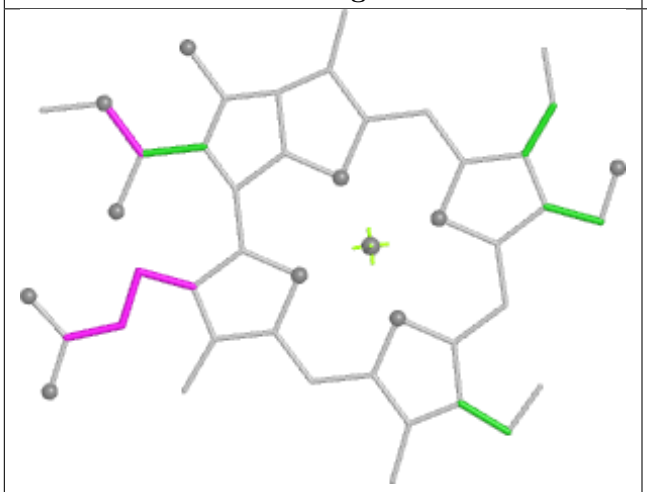
Ligand CHL 4 607



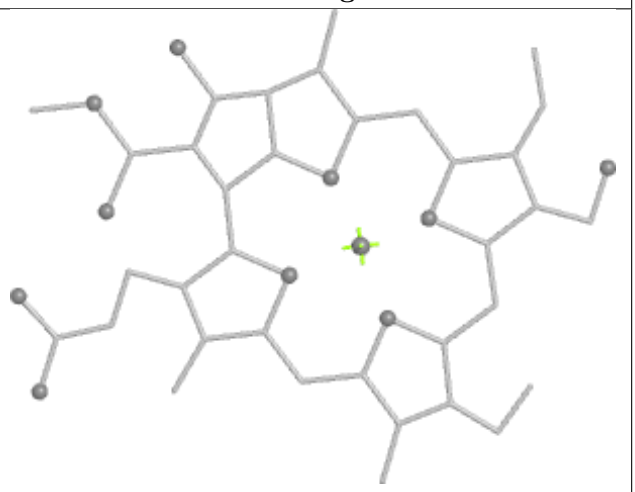
Bond lengths



Bond angles

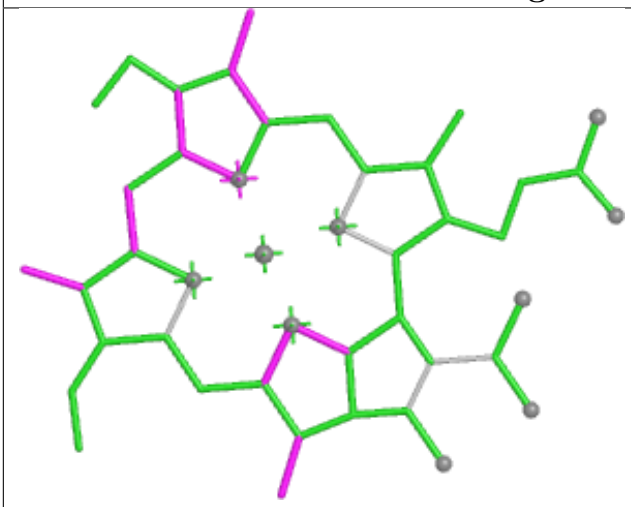


Torsions



Rings

Ligand CLA 1 607



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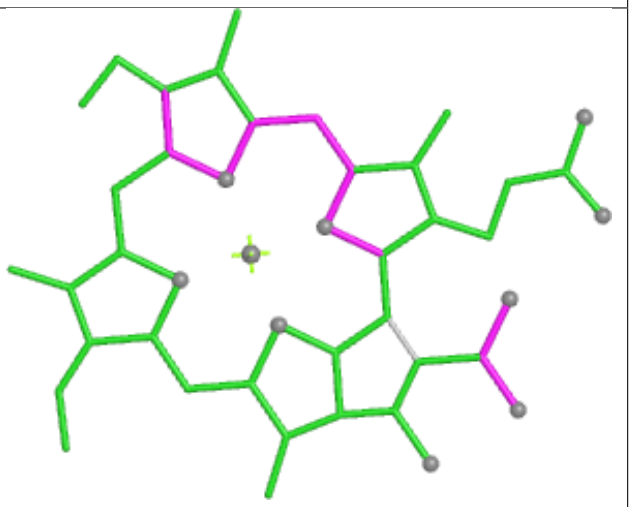
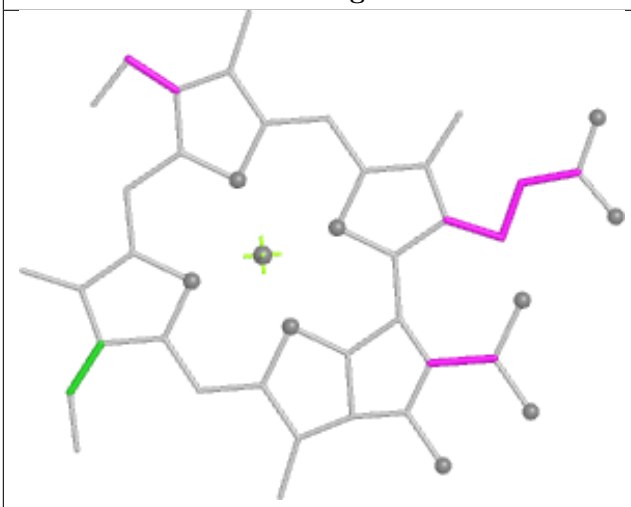
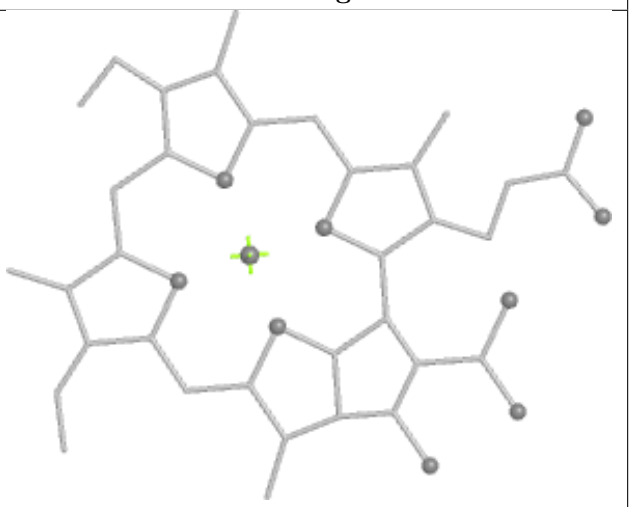


Bond angles

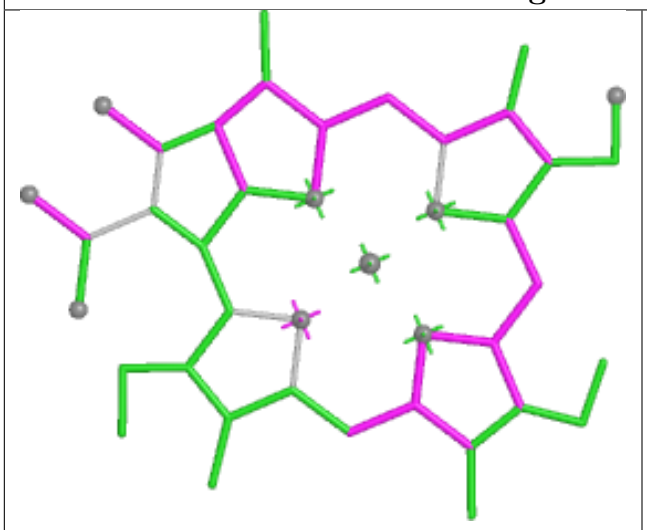


Torsions

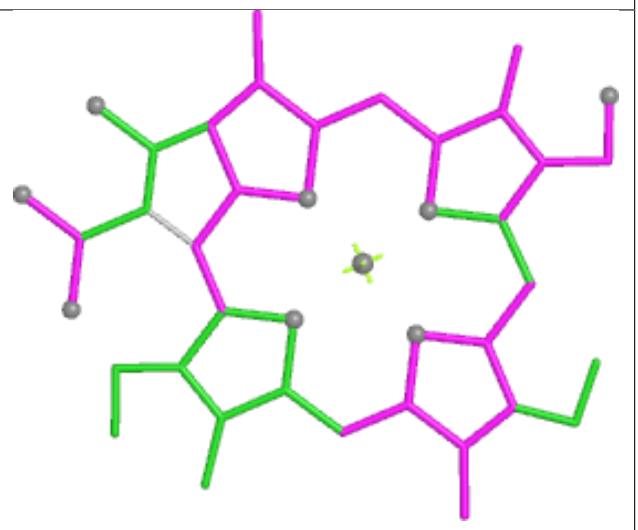


Rings

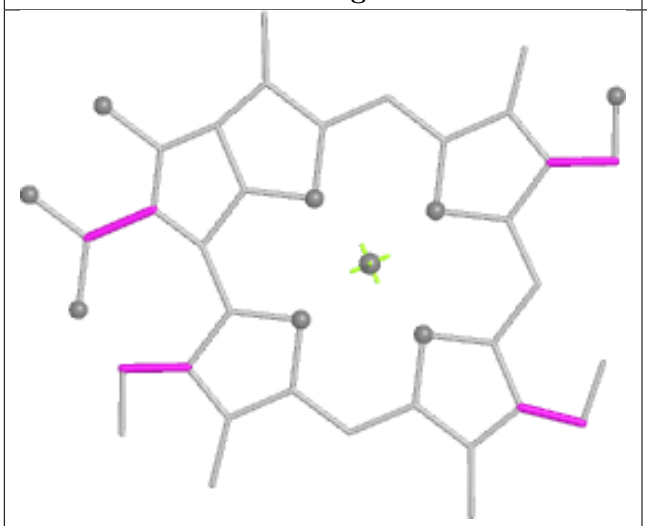
Ligand CHL 4 605



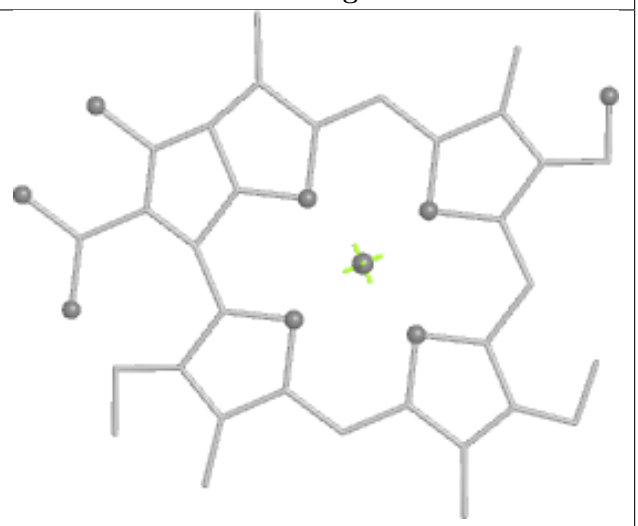
Bond lengths



Bond angles

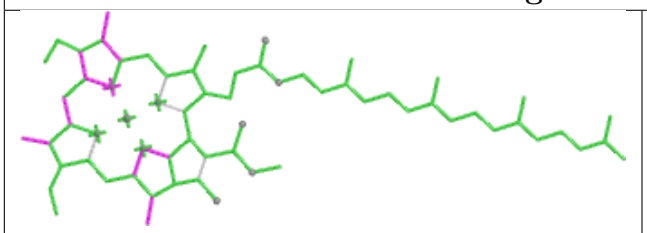


Torsions

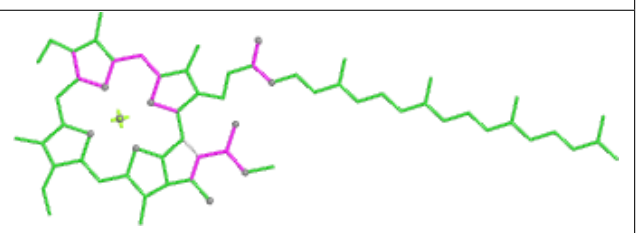


Rings

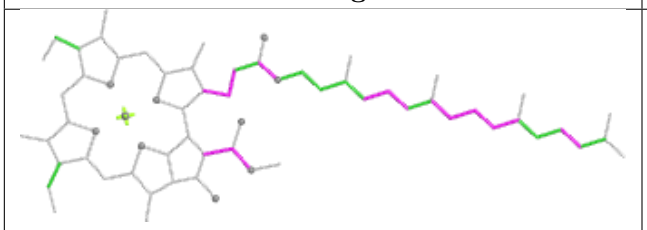
Ligand CLA B 802



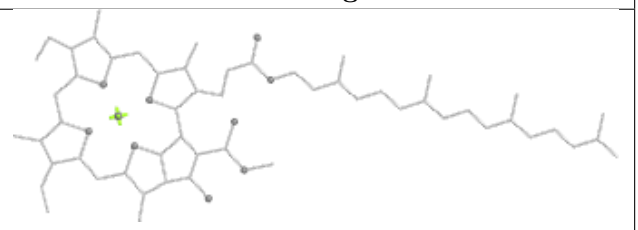
Bond lengths



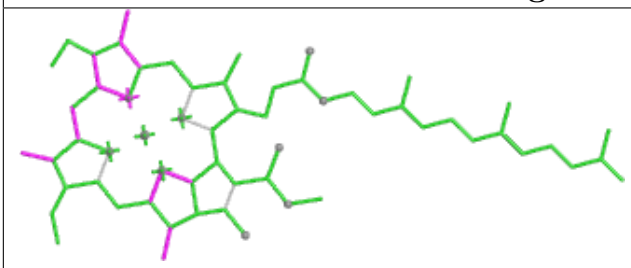
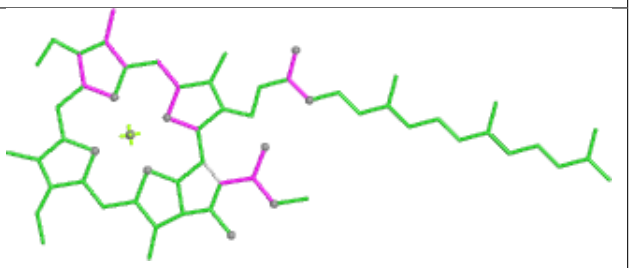
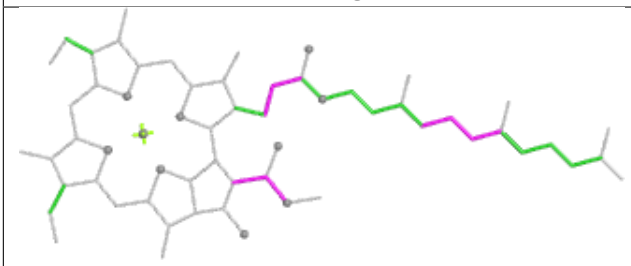
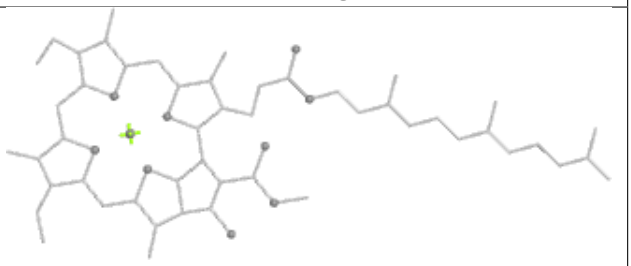
Bond angles

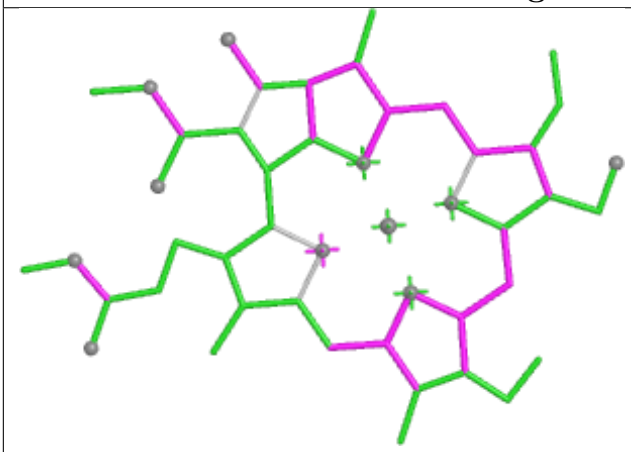
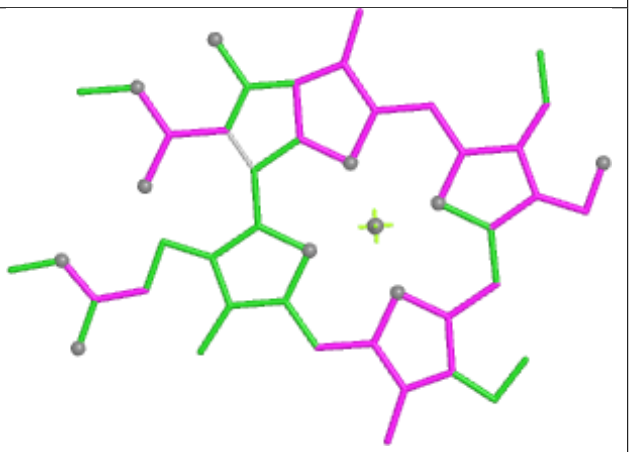
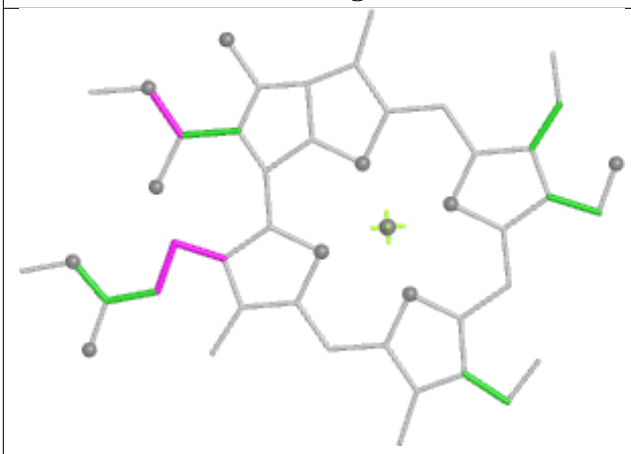


Torsions

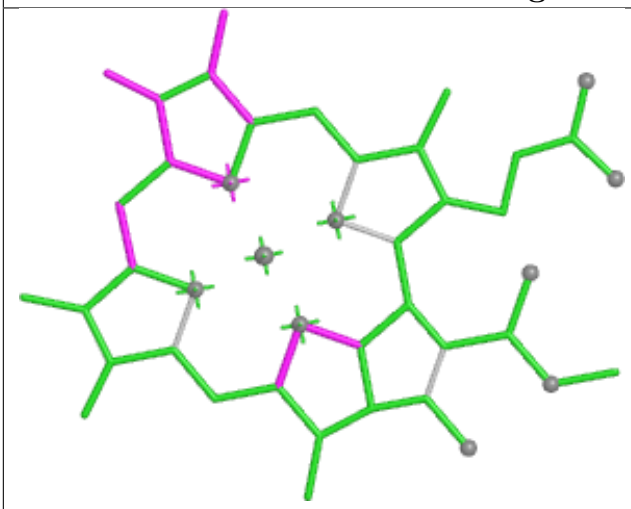


Rings

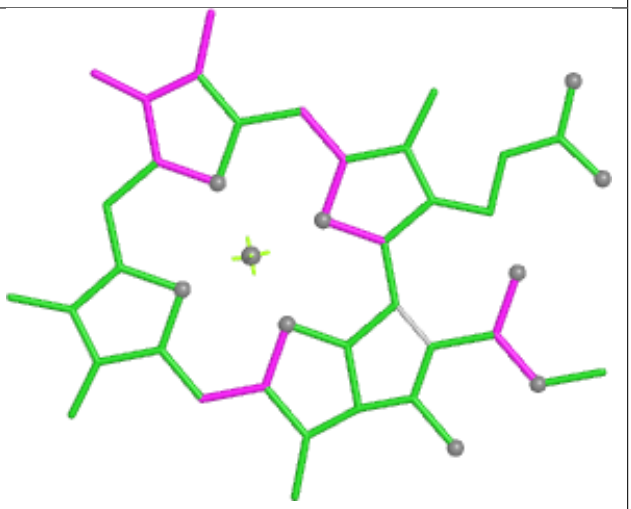
Ligand CLA 4 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 2 601	
 Bond lengths	 Bond angles
 Torsions	Rings

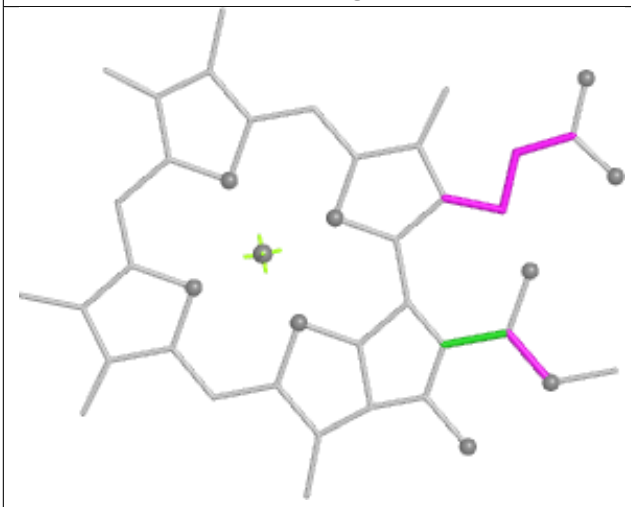
Ligand CLA 4 604



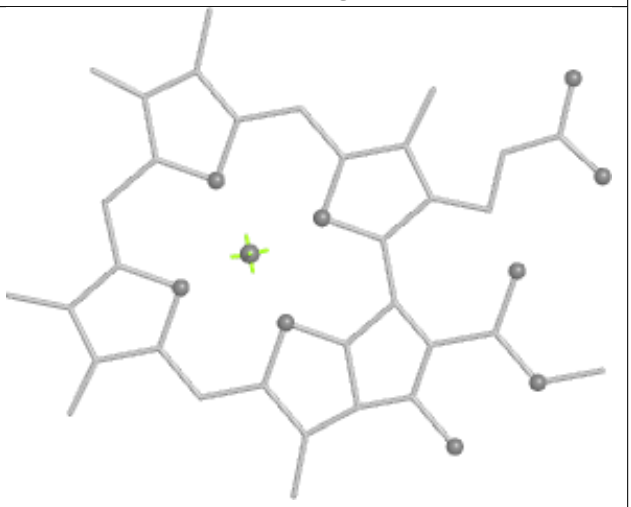
Bond lengths



Bond angles

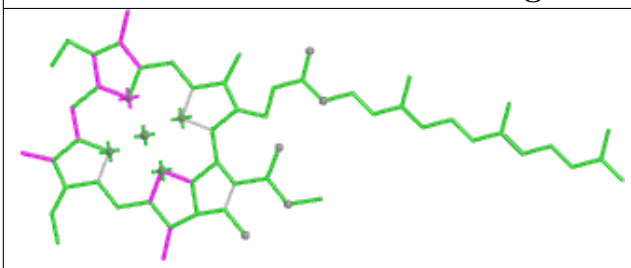


Torsions



Rings

Ligand CLA B 818



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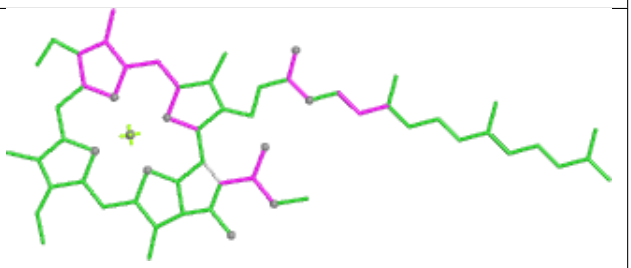
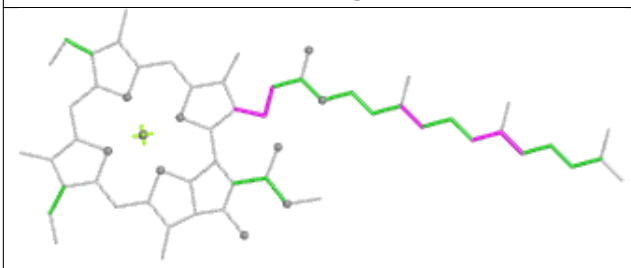


Bond angles



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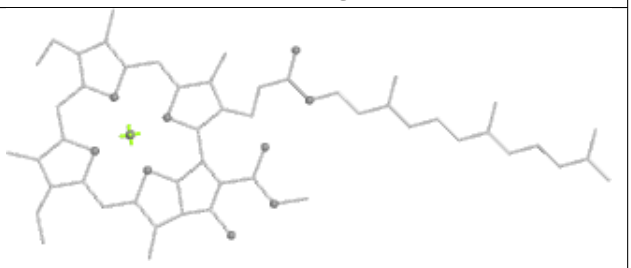
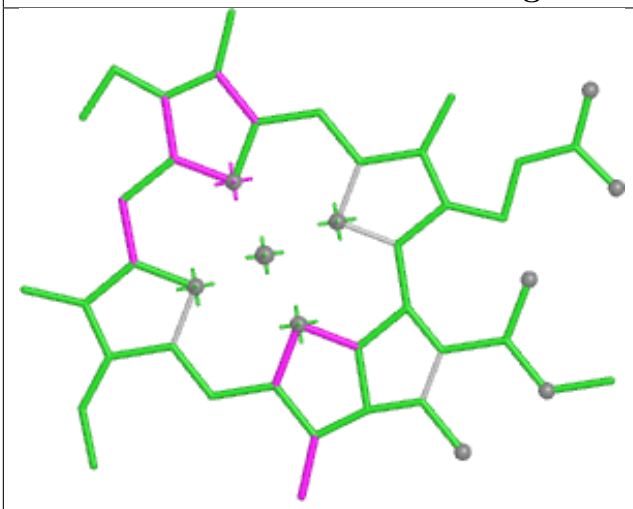


Rings

Ligand CLA G 203



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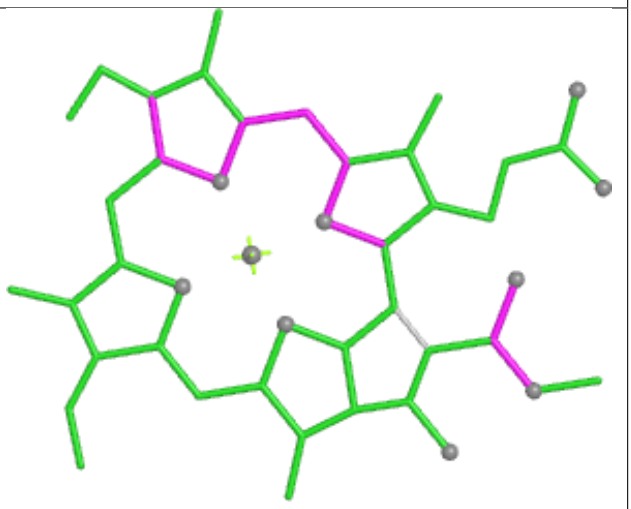
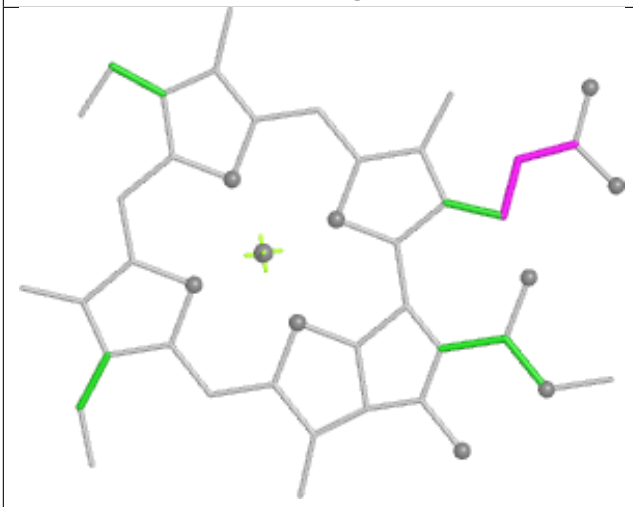


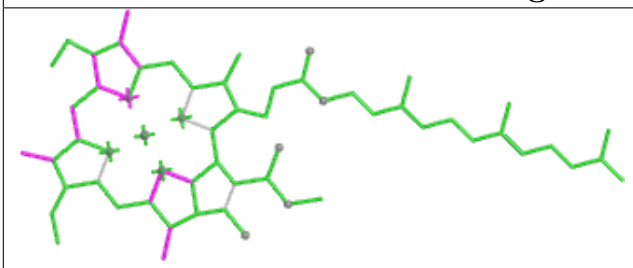
Bond angles



Torsions

Rings

Ligand CLA 3 601



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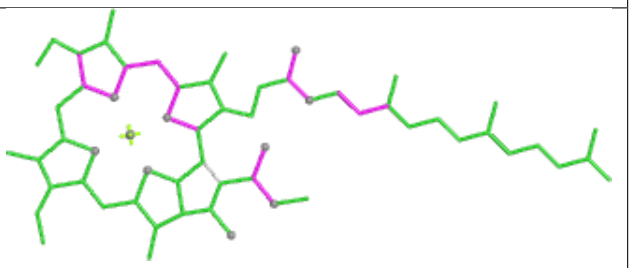
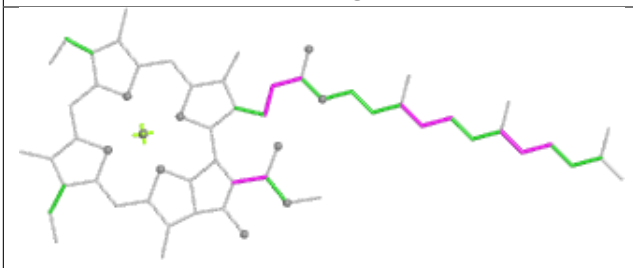


Bond angles



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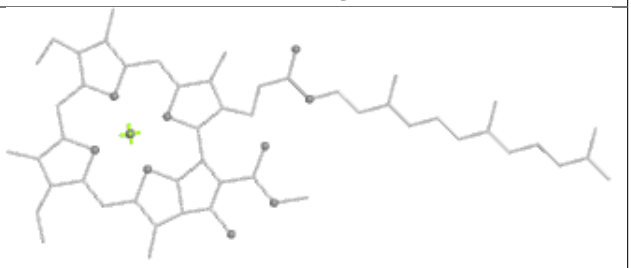
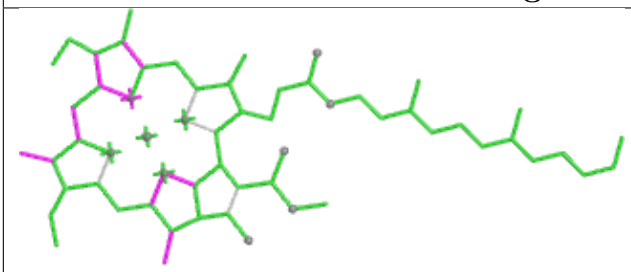
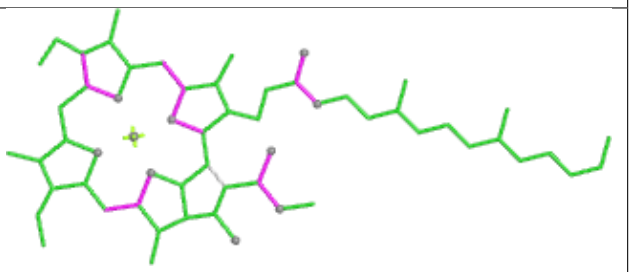
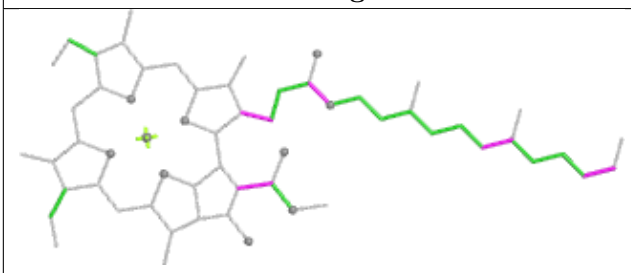
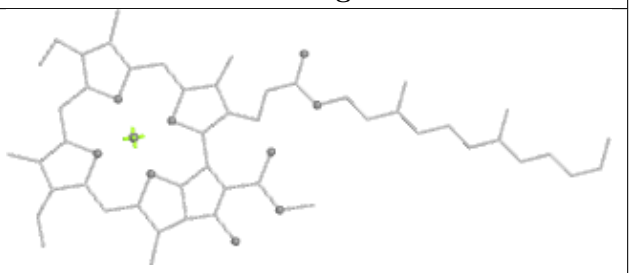
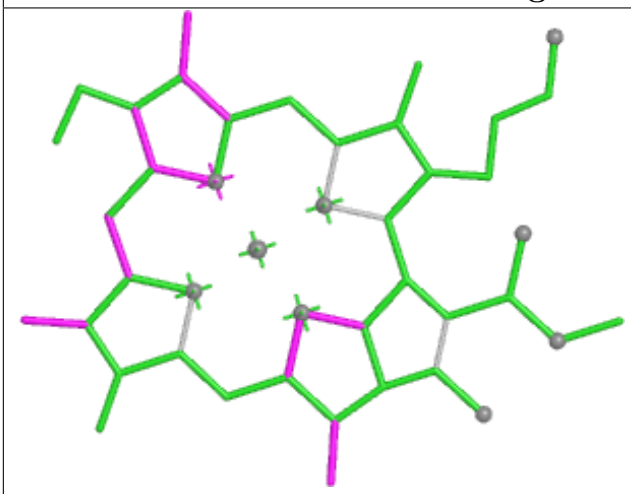
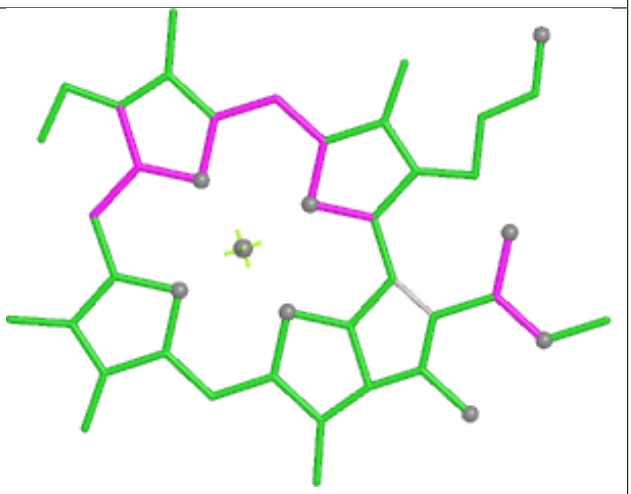
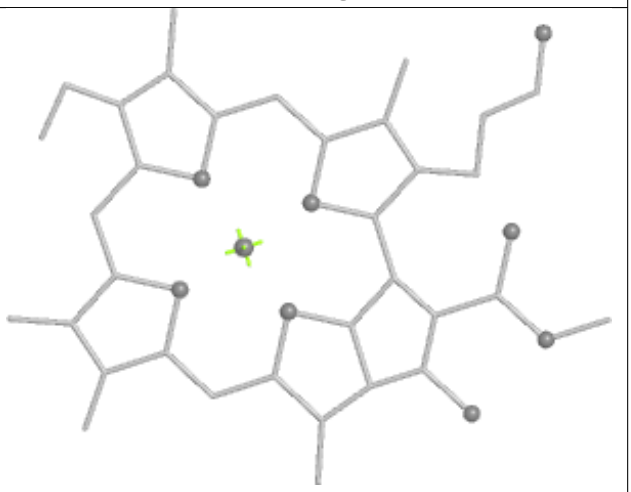
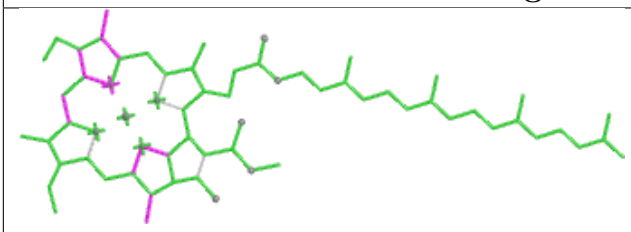


Rings

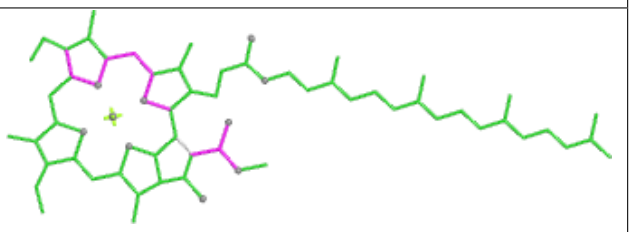
Ligand CLA A 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 604	
 Bond lengths	 Bond angles
Torsions	 Rings

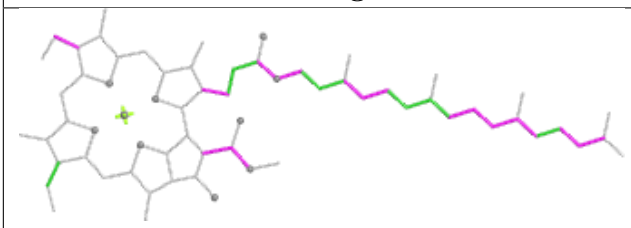
Ligand CLA B 827



Bond lengths



Bond angles



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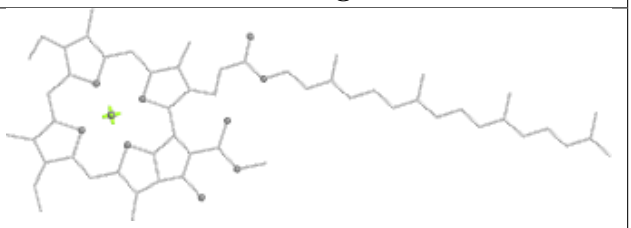
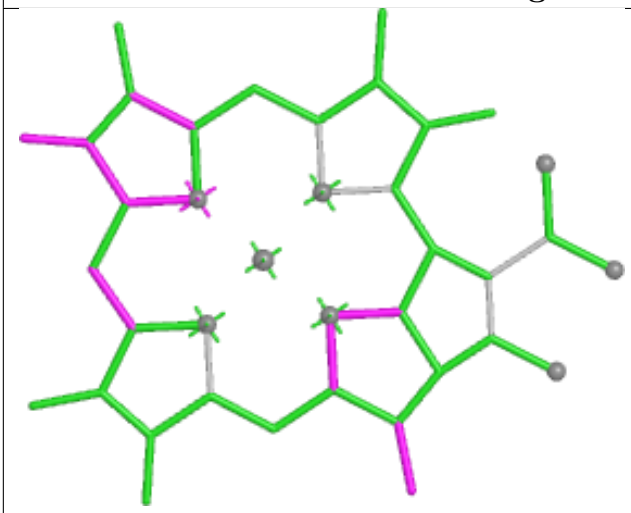


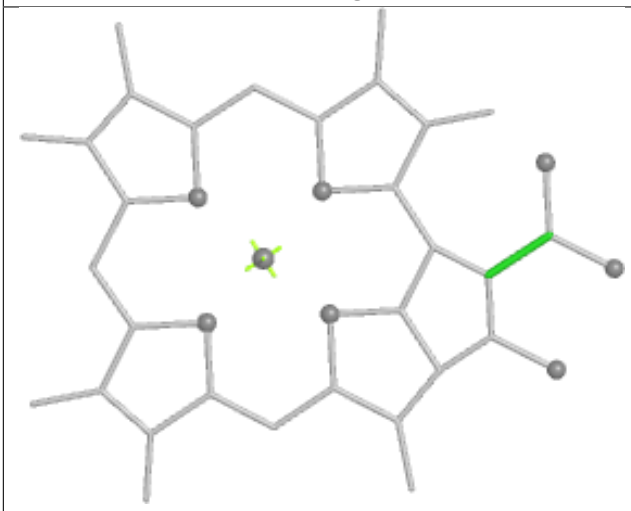
Rings

Ligand CLA 1 610



Bond lengths

Bond angles



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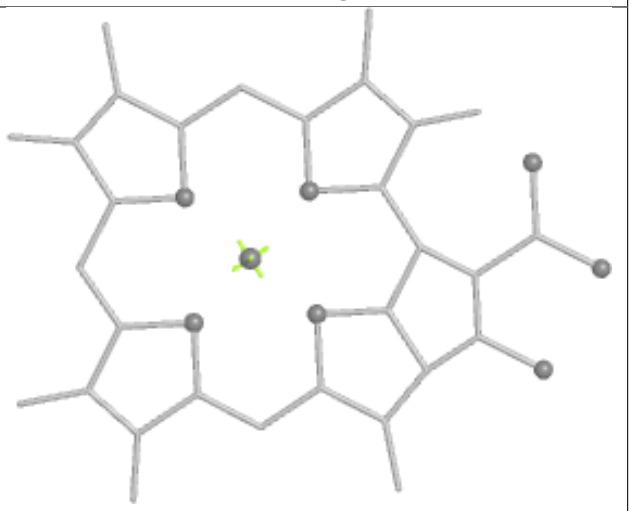
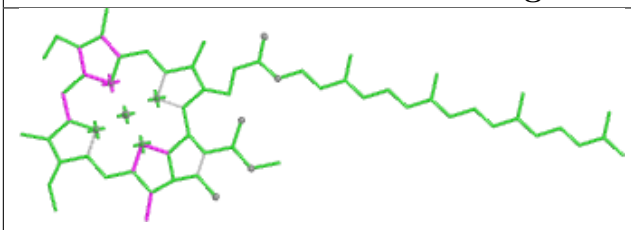
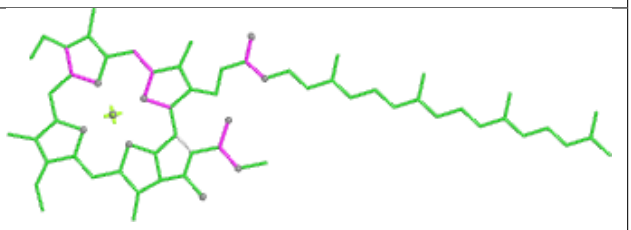
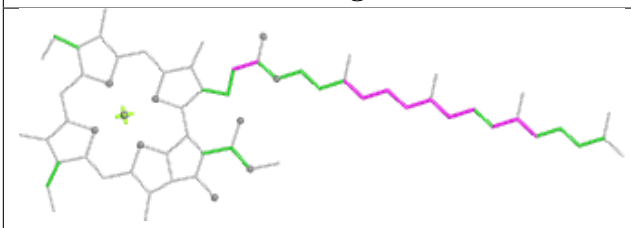
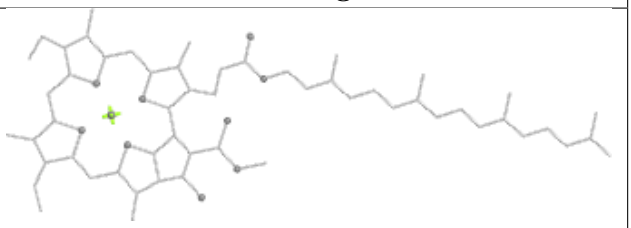
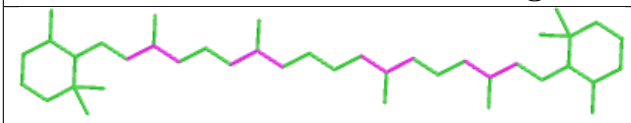
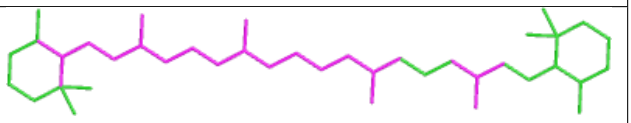
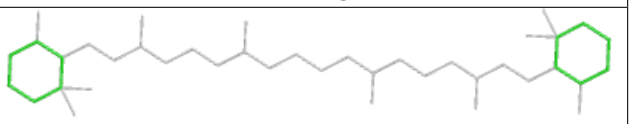
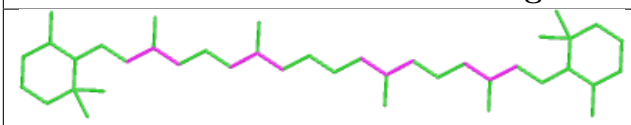
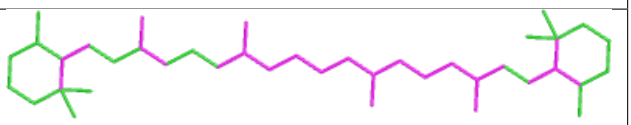
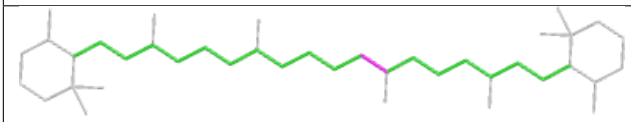
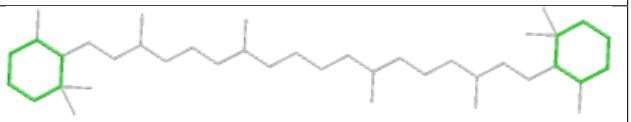
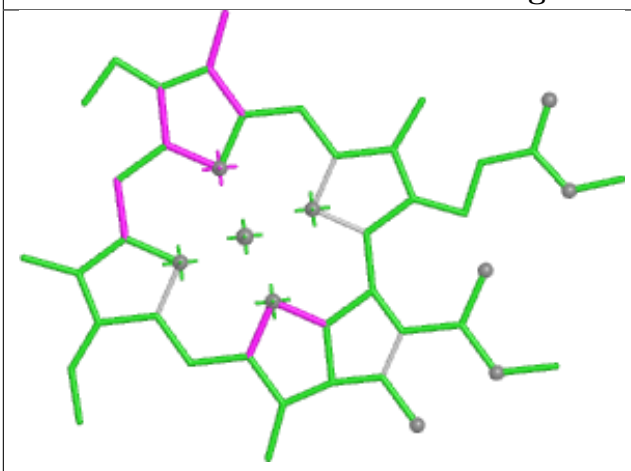
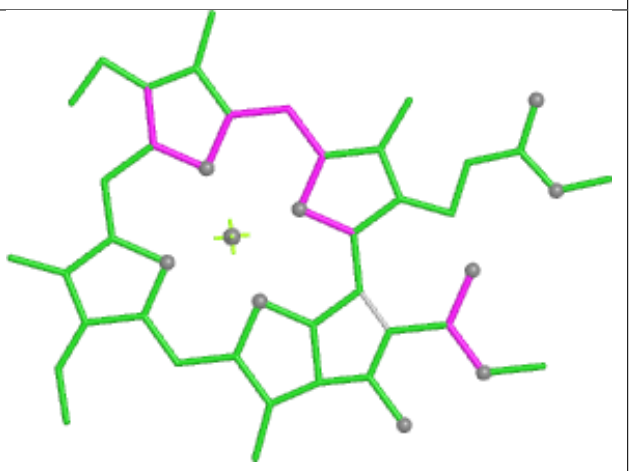
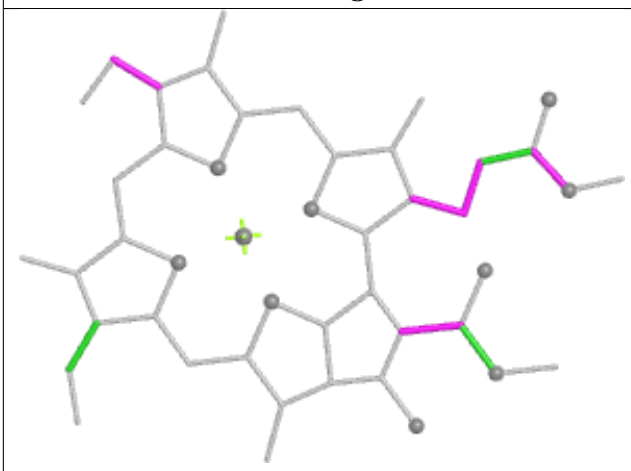
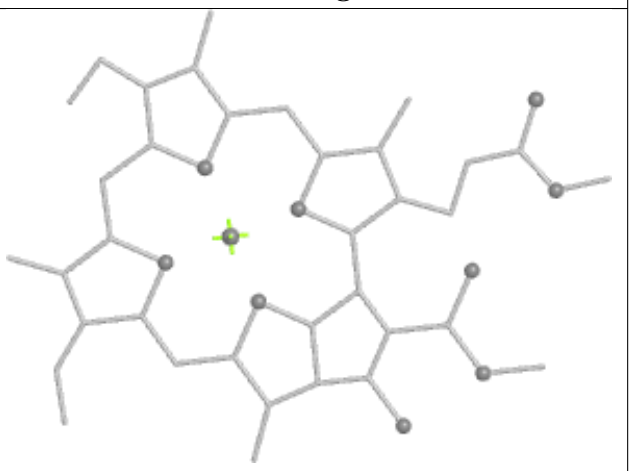


Rings

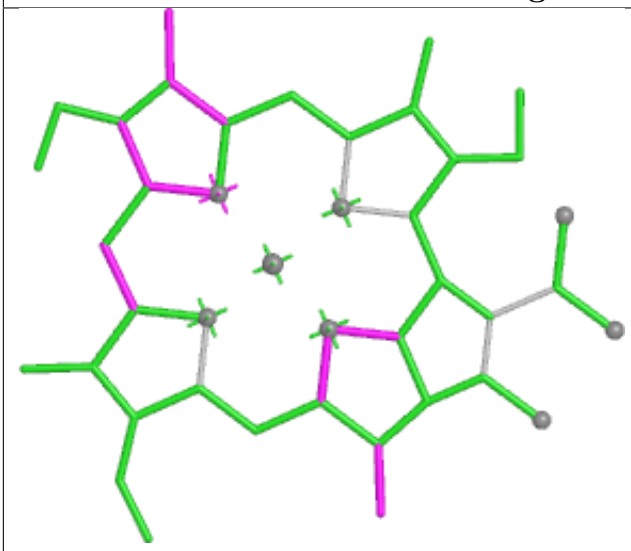
Ligand CLA B 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR J 102	
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand BCR L 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 604



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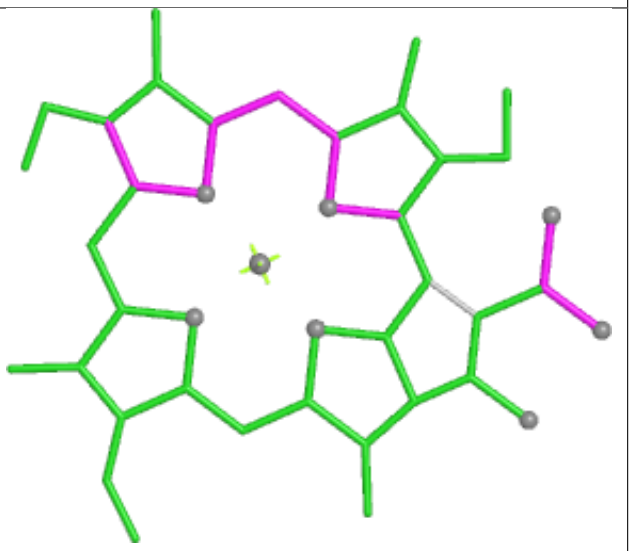

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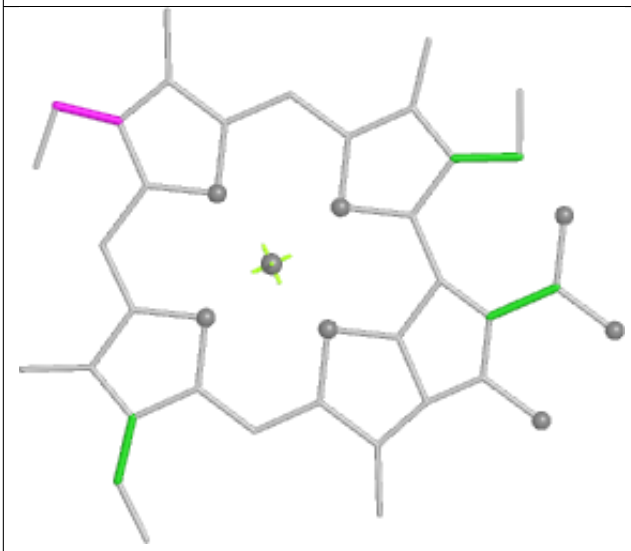

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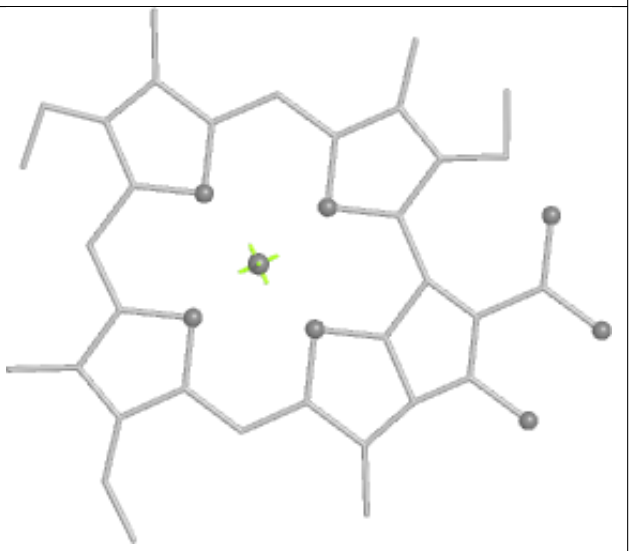
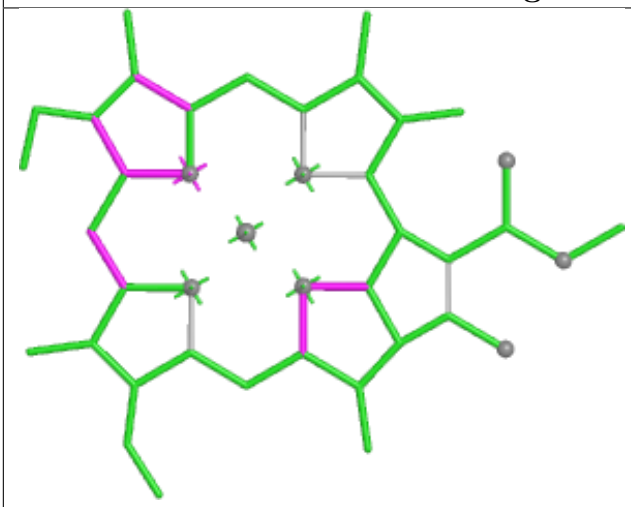


Rings

Ligand CLA A 824



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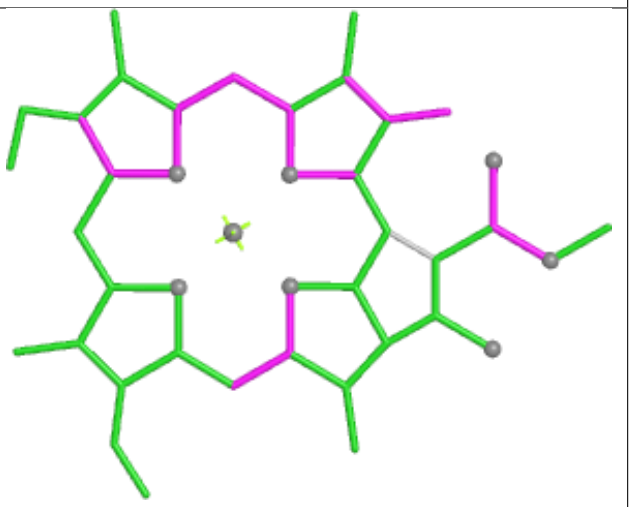

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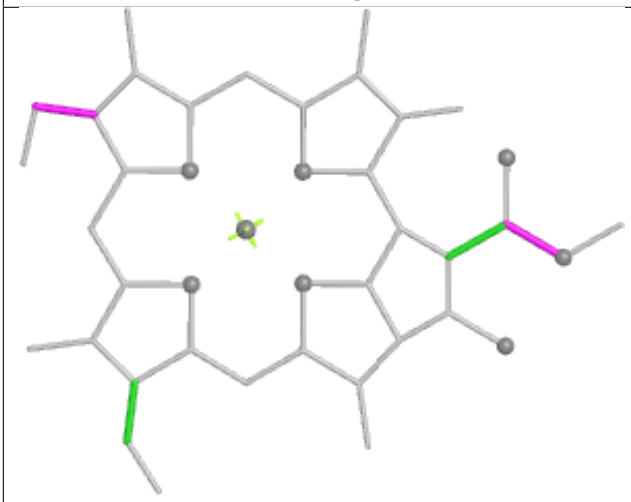

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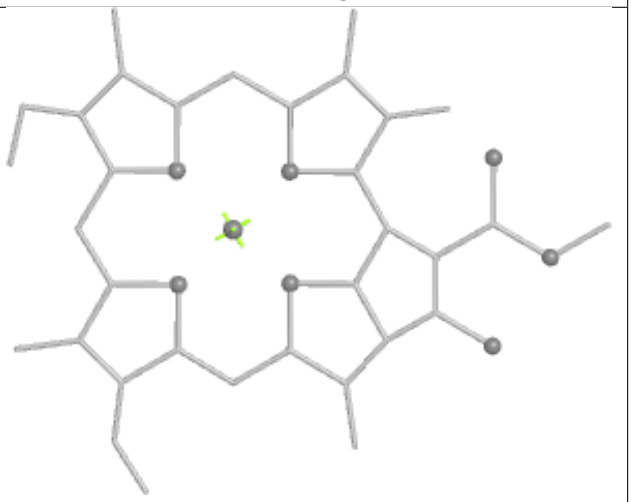
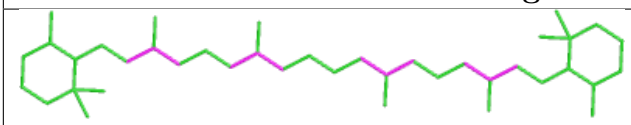


Rings

Ligand BCR B 845



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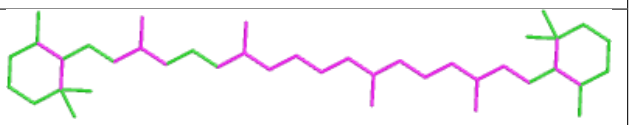

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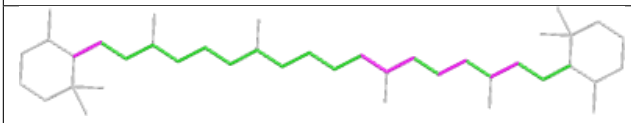

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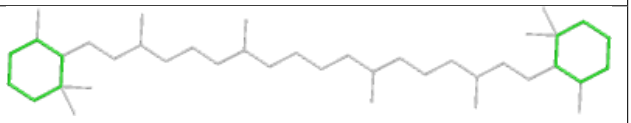
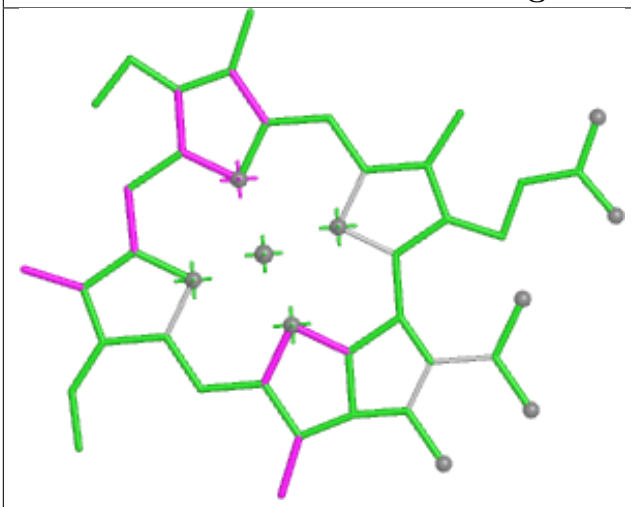


Rings

Ligand CLA 2 603



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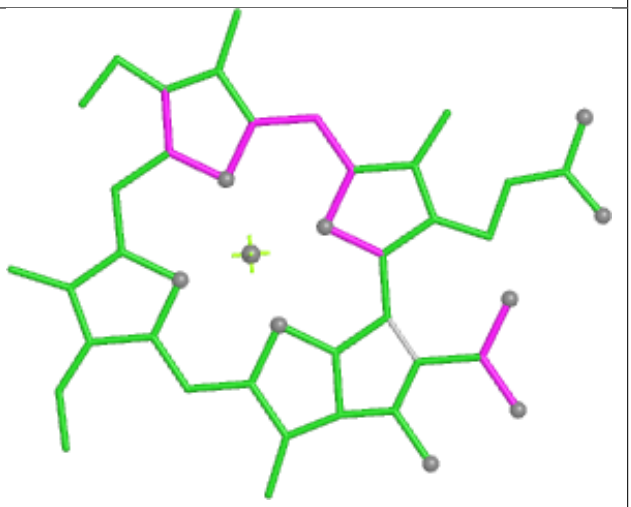

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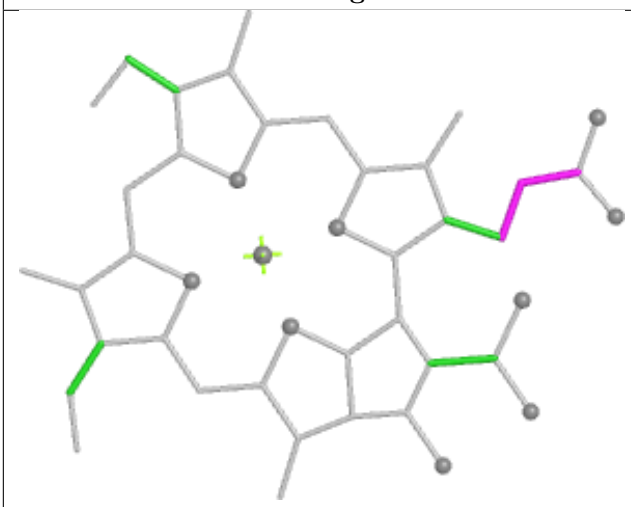

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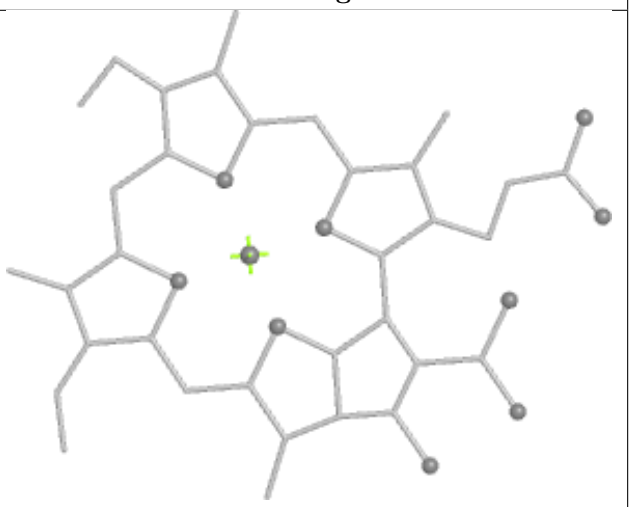

Rings

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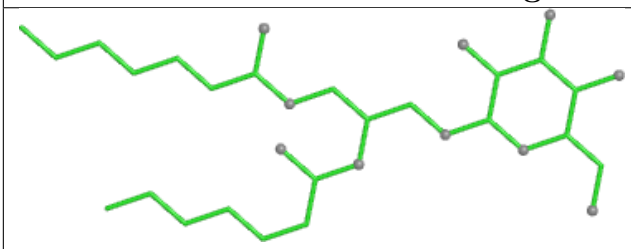

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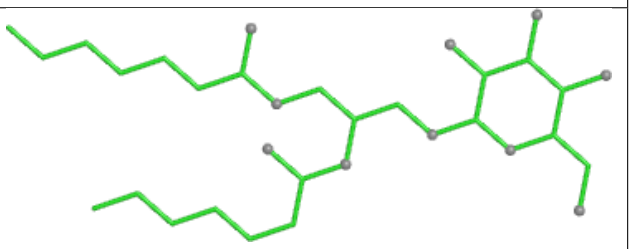

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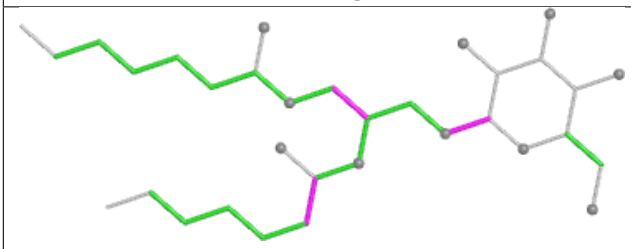

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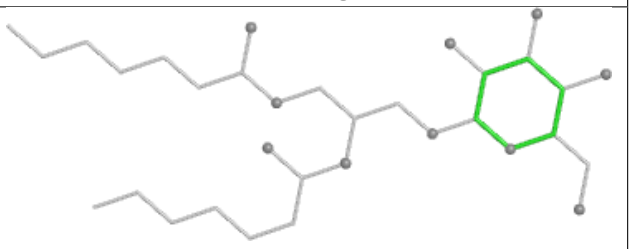
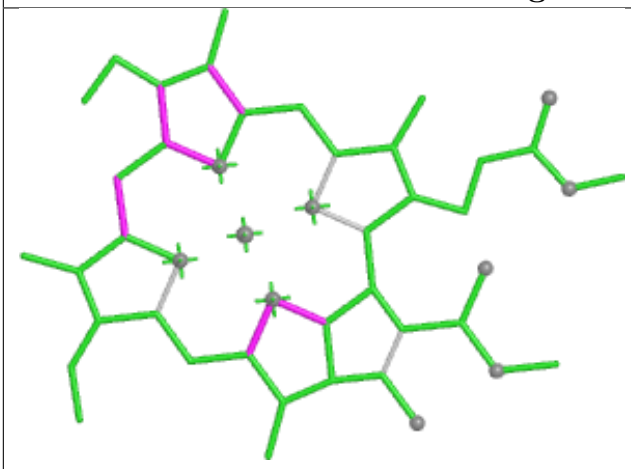


Rings

Ligand CLA 1 605



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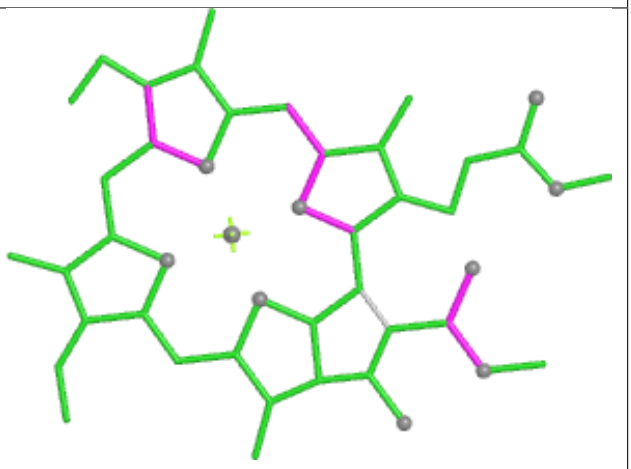

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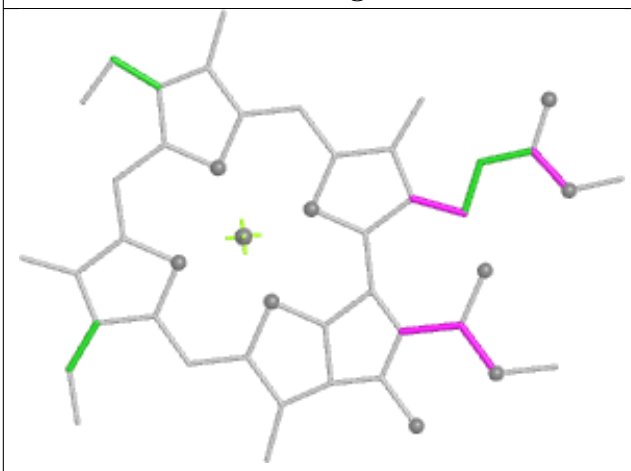

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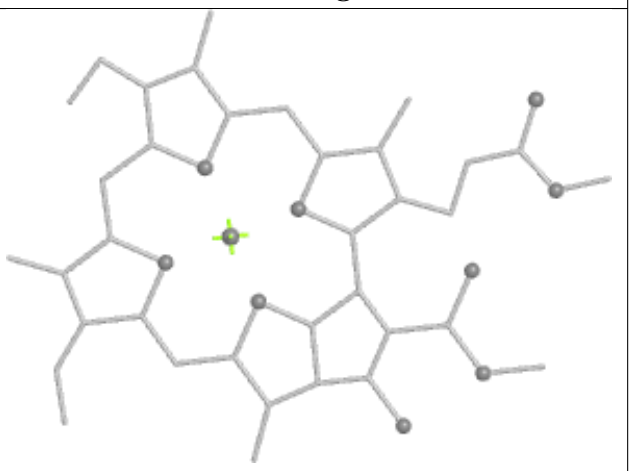
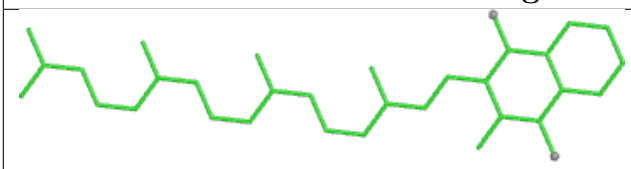


Rings

Ligand PQN B 842



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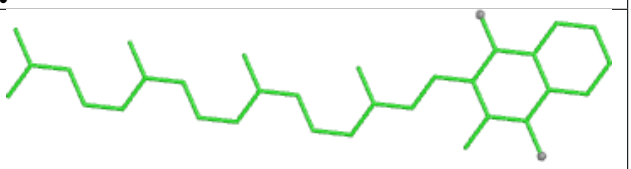

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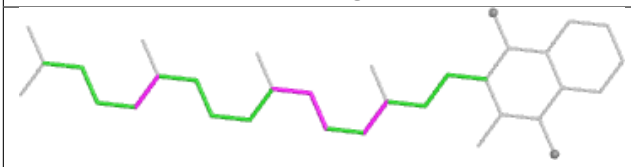

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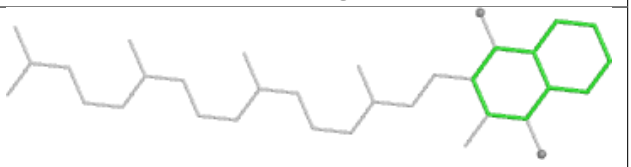
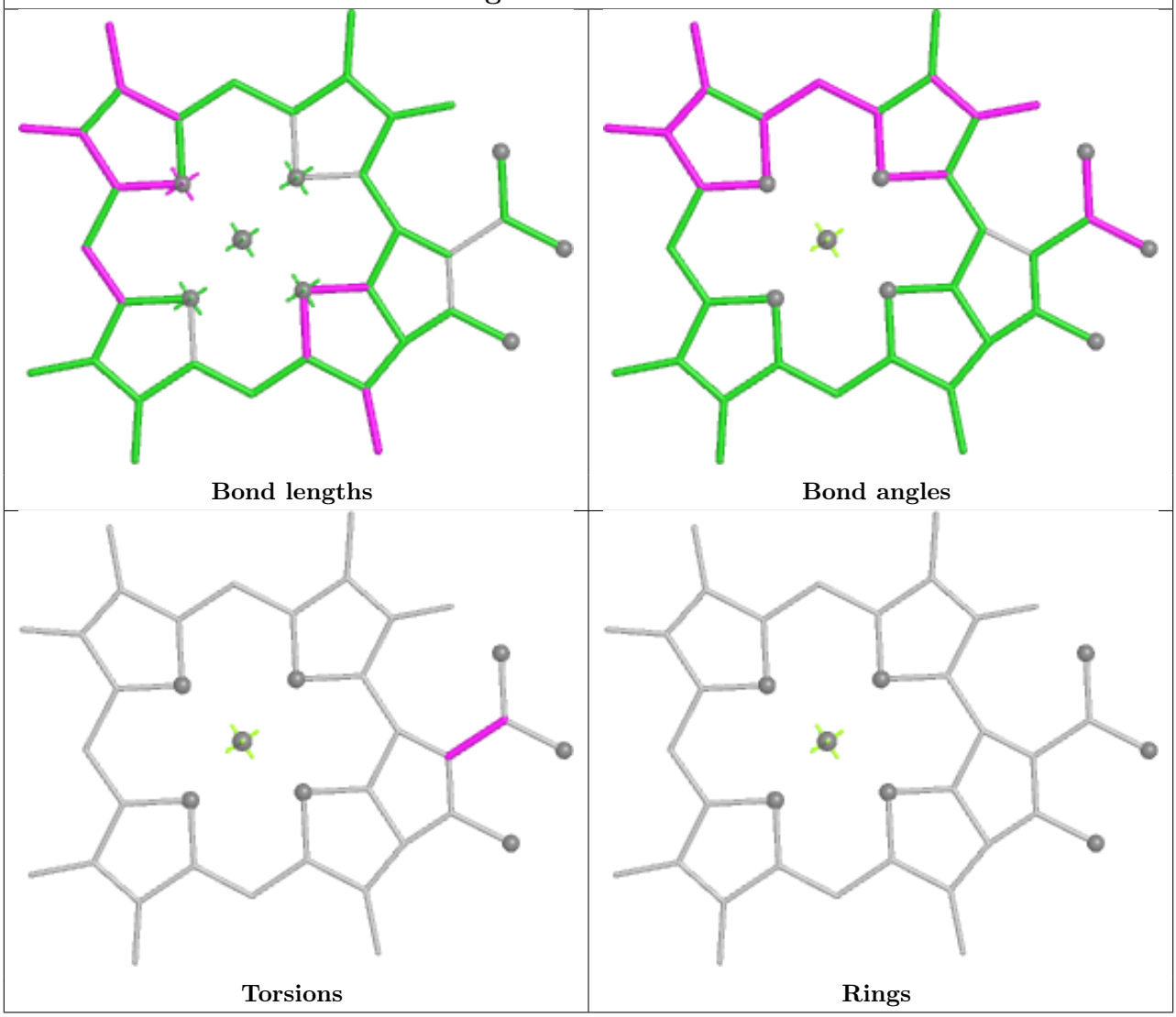


Rings

Ligand CLA 1 613



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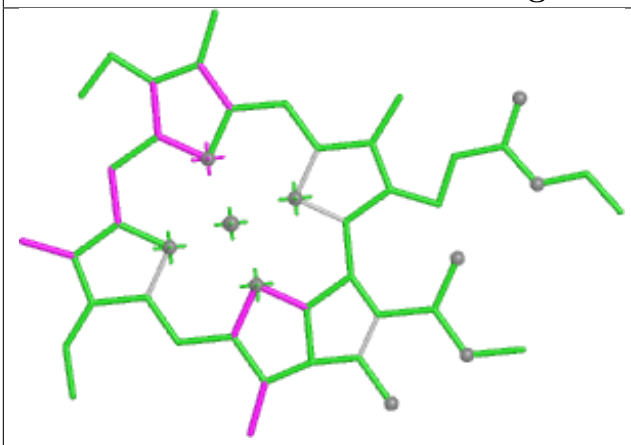
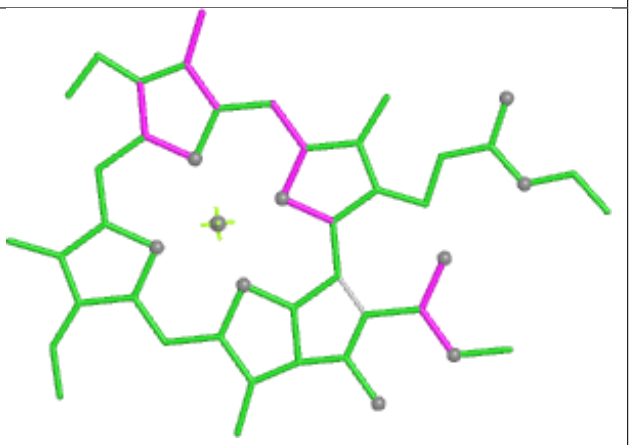
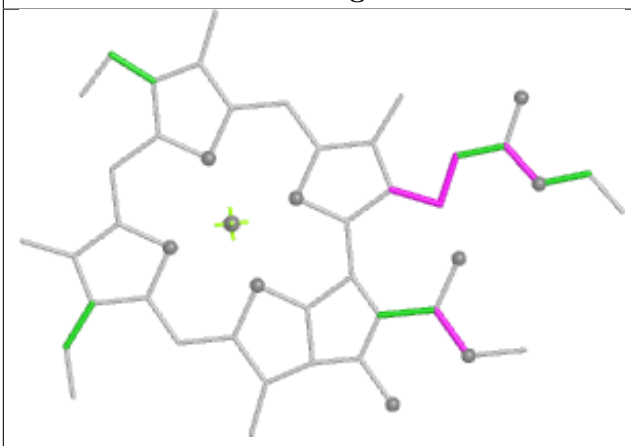
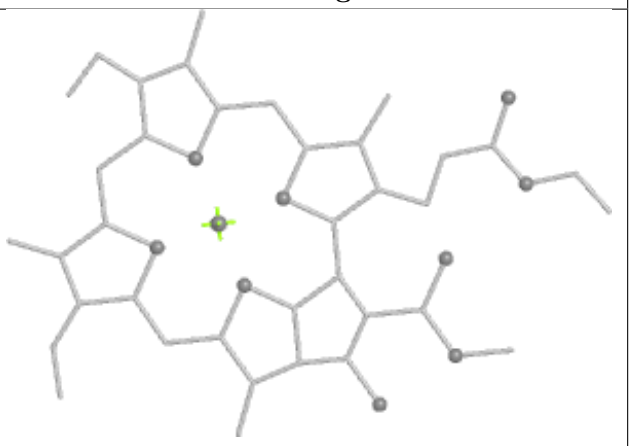
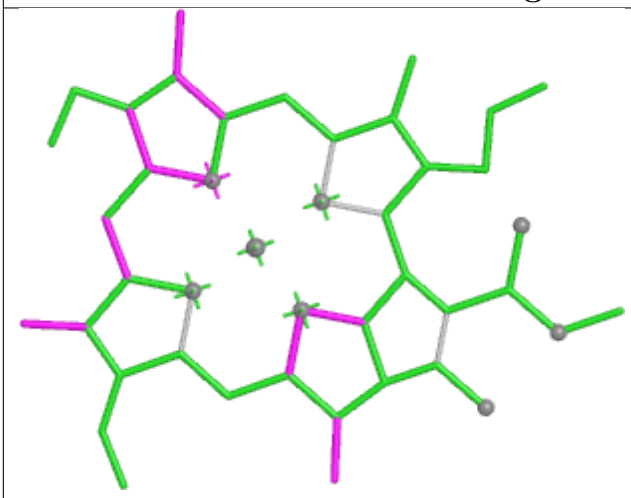
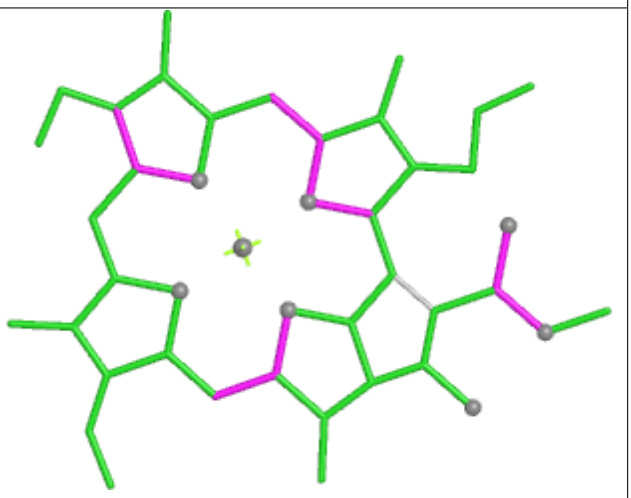
 Bond lengths	 Bond angles
 Torsions	 Rings

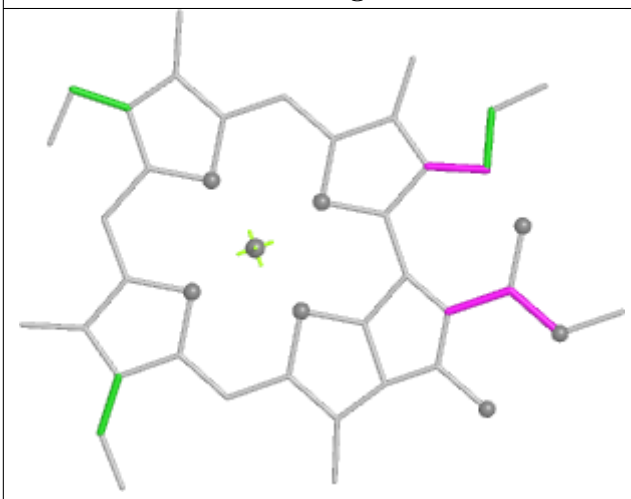
Ligand CLA B 815



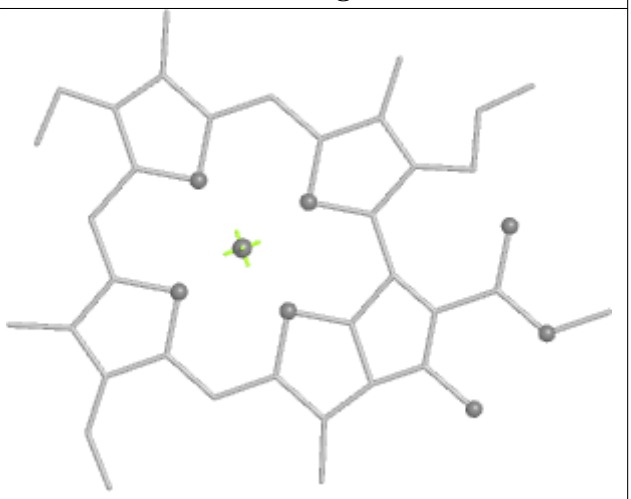
Bond lengths



Bond angles

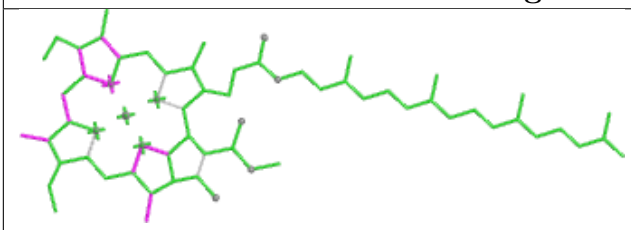


Torsions



Rings

Ligand CLA B 803



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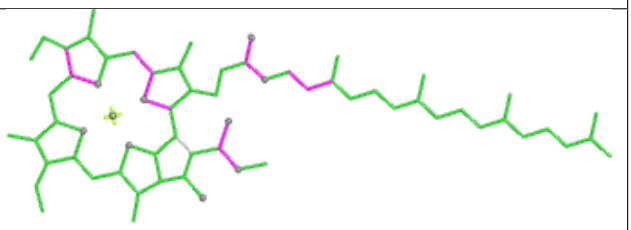

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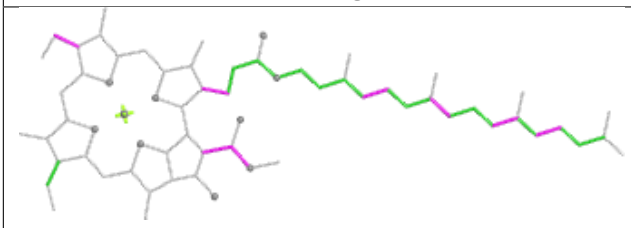

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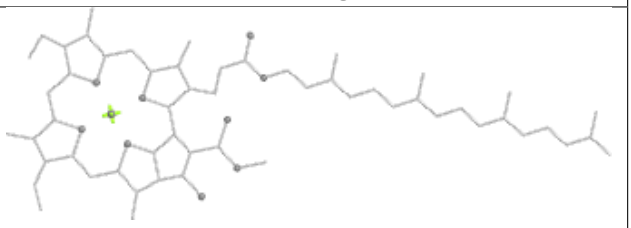
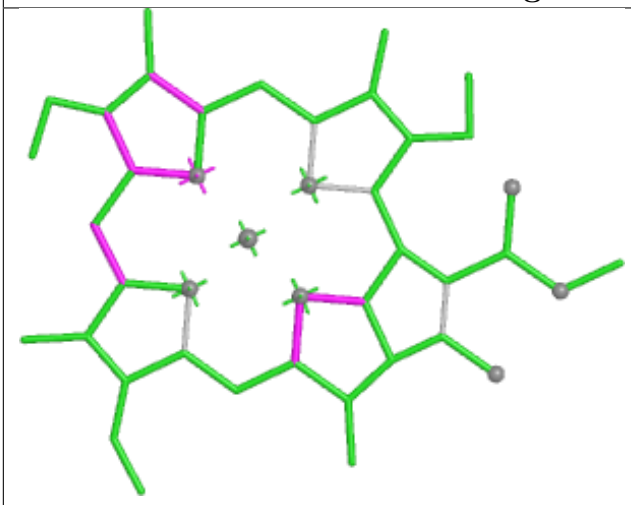


Rings

Ligand CLA A 823



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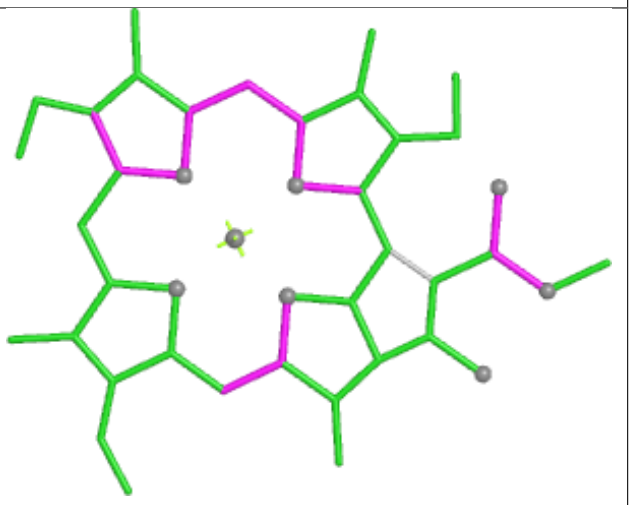
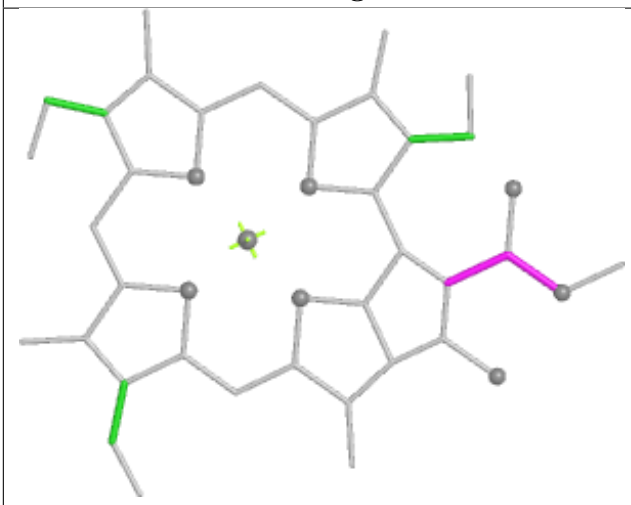


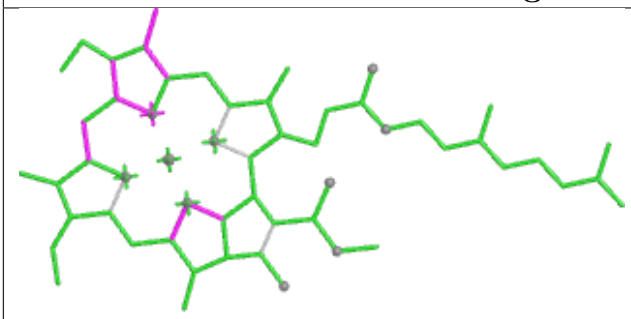
Bond angles



Torsions

Rings

Ligand CLA A 825



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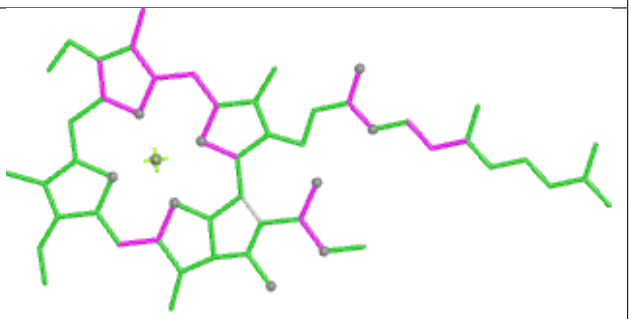
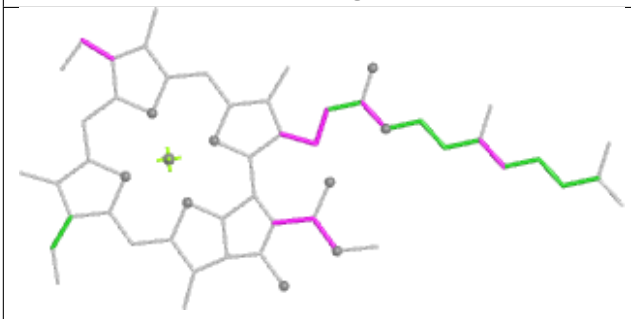


Bond angles



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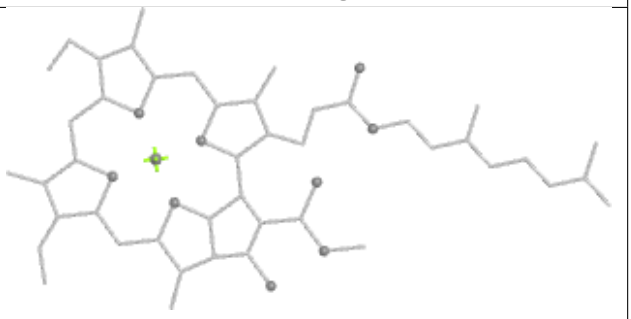
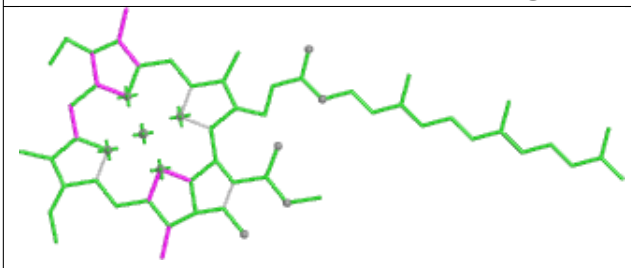


Rings

Ligand CLA B 834



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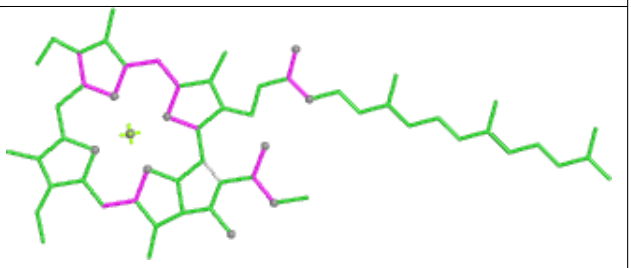
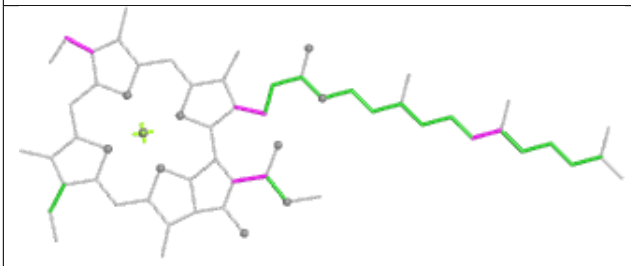
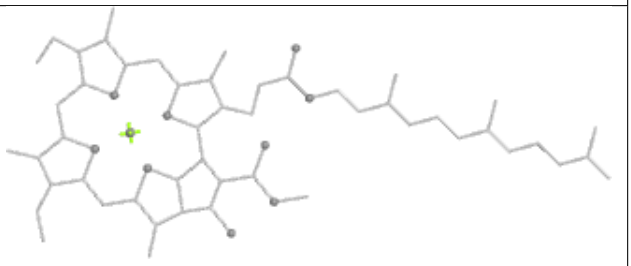


Bond angles



Torsions

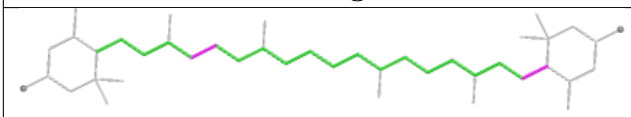


Rings

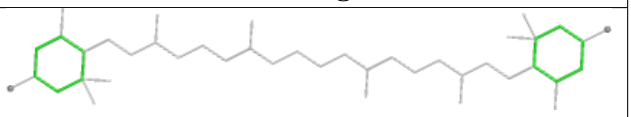
Ligand LUT 1 616

Bond lengths

Bond angles

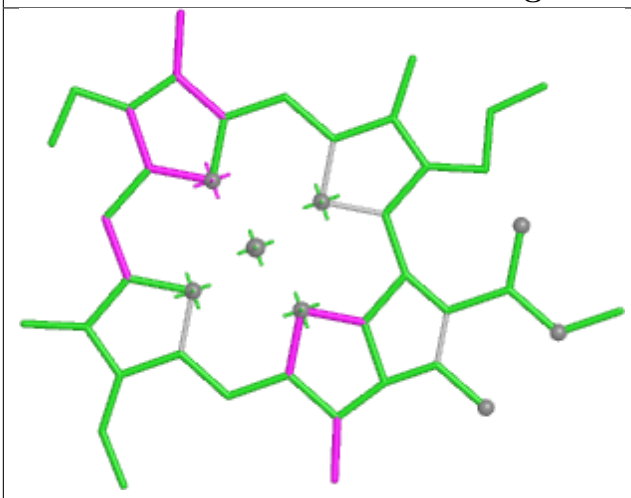


Torsions

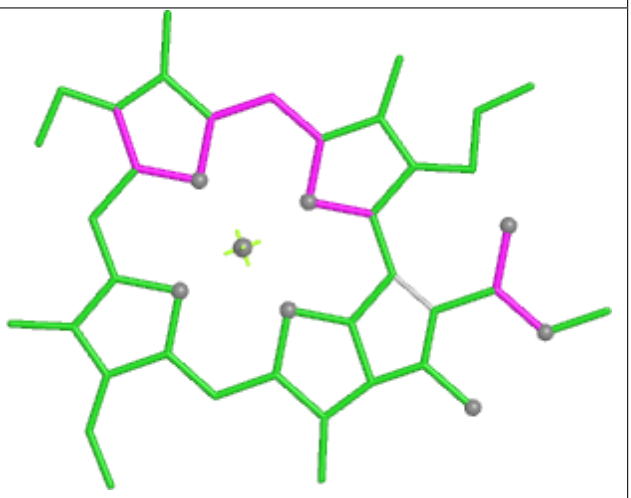


Rings

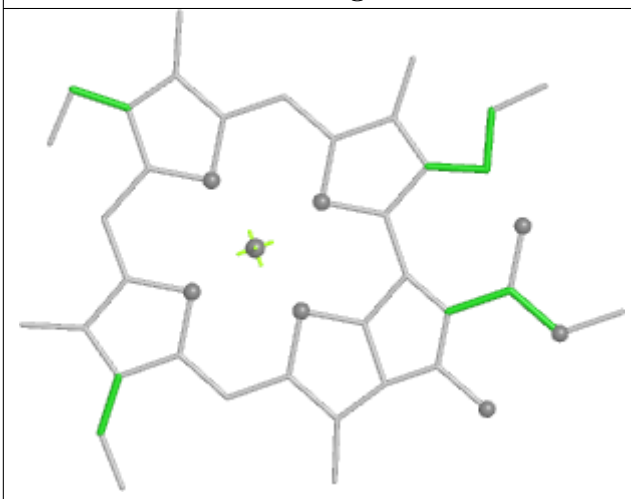
Ligand CLA B 812



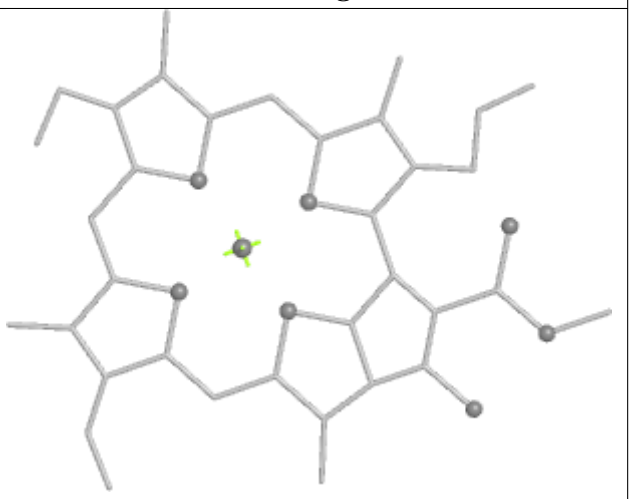
Bond lengths



Bond angles

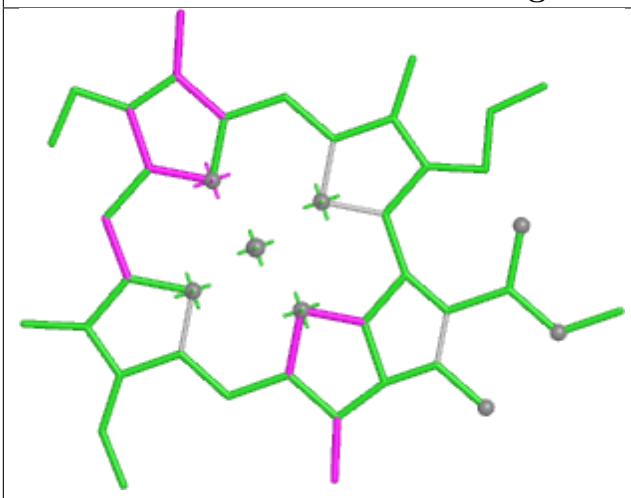


Torsions

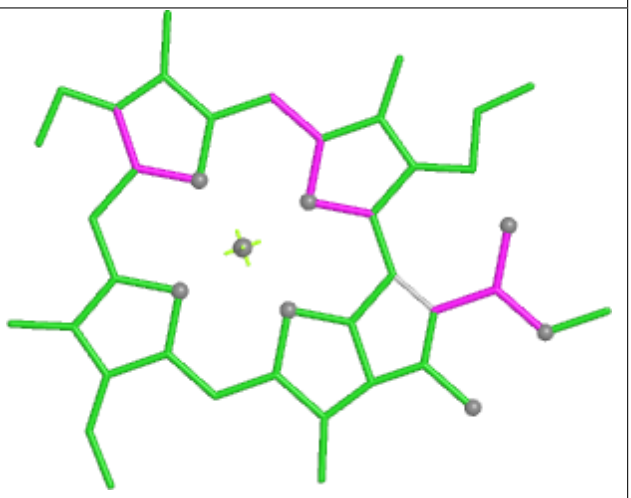


Rings

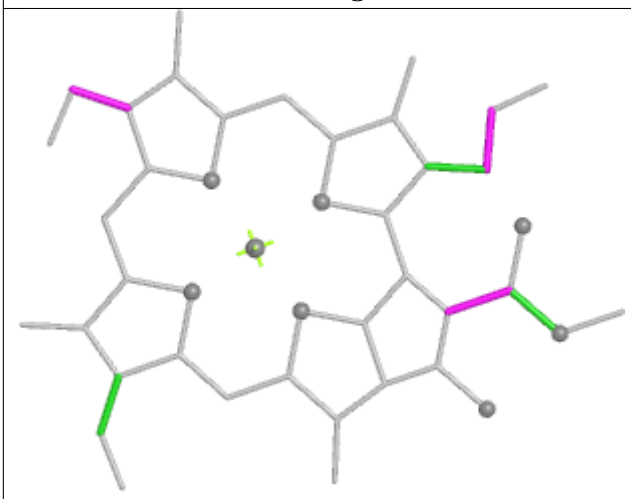
Ligand CLA 2 613



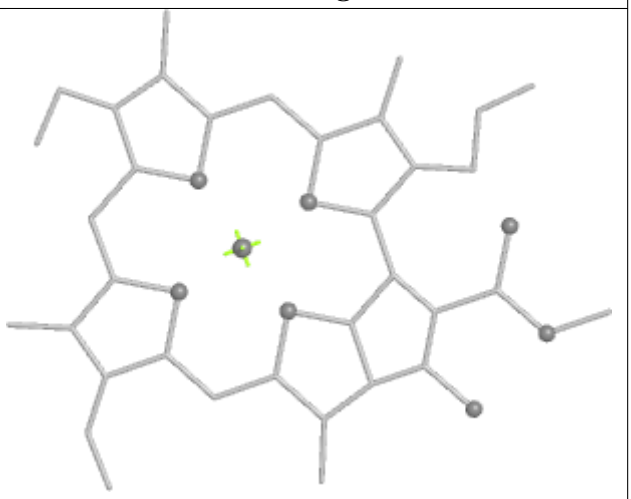
Bond lengths



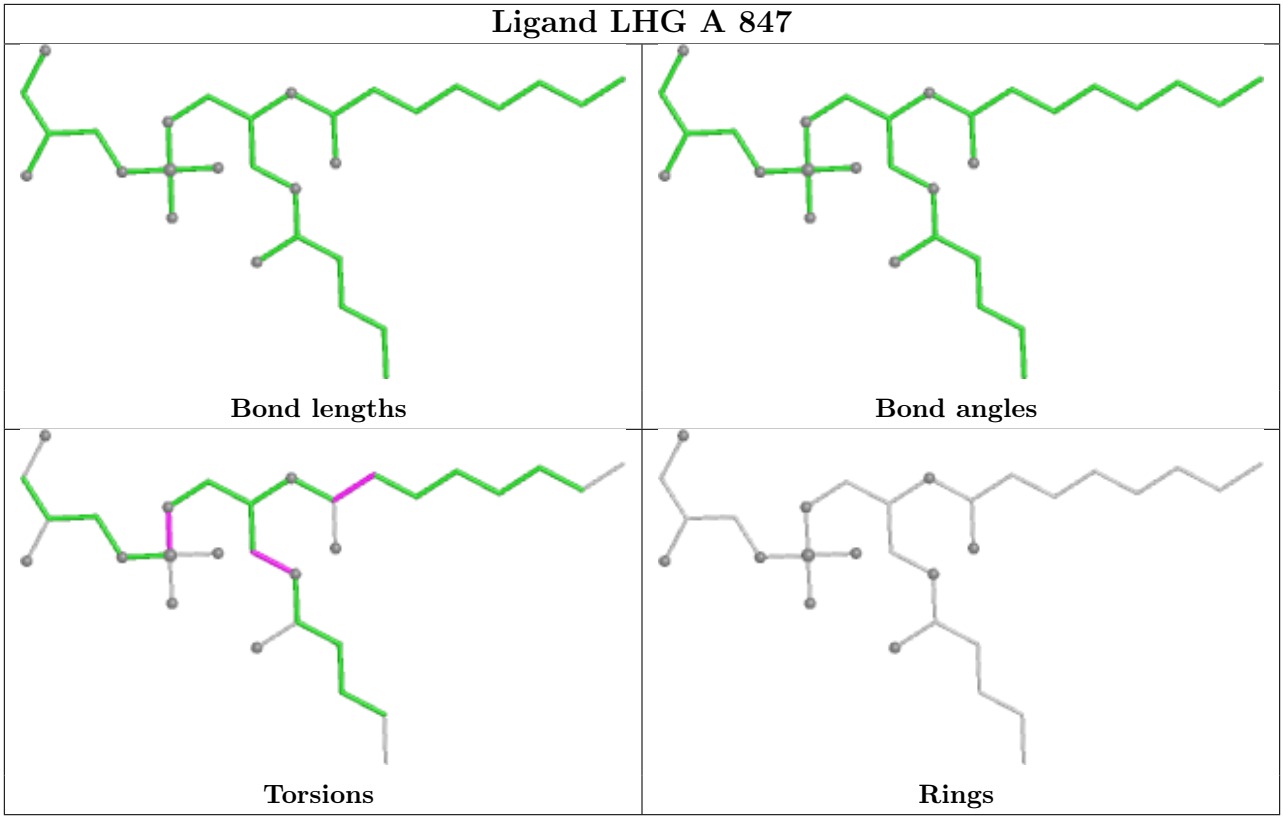
Bond angles



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.

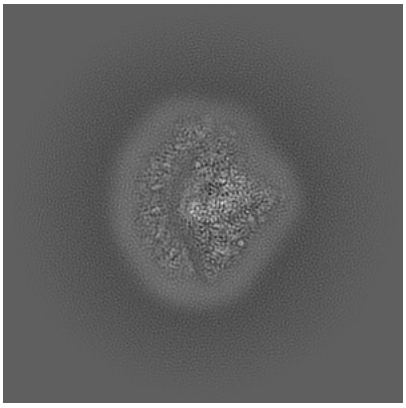
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-36036. These allow visual inspection of the internal detail of the map and identification of artifacts.

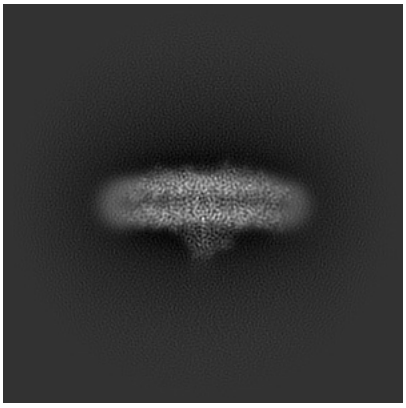
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

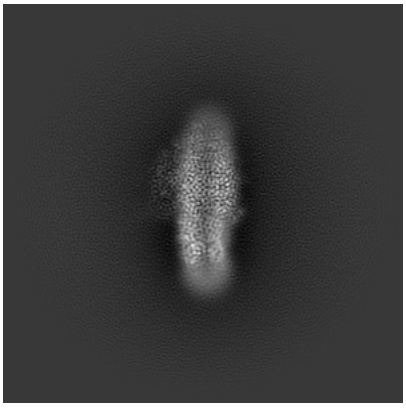
6.1.1 Primary map



X



Y

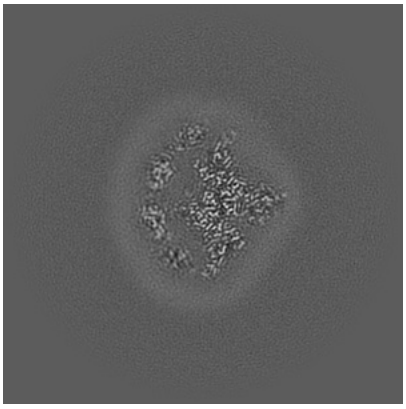


Z

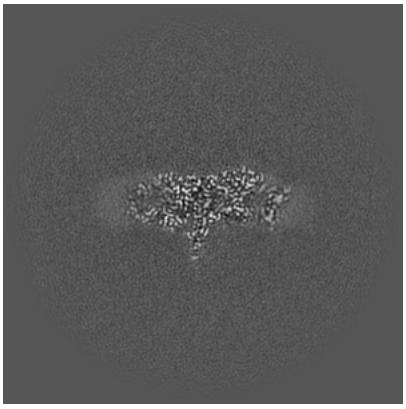
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

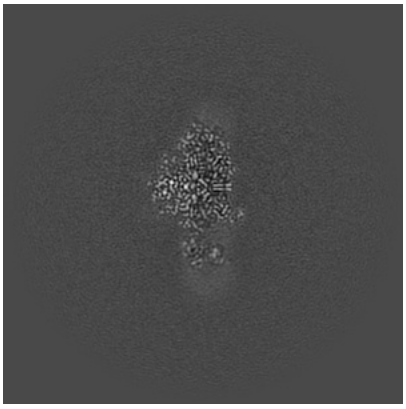
6.2.1 Primary map



X Index: 192



Y Index: 192

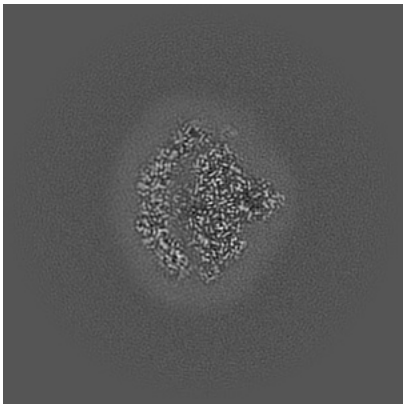


Z Index: 192

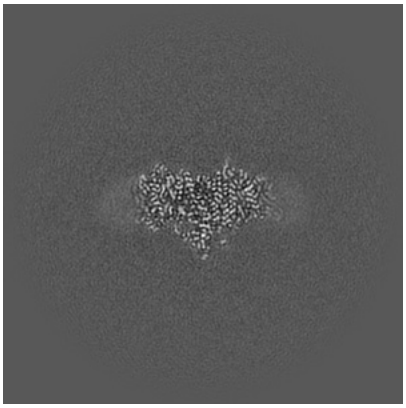
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

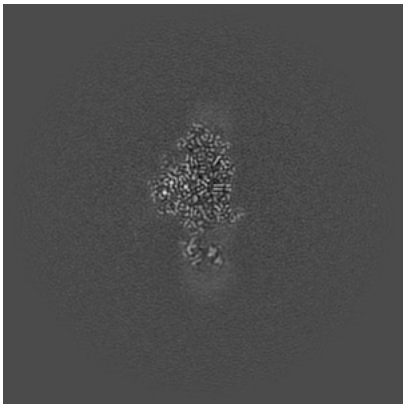
6.3.1 Primary map



X Index: 182



Y Index: 211

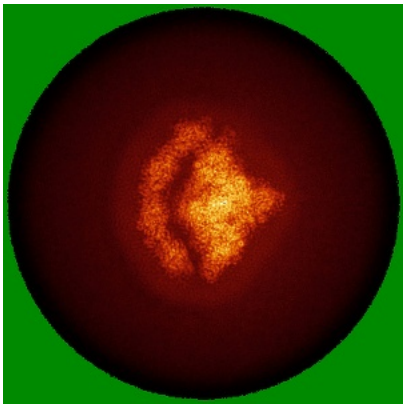


Z Index: 191

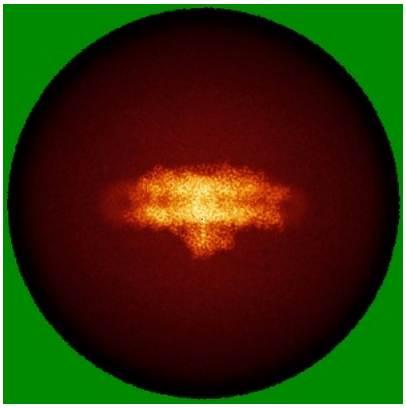
The images above show the largest variance slices of the map in three orthogonal directions.

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

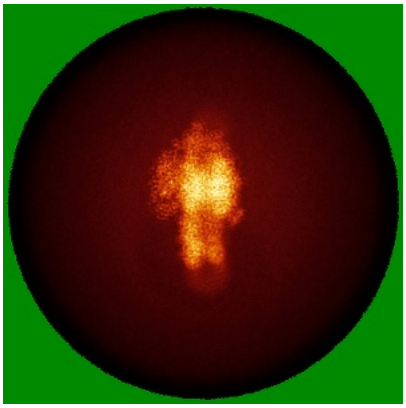
6.4.1 Primary map



X



Y

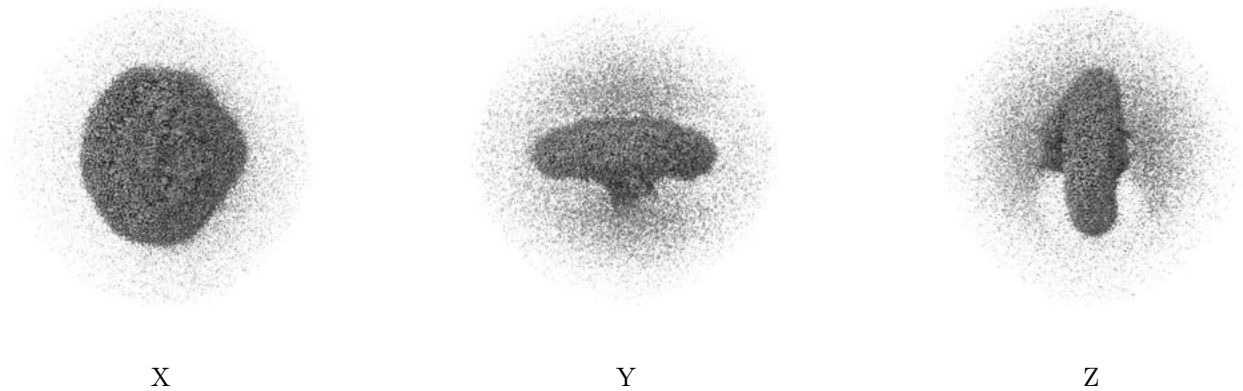


Z

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

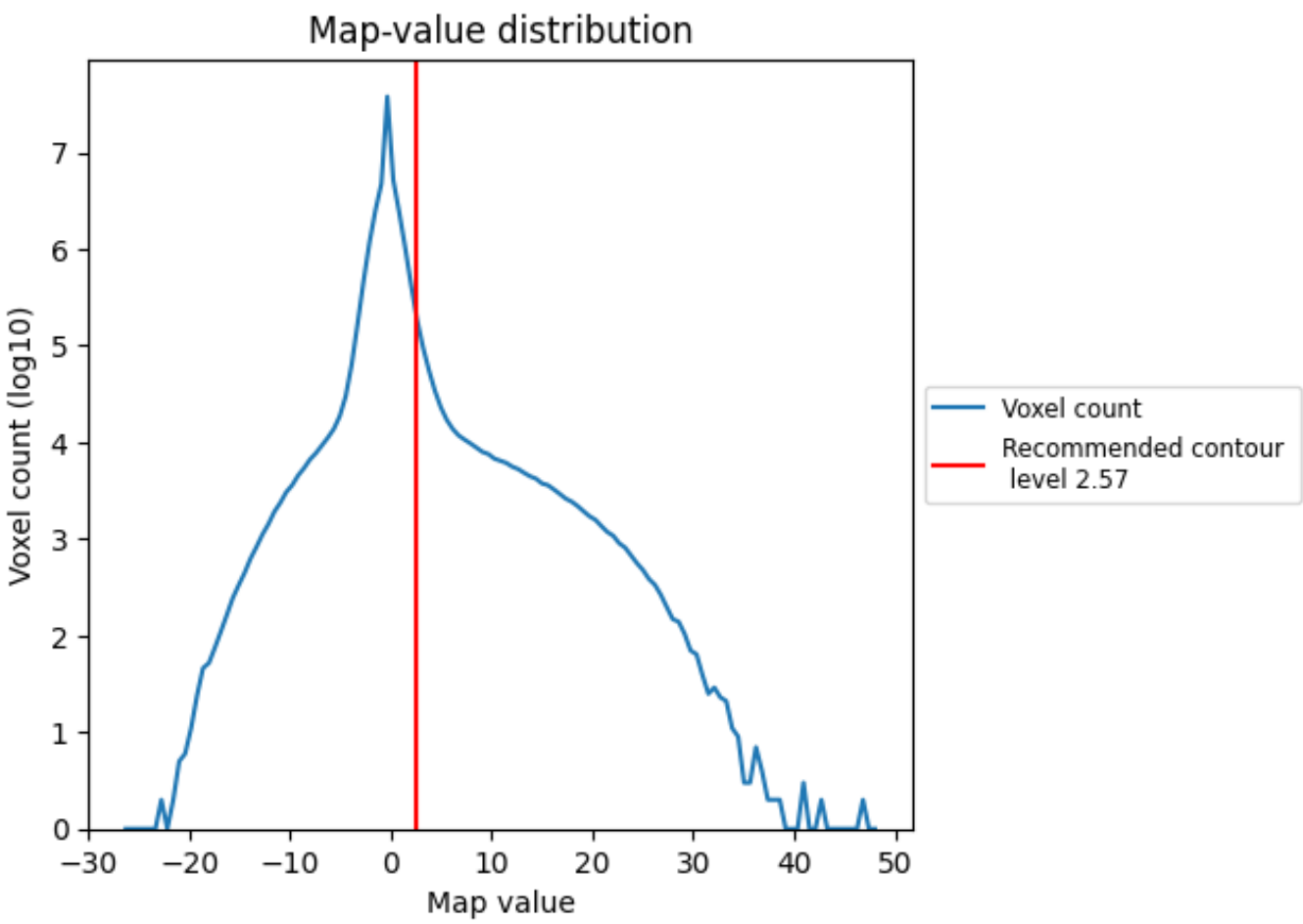
6.6 Mask visualisation (i)

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

7 Map analysis (i)

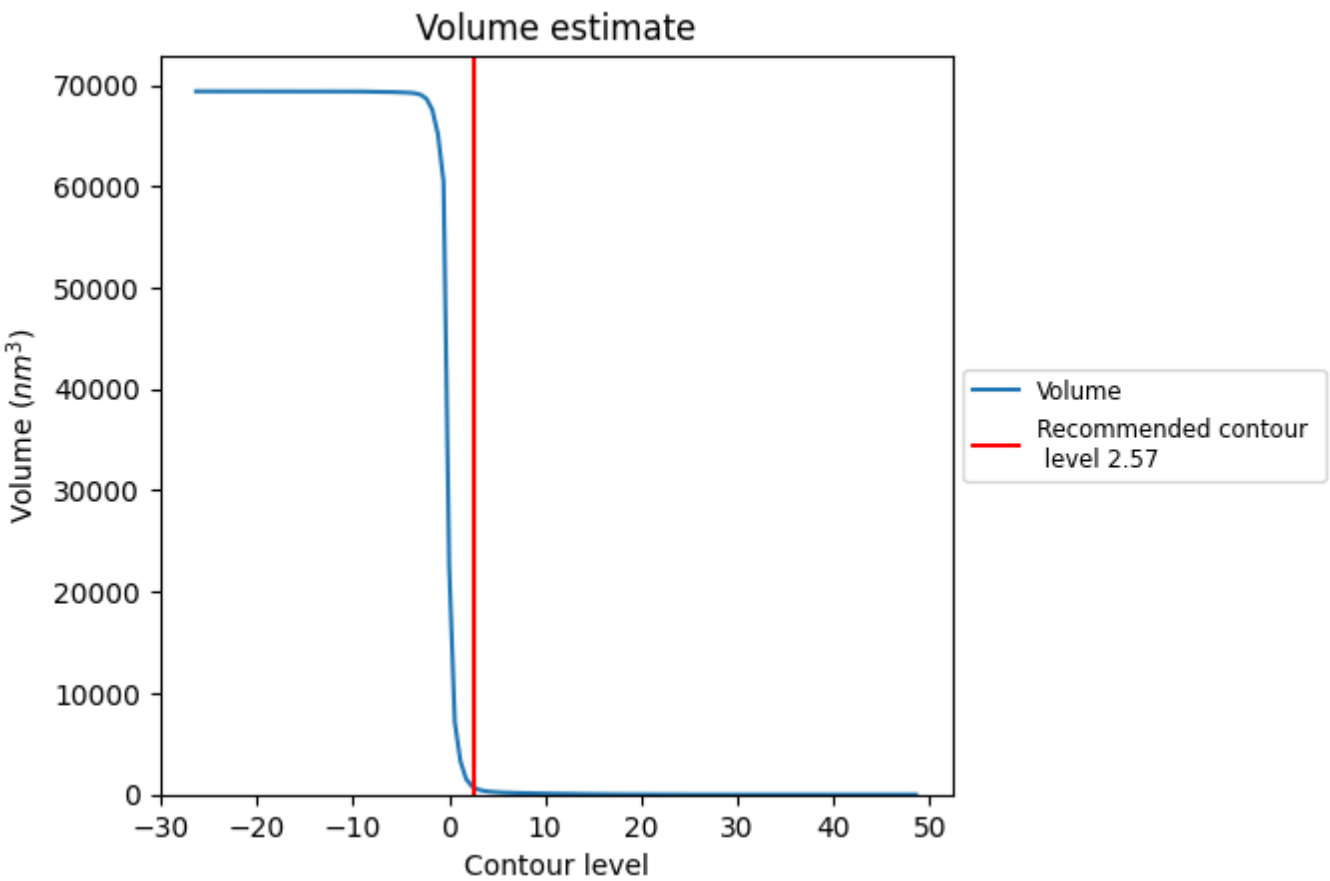
This section contains the results of statistical analysis of the map.

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.

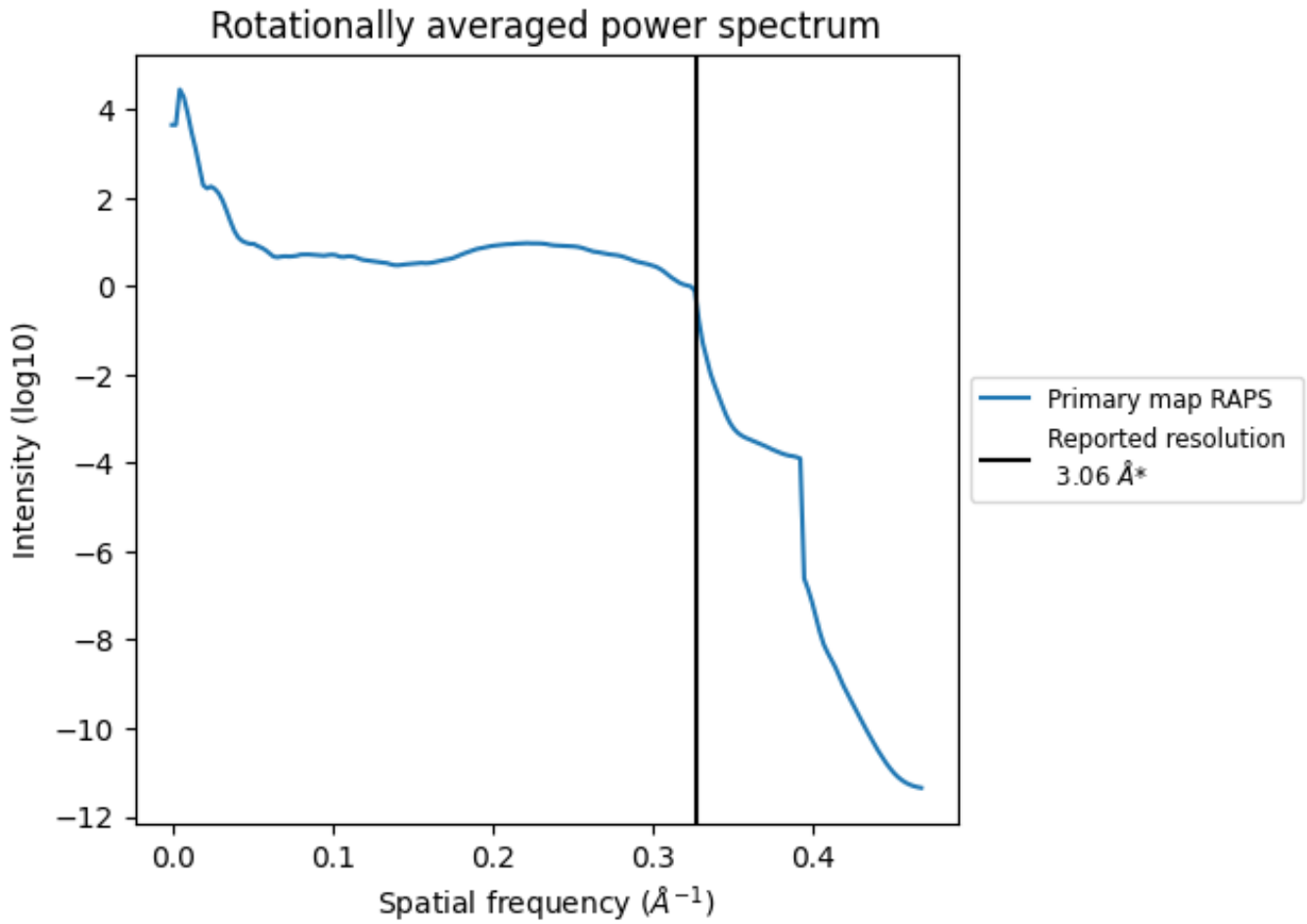
7.2 Volume estimate (i)



The volume at the recommended contour level is 724 nm^3; this corresponds to an approximate mass of 654 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 0.327 Å^{-1}

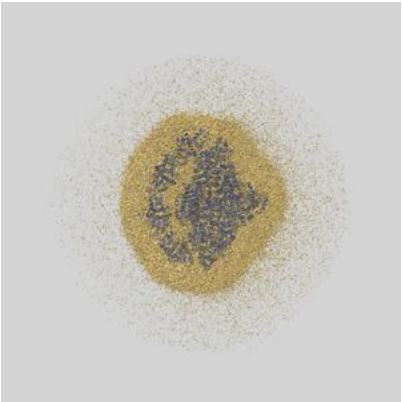
8 Fourier-Shell correlation (i)

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

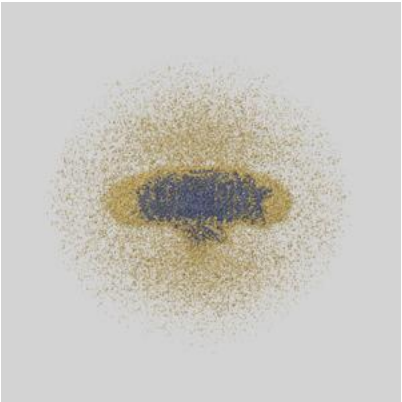
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-36036 and PDB model 8J7A. Per-residue inclusion information can be found in section 3 on page 22.

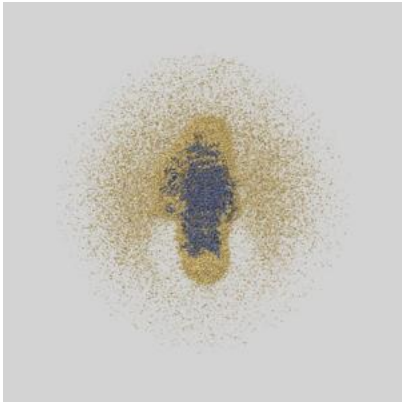
9.1 Map-model overlay (i)



X



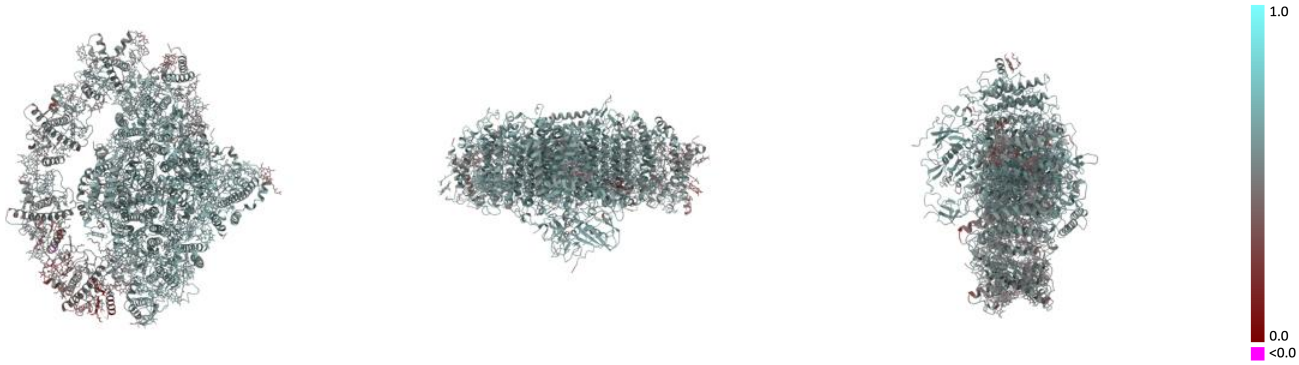
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.57 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.

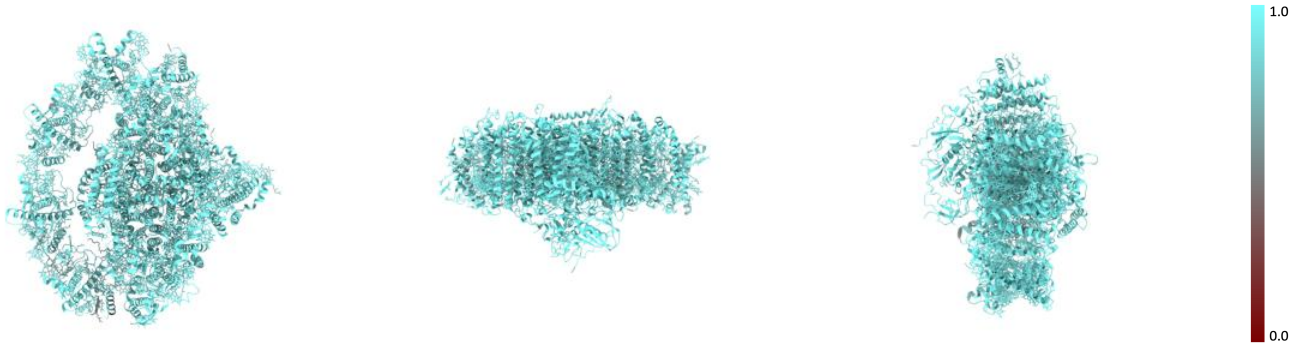
9.2 Q-score mapped to coordinate model (i)



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.

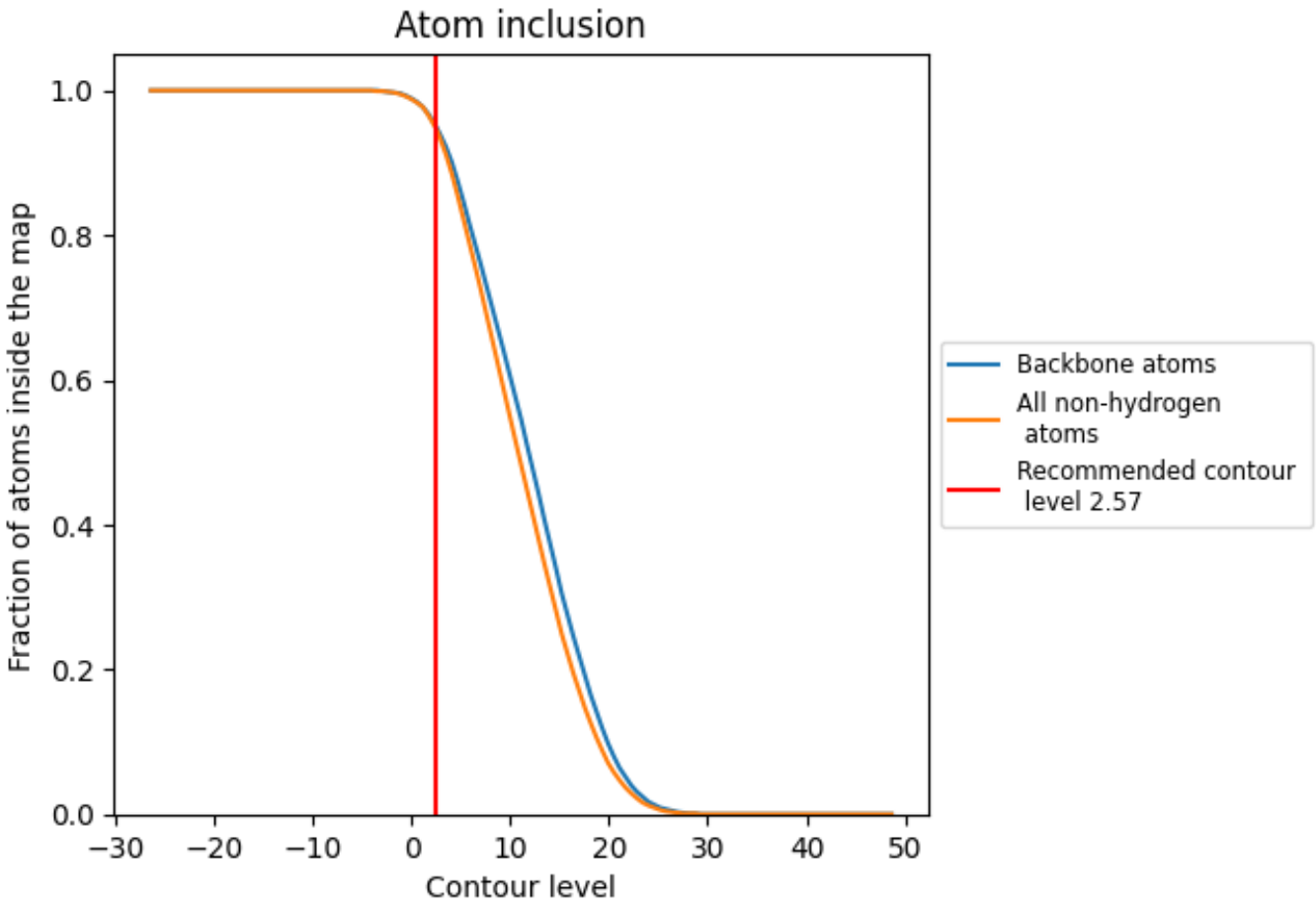
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.57).

9.4 Atom inclusion (i)



At the recommended contour level, 95% 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 (2.57) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.5490
1	0.8790	0.3980
2	0.9350	0.5010
3	0.9320	0.5130
4	0.9280	0.4910
A	0.9570	0.5800
B	0.9640	0.5900
C	0.9870	0.5880
D	0.9750	0.5830
E	0.9880	0.5750
F	0.9370	0.5560
G	0.9340	0.5440
H	0.9420	0.5440
I	0.9610	0.5630
J	0.8390	0.4940
K	0.8610	0.4450
L	0.9580	0.5700