Full wwPDB EM Validation Report ⓘ

Oct 31, 2023 – 02:31 PM JST

PDB ID	:	8J0D
EMDB ID	:	EMD-35899
Title	:	FCP heterodimer, Lhca2, and Lhcf5 together as the M1 side binds to the PSII core in the diatom Thalassiosira pseudonana
Authors	:	Li, Z.; Feng, Y.; Wang, W.; Shen, J.R.
Deposited on	:	2023-04-10
Resolution	:	3.19 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

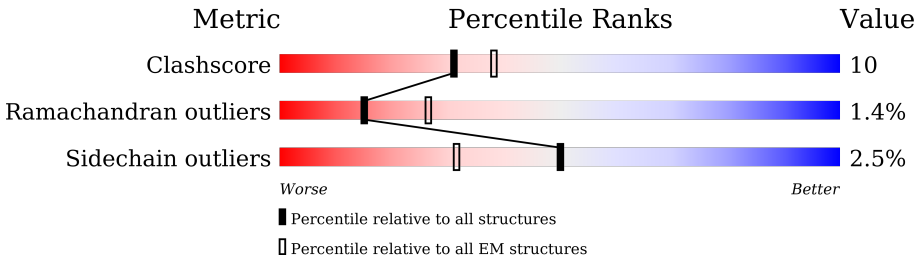
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.19 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	3	220	14% 88% 10%
2	4	163	88% 12%
3	5	160	7% 74% 23%
4	6	168	18% 77% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLA	3	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLA	3	602	X	-	-	-
5	CLA	3	603	X	-	-	-
5	CLA	3	604	X	-	-	-
5	CLA	3	605	X	-	-	-
5	CLA	3	606	X	-	-	-
5	CLA	3	607	X	-	-	-
5	CLA	3	608	X	-	-	-
5	CLA	3	610	X	-	-	-
5	CLA	3	611	X	-	-	-
5	CLA	3	612	X	-	-	-
5	CLA	3	619	X	-	-	-
5	CLA	4	305	X	-	-	-
5	CLA	4	306	X	-	-	-
5	CLA	4	308	X	-	-	-
5	CLA	4	309	X	-	-	-
5	CLA	4	310	X	-	-	-
5	CLA	4	311	X	-	-	-
5	CLA	4	312	X	-	-	-
5	CLA	4	313	X	-	-	-
5	CLA	4	314	X	-	-	-
5	CLA	4	315	X	-	-	-
5	CLA	4	316	X	-	-	-
5	CLA	5	308	X	-	-	-
5	CLA	5	309	X	-	-	-
5	CLA	5	311	X	-	-	-
5	CLA	5	312	X	-	-	-
5	CLA	5	313	X	-	-	-
5	CLA	5	314	X	-	X	-
5	CLA	5	316	X	-	-	-
5	CLA	5	317	X	-	-	-
5	CLA	6	306	X	-	-	-
5	CLA	6	307	X	-	-	-
5	CLA	6	309	X	-	-	-
5	CLA	6	310	X	-	-	-
5	CLA	6	311	X	-	-	-
5	CLA	6	312	X	-	-	-
5	CLA	6	314	X	-	-	-
5	CLA	6	315	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 9105 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 Fucoxanthin chl a/c protein, lhca clade.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	220	Total	C	N	O	S	0	0
			1710	1110	281	315	4		

- Molecule 2 is a protein called Fucoxanthin-chlorophyll a-c binding protein, plastid.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	163	Total	C	N	O	S	0	0
			1249	809	204	232	4		

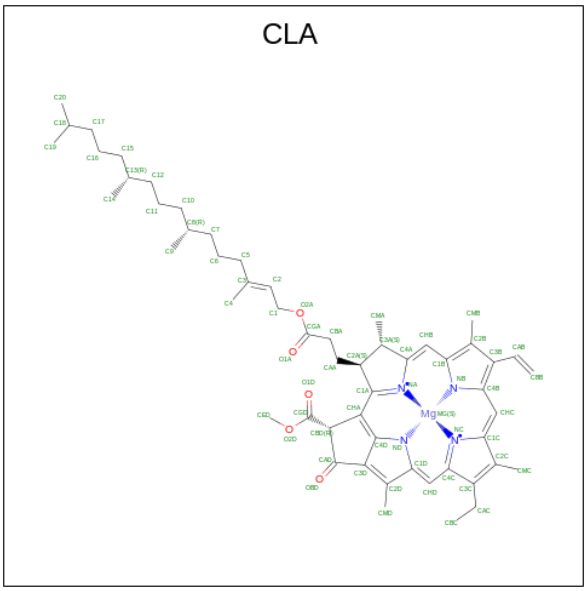
- Molecule 3 is a protein called Fucoxanthin chlorophyll a/c protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	160	Total	C	N	O	S	0	0
			1229	780	217	227	5		

- Molecule 4 is a protein called Fucoxanthin chlorophyll a/c protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	168	Total	C	N	O	S	0	0
			1296	833	219	238	6		

- Molecule 5 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
5	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
5	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
5	3	1	Total 48	C 38	Mg 1	N 4	O 5	0
5	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
5	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
5	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
5	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
5	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
5	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
5	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
5	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
5	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
5	4	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
5	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
5	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
5	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
5	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
5	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
5	5	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
5	6	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
5	6	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
5	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
5	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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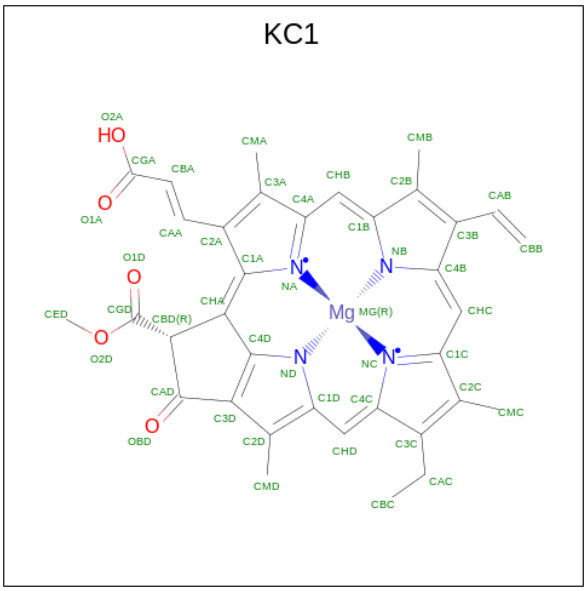
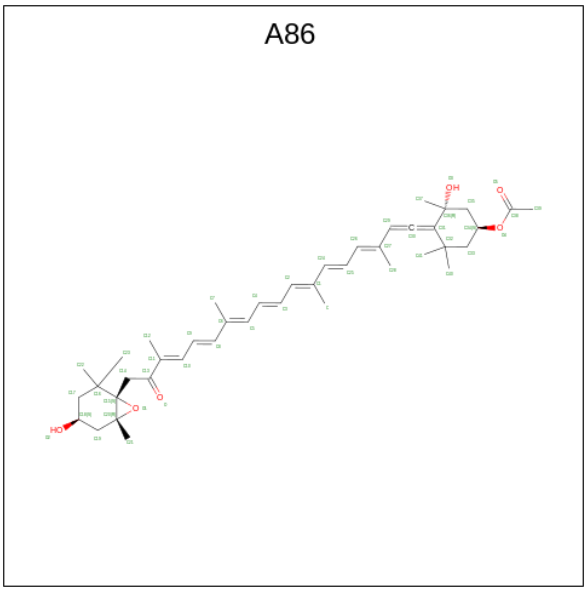
Mol	Chain	Residues	Atoms					AltConf
5	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
5	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
5	6	1	Total	C	Mg	N	O	0
			39	30	1	4	4	

- Molecule 6 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
6	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
6	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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



Mol	Chain	Residues	Atoms	AltConf
7	3	1	Total C O 48 42 6	0
7	4	1	Total C O 48 42 6	0
7	4	1	Total C O 48 42 6	0
7	4	1	Total C O 48 42 6	0
7	5	1	Total C O 48 42 6	0
7	5	1	Total C O 48 42 6	0
7	5	1	Total C O 48 42 6	0
7	5	1	Total C O 48 42 6	0
7	5	1	Total C O 47 41 6	0
7	5	1	Total C O 48 42 6	0
7	5	1	Total C O 48 42 6	0
7	5	1	Total C O 48 42 6	0
7	6	1	Total C O 48 42 6	0
7	6	1	Total C O 48 42 6	0

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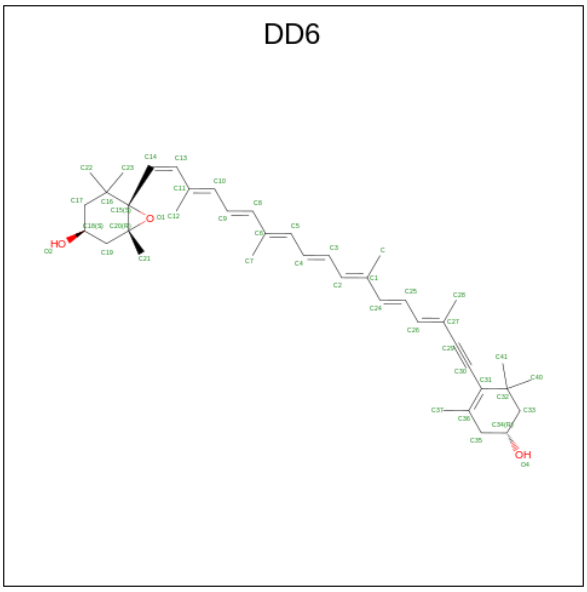
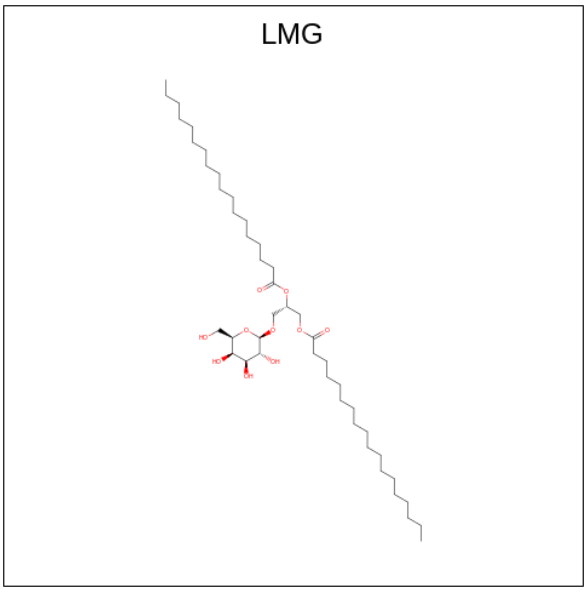
Mol	Chain	Residues	Atoms	AltConf
7	6	1	Total C O 48 42 6	0
7	6	1	Total C O 48 42 6	0
7	6	1	Total C O 48 42 6	0

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



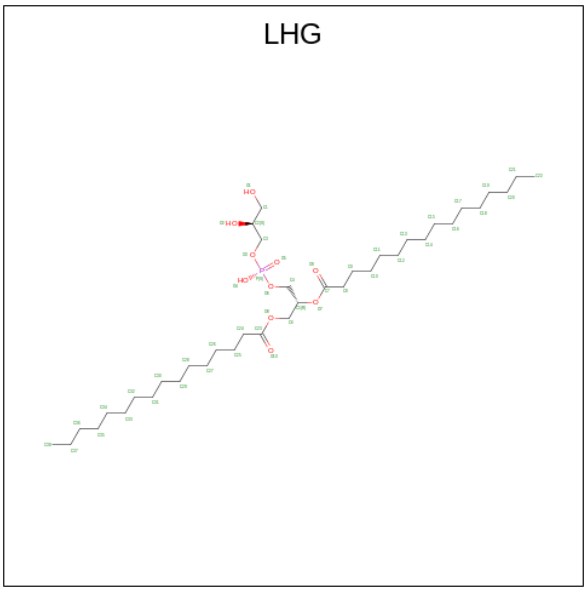
Mol	Chain	Residues	Atoms	AltConf
8	3	1	Total C O 43 40 3	0
8	4	1	Total C O 43 40 3	0

- Molecule 9 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



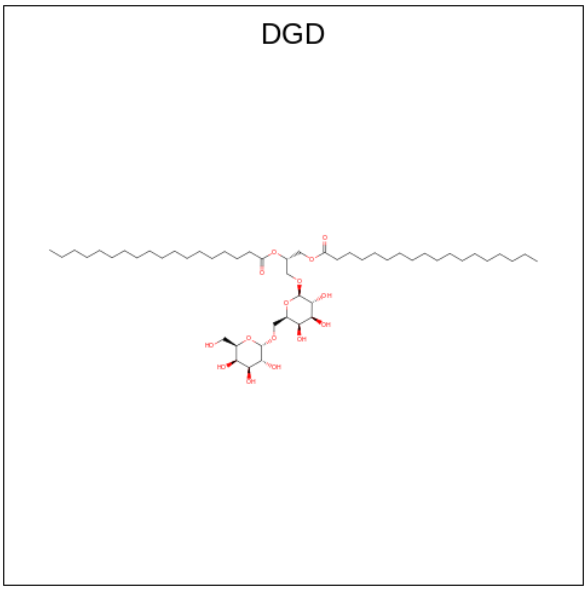
Mol	Chain	Residues	Atoms			AltConf
9	3	1	Total	C	O	0
			31	21	10	
9	3	1	Total	C	O	0
			23	13	10	
9	5	1	Total	C	O	0
			31	21	10	

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



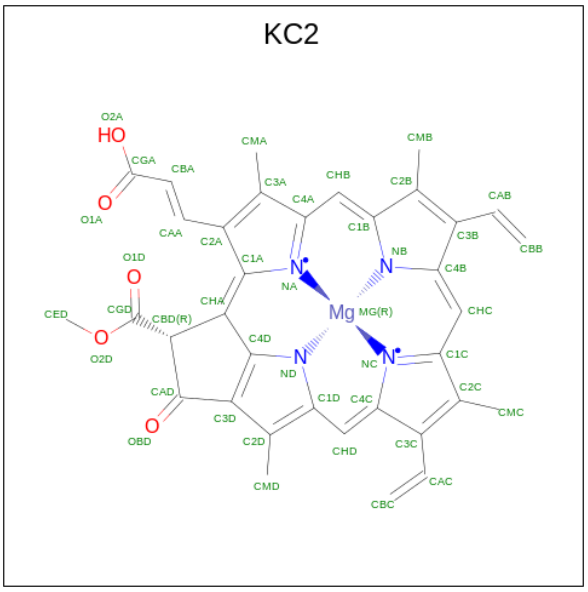
Mol	Chain	Residues	Atoms				AltConf
10	3	1	Total 27	C 16	O 10	P 1	0
10	3	1	Total 49	C 38	O 10	P 1	0
10	4	1	Total 49	C 38	O 10	P 1	0
10	5	1	Total 33	C 24	O 8	P 1	0

- Molecule 11 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



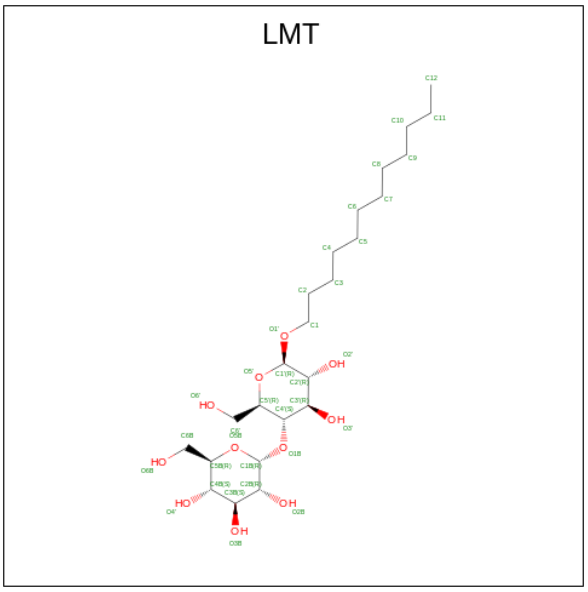
Mol	Chain	Residues	Atoms			AltConf
11	3	1	Total 39	C 34	O 5	0

- Molecule 12 is Chlorophyll c2 (three-letter code: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 13 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



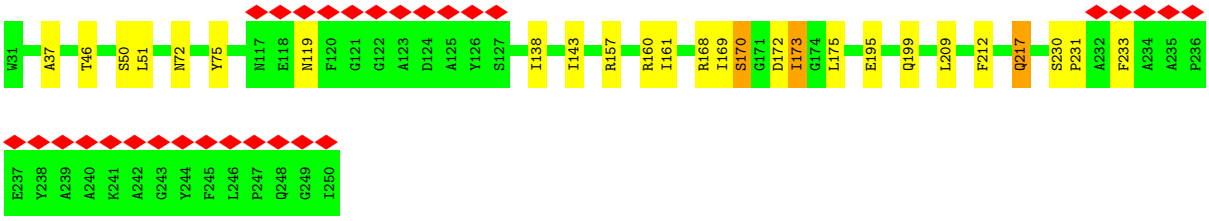
Mol	Chain	Residues	Atoms			AltConf
13	4	1	Total	C	O	0
			35	24	11	
13	5	1	Total	C	O	0
			31	20	11	

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: Fucoxanthin chl a/c protein, lhca clade

Chain 3:

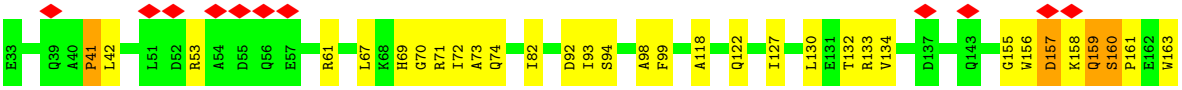


• Molecule 2: Fucoxanthin-chlorophyll a-c binding protein, plastid

Chain 4:

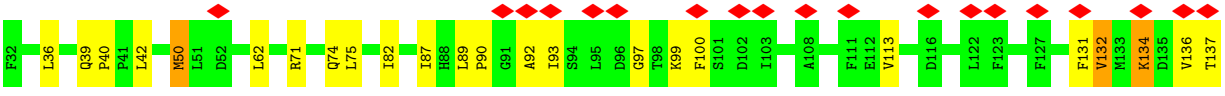
• Molecule 3: Fucoxanthin chlorophyll a/c protein 6

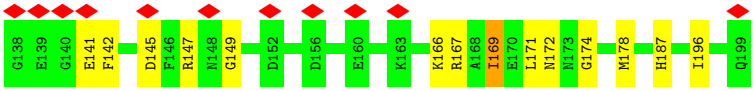
Chain 5:



• Molecule 4: Fucoxanthin chlorophyll a/c protein 5

Chain 6:




G138
E139
G140
E141
F142
D145
F146
R147
N148
G149
D152
D156
E160
K163
K166
R167
A168
I169
E170
L171
N172
N173
G174
M178
H187
I196
Q199

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97098	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.598	Depositor
Minimum map value	-0.249	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KC2, DGD, A86, LHG, LMT, CLA, DD6, LMG, KC1

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	3	0.31	0/1765	0.47	0/2405
2	4	0.31	0/1282	0.47	0/1746
3	5	0.29	0/1255	0.54	1/1696 (0.1%)
4	6	0.29	0/1324	0.48	0/1780
All	All	0.30	0/5626	0.49	1/7627 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	5	41	PRO	N-CA-CB	6.68	111.32	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3	1710	0	1624	17	0
2	4	1249	0	1219	15	0
3	5	1229	0	1184	48	0
4	6	1296	0	1268	30	0
5	3	702	0	698	28	0
5	4	603	0	556	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	5	401	0	340	36	0
5	6	396	0	328	16	0
6	3	45	0	0	0	0
6	5	45	0	0	0	0
6	6	45	0	0	3	0
7	3	48	0	0	1	0
7	4	144	0	0	0	0
7	5	383	0	0	5	0
7	6	240	0	0	2	0
8	3	43	0	0	0	0
8	4	43	0	0	0	0
9	3	54	0	48	1	0
9	5	31	0	32	1	0
10	3	76	0	98	3	0
10	4	49	0	74	2	0
10	5	33	0	42	0	0
11	3	39	0	62	1	0
12	4	45	0	0	0	0
12	5	45	0	0	3	0
12	6	45	0	0	1	0
13	4	35	0	45	0	0
13	5	31	0	34	0	0
All	All	9105	0	7652	163	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 10.

All (163) 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)
3:5:156:TRP:CE3	5:5:314:CLA:HBA1	1.79	1.16
3:5:156:TRP:HE3	5:5:314:CLA:HBA1	1.06	1.13
3:5:167:LYS:CD	5:5:314:CLA:HMA3	1.82	1.07
3:5:167:LYS:CE	5:5:314:CLA:HMA3	1.91	1.00
3:5:156:TRP:HE3	5:5:314:CLA:CBA	1.78	0.95
7:5:304:A86:C37	5:5:314:CLA:H62	2.00	0.91
3:5:167:LYS:HE3	5:5:314:CLA:C4A	2.05	0.87
4:6:187:HIS:HE1	5:6:314:CLA:NA	1.73	0.87
3:5:156:TRP:HB2	5:5:314:CLA:CGA	2.07	0.84
3:5:167:LYS:HD2	5:5:314:CLA:HMA3	1.57	0.84
3:5:69:HIS:HE1	12:5:310:KC2:NC	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:167:LYS:HE3	5:5:314:CLA:HMA3	1.64	0.78
3:5:167:LYS:HE3	5:5:314:CLA:CHB	2.19	0.73
3:5:167:LYS:HG3	5:5:314:CLA:CMA	2.20	0.72
3:5:167:LYS:HE3	5:5:314:CLA:CMA	2.20	0.71
3:5:167:LYS:HG3	5:5:314:CLA:HMA1	1.73	0.71
3:5:174:GLN:HG3	5:5:314:CLA:HBB2	1.74	0.70
3:5:170:ILE:HG22	5:5:314:CLA:HBB1	1.74	0.69
7:5:304:A86:C35	5:5:314:CLA:H62	2.23	0.69
3:5:156:TRP:CE3	5:5:314:CLA:CBA	2.64	0.67
1:3:195:GLU:OE2	1:3:199:GLN:NE2	2.29	0.66
7:5:304:A86:C33	5:5:314:CLA:H93	2.26	0.66
5:3:602:CLA:H43	5:3:602:CLA:HMB2	1.79	0.65
1:3:138:ILE:HG21	5:3:604:CLA:HAA2	1.79	0.65
4:6:89:LEU:HB2	4:6:92:ALA:HB2	1.81	0.62
5:3:612:CLA:HBC2	5:4:314:CLA:HBC3	1.81	0.62
3:5:61:ARG:NH1	12:5:310:KC2:O2A	2.33	0.61
3:5:167:LYS:CG	5:5:314:CLA:HMA3	2.30	0.61
3:5:179:MET:HE3	5:5:309:CLA:HMC3	1.83	0.60
5:3:606:CLA:HBB2	5:3:611:CLA:NA	2.16	0.59
1:3:72:ASN:HB3	1:3:75:TYR:HB2	1.83	0.59
9:3:615:LMG:H292	5:4:312:CLA:H43	1.84	0.59
7:5:306:A86:O3	12:5:310:KC2:O1A	2.20	0.58
5:5:313:CLA:HMB1	5:5:313:CLA:HBB1	1.84	0.58
4:6:75:LEU:HD11	5:6:312:CLA:HBC1	1.86	0.57
2:4:123:PHE:HE2	5:4:314:CLA:HAB	1.70	0.57
5:3:607:CLA:HMB1	5:3:607:CLA:HBB1	1.88	0.56
3:5:92:ASP:HA	3:5:98:ALA:HA	1.88	0.56
4:6:169:ILE:HD11	6:6:313:KC1:CAD	2.35	0.56
3:5:156:TRP:HZ3	3:5:167:LYS:HD2	1.70	0.56
1:3:212:PHE:HE2	5:3:619:CLA:H43	1.71	0.56
4:6:39:GLN:NE2	4:6:172:ASN:OD1	2.38	0.56
3:5:82:ILE:HG21	5:5:311:CLA:HAC2	1.86	0.56
5:4:310:CLA:HMB1	5:4:310:CLA:HBB1	1.87	0.55
3:5:130:LEU:O	3:5:134:VAL:HB	2.07	0.55
4:6:39:GLN:NE2	5:6:306:CLA:O1D	2.39	0.54
3:5:156:TRP:HB2	5:5:314:CLA:CBA	2.38	0.54
4:6:142:PHE:CE1	4:6:145:ASP:HB2	2.43	0.54
3:5:71:ARG:HH12	3:5:171:GLU:CD	2.11	0.54
10:4:318:LHG:H302	10:4:318:LHG:H162	1.89	0.54
5:4:308:CLA:H101	5:4:314:CLA:H43	1.89	0.53
2:4:155:LEU:O	2:4:159:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:169:ILE:O	1:3:170:SER:OG	2.24	0.53
3:5:167:LYS:HE3	5:5:314:CLA:C3A	2.39	0.53
3:5:187:MET:HG3	5:5:316:CLA:HAC2	1.90	0.53
5:3:603:CLA:H93	5:4:308:CLA:H172	1.92	0.52
1:3:138:ILE:HG13	1:3:143:ILE:HD11	1.91	0.52
4:6:62:LEU:HB3	5:6:307:CLA:HMA1	1.92	0.52
3:5:156:TRP:HB2	5:5:314:CLA:HBA1	1.91	0.52
1:3:160:ARG:HD3	1:3:173:ILE:H	1.75	0.52
2:4:140:LEU:HD23	2:4:142:LEU:HD21	1.92	0.52
4:6:82:ILE:HD11	4:6:87:ILE:HD11	1.92	0.52
2:4:90:TYR:OH	5:4:308:CLA:O1A	2.27	0.51
4:6:187:HIS:HE1	5:6:314:CLA:C1A	2.22	0.51
3:5:160:SER:H	3:5:161:PRO:HD2	1.75	0.51
7:5:321:A86:O3	12:6:308:KC2:O1A	2.28	0.51
2:4:145:ASP:N	2:4:145:ASP:OD1	2.43	0.51
5:3:606:CLA:H51	5:3:612:CLA:H12	1.94	0.50
2:4:159:ARG:HH11	5:4:306:CLA:C1D	2.25	0.50
3:5:167:LYS:HZ2	5:5:314:CLA:H2A	1.76	0.50
5:3:603:CLA:HED1	5:3:603:CLA:H8	1.94	0.50
4:6:75:LEU:O	5:6:309:CLA:HMC3	2.12	0.50
5:4:309:CLA:H2	5:4:309:CLA:HED3	1.93	0.49
3:5:164:GLN:OE1	3:5:164:GLN:N	2.40	0.49
4:6:113:VAL:HG23	5:6:315:CLA:HMA1	1.94	0.49
3:5:155:GLY:O	3:5:158:LYS:NZ	2.46	0.48
3:5:156:TRP:CZ2	3:5:164:GLN:HG3	2.49	0.48
4:6:74:GLN:OE1	5:6:312:CLA:HMC3	2.14	0.48
5:3:602:CLA:HMB1	5:3:602:CLA:HBB1	1.96	0.48
1:3:230:SER:HA	1:3:233:PHE:CD2	2.49	0.48
1:3:157:ARG:HH21	5:3:606:CLA:HMA3	1.79	0.47
4:6:131:PHE:O	4:6:132:VAL:HB	2.15	0.47
4:6:93:ILE:HG22	4:6:99:LYS:HA	1.96	0.47
5:4:311:CLA:HBB1	5:4:311:CLA:HMB1	1.96	0.47
3:5:118:ALA:O	3:5:122:GLN:HG3	2.15	0.47
5:3:607:CLA:H72	7:3:613:A86:C29	2.44	0.47
7:6:302:A86:C24	5:6:310:CLA:HMD2	2.45	0.47
5:6:312:CLA:HED3	5:6:312:CLA:HBD	1.72	0.47
1:3:175:LEU:HB2	5:3:607:CLA:CAD	2.45	0.46
1:3:217:GLN:HG3	5:3:610:CLA:C4D	2.45	0.46
4:6:131:PHE:HA	4:6:134:LYS:HE3	1.97	0.46
5:3:606:CLA:H62	5:3:606:CLA:H41	1.58	0.46
3:5:167:LYS:CE	5:5:314:CLA:CMA	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:611:CLA:H41	5:3:611:CLA:H62	1.55	0.46
10:4:318:LHG:H122	10:4:318:LHG:H151	1.58	0.46
1:3:161:ILE:HG12	1:3:168:ARG:HE	1.82	0.45
7:6:301:A86:O	5:6:306:CLA:HAC2	2.17	0.45
10:3:618:LHG:H112	5:3:619:CLA:H2	1.97	0.45
2:4:123:PHE:CE2	5:4:314:CLA:HAB	2.49	0.45
5:3:602:CLA:H102	5:3:602:CLA:H13	1.88	0.45
4:6:145:ASP:OD2	4:6:147:ARG:NH1	2.50	0.45
4:6:178:MET:HE3	5:6:307:CLA:HAB	1.98	0.45
5:5:312:CLA:HBB2	9:5:319:LMG:H131	1.98	0.45
1:3:230:SER:OG	1:3:231:PRO:HD3	2.17	0.45
4:6:166:LYS:NZ	6:6:313:KC1:O1A	2.36	0.44
5:5:311:CLA:H92	5:5:311:CLA:H61	1.79	0.44
5:3:606:CLA:H162	5:3:606:CLA:H121	1.85	0.44
3:5:70:GLY:O	3:5:74:GLN:HG2	2.18	0.44
4:6:92:ALA:HB3	4:6:100:PHE:HB3	2.00	0.44
5:4:308:CLA:H121	5:4:308:CLA:H162	1.74	0.44
3:5:67:LEU:HD21	3:5:71:ARG:HE	1.82	0.44
3:5:72:ILE:HD12	5:5:313:CLA:HMD3	2.00	0.44
10:3:618:LHG:H151	10:3:618:LHG:H182	1.68	0.44
4:6:90:PRO:HA	4:6:100:PHE:CE1	2.52	0.44
1:3:50:SER:OG	1:3:51:LEU:N	2.50	0.43
5:3:611:CLA:H3A	5:3:611:CLA:HBA2	1.72	0.43
2:4:173:SER:HB3	5:4:315:CLA:HMD3	2.00	0.43
5:3:605:CLA:H41	5:3:605:CLA:H61	1.70	0.43
3:5:166:ASN:OD1	3:5:167:LYS:N	2.51	0.43
5:4:315:CLA:HBA1	5:4:315:CLA:H3A	1.84	0.43
3:5:93:ILE:HB	3:5:99:PHE:CE1	2.54	0.43
3:5:127:ILE:O	3:5:130:LEU:HG	2.18	0.43
5:3:602:CLA:H112	5:3:602:CLA:H91	1.78	0.43
11:3:620:DGD:HB71	11:3:620:DGD:HB42	1.54	0.43
5:3:606:CLA:H61	5:3:606:CLA:H93	1.79	0.43
3:5:174:GLN:HG3	5:5:314:CLA:CBB	2.47	0.43
4:6:141:GLU:OE2	4:6:147:ARG:NH2	2.35	0.43
2:4:166:LEU:HA	2:4:166:LEU:HD23	1.80	0.42
3:5:73:ALA:HB1	3:5:179:MET:HA	2.01	0.42
5:3:601:CLA:HBA1	5:3:601:CLA:H3A	1.70	0.42
5:5:312:CLA:H3A	5:5:312:CLA:HBA2	1.29	0.42
5:6:306:CLA:H62	5:6:306:CLA:H41	1.78	0.42
4:6:36:LEU:HD21	4:6:167:ARG:HH21	1.84	0.42
5:3:603:CLA:H112	5:3:603:CLA:H151	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:50:MET:HE3	4:6:50:MET:HB3	1.96	0.42
10:3:618:LHG:H271	10:3:618:LHG:H242	1.66	0.42
2:4:88:PHE:O	2:4:99:THR:OG1	2.32	0.42
2:4:157:HIS:HE1	5:4:312:CLA:C4D	2.33	0.42
3:5:93:ILE:HG23	3:5:94:SER:H	1.83	0.42
3:5:132:THR:HG23	3:5:133:ARG:HG2	2.02	0.42
5:3:603:CLA:H161	5:3:603:CLA:H141	1.73	0.41
4:6:93:ILE:HB	4:6:97:GLY:O	2.20	0.41
5:6:312:CLA:HBB1	5:6:312:CLA:HMB1	2.03	0.41
5:5:313:CLA:H62	5:5:313:CLA:H41	1.75	0.41
1:3:172:ASP:HB3	1:3:173:ILE:H	1.56	0.41
2:4:54:ILE:HB	2:4:55:SER:H	1.69	0.41
4:6:71:ARG:HD3	5:6:312:CLA:CHD	2.51	0.41
4:6:137:THR:HG21	4:6:149:GLY:HA3	2.02	0.41
5:6:307:CLA:H3A	5:6:307:CLA:HBA2	1.44	0.41
2:4:75:LEU:HD23	2:4:75:LEU:HA	1.90	0.41
5:4:311:CLA:H61	5:4:311:CLA:H41	1.54	0.41
3:5:42:LEU:HD12	3:5:42:LEU:O	2.21	0.41
3:5:159:GLN:OE1	3:5:163:TRP:HB3	2.21	0.41
5:5:316:CLA:HED2	5:5:316:CLA:HBD	1.88	0.41
4:6:74:GLN:HE21	4:6:174:GLY:N	2.18	0.41
1:3:175:LEU:HA	1:3:175:LEU:HD23	1.67	0.41
4:6:169:ILE:HD11	6:6:313:KC1:CBD	2.50	0.41
2:4:182:ASP:O	2:4:184:LEU:N	2.54	0.40
5:3:611:CLA:HHC	5:3:611:CLA:HBB1	2.03	0.40
4:6:39:GLN:HG3	4:6:40:PRO:HD2	2.02	0.40
1:3:209:LEU:HD23	1:3:209:LEU:HA	1.92	0.40
5:3:619:CLA:H2A	5:3:619:CLA:O1D	2.22	0.40
2:4:50:LEU:HD13	5:4:306:CLA:H42	2.03	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	3	218/220 (99%)	196 (90%)	19 (9%)	3 (1%)	11 46
2	4	161/163 (99%)	143 (89%)	16 (10%)	2 (1%)	13 49
3	5	158/160 (99%)	141 (89%)	14 (9%)	3 (2%)	8 39
4	6	166/168 (99%)	148 (89%)	16 (10%)	2 (1%)	13 49
All	All	703/711 (99%)	628 (89%)	65 (9%)	10 (1%)	15 46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	173	ILE
3	5	41	PRO
2	4	54	ILE
3	5	157	ASP
4	6	196	ILE
3	5	160	SER
1	3	37	ALA
1	3	170	SER
4	6	132	VAL
2	4	188	ILE

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	3	171/171 (100%)	168 (98%)	3 (2%)	59 82
2	4	128/129 (99%)	127 (99%)	1 (1%)	81 93
3	5	120/123 (98%)	116 (97%)	4 (3%)	38 71
4	6	131/131 (100%)	125 (95%)	6 (5%)	27 63
All	All	550/554 (99%)	536 (98%)	14 (2%)	50 77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	46	THR

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Mol	Chain	Res	Type
1	3	119	ASN
1	3	217	GLN
2	4	126	CYS
3	5	53	ARG
3	5	157	ASP
3	5	159	GLN
3	5	172	LEU
4	6	42	LEU
4	6	50	MET
4	6	134	LYS
4	6	136	VAL
4	6	169	ILE
4	6	171	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	5	173	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

74 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	$\#\|Z\| > 2$
8	DD6	4	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.77	15 (28%)
5	CLA	5	311	-	55,63,73	1.58	5 (9%)	64,101,113	1.48	6 (9%)
6	KC1	5	315	-	48,53,53	1.52	7 (14%)	55,89,89	1.79	11 (20%)
5	CLA	6	307	4	54,62,73	1.60	7 (12%)	62,99,113	1.49	7 (11%)
5	CLA	3	605	-	65,73,73	1.48	6 (9%)	76,113,113	1.35	8 (10%)
7	A86	5	321	-	44,50,50	1.25	4 (9%)	51,76,76	9.10	23 (45%)
5	CLA	6	311	4	65,73,73	1.49	6 (9%)	76,113,113	1.33	6 (7%)
7	A86	5	301	-	44,50,50	1.24	4 (9%)	51,76,76	11.32	26 (50%)
5	CLA	5	313	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	6 (7%)
12	KC2	6	308	-	48,53,53	1.90	9 (18%)	54,89,89	2.19	17 (31%)
5	CLA	3	619	-	55,63,73	1.57	7 (12%)	64,101,113	1.49	7 (10%)
5	CLA	3	603	-	65,73,73	1.48	7 (10%)	76,113,113	1.36	7 (9%)
5	CLA	4	313	2	41,49,73	1.80	6 (14%)	47,84,113	1.70	9 (19%)
12	KC2	4	307	-	48,53,53	1.84	9 (18%)	54,89,89	2.32	15 (27%)
5	CLA	3	607	1	65,73,73	1.45	7 (10%)	76,113,113	1.42	8 (10%)
5	CLA	4	316	-	52,60,73	1.64	7 (13%)	60,97,113	1.52	7 (11%)
7	A86	5	303	-	44,50,50	1.23	3 (6%)	51,76,76	11.73	23 (45%)
5	CLA	4	315	-	47,55,73	1.71	7 (14%)	54,91,113	1.56	7 (12%)
5	CLA	4	308	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	7 (9%)
5	CLA	5	317	-	37,46,73	1.89	6 (16%)	44,80,113	1.77	8 (18%)
6	KC1	3	609	-	48,53,53	1.54	7 (14%)	55,89,89	1.89	9 (16%)
5	CLA	3	606	1	65,73,73	1.49	7 (10%)	76,113,113	1.33	7 (9%)
7	A86	4	302	-	44,50,50	1.24	4 (9%)	51,76,76	12.51	28 (54%)
7	A86	5	305	-	43,49,50	1.42	5 (11%)	48,74,76	7.05	25 (52%)
5	CLA	3	611	-	56,64,73	1.62	7 (12%)	65,102,113	1.47	8 (12%)
5	CLA	4	314	2	56,64,73	1.55	6 (10%)	65,102,113	1.49	8 (12%)
5	CLA	5	316	-	41,49,73	1.84	6 (14%)	47,84,113	1.66	9 (19%)
5	CLA	5	312	3	46,54,73	1.76	7 (15%)	53,90,113	1.53	7 (13%)
11	DGD	3	620	-	38,38,67	0.65	1 (2%)	40,40,81	1.48	6 (15%)
5	CLA	3	601	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	8 (10%)
5	CLA	6	306	-	53,61,73	1.62	7 (13%)	61,98,113	1.52	7 (11%)
6	KC1	6	313	4	48,53,53	1.53	7 (14%)	55,89,89	1.84	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	A86	6	303	-	44,50,50	1.24	4 (9%)	51,76,76	8.48	24 (47%)
7	A86	5	306	-	44,50,50	1.24	4 (9%)	51,76,76	7.71	25 (49%)
9	LMG	3	615	-	31,31,55	0.97	0	39,39,63	1.28	5 (12%)
7	A86	6	305	-	44,50,50	1.21	3 (6%)	51,76,76	8.91	23 (45%)
5	CLA	5	309	3	55,63,73	1.59	7 (12%)	64,101,113	1.52	9 (14%)
9	LMG	3	616	-	23,23,55	1.25	3 (13%)	31,31,63	1.31	5 (16%)
10	LHG	3	618	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
12	KC2	5	310	-	48,53,53	1.85	10 (20%)	54,89,89	2.32	16 (29%)
5	CLA	5	308	-	46,54,73	1.73	6 (13%)	53,90,113	1.56	6 (11%)
5	CLA	6	315	-	38,46,73	2.38	8 (21%)	47,79,113	1.60	9 (19%)
5	CLA	3	612	-	61,69,73	1.50	6 (9%)	71,108,113	1.40	7 (9%)
7	A86	4	301	-	44,50,50	1.25	4 (9%)	51,76,76	9.56	27 (52%)
5	CLA	6	309	-	52,60,73	1.63	6 (11%)	60,97,113	1.51	8 (13%)
7	A86	5	307	-	44,50,50	1.23	4 (9%)	51,76,76	11.49	23 (45%)
5	CLA	3	608	10	51,59,73	1.66	7 (13%)	59,96,113	1.47	7 (11%)
5	CLA	6	312	-	46,54,73	1.73	6 (13%)	53,90,113	1.67	7 (13%)
10	LHG	3	617	5	26,26,48	0.85	1 (3%)	29,32,54	1.38	3 (10%)
7	A86	4	304	-	44,50,50	1.26	5 (11%)	51,76,76	11.03	27 (52%)
10	LHG	5	318	-	32,32,48	0.83	2 (6%)	36,37,54	1.70	6 (16%)
5	CLA	4	310	-	46,54,73	1.69	7 (15%)	53,90,113	1.60	6 (11%)
7	A86	3	613	-	44,50,50	1.25	3 (6%)	51,76,76	2.32	17 (33%)
13	LMT	5	320	-	32,32,36	1.23	5 (15%)	43,43,47	0.93	1 (2%)
5	CLA	4	305	-	55,63,73	1.58	7 (12%)	64,101,113	1.48	7 (10%)
5	CLA	4	306	2	65,73,73	1.45	7 (10%)	76,113,113	1.38	8 (10%)
7	A86	5	304	-	44,50,50	1.22	3 (6%)	51,76,76	11.21	23 (45%)
5	CLA	3	610	1	41,49,73	1.76	8 (19%)	47,84,113	1.75	8 (17%)
5	CLA	6	310	-	46,54,73	1.77	6 (13%)	53,90,113	1.44	7 (13%)
5	CLA	6	314	-	41,49,73	1.85	8 (19%)	47,84,113	1.84	9 (19%)
5	CLA	3	602	-	65,73,73	1.44	7 (10%)	76,113,113	1.45	9 (11%)
7	A86	6	301	-	44,50,50	1.25	5 (11%)	51,76,76	11.60	24 (47%)
5	CLA	3	604	-	48,56,73	1.69	7 (14%)	55,92,113	1.58	8 (14%)
10	LHG	4	318	-	48,48,48	0.62	1 (2%)	51,54,54	1.28	6 (11%)
8	DD6	3	614	-	39,45,45	1.99	3 (7%)	52,67,67	1.98	15 (28%)
7	A86	6	304	-	44,50,50	1.24	3 (6%)	51,76,76	11.87	21 (41%)
7	A86	5	302	-	44,50,50	1.25	5 (11%)	51,76,76	12.11	24 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	A86	6	302	-	44,50,50	1.19	3 (6%)	51,76,76	11.15	25 (49%)
5	CLA	5	314	3	55,63,73	1.62	6 (10%)	64,101,113	1.55	7 (10%)
5	CLA	4	309	2	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
5	CLA	4	311	2	60,68,73	1.50	7 (11%)	70,107,113	1.46	8 (11%)
5	CLA	4	312	-	51,59,73	1.64	6 (11%)	59,96,113	1.61	9 (15%)
13	LMT	4	317	-	36,36,36	1.19	6 (16%)	47,47,47	1.00	1 (2%)
9	LMG	5	319	-	31,31,55	0.96	1 (3%)	39,39,63	1.34	6 (15%)

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
8	DD6	4	303	-	-	3/26/80/80	0/3/3/3
5	CLA	5	311	-	1/1/13/20	8/25/103/115	-
6	KC1	5	315	-	-	6/15/71/71	-
5	CLA	6	307	4	1/1/12/20	5/24/102/115	-
5	CLA	3	605	-	1/1/15/20	13/37/115/115	-
7	A86	5	321	-	-	8/34/90/90	0/3/3/3
5	CLA	6	311	4	1/1/15/20	7/37/115/115	-
7	A86	5	301	-	-	11/34/90/90	0/3/3/3
5	CLA	5	313	-	1/1/15/20	11/37/115/115	-
12	KC2	6	308	-	-	10/15/71/71	-
5	CLA	3	619	-	1/1/13/20	10/25/103/115	-
5	CLA	3	603	-	1/1/15/20	10/37/115/115	-
5	CLA	4	313	2	1/1/10/20	4/8/86/115	-
12	KC2	4	307	-	-	8/15/71/71	-
5	CLA	3	607	1	1/1/15/20	15/37/115/115	-
5	CLA	4	316	-	1/1/12/20	4/22/100/115	-
7	A86	5	303	-	-	9/34/90/90	0/3/3/3
5	CLA	4	315	-	1/1/11/20	4/16/94/115	-
5	CLA	4	308	-	1/1/15/20	9/37/115/115	-
5	CLA	5	317	-	1/1/9/20	0/2/80/115	-
6	KC1	3	609	-	-	9/15/71/71	-
5	CLA	3	606	1	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	A86	4	302	-	-	9/34/90/90	0/3/3/3
7	A86	5	305	-	-	8/33/89/90	0/3/3/3
5	CLA	3	611	-	1/1/13/20	9/27/105/115	-
5	CLA	4	314	2	1/1/13/20	9/27/105/115	-
5	CLA	5	316	-	1/1/10/20	2/8/86/115	-
5	CLA	5	312	3	1/1/11/20	9/15/93/115	-
11	DGD	3	620	-	-	22/40/40/95	-
5	CLA	3	601	-	1/1/15/20	17/37/115/115	-
5	CLA	6	306	-	1/1/12/20	8/23/101/115	-
6	KC1	6	313	4	-	5/15/71/71	-
7	A86	6	303	-	-	8/34/90/90	0/3/3/3
7	A86	5	306	-	-	8/34/90/90	0/3/3/3
9	LMG	3	615	-	-	8/26/46/70	0/1/1/1
7	A86	6	305	-	-	8/34/90/90	0/3/3/3
5	CLA	5	309	3	1/1/13/20	6/25/103/115	-
9	LMG	3	616	-	-	6/16/36/70	0/1/1/1
10	LHG	3	618	-	-	15/53/53/53	-
12	KC2	5	310	-	-	3/15/71/71	-
5	CLA	5	308	-	1/1/11/20	7/15/93/115	-
5	CLA	6	315	-	1/1/9/20	3/8/80/115	-
5	CLA	3	612	-	1/1/14/20	16/33/111/115	-
7	A86	4	301	-	-	10/34/90/90	0/3/3/3
5	CLA	6	309	-	1/1/12/20	8/22/100/115	-
7	A86	5	307	-	-	8/34/90/90	0/3/3/3
5	CLA	3	608	10	1/1/12/20	6/21/99/115	-
5	CLA	6	312	-	1/1/11/20	6/15/93/115	-
10	LHG	3	617	5	-	13/31/31/53	-
7	A86	4	304	-	-	8/34/90/90	0/3/3/3
10	LHG	5	318	-	-	11/34/34/53	-
5	CLA	4	310	-	1/1/11/20	6/15/93/115	-
7	A86	3	613	-	-	5/34/90/90	0/3/3/3
13	LMT	5	320	-	-	8/17/57/61	0/2/2/2
5	CLA	4	305	-	1/1/13/20	7/25/103/115	-
5	CLA	4	306	2	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	A86	5	304	-	-	8/34/90/90	0/3/3/3
5	CLA	3	610	1	1/1/10/20	0/8/86/115	-
5	CLA	6	310	-	1/1/11/20	9/15/93/115	-
5	CLA	6	314	-	1/1/10/20	0/8/86/115	-
5	CLA	3	602	-	1/1/15/20	13/37/115/115	-
7	A86	6	301	-	-	7/34/90/90	0/3/3/3
5	CLA	3	604	-	1/1/11/20	9/17/95/115	-
10	LHG	4	318	-	-	34/53/53/53	-
8	DD6	3	614	-	-	5/26/80/80	0/3/3/3
7	A86	6	304	-	-	9/34/90/90	0/3/3/3
7	A86	5	302	-	-	9/34/90/90	0/3/3/3
7	A86	6	302	-	-	8/34/90/90	0/3/3/3
5	CLA	5	314	3	1/1/13/20	9/25/103/115	-
5	CLA	4	309	2	1/1/15/20	5/37/115/115	-
5	CLA	4	311	2	1/1/14/20	15/31/109/115	-
5	CLA	4	312	-	1/1/12/20	5/21/99/115	-
13	LMT	4	317	-	-	11/21/61/61	0/2/2/2
9	LMG	5	319	-	-	13/26/46/70	0/1/1/1

All (401) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	4	303	DD6	C29-C27	-8.61	1.26	1.42
5	6	315	CLA	C3B-C4B	8.56	1.49	1.39
8	3	614	DD6	C29-C27	-8.43	1.26	1.42
5	3	611	CLA	C4B-NB	7.73	1.42	1.35
5	6	310	CLA	C4B-NB	7.71	1.42	1.35
8	3	614	DD6	C30-C31	-7.71	1.26	1.42
8	4	303	DD6	C30-C31	-7.64	1.26	1.42
5	5	314	CLA	C4B-NB	7.44	1.41	1.35
5	6	315	CLA	C4B-NB	7.40	1.41	1.35
5	6	311	CLA	C4B-NB	7.39	1.41	1.35
5	5	312	CLA	C4B-NB	7.37	1.41	1.35
5	3	605	CLA	C4B-NB	7.34	1.41	1.35
5	5	316	CLA	C4B-NB	7.33	1.41	1.35
5	3	606	CLA	C4B-NB	7.28	1.41	1.35
5	3	603	CLA	C4B-NB	7.26	1.41	1.35
5	5	317	CLA	C4B-NB	7.25	1.41	1.35
5	5	308	CLA	C4B-NB	7.23	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	6	312	CLA	C4B-NB	7.22	1.41	1.35
5	5	309	CLA	C4B-NB	7.21	1.41	1.35
5	6	314	CLA	C4B-NB	7.17	1.41	1.35
5	5	313	CLA	C4B-NB	7.13	1.41	1.35
5	6	309	CLA	C4B-NB	7.12	1.41	1.35
5	4	315	CLA	C4B-NB	7.12	1.41	1.35
5	3	608	CLA	C4B-NB	7.11	1.41	1.35
5	3	604	CLA	C4B-NB	7.11	1.41	1.35
5	3	612	CLA	C4B-NB	7.10	1.41	1.35
5	6	307	CLA	C4B-NB	7.09	1.41	1.35
5	4	305	CLA	C4B-NB	7.08	1.41	1.35
5	6	306	CLA	C4B-NB	7.07	1.41	1.35
5	4	312	CLA	C4B-NB	7.05	1.41	1.35
5	5	311	CLA	C4B-NB	7.05	1.41	1.35
5	4	316	CLA	C4B-NB	7.05	1.41	1.35
5	4	309	CLA	C4B-NB	7.04	1.41	1.35
5	3	607	CLA	C4B-NB	7.01	1.41	1.35
5	3	619	CLA	C4B-NB	7.01	1.41	1.35
5	4	308	CLA	C4B-NB	6.99	1.41	1.35
5	4	313	CLA	C4B-NB	6.98	1.41	1.35
5	3	601	CLA	C4B-NB	6.96	1.41	1.35
5	4	314	CLA	C4B-NB	6.95	1.41	1.35
5	4	306	CLA	C4B-NB	6.93	1.41	1.35
5	4	310	CLA	C4B-NB	6.92	1.41	1.35
6	6	313	KC1	C4D-CHA	-6.90	1.36	1.45
5	4	311	CLA	C4B-NB	6.88	1.41	1.35
5	3	602	CLA	C4B-NB	6.79	1.41	1.35
5	3	610	CLA	C4B-NB	6.68	1.41	1.35
12	6	308	KC2	C4D-CHA	-6.66	1.36	1.45
12	5	310	KC2	C4D-CHA	-6.56	1.36	1.45
6	5	315	KC1	C4D-CHA	-6.54	1.36	1.45
6	3	609	KC1	C4D-CHA	-6.53	1.36	1.45
12	4	307	KC2	C4D-CHA	-6.48	1.37	1.45
7	5	305	A86	O4-C38	5.70	1.45	1.33
12	6	308	KC2	CHD-C4C	5.37	1.48	1.35
12	4	307	KC2	CHD-C4C	5.13	1.48	1.35
12	5	310	KC2	CHD-C4C	5.11	1.48	1.35
6	5	315	KC1	MG-NB	-4.81	1.96	2.05
7	6	302	A86	O4-C38	4.77	1.46	1.35
7	5	302	A86	O4-C38	4.76	1.46	1.35
7	6	304	A86	O4-C38	4.75	1.45	1.35
7	5	304	A86	O4-C38	4.73	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	4	301	A86	O4-C38	4.73	1.45	1.35
7	5	307	A86	O4-C38	4.73	1.45	1.35
7	6	305	A86	O4-C38	4.73	1.45	1.35
7	3	613	A86	O4-C38	4.71	1.45	1.35
7	4	302	A86	O4-C38	4.68	1.45	1.35
7	5	306	A86	O4-C38	4.66	1.45	1.35
7	6	301	A86	O4-C38	4.66	1.45	1.35
7	5	301	A86	O4-C38	4.66	1.45	1.35
7	5	321	A86	O4-C38	4.63	1.45	1.35
7	5	303	A86	O4-C38	4.61	1.45	1.35
7	4	304	A86	O4-C38	4.56	1.45	1.35
6	3	609	KC1	MG-NB	-4.48	1.96	2.05
6	6	313	KC1	MG-NB	-4.46	1.96	2.05
7	6	303	A86	O4-C38	4.46	1.45	1.35
12	6	308	KC2	MG-NB	-4.34	1.97	2.05
12	6	308	KC2	CHC-C4B	4.21	1.46	1.38
12	6	308	KC2	CHC-C1C	4.17	1.48	1.39
12	5	310	KC2	CHC-C4B	4.03	1.46	1.38
5	5	314	CLA	C1D-ND	4.02	1.42	1.37
12	5	310	KC2	MG-NB	-3.99	1.97	2.05
12	4	307	KC2	CHC-C4B	3.97	1.46	1.38
12	4	307	KC2	CHC-C1C	3.91	1.48	1.39
5	6	312	CLA	C1D-ND	3.91	1.42	1.37
12	4	307	KC2	MG-NB	-3.88	1.98	2.05
12	5	310	KC2	CHC-C1C	3.88	1.48	1.39
5	5	317	CLA	C1D-ND	3.87	1.42	1.37
7	6	303	A86	C30-C29	-3.81	1.25	1.32
7	5	301	A86	C30-C29	-3.79	1.25	1.32
7	3	613	A86	C30-C29	-3.78	1.25	1.32
5	3	605	CLA	C1D-ND	3.78	1.42	1.37
5	4	313	CLA	C1D-ND	3.77	1.42	1.37
5	5	312	CLA	C1D-ND	3.77	1.42	1.37
5	6	306	CLA	C1D-ND	3.77	1.42	1.37
7	5	306	A86	C30-C29	-3.75	1.25	1.32
7	5	305	A86	C30-C29	-3.75	1.25	1.32
7	6	301	A86	C30-C29	-3.75	1.25	1.32
5	5	316	CLA	C1D-ND	3.74	1.42	1.37
5	5	308	CLA	C1D-ND	3.73	1.42	1.37
7	5	321	A86	C30-C29	-3.72	1.25	1.32
7	5	307	A86	C30-C29	-3.71	1.25	1.32
5	6	315	CLA	C1D-ND	3.71	1.42	1.37
7	5	302	A86	C30-C29	-3.69	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	4	304	A86	C30-C29	-3.69	1.25	1.32
5	4	315	CLA	C1D-ND	3.69	1.42	1.37
5	6	314	CLA	C1D-ND	3.68	1.42	1.37
5	5	313	CLA	C1D-ND	3.67	1.42	1.37
5	6	309	CLA	C1D-ND	3.66	1.42	1.37
5	5	311	CLA	C1D-ND	3.66	1.42	1.37
7	4	302	A86	C30-C29	-3.66	1.25	1.32
7	5	303	A86	C30-C29	-3.66	1.25	1.32
5	5	309	CLA	C1D-ND	3.64	1.42	1.37
5	6	311	CLA	C1D-ND	3.64	1.42	1.37
5	3	604	CLA	C1D-ND	3.63	1.42	1.37
5	4	309	CLA	C1D-ND	3.62	1.42	1.37
5	6	315	CLA	C4B-CHC	-3.62	1.36	1.43
5	4	306	CLA	C1D-ND	3.62	1.42	1.37
7	6	304	A86	C30-C29	-3.61	1.26	1.32
5	3	603	CLA	C1D-ND	3.60	1.42	1.37
5	3	611	CLA	C1D-ND	3.60	1.42	1.37
5	4	308	CLA	C1D-ND	3.60	1.42	1.37
5	6	307	CLA	C1D-ND	3.59	1.42	1.37
7	4	301	A86	C30-C29	-3.59	1.26	1.32
5	4	316	CLA	C1D-ND	3.58	1.42	1.37
5	4	311	CLA	C1D-ND	3.57	1.42	1.37
5	3	612	CLA	C1D-ND	3.57	1.42	1.37
5	4	310	CLA	C1D-ND	3.55	1.42	1.37
5	3	602	CLA	C1D-ND	3.53	1.42	1.37
5	6	314	CLA	C4D-ND	-3.53	1.32	1.37
5	3	619	CLA	C1D-ND	3.53	1.42	1.37
5	3	608	CLA	C1D-ND	3.53	1.42	1.37
5	3	606	CLA	C1D-ND	3.52	1.42	1.37
5	3	607	CLA	C1D-ND	3.51	1.42	1.37
7	5	304	A86	C30-C29	-3.51	1.26	1.32
5	4	312	CLA	C1D-ND	3.51	1.42	1.37
5	4	314	CLA	C1D-ND	3.50	1.42	1.37
5	3	601	CLA	C1D-ND	3.48	1.42	1.37
7	6	305	A86	C30-C29	-3.48	1.26	1.32
5	4	305	CLA	C1D-ND	3.48	1.42	1.37
7	6	302	A86	C30-C29	-3.45	1.26	1.32
5	6	310	CLA	C1D-ND	3.40	1.42	1.37
5	3	610	CLA	C1D-ND	3.39	1.42	1.37
5	4	312	CLA	C4D-ND	-3.35	1.33	1.37
5	3	607	CLA	C4D-ND	-3.26	1.33	1.37
7	5	305	A86	O4-C34	-3.26	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	6	310	CLA	CHC-C1C	3.25	1.43	1.35
5	3	608	CLA	C4D-ND	-3.24	1.33	1.37
5	4	311	CLA	C4D-ND	-3.22	1.33	1.37
5	3	610	CLA	C4D-ND	-3.21	1.33	1.37
5	4	306	CLA	C4D-ND	-3.20	1.33	1.37
5	3	601	CLA	C4D-ND	-3.19	1.33	1.37
5	3	606	CLA	CHC-C1C	3.16	1.43	1.35
5	4	305	CLA	C4D-ND	-3.16	1.33	1.37
5	3	602	CLA	C4D-ND	-3.16	1.33	1.37
5	4	308	CLA	C4D-ND	-3.15	1.33	1.37
5	4	316	CLA	C4D-ND	-3.14	1.33	1.37
5	5	317	CLA	CHC-C1C	3.13	1.43	1.35
5	3	606	CLA	C4D-ND	-3.13	1.33	1.37
5	6	312	CLA	C4D-ND	-3.12	1.33	1.37
5	6	312	CLA	CHC-C1C	3.12	1.43	1.35
5	4	315	CLA	C4D-ND	-3.11	1.33	1.37
5	4	314	CLA	C4D-ND	-3.11	1.33	1.37
5	5	309	CLA	CHC-C1C	3.11	1.42	1.35
5	3	619	CLA	C4D-ND	-3.11	1.33	1.37
5	5	314	CLA	CHC-C1C	3.11	1.42	1.35
5	3	612	CLA	C4D-ND	-3.10	1.33	1.37
5	6	309	CLA	CHC-C1C	3.10	1.42	1.35
5	4	311	CLA	CHC-C1C	3.10	1.42	1.35
5	6	315	CLA	C4D-ND	-3.10	1.33	1.37
5	6	311	CLA	C4D-ND	-3.10	1.33	1.37
5	3	605	CLA	CHC-C1C	3.10	1.42	1.35
5	6	315	CLA	CHC-C1C	3.10	1.42	1.35
5	4	313	CLA	C4D-ND	-3.09	1.33	1.37
5	4	313	CLA	CHC-C1C	3.09	1.42	1.35
5	5	313	CLA	CHC-C1C	3.09	1.42	1.35
5	3	604	CLA	C4D-ND	-3.09	1.33	1.37
5	5	316	CLA	CHC-C1C	3.09	1.42	1.35
5	4	315	CLA	CHC-C1C	3.08	1.42	1.35
5	4	310	CLA	C4D-ND	-3.08	1.33	1.37
5	5	312	CLA	C4D-ND	-3.08	1.33	1.37
5	4	314	CLA	CHC-C1C	3.08	1.42	1.35
5	6	311	CLA	CHC-C1C	3.07	1.42	1.35
5	6	307	CLA	CHC-C1C	3.07	1.42	1.35
5	4	309	CLA	C4D-ND	-3.07	1.33	1.37
5	4	306	CLA	CHC-C1C	3.07	1.42	1.35
5	4	312	CLA	CHC-C1C	3.06	1.42	1.35
5	3	611	CLA	C4D-ND	-3.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	312	CLA	CHC-C1C	3.06	1.42	1.35
5	3	607	CLA	CHC-C1C	3.06	1.42	1.35
5	4	316	CLA	CHC-C1C	3.06	1.42	1.35
5	6	307	CLA	C4D-ND	-3.06	1.33	1.37
5	3	611	CLA	CHC-C1C	3.05	1.42	1.35
5	5	308	CLA	CHC-C1C	3.05	1.42	1.35
5	5	313	CLA	C4D-ND	-3.05	1.33	1.37
5	3	603	CLA	C4D-ND	-3.05	1.33	1.37
5	5	316	CLA	C4D-ND	-3.04	1.33	1.37
5	4	309	CLA	CHC-C1C	3.04	1.42	1.35
5	5	309	CLA	C4D-ND	-3.04	1.33	1.37
5	5	311	CLA	C4D-ND	-3.04	1.33	1.37
5	5	308	CLA	C4D-ND	-3.03	1.33	1.37
5	3	612	CLA	CHC-C1C	3.03	1.42	1.35
5	3	604	CLA	CHC-C1C	3.03	1.42	1.35
5	4	310	CLA	CHC-C1C	3.03	1.42	1.35
5	5	311	CLA	CHC-C1C	3.02	1.42	1.35
5	4	308	CLA	CHC-C1C	3.01	1.42	1.35
5	3	602	CLA	CHC-C1C	3.01	1.42	1.35
5	3	603	CLA	CHC-C1C	3.01	1.42	1.35
5	4	305	CLA	CHC-C1C	3.00	1.42	1.35
6	3	609	KC1	C4B-NB	-3.00	1.34	1.37
5	6	306	CLA	C4D-ND	-3.00	1.33	1.37
5	3	610	CLA	CHC-C1C	3.00	1.42	1.35
5	6	309	CLA	C4D-ND	-3.00	1.33	1.37
5	3	619	CLA	CHC-C1C	3.00	1.42	1.35
5	3	601	CLA	CHC-C1C	2.99	1.42	1.35
5	3	608	CLA	CHC-C1C	2.99	1.42	1.35
5	6	314	CLA	CHC-C1C	2.97	1.42	1.35
5	5	314	CLA	C4D-ND	-2.97	1.33	1.37
6	3	609	KC1	CBA-CGA	-2.94	1.41	1.48
5	6	306	CLA	CHC-C1C	2.94	1.42	1.35
5	6	310	CLA	C4D-ND	-2.94	1.33	1.37
5	3	605	CLA	C4D-ND	-2.94	1.33	1.37
12	5	310	KC2	CBA-CGA	-2.90	1.41	1.48
5	5	317	CLA	C4D-ND	-2.88	1.33	1.37
6	5	315	KC1	C4B-NB	-2.87	1.34	1.37
9	3	616	LMG	C4-C5	2.87	1.59	1.53
12	4	307	KC2	CBA-CGA	-2.85	1.41	1.48
6	6	313	KC1	CBA-CGA	-2.84	1.41	1.48
6	5	315	KC1	CBA-CGA	-2.82	1.42	1.48
12	6	308	KC2	CBA-CGA	-2.78	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	313	KC1	C4B-NB	-2.69	1.34	1.37
13	5	320	LMT	O3'-C3'	-2.68	1.36	1.43
6	3	609	KC1	C1B-NB	-2.64	1.34	1.37
13	4	317	LMT	O3'-C3'	-2.63	1.36	1.43
8	4	303	DD6	O1-C20	-2.60	1.42	1.46
6	3	609	KC1	C4A-C3A	-2.60	1.39	1.44
5	4	313	CLA	CMB-C2B	-2.60	1.46	1.51
7	4	304	A86	O1-C20	-2.59	1.42	1.46
7	4	301	A86	O1-C20	-2.59	1.42	1.46
5	3	608	CLA	CMB-C2B	-2.58	1.46	1.51
5	3	611	CLA	CMB-C2B	-2.58	1.46	1.51
5	3	606	CLA	CMB-C2B	-2.57	1.46	1.51
5	3	602	CLA	CMB-C2B	-2.56	1.46	1.51
5	4	308	CLA	CMB-C2B	-2.56	1.46	1.51
5	4	312	CLA	CMB-C2B	-2.56	1.46	1.51
5	3	603	CLA	CMB-C2B	-2.55	1.46	1.51
5	6	314	CLA	CMB-C2B	-2.54	1.46	1.51
5	4	306	CLA	CMB-C2B	-2.54	1.46	1.51
5	3	601	CLA	CMB-C2B	-2.53	1.46	1.51
10	3	617	LHG	O7-C5	-2.52	1.40	1.46
5	4	314	CLA	CMB-C2B	-2.51	1.46	1.51
5	4	315	CLA	CMB-C2B	-2.51	1.46	1.51
5	3	619	CLA	CMB-C2B	-2.51	1.46	1.51
5	4	316	CLA	CMB-C2B	-2.50	1.46	1.51
5	4	305	CLA	CMB-C2B	-2.50	1.46	1.51
5	3	612	CLA	CMB-C2B	-2.50	1.46	1.51
5	3	604	CLA	CMB-C2B	-2.50	1.46	1.51
5	4	311	CLA	CMB-C2B	-2.50	1.46	1.51
5	3	607	CLA	CMB-C2B	-2.50	1.46	1.51
12	4	307	KC2	C4A-C3A	-2.50	1.39	1.44
5	5	311	CLA	CMB-C2B	-2.49	1.46	1.51
5	6	307	CLA	CMB-C2B	-2.48	1.46	1.51
5	3	610	CLA	CMB-C2B	-2.48	1.46	1.51
5	5	313	CLA	CMB-C2B	-2.48	1.46	1.51
5	5	314	CLA	CMB-C2B	-2.48	1.46	1.51
5	4	309	CLA	CMB-C2B	-2.47	1.46	1.51
7	5	305	A86	O1-C20	-2.47	1.42	1.46
7	5	321	A86	O1-C20	-2.47	1.42	1.46
5	5	312	CLA	CMB-C2B	-2.46	1.46	1.51
5	5	309	CLA	CMB-C2B	-2.46	1.46	1.51
7	6	301	A86	O1-C20	-2.46	1.42	1.46
5	3	605	CLA	CMB-C2B	-2.45	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3	613	A86	O1-C20	-2.45	1.42	1.46
12	6	308	KC2	C4B-NB	-2.45	1.34	1.37
6	5	315	KC1	C1B-NB	-2.44	1.34	1.37
5	6	311	CLA	CMB-C2B	-2.44	1.46	1.51
12	5	310	KC2	C4B-NB	-2.44	1.34	1.37
5	5	316	CLA	CMB-C2B	-2.44	1.46	1.51
5	4	310	CLA	CMB-C2B	-2.44	1.46	1.51
5	6	306	CLA	CMB-C2B	-2.43	1.46	1.51
13	4	317	LMT	O2'-C2'	-2.42	1.37	1.43
6	6	313	KC1	C1B-NB	-2.41	1.34	1.37
5	5	308	CLA	CMB-C2B	-2.41	1.46	1.51
5	6	309	CLA	CMB-C2B	-2.41	1.46	1.51
13	4	317	LMT	O2B-C2B	-2.39	1.37	1.43
13	4	317	LMT	O3B-C3B	-2.39	1.37	1.43
12	4	307	KC2	C4B-NB	-2.39	1.34	1.37
7	6	303	A86	O1-C20	-2.38	1.42	1.46
5	5	317	CLA	CMB-C2B	-2.38	1.46	1.51
5	6	312	CLA	CMB-C2B	-2.37	1.46	1.51
13	5	320	LMT	O2B-C2B	-2.36	1.37	1.43
7	5	306	A86	O1-C20	-2.36	1.42	1.46
13	5	320	LMT	O2'-C2'	-2.35	1.37	1.43
7	6	304	A86	O1-C20	-2.35	1.42	1.46
5	6	310	CLA	CMB-C2B	-2.34	1.46	1.51
13	5	320	LMT	O3B-C3B	-2.31	1.37	1.43
6	5	315	KC1	CHD-C4C	2.31	1.40	1.35
7	5	307	A86	O1-C20	-2.29	1.42	1.46
5	6	310	CLA	CMD-C2D	-2.29	1.46	1.50
7	4	302	A86	C32-C31	-2.28	1.50	1.54
6	6	313	KC1	C4A-C3A	-2.28	1.40	1.44
5	3	610	CLA	CMC-C2C	-2.27	1.46	1.50
12	6	308	KC2	C4A-C3A	-2.27	1.40	1.44
7	4	304	A86	C32-C31	-2.26	1.50	1.54
5	6	315	CLA	CMB-C2B	-2.26	1.46	1.51
7	5	302	A86	O1-C20	-2.26	1.43	1.46
7	4	302	A86	O1-C20	-2.25	1.43	1.46
12	6	308	KC2	C1D-CHD	2.24	1.47	1.41
7	5	303	A86	O1-C20	-2.24	1.43	1.46
11	3	620	DGD	O1G-C1G	-2.24	1.40	1.45
7	5	304	A86	O1-C20	-2.24	1.43	1.46
5	4	312	CLA	CMC-C2C	-2.22	1.46	1.50
6	5	315	KC1	C4A-C3A	-2.21	1.40	1.44
12	5	310	KC2	C4A-C3A	-2.21	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	317	CLA	CMC-C2C	-2.20	1.46	1.50
5	4	305	CLA	CMD-C2D	-2.20	1.46	1.50
5	3	610	CLA	CMD-C2D	-2.20	1.46	1.50
5	6	314	CLA	CMC-C2C	-2.19	1.46	1.50
5	3	608	CLA	CMD-C2D	-2.18	1.46	1.50
5	6	312	CLA	CMC-C2C	-2.18	1.46	1.50
13	5	320	LMT	O4'-C4B	-2.17	1.37	1.43
13	4	317	LMT	O4'-C4B	-2.17	1.37	1.43
5	3	607	CLA	CMC-C2C	-2.17	1.46	1.50
5	3	606	CLA	CMD-C2D	-2.17	1.46	1.50
5	5	314	CLA	CMC-C2C	-2.16	1.46	1.50
7	5	321	A86	C32-C31	-2.16	1.50	1.54
7	6	302	A86	O1-C20	-2.16	1.43	1.46
7	5	306	A86	C32-C31	-2.15	1.50	1.54
5	4	309	CLA	CMD-C2D	-2.15	1.46	1.50
5	4	311	CLA	CMD-C2D	-2.14	1.46	1.50
5	3	602	CLA	CMD-C2D	-2.14	1.46	1.50
10	5	318	LHG	P-O6	2.14	1.67	1.60
5	3	603	CLA	CMD-C2D	-2.13	1.46	1.50
5	4	308	CLA	CMD-C2D	-2.13	1.46	1.50
5	4	310	CLA	CMD-C2D	-2.13	1.46	1.50
7	5	302	A86	C32-C31	-2.13	1.51	1.54
12	5	310	KC2	C1D-CHD	2.13	1.46	1.41
7	6	305	A86	O1-C20	-2.12	1.43	1.46
5	4	306	CLA	CMD-C2D	-2.12	1.46	1.50
10	5	318	LHG	O7-C5	-2.12	1.41	1.46
7	5	301	A86	O1-C20	-2.12	1.43	1.46
9	3	616	LMG	C4-C3	2.12	1.57	1.52
5	3	602	CLA	CMC-C2C	-2.11	1.46	1.50
5	6	306	CLA	CMC-C2C	-2.11	1.46	1.50
6	6	313	KC1	CHD-C4C	2.11	1.40	1.35
12	5	310	KC2	C1B-NB	-2.11	1.35	1.37
5	3	607	CLA	CMD-C2D	-2.11	1.46	1.50
5	3	611	CLA	CMD-C2D	-2.11	1.46	1.50
5	6	306	CLA	CMD-C2D	-2.11	1.46	1.50
5	4	314	CLA	CMD-C2D	-2.11	1.46	1.50
5	6	311	CLA	CMD-C2D	-2.10	1.46	1.50
5	3	601	CLA	CMD-C2D	-2.10	1.46	1.50
5	3	605	CLA	CMD-C2D	-2.09	1.46	1.50
5	5	312	CLA	CMD-C2D	-2.09	1.46	1.50
5	5	313	CLA	CMD-C2D	-2.09	1.46	1.50
5	6	307	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	317	LMT	O1'-C1'	-2.09	1.36	1.40
5	4	316	CLA	CMD-C2D	-2.08	1.46	1.50
7	6	303	A86	C32-C31	-2.08	1.51	1.54
7	5	305	A86	C32-C31	-2.08	1.51	1.54
5	3	603	CLA	CMC-C2C	-2.08	1.46	1.50
5	4	311	CLA	CMC-C2C	-2.08	1.46	1.50
5	3	619	CLA	CMD-C2D	-2.08	1.46	1.50
5	4	313	CLA	CMC-C2C	-2.07	1.46	1.50
5	4	308	CLA	CMC-C2C	-2.07	1.46	1.50
7	5	301	A86	C32-C31	-2.07	1.51	1.54
8	3	614	DD6	O1-C20	-2.07	1.43	1.46
5	6	307	CLA	CMC-C2C	-2.07	1.46	1.50
7	4	301	A86	C32-C31	-2.07	1.51	1.54
5	4	306	CLA	CMC-C2C	-2.07	1.46	1.50
7	6	301	A86	C32-C31	-2.07	1.51	1.54
5	3	604	CLA	CMD-C2D	-2.06	1.46	1.50
5	3	601	CLA	CMC-C2C	-2.06	1.46	1.50
5	3	606	CLA	CMC-C2C	-2.05	1.46	1.50
5	3	619	CLA	CMC-C2C	-2.05	1.46	1.50
5	4	315	CLA	CMC-C2C	-2.05	1.46	1.50
7	5	307	A86	C32-C31	-2.05	1.51	1.54
5	6	314	CLA	C3B-CAB	-2.05	1.43	1.47
12	4	307	KC2	C1D-CHD	2.04	1.46	1.41
5	4	316	CLA	CMC-C2C	-2.04	1.46	1.50
5	6	314	CLA	C3B-C2B	-2.04	1.37	1.40
5	4	315	CLA	CMD-C2D	-2.04	1.46	1.50
5	3	604	CLA	CMC-C2C	-2.04	1.46	1.50
9	3	616	LMG	O7-C8	-2.04	1.41	1.46
5	6	315	CLA	CMD-C2D	-2.04	1.46	1.50
10	3	618	LHG	O7-C5	-2.03	1.41	1.46
5	5	309	CLA	CMD-C2D	-2.03	1.46	1.50
5	3	608	CLA	C3B-C2B	-2.03	1.37	1.40
5	3	610	CLA	C3B-CAB	-2.03	1.43	1.47
5	3	611	CLA	CMC-C2C	-2.03	1.46	1.50
5	4	305	CLA	CMC-C2C	-2.03	1.46	1.50
5	5	316	CLA	CMD-C2D	-2.02	1.46	1.50
5	3	612	CLA	CMD-C2D	-2.02	1.46	1.50
7	4	304	A86	C13-C11	-2.02	1.45	1.49
6	3	609	KC1	CHD-C4C	2.02	1.40	1.35
7	6	301	A86	C13-C11	-2.02	1.45	1.49
9	5	319	LMG	C4-C5	2.02	1.57	1.53
7	5	302	A86	C13-C11	-2.01	1.45	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	6	309	CLA	CMD-C2D	-2.01	1.46	1.50
5	5	309	CLA	CMC-C2C	-2.01	1.46	1.50
5	5	308	CLA	CMD-C2D	-2.01	1.46	1.50
10	4	318	LHG	O7-C5	-2.01	1.41	1.46
5	4	310	CLA	CMC-C2C	-2.00	1.46	1.50
5	5	312	CLA	CMC-C2C	-2.00	1.46	1.50

All (855) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	5	302	A86	C23-C16-C22	-71.42	2.02	107.37
7	6	304	A86	C23-C16-C22	-71.27	2.25	107.37
7	5	303	A86	C23-C16-C22	-70.78	2.97	107.37
7	4	302	A86	C23-C16-C22	-70.30	3.68	107.37
7	5	307	A86	C23-C16-C22	-68.89	5.75	107.37
7	4	304	A86	C23-C16-C22	-68.27	6.67	107.37
7	6	302	A86	C23-C16-C22	-67.83	7.33	107.37
7	5	304	A86	C23-C16-C22	-66.18	9.75	107.37
7	5	301	A86	C23-C16-C22	-64.86	11.70	107.37
7	6	301	A86	C23-C16-C22	-63.75	13.34	107.37
7	4	301	A86	C23-C16-C22	-57.41	22.69	107.37
7	5	321	A86	C23-C16-C22	-44.89	41.15	107.37
7	6	301	A86	O1-C20-C19	38.30	142.15	113.38
7	6	305	A86	C23-C16-C22	-36.47	53.58	107.37
7	4	302	A86	O1-C20-C19	36.26	140.62	113.38
7	6	303	A86	O1-C20-C19	35.66	140.17	113.38
7	5	306	A86	O1-C20-C19	35.51	140.06	113.38
7	5	321	A86	O1-C20-C19	35.30	139.90	113.38
7	5	304	A86	O1-C15-C14	-33.61	45.77	113.21
7	5	305	A86	O1-C20-C19	32.86	138.07	113.38
7	6	304	A86	O1-C20-C19	32.86	138.07	113.38
7	5	306	A86	C23-C16-C17	-32.29	52.88	108.98
7	6	305	A86	O1-C20-C19	31.72	137.21	113.38
7	6	305	A86	O1-C15-C14	-30.85	51.29	113.21
7	6	303	A86	C23-C16-C17	-30.67	55.69	108.98
7	6	302	A86	O1-C20-C19	-28.39	92.05	113.38
7	5	302	A86	O1-C20-C19	28.18	134.55	113.38
7	6	303	A86	C34-O4-C38	27.43	169.02	117.90
7	5	303	A86	O1-C15-C14	-27.22	58.59	113.21
7	5	301	A86	O1-C20-C19	26.24	133.09	113.38
7	5	302	A86	O1-C15-C14	-24.60	63.84	113.21
7	5	302	A86	C34-O4-C38	23.98	162.59	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	5	307	A86	O1-C20-C19	23.68	131.17	113.38
7	5	303	A86	C34-O4-C38	23.46	161.61	117.90
7	5	301	A86	O1-C15-C14	-23.20	66.66	113.21
7	4	304	A86	O1-C20-C19	22.42	130.23	113.38
7	5	307	A86	C34-O4-C38	21.95	158.80	117.90
7	5	307	A86	O1-C15-C14	-21.51	70.04	113.21
7	5	304	A86	O1-C20-C19	20.69	128.93	113.38
7	4	302	A86	O4-C34-C35	-20.31	57.00	107.59
7	6	302	A86	O1-C15-C14	-20.27	72.54	113.21
7	5	305	A86	C23-C16-C22	20.11	137.03	107.37
7	6	304	A86	O1-C15-C14	-19.44	74.20	113.21
7	5	321	A86	C23-C16-C17	-18.53	76.79	108.98
7	6	301	A86	C35-C34-C33	-18.42	77.74	109.88
7	4	302	A86	O4-C34-C33	18.19	152.89	107.59
7	5	303	A86	O1-C20-C19	18.04	126.94	113.38
7	5	301	A86	C34-O4-C38	17.40	150.32	117.90
7	4	304	A86	C34-O4-C38	17.34	150.22	117.90
7	5	305	A86	O1-C15-C14	-16.31	80.47	113.21
7	6	304	A86	C34-O4-C38	15.83	147.40	117.90
7	4	301	A86	C23-C16-C17	-15.31	82.39	108.98
7	5	301	A86	C35-C34-C33	-15.07	83.58	109.88
7	4	301	A86	C35-C34-C33	-14.77	84.10	109.88
7	6	303	A86	O1-C15-C14	-14.59	83.92	113.21
7	5	321	A86	O1-C15-C14	-13.15	86.83	113.21
7	4	302	A86	C34-O4-C38	-12.69	94.25	117.90
7	6	305	A86	C34-O4-C38	12.58	141.35	117.90
7	6	305	A86	C23-C16-C17	-12.33	87.57	108.98
7	6	301	A86	O4-C34-C33	11.91	137.26	107.59
7	6	301	A86	O4-C34-C35	11.84	137.07	107.59
7	5	307	A86	C35-C34-C33	-11.71	89.45	109.88
7	4	301	A86	C34-O4-C38	11.56	139.45	117.90
7	6	301	A86	C20-C19-C18	-11.21	90.58	112.75
7	6	301	A86	C23-C16-C17	-11.09	89.71	108.98
7	5	305	A86	C35-C34-C33	-11.00	90.67	109.88
7	5	306	A86	C35-C34-C33	-10.69	91.23	109.88
7	4	301	A86	O1-C20-C19	10.64	121.38	113.38
7	4	304	A86	C23-C16-C17	-10.64	90.49	108.98
7	5	306	A86	C23-C16-C22	10.61	123.02	107.37
7	6	301	A86	O1-C15-C14	-10.56	92.02	113.21
7	4	301	A86	C22-C16-C17	-10.43	90.86	108.98
7	6	302	A86	C35-C34-C33	-10.43	91.68	109.88
7	4	302	A86	C33-C32-C31	10.20	119.13	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	6	303	A86	C23-C16-C22	-10.20	92.32	107.37
7	5	301	A86	O4-C34-C33	10.17	132.93	107.59
7	5	301	A86	O4-C34-C35	10.10	132.74	107.59
7	4	301	A86	O4-C34-C35	10.06	132.64	107.59
7	4	304	A86	C22-C16-C17	-10.02	91.58	108.98
7	4	302	A86	C23-C16-C17	-9.78	91.99	108.98
7	4	301	A86	O4-C34-C33	9.75	131.88	107.59
7	4	302	A86	C20-C19-C18	-9.72	93.51	112.75
7	5	304	A86	C35-C34-C33	-9.47	93.36	109.88
7	5	304	A86	C14-C15-C16	9.42	154.81	118.75
7	6	305	A86	C35-C34-C33	-9.40	93.46	109.88
7	4	302	A86	C22-C16-C17	-9.26	92.89	108.98
8	4	303	DD6	C10-C9-C8	9.23	152.01	123.22
7	4	302	A86	O1-C15-C14	-9.22	94.70	113.21
7	5	321	A86	C35-C34-C33	-9.08	94.04	109.88
7	4	304	A86	C33-C32-C31	9.05	118.01	109.21
7	5	305	A86	C19-C18-C17	-8.89	93.60	110.77
7	5	306	A86	C20-C19-C18	-8.67	95.61	112.75
7	5	306	A86	C22-C16-C17	-8.50	94.21	108.98
8	4	303	DD6	C9-C10-C11	8.41	139.32	127.31
7	6	301	A86	C22-C16-C17	-8.33	94.51	108.98
7	5	306	A86	O1-C15-C14	-8.22	96.71	113.21
7	4	302	A86	C41-C32-C40	-8.17	83.46	108.53
7	6	305	A86	C14-C15-C16	8.12	149.86	118.75
7	4	304	A86	C41-C32-C40	-7.98	84.04	108.53
7	5	302	A86	C35-C34-C33	-7.97	95.97	109.88
7	5	321	A86	C22-C16-C17	-7.86	95.32	108.98
7	4	301	A86	C19-C18-C17	-7.80	95.72	110.77
7	5	301	A86	C23-C16-C17	-7.78	95.47	108.98
7	5	303	A86	C35-C34-C33	-7.78	96.31	109.88
7	4	304	A86	C21-C20-C19	-7.67	105.65	114.28
7	5	303	A86	C14-C15-C16	7.66	148.10	118.75
8	4	303	DD6	C9-C8-C6	7.66	147.93	126.42
7	6	304	A86	C20-C19-C18	-7.47	97.98	112.75
7	6	303	A86	C35-C34-C33	-7.46	96.85	109.88
7	5	305	A86	C22-C16-C17	-7.44	96.05	108.98
7	5	321	A86	C20-C19-C18	-7.39	98.12	112.75
12	6	308	KC2	CHB-C1B-NB	7.14	131.02	124.45
5	5	314	CLA	C4A-NA-C1A	7.12	109.91	106.71
12	4	307	KC2	CHB-C1B-NB	7.09	130.97	124.45
7	3	613	A86	O1-C20-C19	-7.08	108.06	113.38
7	6	305	A86	C22-C16-C17	-7.06	96.71	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	5	305	A86	O4-C34-C35	-7.03	97.51	107.66
7	5	306	A86	C34-O4-C38	7.01	130.96	117.90
7	6	305	A86	C19-C18-C17	-6.99	97.28	110.77
5	5	317	CLA	C4A-NA-C1A	6.94	109.83	106.71
5	4	308	CLA	C4A-NA-C1A	6.94	109.83	106.71
5	6	314	CLA	C4A-NA-C1A	6.92	109.82	106.71
12	5	310	KC2	CHB-C1B-NB	6.90	130.80	124.45
7	6	302	A86	C20-C19-C18	6.90	126.40	112.75
5	6	312	CLA	C4A-NA-C1A	6.85	109.78	106.71
5	6	306	CLA	C4A-NA-C1A	6.82	109.77	106.71
12	5	310	KC2	CHC-C4B-NB	6.81	130.71	124.45
5	3	601	CLA	C4A-NA-C1A	6.80	109.77	106.71
7	4	304	A86	O1-C15-C14	-6.76	99.64	113.21
12	6	308	KC2	CHC-C4B-NB	6.75	130.66	124.45
5	5	309	CLA	C4A-NA-C1A	6.75	109.74	106.71
12	4	307	KC2	CHC-C4B-NB	6.72	130.63	124.45
5	3	612	CLA	C4A-NA-C1A	6.71	109.72	106.71
5	3	619	CLA	C4A-NA-C1A	6.69	109.71	106.71
5	3	611	CLA	C4A-NA-C1A	6.68	109.71	106.71
5	6	309	CLA	C4A-NA-C1A	6.67	109.71	106.71
7	6	302	A86	C34-O4-C38	6.65	130.29	117.90
5	3	604	CLA	C4A-NA-C1A	6.64	109.69	106.71
5	4	306	CLA	C4A-NA-C1A	6.63	109.69	106.71
6	3	609	KC1	CHB-C1B-NB	6.62	130.54	124.45
5	5	308	CLA	C4A-NA-C1A	6.61	109.68	106.71
7	4	304	A86	O1-C20-C21	-6.60	107.15	115.06
5	4	305	CLA	C4A-NA-C1A	6.59	109.67	106.71
5	5	311	CLA	C4A-NA-C1A	6.59	109.67	106.71
5	4	315	CLA	C4A-NA-C1A	6.53	109.64	106.71
5	3	610	CLA	C4A-NA-C1A	6.51	109.63	106.71
7	4	301	A86	O1-C20-C21	-6.51	107.26	115.06
5	4	309	CLA	C4A-NA-C1A	6.49	109.62	106.71
5	5	312	CLA	C4A-NA-C1A	6.47	109.61	106.71
7	6	303	A86	C4-C3-C2	-6.46	110.23	123.47
5	6	307	CLA	C4A-NA-C1A	6.46	109.61	106.71
7	6	303	A86	C22-C16-C17	-6.46	97.76	108.98
5	4	310	CLA	C4A-NA-C1A	6.45	109.61	106.71
5	3	602	CLA	C4A-NA-C1A	6.44	109.60	106.71
5	4	312	CLA	C4A-NA-C1A	6.38	109.58	106.71
5	4	311	CLA	C4A-NA-C1A	6.38	109.57	106.71
5	5	313	CLA	C4A-NA-C1A	6.35	109.56	106.71
7	4	302	A86	C35-C34-C33	6.34	120.93	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	5	315	KC1	CHC-C4B-NB	6.33	130.27	124.45
5	4	313	CLA	C4A-NA-C1A	6.33	109.55	106.71
5	5	316	CLA	C4A-NA-C1A	6.32	109.55	106.71
5	3	605	CLA	C4A-NA-C1A	6.31	109.54	106.71
5	6	315	CLA	C4A-NA-C1A	6.29	109.53	106.71
5	3	606	CLA	C4A-NA-C1A	6.28	109.53	106.71
5	4	314	CLA	C4A-NA-C1A	6.27	109.53	106.71
5	4	316	CLA	C4A-NA-C1A	6.26	109.52	106.71
5	6	311	CLA	C4A-NA-C1A	6.24	109.51	106.71
5	3	608	CLA	C4A-NA-C1A	6.23	109.51	106.71
5	3	607	CLA	C4A-NA-C1A	6.21	109.50	106.71
7	5	307	A86	C20-C19-C18	-6.20	100.49	112.75
7	6	304	A86	C35-C34-C33	-6.11	99.22	109.88
7	5	305	A86	O1-C20-C21	-6.07	107.78	115.06
6	6	313	KC1	CHB-C1B-NB	6.06	130.03	124.45
5	6	310	CLA	C4A-NA-C1A	6.05	109.43	106.71
7	6	301	A86	C34-O4-C38	6.05	129.17	117.90
5	3	603	CLA	C4A-NA-C1A	6.01	109.41	106.71
7	5	301	A86	C14-C15-C16	5.98	141.65	118.75
7	6	302	A86	C4-C3-C2	-5.95	111.29	123.47
7	6	301	A86	O1-C20-C21	-5.92	107.96	115.06
6	6	313	KC1	CHC-C4B-NB	5.90	129.87	124.45
7	4	301	A86	C21-C20-C19	-5.86	107.69	114.28
7	5	305	A86	C25-C26-C27	-5.85	118.96	127.31
7	6	303	A86	C20-C19-C18	-5.75	101.38	112.75
7	5	321	A86	O1-C20-C21	-5.73	108.19	115.06
10	5	318	LHG	O4-P-O5	5.67	132.87	110.68
7	6	304	A86	C22-C16-C17	-5.66	99.14	108.98
7	5	302	A86	C14-C15-C16	5.65	140.39	118.75
7	6	304	A86	C23-C16-C17	-5.65	99.16	108.98
6	5	315	KC1	CHB-C1B-NB	5.65	129.65	124.45
6	3	609	KC1	CHC-C4B-NB	5.59	129.59	124.45
7	6	304	A86	O1-C20-C21	-5.57	108.38	115.06
7	5	307	A86	O1-C20-C21	-5.56	108.40	115.06
7	5	306	A86	O1-C20-C21	-5.47	108.50	115.06
7	5	302	A86	C3-C2-C1	-5.40	119.61	127.31
7	5	302	A86	O1-C20-C21	-5.39	108.60	115.06
7	5	305	A86	C3-C2-C1	-5.37	119.65	127.31
7	5	321	A86	C3-C2-C1	-5.35	119.67	127.31
7	5	307	A86	C19-C18-C17	5.33	121.08	110.77
7	5	304	A86	C25-C26-C27	-5.30	119.74	127.31
7	4	301	A86	C14-C15-C16	-5.30	98.47	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	5	303	A86	C22-C16-C17	-5.28	99.81	108.98
7	5	307	A86	C25-C26-C27	-5.27	119.79	127.31
7	5	321	A86	C25-C26-C27	-5.27	119.79	127.31
7	5	304	A86	C22-C16-C17	-5.26	99.84	108.98
7	6	302	A86	C14-C15-C16	5.22	138.76	118.75
7	5	302	A86	C4-C5-C6	-5.21	119.88	127.31
7	4	302	A86	O1-C20-C21	-5.18	108.86	115.06
7	5	303	A86	C23-C16-C17	-5.17	100.00	108.98
7	5	305	A86	O4-C38-O5	-5.17	118.99	125.57
7	5	302	A86	C21-C20-C19	-5.14	108.50	114.28
7	5	302	A86	C20-C19-C18	-5.10	102.66	112.75
7	5	305	A86	C4-C5-C6	-5.08	120.06	127.31
7	6	302	A86	C22-C16-C17	5.08	117.81	108.98
7	5	307	A86	C3-C2-C1	-5.08	120.06	127.31
8	3	614	DD6	C4-C5-C6	-5.07	120.08	127.31
7	5	305	A86	C23-C16-C17	-5.06	100.19	108.98
8	4	303	DD6	C37-C36-C31	-5.05	117.48	124.35
7	6	303	A86	O1-C20-C21	-5.05	109.01	115.06
7	4	302	A86	C3-C2-C1	-5.04	120.12	127.31
7	6	303	A86	C3-C2-C1	-5.01	120.15	127.31
7	6	302	A86	C25-C26-C27	-5.01	120.16	127.31
7	6	302	A86	C3-C2-C1	-5.01	120.16	127.31
7	5	305	A86	O4-C34-C33	-5.00	100.45	107.66
7	5	302	A86	C25-C26-C27	-4.97	120.21	127.31
7	5	301	A86	C25-C26-C27	-4.95	120.25	127.31
7	4	302	A86	C21-C20-C19	-4.94	108.72	114.28
7	3	613	A86	C3-C2-C1	-4.93	120.27	127.31
7	6	302	A86	C4-C5-C6	-4.92	120.28	127.31
7	6	305	A86	C25-C26-C27	-4.91	120.30	127.31
7	4	301	A86	C3-C2-C1	-4.91	120.30	127.31
12	4	307	KC2	CHD-C4C-NC	4.91	131.65	124.20
7	5	301	A86	C20-C19-C18	-4.91	103.04	112.75
8	3	614	DD6	C21-C20-C19	4.91	119.80	114.28
7	6	301	A86	C21-C20-C19	-4.88	108.79	114.28
7	5	301	A86	C3-C2-C1	-4.88	120.35	127.31
8	4	303	DD6	C4-C5-C6	-4.87	120.36	127.31
7	4	302	A86	C4-C3-C2	-4.86	113.51	123.47
7	4	301	A86	C25-C26-C27	-4.84	120.40	127.31
7	5	305	A86	C21-C20-C19	-4.83	108.84	114.28
7	5	303	A86	O1-C20-C21	-4.81	109.29	115.06
12	5	310	KC2	O2D-CGD-CBD	4.81	119.81	111.27
7	6	301	A86	C19-C18-C17	4.80	120.03	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	5	306	A86	C25-C26-C27	-4.79	120.47	127.31
7	4	304	A86	C4-C3-C2	-4.79	113.67	123.47
7	6	304	A86	C21-C20-C19	-4.78	108.90	114.28
7	6	304	A86	C3-C2-C1	-4.77	120.50	127.31
7	4	302	A86	C25-C26-C27	-4.77	120.50	127.31
7	5	301	A86	C4-C5-C6	-4.75	120.53	127.31
7	5	304	A86	C19-C18-C17	-4.75	101.60	110.77
7	5	304	A86	C3-C2-C1	-4.73	120.56	127.31
7	5	306	A86	C3-C2-C1	-4.72	120.57	127.31
7	5	301	A86	C21-C20-C19	-4.72	108.97	114.28
7	5	307	A86	C21-C20-C19	-4.71	108.98	114.28
12	5	310	KC2	CHD-C4C-NC	4.70	131.34	124.20
8	4	303	DD6	C21-C20-C19	4.68	119.55	114.28
7	5	307	A86	C4-C5-C6	-4.68	120.63	127.31
7	4	301	A86	C4-C5-C6	-4.67	120.64	127.31
7	6	301	A86	C25-C26-C27	-4.67	120.64	127.31
7	6	302	A86	O1-C20-C21	-4.67	109.47	115.06
7	6	305	A86	C3-C2-C1	-4.66	120.66	127.31
7	5	304	A86	C4-C3-C2	4.66	133.01	123.47
7	6	301	A86	C3-C2-C1	-4.65	120.67	127.31
7	5	305	A86	C20-C19-C18	4.64	121.92	112.75
7	6	303	A86	C25-C26-C27	-4.63	120.70	127.31
6	6	313	KC1	O2D-CGD-CBD	4.62	119.47	111.27
12	4	307	KC2	C4B-CHC-C1C	-4.60	116.14	126.06
7	6	302	A86	C17-C16-C15	4.59	113.84	109.16
7	4	304	A86	O4-C38-C39	4.59	119.53	111.09
6	3	609	KC1	O2D-CGD-CBD	4.58	119.41	111.27
8	3	614	DD6	C3-C2-C1	-4.58	120.77	127.31
7	5	321	A86	C4-C3-C2	-4.58	114.09	123.47
7	6	301	A86	O4-C38-C39	4.58	119.51	111.09
7	5	303	A86	C3-C2-C1	-4.57	120.79	127.31
7	5	302	A86	O4-C38-C39	4.56	119.47	111.09
12	6	308	KC2	CHD-C4C-NC	4.54	131.10	124.20
7	4	301	A86	O4-C38-C39	4.52	119.41	111.09
7	6	305	A86	O4-C38-C39	4.50	119.36	111.09
7	6	304	A86	O4-C38-C39	4.49	119.36	111.09
7	4	302	A86	O4-C38-C39	4.48	119.34	111.09
12	5	310	KC2	C4B-CHC-C1C	-4.48	116.39	126.06
7	5	304	A86	O4-C38-C39	4.48	119.33	111.09
7	4	304	A86	C3-C2-C1	-4.47	120.92	127.31
6	5	315	KC1	O2D-CGD-CBD	4.47	119.21	111.27
5	6	312	CLA	CMB-C2B-C1B	-4.46	121.61	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	5	321	A86	O4-C38-C39	4.45	119.28	111.09
7	5	301	A86	O4-C38-C39	4.45	119.28	111.09
7	6	305	A86	C4-C5-C6	-4.45	120.96	127.31
7	3	613	A86	C17-C16-C15	4.44	113.69	109.16
7	3	613	A86	C4-C5-C6	-4.43	120.99	127.31
7	6	302	A86	O4-C38-C39	4.42	119.23	111.09
7	5	304	A86	C4-C5-C6	-4.42	121.00	127.31
7	5	303	A86	O4-C38-C39	4.42	119.22	111.09
7	5	307	A86	O4-C38-C39	4.42	119.22	111.09
10	5	318	LHG	O3-P-O6	-4.41	94.99	106.73
5	5	313	CLA	CMB-C2B-C1B	-4.39	121.71	128.46
5	4	310	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
5	3	607	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
7	5	303	A86	C25-C26-C27	-4.36	121.09	127.31
7	6	304	A86	C25-C26-C27	-4.36	121.09	127.31
7	4	304	A86	O4-C34-C35	4.36	118.44	107.59
8	3	614	DD6	C20-C19-C18	-4.34	104.16	112.75
7	5	303	A86	C21-C20-C19	-4.34	109.40	114.28
7	5	303	A86	C4-C5-C6	-4.33	121.13	127.31
12	6	308	KC2	O2D-CGD-CBD	4.32	118.95	111.27
5	4	311	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
7	6	304	A86	C4-C5-C6	-4.30	121.18	127.31
7	5	301	A86	O1-C20-C21	-4.29	109.92	115.06
11	3	620	DGD	O3G-C3G-C2G	-4.29	100.41	111.78
7	5	301	A86	C22-C16-C17	-4.29	101.53	108.98
7	5	306	A86	O4-C38-C39	4.27	118.94	111.09
12	4	307	KC2	O2D-CGD-CBD	4.26	118.83	111.27
10	3	617	LHG	O4-P-O5	4.25	133.23	112.24
7	3	613	A86	O4-C38-C39	4.22	118.86	111.09
10	3	618	LHG	O4-P-O5	4.20	133.00	112.24
10	4	318	LHG	O4-P-O5	4.19	132.95	112.24
7	5	321	A86	C21-C20-C19	-4.15	109.61	114.28
7	4	302	A86	C4-C5-C6	-4.13	121.41	127.31
7	5	304	A86	O1-C20-C21	-4.12	110.12	115.06
5	3	602	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
7	5	307	A86	C14-C15-C16	4.09	134.42	118.75
5	4	314	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
7	4	304	A86	C40-C32-C31	4.05	114.10	110.47
7	3	613	A86	O1-C20-C21	-4.05	110.21	115.06
7	5	301	A86	C17-C16-C15	4.04	113.29	109.16
7	5	321	A86	C4-C5-C6	-4.03	121.55	127.31
7	6	303	A86	O4-C38-C39	4.00	118.45	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	310	KC2	C1A-NA-C4A	-3.99	104.91	106.71
7	6	304	A86	C19-C18-C17	3.99	118.48	110.77
7	6	303	A86	C21-C20-C19	-3.98	109.80	114.28
5	3	604	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
12	6	308	KC2	C4B-CHC-C1C	-3.97	117.50	126.06
7	5	306	A86	C21-C20-C19	-3.96	109.82	114.28
5	4	312	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
7	6	301	A86	C17-C16-C15	3.93	113.17	109.16
12	5	310	KC2	CHC-C4B-C3B	-3.91	118.57	125.26
5	5	309	CLA	CMB-C2B-C1B	-3.90	122.46	128.46
5	3	619	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
5	5	311	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
5	3	603	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
5	6	307	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
7	5	306	A86	C4-C5-C6	-3.86	121.80	127.31
5	4	306	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
8	4	303	DD6	C14-C13-C11	-3.85	119.55	125.53
7	4	301	A86	O1-C15-C14	-3.85	105.48	113.21
7	5	304	A86	C23-C16-C17	-3.83	102.32	108.98
7	5	304	A86	C21-C20-C19	-3.83	109.97	114.28
5	4	309	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
7	4	304	A86	C25-C26-C27	-3.83	121.85	127.31
5	4	308	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
5	4	315	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
5	6	314	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
7	6	301	A86	C4-C5-C6	-3.80	121.89	127.31
7	3	613	A86	C36-C31-C32	3.80	123.47	119.70
7	5	307	A86	O4-C34-C35	-3.80	98.13	107.59
5	5	317	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
12	5	310	KC2	C3D-CAD-CBD	-3.79	102.62	107.61
7	5	305	A86	C33-C32-C31	-3.78	105.54	109.21
5	4	316	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
5	6	312	CLA	CMB-C2B-C3B	3.77	131.73	124.68
7	6	305	A86	O1-C20-C21	-3.76	110.55	115.06
5	4	313	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
7	5	301	A86	C4-C3-C2	3.74	131.14	123.47
5	5	308	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
8	3	614	DD6	C9-C10-C11	-3.72	122.00	127.31
7	6	303	A86	C17-C16-C15	3.71	112.95	109.16
7	4	304	A86	O4-C34-C33	-3.70	98.36	107.59
5	6	309	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
7	4	304	A86	C19-C18-C17	-3.70	103.64	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	3	612	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
7	4	304	A86	C4-C5-C6	-3.68	122.05	127.31
7	5	302	A86	C17-C16-C15	3.68	112.92	109.16
8	4	303	DD6	C37-C36-C35	3.68	121.18	114.36
5	5	313	CLA	CMB-C2B-C3B	3.67	131.55	124.68
7	5	304	A86	C34-O4-C38	3.66	124.72	117.90
5	4	310	CLA	CMB-C2B-C3B	3.65	131.51	124.68
5	5	314	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
5	3	601	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
5	4	311	CLA	CMB-C2B-C3B	3.64	131.48	124.68
5	5	316	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
5	3	607	CLA	CMB-C2B-C3B	3.62	131.46	124.68
7	4	302	A86	C17-C16-C15	3.61	112.85	109.16
7	5	306	A86	O4-C34-C35	-3.61	98.61	107.59
5	6	311	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
12	4	307	KC2	CHC-C4B-C3B	-3.59	119.12	125.26
5	6	306	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
7	3	613	A86	C33-C32-C31	3.56	112.67	109.21
5	3	606	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
5	3	611	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
12	4	307	KC2	CHB-C1B-C2B	-3.54	118.05	125.48
12	5	310	KC2	CHB-C1B-C2B	-3.54	118.06	125.48
7	4	301	A86	C4-C3-C2	-3.53	116.24	123.47
7	6	304	A86	C4-C3-C2	-3.53	116.25	123.47
12	4	307	KC2	C1A-NA-C4A	-3.53	105.12	106.71
5	4	314	CLA	CMB-C2B-C3B	3.52	131.26	124.68
7	5	302	A86	C23-C16-C17	-3.50	102.90	108.98
7	6	303	A86	C4-C5-C6	-3.49	122.33	127.31
7	5	307	A86	O4-C34-C33	-3.48	98.92	107.59
5	3	602	CLA	CMB-C2B-C3B	3.48	131.19	124.68
5	3	608	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
7	6	305	A86	C17-C16-C15	3.47	112.71	109.16
5	4	305	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
5	3	610	CLA	CAA-C2A-C3A	-3.44	108.08	116.10
7	5	306	A86	O4-C34-C33	-3.43	99.06	107.59
5	4	312	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
7	6	305	A86	C21-C20-C19	-3.40	110.45	114.28
6	3	609	KC1	C4B-CHC-C1C	-3.39	118.74	126.06
5	6	314	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
5	3	605	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
5	5	312	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
6	3	609	KC1	C3D-CAD-CBD	-3.36	103.17	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	4	304	A86	C14-C15-C16	-3.32	106.02	118.75
5	3	604	CLA	CMB-C2B-C3B	3.32	130.89	124.68
5	3	610	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
5	6	314	CLA	CHD-C1D-ND	-3.29	121.43	124.45
7	5	306	A86	C4-C3-C2	-3.29	116.73	123.47
10	3	617	LHG	O8-C23-C24	3.29	120.00	111.38
5	5	309	CLA	CMB-C2B-C3B	3.27	130.79	124.68
5	5	311	CLA	CMB-C2B-C3B	3.27	130.79	124.68
12	4	307	KC2	C3D-CAD-CBD	-3.26	103.31	107.61
7	6	303	A86	C33-C32-C31	-3.25	106.05	109.21
5	3	603	CLA	CMB-C2B-C3B	3.25	130.75	124.68
5	6	307	CLA	CMB-C2B-C3B	3.25	130.75	124.68
5	4	306	CLA	CMB-C2B-C3B	3.24	130.74	124.68
7	5	307	A86	C17-C16-C15	3.23	112.46	109.16
5	5	317	CLA	CMB-C2B-C3B	3.23	130.72	124.68
7	6	302	A86	C21-C20-C19	-3.23	110.65	114.28
12	6	308	KC2	CHB-C1B-C2B	-3.22	118.72	125.48
12	6	308	KC2	CHC-C4B-C3B	-3.22	119.74	125.26
5	4	312	CLA	CMB-C2B-C3B	3.22	130.71	124.68
7	4	302	A86	C40-C32-C31	3.22	113.36	110.47
5	3	619	CLA	CMB-C2B-C3B	3.22	130.70	124.68
7	4	301	A86	C20-C19-C18	3.20	119.08	112.75
7	5	303	A86	C20-C19-C18	-3.20	106.42	112.75
5	4	309	CLA	CMB-C2B-C3B	3.19	130.65	124.68
5	4	308	CLA	CMB-C2B-C3B	3.18	130.63	124.68
12	4	307	KC2	C4C-C3C-C2C	-3.18	104.59	107.11
5	4	316	CLA	CMB-C2B-C3B	3.17	130.61	124.68
5	6	310	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
5	4	315	CLA	CMB-C2B-C3B	3.16	130.60	124.68
5	4	314	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
7	3	613	A86	C40-C32-C31	-3.14	107.66	110.47
5	4	313	CLA	CMB-C2B-C3B	3.14	130.55	124.68
5	3	610	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
5	3	611	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
9	3	615	LMG	C1-C2-C3	-3.12	103.49	110.00
5	5	308	CLA	CMB-C2B-C3B	3.12	130.51	124.68
12	5	310	KC2	C4C-C3C-C2C	-3.11	104.64	107.11
7	5	302	A86	C4-C3-C2	-3.11	117.11	123.47
8	3	614	DD6	C37-C36-C31	-3.10	120.13	124.35
5	6	309	CLA	CMB-C2B-C3B	3.10	130.47	124.68
5	4	312	CLA	CHB-C4A-NA	3.10	128.79	124.51
8	4	303	DD6	C33-C34-C35	-3.09	106.07	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	6	314	CLA	CAA-C2A-C3A	-3.09	108.88	116.10
6	3	609	KC1	CHB-C1B-C2B	-3.08	119.02	125.48
5	3	619	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
5	6	311	CLA	CMB-C2B-C3B	3.07	130.43	124.68
5	4	305	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
7	6	302	A86	O4-C34-C33	-3.07	99.95	107.59
5	3	612	CLA	CMB-C2B-C3B	3.07	130.42	124.68
5	3	601	CLA	CMB-C2B-C3B	3.04	130.36	124.68
7	5	303	A86	C17-C16-C15	3.04	112.26	109.16
7	6	303	A86	O4-C34-C33	-3.03	100.04	107.59
5	5	314	CLA	CMB-C2B-C3B	3.03	130.35	124.68
8	4	303	DD6	C4-C3-C2	-3.01	117.30	123.47
5	3	601	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
5	5	317	CLA	CBD-CHA-C1A	3.00	132.24	127.43
7	6	302	A86	O4-C34-C35	-3.00	100.12	107.59
13	4	317	LMT	C1'-O5'-C5'	-3.00	107.81	113.69
7	6	301	A86	C33-C32-C31	-2.99	106.30	109.21
5	4	313	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
5	5	316	CLA	CMB-C2B-C3B	2.98	130.25	124.68
5	5	317	CLA	CAA-C2A-C3A	-2.98	109.15	116.10
5	3	607	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
12	6	308	KC2	C3D-CAD-CBD	-2.97	103.70	107.61
7	5	307	A86	C22-C16-C17	-2.96	103.84	108.98
5	6	306	CLA	CMB-C2B-C3B	2.96	130.22	124.68
5	4	309	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
8	3	614	DD6	C21-C20-C15	-2.96	117.30	122.26
5	3	610	CLA	CMB-C2B-C3B	2.95	130.19	124.68
7	4	304	A86	C36-C31-C32	-2.94	116.78	119.70
7	6	304	A86	C14-C15-C16	2.94	130.00	118.75
5	6	314	CLA	CMB-C2B-C3B	2.93	130.16	124.68
7	5	302	A86	C19-C18-C17	2.92	116.41	110.77
5	6	306	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
5	3	603	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
5	3	606	CLA	CMB-C2B-C3B	2.90	130.11	124.68
5	4	306	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
7	5	306	A86	C14-C15-C16	-2.90	107.67	118.75
5	6	312	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
5	4	313	CLA	CAA-C2A-C3A	-2.88	109.38	116.10
5	4	316	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
5	5	309	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
7	5	305	A86	C25-C24-C1	-2.86	118.38	126.42
5	4	305	CLA	CMB-C2B-C3B	2.86	130.03	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	312	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
5	6	307	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
5	6	309	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
5	4	308	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
6	6	313	KC1	CHC-C4B-C3B	-2.82	120.43	125.26
5	3	608	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
6	6	313	KC1	CHB-C1B-C2B	-2.82	119.58	125.48
7	3	613	A86	C9-C8-C6	-2.81	118.51	126.42
7	5	304	A86	O4-C34-C35	-2.81	100.59	107.59
5	3	602	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
5	5	316	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
12	6	308	KC2	C4C-C3C-C2C	-2.81	104.88	107.11
5	4	311	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
7	5	302	A86	C33-C32-C31	-2.80	106.49	109.21
7	5	321	A86	O4-C34-C33	-2.79	100.63	107.59
5	3	612	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
5	5	314	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
5	5	313	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
6	5	315	KC1	CHC-C4B-C3B	-2.77	120.51	125.26
5	3	610	CLA	CHB-C4A-NA	2.77	128.34	124.51
10	4	318	LHG	O8-C23-C24	2.77	120.60	111.91
5	5	311	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
5	3	605	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
5	4	315	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
5	3	605	CLA	CMB-C2B-C3B	2.76	129.84	124.68
5	3	611	CLA	CMB-C2B-C3B	2.75	129.82	124.68
9	3	616	LMG	O6-C1-O1	-2.75	103.47	109.97
8	3	614	DD6	C15-C14-C13	-2.74	120.19	125.99
7	6	303	A86	O4-C34-C35	-2.74	100.77	107.59
5	5	314	CLA	CHD-C1D-ND	-2.74	121.94	124.45
6	6	313	KC1	C4B-CHC-C1C	-2.74	120.16	126.06
5	6	315	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
5	3	604	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
5	6	311	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
7	6	304	A86	C17-C16-C15	2.73	111.95	109.16
5	5	308	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
6	3	609	KC1	CHC-C4B-C3B	-2.72	120.60	125.26
5	3	608	CLA	CMB-C2B-C3B	2.72	129.77	124.68
5	5	312	CLA	CMB-C2B-C3B	2.72	129.76	124.68
7	5	302	A86	C9-C10-C11	-2.71	118.63	126.61
12	4	307	KC2	O1D-CGD-CBD	-2.71	118.94	124.48
7	6	305	A86	O4-C34-C35	-2.71	100.85	107.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	6	313	KC1	C3D-CAD-CBD	-2.70	104.05	107.61
11	3	620	DGD	CDB-CCB-CBB	-2.70	100.71	114.42
5	4	310	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
7	5	305	A86	C14-C15-C16	-2.70	108.43	118.75
7	5	302	A86	C9-C8-C6	-2.68	118.88	126.42
7	5	306	A86	C17-C16-C15	2.68	111.89	109.16
7	3	613	A86	O1-C15-C14	-2.67	107.85	113.21
10	3	618	LHG	O8-C23-C24	2.67	120.28	111.91
7	5	307	A86	C23-C16-C17	-2.65	104.38	108.98
6	5	315	KC1	C4B-CHC-C1C	-2.65	120.35	126.06
7	5	305	A86	C12-C11-C13	2.64	120.46	116.02
12	4	307	KC2	C1B-CHB-C4A	-2.64	120.36	126.06
8	3	614	DD6	C37-C36-C35	2.63	119.23	114.36
9	5	319	LMG	O6-C5-C4	2.63	114.47	109.69
10	5	318	LHG	O8-C23-C24	2.63	120.16	111.91
7	5	321	A86	C17-C16-C15	2.62	111.84	109.16
5	3	606	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
5	6	315	CLA	CMB-C2B-C3B	2.62	129.72	124.93
5	5	317	CLA	CHB-C4A-NA	2.62	128.13	124.51
5	6	310	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
7	5	303	A86	C12-C11-C13	2.60	120.39	116.02
5	4	312	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
5	6	312	CLA	CHB-C4A-NA	2.60	128.10	124.51
7	5	302	A86	C25-C24-C1	-2.60	119.12	126.42
7	5	302	A86	C22-C16-C17	-2.59	104.49	108.98
5	5	314	CLA	C1-C2-C3	-2.59	121.57	126.04
7	3	613	A86	C34-O4-C38	-2.58	113.08	117.90
5	4	311	CLA	CHB-C4A-NA	2.58	128.08	124.51
7	5	307	A86	C12-C11-C13	2.58	120.35	116.02
7	5	303	A86	O4-C34-C35	-2.58	101.18	107.59
7	5	301	A86	C12-C11-C13	2.57	120.35	116.02
5	5	313	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
7	5	321	A86	C12-C11-C13	2.57	120.33	116.02
7	6	302	A86	C9-C8-C6	-2.57	119.21	126.42
5	3	612	CLA	CHB-C4A-NA	2.56	128.05	124.51
5	6	310	CLA	CMB-C2B-C3B	2.56	129.47	124.68
5	4	311	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
5	4	306	CLA	CHB-C4A-NA	2.55	128.04	124.51
5	5	316	CLA	CAA-C2A-C3A	-2.55	110.14	116.10
5	3	611	CLA	C1-C2-C3	-2.55	121.63	126.04
5	5	312	CLA	CHB-C4A-NA	2.55	128.04	124.51
7	6	301	A86	C14-C15-C16	-2.55	108.99	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	3	616	LMG	O6-C5-C4	2.55	114.32	109.69
9	3	615	LMG	O6-C1-O1	-2.54	103.95	109.97
5	5	309	CLA	CHB-C4A-NA	2.54	128.03	124.51
8	3	614	DD6	C32-C31-C36	-2.54	119.05	122.63
8	4	303	DD6	C12-C11-C10	-2.54	119.37	122.92
5	3	606	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
5	4	308	CLA	CHB-C4A-NA	2.54	128.02	124.51
5	4	313	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
7	4	301	A86	C33-C32-C31	-2.53	106.75	109.21
6	5	315	KC1	O1D-CGD-CBD	-2.53	119.31	124.48
12	5	310	KC2	C1B-CHB-C4A	-2.53	120.61	126.06
5	4	309	CLA	CHB-C4A-NA	2.53	128.01	124.51
5	6	311	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
5	3	604	CLA	CHB-C4A-NA	2.52	128.00	124.51
10	4	318	LHG	C11-C10-C9	-2.52	101.62	114.42
5	6	306	CLA	CHB-C4A-NA	2.52	128.00	124.51
7	5	301	A86	C33-C32-C31	-2.52	106.76	109.21
7	6	304	A86	C12-C11-C13	2.52	120.25	116.02
7	6	302	A86	C9-C10-C11	-2.51	119.22	126.61
9	3	616	LMG	O1-C7-C8	-2.51	104.84	110.90
8	4	303	DD6	C3-C2-C1	-2.51	123.73	127.31
5	4	315	CLA	CHB-C4A-NA	2.51	127.98	124.51
7	5	306	A86	C19-C18-C17	2.50	115.61	110.77
5	6	307	CLA	CHB-C4A-NA	2.50	127.97	124.51
8	3	614	DD6	C7-C6-C5	-2.50	119.43	122.92
5	3	602	CLA	CHB-C4A-NA	2.50	127.96	124.51
5	3	619	CLA	CHB-C4A-NA	2.50	127.96	124.51
7	6	303	A86	C12-C11-C13	2.49	120.21	116.02
5	5	308	CLA	CHB-C4A-NA	2.49	127.96	124.51
5	6	314	CLA	CAC-C3C-C4C	2.49	128.04	124.81
5	3	603	CLA	CHB-C4A-NA	2.49	127.95	124.51
5	4	314	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
5	4	305	CLA	CHB-C4A-NA	2.49	127.95	124.51
8	3	614	DD6	C-C1-C2	-2.49	119.44	122.92
5	5	311	CLA	CHB-C4A-NA	2.48	127.94	124.51
7	5	302	A86	O4-C34-C35	-2.48	101.41	107.59
7	3	613	A86	C41-C32-C31	-2.48	108.25	110.47
6	5	315	KC1	CBD-CHA-C1A	2.47	133.49	128.88
5	5	316	CLA	CMA-C3A-C2A	-2.47	110.34	116.10
12	4	307	KC2	CHD-C4C-C3C	-2.47	117.17	126.11
5	4	313	CLA	CMA-C3A-C2A	-2.47	110.34	116.10
8	3	614	DD6	C25-C24-C1	-2.46	119.50	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	6	314	CLA	O2D-CGD-CBD	2.46	115.63	111.27
5	3	601	CLA	CHB-C4A-NA	2.45	127.90	124.51
7	5	306	A86	C12-C11-C13	2.45	120.14	116.02
5	3	605	CLA	CHB-C4A-NA	2.44	127.89	124.51
5	4	313	CLA	CHD-C1D-ND	-2.44	122.21	124.45
10	3	618	LHG	C11-C10-C9	-2.44	102.05	114.42
5	6	309	CLA	CHB-C4A-NA	2.44	127.88	124.51
12	6	308	KC2	CBD-CHA-C1A	2.43	133.41	128.88
7	3	613	A86	C12-C11-C13	2.43	120.10	116.02
5	3	611	CLA	CHB-C4A-NA	2.43	127.87	124.51
5	4	314	CLA	CHB-C4A-NA	2.43	127.87	124.51
7	5	307	A86	C25-C24-C1	-2.43	119.60	126.42
5	5	313	CLA	CHB-C4A-NA	2.42	127.86	124.51
7	3	613	A86	C35-C34-C33	-2.41	105.67	109.88
5	3	607	CLA	CHB-C4A-NA	2.40	127.83	124.51
5	3	619	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
10	4	318	LHG	C20-C19-C18	-2.40	102.25	114.42
6	5	315	KC1	C3D-CAD-CBD	-2.40	104.45	107.61
7	5	321	A86	O4-C34-C35	-2.40	101.63	107.59
7	4	302	A86	C12-C11-C13	2.39	120.04	116.02
5	4	310	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
8	4	303	DD6	O1-C20-C21	-2.39	112.20	115.06
5	6	315	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
5	3	607	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
8	4	303	DD6	C26-C25-C24	-2.38	115.78	123.22
10	3	618	LHG	C20-C19-C18	-2.38	102.33	114.42
5	3	608	CLA	CHB-C4A-NA	2.38	127.80	124.51
5	6	312	CLA	CHD-C1D-ND	-2.38	122.27	124.45
7	5	305	A86	C28-C27-C26	-2.37	119.60	122.92
7	6	303	A86	C3-C4-C5	-2.37	118.62	123.47
5	5	314	CLA	CHB-C4A-NA	2.37	127.79	124.51
12	4	307	KC2	CHB-C4A-C3A	-2.37	121.28	124.98
12	5	310	KC2	CHD-C4C-C3C	-2.37	117.52	126.11
5	4	316	CLA	CHB-C4A-NA	2.37	127.79	124.51
5	6	312	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
7	4	302	A86	C36-C31-C32	-2.36	117.35	119.70
5	3	602	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
5	4	306	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
5	4	308	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
5	4	309	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
5	5	317	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
7	5	321	A86	C25-C24-C1	-2.36	119.79	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	6	308	KC2	O1D-CGD-CBD	-2.36	119.66	124.48
13	5	320	LMT	C1'-O5'-C5'	-2.35	109.07	113.69
7	4	301	A86	O4-C38-O5	-2.35	118.29	122.96
7	6	305	A86	O4-C38-O5	-2.35	118.29	122.96
10	5	318	LHG	C20-C19-C18	-2.35	102.49	114.42
5	3	610	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
7	6	301	A86	C12-C11-C13	2.35	119.97	116.02
5	3	603	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
10	3	617	LHG	C11-C10-C9	-2.35	102.51	114.42
5	5	311	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
5	5	316	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
5	5	309	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
5	4	310	CLA	CHB-C4A-NA	2.34	127.75	124.51
5	4	305	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
5	6	309	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
12	5	310	KC2	O1D-CGD-CBD	-2.34	119.70	124.48
6	6	313	KC1	C1B-CHB-C4A	-2.34	121.02	126.06
5	3	604	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
5	5	316	CLA	CHB-C4A-NA	2.33	127.74	124.51
7	5	301	A86	O4-C38-O5	-2.33	118.33	122.96
5	6	310	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
5	4	316	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
10	5	318	LHG	C11-C10-C9	-2.32	102.65	114.42
7	6	305	A86	O4-C34-C33	-2.32	101.82	107.59
7	6	305	A86	C12-C11-C13	2.32	119.92	116.02
5	5	312	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
5	4	315	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
5	4	311	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
5	3	611	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
7	4	304	A86	O4-C38-O5	-2.31	118.38	122.96
7	5	321	A86	O4-C38-O5	-2.31	118.38	122.96
9	5	319	LMG	O3-C3-C2	-2.31	105.02	110.35
7	6	304	A86	O4-C38-O5	-2.30	118.39	122.96
7	5	302	A86	O4-C38-O5	-2.30	118.39	122.96
7	5	304	A86	C25-C24-C1	-2.30	119.95	126.42
5	3	612	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
7	5	304	A86	O4-C38-O5	-2.30	118.39	122.96
5	3	606	CLA	CHB-C4A-NA	2.30	127.69	124.51
5	6	315	CLA	C4B-CHC-C1C	-2.30	126.10	129.64
5	4	314	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
12	6	308	KC2	C1A-NA-C4A	-2.30	105.67	106.71
7	4	302	A86	O4-C38-O5	-2.30	118.40	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	4	312	CLA	O2D-CGD-CBD	2.29	115.35	111.27
5	6	307	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
7	5	301	A86	C9-C8-C6	-2.29	119.97	126.42
7	5	307	A86	O4-C38-O5	-2.29	118.41	122.96
7	5	301	A86	C25-C24-C1	-2.29	119.98	126.42
5	6	311	CLA	CHB-C4A-NA	2.29	127.68	124.51
7	6	302	A86	O4-C38-O5	-2.29	118.41	122.96
7	5	303	A86	C33-C32-C31	-2.28	106.99	109.21
6	5	315	KC1	CHB-C1B-C2B	-2.28	120.69	125.48
7	5	306	A86	C33-C32-C31	-2.28	107.00	109.21
5	5	308	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
6	5	315	KC1	O2D-CGD-O1D	-2.28	119.39	123.84
7	5	303	A86	O4-C38-O5	-2.28	118.44	122.96
7	4	304	A86	C17-C16-C15	2.28	111.48	109.16
5	3	601	CLA	C1-C2-C3	-2.27	122.11	126.04
5	3	602	CLA	C1-C2-C3	-2.27	122.11	126.04
12	5	310	KC2	CHB-C4A-C3A	-2.27	121.43	124.98
5	3	605	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
7	4	302	A86	C9-C10-C11	-2.27	119.93	126.61
7	6	301	A86	O4-C38-O5	-2.27	118.45	122.96
7	5	306	A86	O4-C38-O5	-2.27	118.46	122.96
5	3	608	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
10	3	618	LHG	C18-C17-C16	-2.26	102.94	114.42
7	5	321	A86	C28-C27-C26	-2.26	119.76	122.92
9	5	319	LMG	O1-C7-C8	-2.25	105.46	110.90
11	3	620	DGD	CBB-CAB-C9B	-2.25	102.98	114.42
7	6	301	A86	C3-C4-C5	-2.25	118.86	123.47
5	5	309	CLA	C1-C2-C3	-2.25	122.15	126.04
9	5	319	LMG	C4-C3-C2	-2.24	106.91	110.82
5	5	309	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
7	5	305	A86	C17-C16-C15	2.23	111.44	109.16
5	3	601	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
5	6	315	CLA	CBD-CHA-C1A	2.23	131.12	128.50
5	6	306	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
7	3	613	A86	C26-C25-C24	-2.22	116.28	123.22
5	3	602	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
5	4	313	CLA	CHB-C4A-NA	2.22	127.58	124.51
10	4	318	LHG	C27-C26-C25	-2.22	103.16	114.42
11	3	620	DGD	CFB-CEB-CDB	-2.22	103.17	114.42
7	5	303	A86	O4-C34-C33	-2.21	102.08	107.59
7	4	304	A86	C12-C11-C13	2.21	119.74	116.02
6	6	313	KC1	C1A-NA-C4A	-2.21	105.71	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	5	319	LMG	O2-C2-C1	-2.21	104.69	110.05
5	6	310	CLA	CHB-C4A-NA	2.20	127.56	124.51
10	4	318	LHG	C18-C17-C16	-2.20	103.23	114.42
5	3	611	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
7	6	303	A86	C25-C24-C1	-2.20	120.23	126.42
9	3	615	LMG	O3-C3-C2	-2.20	105.26	110.35
7	6	301	A86	C25-C24-C1	-2.20	120.23	126.42
7	5	304	A86	C28-C27-C26	-2.20	119.84	122.92
7	4	302	A86	C3-C4-C5	-2.20	118.97	123.47
10	5	318	LHG	C18-C17-C16	-2.20	103.28	114.42
12	6	308	KC2	C1B-CHB-C4A	-2.19	121.33	126.06
7	5	304	A86	O4-C34-C33	-2.19	102.14	107.59
7	4	301	A86	C12-C11-C13	2.19	119.70	116.02
5	4	316	CLA	C1-C2-C3	-2.19	122.26	126.04
5	6	315	CLA	CHD-C1D-ND	-2.18	122.45	124.45
7	5	307	A86	C28-C27-C26	-2.18	119.87	122.92
5	6	315	CLA	C1B-NB-C4B	2.18	108.32	106.32
7	6	302	A86	C23-C16-C17	2.18	112.77	108.98
5	6	315	CLA	CHB-C4A-NA	2.18	127.52	124.51
6	5	315	KC1	C2A-C3A-C4A	2.17	108.10	106.49
7	4	304	A86	C20-C19-C18	-2.17	108.45	112.75
7	6	305	A86	C25-C24-C1	-2.17	120.33	126.42
7	4	304	A86	C3-C4-C5	-2.16	119.05	123.47
5	3	601	CLA	CAA-CBA-CGA	-2.16	106.95	113.25
9	3	616	LMG	O3-C3-C2	-2.16	105.36	110.35
7	5	304	A86	C-C1-C2	-2.16	119.90	122.92
5	3	606	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
5	3	607	CLA	CHD-C1D-ND	-2.15	122.47	124.45
12	6	308	KC2	C1A-C2A-C3A	-2.15	105.41	107.11
8	4	303	DD6	C21-C20-C15	-2.15	118.66	122.26
7	5	305	A86	C9-C8-C6	-2.14	120.39	126.42
6	6	313	KC1	O1D-CGD-CBD	-2.14	120.10	124.48
5	6	309	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
5	4	305	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
7	5	306	A86	C3-C4-C5	-2.13	119.10	123.47
5	6	309	CLA	C1-C2-C3	-2.13	122.35	126.04
6	3	609	KC1	C2A-C3A-C4A	2.13	108.07	106.49
5	3	604	CLA	CHD-C1D-ND	-2.13	122.50	124.45
9	3	616	LMG	O2-C2-C1	-2.12	104.88	110.05
7	5	321	A86	C-C1-C2	-2.12	119.95	122.92
7	4	301	A86	C25-C24-C1	-2.12	120.46	126.42
5	5	309	CLA	CHD-C1D-ND	-2.12	122.51	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	3	602	CLA	CHD-C1D-ND	-2.11	122.51	124.45
7	5	303	A86	C19-C18-C17	-2.11	106.70	110.77
5	3	610	CLA	CMA-C3A-C2A	-2.11	111.18	116.10
10	3	618	LHG	C27-C26-C25	-2.10	103.74	114.42
5	6	310	CLA	CHD-C1D-ND	-2.10	122.52	124.45
7	5	301	A86	C9-C10-C11	-2.10	120.43	126.61
7	6	305	A86	C-C1-C2	-2.10	119.98	122.92
6	6	313	KC1	CBD-CHA-C1A	2.10	132.79	128.88
5	3	612	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
12	6	308	KC2	CHD-C4C-C3C	-2.09	118.52	126.11
11	3	620	DGD	C1G-C2G-C3G	-2.09	106.90	111.80
5	6	307	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
5	4	306	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
7	4	304	A86	O1-C15-C20	-2.08	57.37	59.40
7	3	613	A86	C-C1-C2	-2.08	120.01	122.92
12	5	310	KC2	O2D-CGD-O1D	-2.08	119.78	123.84
7	5	306	A86	C28-C27-C26	-2.08	120.02	122.92
7	4	302	A86	C-C1-C2	-2.07	120.02	122.92
9	5	319	LMG	C1-C2-C3	-2.07	105.68	110.00
7	6	302	A86	C25-C24-C1	-2.07	120.60	126.42
6	3	609	KC1	O2D-CGD-O1D	-2.07	119.80	123.84
7	4	302	A86	C25-C24-C1	-2.06	120.62	126.42
12	4	307	KC2	O2D-CGD-O1D	-2.06	119.81	123.84
5	3	604	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
7	5	303	A86	C3-C4-C5	-2.05	119.27	123.47
5	4	314	CLA	CHD-C1D-ND	-2.05	122.57	124.45
8	3	614	DD6	C32-C33-C34	-2.05	109.01	113.64
9	3	615	LMG	O1-C7-C8	-2.05	105.96	110.90
5	5	316	CLA	CHD-C1D-ND	-2.04	122.58	124.45
5	3	605	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
7	5	301	A86	C3-C4-C5	-2.04	119.30	123.47
7	6	304	A86	C3-C4-C5	-2.04	119.30	123.47
5	6	314	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
5	3	607	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
5	3	603	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
5	5	317	CLA	CHD-C1D-ND	-2.03	122.58	124.45
5	3	605	CLA	C1-C2-C3	-2.03	122.53	126.04
5	3	608	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
5	4	312	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
5	6	306	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
12	6	308	KC2	O2D-CGD-O1D	-2.03	119.87	123.84
7	4	301	A86	O1-C15-C20	-2.03	57.42	59.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	312	CLA	CHD-C1D-ND	-2.03	122.59	124.45
7	5	305	A86	C-C1-C2	-2.02	120.09	122.92
7	6	303	A86	O4-C38-O5	-2.02	118.94	122.96
7	5	304	A86	C17-C16-C15	2.02	111.23	109.16
9	3	615	LMG	O2-C2-C1	-2.02	105.14	110.05
7	6	303	A86	C10-C9-C8	-2.02	116.91	123.22
11	3	620	DGD	CAB-C9B-C8B	-2.02	104.18	114.42
5	4	309	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
7	6	302	A86	C28-C27-C26	-2.02	120.10	122.92
7	5	321	A86	C3-C4-C5	-2.02	119.34	123.47
5	4	315	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
5	4	306	CLA	CHD-C1D-ND	-2.02	122.60	124.45
7	5	305	A86	C9-C10-C11	-2.01	120.68	126.61
5	4	311	CLA	CHD-C1D-ND	-2.01	122.60	124.45
8	3	614	DD6	C9-C8-C6	-2.01	120.76	126.42
12	5	310	KC2	C1A-C2A-C3A	-2.01	105.52	107.11
5	3	619	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
7	4	301	A86	C9-C8-C6	-2.01	120.77	126.42
7	6	302	A86	C7-C6-C5	-2.01	120.11	122.92
7	4	301	A86	C28-C27-C26	-2.01	120.11	122.92
7	6	305	A86	C28-C27-C26	-2.01	120.11	122.92
7	4	301	A86	C9-C10-C11	-2.01	120.71	126.61
5	4	312	CLA	CHA-C1A-NA	-2.01	121.81	126.40
12	6	308	KC2	CHB-C4A-C3A	-2.00	121.85	124.98
5	4	308	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (39) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	3	601	CLA	ND
5	3	602	CLA	ND
5	3	603	CLA	ND
5	3	604	CLA	ND
5	3	605	CLA	ND
5	3	606	CLA	ND
5	3	607	CLA	ND
5	3	608	CLA	ND
5	3	610	CLA	ND
5	3	611	CLA	ND
5	3	612	CLA	ND
5	3	619	CLA	ND
5	4	305	CLA	ND

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Mol	Chain	Res	Type	Atom
5	4	306	CLA	ND
5	4	308	CLA	ND
5	4	309	CLA	ND
5	4	310	CLA	ND
5	4	311	CLA	ND
5	4	312	CLA	ND
5	4	313	CLA	ND
5	4	314	CLA	ND
5	4	315	CLA	ND
5	4	316	CLA	ND
5	5	308	CLA	ND
5	5	309	CLA	ND
5	5	311	CLA	ND
5	5	312	CLA	ND
5	5	313	CLA	ND
5	5	314	CLA	ND
5	5	316	CLA	ND
5	5	317	CLA	ND
5	6	306	CLA	ND
5	6	307	CLA	ND
5	6	309	CLA	ND
5	6	310	CLA	ND
5	6	311	CLA	ND
5	6	312	CLA	ND
5	6	314	CLA	ND
5	6	315	CLA	ND

All (637) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	3	601	CLA	C1A-C2A-CAA-CBA
5	3	602	CLA	CHA-CBD-CGD-O1D
5	3	602	CLA	CHA-CBD-CGD-O2D
5	3	604	CLA	CHA-CBD-CGD-O1D
5	3	604	CLA	CHA-CBD-CGD-O2D
5	3	606	CLA	C2-C3-C5-C6
5	3	606	CLA	C4-C3-C5-C6
5	3	608	CLA	C2-C3-C5-C6
5	3	608	CLA	C4-C3-C5-C6
5	3	611	CLA	C2-C3-C5-C6
5	3	611	CLA	C4-C3-C5-C6
5	3	612	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
5	3	619	CLA	CAD-CBD-CGD-O1D
5	3	619	CLA	CAD-CBD-CGD-O2D
5	3	619	CLA	CBD-CGD-O2D-CED
5	4	310	CLA	CBA-CGA-O2A-C1
5	4	310	CLA	CBD-CGD-O2D-CED
5	4	311	CLA	CHA-CBD-CGD-O1D
5	4	311	CLA	CHA-CBD-CGD-O2D
5	4	312	CLA	C2-C3-C5-C6
5	4	312	CLA	C4-C3-C5-C6
5	4	313	CLA	CHA-CBD-CGD-O1D
5	4	313	CLA	CHA-CBD-CGD-O2D
5	4	313	CLA	CBD-CGD-O2D-CED
5	4	315	CLA	C1A-C2A-CAA-CBA
5	5	308	CLA	CBA-CGA-O2A-C1
5	5	312	CLA	C1A-C2A-CAA-CBA
5	5	312	CLA	C3A-C2A-CAA-CBA
5	5	312	CLA	CBA-CGA-O2A-C1
5	5	314	CLA	CHA-CBD-CGD-O1D
5	5	314	CLA	CHA-CBD-CGD-O2D
5	5	314	CLA	CBD-CGD-O2D-CED
5	5	316	CLA	CBD-CGD-O2D-CED
5	6	306	CLA	CHA-CBD-CGD-O1D
5	6	306	CLA	CHA-CBD-CGD-O2D
5	6	307	CLA	C1A-C2A-CAA-CBA
5	6	307	CLA	C3A-C2A-CAA-CBA
5	6	310	CLA	CBD-CGD-O2D-CED
5	6	310	CLA	O1D-CGD-O2D-CED
5	6	311	CLA	CBD-CGD-O2D-CED
5	6	312	CLA	CBD-CGD-O2D-CED
5	6	315	CLA	CBD-CGD-O2D-CED
6	3	609	KC1	C1A-C2A-CAA-CBA
6	3	609	KC1	C3A-C2A-CAA-CBA
6	3	609	KC1	C2B-C3B-CAB-CBB
6	3	609	KC1	C4B-C3B-CAB-CBB
6	3	609	KC1	C2A-CAA-CBA-CGA
6	3	609	KC1	CBD-CGD-O2D-CED
6	5	315	KC1	C1A-C2A-CAA-CBA
6	5	315	KC1	C3A-C2A-CAA-CBA
6	5	315	KC1	C2B-C3B-CAB-CBB
6	5	315	KC1	C4B-C3B-CAB-CBB
6	6	313	KC1	C1A-C2A-CAA-CBA
6	6	313	KC1	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	6	313	KC1	C2A-CAA-CBA-CGA
7	4	301	A86	C12-C11-C13-O
7	4	301	A86	C12-C11-C13-C14
7	4	301	A86	C13-C14-C15-C16
7	4	301	A86	C13-C14-C15-C20
7	4	301	A86	C13-C14-C15-O1
7	4	302	A86	C10-C11-C13-O
7	4	302	A86	C12-C11-C13-O
7	4	304	A86	C13-C14-C15-C20
7	4	304	A86	C13-C14-C15-O1
7	5	301	A86	C12-C11-C13-C14
7	5	301	A86	C13-C14-C15-C16
7	5	301	A86	C35-C34-O4-C38
7	5	302	A86	C10-C11-C13-O
7	5	302	A86	C12-C11-C13-O
7	5	302	A86	C13-C14-C15-C16
7	5	302	A86	C35-C34-O4-C38
7	5	302	A86	O5-C38-O4-C34
7	5	303	A86	C12-C11-C13-O
7	5	303	A86	C13-C14-C15-C16
7	5	303	A86	C35-C34-O4-C38
7	5	304	A86	C12-C11-C13-C14
7	5	304	A86	C13-C14-C15-C16
7	5	305	A86	C12-C11-C13-C14
7	5	305	A86	C13-C14-C15-C20
7	5	305	A86	C13-C14-C15-O1
7	5	305	A86	C35-C34-O4-C38
7	5	305	A86	O5-C38-O4-C34
7	5	306	A86	C12-C11-C13-O
7	5	306	A86	C12-C11-C13-C14
7	5	306	A86	C13-C14-C15-C16
7	5	306	A86	C39-C38-O4-C34
7	5	307	A86	C12-C11-C13-C14
7	5	307	A86	C13-C14-C15-C16
7	5	307	A86	C39-C38-O4-C34
7	5	321	A86	C10-C11-C13-O
7	5	321	A86	C12-C11-C13-O
7	5	321	A86	C13-C14-C15-C16
7	6	301	A86	C10-C11-C13-O
7	6	302	A86	C12-C11-C13-O
7	6	303	A86	C10-C11-C13-O
7	6	303	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
7	6	303	A86	C13-C14-C15-C16
7	6	304	A86	C10-C11-C13-O
7	6	304	A86	C12-C11-C13-O
7	6	304	A86	C13-C14-C15-C16
7	6	305	A86	C12-C11-C13-C14
7	6	305	A86	C13-C14-C15-C16
8	3	614	DD6	C10-C11-C13-C14
8	3	614	DD6	C12-C11-C13-C14
8	4	303	DD6	C12-C11-C13-C14
9	3	616	LMG	O7-C8-C9-O8
9	5	319	LMG	C2-C1-O1-C7
9	5	319	LMG	O6-C1-O1-C7
9	5	319	LMG	O7-C8-C9-O8
10	3	617	LHG	C3-O3-P-O6
10	3	617	LHG	C4-O6-P-O5
10	3	618	LHG	C3-O3-P-O5
10	3	618	LHG	C4-O6-P-O4
10	4	318	LHG	O1-C1-C2-C3
10	4	318	LHG	C3-O3-P-O5
10	4	318	LHG	C4-O6-P-O3
10	4	318	LHG	C4-O6-P-O4
10	4	318	LHG	C4-O6-P-O5
10	5	318	LHG	C8-C7-O7-C5
11	3	620	DGD	O2G-C2G-C3G-O3G
12	4	307	KC2	C1A-C2A-CAA-CBA
12	4	307	KC2	C3A-C2A-CAA-CBA
12	4	307	KC2	C2B-C3B-CAB-CBB
12	4	307	KC2	C4B-C3B-CAB-CBB
12	4	307	KC2	C2C-C3C-CAC-CBC
12	4	307	KC2	C2A-CAA-CBA-CGA
12	5	310	KC2	C2C-C3C-CAC-CBC
12	6	308	KC2	C2B-C3B-CAB-CBB
12	6	308	KC2	C4B-C3B-CAB-CBB
12	6	308	KC2	C2C-C3C-CAC-CBC
13	5	320	LMT	C2-C1-O1'-C1'
7	4	301	A86	C39-C38-O4-C34
7	4	302	A86	C39-C38-O4-C34
7	4	304	A86	O5-C38-O4-C34
7	5	301	A86	C39-C38-O4-C34
7	5	302	A86	C39-C38-O4-C34
7	5	304	A86	C39-C38-O4-C34
7	5	321	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
7	6	302	A86	C39-C38-O4-C34
7	6	305	A86	C39-C38-O4-C34
9	3	616	LMG	C11-C10-O7-C8
5	4	310	CLA	O1D-CGD-O2D-CED
5	5	316	CLA	O1D-CGD-O2D-CED
5	6	315	CLA	O1D-CGD-O2D-CED
7	4	302	A86	O5-C38-O4-C34
7	4	304	A86	C39-C38-O4-C34
5	6	311	CLA	O1D-CGD-O2D-CED
5	6	312	CLA	O1D-CGD-O2D-CED
5	3	604	CLA	CBD-CGD-O2D-CED
5	3	605	CLA	CBD-CGD-O2D-CED
5	3	608	CLA	CBD-CGD-O2D-CED
5	3	612	CLA	CBD-CGD-O2D-CED
5	5	311	CLA	CBD-CGD-O2D-CED
5	5	313	CLA	CBD-CGD-O2D-CED
5	4	305	CLA	O1A-CGA-O2A-C1
5	5	311	CLA	O1A-CGA-O2A-C1
5	4	310	CLA	O1A-CGA-O2A-C1
7	4	301	A86	O5-C38-O4-C34
7	5	303	A86	C39-C38-O4-C34
5	4	313	CLA	O1D-CGD-O2D-CED
5	5	314	CLA	O1D-CGD-O2D-CED
7	5	303	A86	O5-C38-O4-C34
6	3	609	KC1	O1D-CGD-O2D-CED
5	3	601	CLA	CBA-CGA-O2A-C1
5	5	311	CLA	CBA-CGA-O2A-C1
5	4	305	CLA	CBD-CGD-O2D-CED
5	4	306	CLA	CBD-CGD-O2D-CED
5	5	308	CLA	CBD-CGD-O2D-CED
6	5	315	KC1	CBD-CGD-O2D-CED
12	6	308	KC2	CBD-CGD-O2D-CED
7	5	301	A86	O5-C38-O4-C34
5	3	601	CLA	O1A-CGA-O2A-C1
5	3	603	CLA	O1A-CGA-O2A-C1
5	4	314	CLA	O1A-CGA-O2A-C1
5	6	311	CLA	O1A-CGA-O2A-C1
10	3	617	LHG	O10-C23-O8-C6
10	3	618	LHG	O10-C23-O8-C6
10	4	318	LHG	O10-C23-O8-C6
5	5	308	CLA	O1A-CGA-O2A-C1
5	3	619	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
7	6	302	A86	O5-C38-O4-C34
7	6	305	A86	O5-C38-O4-C34
5	3	601	CLA	CBD-CGD-O2D-CED
10	4	318	LHG	O9-C7-O7-C5
10	5	318	LHG	O9-C7-O7-C5
11	3	620	DGD	O1B-C1B-O2G-C2G
5	5	314	CLA	O1A-CGA-O2A-C1
5	3	601	CLA	C3-C5-C6-C7
5	4	305	CLA	C3-C5-C6-C7
5	4	305	CLA	CBA-CGA-O2A-C1
5	4	314	CLA	CBA-CGA-O2A-C1
10	3	618	LHG	C24-C23-O8-C6
10	4	318	LHG	C24-C23-O8-C6
5	4	311	CLA	CBD-CGD-O2D-CED
7	5	307	A86	O5-C38-O4-C34
5	5	312	CLA	O1A-CGA-O2A-C1
7	5	306	A86	O5-C38-O4-C34
6	3	609	KC1	CAA-CBA-CGA-O2A
7	5	304	A86	O5-C38-O4-C34
5	3	607	CLA	C4-C3-C5-C6
5	3	612	CLA	C4-C3-C5-C6
5	4	311	CLA	C4-C3-C5-C6
5	4	311	CLA	C2-C3-C5-C6
5	3	606	CLA	CBD-CGD-O2D-CED
7	5	321	A86	O5-C38-O4-C34
5	3	603	CLA	CBA-CGA-O2A-C1
5	3	608	CLA	CBA-CGA-O2A-C1
5	3	612	CLA	CBA-CGA-O2A-C1
5	5	313	CLA	CBA-CGA-O2A-C1
5	5	314	CLA	CBA-CGA-O2A-C1
5	6	311	CLA	CBA-CGA-O2A-C1
10	3	617	LHG	C24-C23-O8-C6
5	5	313	CLA	O1D-CGD-O2D-CED
5	3	605	CLA	O1D-CGD-O2D-CED
5	3	612	CLA	O1D-CGD-O2D-CED
5	3	608	CLA	O1A-CGA-O2A-C1
5	5	313	CLA	O1A-CGA-O2A-C1
5	5	311	CLA	O1D-CGD-O2D-CED
13	5	320	LMT	O5B-C5B-C6B-O6B
7	6	301	A86	C39-C38-O4-C34
5	3	603	CLA	CBD-CGD-O2D-CED
5	4	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
10	3	618	LHG	O2-C2-C3-O3
5	3	612	CLA	C3-C5-C6-C7
5	3	607	CLA	CBA-CGA-O2A-C1
5	6	306	CLA	CBA-CGA-O2A-C1
7	6	301	A86	O5-C38-O4-C34
7	6	303	A86	C39-C38-O4-C34
7	6	304	A86	C39-C38-O4-C34
9	3	616	LMG	O9-C10-O7-C8
13	5	320	LMT	C5'-C4'-O1B-C1B
5	3	604	CLA	O1D-CGD-O2D-CED
5	3	608	CLA	O1D-CGD-O2D-CED
11	3	620	DGD	C2B-C1B-O2G-C2G
7	6	303	A86	O5-C38-O4-C34
7	6	304	A86	O5-C38-O4-C34
5	6	310	CLA	CBA-CGA-O2A-C1
9	5	319	LMG	O6-C5-C6-O5
9	5	319	LMG	C4-C5-C6-O5
5	6	306	CLA	O1A-CGA-O2A-C1
5	3	619	CLA	C3-C5-C6-C7
5	5	309	CLA	C3-C5-C6-C7
5	4	316	CLA	C3-C5-C6-C7
13	5	320	LMT	C4B-C5B-C6B-O6B
5	3	612	CLA	C2-C3-C5-C6
5	3	607	CLA	O1A-CGA-O2A-C1
5	3	612	CLA	O1A-CGA-O2A-C1
5	3	611	CLA	CBA-CGA-O2A-C1
5	5	308	CLA	O1D-CGD-O2D-CED
7	5	321	A86	C33-C34-O4-C38
5	3	611	CLA	O1A-CGA-O2A-C1
5	3	606	CLA	CBA-CGA-O2A-C1
6	3	609	KC1	CAA-CBA-CGA-O1A
5	3	606	CLA	O1A-CGA-O2A-C1
5	3	607	CLA	C2-C3-C5-C6
7	3	613	A86	C7-C6-C8-C9
7	3	613	A86	C5-C6-C8-C9
12	6	308	KC2	CAA-CBA-CGA-O2A
5	4	311	CLA	CBA-CGA-O2A-C1
5	3	601	CLA	C10-C11-C12-C13
5	4	306	CLA	O1D-CGD-O2D-CED
10	3	618	LHG	C23-C24-C25-C26
10	4	318	LHG	C23-C24-C25-C26
7	5	306	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
10	5	318	LHG	C23-C24-C25-C26
5	4	308	CLA	C12-C13-C15-C16
7	3	613	A86	C11-C10-C9-C8
5	4	305	CLA	O1D-CGD-O2D-CED
5	6	306	CLA	CBD-CGD-O2D-CED
10	4	318	LHG	C7-C8-C9-C10
10	4	318	LHG	O2-C2-C3-O3
5	6	310	CLA	O1A-CGA-O2A-C1
5	3	601	CLA	O1D-CGD-O2D-CED
13	4	317	LMT	C4B-C5B-C6B-O6B
10	3	618	LHG	C3-O3-P-O6
10	3	618	LHG	C4-O6-P-O3
10	4	318	LHG	C3-O3-P-O6
5	4	311	CLA	O1D-CGD-O2D-CED
5	4	311	CLA	O1A-CGA-O2A-C1
10	4	318	LHG	C1-C2-C3-O3
5	3	602	CLA	C4-C3-C5-C6
5	4	314	CLA	C4-C3-C5-C6
5	6	306	CLA	C4-C3-C5-C6
5	3	606	CLA	C5-C6-C7-C8
5	3	604	CLA	C2A-CAA-CBA-CGA
5	3	606	CLA	O1D-CGD-O2D-CED
5	4	311	CLA	C11-C12-C13-C15
5	4	308	CLA	O1D-CGD-O2D-CED
5	3	602	CLA	C3-C5-C6-C7
5	4	308	CLA	C13-C15-C16-C17
11	3	620	DGD	C5A-C6A-C7A-C8A
11	3	620	DGD	C6A-C7A-C8A-C9A
5	3	603	CLA	C14-C13-C15-C16
5	4	309	CLA	C6-C7-C8-C9
10	4	318	LHG	C32-C33-C34-C35
5	3	605	CLA	C15-C16-C17-C18
5	5	312	CLA	C2A-CAA-CBA-CGA
10	4	318	LHG	C27-C28-C29-C30
5	3	603	CLA	O1D-CGD-O2D-CED
13	4	317	LMT	O5B-C5B-C6B-O6B
5	4	311	CLA	C11-C12-C13-C14
5	6	312	CLA	CBA-CGA-O2A-C1
5	3	603	CLA	C3A-C2A-CAA-CBA
5	4	309	CLA	C3A-C2A-CAA-CBA
5	4	312	CLA	C3A-C2A-CAA-CBA
5	6	310	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	3	620	DGD	C4A-C5A-C6A-C7A
7	6	305	A86	C35-C34-O4-C38
10	5	318	LHG	C11-C12-C13-C14
11	3	620	DGD	C6B-C7B-C8B-C9B
5	3	601	CLA	C8-C10-C11-C12
5	4	316	CLA	CBA-CGA-O2A-C1
9	5	319	LMG	C11-C10-O7-C8
10	4	318	LHG	O1-C1-C2-O2
5	4	311	CLA	C10-C11-C12-C13
5	3	601	CLA	C16-C17-C18-C20
13	4	317	LMT	C6-C7-C8-C9
5	3	612	CLA	C8-C10-C11-C12
10	4	318	LHG	C10-C11-C12-C13
5	3	603	CLA	C2-C1-O2A-CGA
10	3	618	LHG	C27-C28-C29-C30
9	3	615	LMG	C28-C29-C30-C31
5	3	605	CLA	C4-C3-C5-C6
5	3	612	CLA	C11-C12-C13-C15
5	5	313	CLA	C11-C10-C8-C7
7	4	302	A86	C35-C34-O4-C38
11	3	620	DGD	C1A-C2A-C3A-C4A
5	4	311	CLA	C5-C6-C7-C8
6	6	313	KC1	C2B-C3B-CAB-CBB
5	3	611	CLA	C3-C5-C6-C7
5	4	316	CLA	O1A-CGA-O2A-C1
10	3	618	LHG	C8-C7-O7-C5
10	4	318	LHG	C8-C7-O7-C5
6	6	313	KC1	C4B-C3B-CAB-CBB
12	4	307	KC2	C4C-C3C-CAC-CBC
12	5	310	KC2	C4C-C3C-CAC-CBC
12	6	308	KC2	C4C-C3C-CAC-CBC
10	3	617	LHG	O7-C5-C6-O8
5	3	602	CLA	C2-C3-C5-C6
5	4	314	CLA	C2-C3-C5-C6
5	6	306	CLA	C2-C3-C5-C6
5	5	313	CLA	C11-C10-C8-C9
9	3	615	LMG	O6-C5-C6-O5
5	3	607	CLA	C2A-CAA-CBA-CGA
13	4	317	LMT	C5'-C4'-O1B-C1B
5	3	602	CLA	C1A-C2A-CAA-CBA
5	3	603	CLA	C1A-C2A-CAA-CBA
5	4	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	4	310	CLA	C1A-C2A-CAA-CBA
5	4	312	CLA	C1A-C2A-CAA-CBA
5	5	311	CLA	C1A-C2A-CAA-CBA
5	6	310	CLA	C1A-C2A-CAA-CBA
5	6	311	CLA	C1A-C2A-CAA-CBA
5	3	601	CLA	C16-C17-C18-C19
10	4	318	LHG	O6-C4-C5-C6
13	4	317	LMT	O5'-C5'-C6'-O6'
11	3	620	DGD	C3A-C4A-C5A-C6A
9	3	615	LMG	O1-C7-C8-C9
9	3	616	LMG	O1-C7-C8-C9
9	5	319	LMG	C7-C8-C9-O8
9	3	615	LMG	C8-C7-O1-C1
9	5	319	LMG	C8-C7-O1-C1
5	3	604	CLA	O2A-C1-C2-C3
5	3	602	CLA	C10-C11-C12-C13
10	5	318	LHG	C12-C13-C14-C15
11	3	620	DGD	CEB-CFB-CGB-CHB
5	5	311	CLA	C5-C6-C7-C8
5	3	619	CLA	CBA-CGA-O2A-C1
11	3	620	DGD	C1G-C2G-O2G-C1B
10	5	318	LHG	C4-O6-P-O5
9	3	615	LMG	C30-C31-C32-C33
5	3	612	CLA	C10-C11-C12-C13
5	6	306	CLA	O1D-CGD-O2D-CED
9	5	319	LMG	C30-C31-C32-C33
5	3	602	CLA	C11-C12-C13-C15
5	4	311	CLA	C6-C7-C8-C10
5	3	611	CLA	C6-C7-C8-C9
5	4	311	CLA	C6-C7-C8-C9
5	4	314	CLA	C6-C7-C8-C9
13	4	317	LMT	C3-C4-C5-C6
5	3	602	CLA	C2A-CAA-CBA-CGA
8	3	614	DD6	C-C1-C24-C25
8	4	303	DD6	C10-C11-C13-C14
13	5	320	LMT	O1'-C1-C2-C3
5	3	604	CLA	CBA-CGA-O2A-C1
10	4	318	LHG	C2-C3-O3-P
5	3	601	CLA	C3A-C2A-CAA-CBA
5	4	315	CLA	C3A-C2A-CAA-CBA
13	5	320	LMT	C3'-C4'-O1B-C1B
5	5	314	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	4	317	LMT	C3'-C4'-O1B-C1B
7	5	301	A86	C33-C34-O4-C38
5	3	605	CLA	C2-C3-C5-C6
5	4	306	CLA	C13-C15-C16-C17
5	3	619	CLA	O1A-CGA-O2A-C1
5	3	606	CLA	C3-C5-C6-C7
10	4	318	LHG	C9-C10-C11-C12
10	4	318	LHG	C33-C34-C35-C36
10	4	318	LHG	O6-C4-C5-O7
10	3	618	LHG	C11-C12-C13-C14
5	6	312	CLA	O1A-CGA-O2A-C1
9	3	615	LMG	O1-C7-C8-O7
9	3	616	LMG	O1-C7-C8-O7
5	3	603	CLA	C13-C15-C16-C17
7	4	301	A86	C10-C11-C13-C14
7	5	301	A86	C10-C11-C13-C14
7	5	302	A86	C10-C11-C13-C14
7	5	303	A86	C10-C11-C13-C14
7	5	304	A86	C10-C11-C13-C14
7	5	305	A86	C10-C11-C13-C14
7	5	306	A86	C10-C11-C13-C14
7	5	307	A86	C10-C11-C13-C14
7	6	305	A86	C10-C11-C13-C14
10	3	618	LHG	C1-C2-C3-O3
9	5	319	LMG	C11-C12-C13-C14
5	3	602	CLA	C11-C12-C13-C14
10	4	318	LHG	C18-C19-C20-C21
5	4	311	CLA	C2A-CAA-CBA-CGA
10	4	318	LHG	C17-C18-C19-C20
9	5	319	LMG	O9-C10-O7-C8
10	4	318	LHG	C24-C25-C26-C27
5	3	601	CLA	C6-C7-C8-C10
5	3	607	CLA	C11-C10-C8-C7
5	3	611	CLA	C6-C7-C8-C10
5	3	612	CLA	C11-C10-C8-C7
5	6	311	CLA	C3-C5-C6-C7
13	5	320	LMT	O5B-C1B-O1B-C4'
5	4	309	CLA	CBA-CGA-O2A-C1
5	6	307	CLA	CBA-CGA-O2A-C1
10	5	318	LHG	C10-C11-C12-C13
13	5	320	LMT	C2B-C1B-O1B-C4'
5	3	601	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
5	3	607	CLA	CAD-CBD-CGD-O2D
5	4	310	CLA	CAD-CBD-CGD-O2D
5	4	314	CLA	CAD-CBD-CGD-O2D
5	3	607	CLA	C10-C11-C12-C13
5	3	604	CLA	O1A-CGA-O2A-C1
7	4	304	A86	C12-C11-C13-O
7	5	301	A86	C12-C11-C13-O
7	5	304	A86	C12-C11-C13-O
7	5	305	A86	C12-C11-C13-O
7	5	307	A86	C12-C11-C13-O
7	6	301	A86	C12-C11-C13-O
7	6	305	A86	C12-C11-C13-O
9	3	616	LMG	C7-C8-C9-O8
11	3	620	DGD	O1G-C1G-C2G-C3G
5	6	307	CLA	O1A-CGA-O2A-C1
5	3	607	CLA	C8-C10-C11-C12
7	6	302	A86	C35-C34-O4-C38
11	3	620	DGD	C2B-C3B-C4B-C5B
5	5	312	CLA	CBD-CGD-O2D-CED
10	3	617	LHG	O2-C2-C3-O3
5	6	309	CLA	CHA-CBD-CGD-O1D
5	6	309	CLA	CHA-CBD-CGD-O2D
12	4	307	KC2	CBD-CGD-O2D-CED
11	3	620	DGD	O1G-C1G-C2G-O2G
10	5	318	LHG	C24-C25-C26-C27
7	4	301	A86	C10-C11-C13-O
7	4	304	A86	C10-C11-C13-O
7	5	301	A86	C10-C11-C13-O
7	5	303	A86	C10-C11-C13-O
7	5	304	A86	C10-C11-C13-O
7	5	305	A86	C10-C11-C13-O
7	5	306	A86	C10-C11-C13-O
7	5	307	A86	C10-C11-C13-O
7	6	302	A86	C10-C11-C13-O
7	6	305	A86	C10-C11-C13-O
8	4	303	DD6	C27-C29-C30-C31
5	3	601	CLA	C6-C7-C8-C9
11	3	620	DGD	C7B-C8B-C9B-CAB
5	4	309	CLA	O1A-CGA-O2A-C1
10	4	318	LHG	C29-C30-C31-C32
8	3	614	DD6	C2-C1-C24-C25
5	5	313	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	4	314	CLA	C2-C1-O2A-CGA
10	4	318	LHG	C26-C27-C28-C29
10	5	318	LHG	C11-C10-C9-C8
10	3	617	LHG	C3-O3-P-O5
10	4	318	LHG	C3-O3-P-O4
5	3	606	CLA	C16-C17-C18-C20
5	3	602	CLA	C13-C15-C16-C17
10	5	318	LHG	O6-C4-C5-C6
5	3	604	CLA	CAD-CBD-CGD-O1D
5	5	314	CLA	CAD-CBD-CGD-O1D
5	6	309	CLA	CAD-CBD-CGD-O1D
11	3	620	DGD	CAB-CBB-CCB-CDB
10	3	617	LHG	C1-C2-C3-O3
5	3	605	CLA	C11-C10-C8-C7
5	4	306	CLA	C11-C10-C8-C7
10	5	318	LHG	O6-C4-C5-O7
5	3	606	CLA	C10-C11-C12-C13
5	6	309	CLA	C2A-CAA-CBA-CGA
13	4	317	LMT	C7-C8-C9-C10
9	5	319	LMG	O1-C7-C8-C9
7	6	301	A86	C33-C34-O4-C38
7	4	302	A86	C13-C14-C15-C20
7	5	301	A86	C13-C14-C15-C20
7	5	302	A86	C13-C14-C15-C20
7	5	303	A86	C13-C14-C15-C20
7	6	304	A86	C13-C14-C15-C20
5	3	607	CLA	C11-C10-C8-C9
5	3	612	CLA	C6-C7-C8-C9
5	4	306	CLA	C11-C10-C8-C9
5	3	605	CLA	C3-C5-C6-C7
11	3	620	DGD	C9A-CAA-CBA-CCA
10	4	318	LHG	C6-C5-O7-C7
7	4	301	A86	C33-C34-O4-C38
5	5	312	CLA	O1D-CGD-O2D-CED
10	4	318	LHG	C13-C14-C15-C16
7	4	302	A86	C12-C11-C13-C14
7	4	304	A86	C12-C11-C13-C14
7	5	302	A86	C12-C11-C13-C14
7	5	303	A86	C12-C11-C13-C14
7	5	321	A86	C12-C11-C13-C14
7	6	301	A86	C12-C11-C13-C14
7	6	302	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
7	6	303	A86	C12-C11-C13-C14
7	6	304	A86	C12-C11-C13-C14
5	5	313	CLA	C10-C11-C12-C13
7	3	613	A86	C39-C38-O4-C34
5	3	606	CLA	C16-C17-C18-C19
10	3	617	LHG	C4-C5-C6-O8
10	4	318	LHG	C28-C29-C30-C31
5	4	308	CLA	C14-C13-C15-C16
10	3	618	LHG	C32-C33-C34-C35
12	6	308	KC2	CAA-CBA-CGA-O1A
5	5	309	CLA	C6-C7-C8-C9
10	3	618	LHG	C5-C4-O6-P
10	4	318	LHG	C30-C31-C32-C33
10	3	618	LHG	C24-C25-C26-C27
10	3	617	LHG	O6-C4-C5-C6
11	3	620	DGD	C8A-C9A-CAA-CBA
5	5	313	CLA	C4-C3-C5-C6
5	3	612	CLA	C2-C1-O2A-CGA
7	5	307	A86	C35-C34-O4-C38
11	3	620	DGD	C5B-C6B-C7B-C8B
5	5	313	CLA	C6-C7-C8-C9
5	5	308	CLA	C2A-CAA-CBA-CGA
12	6	308	KC2	C2A-CAA-CBA-CGA
5	5	309	CLA	C6-C7-C8-C10
11	3	620	DGD	C1B-C2B-C3B-C4B
7	6	304	A86	C35-C34-O4-C38
5	4	314	CLA	C1A-C2A-CAA-CBA
5	4	306	CLA	C2A-CAA-CBA-CGA
5	4	308	CLA	C2A-CAA-CBA-CGA
7	4	302	A86	C13-C14-C15-C16
7	6	302	A86	C13-C14-C15-C16
7	5	304	A86	C35-C34-O4-C38
7	6	303	A86	C35-C34-O4-C38
7	4	302	A86	C10-C11-C13-C14
7	4	304	A86	C10-C11-C13-C14
7	5	321	A86	C10-C11-C13-C14
7	6	301	A86	C10-C11-C13-C14
7	6	302	A86	C10-C11-C13-C14
7	6	303	A86	C10-C11-C13-C14
7	6	304	A86	C10-C11-C13-C14
11	3	620	DGD	C1G-C2G-C3G-O3G
5	6	309	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	6	308	KC2	O1D-CGD-O2D-CED
5	3	605	CLA	O1A-CGA-O2A-C1
5	3	605	CLA	CBA-CGA-O2A-C1
5	6	309	CLA	CBD-CGD-O2D-CED
5	3	605	CLA	C13-C15-C16-C17
10	3	617	LHG	O6-C4-C5-O7
5	5	314	CLA	C4-C3-C5-C6
5	6	309	CLA	C2-C3-C5-C6
7	3	613	A86	O5-C38-O4-C34
9	5	319	LMG	O1-C7-C8-O7
5	3	607	CLA	O1D-CGD-O2D-CED
5	3	601	CLA	CAA-CBA-CGA-O2A
13	4	317	LMT	C1-C2-C3-C4
5	3	605	CLA	C11-C10-C8-C9
5	6	311	CLA	C6-C7-C8-C9
5	3	611	CLA	C3A-C2A-CAA-CBA
5	6	312	CLA	C3A-C2A-CAA-CBA
13	4	317	LMT	C11-C10-C9-C8
5	3	603	CLA	CAD-CBD-CGD-O2D
5	5	309	CLA	CAD-CBD-CGD-O2D
7	5	301	A86	C28-C27-C29-C30
12	5	310	KC2	CAD-CBD-CGD-O2D
5	3	606	CLA	C13-C15-C16-C17
9	3	615	LMG	O8-C28-C29-C30
6	5	315	KC1	CAA-CBA-CGA-O2A
8	3	614	DD6	C13-C14-C15-O1
5	3	607	CLA	CBD-CGD-O2D-CED
5	4	314	CLA	C2A-CAA-CBA-CGA
5	5	309	CLA	C2A-CAA-CBA-CGA
5	3	602	CLA	CAA-CBA-CGA-O2A
5	3	605	CLA	CHA-CBD-CGD-O1D
5	3	605	CLA	CHA-CBD-CGD-O2D
5	3	612	CLA	CHA-CBD-CGD-O1D
5	3	619	CLA	CHA-CBD-CGD-O1D
5	3	619	CLA	CHA-CBD-CGD-O2D
5	4	306	CLA	CHA-CBD-CGD-O1D
5	4	306	CLA	CHA-CBD-CGD-O2D
5	4	312	CLA	CHA-CBD-CGD-O1D
5	4	315	CLA	CHA-CBD-CGD-O1D
5	4	315	CLA	CHA-CBD-CGD-O2D
5	6	307	CLA	CHA-CBD-CGD-O2D
12	6	308	KC2	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
5	3	607	CLA	CAA-CBA-CGA-O2A
5	5	312	CLA	CAA-CBA-CGA-O2A
10	4	318	LHG	C5-C4-O6-P
5	4	305	CLA	C4-C3-C5-C6
5	3	601	CLA	CAA-CBA-CGA-O1A
5	3	606	CLA	C1A-C2A-CAA-CBA
5	3	607	CLA	C1A-C2A-CAA-CBA
5	3	611	CLA	C1A-C2A-CAA-CBA
5	4	308	CLA	C1A-C2A-CAA-CBA
5	4	316	CLA	C1A-C2A-CAA-CBA
5	5	309	CLA	C1A-C2A-CAA-CBA
5	6	312	CLA	C1A-C2A-CAA-CBA
5	5	311	CLA	C2-C1-O2A-CGA
5	3	601	CLA	C15-C16-C17-C18
5	6	309	CLA	C4-C3-C5-C6
5	3	607	CLA	CAA-CBA-CGA-O1A
5	3	602	CLA	CAA-CBA-CGA-O1A
9	3	615	LMG	O10-C28-C29-C30
5	3	619	CLA	C5-C6-C7-C8
10	3	617	LHG	C11-C10-C9-C8
5	6	310	CLA	CAD-CBD-CGD-O1D
5	6	315	CLA	CAD-CBD-CGD-O1D
5	3	612	CLA	C11-C12-C13-C14
5	4	308	CLA	CAA-CBA-CGA-O2A
5	5	308	CLA	CAA-CBA-CGA-O2A
5	6	310	CLA	CAA-CBA-CGA-O2A
5	4	305	CLA	CAA-CBA-CGA-O2A
5	5	311	CLA	CAA-CBA-CGA-O2A
5	3	606	CLA	C11-C10-C8-C7
5	5	313	CLA	C2-C3-C5-C6
5	5	312	CLA	CAA-CBA-CGA-O1A
11	3	620	DGD	C4B-C5B-C6B-C7B
10	3	617	LHG	O8-C23-C24-C25
5	6	310	CLA	CAA-CBA-CGA-O1A
13	4	317	LMT	C2-C1-O1'-C1'
5	4	308	CLA	CAA-CBA-CGA-O1A
5	5	308	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

46 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	5	311	CLA	2	0
5	6	307	CLA	3	0
5	3	605	CLA	1	0
7	5	321	A86	1	0
5	5	313	CLA	3	0
12	6	308	KC2	1	0
5	3	619	CLA	3	0
5	3	603	CLA	4	0
5	3	607	CLA	3	0
5	4	315	CLA	2	0
5	4	308	CLA	4	0
5	3	606	CLA	6	0
5	3	611	CLA	4	0
5	4	314	CLA	4	0
5	5	316	CLA	2	0
5	5	312	CLA	2	0
11	3	620	DGD	1	0
5	3	601	CLA	1	0
5	6	306	CLA	3	0
6	6	313	KC1	3	0
7	5	306	A86	1	0
9	3	615	LMG	1	0
5	5	309	CLA	1	0
10	3	618	LHG	3	0
12	5	310	KC2	3	0
5	6	315	CLA	1	0
5	3	612	CLA	2	0
5	6	309	CLA	1	0
5	6	312	CLA	5	0
5	4	310	CLA	1	0
7	3	613	A86	1	0
5	4	306	CLA	2	0
7	5	304	A86	3	0
5	3	610	CLA	1	0
5	6	310	CLA	1	0
5	6	314	CLA	2	0
5	3	602	CLA	4	0
7	6	301	A86	1	0
5	3	604	CLA	1	0
10	4	318	LHG	2	0
7	6	302	A86	1	0
5	5	314	CLA	26	0
5	4	309	CLA	1	0

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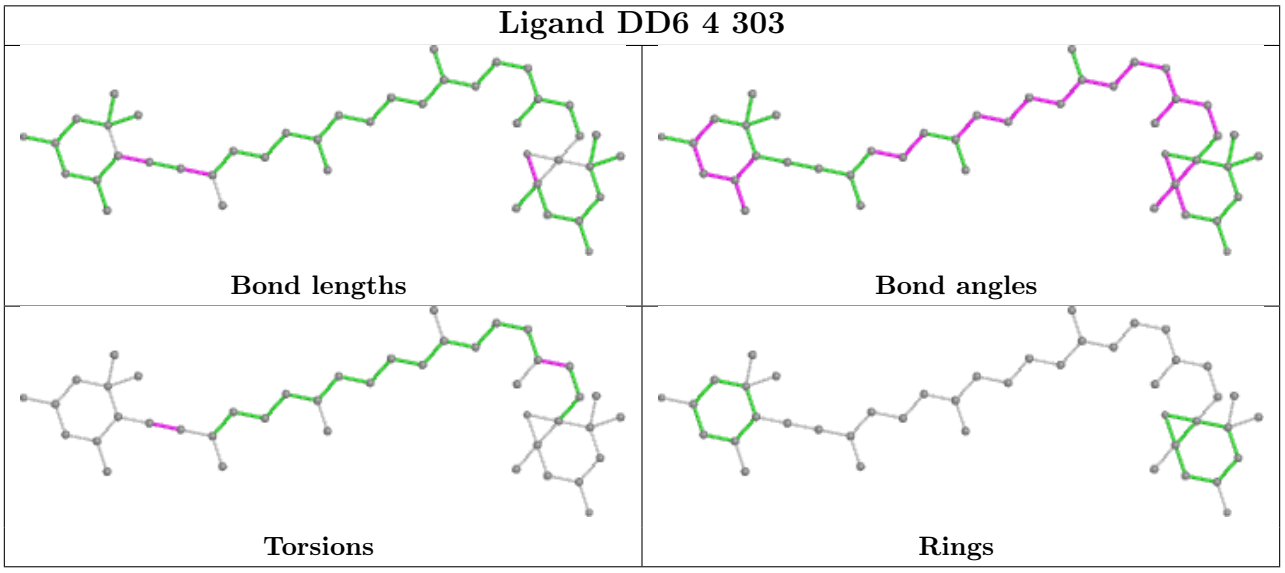
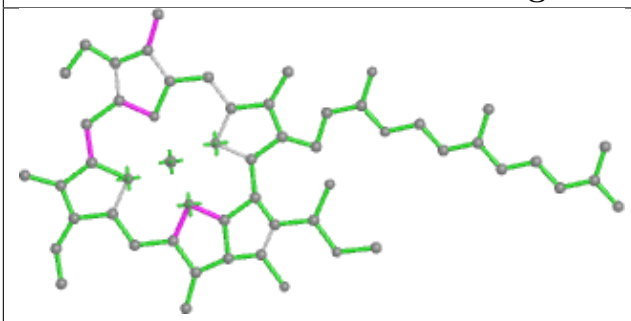
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	4	311	CLA	2	0
5	4	312	CLA	2	0
9	5	319	LMG	1	0

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

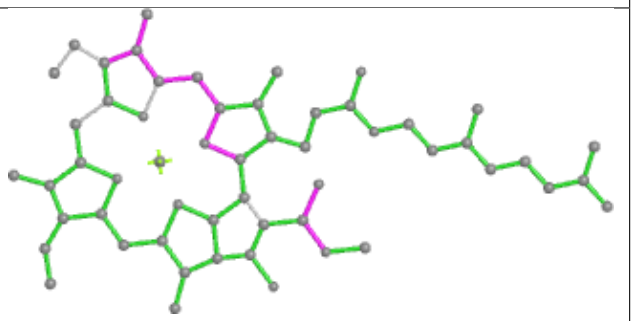
Ligand DD6 4 303



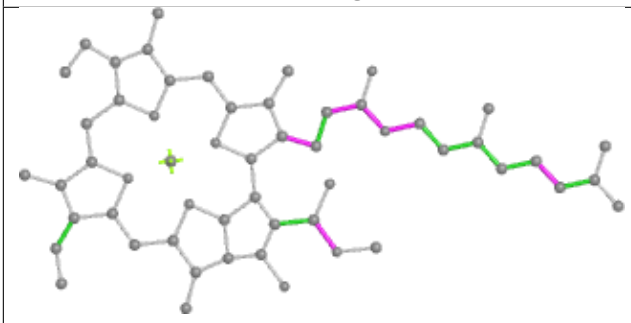
Ligand CLA 5 311



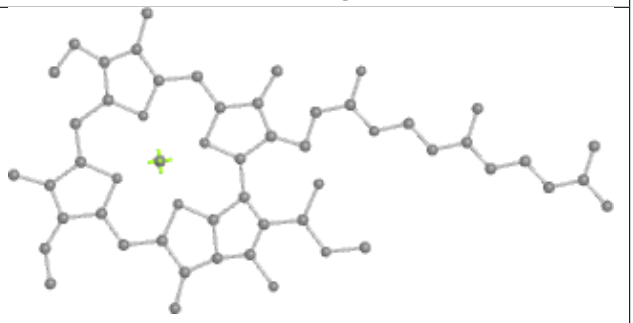
Bond lengths



Bond angles

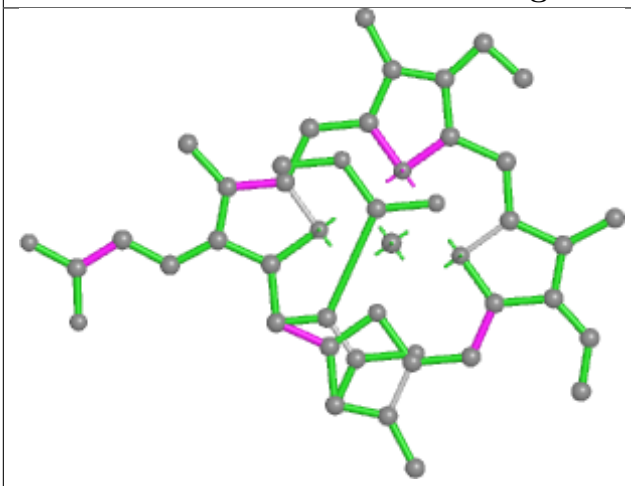


Torsions

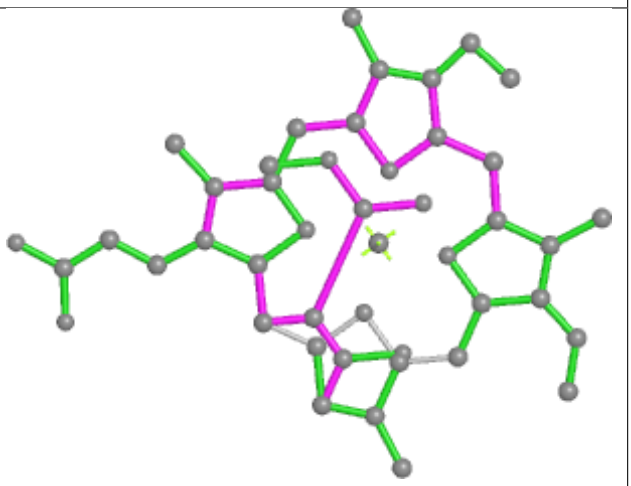


Rings

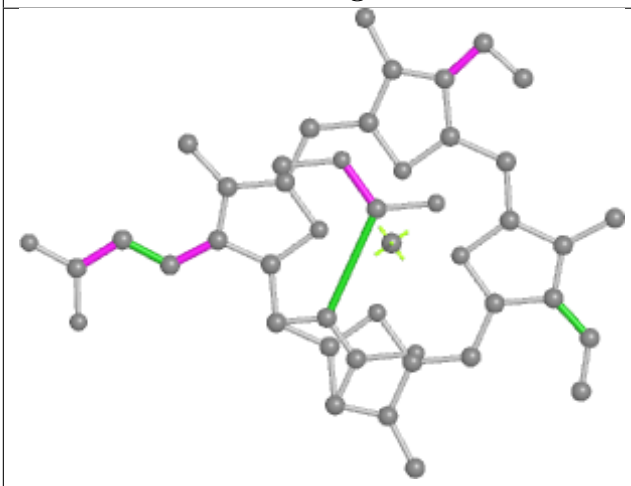
Ligand KC1 5 315



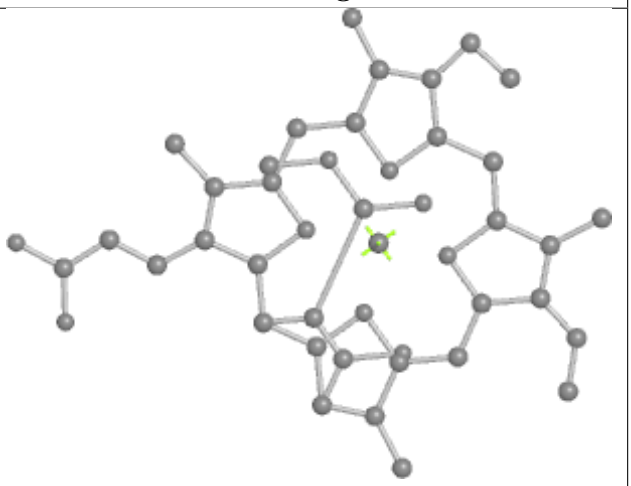
Bond lengths



Bond angles

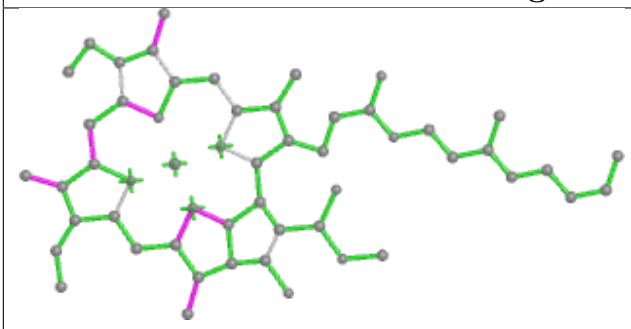


Torsions

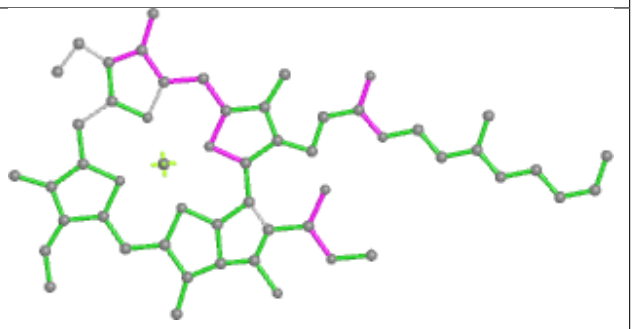


Rings

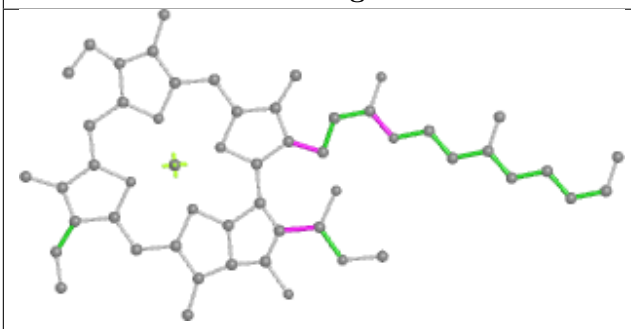
Ligand CLA 6 307



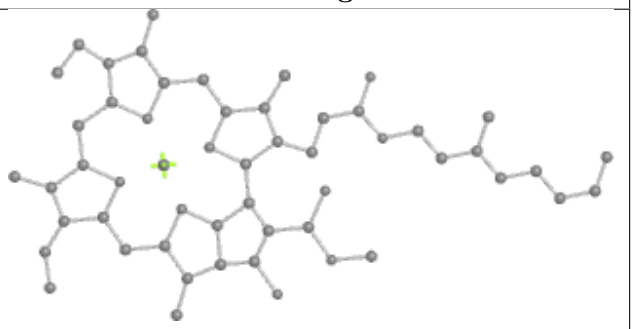
Bond lengths



Bond angles

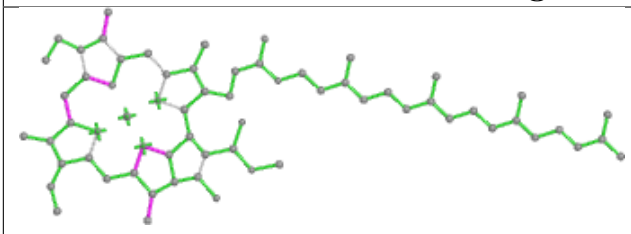


Torsions

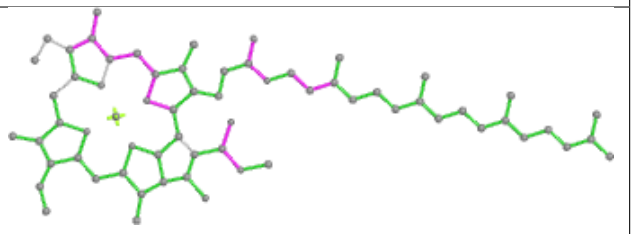


Rings

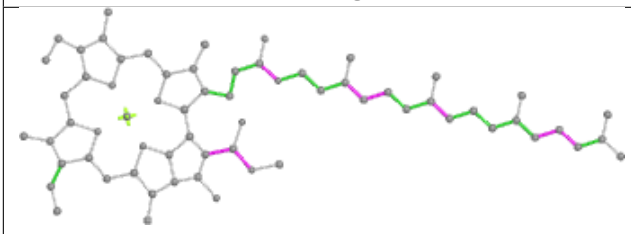
Ligand CLA 3 605



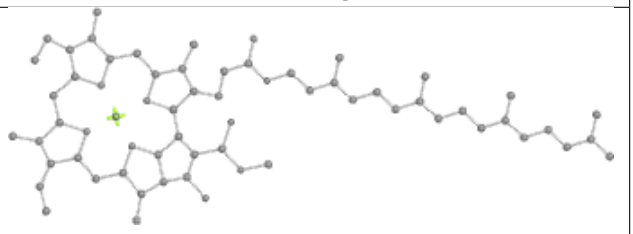
Bond lengths



Bond angles

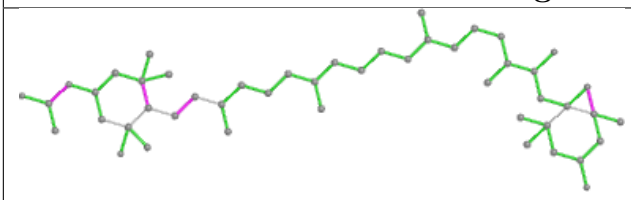


Torsions

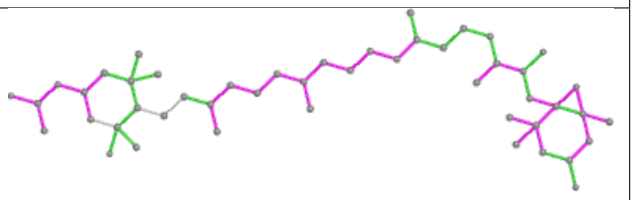


Rings

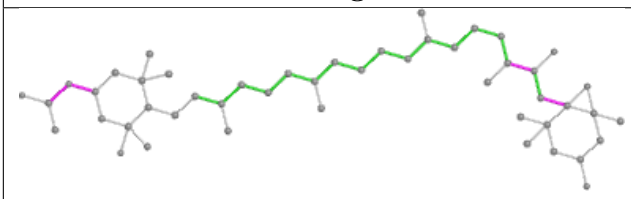
Ligand A86 5 321



Bond lengths



Bond angles



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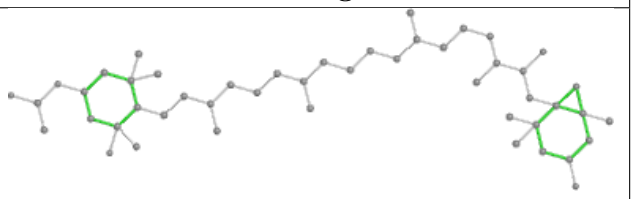
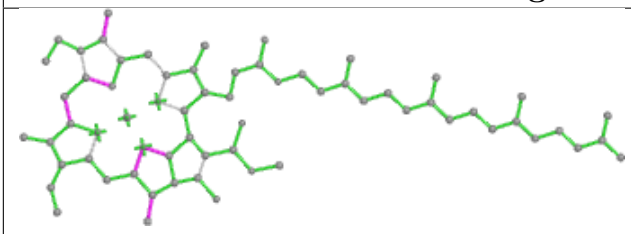
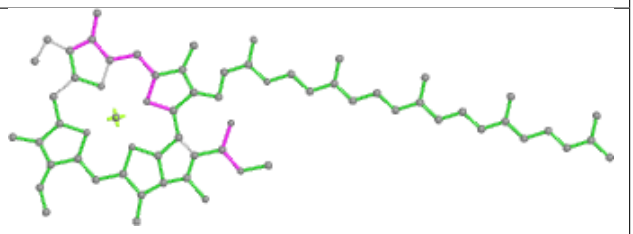


Rings

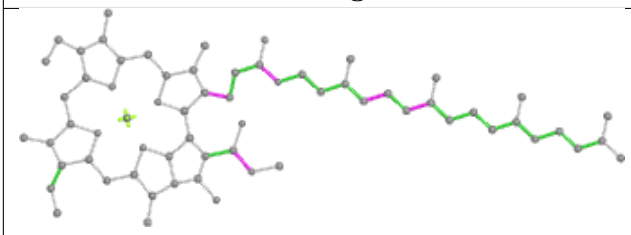
Ligand CLA 6 311



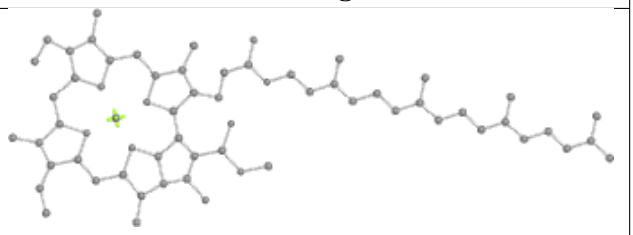
Bond lengths



Bond angles

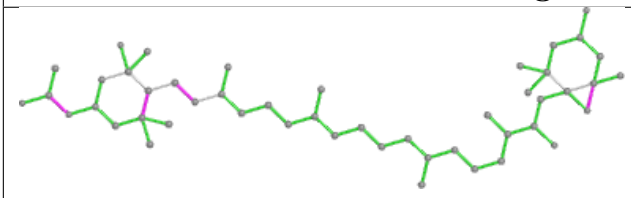


Torsions

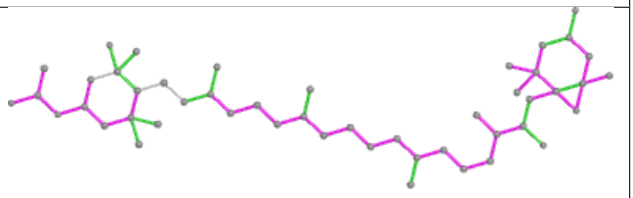


Rings

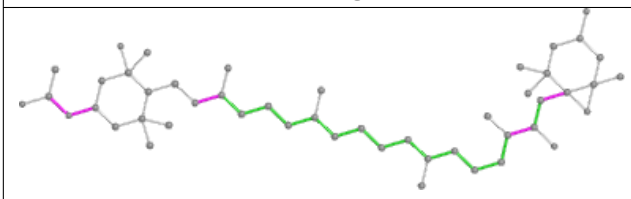
Ligand A86 5 301



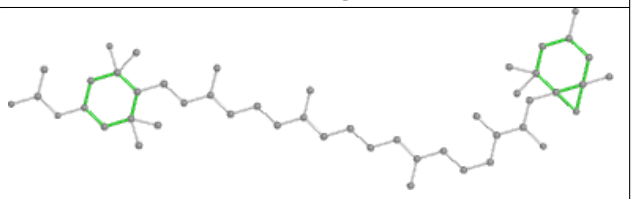
Bond lengths



Bond angles

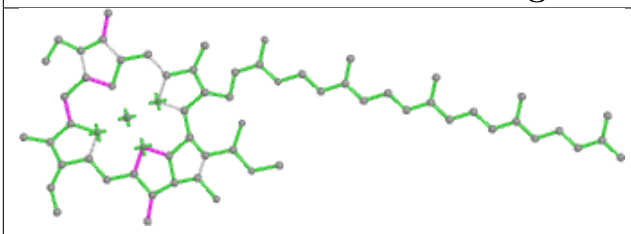


Torsions

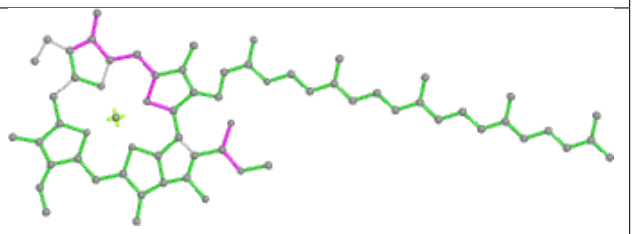


Rings

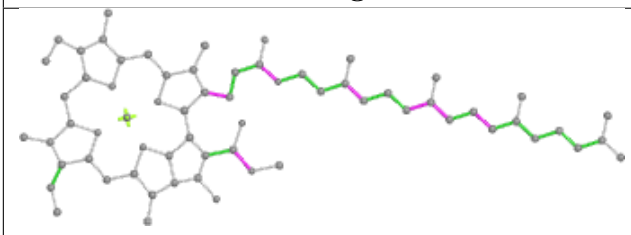
Ligand CLA 5 313



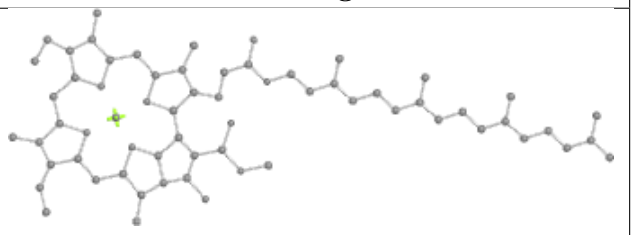
Bond lengths



Bond angles

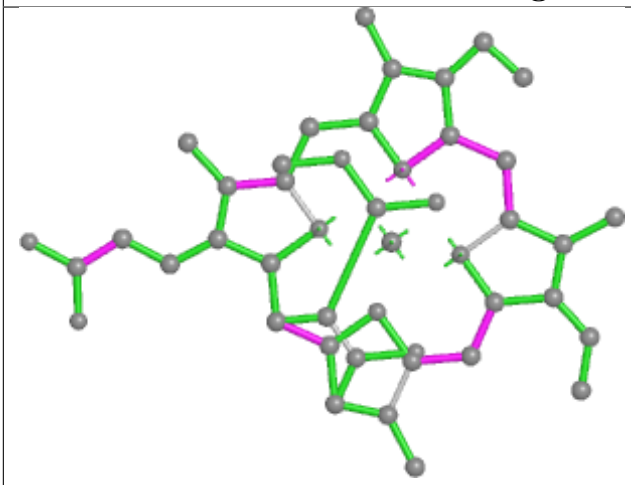


Torsions

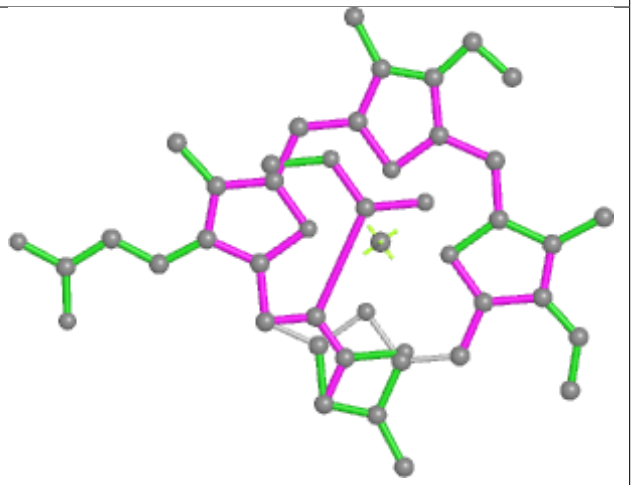


Rings

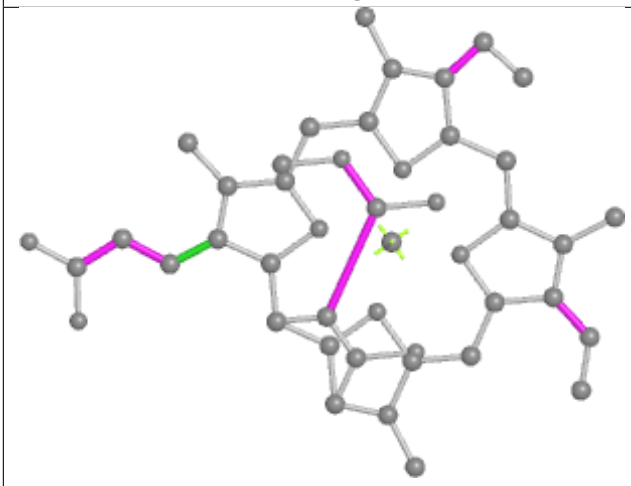
Ligand KC2 6 308



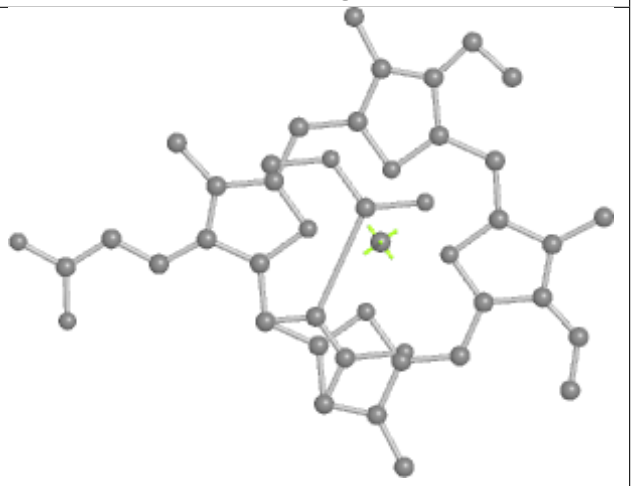
Bond lengths



Bond angles

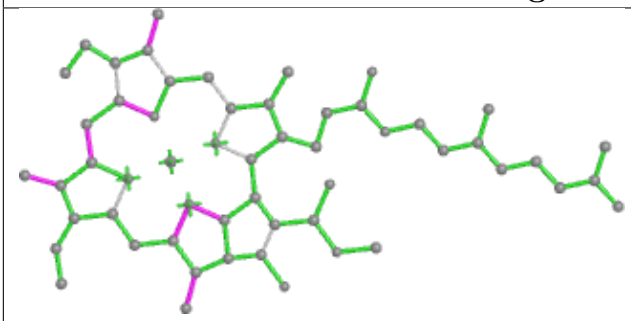


Torsions

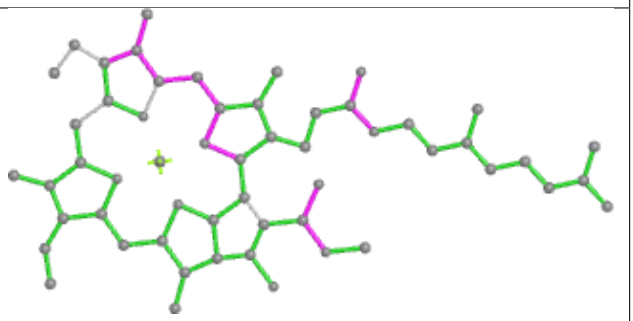


Rings

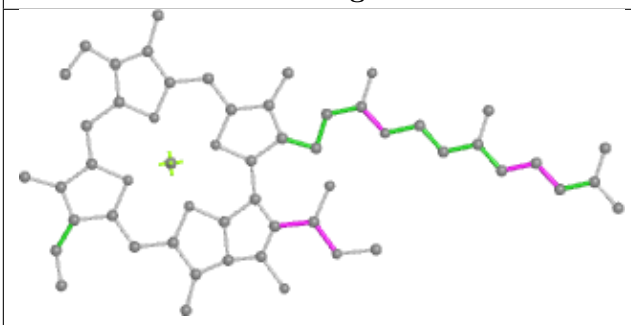
Ligand CLA 3 619



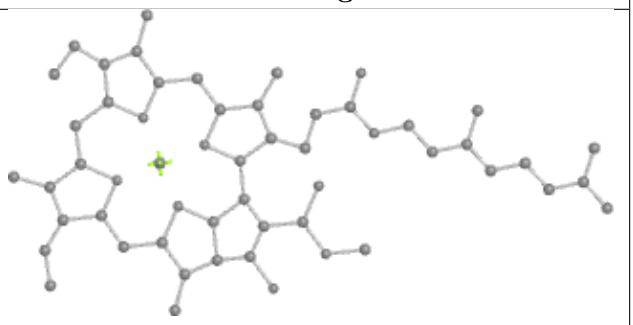
Bond lengths



Bond angles

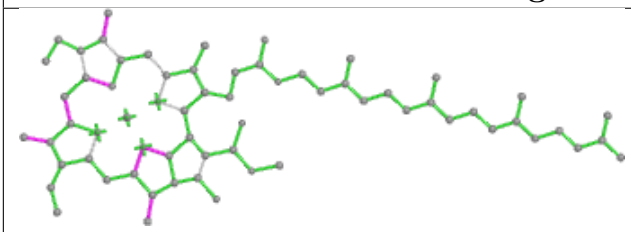


Torsions

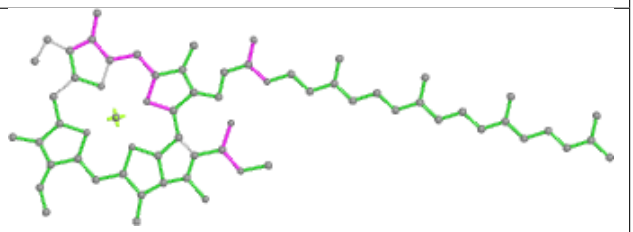


Rings

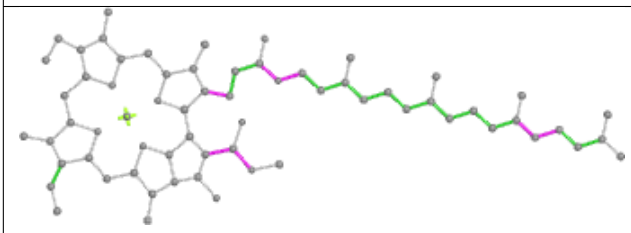
Ligand CLA 3 603



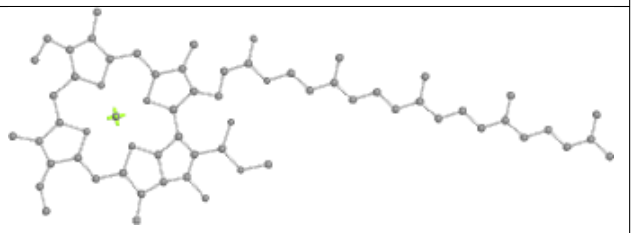
Bond lengths



Bond angles

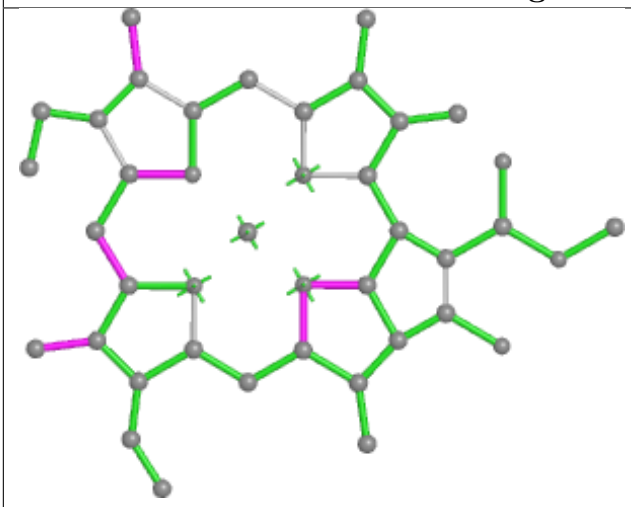


Torsions



Rings

Ligand CLA 4 313



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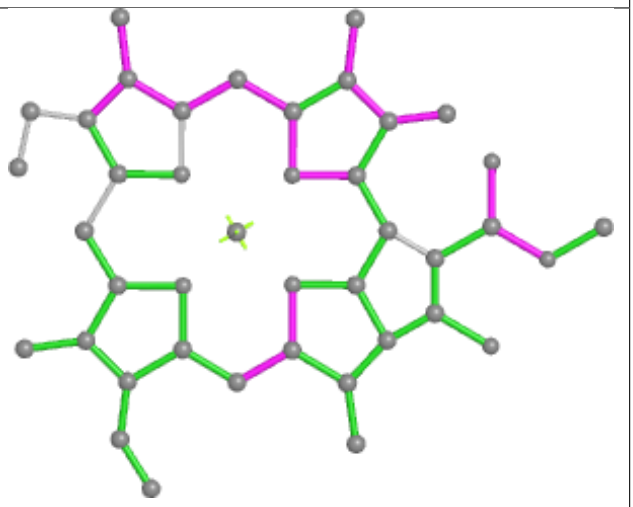
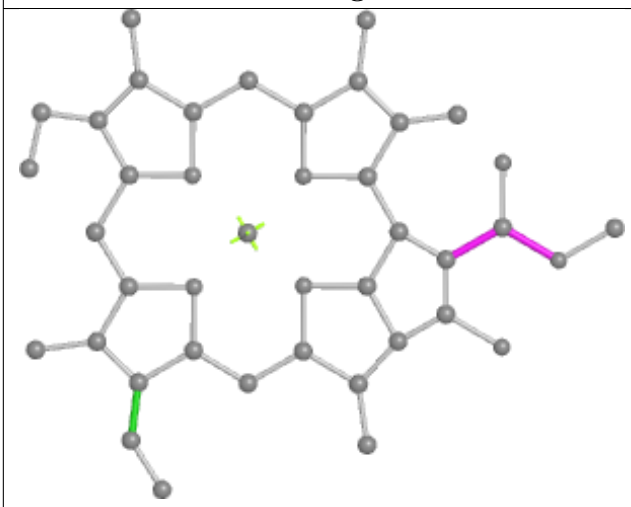
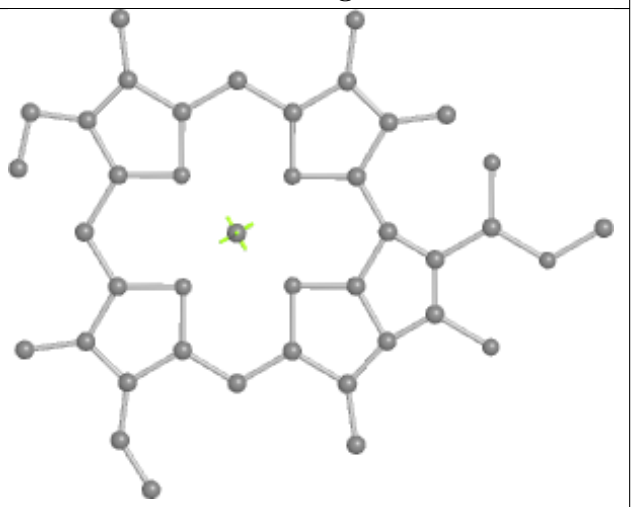


Bond angles

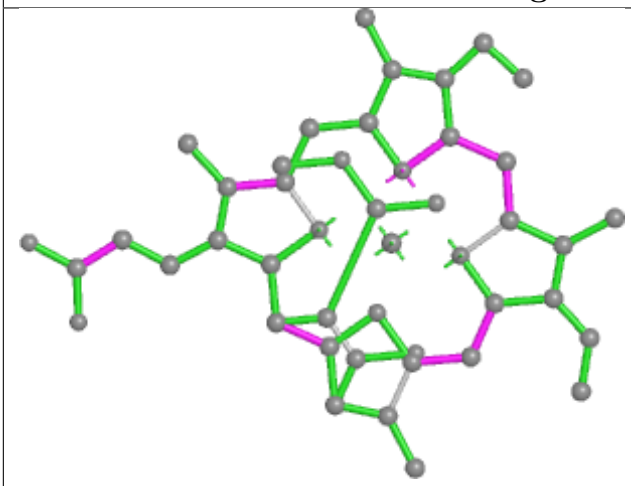


Torsions



Rings

Ligand KC2 4 307



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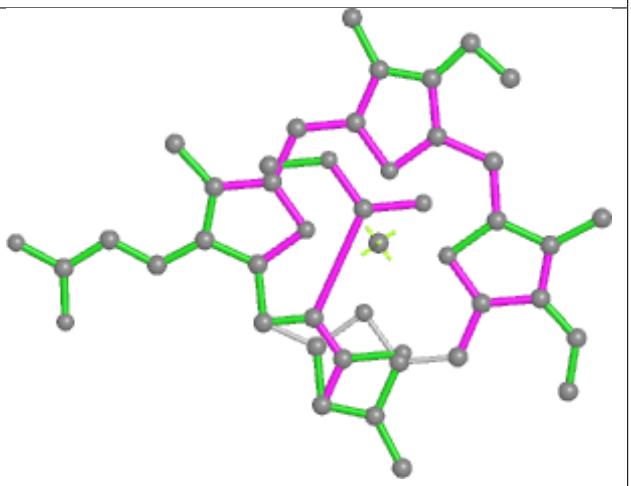
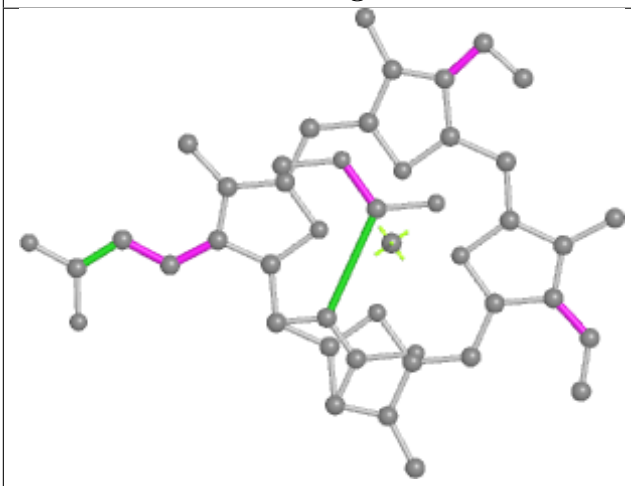
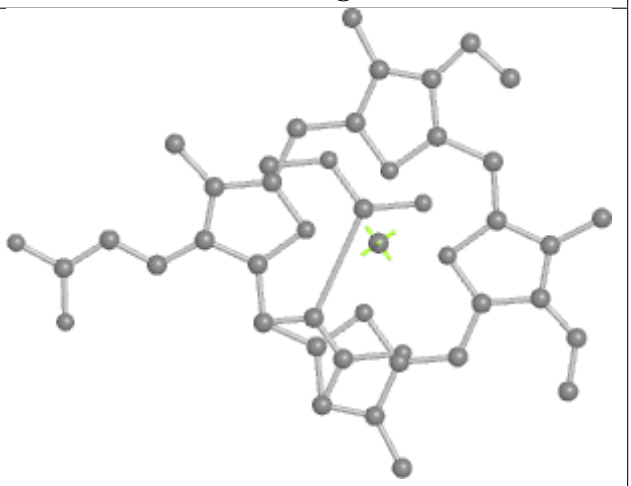


Bond angles

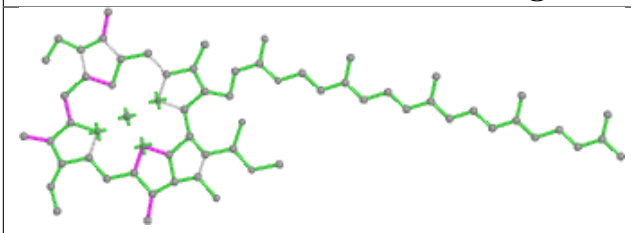


Torsions



Rings

Ligand CLA 3 607



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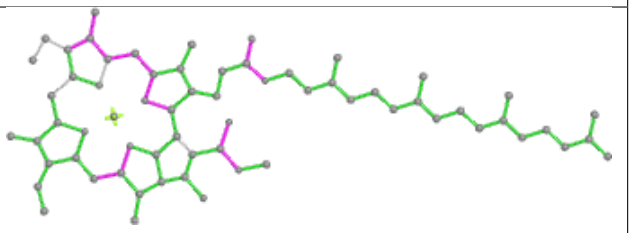
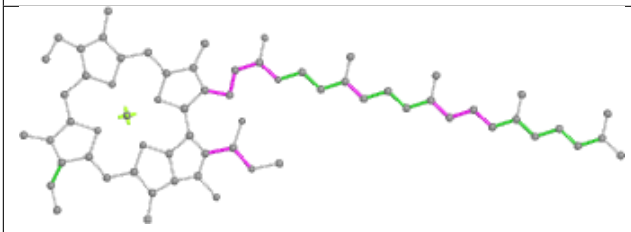
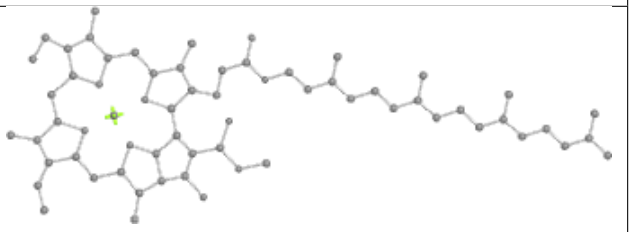


Bond angles

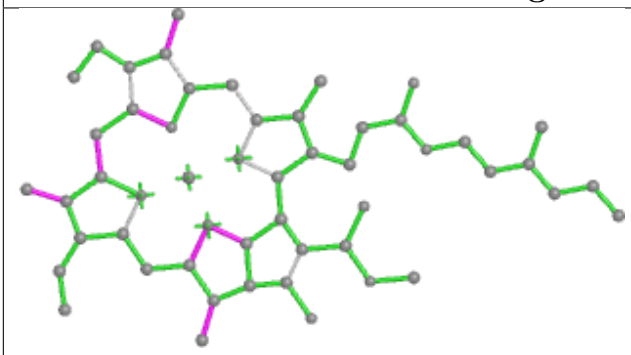


Torsions



Rings

Ligand CLA 4 316



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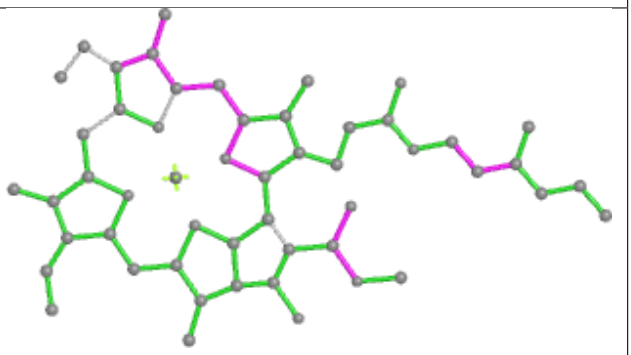
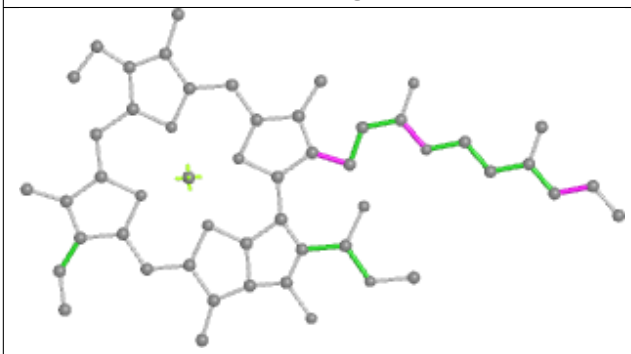


Bond angles



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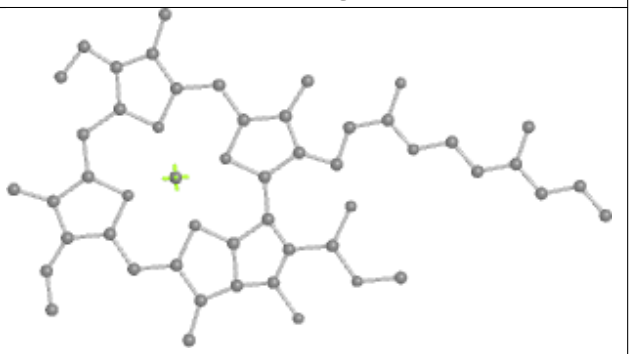
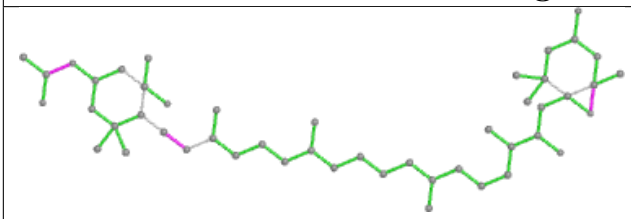


Rings

Ligand A86 5 303



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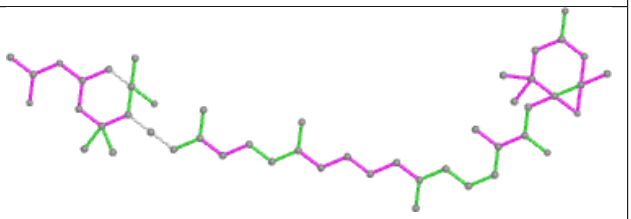

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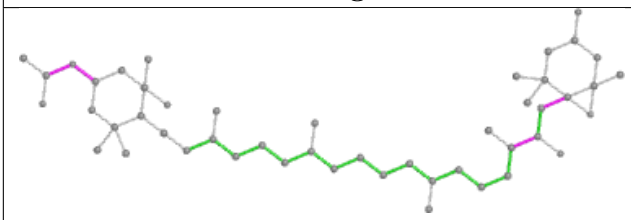
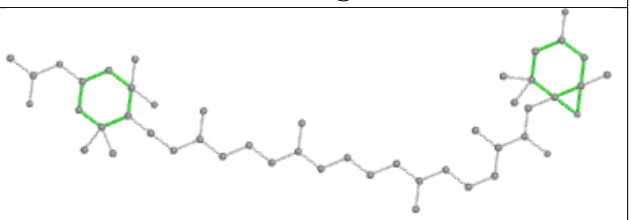
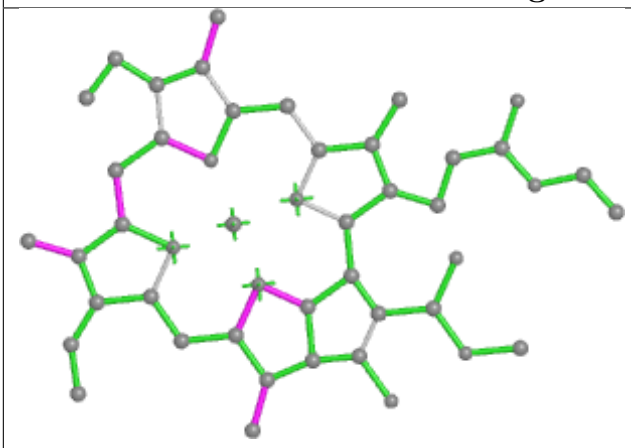


Torsions



Rings

Ligand CLA 4 315



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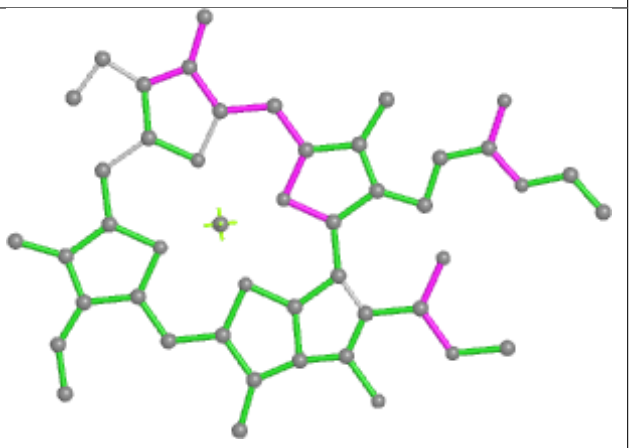
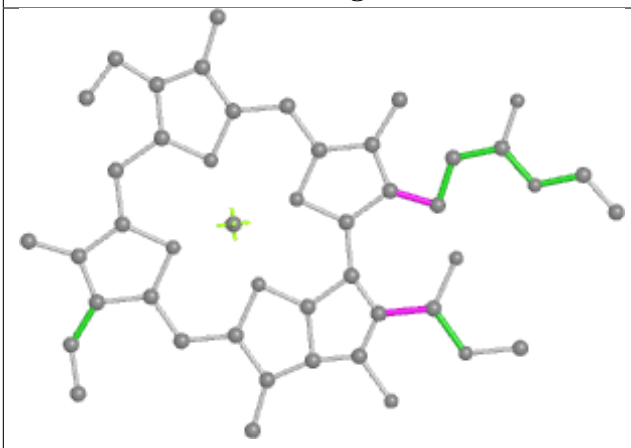
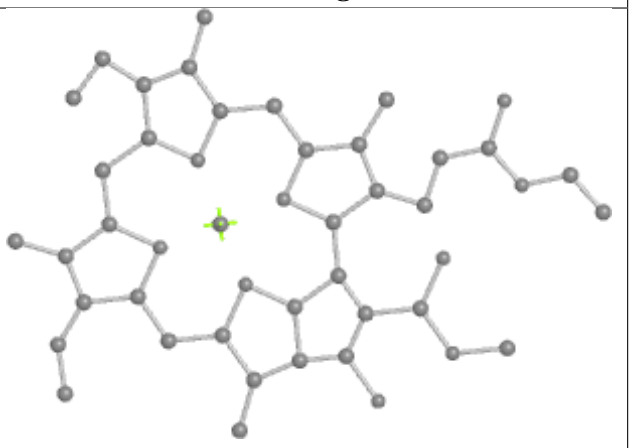


Bond angles

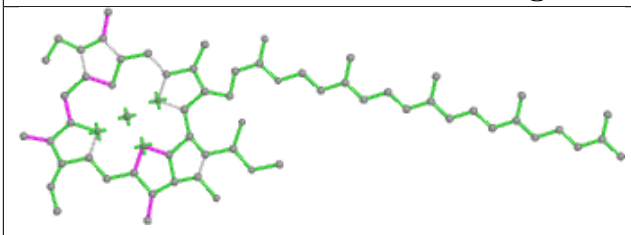


Torsions



Rings

Ligand CLA 4 308



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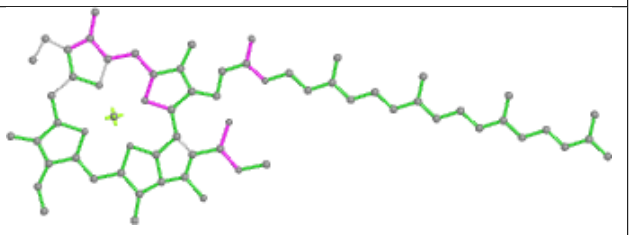
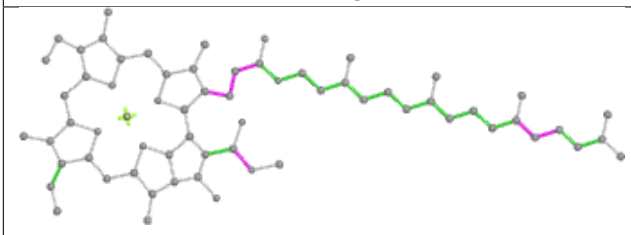
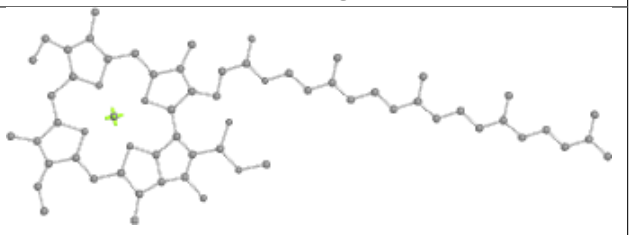


Bond angles

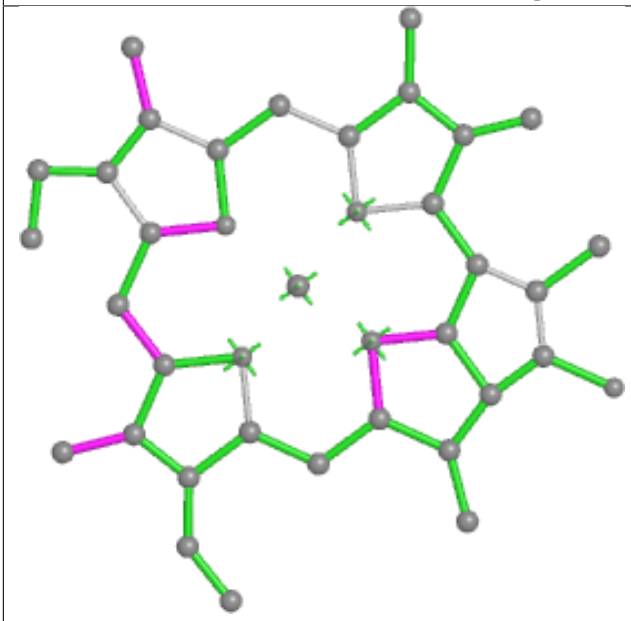


Torsions



Rings

Ligand CLA 5 317



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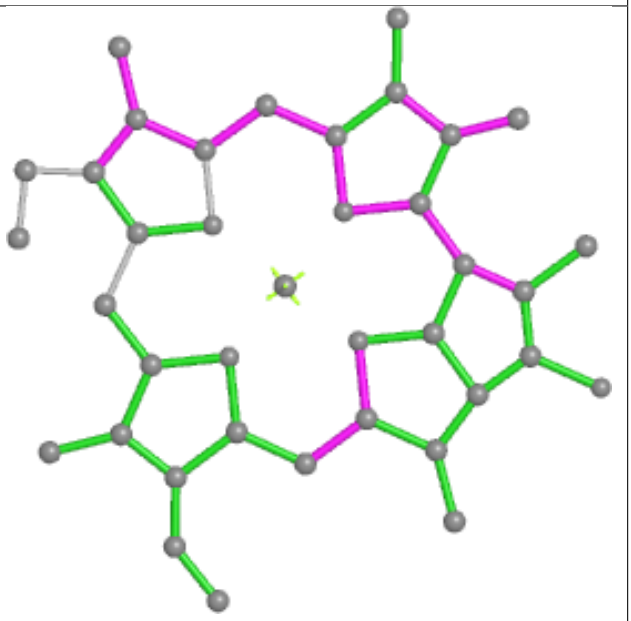
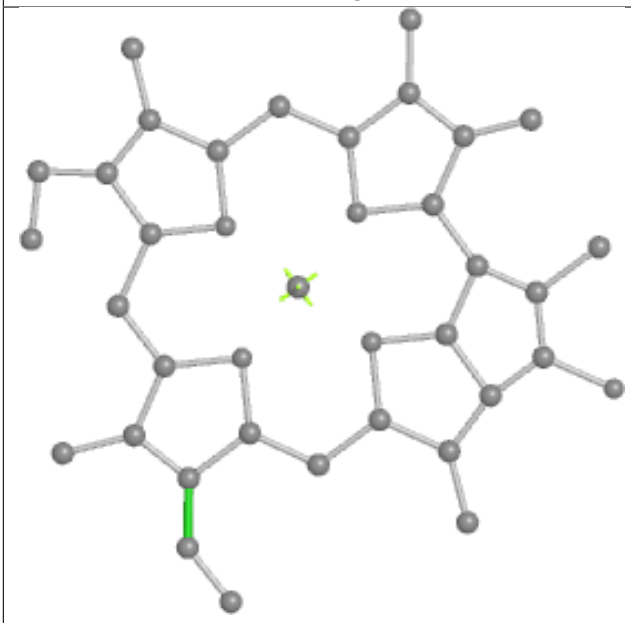
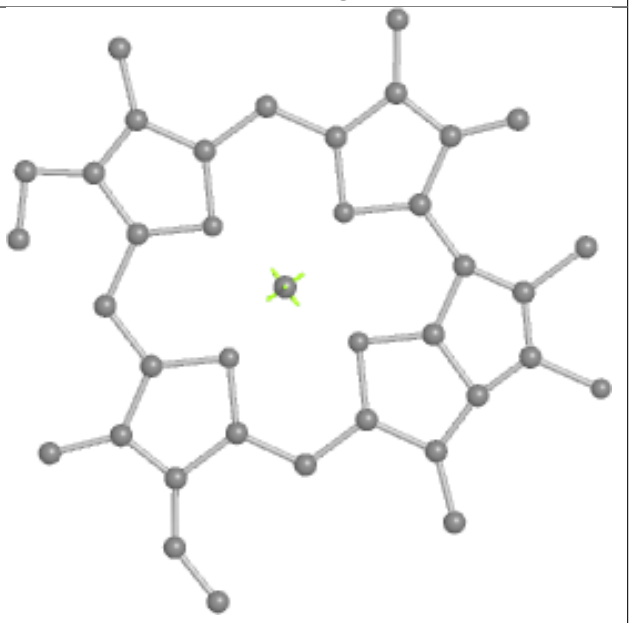


Bond angles

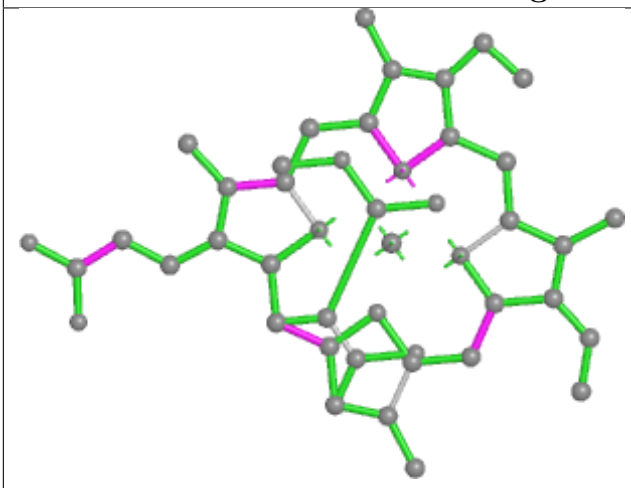


Torsions



Rings

Ligand KC1 3 609



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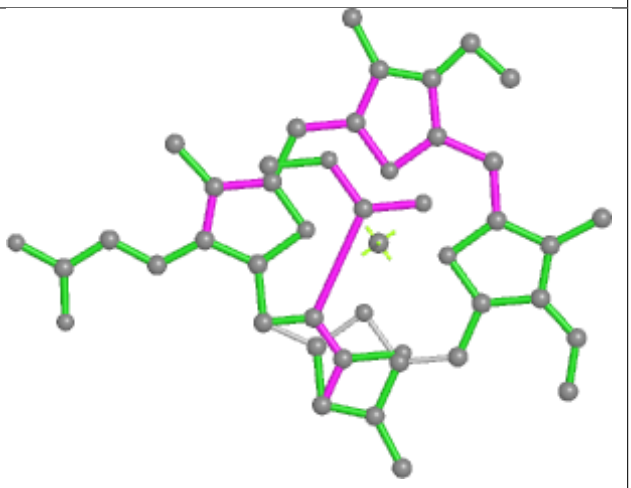
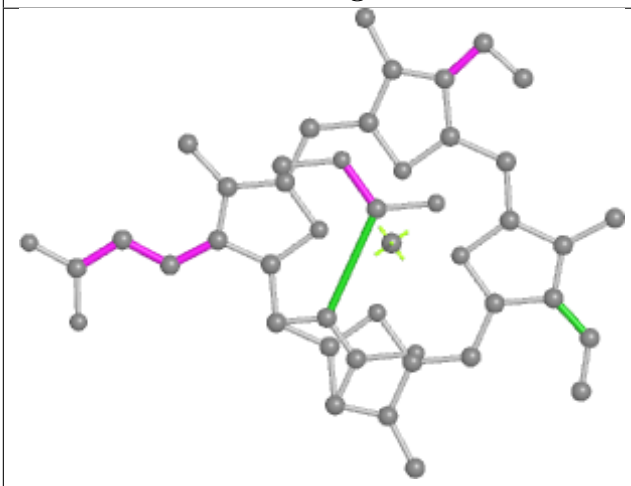
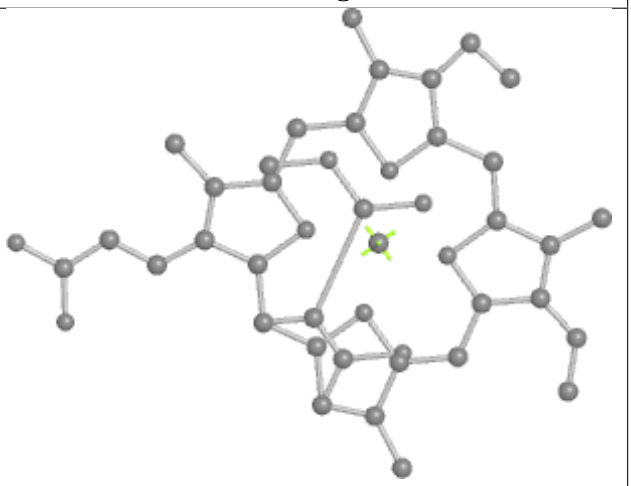


Bond angles

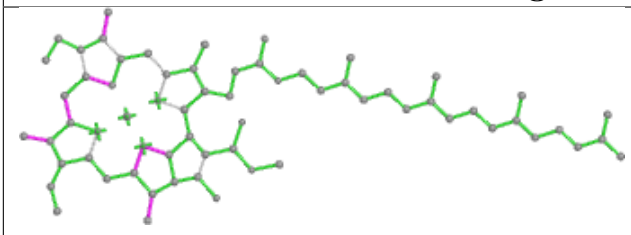


Torsions



Rings

Ligand CLA 3 606



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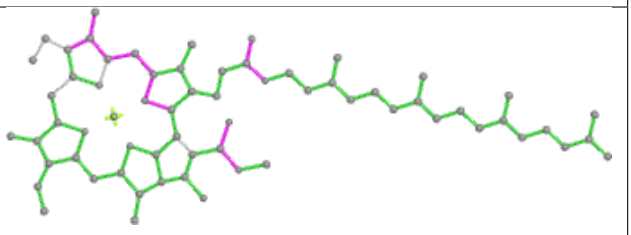
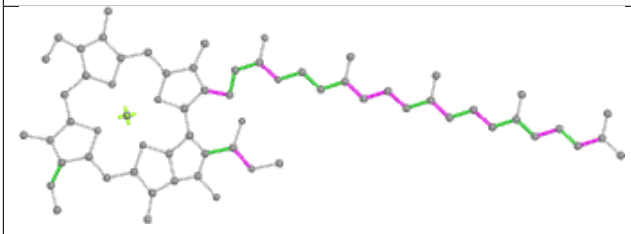
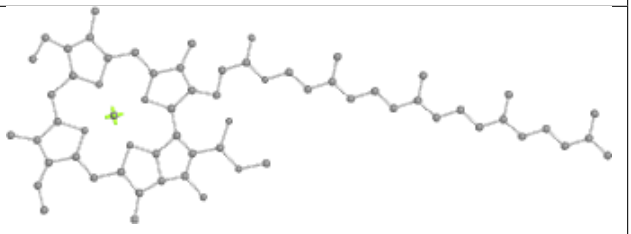


Bond angles

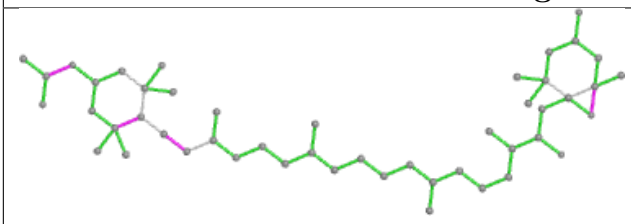


Torsions

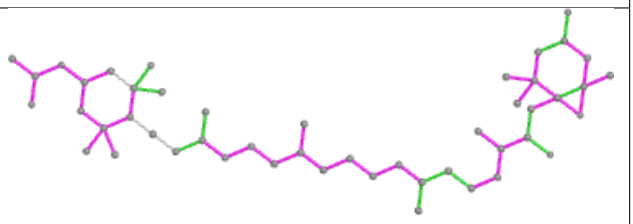


Rings

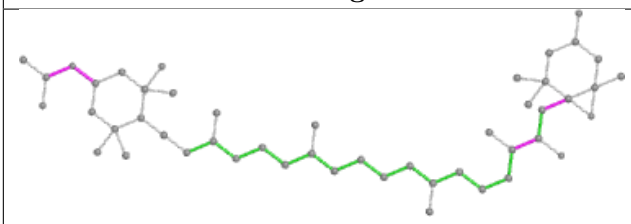
Ligand A86 4 302



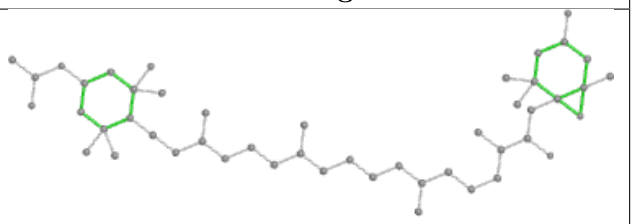
Bond lengths



Bond angles

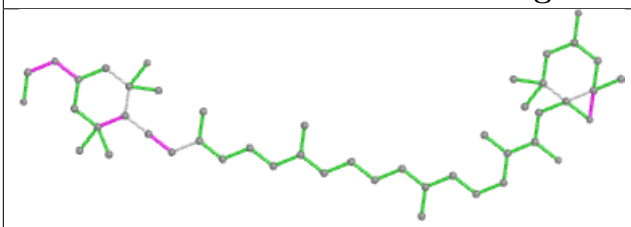


Torsions

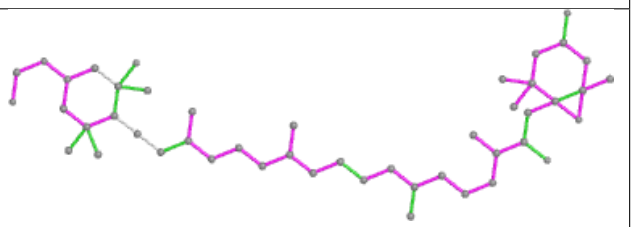


Rings

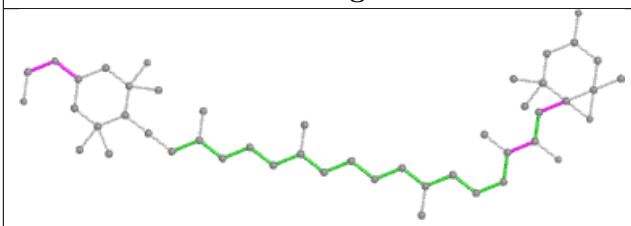
Ligand A86 5 305



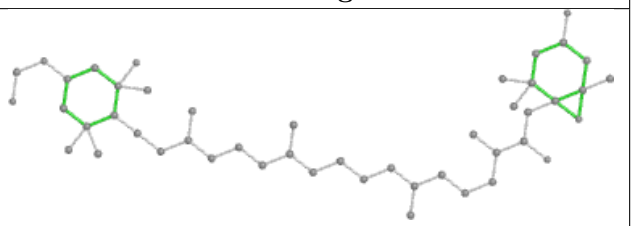
Bond lengths



Bond angles

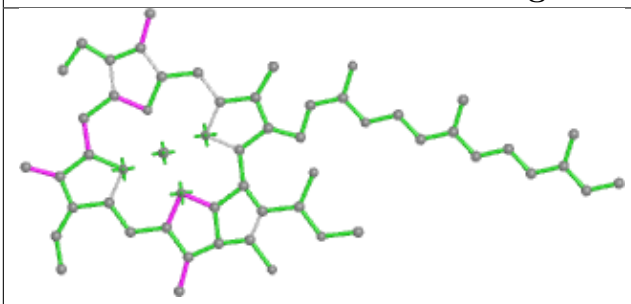


Torsions

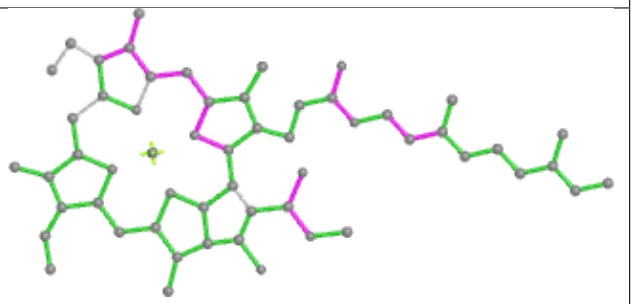


Rings

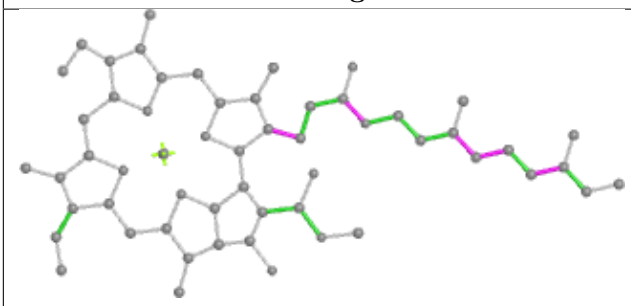
Ligand CLA 3 611



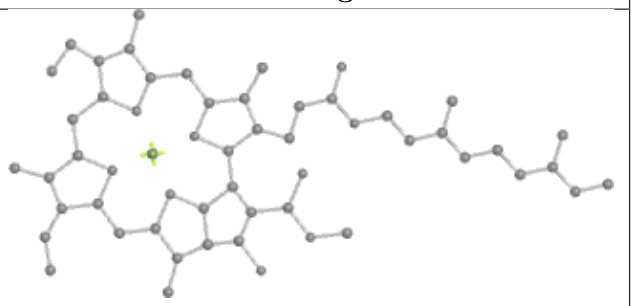
Bond lengths



Bond angles

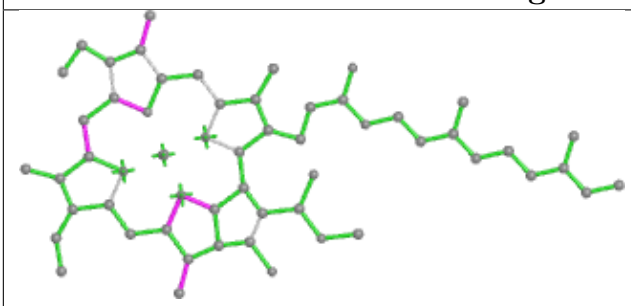


Torsions

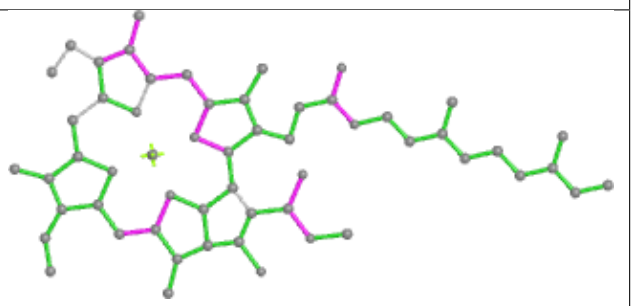


Rings

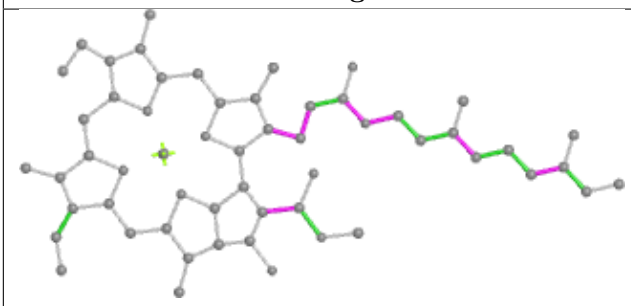
Ligand CLA 4 314



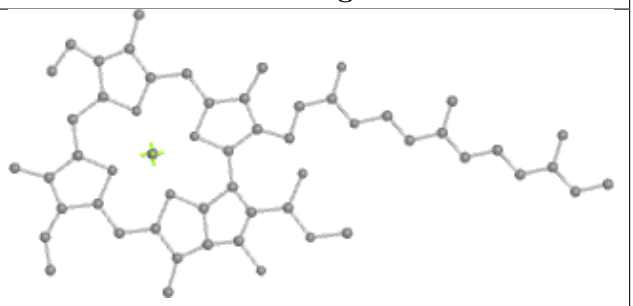
Bond lengths



Bond angles

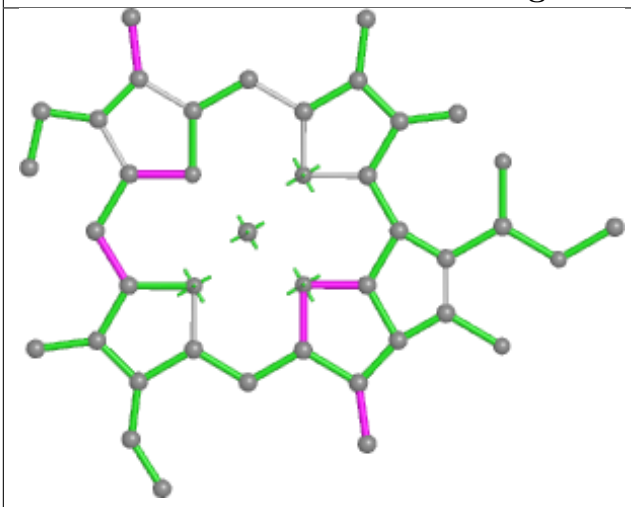


Torsions

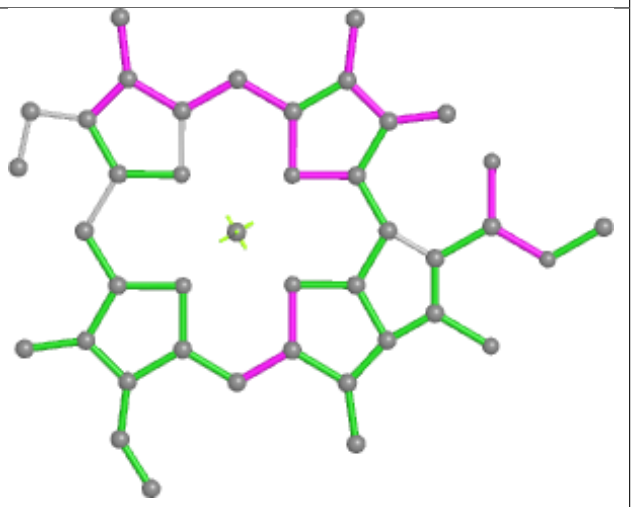


Rings

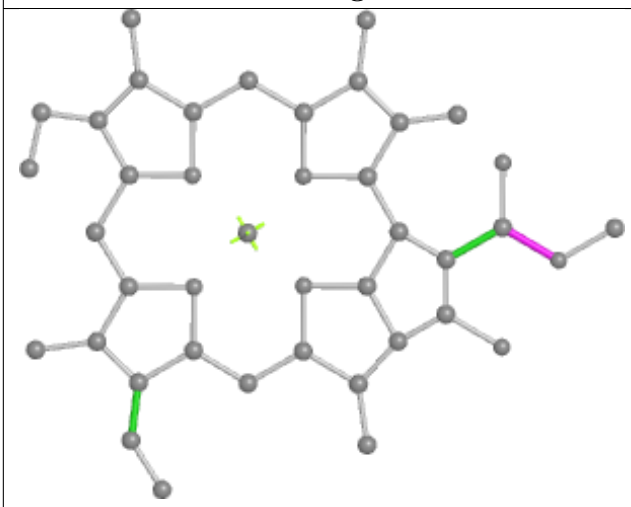
Ligand CLA 5 316



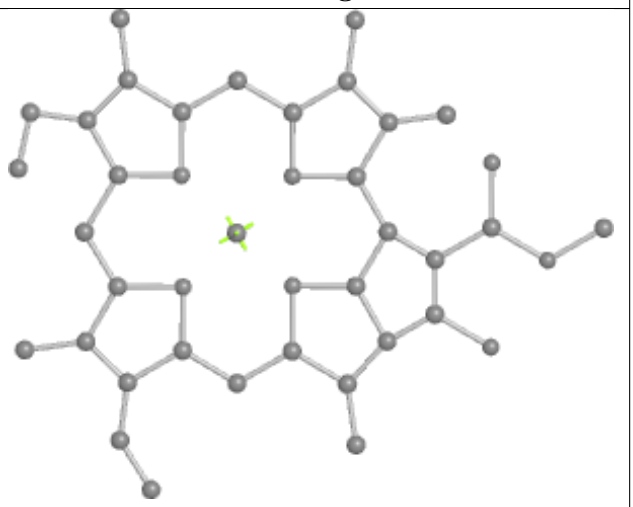
Bond lengths



Bond angles

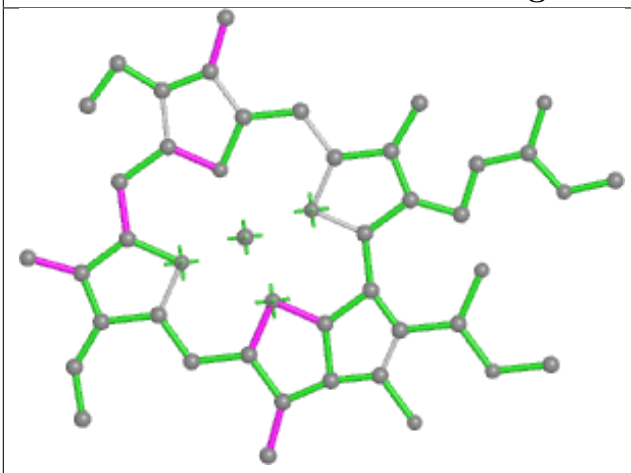


Torsions

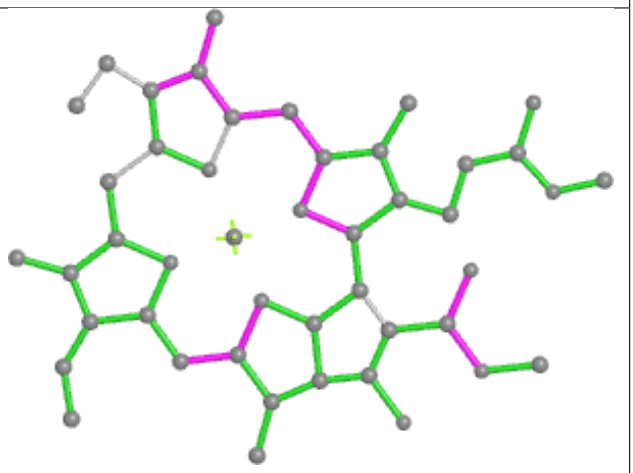


Rings

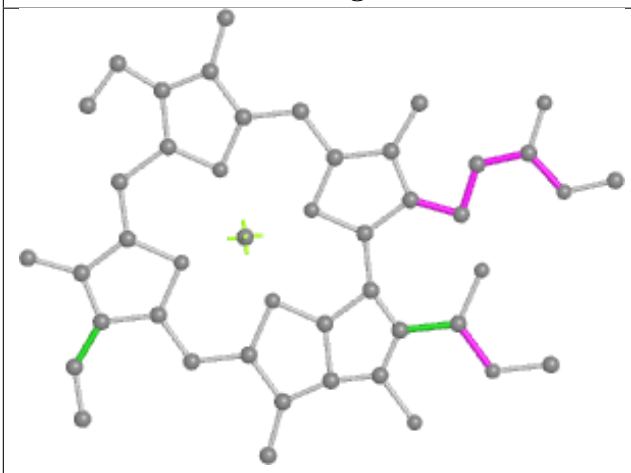
Ligand CLA 5 312



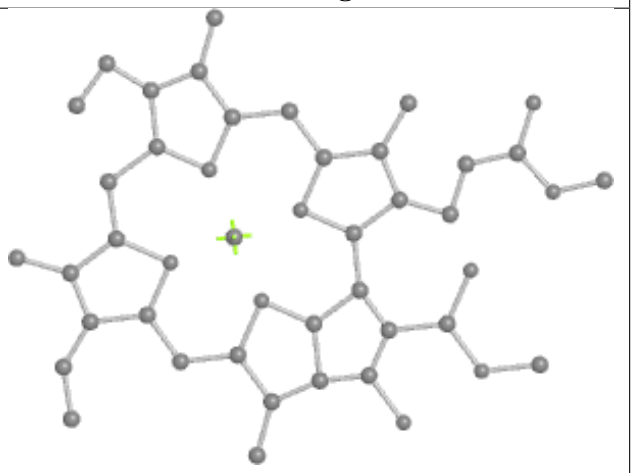
Bond lengths



Bond angles

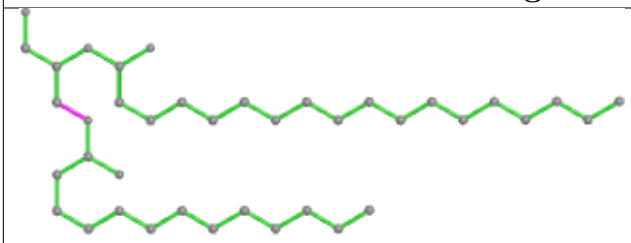


Torsions

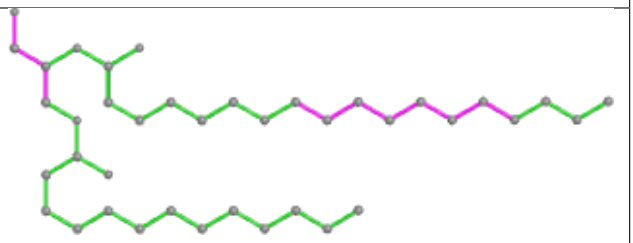


Rings

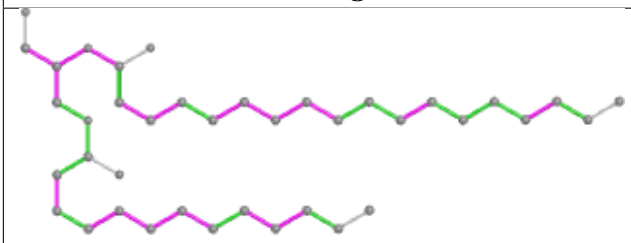
Ligand DGD 3 620



Bond lengths



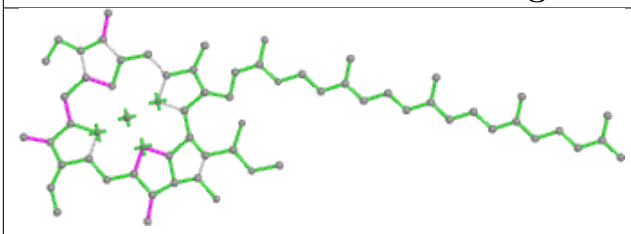
Bond angles



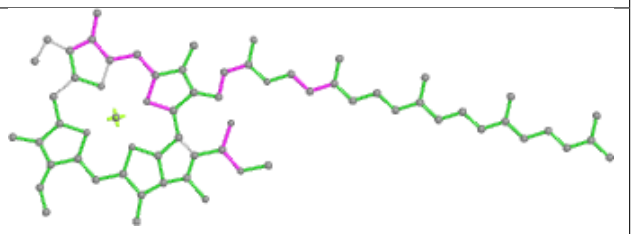
Torsions

Rings

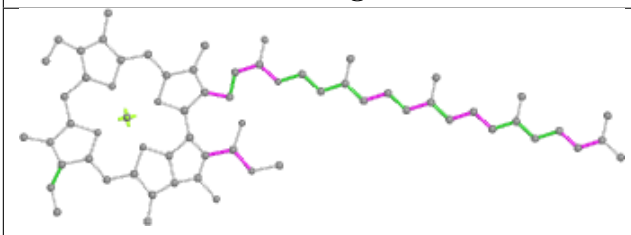
Ligand CLA 3 601



Bond lengths



Bond angles



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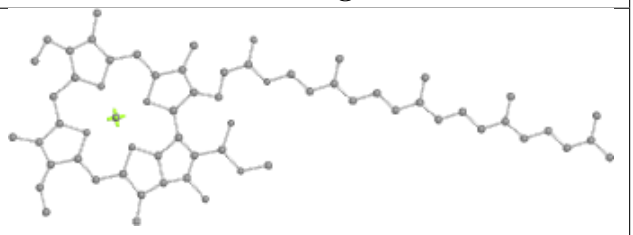
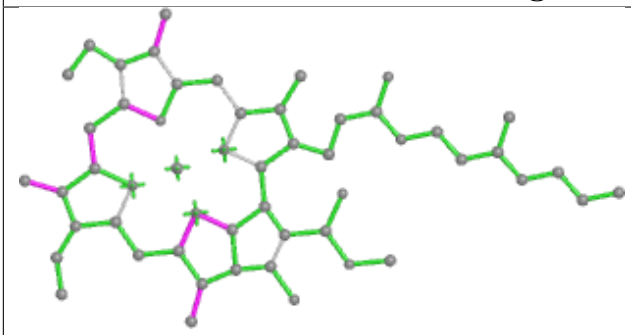
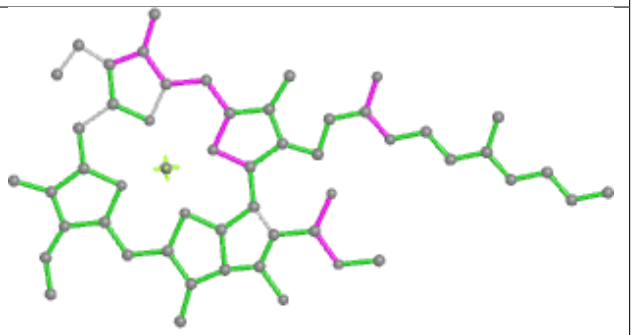


Rings

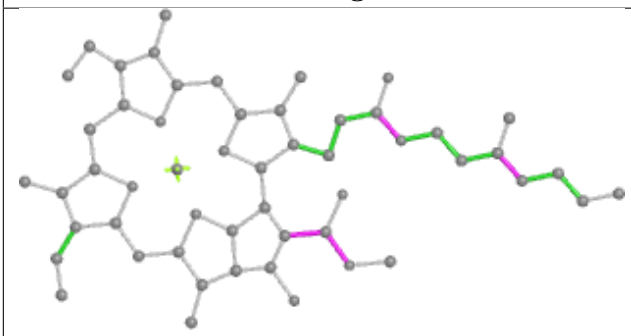
Ligand CLA 6 306



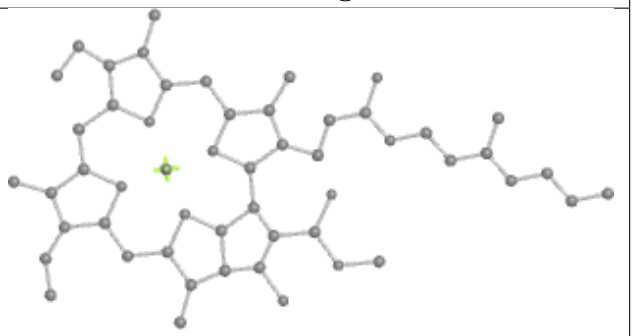
Bond lengths



Bond angles

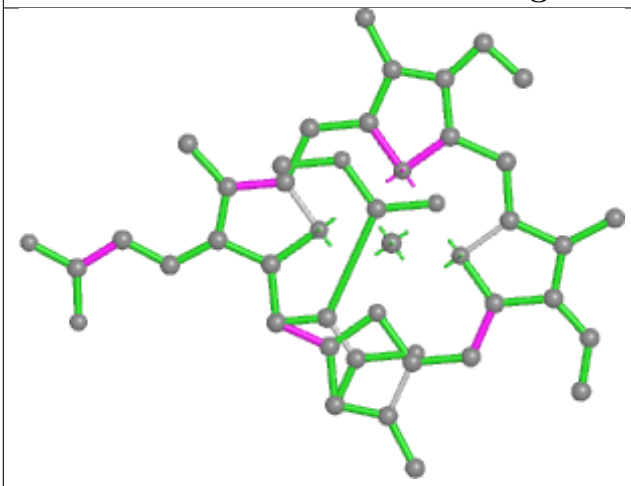


Torsions

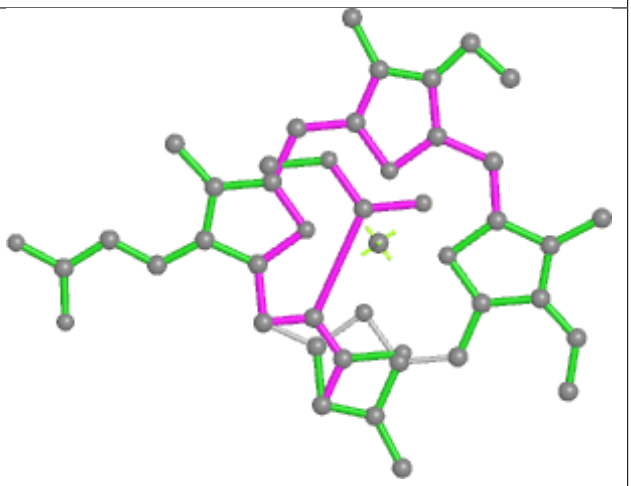


Rings

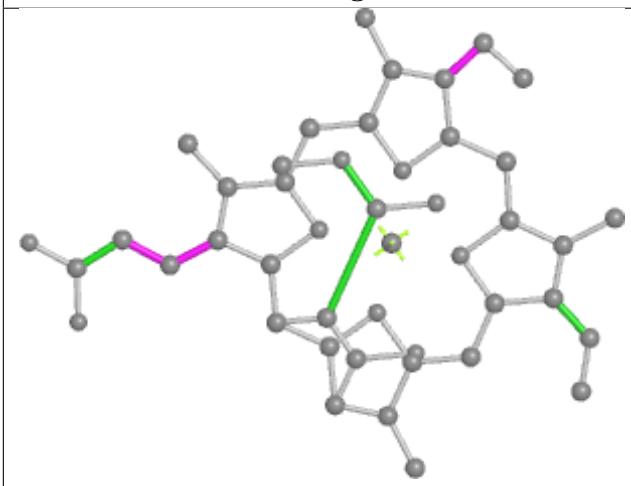
Ligand KC1 6 313



Bond lengths



Bond angles



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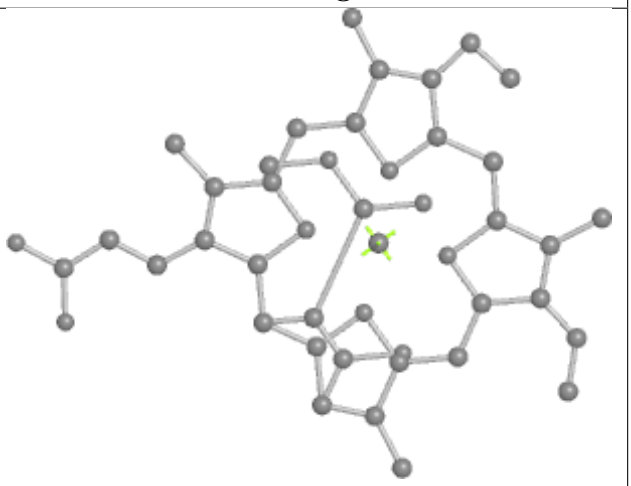
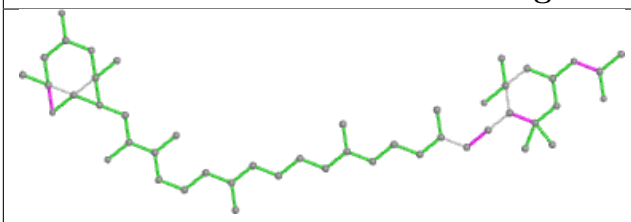
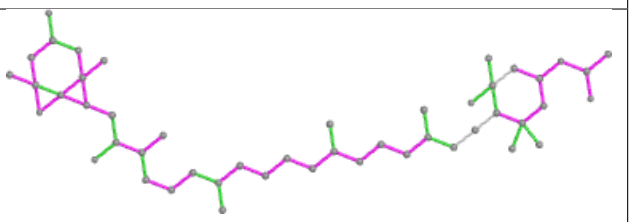


Rings

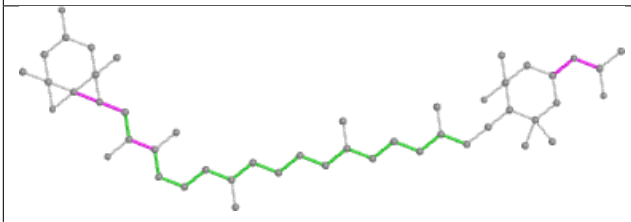
Ligand A86 6 303



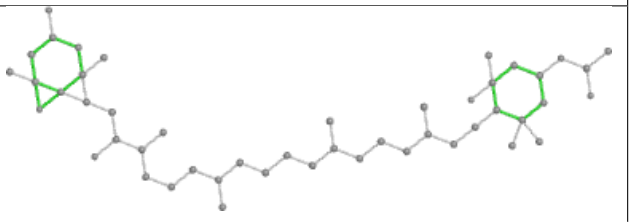
Bond lengths



Bond angles

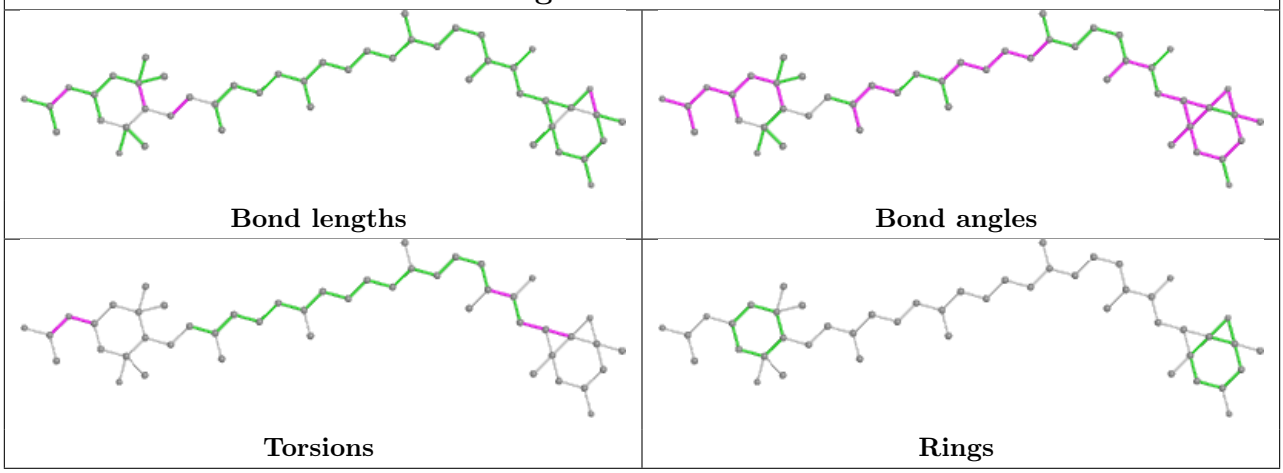


Torsions

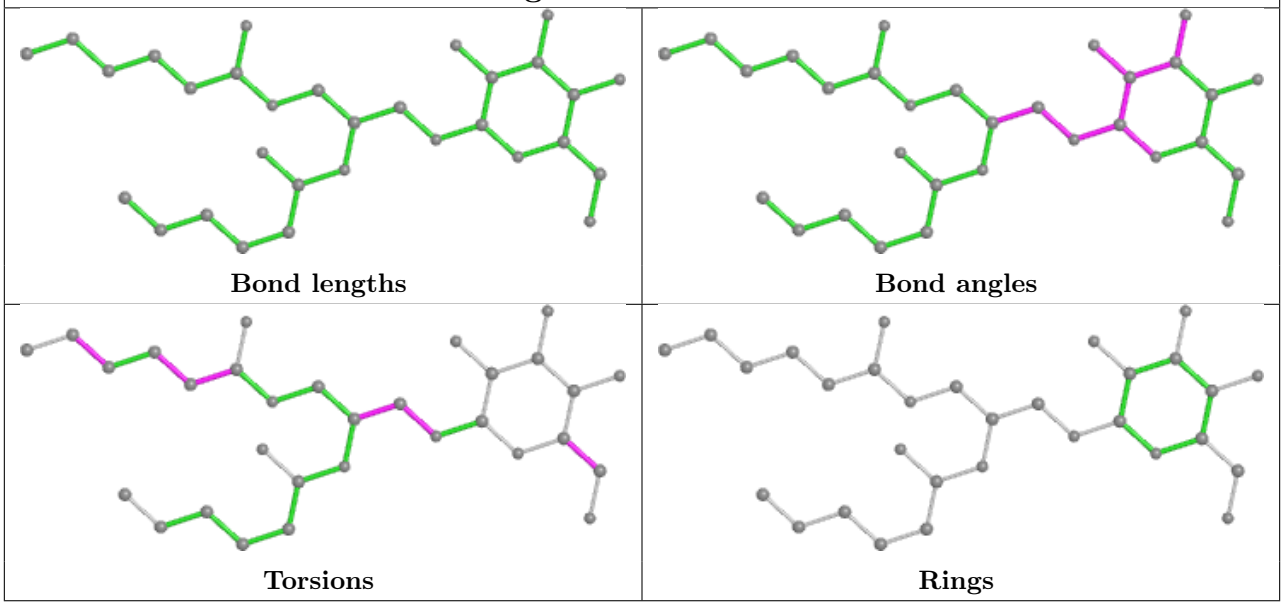


Rings

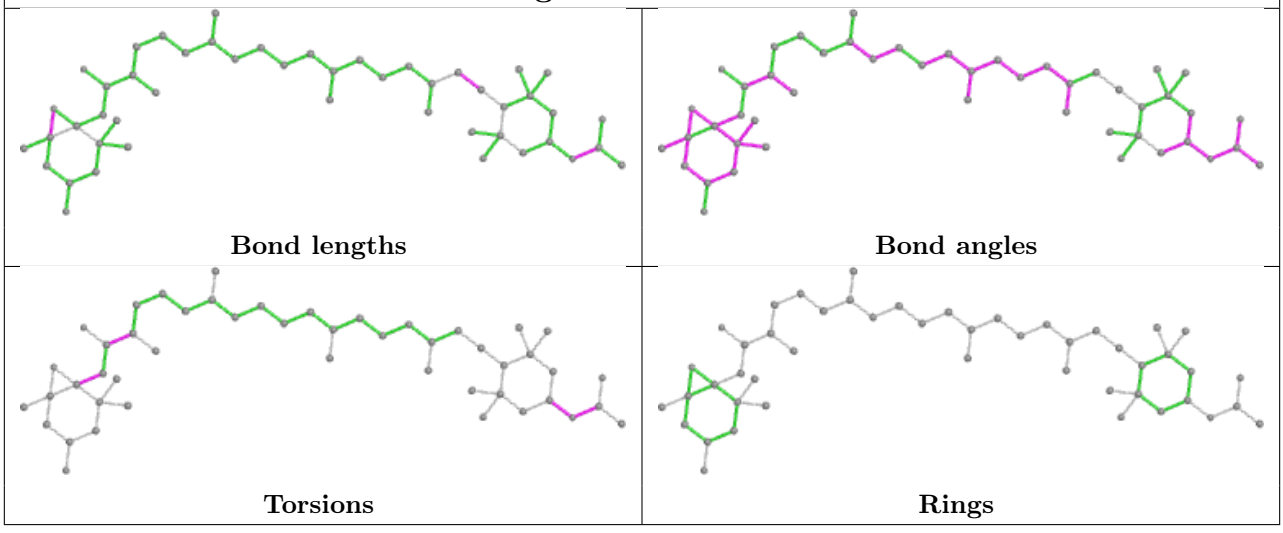
Ligand A86 5 306



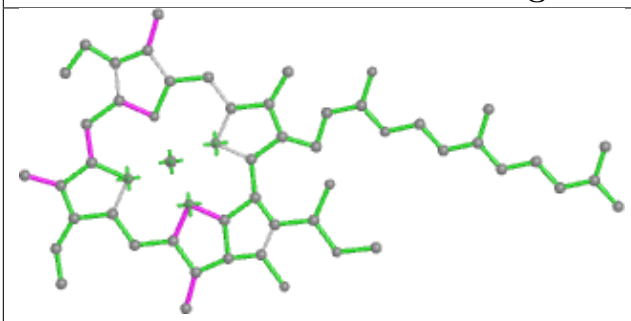
Ligand LMG 3 615



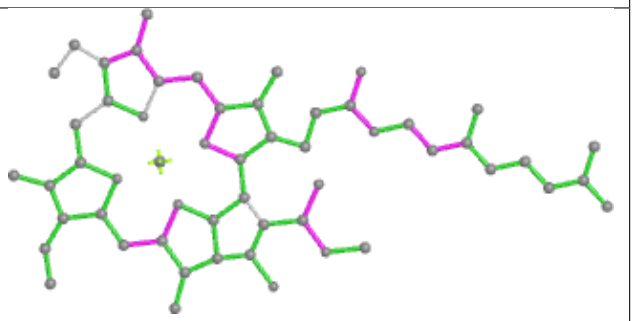
Ligand A86 6 305



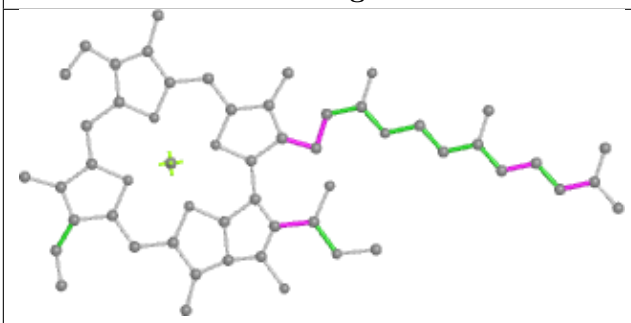
Ligand CLA 5 309



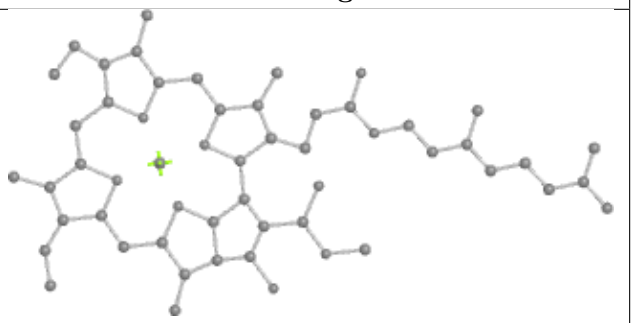
Bond lengths



Bond angles

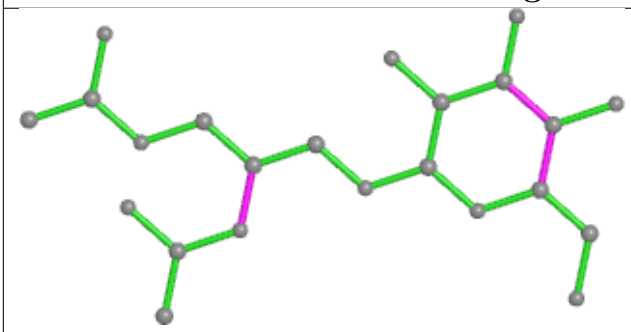


Torsions



Rings

Ligand LMG 3 616



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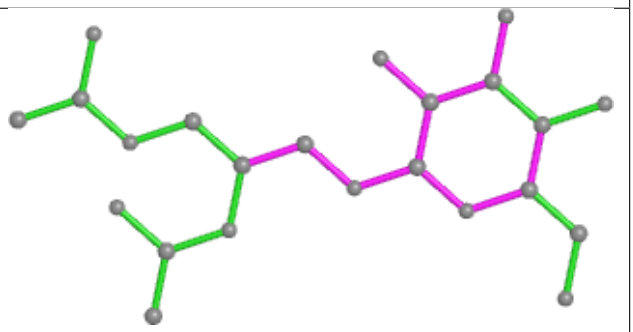
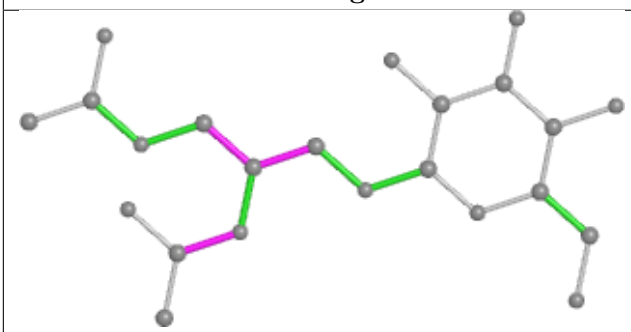


Bond angles



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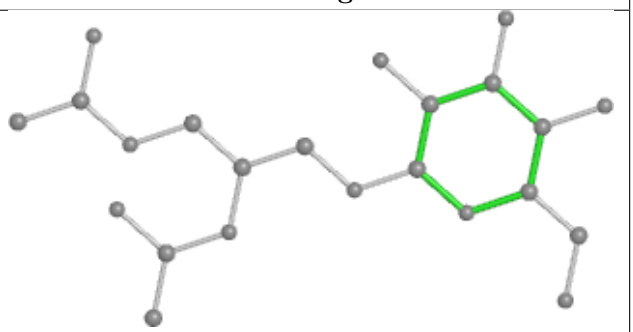
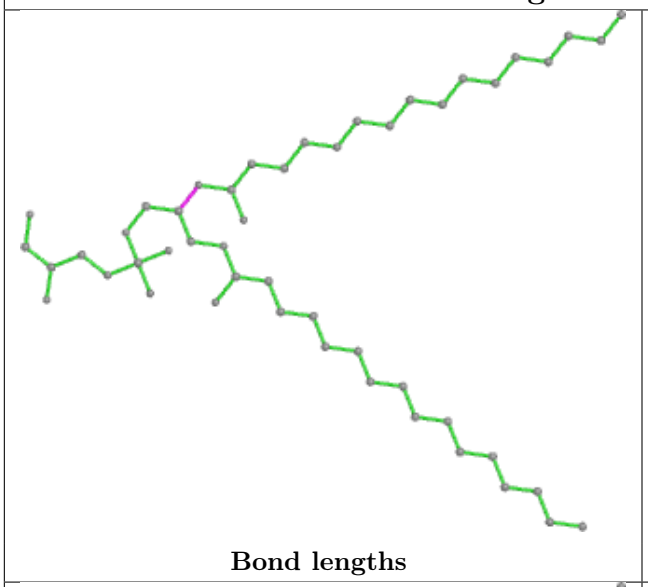
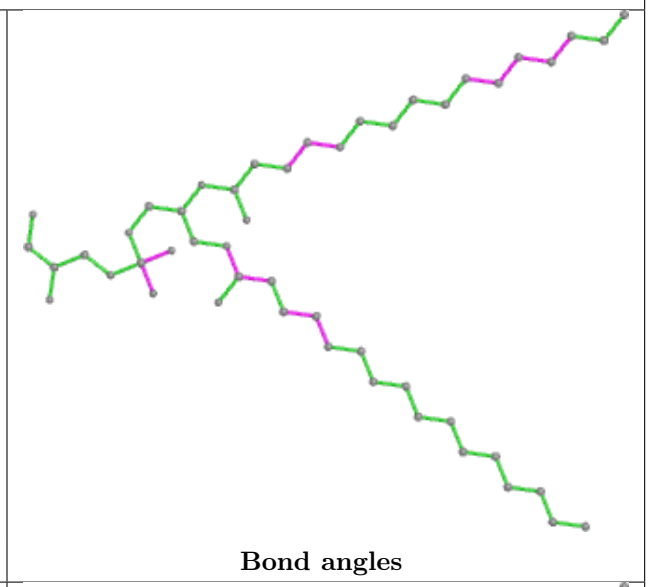


Rings

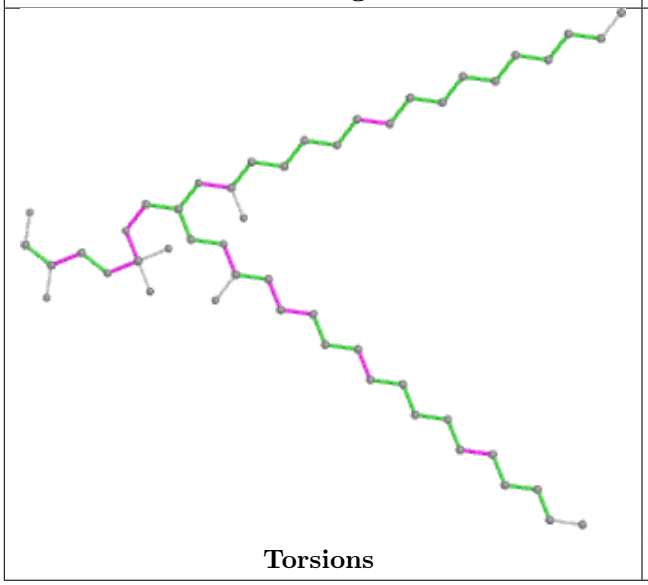
Ligand LHG 3 618



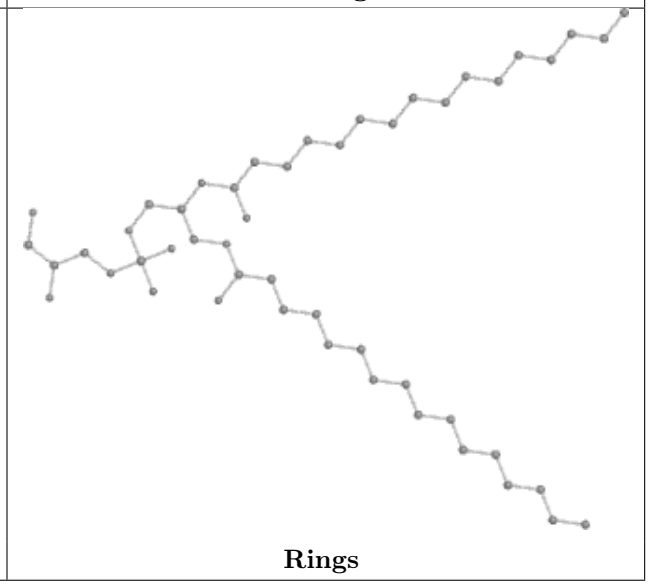
Bond lengths



Bond angles

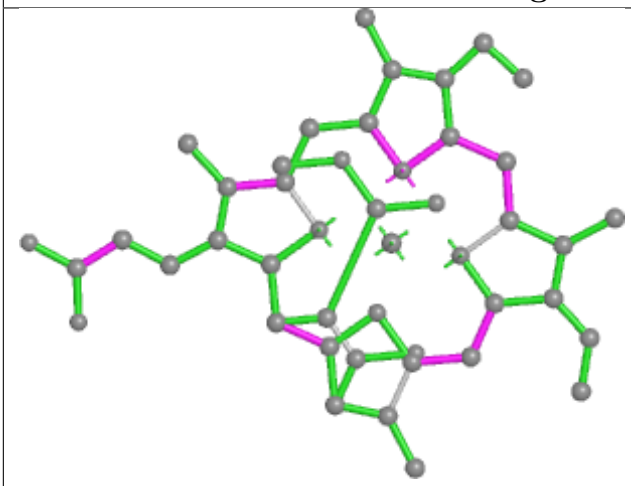


Torsions

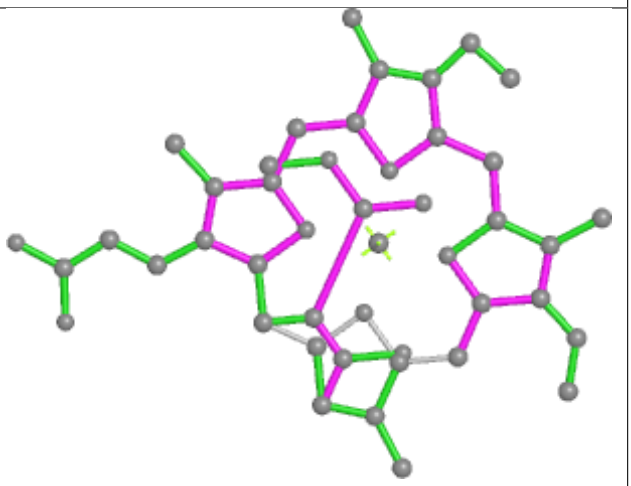


Rings

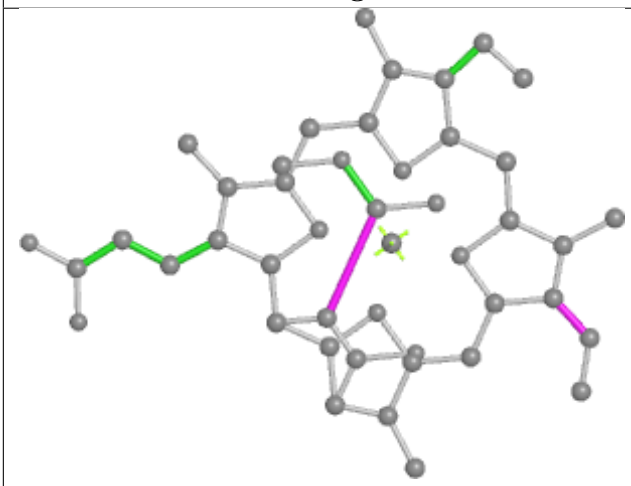
Ligand KC2 5 310



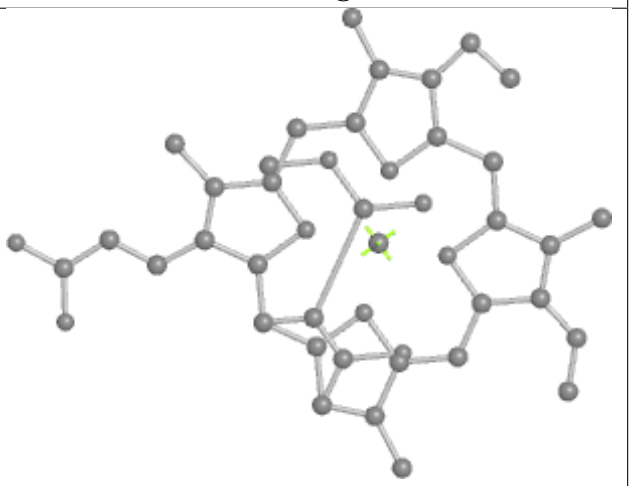
Bond lengths



Bond angles

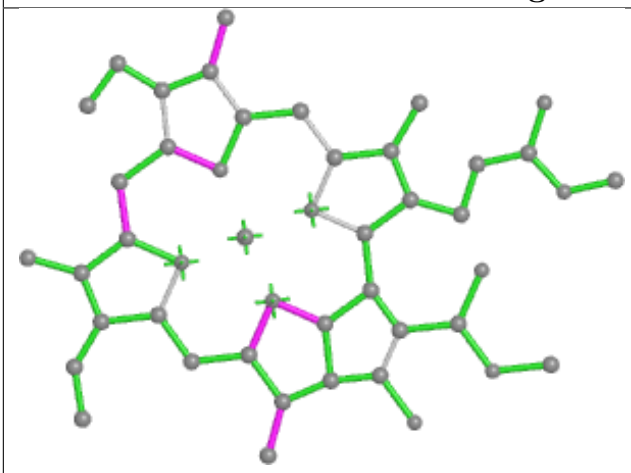


Torsions

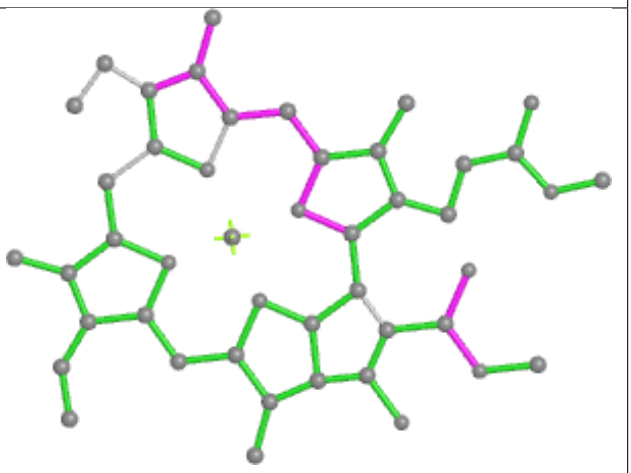


Rings

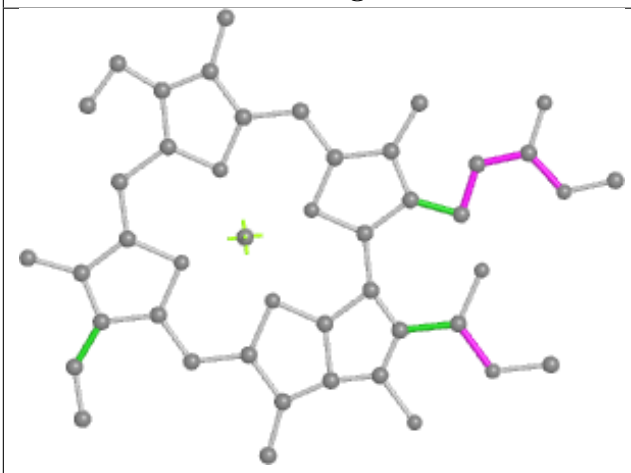
Ligand CLA 5 308



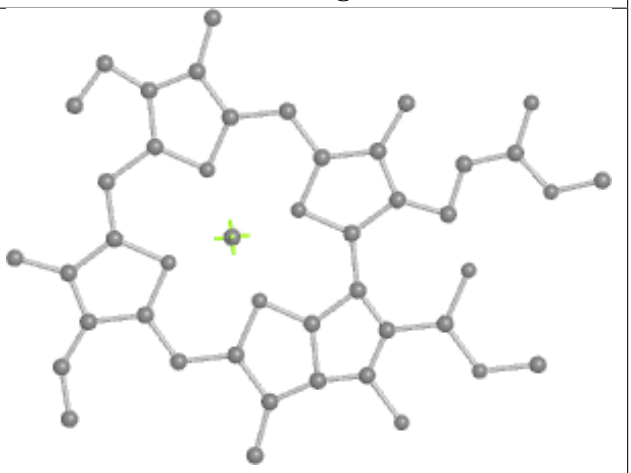
Bond lengths



Bond angles

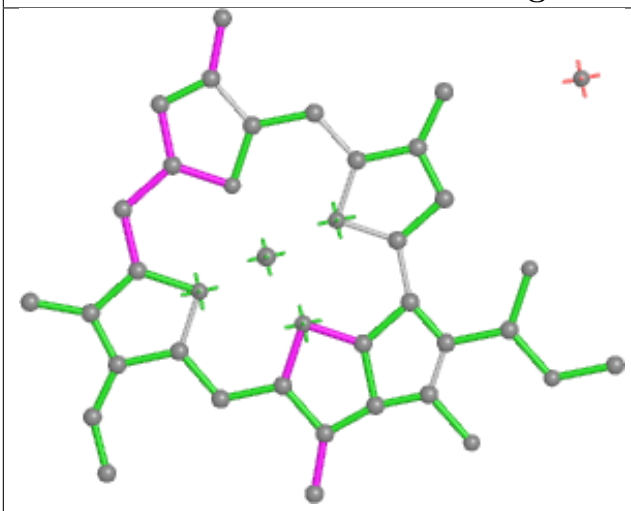


Torsions

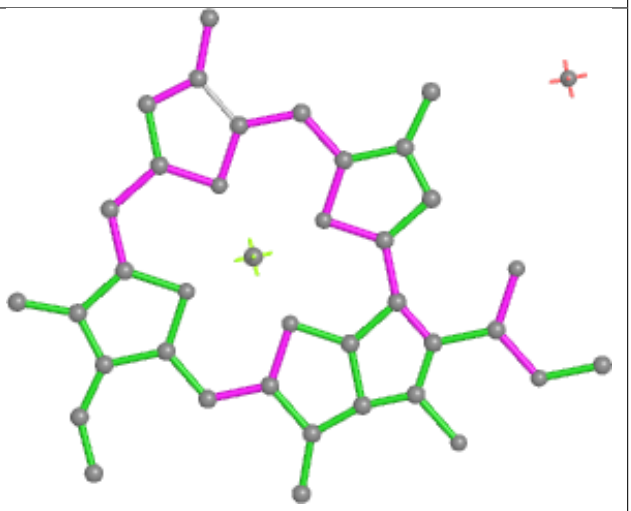


Rings

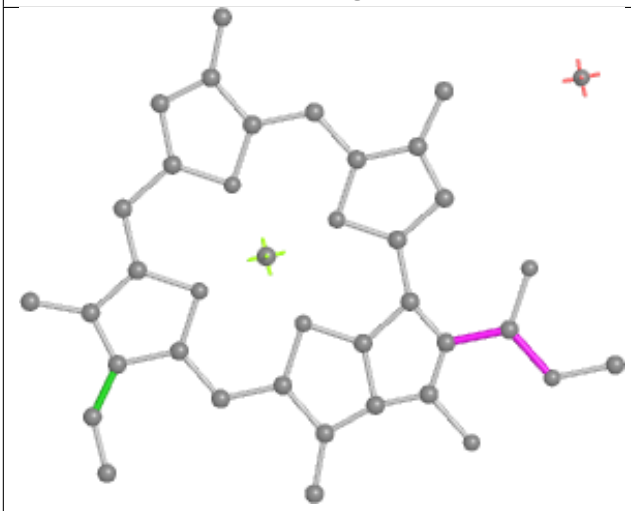
Ligand CLA 6 315



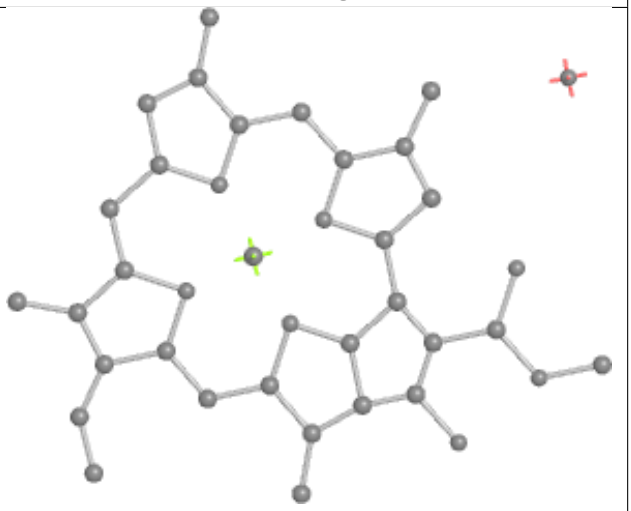
Bond lengths



Bond angles

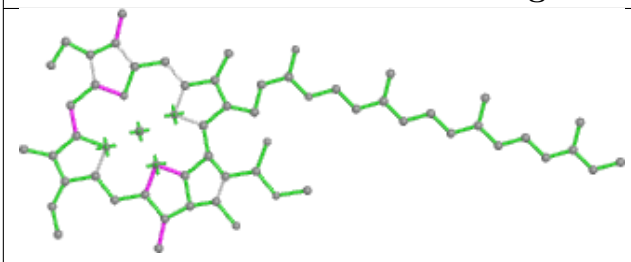


Torsions

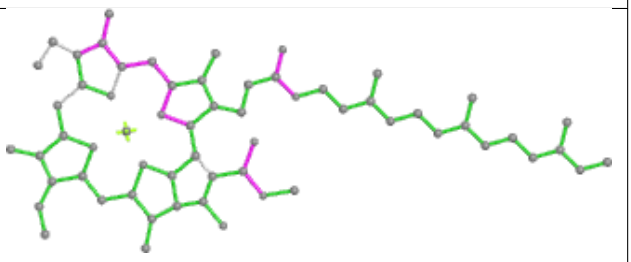


Rings

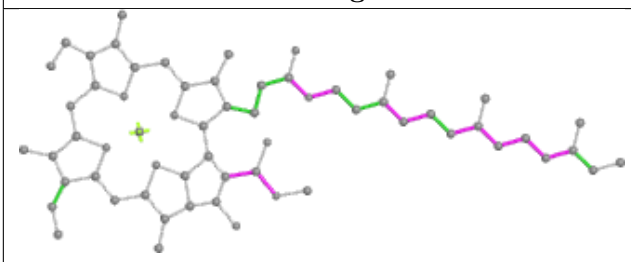
Ligand CLA 3 612



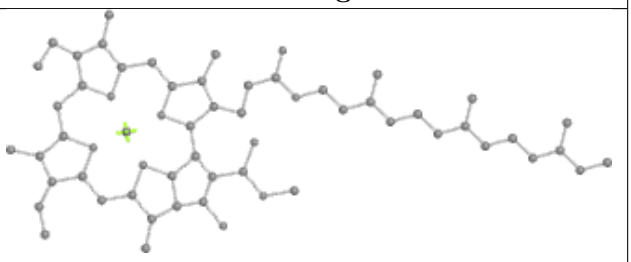
Bond lengths



Bond angles

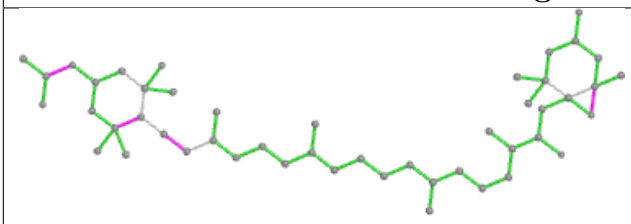


Torsions

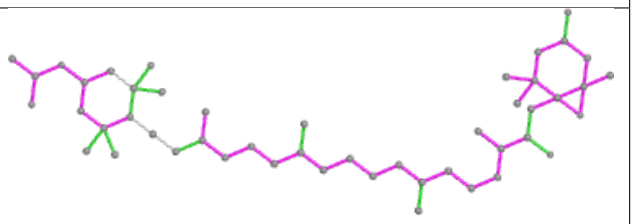


Rings

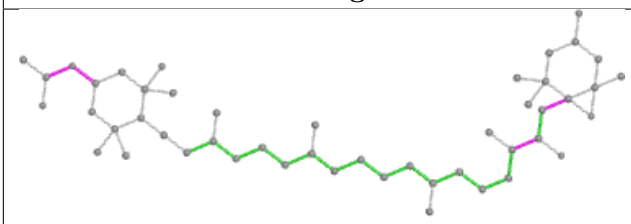
Ligand A86 4 301



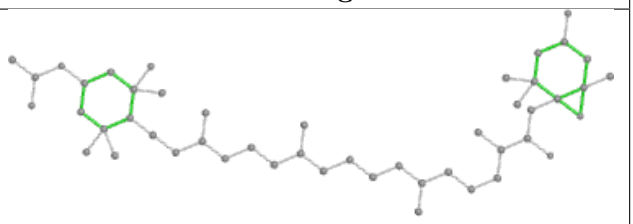
Bond lengths



Bond angles

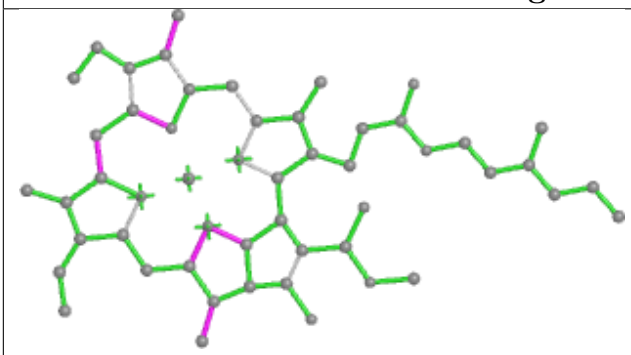


Torsions

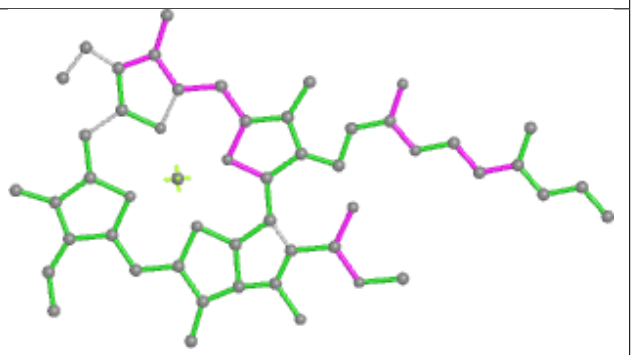


Rings

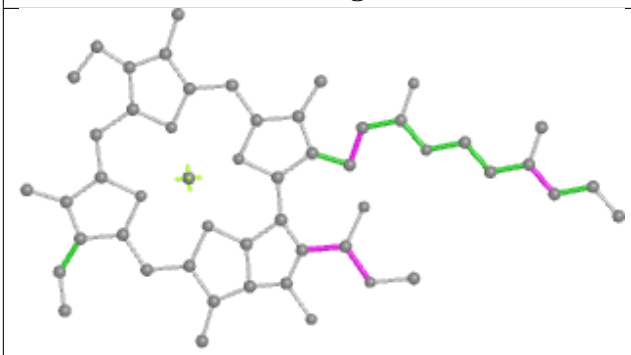
Ligand CLA 6 309



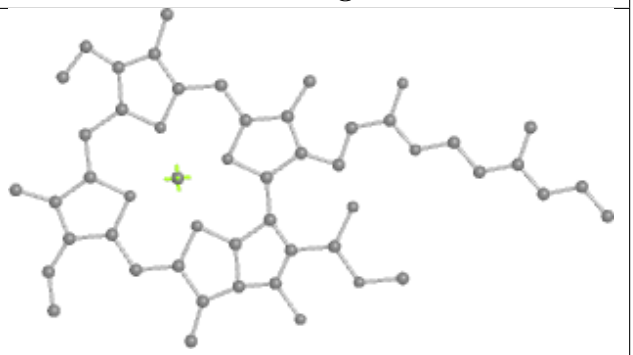
Bond lengths



Bond angles

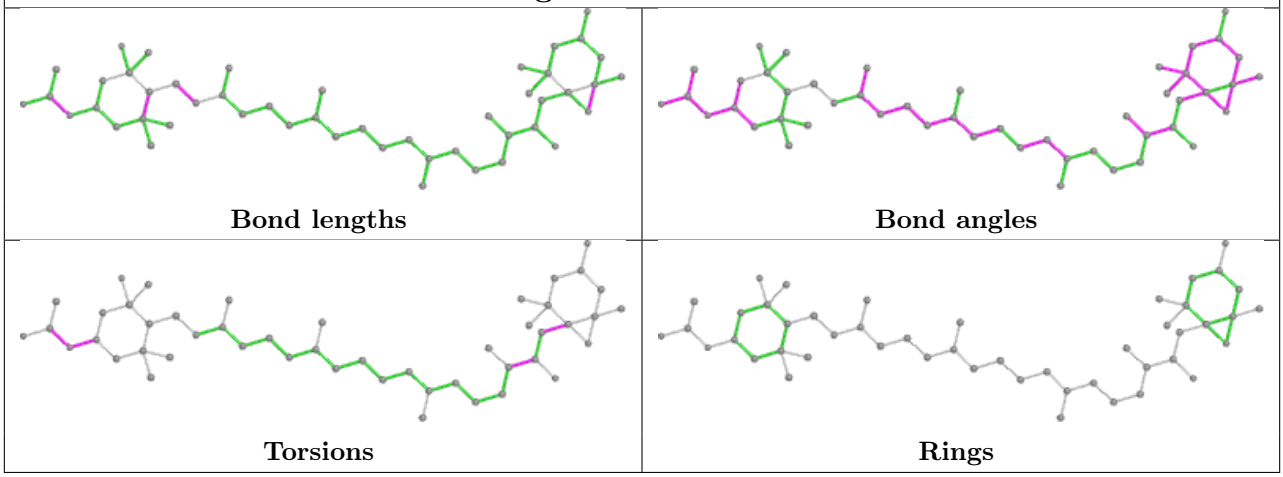


Torsions

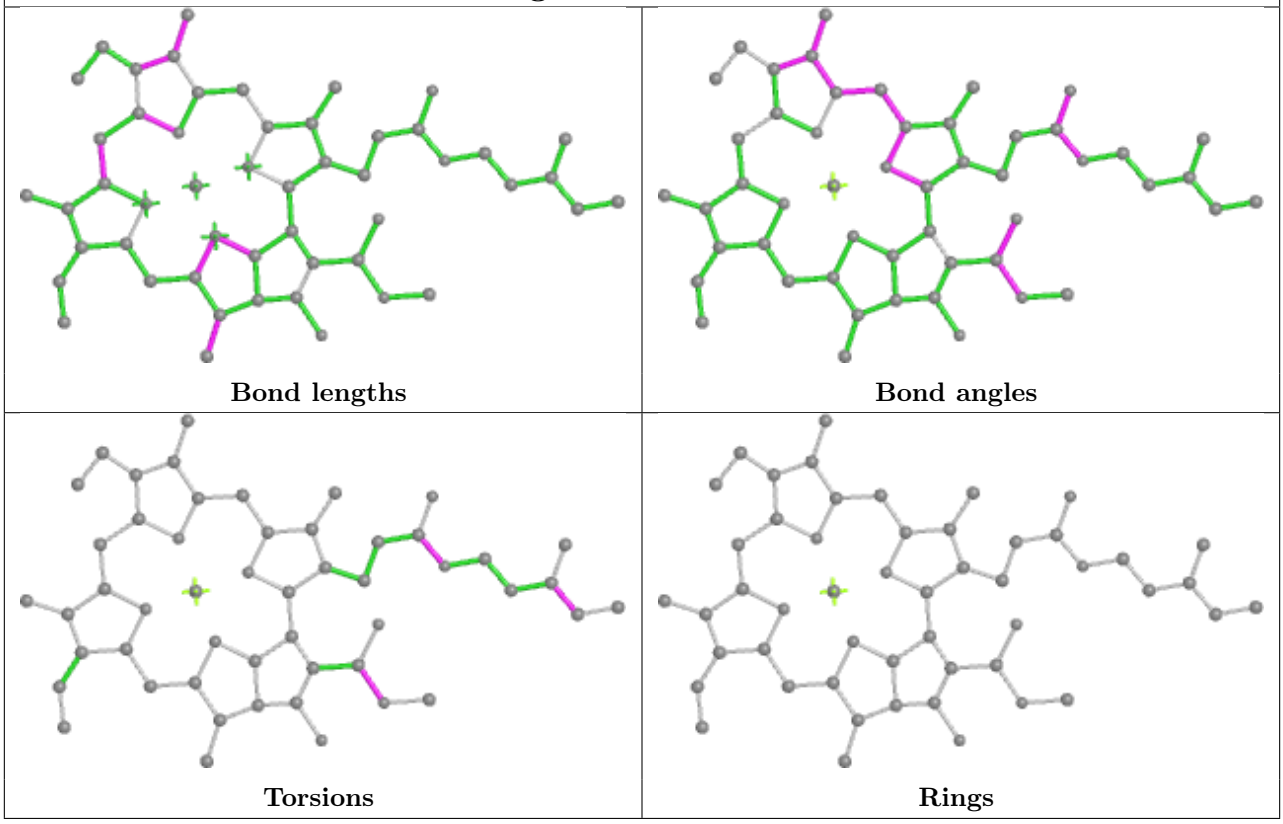


Rings

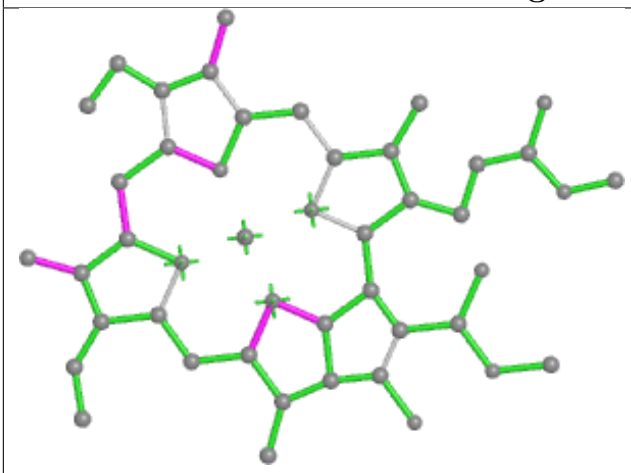
Ligand A86 5 307



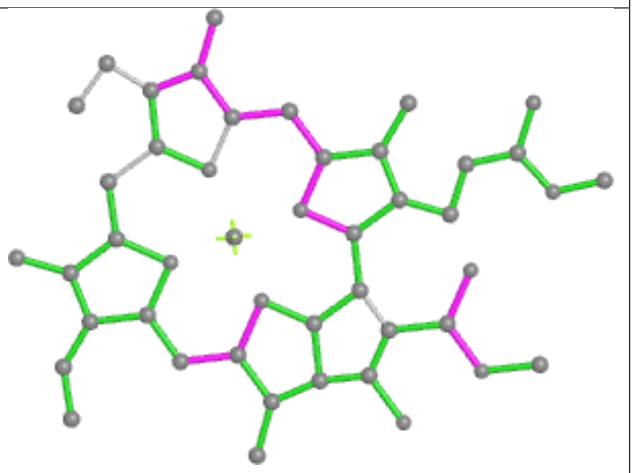
Ligand CLA 3 608



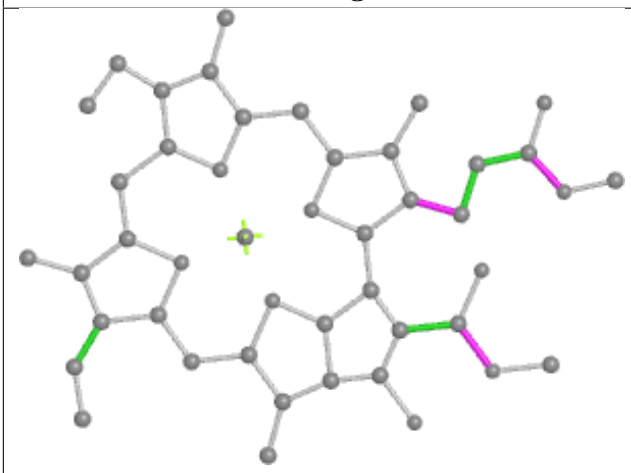
Ligand CLA 6 312



Bond lengths



Bond angles



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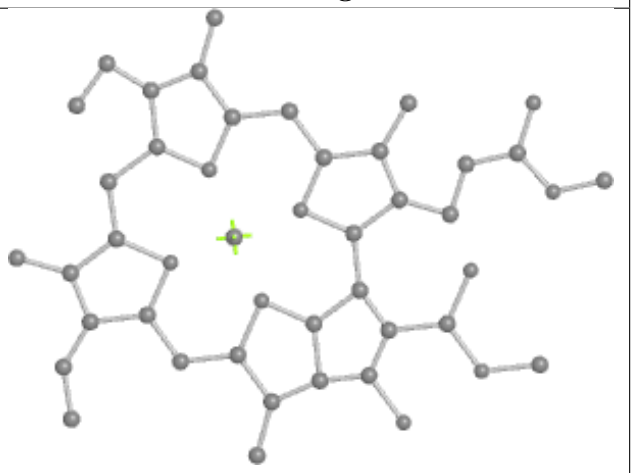
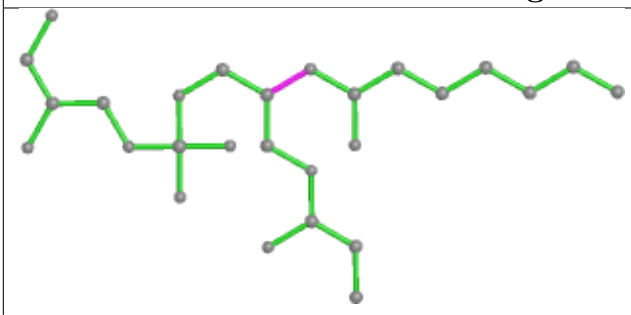
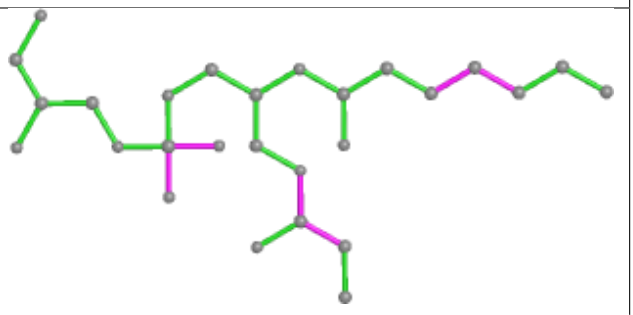


Rings

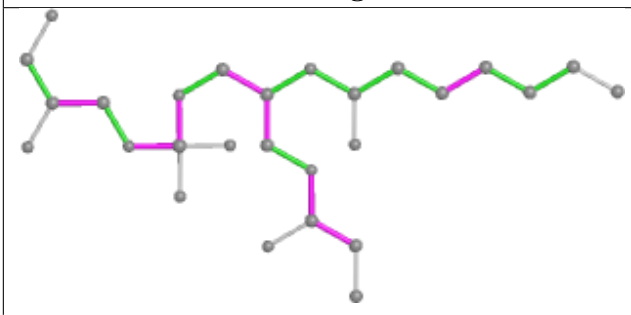
Ligand LHG 3 617



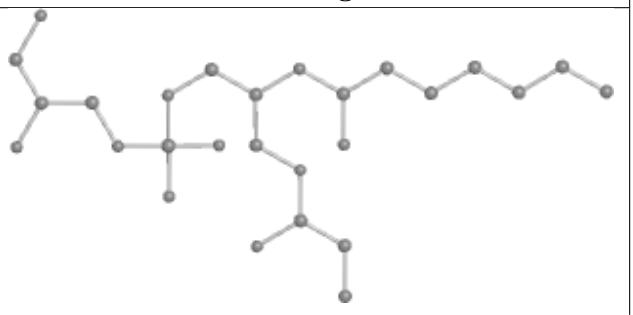
Bond lengths



Bond angles

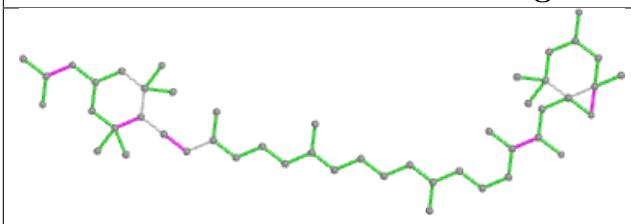


Torsions



Rings

Ligand A86 4 304



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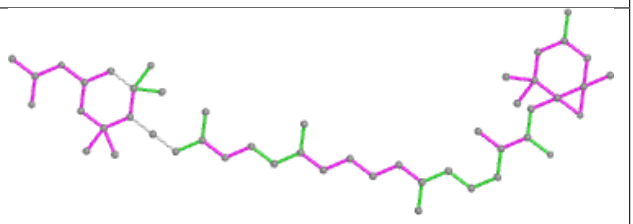
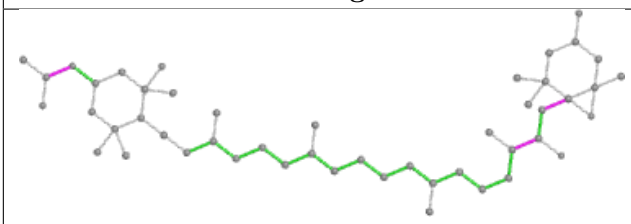


Bond angles



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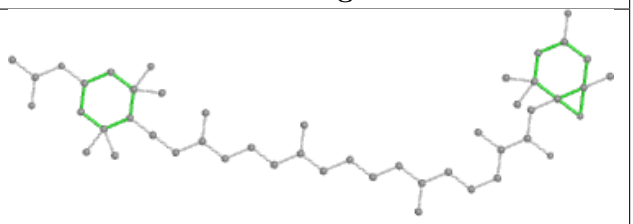
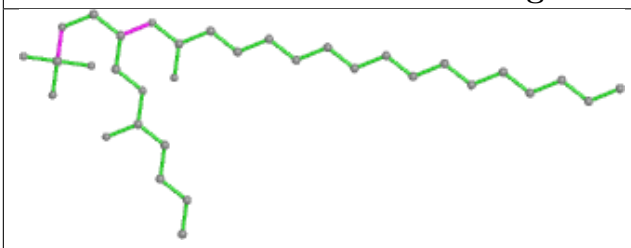
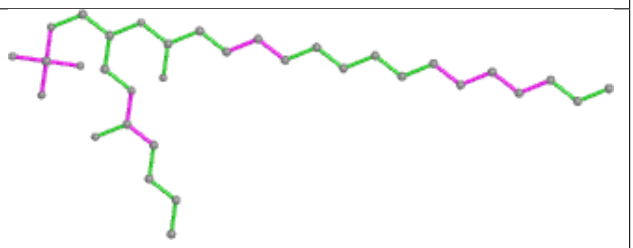


Rings

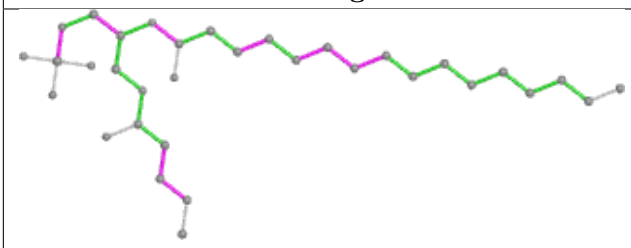
Ligand LHG 5 318



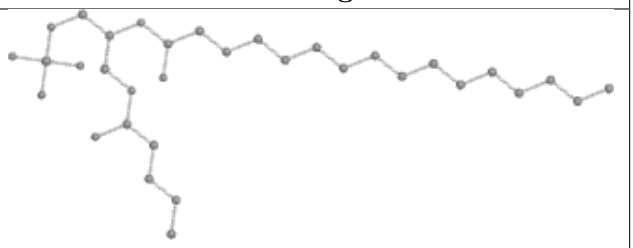
Bond lengths



Bond angles

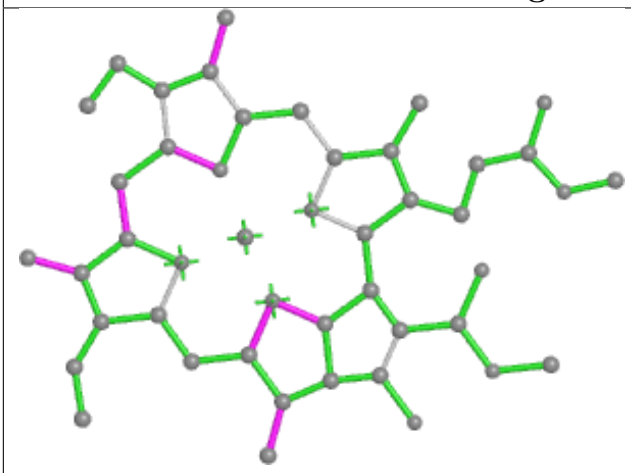


Torsions



Rings

Ligand CLA 4 310



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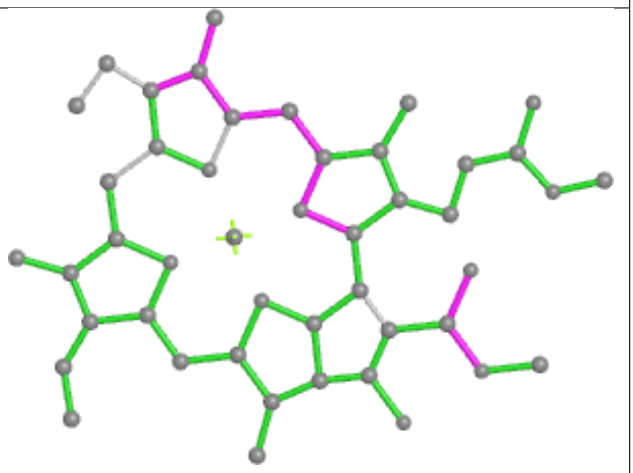
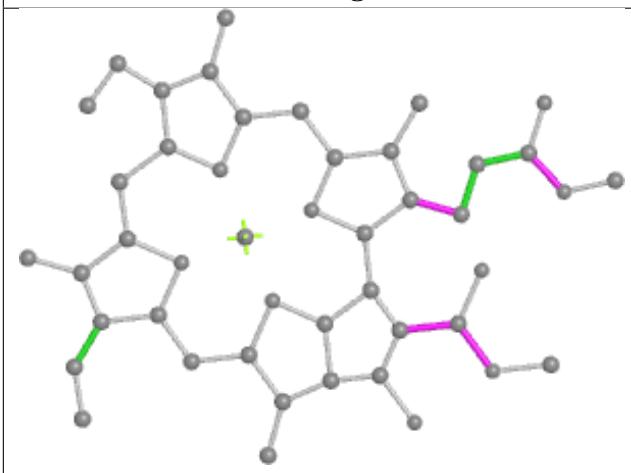
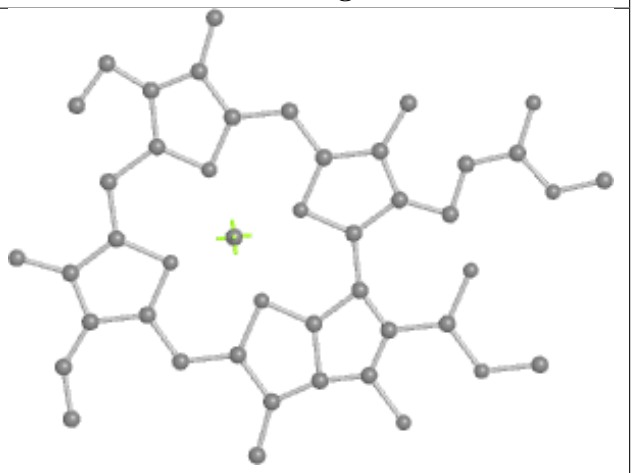


Bond angles

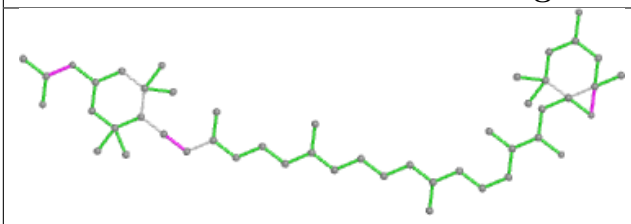


Torsions



Rings

Ligand A86 3 613



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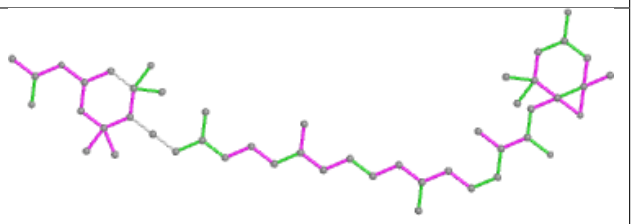
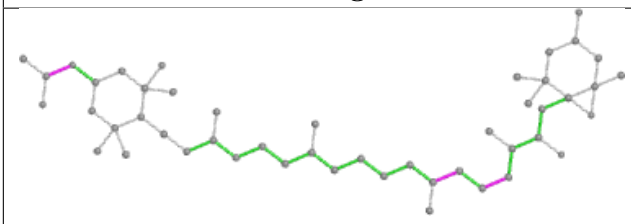
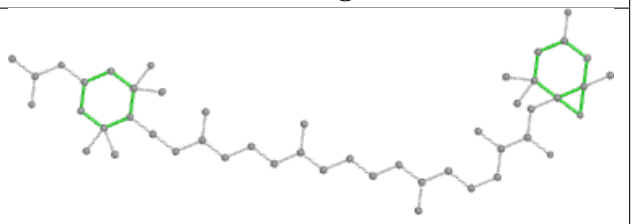


Bond angles

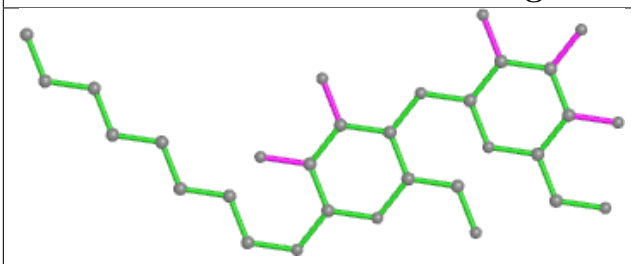


Torsions



Rings

Ligand LMT 5 320



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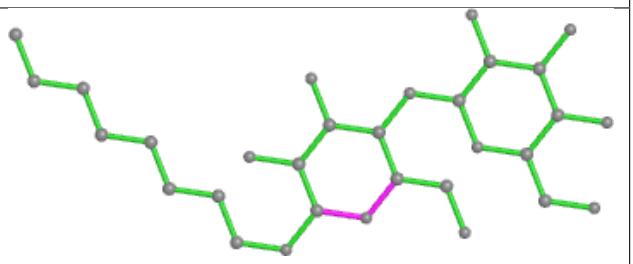
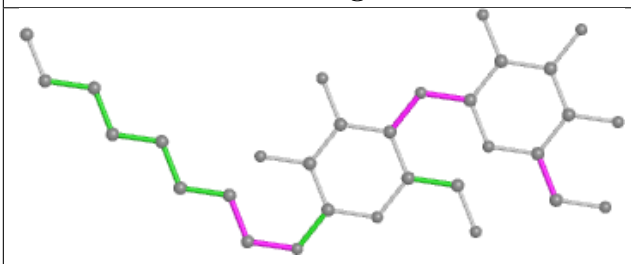
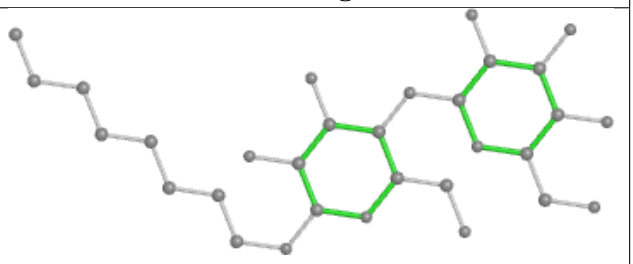


Bond angles

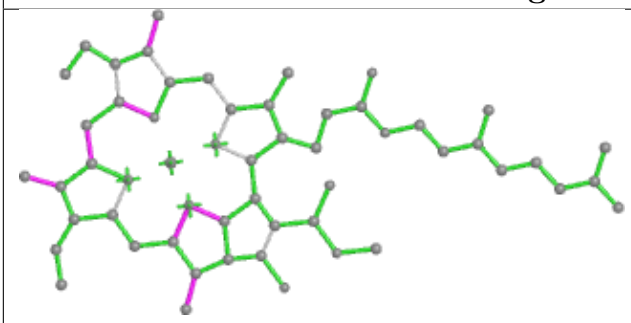


Torsions

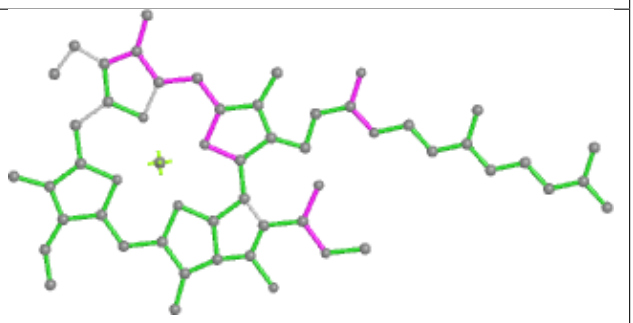


Rings

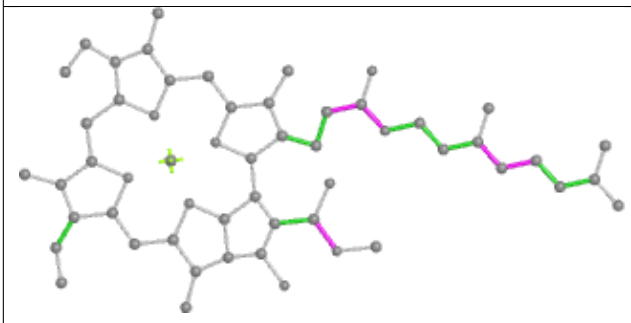
Ligand CLA 4 305



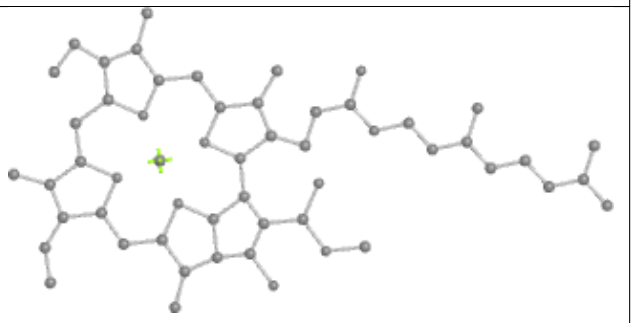
Bond lengths



Bond angles

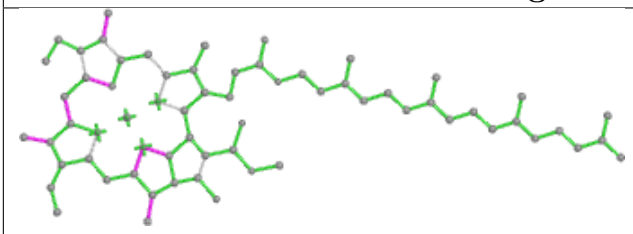


Torsions

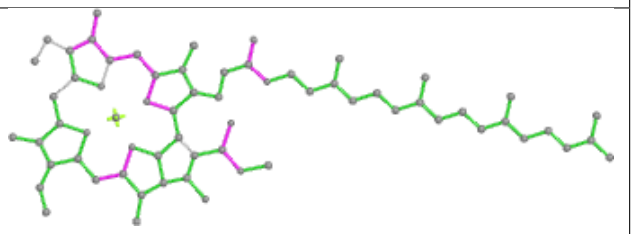


Rings

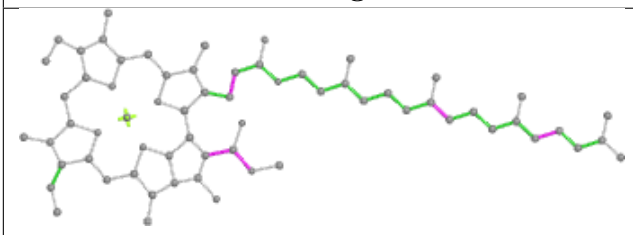
Ligand CLA 4 306



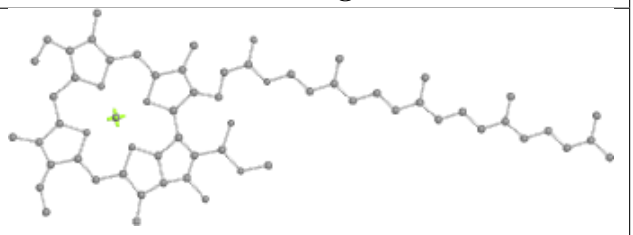
Bond lengths



Bond angles

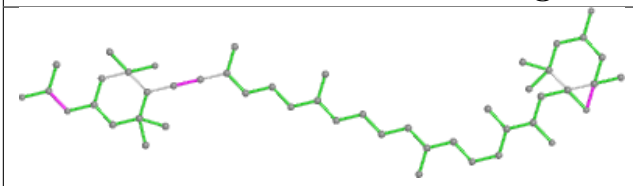


Torsions

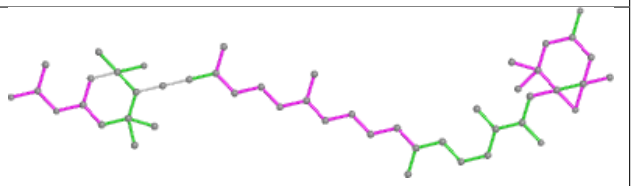


Rings

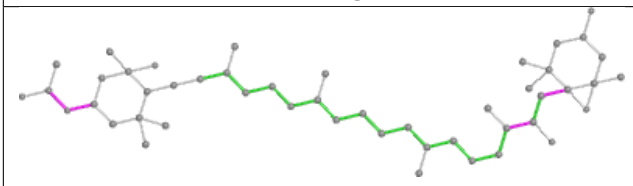
Ligand A86 5 304



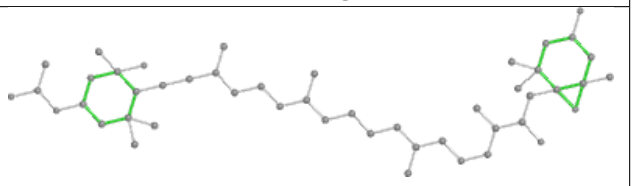
Bond lengths



Bond angles

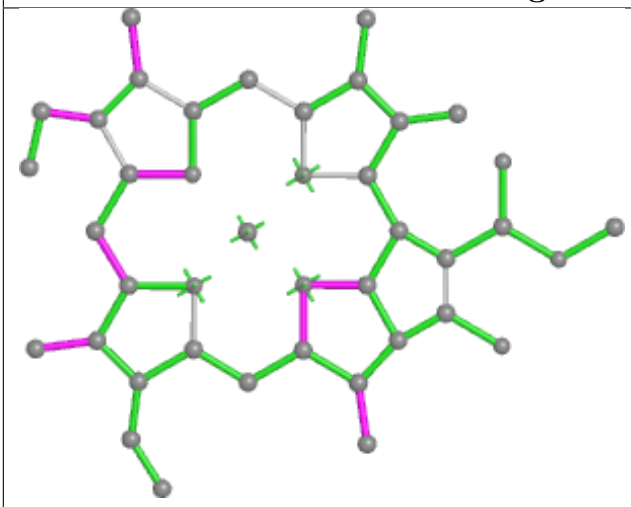


Torsions

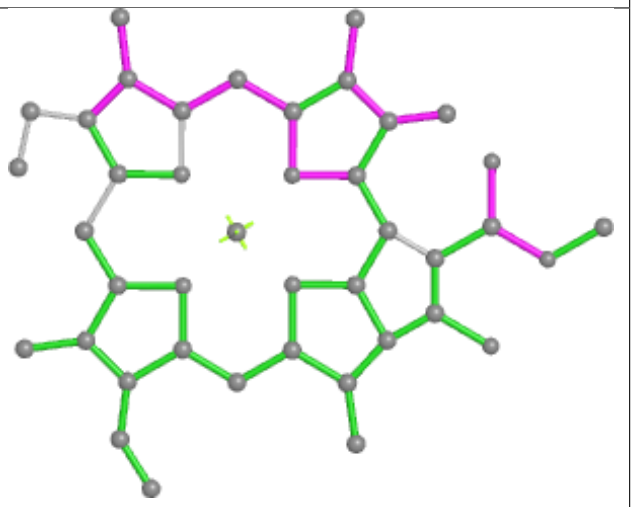


Rings

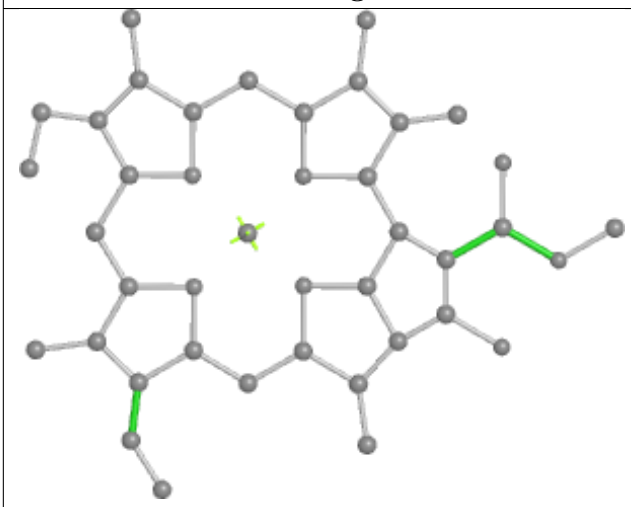
Ligand CLA 3 610



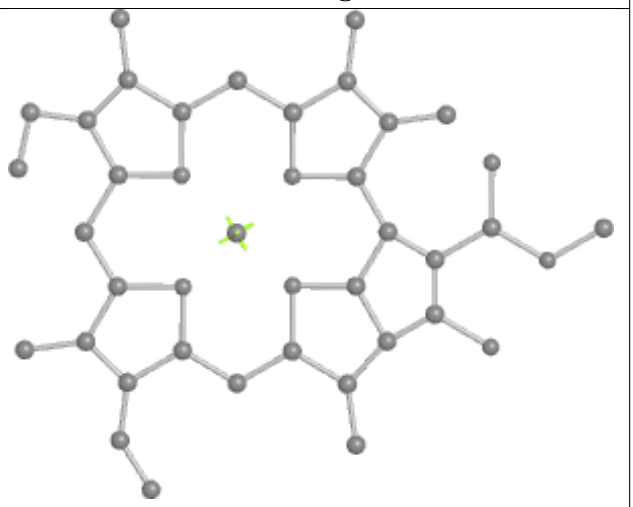
Bond lengths



Bond angles

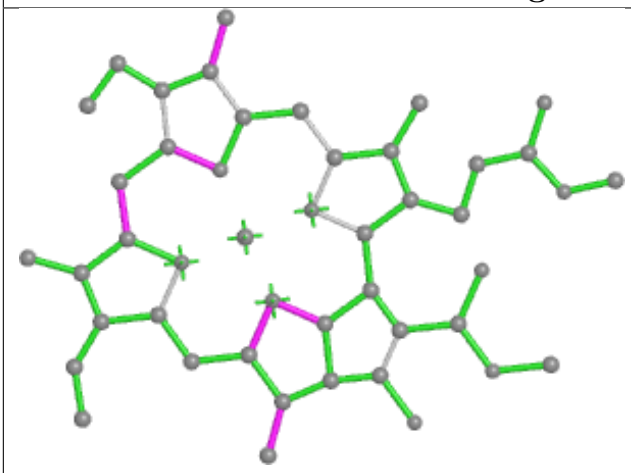


Torsions

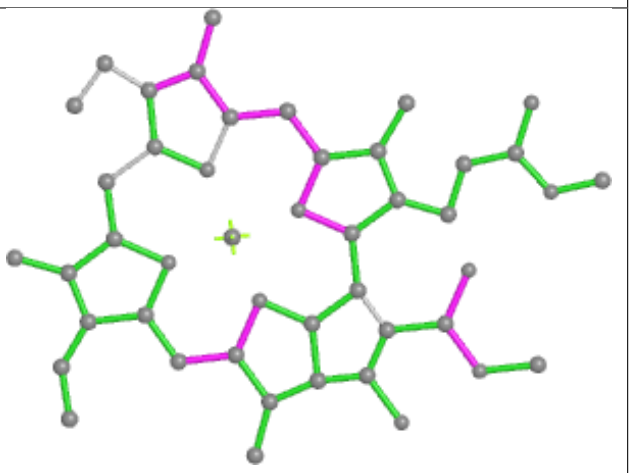


Rings

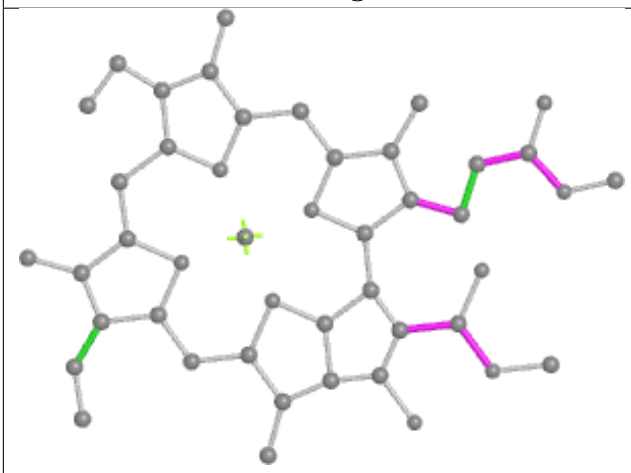
Ligand CLA 6 310



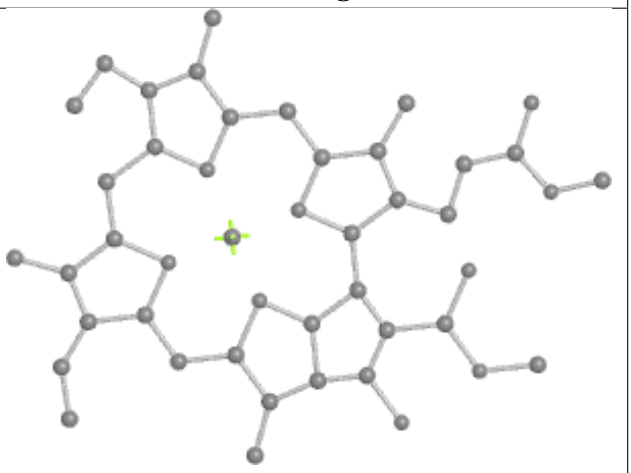
Bond lengths



Bond angles

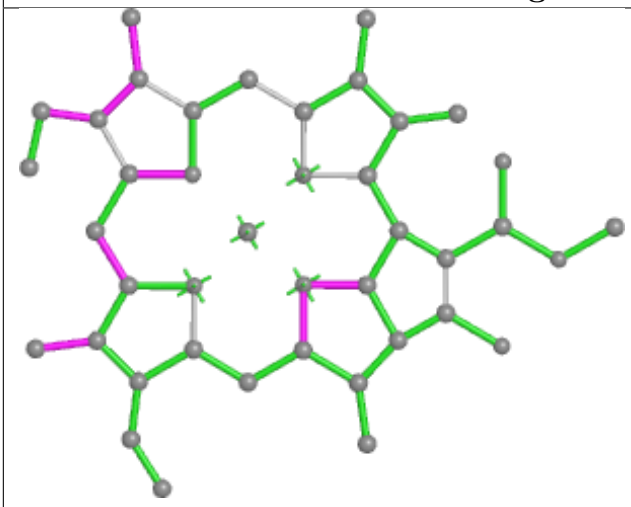


Torsions

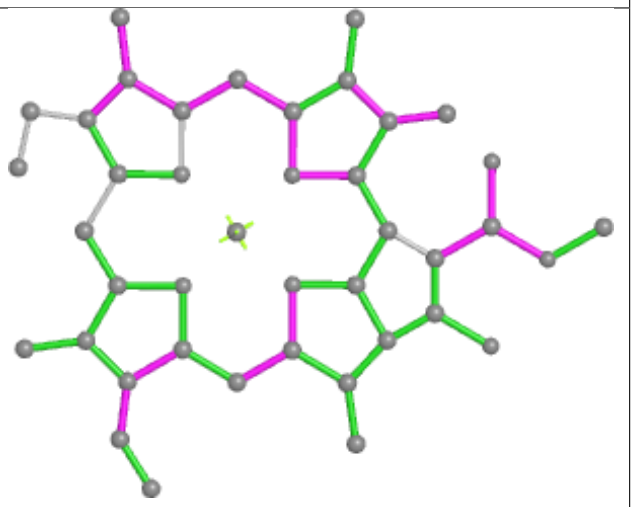


Rings

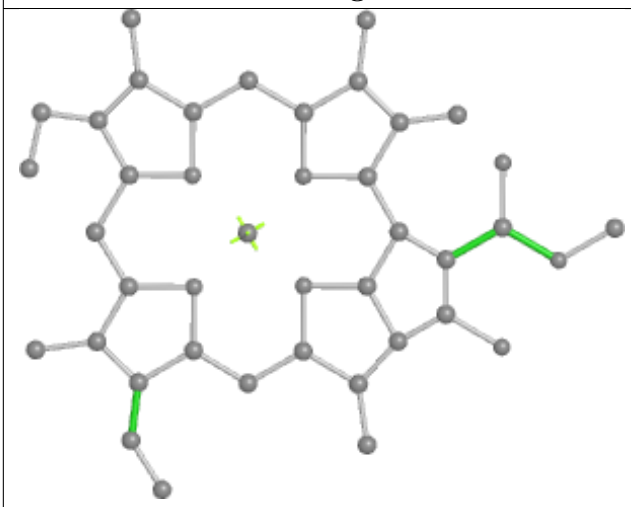
Ligand CLA 6 314



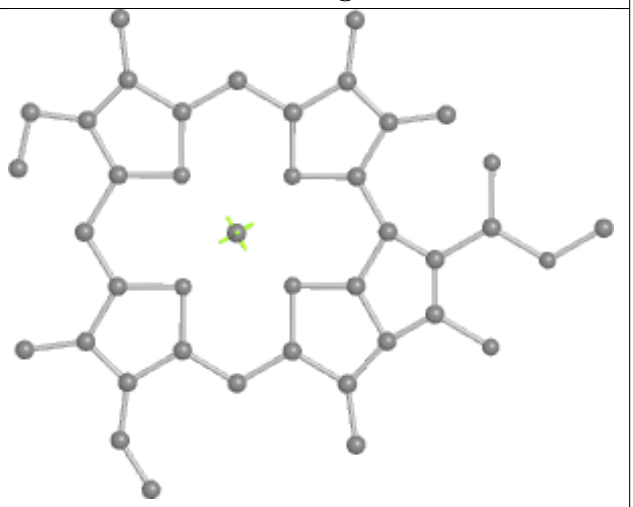
Bond lengths



Bond angles

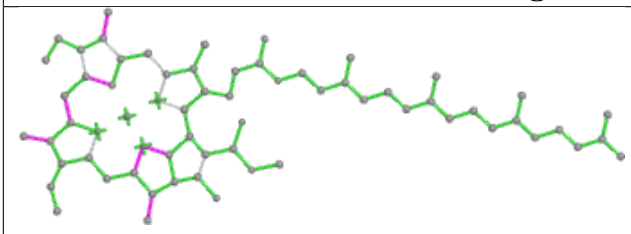


Torsions

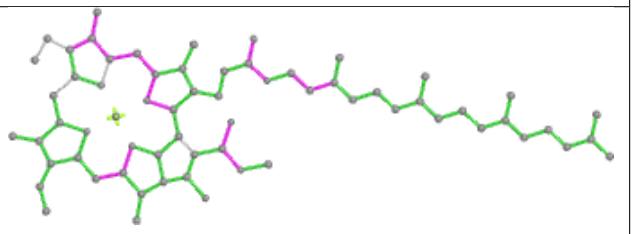


Rings

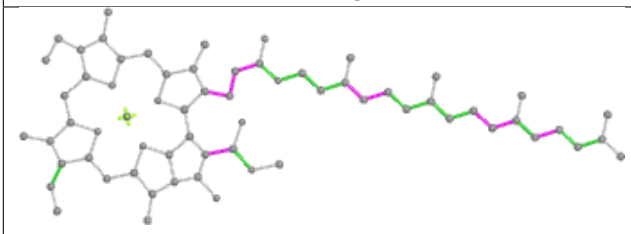
Ligand CLA 3 602



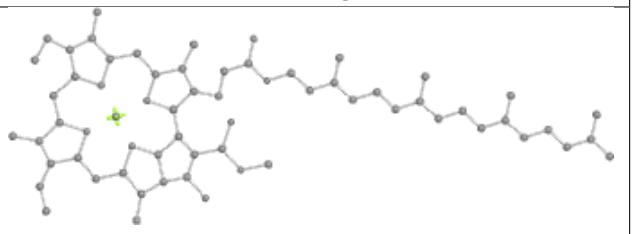
Bond lengths



Bond angles

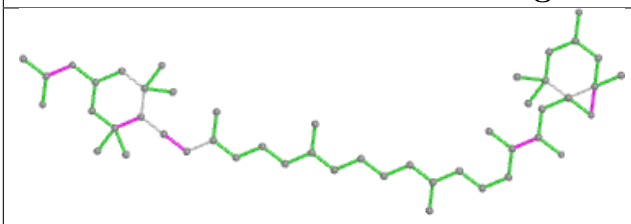


Torsions



Rings

Ligand A86 6 301



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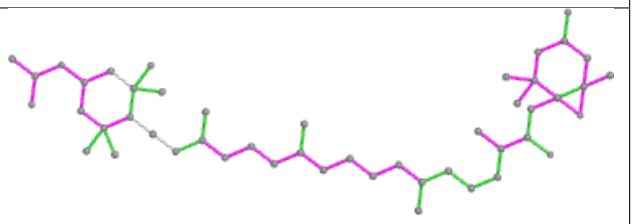
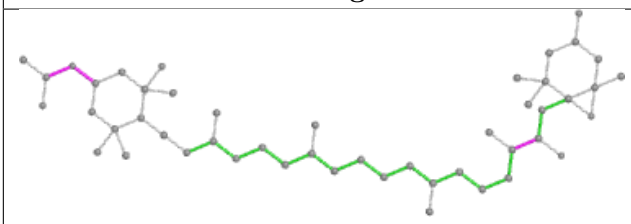
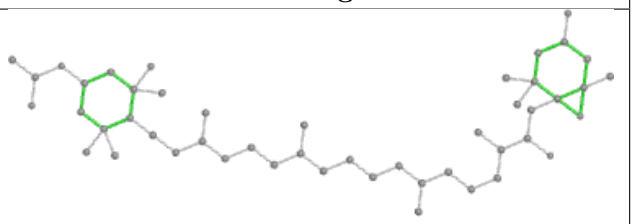


Bond angles

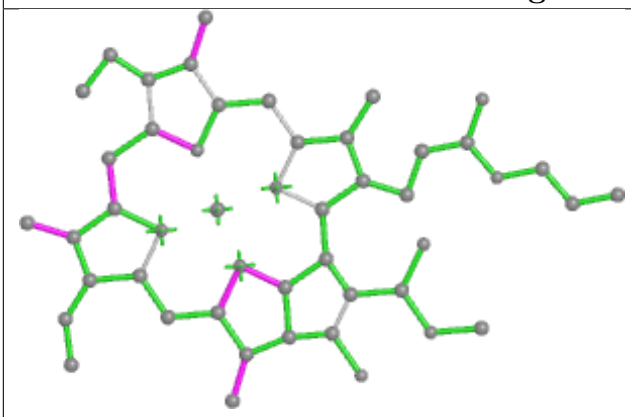


Torsions

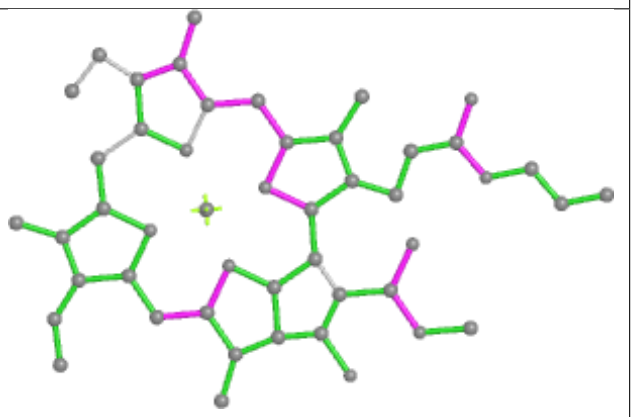


Rings

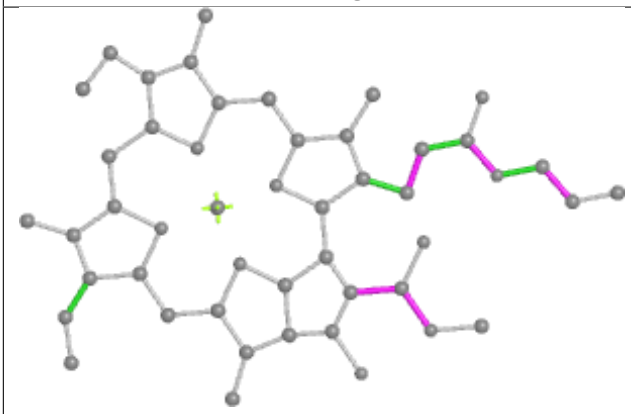
Ligand CLA 3 604



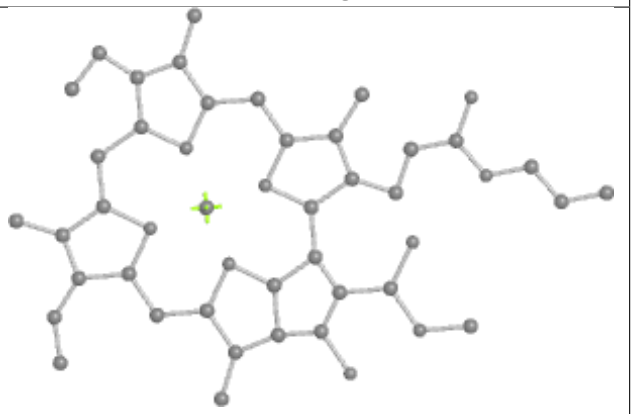
Bond lengths



Bond angles

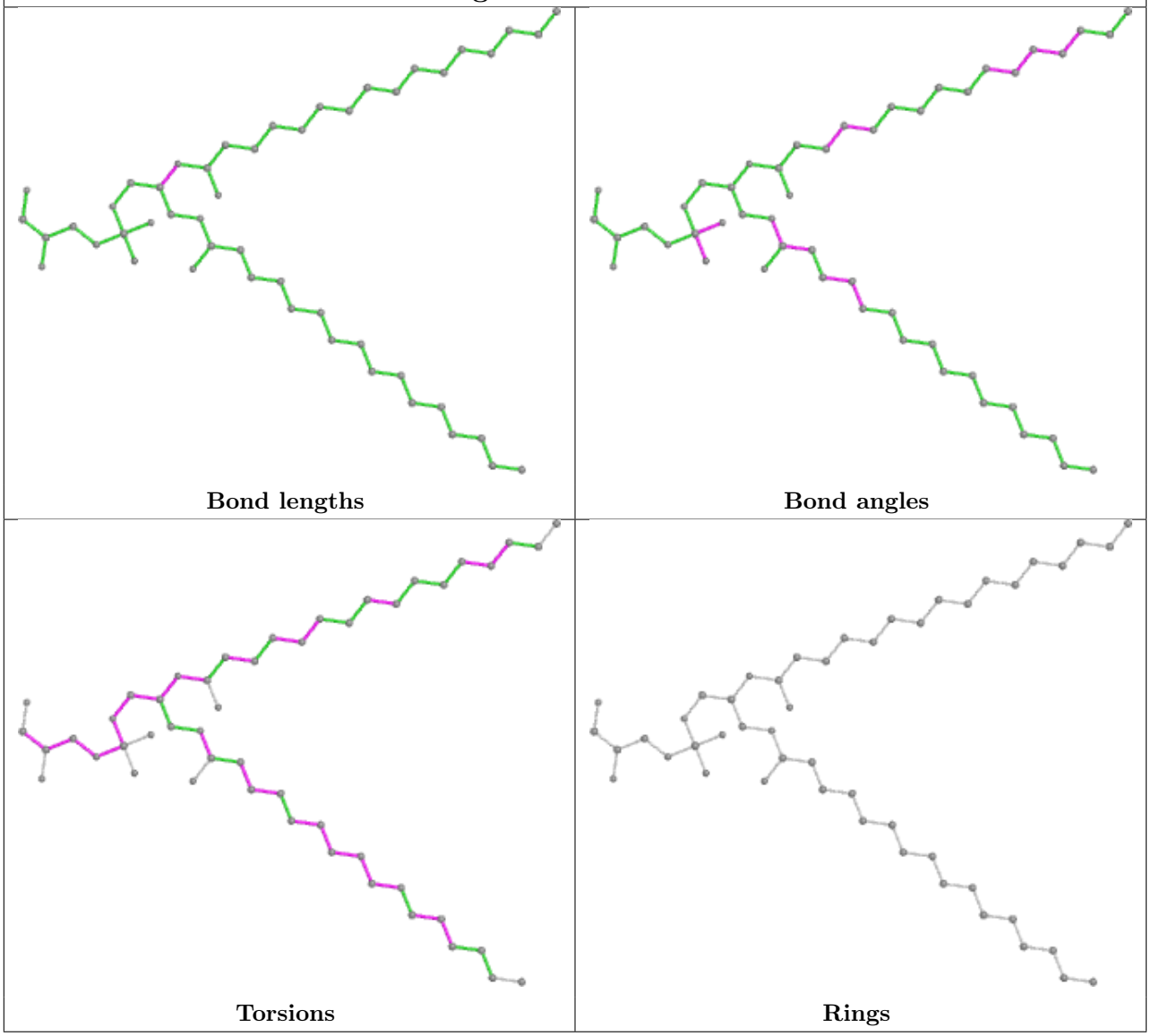


Torsions

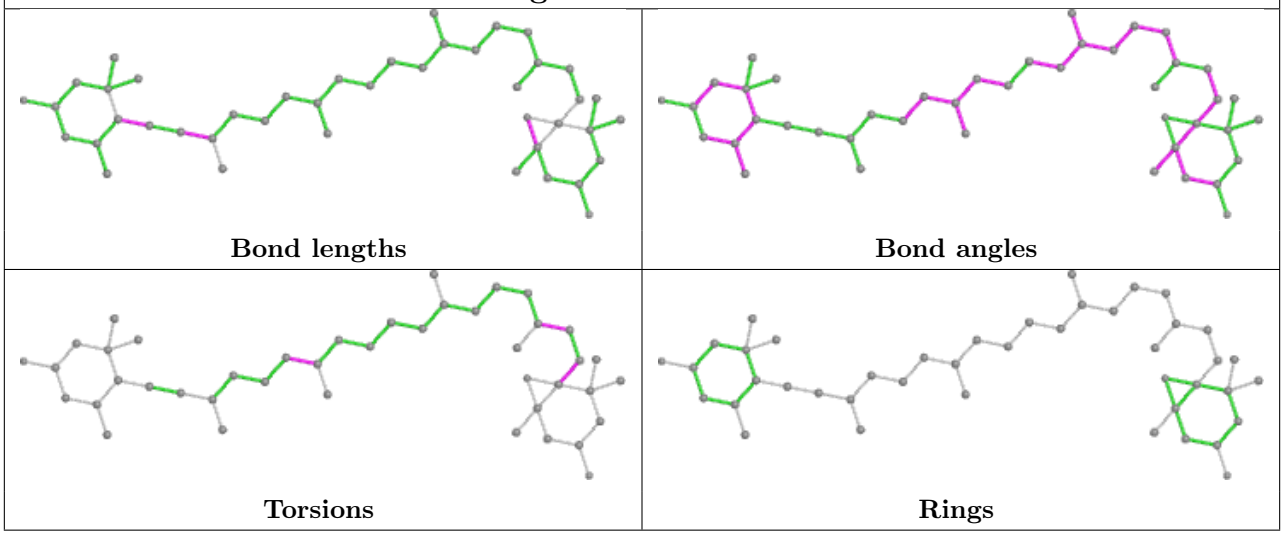


Rings

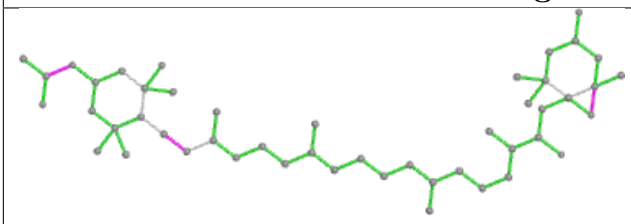
Ligand LHG 4 318



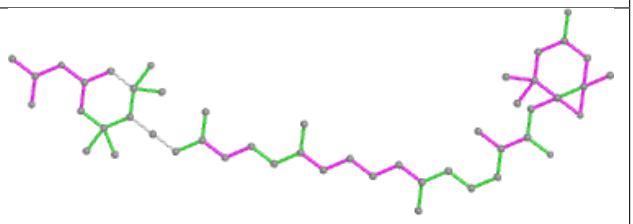
Ligand DD6 3 614



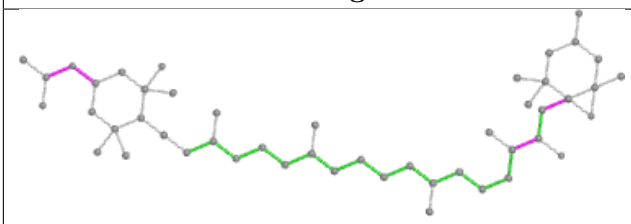
Ligand A86 6 304



Bond lengths



Bond angles



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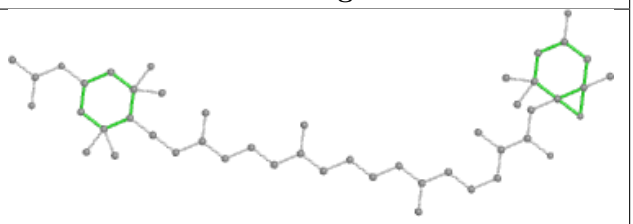
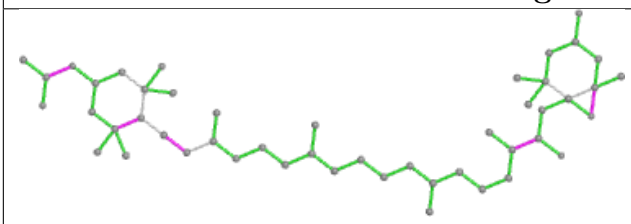
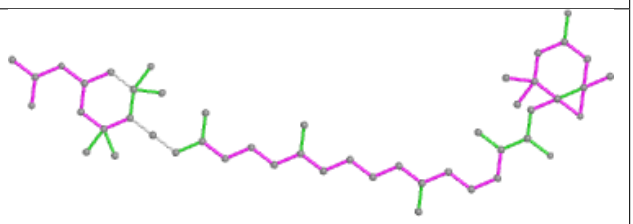


Rings

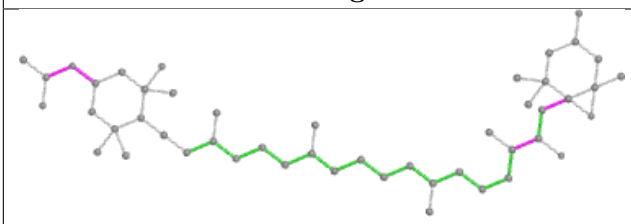
Ligand A86 5 302



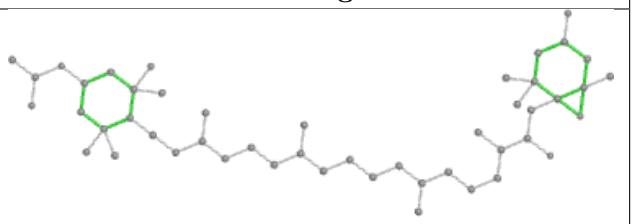
Bond lengths



Bond angles

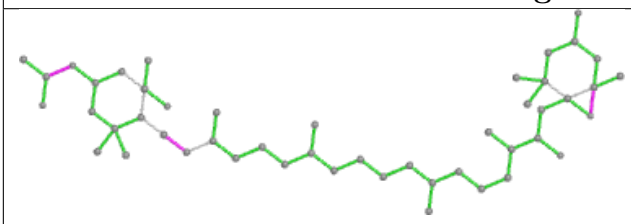


Torsions

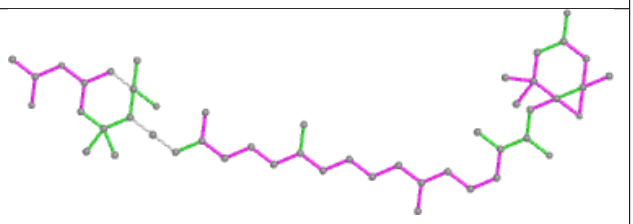


Rings

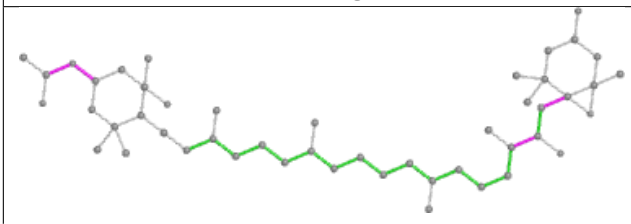
Ligand A86 6 302



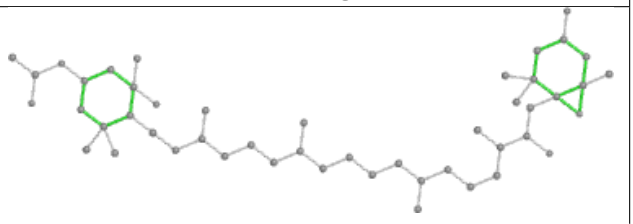
Bond lengths



Bond angles

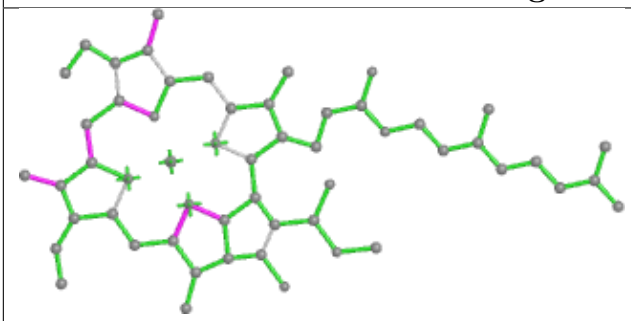


Torsions



Rings

Ligand CLA 5 314



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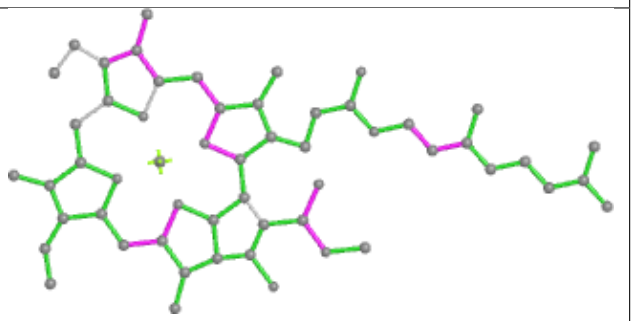
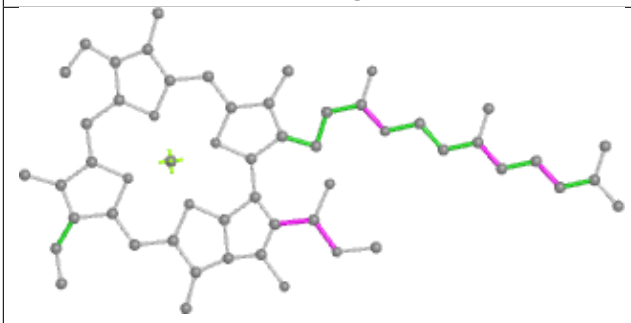
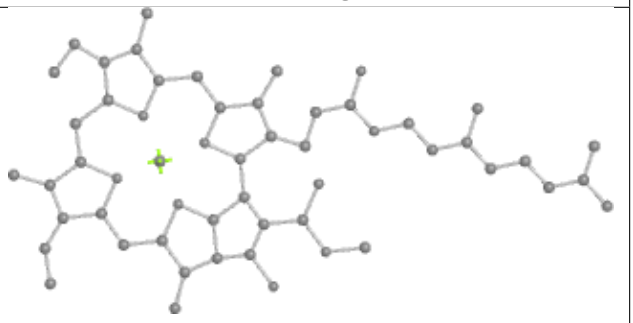


Bond angles

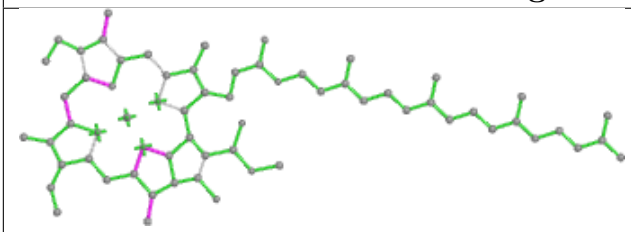


Torsions



Rings

Ligand CLA 4 309



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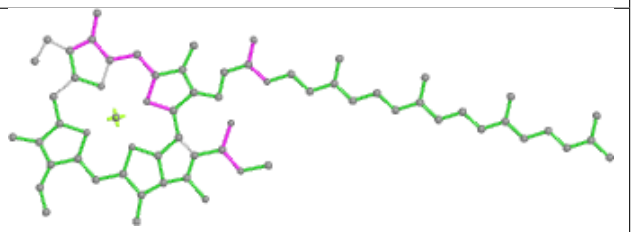
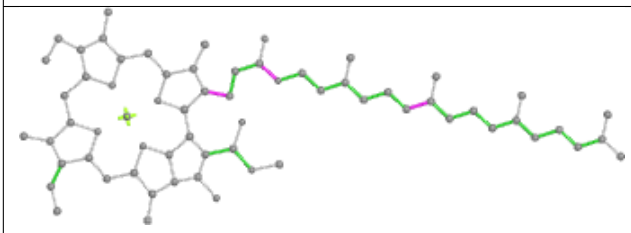
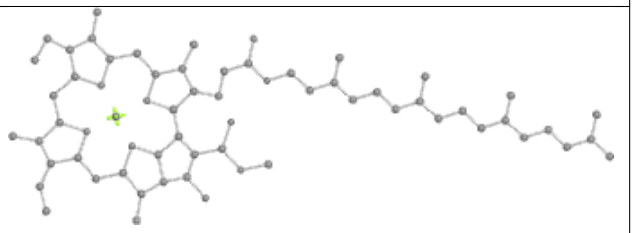


Bond angles

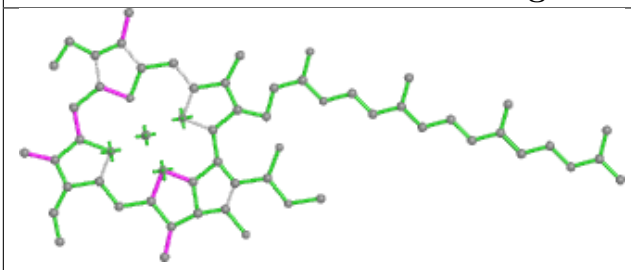


Torsions

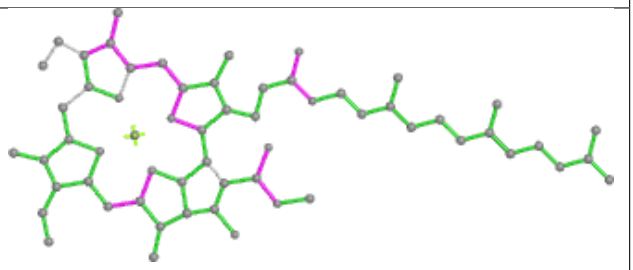


Rings

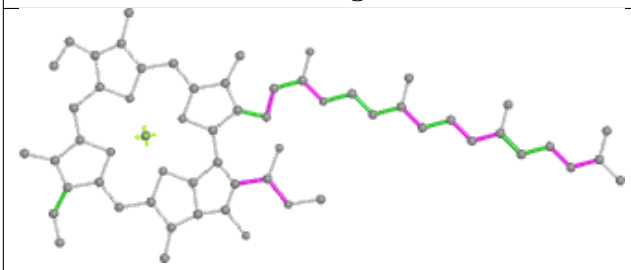
Ligand CLA 4 311



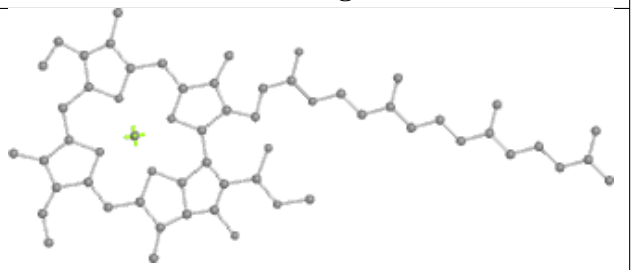
Bond lengths



Bond angles

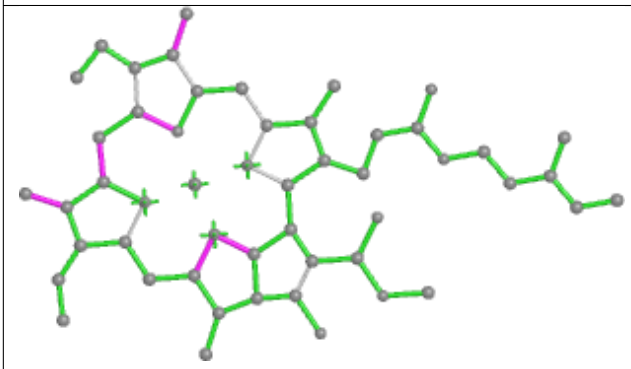


Torsions

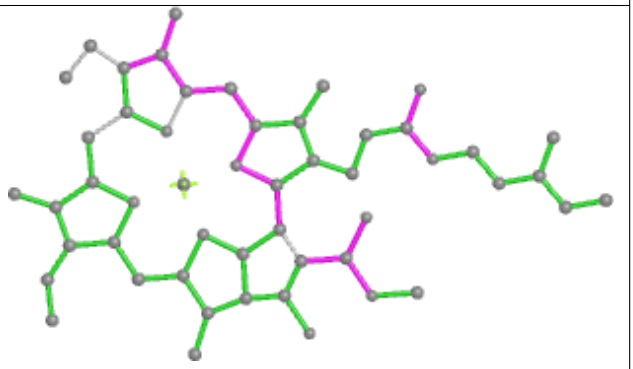


Rings

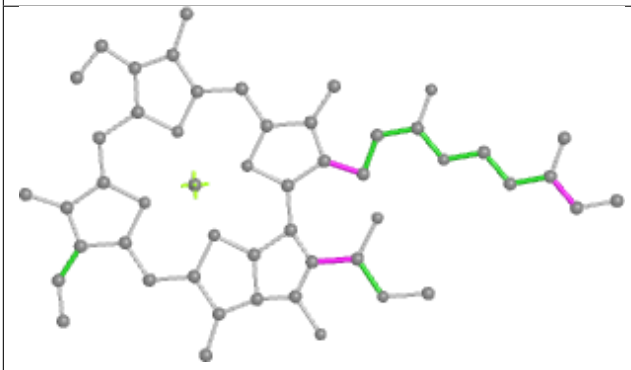
Ligand CLA 4 312



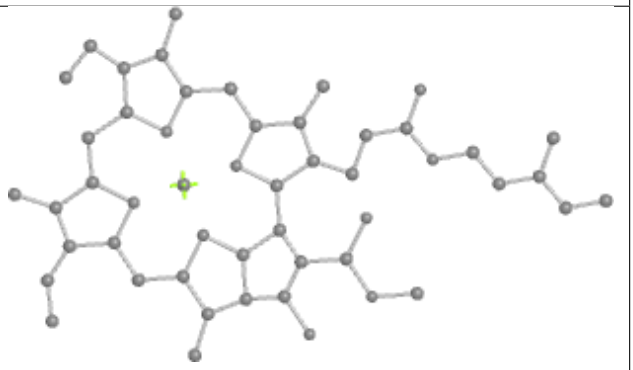
Bond lengths



Bond angles

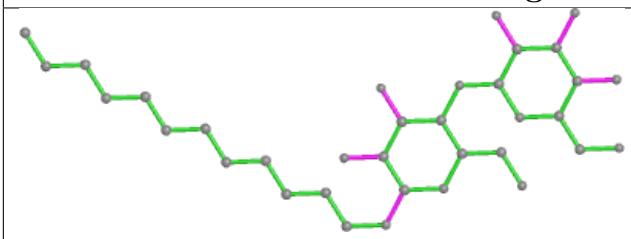


Torsions

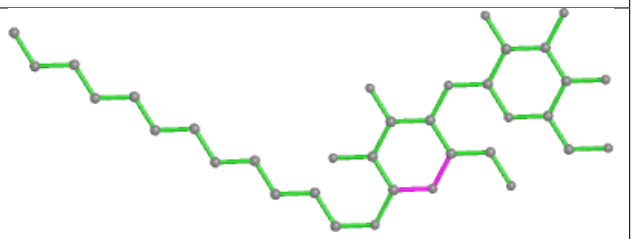


Rings

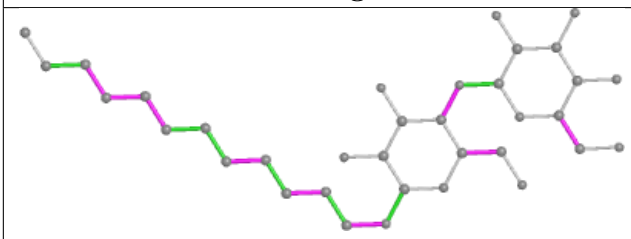
Ligand LMT 4 317



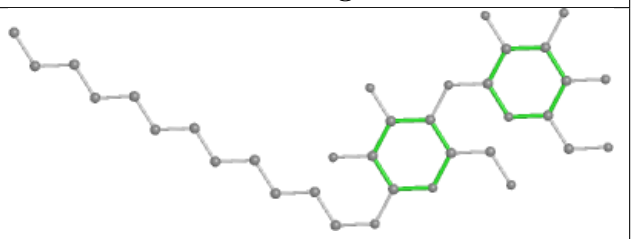
Bond lengths



Bond angles

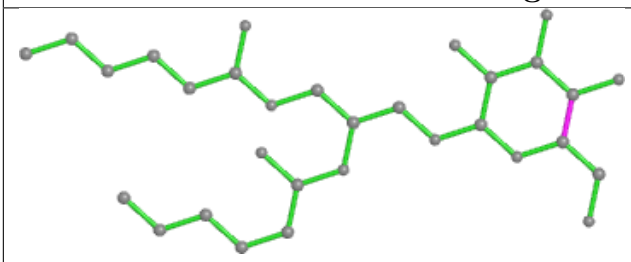


Torsions

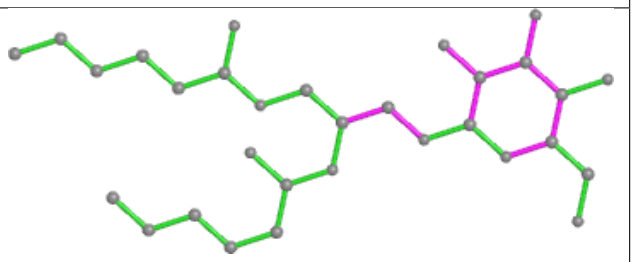


Rings

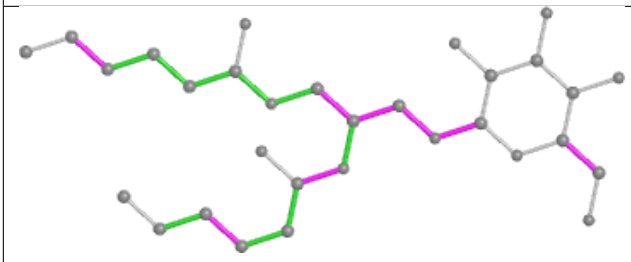
Ligand LMG 5 319



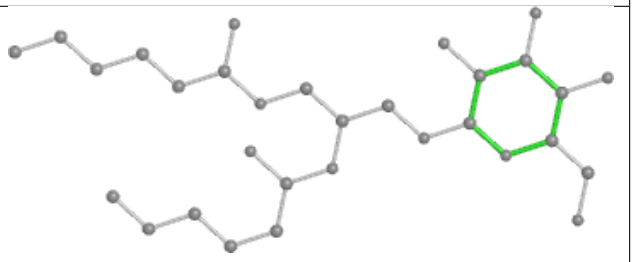
Bond lengths



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.

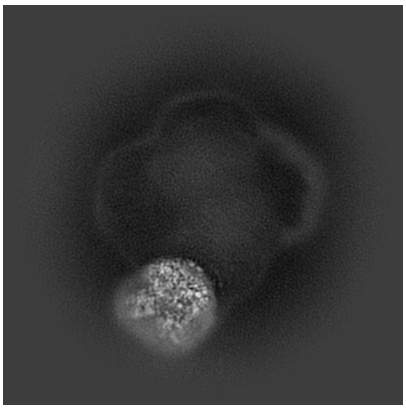
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35899. These allow visual inspection of the internal detail of the map and identification of artifacts.

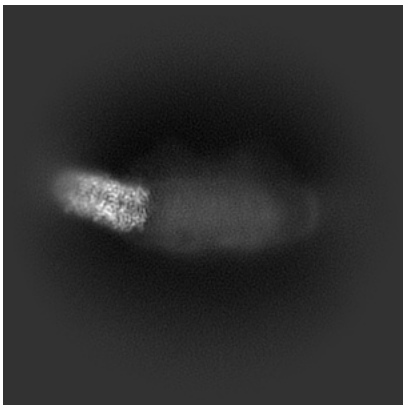
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

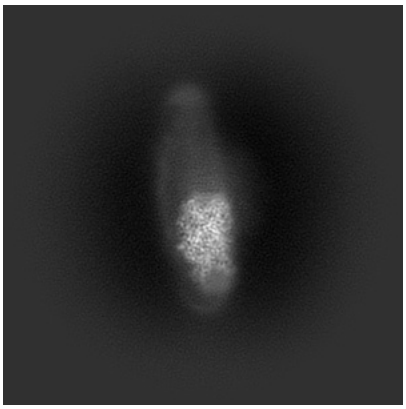
6.1.1 Primary map



X

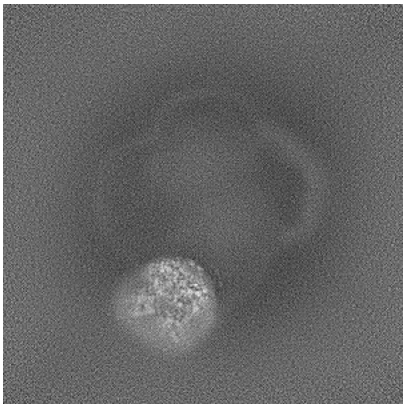


Y

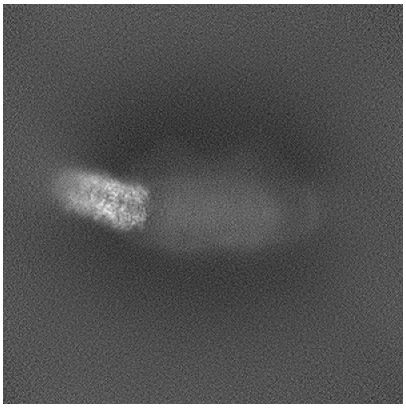


Z

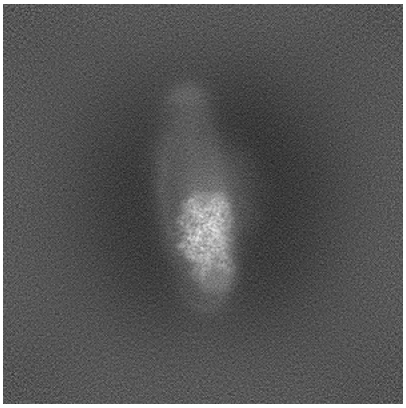
6.1.2 Raw map



X



Y

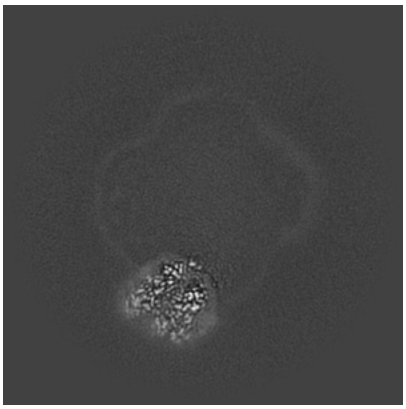


Z

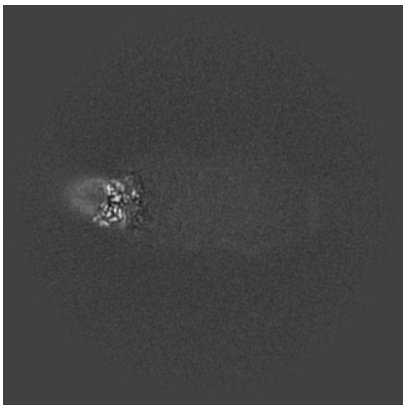
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

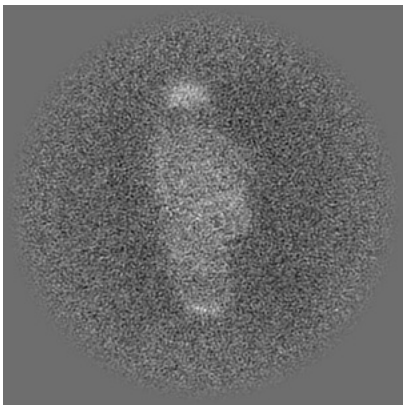
6.2.1 Primary map



X Index: 250

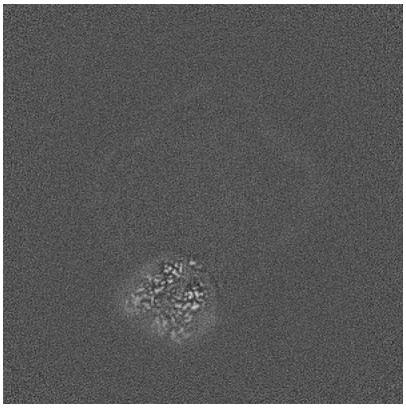


Y Index: 250

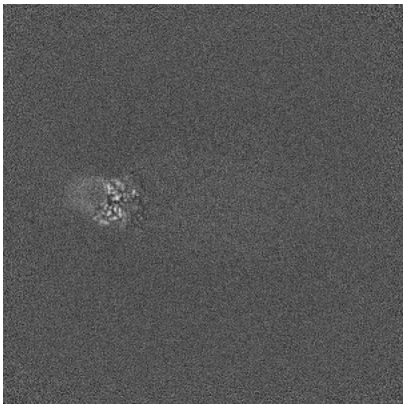


Z Index: 250

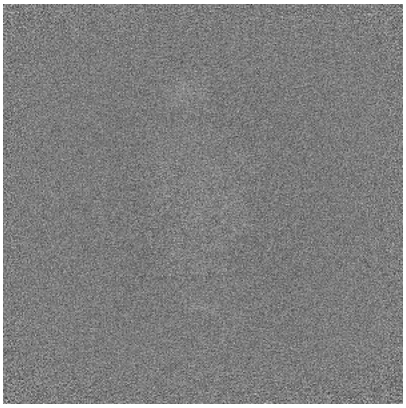
6.2.2 Raw map



X Index: 250



Y Index: 250

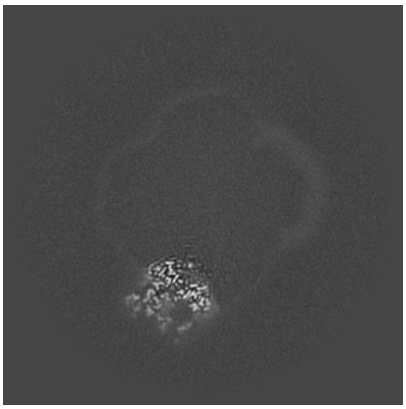


Z Index: 250

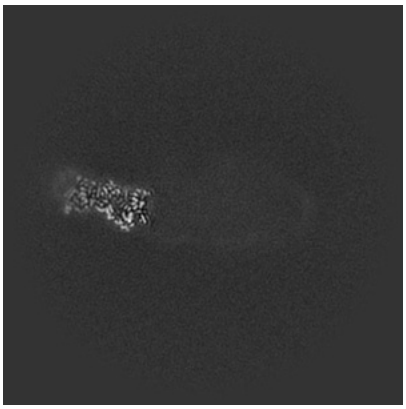
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

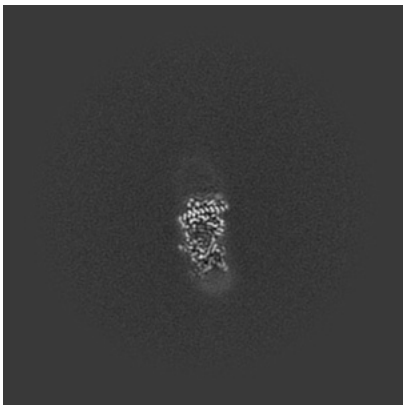
6.3.1 Primary map



X Index: 238

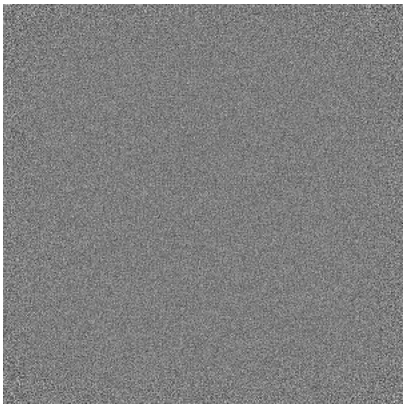


Y Index: 216

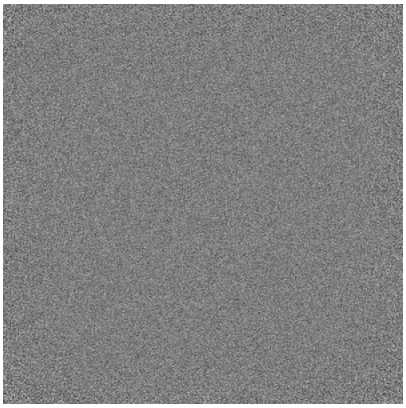


Z Index: 139

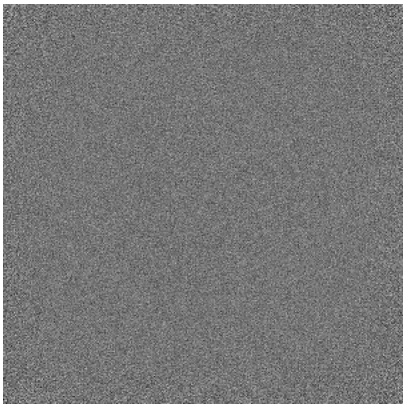
6.3.2 Raw map



X Index: 0



Y Index: 0

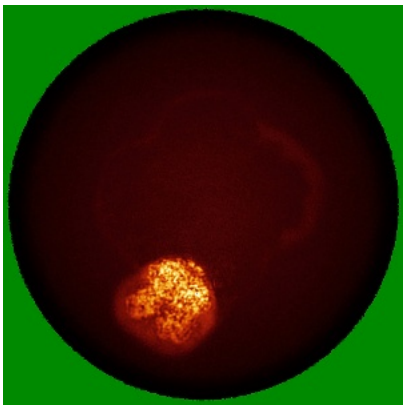


Z Index: 0

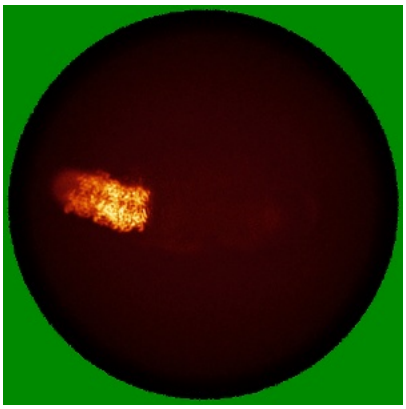
The images above show the largest variance slices of the map in three orthogonal directions.

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

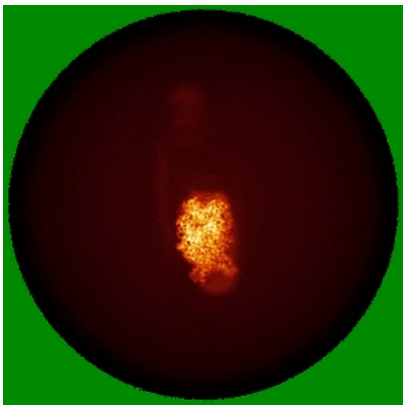
6.4.1 Primary map



X

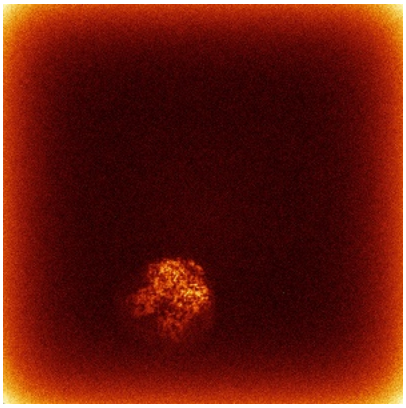


Y

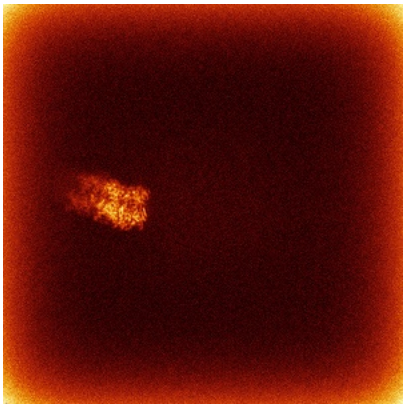


Z

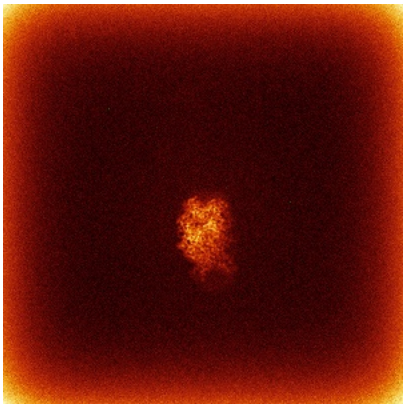
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

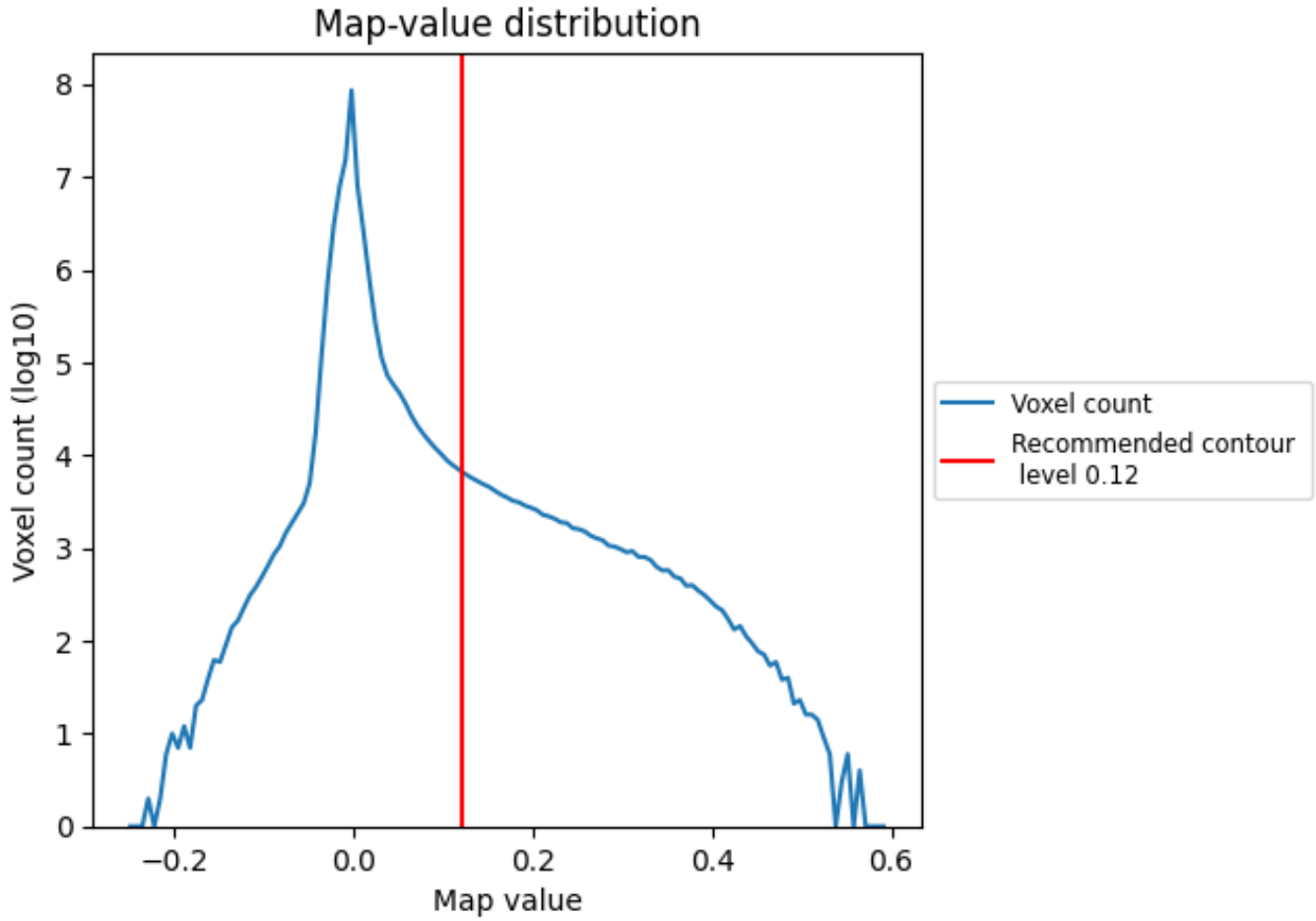
6.6 Mask visualisation (i)

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

7 Map analysis

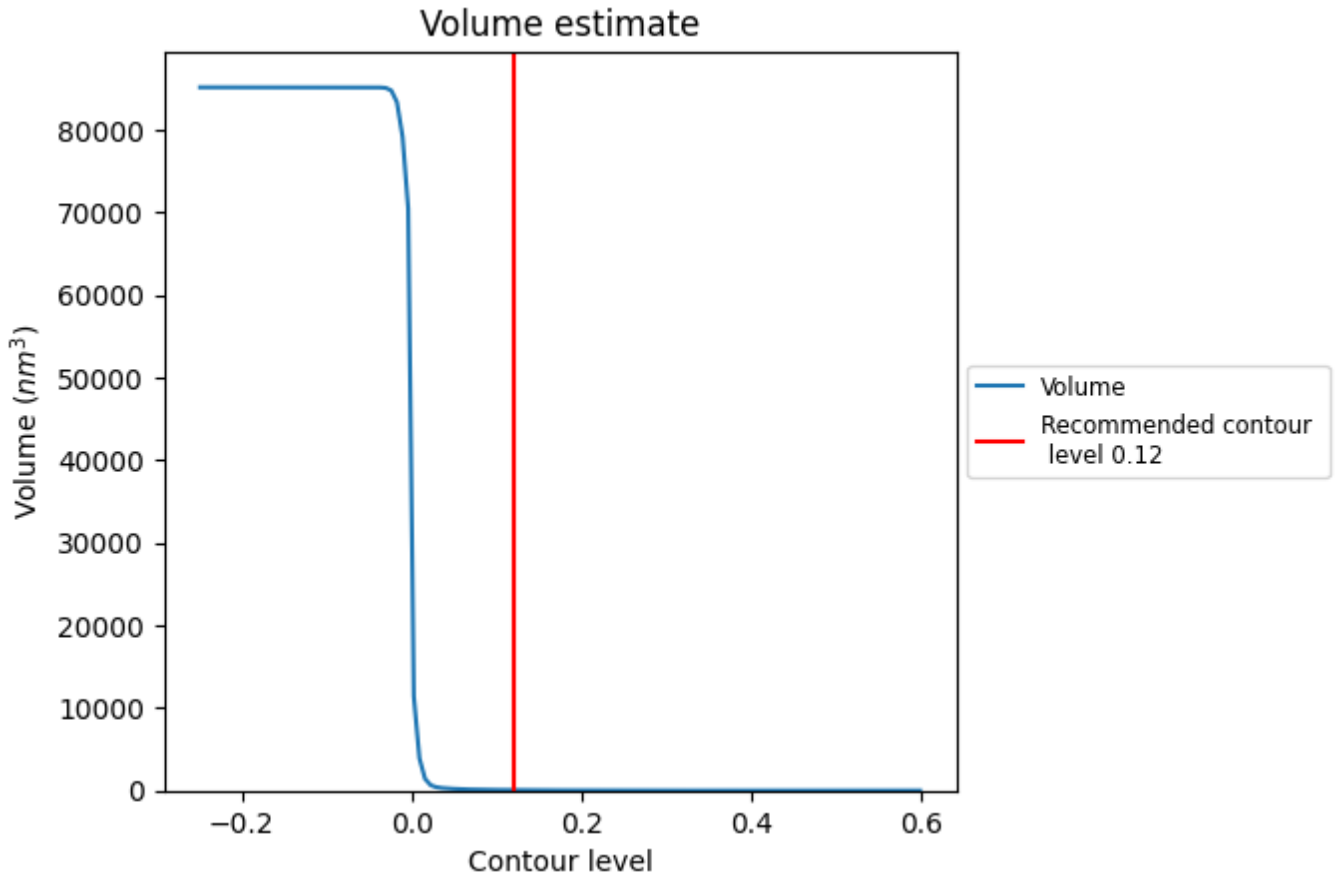
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

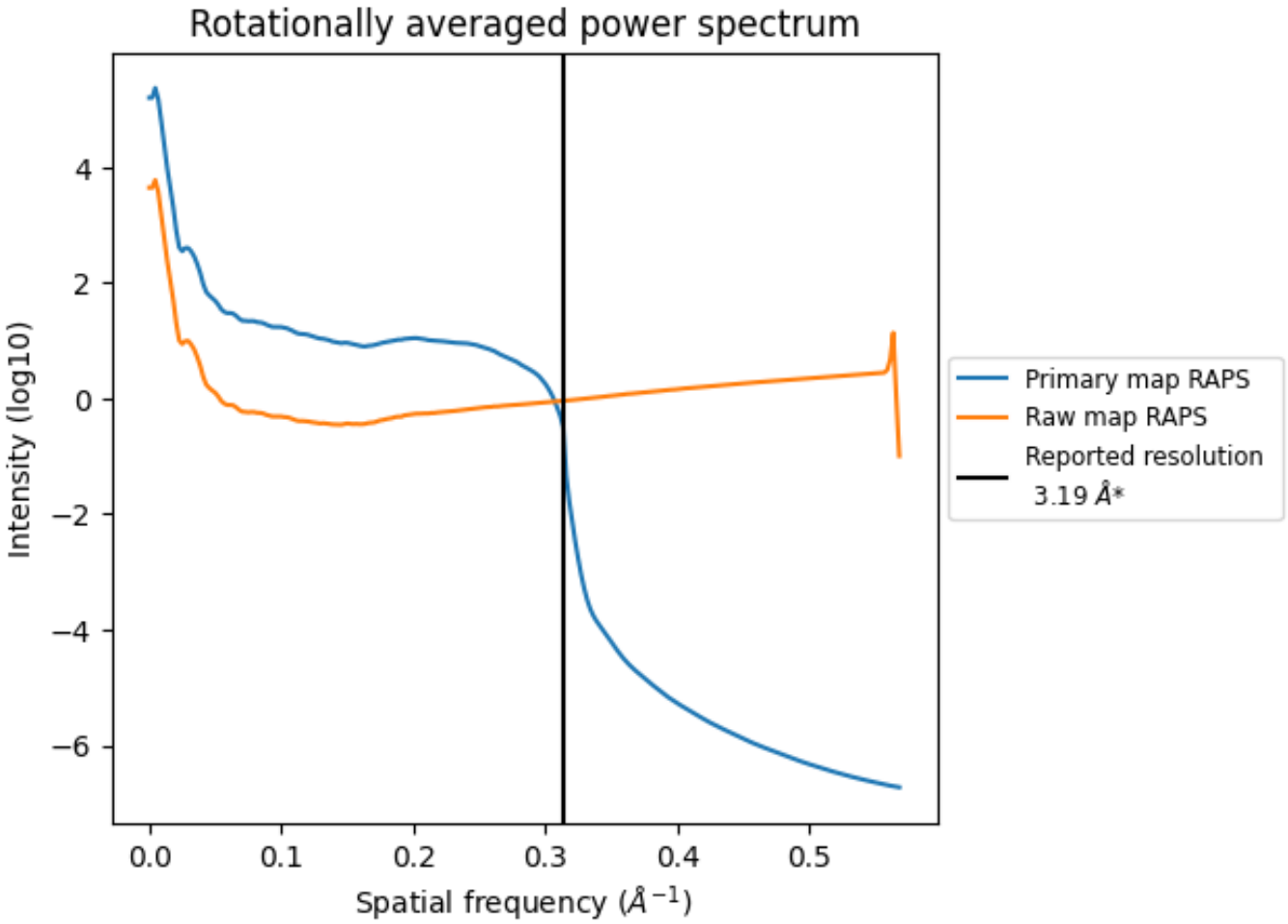
7.2 Volume estimate



The volume at the recommended contour level is 61 nm^3; this corresponds to an approximate mass of 55 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)

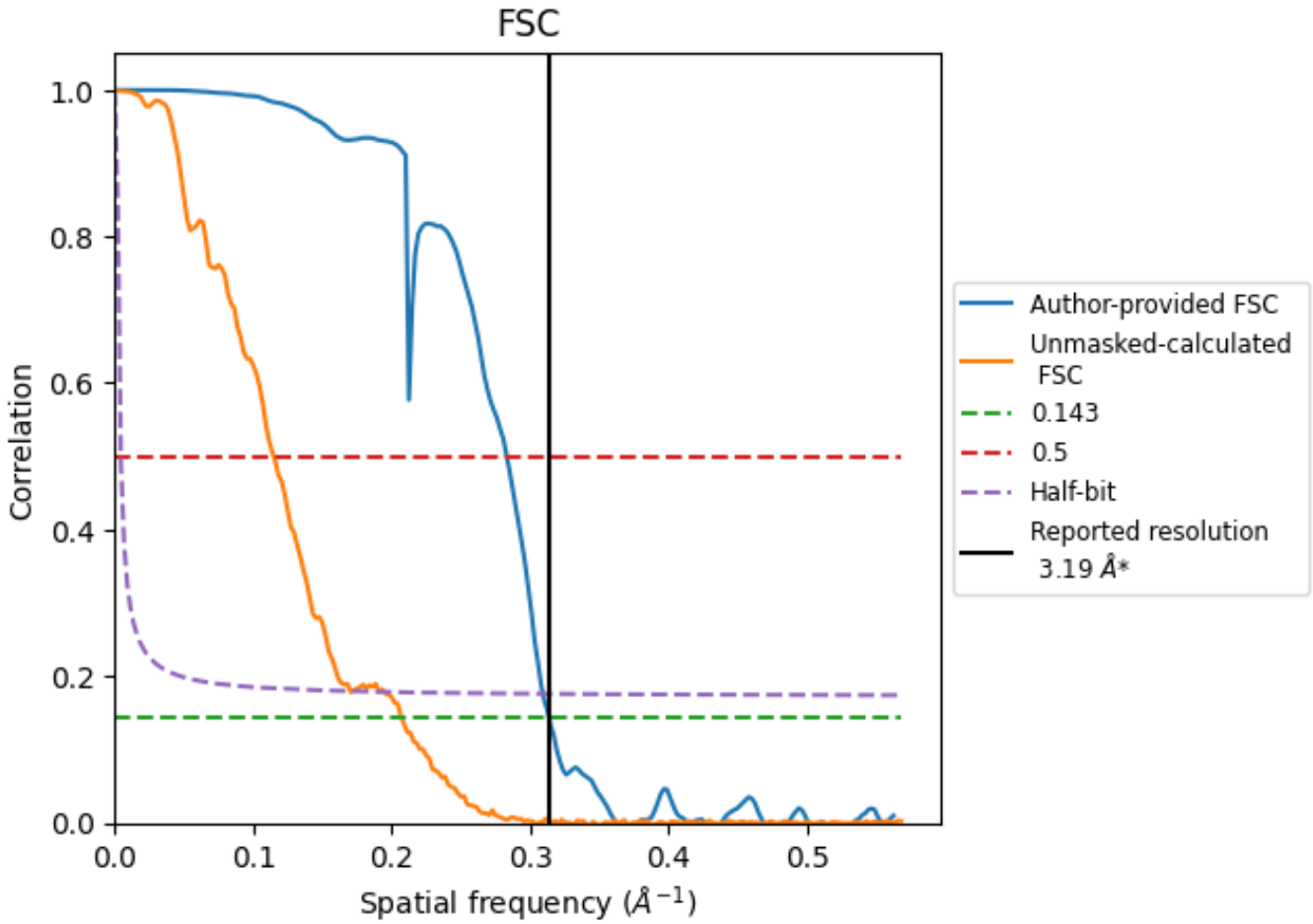


*Reported resolution corresponds to spatial frequency of 0.313 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.313 Å^{-1}

8.2 Resolution estimates (i)

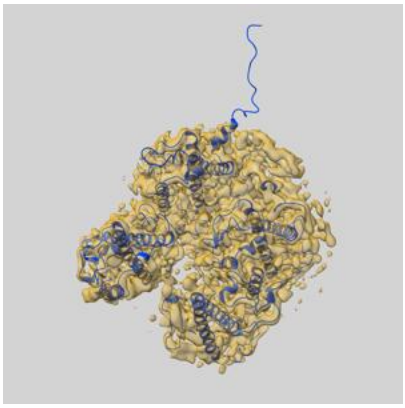
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.19	-	-
Author-provided FSC curve	3.19	3.53	3.23
Unmasked-calculated*	4.83	8.70	5.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.83 differs from the reported value 3.19 by more than 10 %

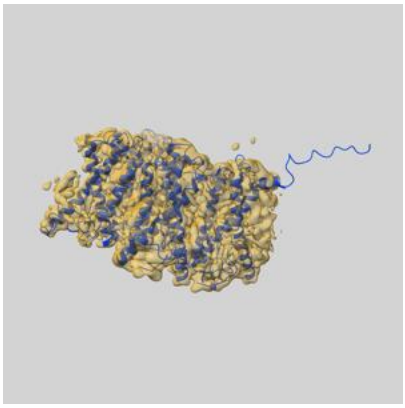
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35899 and PDB model 8J0D. Per-residue inclusion information can be found in section 3 on page 14.

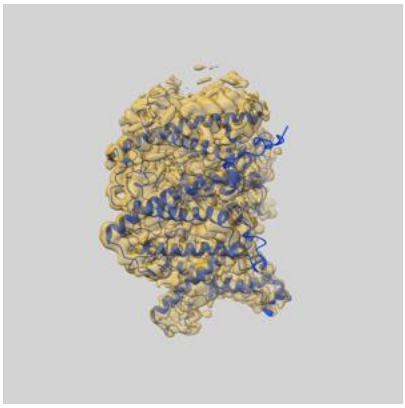
9.1 Map-model overlay



X



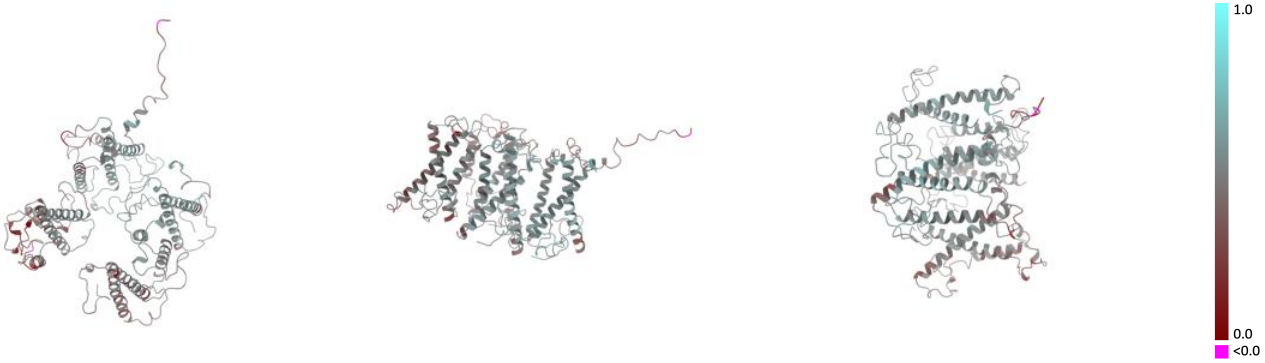
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

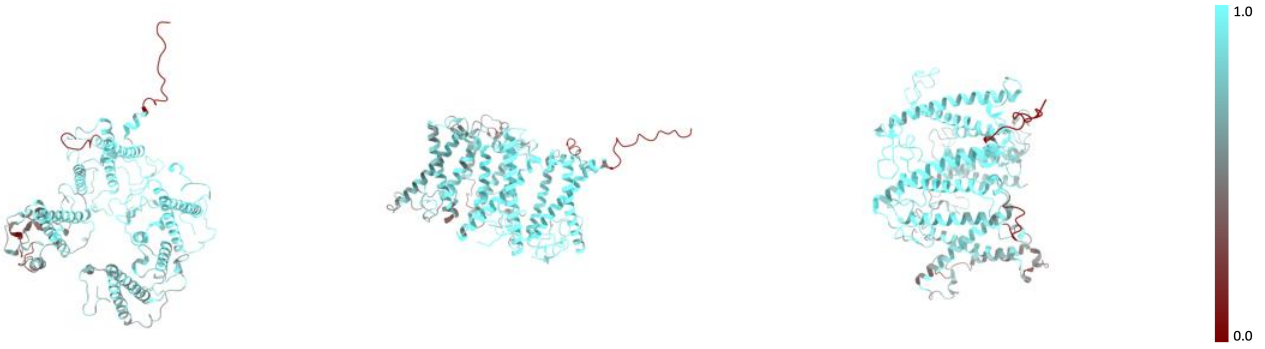
9.2 Q-score mapped to coordinate model



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.

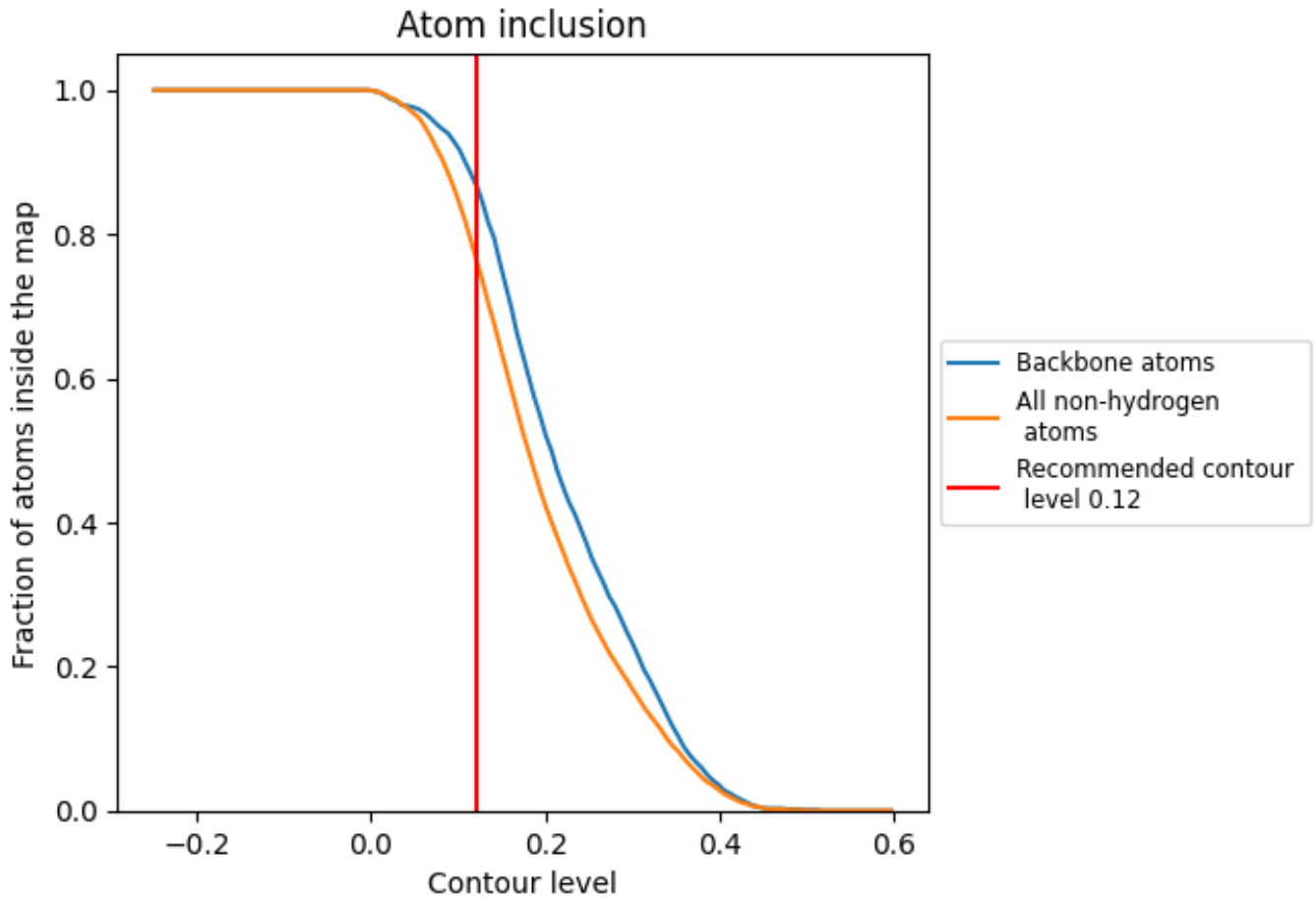
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.4980
3	0.8220	0.5230
4	0.9060	0.5420
5	0.6710	0.4700
6	0.6570	0.4470