Full wwPDB EM Validation Report ⓘ

Jul 25, 2024 – 10:26 AM JST

PDB ID	:	8WCL
EMDB ID	:	EMD-37442
Title	:	FCP pentamer in Chaetoceros gracilis
Authors	:	Feng, Y.; Li, Z.; Zhou, C.; Liu, C.; Shen, J.-R.; Wang, W.
Deposited on	:	2023-09-12
Resolution	:	2.65 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:

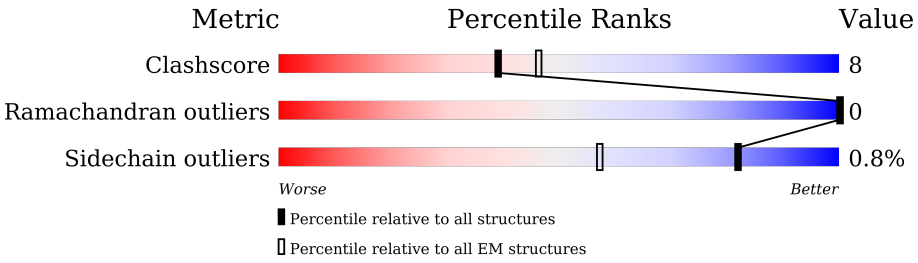
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	6	211	64% 14% 22%
2	5	207	67% 15% 18%
2	8	207	70% 12% 18%
3	9	195	63% 22% 15%
4	7	207	74% 12% 14%

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
6	CLA	5	306	X	-	-	-
6	CLA	5	307	X	-	-	-
6	CLA	5	309	X	-	-	-
6	CLA	5	312	X	-	-	-
6	CLA	5	314	X	-	-	-
6	CLA	5	315	X	-	-	-
6	CLA	6	305	X	-	-	-
6	CLA	6	306	X	-	-	-
6	CLA	6	308	X	-	-	-
6	CLA	6	311	X	-	-	-
6	CLA	6	313	X	-	-	-
6	CLA	6	314	X	-	-	-
6	CLA	7	308	X	-	-	-
6	CLA	7	309	X	-	-	-
6	CLA	7	311	X	-	-	-
6	CLA	7	314	X	-	-	-
6	CLA	7	316	X	-	-	-
6	CLA	8	307	X	-	-	-
6	CLA	8	309	X	-	-	-
6	CLA	8	312	X	-	-	-
6	CLA	8	314	X	-	-	-
6	CLA	8	315	X	-	-	-
6	CLA	9	308	X	-	-	-
6	CLA	9	309	X	-	-	-
6	CLA	9	311	X	-	-	-
6	CLA	9	312	X	-	-	-
6	CLA	9	313	X	-	-	-
6	CLA	9	314	X	-	-	-
6	CLA	9	316	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10662 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a/c-binding protein Lhcf6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	6	165	Total	C	N	O	S	0	0
			1281	821	216	238	6		

- Molecule 2 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	8	169	Total	C	N	O	S	0	0
			1300	829	220	244	7		
2	5	170	Total	C	N	O	S	0	0
			1306	832	221	246	7		

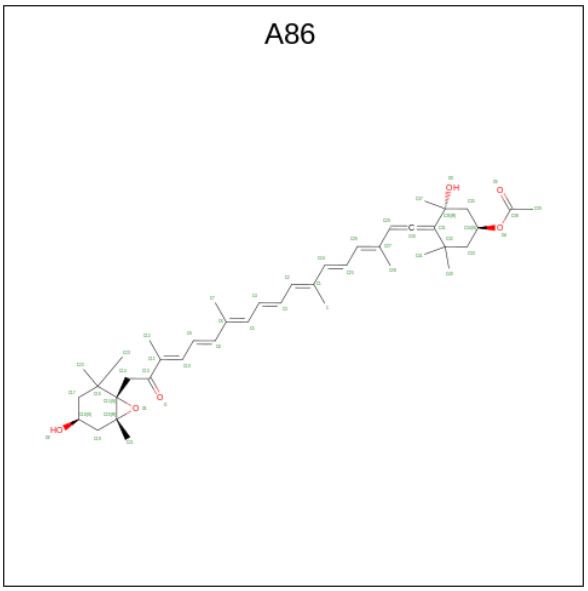
- Molecule 3 is a protein called Fucoxanthin-chlorophyll a/c protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	9	165	Total	C	N	O	S	1	0
			1290	842	210	233	5		

- Molecule 4 is a protein called Chlorophyll a/c-binding protein Lhcf7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	178	Total	C	N	O	S	0	0
			1371	876	229	260	6		

- Molecule 5 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
5	6	1	Total C O 48 42 6	0
5	6	1	Total C O 48 42 6	0
5	6	1	Total C O 48 42 6	0
5	6	1	Total C O 48 42 6	0
5	8	1	Total C O 48 42 6	0
5	8	1	Total C O 48 42 6	0
5	8	1	Total C O 48 42 6	0
5	8	1	Total C O 48 42 6	0
5	8	1	Total C O 48 42 6	0
5	8	1	Total C O 48 42 6	0
5	9	1	Total C O 48 42 6	0
5	9	1	Total C O 48 42 6	0
5	9	1	Total C O 48 42 6	0
5	9	1	Total C O 48 42 6	0

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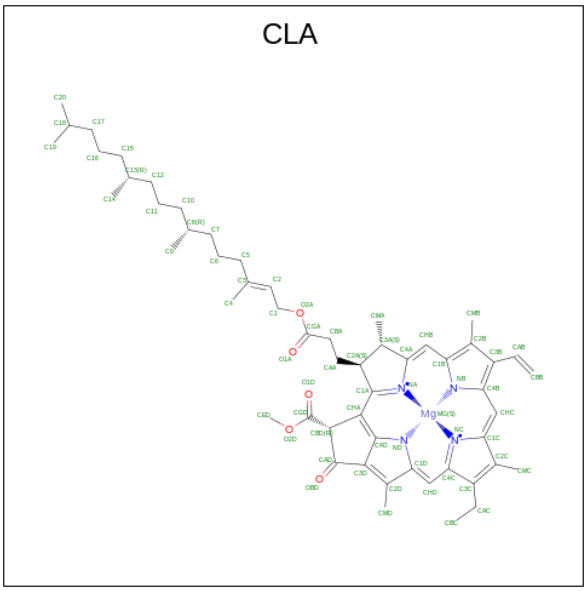
Mol	Chain	Residues	Atoms	AltConf
5	9	1	Total C O 48 42 6	0
5	9	1	Total C O 48 42 6	0
5	9	1	Total C O 48 42 6	0
5	5	1	Total C O 48 42 6	0
5	5	1	Total C O 48 42 6	0
5	5	1	Total C O 48 42 6	0
5	5	1	Total C O 48 42 6	0
5	5	1	Total C O 48 42 6	0
5	5	1	Total C O 48 42 6	0
5	7	1	Total C O 48 42 6	0
5	7	1	Total C O 48 42 6	0
5	7	1	Total C O 48 42 6	0
5	7	1	Total C O 48 42 6	0
5	7	1	Total C O 48 42 6	0
5	7	1	Total C O 48 42 6	0

- Molecule 6 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
6	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
6	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
6	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
6	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
6	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
6	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
6	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
6	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
6	8	1	Total 47	C 37	Mg 1	N 4	O 5	0
6	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
6	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
6	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
6	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
6	9	1	Total 65	C 55	Mg 1	N 4	O 5	0

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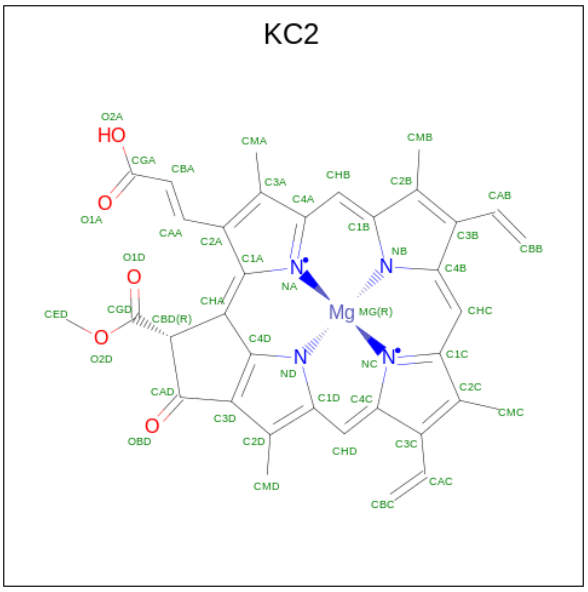
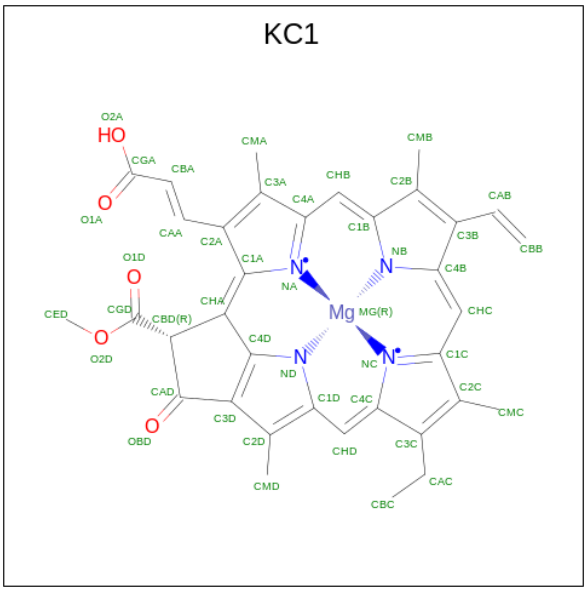
Mol	Chain	Residues	Atoms					AltConf
6	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
6	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
6	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
6	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
6	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
6	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
6	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
6	5	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
6	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
6	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
6	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
6	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
6	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
6	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
6	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 7 is Chlorophyll c2 (three-letter code: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



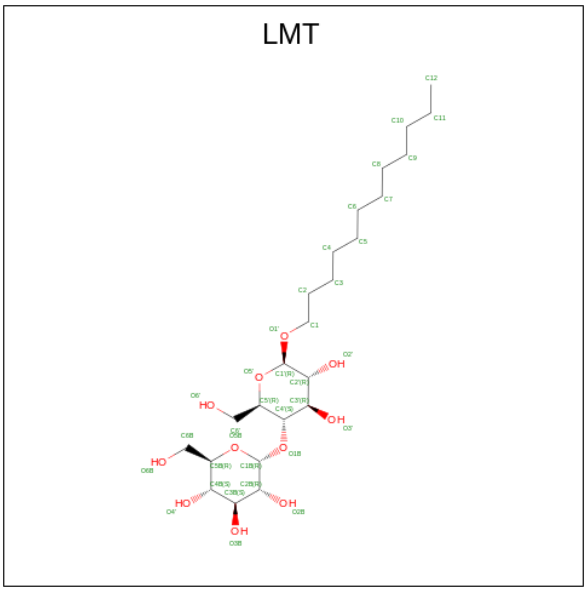
Mol	Chain	Residues	Atoms					AltConf
7	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
7	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
7	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
7	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
7	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
7	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
7	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
7	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
7	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 8 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



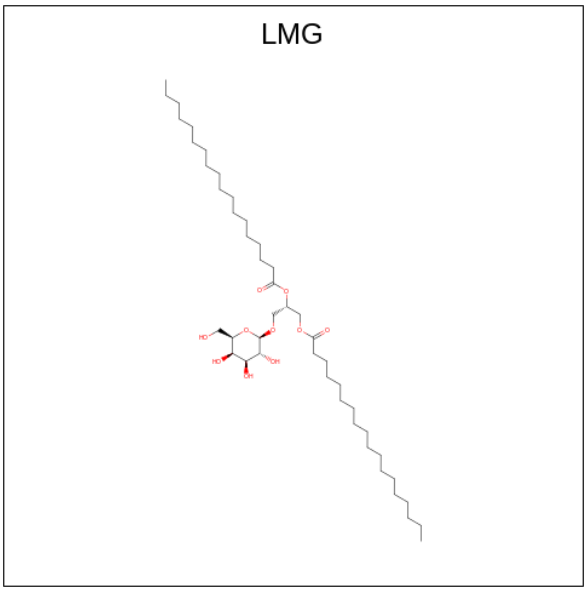
Mol	Chain	Residues	Atoms					AltConf
8	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 9 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
9	8	1	Total 35	C 24	O 11	0
9	5	1	Total 31	C 20	O 11	0
9	5	1	Total 35	C 24	O 11	0
9	7	1	Total 31	C 20	O 11	0
9	7	1	Total 35	C 24	O 11	0

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



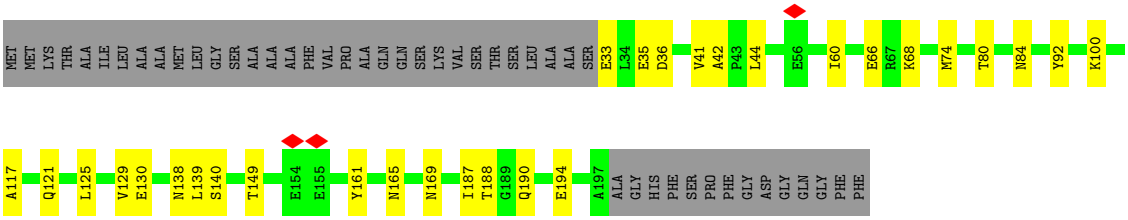
Mol	Chain	Residues	Atoms			AltConf
10	9	1	Total	C	O	0
			34	24	10	
10	7	1	Total	C	O	0
			47	37	10	

3 Residue-property plots (i)

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

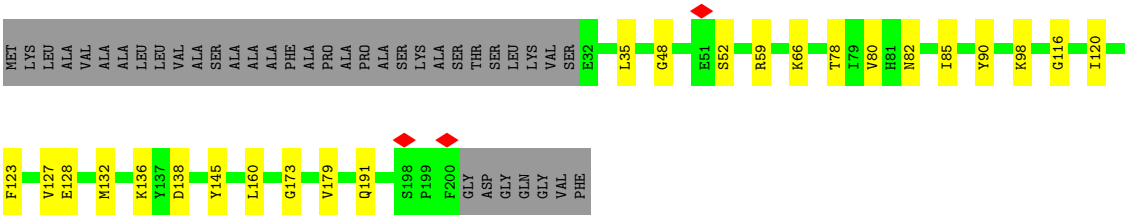
• Molecule 1: Chlorophyll a/c-binding protein Lhcf6

Chain 6:



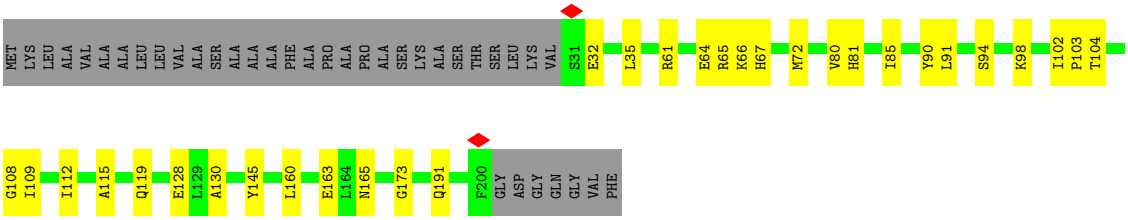
• Molecule 2: Chlorophyll a/b-binding protein

Chain 8:



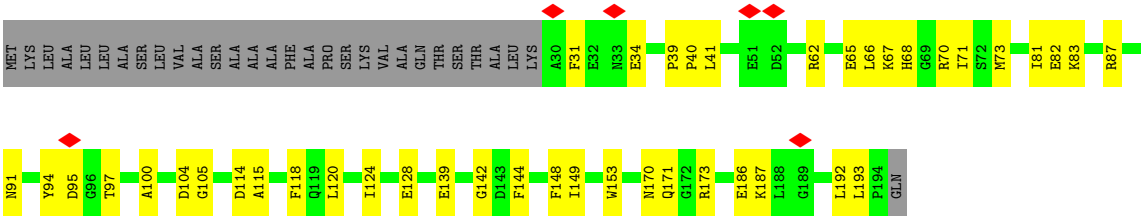
• Molecule 2: Chlorophyll a/b-binding protein

Chain 5:



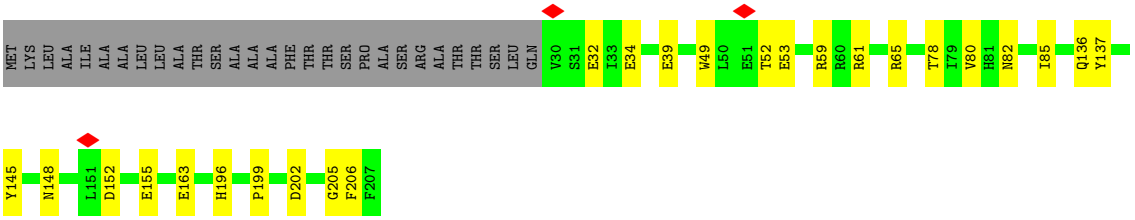
• Molecule 3: Fucoxanthin-chlorophyll a/c protein

Chain 9:



• Molecule 4: Chlorophyll a/c-binding protein Lhcf7

Chain 7:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	681510	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 (6k x 4k)	Depositor
Maximum map value	1.187	Depositor
Minimum map value	-0.526	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	6	0.28	0/1314	0.44	0/1781
2	5	0.28	0/1336	0.45	0/1812
2	8	0.28	0/1330	0.46	0/1804
3	9	0.28	0/1319	0.46	0/1776
4	7	0.28	0/1405	0.45	0/1905
All	All	0.28	0/6704	0.45	0/9078

There are no bond length outliers.

There are no bond angle outliers.

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	6	1281	0	1230	19	0
2	5	1306	0	1273	23	0
2	8	1300	0	1268	17	0
3	9	1290	0	1285	36	0
4	7	1371	0	1310	18	0
5	5	288	0	0	2	0
5	6	192	0	0	1	0
5	7	336	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	8	288	0	0	2	0
5	9	336	0	0	3	0
6	5	324	0	294	13	0
6	6	357	0	357	11	0
6	7	297	0	300	17	0
6	8	259	0	222	12	0
6	9	379	0	355	22	0
7	5	90	0	0	2	0
7	6	90	0	0	0	0
7	7	90	0	0	0	0
7	8	90	0	0	0	0
7	9	45	0	0	0	0
8	5	90	0	0	0	0
8	6	90	0	0	0	0
8	7	90	0	0	0	0
8	8	90	0	0	2	0
8	9	45	0	0	0	0
9	5	66	0	79	0	0
9	7	66	0	79	4	0
9	8	35	0	45	1	0
10	7	47	0	67	6	0
10	9	34	0	38	3	0
All	All	10662	0	8202	148	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 8.

All (148) 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)
2:5:61:ARG:NH1	2:5:64:GLU:OE1	2.24	0.70
2:8:35:LEU:HD21	2:8:160:LEU:HD13	1.73	0.69
4:7:32:GLU:OE2	4:7:65:ARG:NH2	2.28	0.67
1:6:169:ASN:ND2	6:6:305:CLA:O1D	2.28	0.66
3:9:87:ARG:NH2	3:9:104:ASP:OD1	2.24	0.64
2:8:59:ARG:NH1	8:8:311:KC1:O1A	2.31	0.64
2:5:91:LEU:HD22	2:5:102:ILE:HD11	1.81	0.62
1:6:68:LYS:NZ	1:6:130:GLU:OE2	2.25	0.62
2:8:145:TYR:HB2	6:8:312:CLA:HAA1	1.81	0.61
4:7:145:TYR:HB2	6:7:314:CLA:H3A	1.81	0.61
3:9:83:LYS:HD3	3:9:193:LEU:HD22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:161:TYR:O	1:6:165:ASN:ND2	2.33	0.60
3:9:39:PRO:HB2	6:9:308:CLA:HMB3	1.84	0.59
3:9:171:GLN:NE2	6:9:308:CLA:OBD	2.34	0.59
2:5:35:LEU:O	2:5:61:ARG:NH2	2.36	0.59
2:5:191:GLN:NE2	6:5:314:CLA:O1D	2.34	0.58
4:7:78:THR:O	4:7:82:ASN:ND2	2.36	0.58
2:8:66:LYS:NZ	2:8:128:GLU:OE2	2.28	0.58
3:9:91:ASN:O	5:9:302:A86:O3	2.21	0.58
3:9:62:ARG:NH2	6:9:309:CLA:O1D	2.37	0.58
10:9:317:LMG:H151	6:7:316:CLA:H12	1.86	0.57
2:8:78:THR:O	2:8:82:ASN:ND2	2.36	0.57
6:9:312:CLA:O1A	6:9:312:CLA:H2A	2.04	0.57
1:6:190:GLN:HB2	1:6:194:GLU:HG3	1.86	0.56
2:5:112:ILE:HD11	6:5:309:CLA:H3A	1.88	0.56
3:9:139:GLU:OE1	3:9:139:GLU:N	2.34	0.56
2:5:66:LYS:NZ	2:5:128:GLU:OE2	2.31	0.56
5:6:301:A86:O	6:6:305:CLA:HAC2	2.06	0.55
4:7:137:TYR:HH	9:7:319:LMT:H6'	1.55	0.55
6:7:316:CLA:H71	10:7:317:LMG:H132	1.88	0.55
1:6:92:TYR:HA	1:6:100:LYS:HA	1.89	0.54
2:5:115:ALA:O	2:5:119:GLN:HG3	2.08	0.54
3:9:67:LYS:NZ	3:9:128:GLU:OE1	2.39	0.54
3:9:192:LEU:O	5:9:305:A86:O2	2.26	0.54
1:6:41:VAL:HG21	1:6:169:ASN:HD21	1.72	0.54
5:5:301:A86:O	6:5:306:CLA:HAC2	2.08	0.54
4:7:206:PHE:N	10:7:317:LMG:O3	2.41	0.54
1:6:149:THR:OG1	9:7:318:LMT:O6B	2.26	0.53
3:9:153:TRP:CD1	6:9:314:CLA:HAA2	2.44	0.53
2:8:59:ARG:HD3	9:8:316:LMT:H3B	1.91	0.53
3:9:144:PHE:HB2	6:9:314:CLA:HMD1	1.90	0.52
1:6:80:THR:O	1:6:84:ASN:ND2	2.37	0.52
4:7:196:HIS:NE2	4:7:202:ASP:OD2	2.38	0.52
6:7:316:CLA:H51	10:7:317:LMG:H182	1.92	0.52
2:8:128:GLU:HG2	8:8:311:KC1:C1B	2.40	0.51
3:9:118:PHE:HD1	10:9:317:LMG:H141	1.75	0.51
2:8:123:PHE:O	2:8:127:VAL:HG23	2.10	0.51
6:9:313:CLA:H3A	10:7:317:LMG:H242	1.91	0.51
2:5:165:ASN:ND2	6:5:306:CLA:O1D	2.44	0.51
2:5:173:GLY:HA2	6:5:314:CLA:HBB1	1.92	0.51
1:6:33:GLU:N	1:6:35:GLU:OE2	2.44	0.50
2:5:32:GLU:OE2	2:5:65:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:81:ILE:HD11	6:9:311:CLA:CHD	2.41	0.50
4:7:61:ARG:NH2	6:7:309:CLA:O1D	2.45	0.50
4:7:52:THR:HG23	4:7:53:GLU:HG3	1.93	0.50
3:9:81:ILE:HD11	6:9:311:CLA:HHD	1.94	0.49
2:8:90:TYR:HA	2:8:98:LYS:HA	1.95	0.49
2:5:72:MET:HE2	6:5:312:CLA:HHC	1.94	0.49
3:9:94:TYR:H	6:9:312:CLA:HBA1	1.77	0.48
3:9:115:ALA:HB3	6:9:312:CLA:HED2	1.95	0.48
4:7:152:ASP:HB3	4:7:155:GLU:HB3	1.95	0.48
2:5:80:VAL:HG13	2:5:85:ILE:HB	1.96	0.48
6:8:312:CLA:HBB1	6:8:312:CLA:HMB1	1.95	0.47
2:8:116:GLY:O	2:8:120:ILE:HG12	2.14	0.47
3:9:118:PHE:CZ	2:5:119:GLN:HG2	2.49	0.47
4:7:80:VAL:HG13	4:7:85:ILE:HB	1.96	0.47
4:7:148:ASN:HB3	9:7:318:LMT:H6'2	1.96	0.47
1:6:42:ALA:HB1	6:6:305:CLA:HMB3	1.97	0.46
1:6:138:ASN:OD1	1:6:140:SER:OG	2.24	0.46
6:7:309:CLA:H92	6:7:309:CLA:H61	1.74	0.46
6:6:311:CLA:H3A	6:6:311:CLA:HBA2	1.55	0.46
6:6:305:CLA:H162	6:6:305:CLA:H141	1.72	0.46
3:9:73:MET:SD	6:9:314:CLA:HMC3	2.55	0.46
2:8:191:GLN:NE2	6:8:314:CLA:O1D	2.49	0.46
2:8:179:VAL:HG12	6:8:314:CLA:HMD3	1.97	0.46
1:6:125:LEU:O	1:6:129:VAL:HG12	2.16	0.45
1:6:66:GLU:HB2	6:6:306:CLA:C1B	2.47	0.45
6:7:316:CLA:H71	10:7:317:LMG:H161	1.98	0.45
6:7:316:CLA:HBB1	6:7:316:CLA:HHC	1.99	0.45
5:8:304:A86:C24	6:8:312:CLA:HAB	2.47	0.45
3:9:114:ASP:OD2	10:9:317:LMG:O4	2.28	0.45
3:9:87:ARG:HG3	3:9:100:ALA:HA	1.99	0.45
3:9:170:ASN:ND2	6:9:308:CLA:O1D	2.30	0.45
5:5:304:A86:C24	6:5:312:CLA:HAB	2.47	0.45
4:7:205:GLY:HA3	10:7:317:LMG:HC4	1.99	0.45
2:5:145:TYR:HB2	6:5:312:CLA:H3A	1.99	0.45
4:7:199:PRO:HG3	6:7:316:CLA:HBD	1.99	0.45
3:9:39:PRO:N	3:9:40:PRO:HD2	2.32	0.44
6:6:311:CLA:H111	6:6:311:CLA:H91	1.70	0.44
6:6:311:CLA:H141	6:6:311:CLA:H161	1.76	0.44
6:5:306:CLA:H93	6:5:306:CLA:H111	1.76	0.44
3:9:68:HIS:CE1	6:9:313:CLA:HMD1	2.52	0.44
6:7:309:CLA:H143	6:7:309:CLA:H112	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:67:HIS:HE1	7:5:308:KC2:NA	2.14	0.44
5:7:304:A86:C25	6:7:309:CLA:HMC2	2.48	0.44
5:7:305:A86:C24	6:7:314:CLA:HAB	2.48	0.44
3:9:66:LEU:HD23	3:9:142:GLY:HA3	2.00	0.44
4:7:163:GLU:HB2	6:7:314:CLA:C1B	2.48	0.44
1:6:36:ASP:HB3	1:6:161:TYR:HE1	1.83	0.44
3:9:124:ILE:HG21	6:9:313:CLA:HMC3	2.00	0.44
3:9:187:LYS:HE3	4:7:206:PHE:CE1	2.53	0.44
2:5:81:HIS:HB3	2:5:104:THR:HG23	1.99	0.43
6:9:314:CLA:HBB1	6:9:314:CLA:HMB1	1.99	0.43
1:6:117:ALA:O	1:6:121:GLN:HG3	2.18	0.43
6:6:311:CLA:H101	6:6:311:CLA:H61	1.61	0.43
6:5:307:CLA:H93	6:5:307:CLA:H61	1.86	0.43
2:8:48:GLY:O	2:8:52:SER:OG	2.30	0.43
3:9:34:GLU:OE1	3:9:34:GLU:N	2.52	0.43
2:5:109:ILE:HD12	2:5:112:ILE:HD12	2.01	0.43
4:7:39:GLU:HB3	6:7:308:CLA:HMB3	2.01	0.43
3:9:65:GLU:OE2	3:9:173:ARG:NE	2.45	0.43
6:5:307:CLA:H162	6:5:307:CLA:H141	1.77	0.43
2:5:103:PRO:HG2	2:5:108:GLY:HA2	2.01	0.42
3:9:105:GLY:HA3	3:9:186:GLU:OE2	2.18	0.42
3:9:120:LEU:O	3:9:124:ILE:HG12	2.19	0.42
6:7:309:CLA:H62	6:7:309:CLA:H41	1.91	0.42
6:7:308:CLA:H93	6:7:308:CLA:H111	1.75	0.42
4:7:49:TRP:HA	4:7:52:THR:HG22	2.02	0.42
1:6:187:ILE:HG13	1:6:188:THR:HG23	2.00	0.42
4:7:59:ARG:NH1	9:7:319:LMT:H3'	2.34	0.42
6:9:311:CLA:H111	6:9:311:CLA:H91	1.67	0.42
6:8:307:CLA:H8	6:8:307:CLA:H52	1.56	0.42
2:8:136:LYS:HG2	2:8:138:ASP:OD1	2.20	0.41
3:9:70:ARG:HA	3:9:73:MET:HG2	2.02	0.41
5:9:303:A86:C25	6:9:309:CLA:HMC2	2.50	0.41
6:8:315:CLA:HBA1	6:8:315:CLA:H3A	1.86	0.41
3:9:39:PRO:HG2	6:9:308:CLA:HMA1	2.03	0.41
2:5:35:LEU:HD21	2:5:160:LEU:HB3	2.02	0.41
3:9:71:ILE:HD12	6:9:313:CLA:HMD3	2.01	0.41
6:9:314:CLA:HBA1	6:9:314:CLA:H3A	1.93	0.41
2:5:130:ALA:HB1	6:7:308:CLA:C2B	2.50	0.41
3:9:148:PHE:CD2	3:9:149:ILE:HG13	2.56	0.41
2:8:132:MET:HG3	6:5:306:CLA:H12	2.03	0.41
1:6:60:ILE:HG22	1:6:139:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:90:TYR:CZ	2:5:98:LYS:HE3	2.56	0.41
1:6:42:ALA:HB3	6:6:305:CLA:HMA1	2.02	0.41
2:8:80:VAL:HG13	2:8:85:ILE:HB	2.02	0.41
2:5:94:SER:OG	7:5:310:KC2:O1A	2.31	0.41
5:8:303:A86:C25	6:8:307:CLA:HMC2	2.51	0.40
6:8:307:CLA:H41	6:8:307:CLA:H61	1.82	0.40
2:5:163:GLU:HB2	6:5:312:CLA:C1B	2.51	0.40
3:9:82:GLU:O	3:9:87:ARG:NH1	2.50	0.40
2:8:173:GLY:HA2	6:8:314:CLA:HBB1	2.04	0.40
6:8:307:CLA:H43	6:8:307:CLA:HMB2	2.03	0.40
6:8:309:CLA:HBB1	6:8:309:CLA:HMB1	2.03	0.40
1:6:74:MET:HE2	6:6:311:CLA:HHC	2.02	0.40
3:9:95:ASP:OD1	3:9:97:THR:HG22	2.21	0.40
6:9:314:CLA:H92	6:9:314:CLA:H61	1.69	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	6	163/211 (77%)	158 (97%)	5 (3%)	0	100	100
2	5	168/207 (81%)	165 (98%)	3 (2%)	0	100	100
2	8	167/207 (81%)	165 (99%)	2 (1%)	0	100	100
3	9	164/195 (84%)	155 (94%)	9 (6%)	0	100	100
4	7	176/207 (85%)	174 (99%)	2 (1%)	0	100	100
All	All	838/1027 (82%)	817 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	6	128/159 (80%)	127 (99%)	1 (1%)	81 89
2	5	134/158 (85%)	134 (100%)	0	100 100
2	8	133/158 (84%)	133 (100%)	0	100 100
3	9	132/152 (87%)	129 (98%)	3 (2%)	50 68
4	7	139/159 (87%)	137 (99%)	2 (1%)	67 81
All	All	666/786 (85%)	660 (99%)	6 (1%)	82 87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	6	44	LEU
3	9	31	PHE
3	9	41[A]	LEU
3	9	41[B]	LEU
4	7	34	GLU
4	7	136	GLN

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

Mol	Chain	Res	Type
2	8	67	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

84 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	$\#\|Z\| > 2$
5	A86	9	305	-	44,50,50	1.24	4 (9%)	51,76,76	2.98	18 (35%)
6	CLA	6	313	-	46,54,73	1.73	6 (13%)	53,90,113	1.57	7 (13%)
8	KC1	8	313	2	48,53,53	1.57	7 (14%)	55,89,89	1.86	12 (21%)
5	A86	9	301	-	44,50,50	1.23	4 (9%)	51,76,76	3.97	18 (35%)
5	A86	5	303	-	44,50,50	1.23	4 (9%)	51,76,76	3.66	19 (37%)
6	CLA	6	311	1	65,73,73	1.46	6 (9%)	76,113,113	1.37	8 (10%)
6	CLA	7	309	4	65,73,73	1.45	6 (9%)	76,113,113	1.42	7 (9%)
6	CLA	5	306	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
8	KC1	6	310	1	48,53,53	1.54	7 (14%)	55,89,89	1.86	11 (20%)
7	KC2	6	309	1	48,53,53	1.88	10 (20%)	54,89,89	2.09	14 (25%)
6	CLA	9	314	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	9 (11%)
5	A86	7	305	-	44,50,50	1.23	4 (9%)	51,76,76	4.60	21 (41%)
5	A86	9	302	-	44,50,50	1.24	4 (9%)	51,76,76	10.45	20 (39%)
7	KC2	6	307	-	48,53,53	1.88	11 (22%)	54,89,89	2.15	14 (25%)
9	LMT	8	316	-	36,36,36	1.19	6 (16%)	47,47,47	0.98	2 (4%)
6	CLA	5	315	-	46,54,73	1.79	6 (13%)	53,90,113	1.51	6 (11%)
5	A86	6	301	-	44,50,50	1.21	3 (6%)	51,76,76	3.21	15 (29%)
5	A86	6	303	-	44,50,50	1.26	4 (9%)	51,76,76	4.47	20 (39%)
8	KC1	9	315	3	48,53,53	1.54	7 (14%)	55,89,89	1.81	11 (20%)
5	A86	5	301	-	44,50,50	1.23	4 (9%)	51,76,76	3.98	19 (37%)
5	A86	7	304	-	44,50,50	1.23	4 (9%)	51,76,76	3.21	16 (31%)
6	CLA	8	314	-	46,54,73	1.74	6 (13%)	53,90,113	1.53	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	A86	7	302	-	44,50,50	1.23	3 (6%)	51,76,76	4.43	15 (29%)
7	KC2	7	310	-	48,53,53	1.89	11 (22%)	54,89,89	2.13	13 (24%)
5	A86	6	302	-	44,50,50	1.22	3 (6%)	51,76,76	2.82	18 (35%)
5	A86	8	302	-	44,50,50	1.24	4 (9%)	51,76,76	2.77	14 (27%)
6	CLA	9	316	-	41,49,73	1.82	6 (14%)	47,84,113	1.71	7 (14%)
5	A86	7	301	-	44,50,50	1.23	4 (9%)	51,76,76	2.89	17 (33%)
5	A86	7	307	-	44,50,50	1.27	4 (9%)	51,76,76	4.07	20 (39%)
6	CLA	7	311	-	55,63,73	1.56	6 (10%)	64,101,113	1.50	9 (14%)
6	CLA	8	309	-	55,63,73	1.57	6 (10%)	64,101,113	1.53	9 (14%)
6	CLA	7	314	-	47,55,73	1.72	6 (12%)	54,91,113	1.61	7 (12%)
6	CLA	5	309	-	55,63,73	1.61	6 (10%)	64,101,113	1.45	9 (14%)
5	A86	8	303	-	44,50,50	1.19	3 (6%)	51,76,76	10.37	18 (35%)
6	CLA	8	312	2	47,55,73	1.70	6 (12%)	54,91,113	1.64	8 (14%)
5	A86	7	306	-	44,50,50	1.23	3 (6%)	51,76,76	4.53	20 (39%)
8	KC1	6	312	1	48,53,53	1.56	7 (14%)	55,89,89	1.86	11 (20%)
5	A86	5	318	-	44,50,50	1.27	3 (6%)	51,76,76	4.32	18 (35%)
8	KC1	7	315	4	48,53,53	1.56	7 (14%)	55,89,89	1.86	12 (21%)
5	A86	5	305	-	44,50,50	1.22	3 (6%)	51,76,76	4.92	19 (37%)
6	CLA	9	313	3	60,68,73	1.51	6 (10%)	70,107,113	1.43	6 (8%)
5	A86	5	304	-	44,50,50	1.21	3 (6%)	51,76,76	5.32	20 (39%)
7	KC2	8	308	-	48,53,53	1.89	10 (20%)	54,89,89	2.12	15 (27%)
5	A86	6	304	-	44,50,50	1.23	4 (9%)	51,76,76	3.17	18 (35%)
8	KC1	5	313	2	48,53,53	1.56	7 (14%)	55,89,89	1.88	12 (21%)
6	CLA	5	312	-	47,55,73	1.71	6 (12%)	54,91,113	1.62	8 (14%)
5	A86	8	306	-	44,50,50	1.35	4 (9%)	51,76,76	4.93	20 (39%)
6	CLA	6	306	-	60,68,73	1.51	6 (10%)	70,107,113	1.44	7 (10%)
7	KC2	8	310	-	48,53,53	1.88	10 (20%)	54,89,89	2.11	14 (25%)
6	CLA	9	308	-	42,50,73	1.80	6 (14%)	48,85,113	1.62	6 (12%)
5	A86	5	302	-	44,50,50	1.23	4 (9%)	51,76,76	3.26	17 (33%)
10	LMG	9	317	-	34,34,55	0.25	0	42,42,63	0.30	0
7	KC2	5	308	-	48,53,53	1.89	11 (22%)	54,89,89	2.14	13 (24%)
6	CLA	5	307	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	8 (10%)
6	CLA	8	307	2	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
7	KC2	5	310	-	48,53,53	1.89	10 (20%)	54,89,89	2.14	15 (27%)
8	KC1	7	313	4	48,53,53	1.53	7 (14%)	55,89,89	1.79	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	A86	9	304	-	44,50,50	1.20	3 (6%)	51,76,76	3.80	12 (23%)
7	KC2	7	312	-	48,53,53	1.89	10 (20%)	54,89,89	2.12	14 (25%)
6	CLA	6	314	-	65,73,73	1.45	6 (9%)	76,113,113	1.45	6 (7%)
7	KC2	9	310	-	48,53,53	1.89	11 (22%)	54,89,89	2.14	14 (25%)
9	LMT	5	316	-	32,32,36	1.24	5 (15%)	43,43,47	1.01	2 (4%)
6	CLA	8	315	-	46,54,73	1.78	5 (10%)	53,90,113	1.53	7 (13%)
8	KC1	8	311	2	48,53,53	1.54	7 (14%)	55,89,89	1.87	11 (20%)
6	CLA	9	311	-	65,73,73	1.45	7 (10%)	76,113,113	1.40	9 (11%)
9	LMT	7	318	-	32,32,36	1.26	6 (18%)	43,43,47	1.04	2 (4%)
9	LMT	5	317	-	36,36,36	1.18	5 (13%)	47,47,47	0.99	2 (4%)
5	A86	8	305	-	44,50,50	1.22	3 (6%)	51,76,76	4.60	20 (39%)
5	A86	9	306	-	44,50,50	1.22	3 (6%)	51,76,76	4.00	19 (37%)
10	LMG	7	317	-	47,47,55	0.22	0	55,55,63	0.43	1 (1%)
6	CLA	7	316	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
5	A86	8	301	-	44,50,50	1.23	4 (9%)	51,76,76	4.36	16 (31%)
5	A86	9	307	-	44,50,50	1.22	3 (6%)	51,76,76	5.17	21 (41%)
6	CLA	5	314	-	46,54,73	1.73	6 (13%)	53,90,113	1.52	6 (11%)
8	KC1	5	311	2	48,53,53	1.56	7 (14%)	55,89,89	1.91	12 (21%)
6	CLA	9	309	-	60,68,73	1.51	7 (11%)	70,107,113	1.43	8 (11%)
5	A86	7	303	-	44,50,50	1.23	3 (6%)	51,76,76	3.58	19 (37%)
6	CLA	6	305	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
9	LMT	7	319	-	36,36,36	1.20	6 (16%)	47,47,47	0.96	1 (2%)
5	A86	8	304	-	44,50,50	1.21	3 (6%)	51,76,76	5.22	19 (37%)
6	CLA	7	308	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	8 (10%)
6	CLA	6	308	-	55,63,73	1.57	7 (12%)	64,101,113	1.51	9 (14%)
5	A86	9	303	-	44,50,50	1.23	4 (9%)	51,76,76	3.23	17 (33%)
6	CLA	9	312	-	46,54,73	1.74	6 (13%)	53,90,113	1.59	6 (11%)

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
5	A86	9	305	-	-	9/34/90/90	0/3/3/3
6	CLA	6	313	-	1/1/11/20	8/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	KC1	8	313	2	-	8/15/71/71	-
5	A86	9	301	-	-	10/34/90/90	0/3/3/3
5	A86	5	303	-	-	10/34/90/90	0/3/3/3
6	CLA	6	311	1	1/1/15/20	17/37/115/115	-
6	CLA	7	309	4	1/1/15/20	13/37/115/115	-
6	CLA	5	306	-	1/1/15/20	13/37/115/115	-
8	KC1	6	310	1	-	4/15/71/71	-
7	KC2	6	309	1	-	8/15/71/71	-
6	CLA	9	314	-	1/1/15/20	14/37/115/115	-
5	A86	7	305	-	-	10/34/90/90	0/3/3/3
5	A86	9	302	-	-	7/34/90/90	0/3/3/3
7	KC2	6	307	-	-	9/15/71/71	-
9	LMT	8	316	-	-	1/21/61/61	0/2/2/2
6	CLA	5	315	-	1/1/11/20	6/15/93/115	-
5	A86	6	301	-	-	8/34/90/90	0/3/3/3
5	A86	6	303	-	-	9/34/90/90	0/3/3/3
8	KC1	9	315	3	-	5/15/71/71	-
5	A86	5	301	-	-	9/34/90/90	0/3/3/3
5	A86	7	304	-	-	8/34/90/90	0/3/3/3
6	CLA	8	314	-	1/1/11/20	6/15/93/115	-
5	A86	7	302	-	-	8/34/90/90	0/3/3/3
7	KC2	7	310	-	-	6/15/71/71	-
5	A86	6	302	-	-	9/34/90/90	0/3/3/3
6	CLA	9	316	-	1/1/10/20	2/8/86/115	-
5	A86	8	302	-	-	9/34/90/90	0/3/3/3
5	A86	7	301	-	-	7/34/90/90	0/3/3/3
5	A86	7	307	-	-	9/34/90/90	0/3/3/3
6	CLA	7	311	-	1/1/13/20	5/25/103/115	-
6	CLA	8	309	-	1/1/13/20	5/25/103/115	-
6	CLA	7	314	-	1/1/11/20	7/16/94/115	-
6	CLA	5	309	-	1/1/13/20	5/25/103/115	-
5	A86	8	303	-	-	12/34/90/90	0/3/3/3
6	CLA	8	312	2	1/1/11/20	7/16/94/115	-
5	A86	7	306	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	KC1	6	312	1	-	6/15/71/71	-
5	A86	5	318	-	-	12/34/90/90	0/3/3/3
8	KC1	7	315	4	-	5/15/71/71	-
5	A86	5	305	-	-	8/34/90/90	0/3/3/3
6	CLA	9	313	3	1/1/14/20	7/31/109/115	-
5	A86	5	304	-	-	8/34/90/90	0/3/3/3
7	KC2	8	308	-	-	8/15/71/71	-
5	A86	6	304	-	-	9/34/90/90	0/3/3/3
8	KC1	5	313	2	-	5/15/71/71	-
6	CLA	5	312	-	1/1/11/20	8/16/94/115	-
5	A86	8	306	-	-	13/34/90/90	0/3/3/3
6	CLA	6	306	-	1/1/14/20	6/31/109/115	-
7	KC2	8	310	-	-	6/15/71/71	-
6	CLA	9	308	-	1/1/10/20	4/10/88/115	-
5	A86	5	302	-	-	9/34/90/90	0/3/3/3
10	LMG	9	317	-	-	7/29/49/70	0/1/1/1
7	KC2	5	308	-	-	7/15/71/71	-
6	CLA	5	307	-	1/1/15/20	11/37/115/115	-
6	CLA	8	307	2	1/1/15/20	9/37/115/115	-
7	KC2	5	310	-	-	9/15/71/71	-
8	KC1	7	313	4	-	4/15/71/71	-
5	A86	9	304	-	-	10/34/90/90	0/3/3/3
7	KC2	7	312	-	-	7/15/71/71	-
6	CLA	6	314	-	1/1/15/20	13/37/115/115	-
7	KC2	9	310	-	-	11/15/71/71	-
9	LMT	5	316	-	-	6/17/57/61	0/2/2/2
6	CLA	8	315	-	1/1/11/20	6/15/93/115	-
8	KC1	8	311	2	-	8/15/71/71	-
6	CLA	9	311	-	1/1/15/20	6/37/115/115	-
9	LMT	7	318	-	-	8/17/57/61	0/2/2/2
9	LMT	5	317	-	-	6/21/61/61	0/2/2/2
5	A86	8	305	-	-	8/34/90/90	0/3/3/3
5	A86	9	306	-	-	10/34/90/90	0/3/3/3
10	LMG	7	317	-	-	6/42/62/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	7	316	-	1/1/15/20	12/37/115/115	-
5	A86	8	301	-	-	10/34/90/90	0/3/3/3
5	A86	9	307	-	-	8/34/90/90	0/3/3/3
6	CLA	5	314	-	1/1/11/20	8/15/93/115	-
8	KC1	5	311	2	-	4/15/71/71	-
6	CLA	9	309	-	1/1/14/20	13/31/109/115	-
5	A86	7	303	-	-	9/34/90/90	0/3/3/3
6	CLA	6	305	-	1/1/15/20	8/37/115/115	-
9	LMT	7	319	-	-	10/21/61/61	0/2/2/2
6	CLA	7	308	-	1/1/15/20	11/37/115/115	-
5	A86	8	304	-	-	9/34/90/90	0/3/3/3
6	CLA	6	308	-	1/1/13/20	5/25/103/115	-
5	A86	9	303	-	-	9/34/90/90	0/3/3/3
6	CLA	9	312	-	1/1/11/20	8/15/93/115	-

All (469) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	315	CLA	C4B-NB	7.63	1.42	1.35
6	8	315	CLA	C4B-NB	7.61	1.42	1.35
6	6	313	CLA	C4B-NB	7.38	1.41	1.35
6	7	316	CLA	C4B-NB	7.35	1.41	1.35
6	5	309	CLA	C4B-NB	7.30	1.41	1.35
6	8	314	CLA	C4B-NB	7.30	1.41	1.35
6	9	316	CLA	C4B-NB	7.29	1.41	1.35
6	9	312	CLA	C4B-NB	7.26	1.41	1.35
6	7	314	CLA	C4B-NB	7.25	1.41	1.35
6	9	308	CLA	C4B-NB	7.24	1.41	1.35
6	7	308	CLA	C4B-NB	7.21	1.41	1.35
6	5	314	CLA	C4B-NB	7.18	1.41	1.35
6	6	305	CLA	C4B-NB	7.14	1.41	1.35
6	5	306	CLA	C4B-NB	7.13	1.41	1.35
6	8	312	CLA	C4B-NB	7.11	1.41	1.35
6	9	314	CLA	C4B-NB	7.09	1.41	1.35
6	7	309	CLA	C4B-NB	7.09	1.41	1.35
6	6	311	CLA	C4B-NB	7.09	1.41	1.35
6	6	306	CLA	C4B-NB	7.08	1.41	1.35
6	8	309	CLA	C4B-NB	7.08	1.41	1.35
6	9	313	CLA	C4B-NB	7.08	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	314	CLA	C4B-NB	7.07	1.41	1.35
6	5	312	CLA	C4B-NB	7.07	1.41	1.35
6	8	307	CLA	C4B-NB	7.05	1.41	1.35
6	9	311	CLA	C4B-NB	7.05	1.41	1.35
6	9	309	CLA	C4B-NB	7.03	1.41	1.35
6	7	311	CLA	C4B-NB	7.02	1.41	1.35
6	6	308	CLA	C4B-NB	6.96	1.41	1.35
6	5	307	CLA	C4B-NB	6.95	1.41	1.35
8	7	315	KC1	C4D-CHA	-6.95	1.36	1.45
8	8	313	KC1	C4D-CHA	-6.94	1.36	1.45
8	6	312	KC1	C4D-CHA	-6.93	1.36	1.45
7	7	312	KC2	C4D-CHA	-6.92	1.36	1.45
8	5	313	KC1	C4D-CHA	-6.92	1.36	1.45
7	7	310	KC2	C4D-CHA	-6.89	1.36	1.45
7	8	308	KC2	C4D-CHA	-6.84	1.36	1.45
7	5	308	KC2	C4D-CHA	-6.83	1.36	1.45
7	9	310	KC2	C4D-CHA	-6.81	1.36	1.45
7	5	310	KC2	C4D-CHA	-6.81	1.36	1.45
8	9	315	KC1	C4D-CHA	-6.80	1.36	1.45
7	8	310	KC2	C4D-CHA	-6.79	1.36	1.45
7	6	309	KC2	C4D-CHA	-6.75	1.36	1.45
7	6	307	KC2	C4D-CHA	-6.70	1.36	1.45
8	8	311	KC1	C4D-CHA	-6.64	1.36	1.45
8	5	311	KC1	C4D-CHA	-6.60	1.36	1.45
8	6	310	KC1	C4D-CHA	-6.55	1.36	1.45
8	7	313	KC1	C4D-CHA	-6.46	1.37	1.45
7	8	308	KC2	CHD-C4C	5.51	1.49	1.35
7	5	310	KC2	CHD-C4C	5.42	1.48	1.35
7	9	310	KC2	CHD-C4C	5.41	1.48	1.35
7	6	307	KC2	CHD-C4C	5.41	1.48	1.35
7	6	309	KC2	CHD-C4C	5.41	1.48	1.35
7	7	310	KC2	CHD-C4C	5.39	1.48	1.35
7	5	308	KC2	CHD-C4C	5.39	1.48	1.35
7	8	310	KC2	CHD-C4C	5.39	1.48	1.35
7	7	312	KC2	CHD-C4C	5.36	1.48	1.35
8	5	311	KC1	MG-NB	-4.95	1.96	2.05
8	6	310	KC1	MG-NB	-4.82	1.96	2.05
8	7	313	KC1	MG-NB	-4.78	1.96	2.05
5	9	305	A86	O4-C38	4.77	1.46	1.35
5	8	305	A86	O4-C38	4.77	1.46	1.35
5	5	305	A86	O4-C38	4.77	1.46	1.35
8	5	313	KC1	MG-NB	-4.76	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	8	313	KC1	MG-NB	-4.75	1.96	2.05
5	7	306	A86	O4-C38	4.75	1.45	1.35
5	9	301	A86	O4-C38	4.75	1.45	1.35
5	6	301	A86	O4-C38	4.74	1.45	1.35
8	6	312	KC1	MG-NB	-4.74	1.96	2.05
5	6	303	A86	O4-C38	4.72	1.45	1.35
5	9	302	A86	O4-C38	4.71	1.45	1.35
8	7	315	KC1	MG-NB	-4.70	1.96	2.05
5	5	301	A86	O4-C38	4.70	1.45	1.35
5	8	301	A86	O4-C38	4.70	1.45	1.35
5	5	318	A86	O4-C38	4.69	1.45	1.35
8	8	311	KC1	MG-NB	-4.68	1.96	2.05
5	9	303	A86	O4-C38	4.68	1.45	1.35
5	5	303	A86	O4-C38	4.68	1.45	1.35
5	9	304	A86	O4-C38	4.67	1.45	1.35
5	7	307	A86	O4-C38	4.67	1.45	1.35
5	8	306	A86	O4-C38	4.67	1.45	1.35
8	9	315	KC1	MG-NB	-4.66	1.96	2.05
5	7	303	A86	O4-C38	4.65	1.45	1.35
5	9	306	A86	O4-C38	4.64	1.45	1.35
5	7	302	A86	O4-C38	4.64	1.45	1.35
5	7	301	A86	O4-C38	4.63	1.45	1.35
5	8	302	A86	O4-C38	4.63	1.45	1.35
5	9	307	A86	O4-C38	4.63	1.45	1.35
5	8	304	A86	O4-C38	4.63	1.45	1.35
5	6	304	A86	O4-C38	4.63	1.45	1.35
5	7	304	A86	O4-C38	4.63	1.45	1.35
5	6	302	A86	O4-C38	4.62	1.45	1.35
5	7	305	A86	O4-C38	4.61	1.45	1.35
5	8	303	A86	O4-C38	4.58	1.45	1.35
5	5	304	A86	O4-C38	4.57	1.45	1.35
5	5	302	A86	O4-C38	4.56	1.45	1.35
7	5	310	KC2	MG-NB	-4.22	1.97	2.05
7	7	310	KC2	MG-NB	-4.21	1.97	2.05
7	9	310	KC2	MG-NB	-4.19	1.97	2.05
7	5	308	KC2	MG-NB	-4.17	1.97	2.05
7	6	309	KC2	MG-NB	-4.15	1.97	2.05
7	8	310	KC2	MG-NB	-4.15	1.97	2.05
7	6	309	KC2	CHC-C1C	4.15	1.48	1.39
7	8	308	KC2	MG-NB	-4.14	1.97	2.05
7	6	307	KC2	MG-NB	-4.14	1.97	2.05
7	8	310	KC2	CHC-C1C	4.11	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	312	KC2	CHC-C1C	4.10	1.48	1.39
7	7	312	KC2	MG-NB	-4.09	1.97	2.05
7	9	310	KC2	CHC-C1C	4.09	1.48	1.39
7	7	312	KC2	CHC-C4B	4.06	1.46	1.38
7	8	308	KC2	CHC-C1C	4.05	1.48	1.39
7	5	308	KC2	CHC-C1C	4.04	1.48	1.39
7	6	309	KC2	CHC-C4B	4.03	1.46	1.38
7	6	307	KC2	CHC-C1C	4.03	1.48	1.39
7	7	310	KC2	CHC-C1C	4.02	1.48	1.39
7	5	310	KC2	CHC-C1C	4.01	1.48	1.39
7	8	310	KC2	CHC-C4B	3.97	1.46	1.38
7	8	308	KC2	CHC-C4B	3.96	1.46	1.38
7	9	310	KC2	CHC-C4B	3.94	1.46	1.38
7	5	308	KC2	CHC-C4B	3.94	1.46	1.38
7	6	307	KC2	CHC-C4B	3.94	1.46	1.38
7	5	310	KC2	CHC-C4B	3.92	1.46	1.38
7	7	310	KC2	CHC-C4B	3.87	1.45	1.38
6	5	315	CLA	C1D-ND	3.86	1.42	1.37
6	9	312	CLA	C1D-ND	3.85	1.42	1.37
6	6	305	CLA	C1D-ND	3.83	1.42	1.37
6	5	306	CLA	C1D-ND	3.80	1.42	1.37
6	8	315	CLA	C1D-ND	3.79	1.42	1.37
6	7	316	CLA	C1D-ND	3.79	1.42	1.37
5	8	306	A86	O1-C20	-3.73	1.40	1.46
5	5	318	A86	C30-C29	-3.72	1.25	1.32
5	7	307	A86	C30-C29	-3.71	1.25	1.32
6	5	314	CLA	C1D-ND	3.71	1.42	1.37
6	9	308	CLA	C1D-ND	3.70	1.42	1.37
6	5	312	CLA	C1D-ND	3.70	1.42	1.37
6	8	307	CLA	C1D-ND	3.70	1.42	1.37
6	9	316	CLA	C1D-ND	3.70	1.42	1.37
6	6	314	CLA	C1D-ND	3.69	1.42	1.37
6	7	308	CLA	C1D-ND	3.69	1.42	1.37
6	7	309	CLA	C1D-ND	3.68	1.42	1.37
5	7	306	A86	C30-C29	-3.68	1.25	1.32
6	6	308	CLA	C1D-ND	3.67	1.42	1.37
6	8	312	CLA	C1D-ND	3.67	1.42	1.37
6	7	314	CLA	C1D-ND	3.66	1.42	1.37
6	5	307	CLA	C1D-ND	3.66	1.42	1.37
6	6	313	CLA	C1D-ND	3.65	1.42	1.37
6	9	314	CLA	C1D-ND	3.65	1.42	1.37
6	8	314	CLA	C1D-ND	3.65	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	8	309	CLA	C1D-ND	3.64	1.42	1.37
5	9	302	A86	C30-C29	-3.63	1.25	1.32
5	8	305	A86	C30-C29	-3.62	1.25	1.32
6	9	309	CLA	C1D-ND	3.62	1.42	1.37
6	5	309	CLA	C1D-ND	3.62	1.42	1.37
6	9	311	CLA	C1D-ND	3.62	1.42	1.37
6	6	311	CLA	C1D-ND	3.61	1.42	1.37
6	7	311	CLA	C1D-ND	3.60	1.42	1.37
5	6	303	A86	C30-C29	-3.60	1.26	1.32
6	9	313	CLA	C1D-ND	3.60	1.42	1.37
5	7	301	A86	C30-C29	-3.59	1.26	1.32
5	7	304	A86	C30-C29	-3.59	1.26	1.32
5	5	305	A86	C30-C29	-3.59	1.26	1.32
5	8	306	A86	C30-C29	-3.58	1.26	1.32
5	7	302	A86	C30-C29	-3.57	1.26	1.32
5	5	302	A86	C30-C29	-3.56	1.26	1.32
5	6	304	A86	C30-C29	-3.56	1.26	1.32
5	9	301	A86	C30-C29	-3.54	1.26	1.32
6	6	306	CLA	C1D-ND	3.54	1.42	1.37
5	8	302	A86	C30-C29	-3.54	1.26	1.32
5	9	307	A86	C30-C29	-3.53	1.26	1.32
5	9	305	A86	C30-C29	-3.52	1.26	1.32
5	6	302	A86	C30-C29	-3.51	1.26	1.32
5	5	303	A86	C30-C29	-3.51	1.26	1.32
5	5	301	A86	C30-C29	-3.51	1.26	1.32
5	9	303	A86	C30-C29	-3.50	1.26	1.32
5	8	301	A86	C30-C29	-3.48	1.26	1.32
5	6	301	A86	C30-C29	-3.45	1.26	1.32
5	7	305	A86	C30-C29	-3.44	1.26	1.32
5	7	303	A86	C30-C29	-3.43	1.26	1.32
5	9	306	A86	C30-C29	-3.42	1.26	1.32
5	9	304	A86	C30-C29	-3.41	1.26	1.32
5	8	303	A86	C30-C29	-3.36	1.26	1.32
5	5	304	A86	C30-C29	-3.34	1.26	1.32
5	8	304	A86	C30-C29	-3.30	1.26	1.32
6	9	309	CLA	CHC-C1C	3.15	1.43	1.35
6	6	311	CLA	CHC-C1C	3.14	1.43	1.35
6	8	315	CLA	CHC-C1C	3.14	1.43	1.35
6	7	309	CLA	CHC-C1C	3.14	1.43	1.35
6	9	314	CLA	CHC-C1C	3.13	1.43	1.35
6	9	309	CLA	C4D-ND	-3.13	1.33	1.37
6	6	313	CLA	CHC-C1C	3.13	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	306	CLA	C4D-ND	-3.13	1.33	1.37
6	9	308	CLA	CHC-C1C	3.12	1.43	1.35
6	5	315	CLA	CHC-C1C	3.11	1.43	1.35
6	5	309	CLA	CHC-C1C	3.11	1.42	1.35
6	8	312	CLA	CHC-C1C	3.11	1.42	1.35
6	8	307	CLA	CHC-C1C	3.10	1.42	1.35
6	6	308	CLA	C4D-ND	-3.10	1.33	1.37
6	9	314	CLA	C4D-ND	-3.09	1.33	1.37
6	6	306	CLA	CHC-C1C	3.09	1.42	1.35
8	5	313	KC1	C4B-NB	-3.08	1.34	1.37
6	9	311	CLA	C4D-ND	-3.07	1.33	1.37
6	6	311	CLA	C4D-ND	-3.07	1.33	1.37
6	7	308	CLA	C4D-ND	-3.07	1.33	1.37
6	5	307	CLA	C4D-ND	-3.07	1.33	1.37
6	8	309	CLA	C4D-ND	-3.07	1.33	1.37
6	8	307	CLA	C4D-ND	-3.07	1.33	1.37
6	9	313	CLA	CHC-C1C	3.07	1.42	1.35
6	6	314	CLA	C4D-ND	-3.07	1.33	1.37
6	7	309	CLA	C4D-ND	-3.07	1.33	1.37
8	6	310	KC1	C4B-NB	-3.06	1.34	1.37
8	5	311	KC1	C4B-NB	-3.06	1.34	1.37
6	5	306	CLA	C4D-ND	-3.06	1.33	1.37
6	5	314	CLA	CHC-C1C	3.06	1.42	1.35
6	7	314	CLA	CHC-C1C	3.05	1.42	1.35
6	7	316	CLA	C4D-ND	-3.05	1.33	1.37
6	8	309	CLA	CHC-C1C	3.05	1.42	1.35
6	6	308	CLA	CHC-C1C	3.04	1.42	1.35
6	7	311	CLA	CHC-C1C	3.04	1.42	1.35
6	7	308	CLA	CHC-C1C	3.04	1.42	1.35
6	9	311	CLA	CHC-C1C	3.03	1.42	1.35
6	9	313	CLA	C4D-ND	-3.03	1.33	1.37
6	5	306	CLA	CHC-C1C	3.03	1.42	1.35
6	8	314	CLA	C4D-ND	-3.02	1.33	1.37
6	5	309	CLA	C4D-ND	-3.02	1.33	1.37
6	5	307	CLA	CHC-C1C	3.01	1.42	1.35
6	5	314	CLA	C4D-ND	-3.01	1.33	1.37
6	9	312	CLA	CHC-C1C	3.01	1.42	1.35
6	6	305	CLA	C4D-ND	-3.01	1.33	1.37
6	9	308	CLA	C4D-ND	-3.00	1.33	1.37
6	7	316	CLA	CHC-C1C	3.00	1.42	1.35
6	8	312	CLA	C4D-ND	-2.99	1.33	1.37
6	7	311	CLA	C4D-ND	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	314	CLA	CHC-C1C	2.99	1.42	1.35
6	9	316	CLA	CHC-C1C	2.98	1.42	1.35
8	8	313	KC1	C4B-NB	-2.98	1.34	1.37
6	5	312	CLA	CHC-C1C	2.97	1.42	1.35
6	6	305	CLA	CHC-C1C	2.97	1.42	1.35
6	8	314	CLA	CHC-C1C	2.96	1.42	1.35
8	7	313	KC1	C4B-NB	-2.96	1.34	1.37
6	9	316	CLA	C4D-ND	-2.95	1.33	1.37
8	7	315	KC1	C4B-NB	-2.95	1.34	1.37
6	7	314	CLA	C4D-ND	-2.94	1.33	1.37
6	5	315	CLA	C4D-ND	-2.94	1.33	1.37
6	5	312	CLA	C4D-ND	-2.93	1.33	1.37
8	8	311	KC1	C4B-NB	-2.93	1.34	1.37
6	9	312	CLA	C4D-ND	-2.92	1.33	1.37
6	6	313	CLA	C4D-ND	-2.92	1.33	1.37
6	8	315	CLA	C4D-ND	-2.92	1.33	1.37
8	8	311	KC1	CBA-CGA	-2.90	1.41	1.48
8	9	315	KC1	C4B-NB	-2.90	1.34	1.37
8	6	310	KC1	CBA-CGA	-2.89	1.41	1.48
8	7	313	KC1	CBA-CGA	-2.88	1.41	1.48
7	7	312	KC2	CBA-CGA	-2.87	1.41	1.48
8	6	312	KC1	CBA-CGA	-2.87	1.41	1.48
8	8	313	KC1	CBA-CGA	-2.87	1.41	1.48
8	5	311	KC1	CBA-CGA	-2.86	1.41	1.48
8	7	315	KC1	CBA-CGA	-2.86	1.41	1.48
7	8	310	KC2	CBA-CGA	-2.86	1.41	1.48
7	5	310	KC2	CBA-CGA	-2.86	1.41	1.48
8	6	312	KC1	C4B-NB	-2.86	1.34	1.37
7	9	310	KC2	CBA-CGA	-2.85	1.41	1.48
8	9	315	KC1	CBA-CGA	-2.84	1.41	1.48
8	5	313	KC1	CBA-CGA	-2.83	1.42	1.48
7	6	307	KC2	CBA-CGA	-2.83	1.42	1.48
7	5	308	KC2	CBA-CGA	-2.82	1.42	1.48
7	7	310	KC2	CBA-CGA	-2.82	1.42	1.48
7	6	309	KC2	CBA-CGA	-2.80	1.42	1.48
7	8	308	KC2	CBA-CGA	-2.79	1.42	1.48
9	7	318	LMT	O3'-C3'	-2.74	1.36	1.43
9	8	316	LMT	O3'-C3'	-2.71	1.36	1.43
9	5	316	LMT	O3'-C3'	-2.69	1.36	1.43
5	7	304	A86	O1-C20	-2.68	1.42	1.46
9	7	319	LMT	O3'-C3'	-2.67	1.36	1.43
9	5	317	LMT	O3'-C3'	-2.66	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	310	KC2	C4B-NB	-2.64	1.34	1.37
7	5	308	KC2	C4B-NB	-2.63	1.34	1.37
7	5	310	KC2	C4B-NB	-2.62	1.34	1.37
5	9	306	A86	O1-C20	-2.62	1.42	1.46
7	6	309	KC2	C4B-NB	-2.62	1.34	1.37
7	6	307	KC2	C4B-NB	-2.60	1.34	1.37
7	9	310	KC2	C4B-NB	-2.59	1.34	1.37
5	5	304	A86	O1-C20	-2.59	1.42	1.46
9	5	316	LMT	O2'-C2'	-2.58	1.36	1.43
5	9	301	A86	O1-C20	-2.56	1.42	1.46
5	8	304	A86	O1-C20	-2.56	1.42	1.46
7	7	312	KC2	C4B-NB	-2.56	1.34	1.37
7	8	308	KC2	C4B-NB	-2.55	1.34	1.37
8	5	311	KC1	C1B-NB	-2.55	1.34	1.37
7	8	310	KC2	C4B-NB	-2.53	1.34	1.37
8	8	313	KC1	C1B-NB	-2.53	1.34	1.37
5	7	306	A86	O1-C20	-2.53	1.42	1.46
8	6	312	KC1	C1B-NB	-2.53	1.34	1.37
5	9	305	A86	O1-C20	-2.53	1.42	1.46
5	7	307	A86	O1-C20	-2.53	1.42	1.46
9	7	318	LMT	O2B-C2B	-2.53	1.37	1.43
8	6	310	KC1	C1B-NB	-2.52	1.34	1.37
8	7	313	KC1	C1B-NB	-2.51	1.34	1.37
6	5	309	CLA	CMB-C2B	-2.50	1.46	1.51
6	6	314	CLA	CMB-C2B	-2.50	1.46	1.51
8	5	313	KC1	C1B-NB	-2.49	1.34	1.37
6	5	312	CLA	CMB-C2B	-2.49	1.46	1.51
5	5	318	A86	O1-C20	-2.49	1.42	1.46
5	7	302	A86	O1-C20	-2.49	1.42	1.46
8	7	315	KC1	C1B-NB	-2.49	1.34	1.37
6	5	315	CLA	CMB-C2B	-2.48	1.46	1.51
6	8	315	CLA	CMB-C2B	-2.48	1.46	1.51
6	6	306	CLA	CMB-C2B	-2.48	1.46	1.51
6	6	311	CLA	CMB-C2B	-2.48	1.46	1.51
6	9	312	CLA	CMB-C2B	-2.48	1.46	1.51
6	7	316	CLA	CMB-C2B	-2.47	1.46	1.51
6	8	312	CLA	CMB-C2B	-2.47	1.46	1.51
9	7	318	LMT	O2'-C2'	-2.47	1.37	1.43
6	9	311	CLA	CMB-C2B	-2.46	1.46	1.51
6	8	314	CLA	CMB-C2B	-2.46	1.46	1.51
5	9	302	A86	O1-C20	-2.45	1.42	1.46
6	5	314	CLA	CMB-C2B	-2.44	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	308	CLA	CMB-C2B	-2.44	1.46	1.51
8	8	311	KC1	C1B-NB	-2.44	1.34	1.37
5	7	305	A86	O1-C20	-2.43	1.42	1.46
6	9	308	CLA	CMB-C2B	-2.43	1.46	1.51
6	7	314	CLA	CMB-C2B	-2.43	1.46	1.51
9	7	318	LMT	O3B-C3B	-2.43	1.37	1.43
9	8	316	LMT	O2B-C2B	-2.43	1.37	1.43
6	8	307	CLA	CMB-C2B	-2.43	1.46	1.51
6	5	306	CLA	CMB-C2B	-2.42	1.46	1.51
6	9	316	CLA	CMB-C2B	-2.42	1.46	1.51
6	8	309	CLA	CMB-C2B	-2.41	1.46	1.51
6	5	307	CLA	CMB-C2B	-2.41	1.46	1.51
8	9	315	KC1	C1B-NB	-2.41	1.34	1.37
6	9	309	CLA	CMB-C2B	-2.41	1.46	1.51
6	9	314	CLA	CMB-C2B	-2.41	1.46	1.51
6	7	309	CLA	CMB-C2B	-2.41	1.46	1.51
5	8	305	A86	O1-C20	-2.41	1.42	1.46
5	7	301	A86	O1-C20	-2.41	1.42	1.46
6	6	305	CLA	CMB-C2B	-2.40	1.46	1.51
5	6	301	A86	O1-C20	-2.40	1.42	1.46
5	8	302	A86	O1-C20	-2.39	1.42	1.46
6	7	308	CLA	CMB-C2B	-2.39	1.46	1.51
6	7	311	CLA	CMB-C2B	-2.39	1.46	1.51
9	7	319	LMT	O2'-C2'	-2.39	1.37	1.43
9	7	319	LMT	O2B-C2B	-2.39	1.37	1.43
6	9	313	CLA	CMB-C2B	-2.38	1.46	1.51
9	5	317	LMT	O3B-C3B	-2.37	1.37	1.43
7	9	310	KC2	C4A-C3A	-2.37	1.40	1.44
9	5	316	LMT	O3B-C3B	-2.37	1.37	1.43
5	6	304	A86	O1-C20	-2.37	1.42	1.46
9	8	316	LMT	O2'-C2'	-2.36	1.37	1.43
6	6	313	CLA	CMB-C2B	-2.36	1.46	1.51
9	7	319	LMT	O3B-C3B	-2.36	1.37	1.43
5	8	303	A86	O1-C20	-2.36	1.42	1.46
9	5	317	LMT	O2'-C2'	-2.36	1.37	1.43
9	8	316	LMT	O3B-C3B	-2.35	1.37	1.43
5	5	302	A86	O1-C20	-2.35	1.42	1.46
9	5	316	LMT	O2B-C2B	-2.34	1.37	1.43
7	6	307	KC2	C4A-C3A	-2.34	1.40	1.44
7	5	310	KC2	C4A-C3A	-2.34	1.40	1.44
5	7	303	A86	O1-C20	-2.34	1.42	1.46
9	5	317	LMT	O2B-C2B	-2.33	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	9	315	KC1	CHD-C4C	2.33	1.40	1.35
8	6	312	KC1	CHD-C4C	2.33	1.40	1.35
7	8	310	KC2	C4A-C3A	-2.31	1.40	1.44
7	5	308	KC2	C4A-C3A	-2.30	1.40	1.44
8	8	311	KC1	C4A-C3A	-2.30	1.40	1.44
8	8	313	KC1	CHD-C4C	2.30	1.40	1.35
5	6	302	A86	O1-C20	-2.30	1.42	1.46
7	7	310	KC2	C4A-C3A	-2.30	1.40	1.44
8	5	313	KC1	CHD-C4C	2.30	1.40	1.35
8	5	311	KC1	C4A-C3A	-2.29	1.40	1.44
8	6	310	KC1	C4A-C3A	-2.29	1.40	1.44
7	8	308	KC2	C4A-C3A	-2.28	1.40	1.44
5	5	301	A86	O1-C20	-2.28	1.43	1.46
7	7	312	KC2	C4A-C3A	-2.28	1.40	1.44
8	7	313	KC1	C4A-C3A	-2.27	1.40	1.44
8	7	315	KC1	CHD-C4C	2.27	1.40	1.35
8	7	313	KC1	CHD-C4C	2.27	1.40	1.35
5	9	303	A86	O1-C20	-2.26	1.43	1.46
7	6	309	KC2	C4A-C3A	-2.26	1.40	1.44
5	5	303	A86	O1-C20	-2.23	1.43	1.46
5	9	307	A86	O1-C20	-2.23	1.43	1.46
8	6	310	KC1	CHD-C4C	2.22	1.40	1.35
5	8	301	A86	O1-C20	-2.22	1.43	1.46
8	8	311	KC1	CHD-C4C	2.22	1.40	1.35
9	7	318	LMT	O4'-C4B	-2.21	1.37	1.43
7	5	308	KC2	C1C-C2C	-2.19	1.40	1.44
9	7	319	LMT	O4'-C4B	-2.19	1.37	1.43
7	8	308	KC2	C1C-C2C	-2.19	1.40	1.44
7	6	307	KC2	C1C-C2C	-2.18	1.40	1.44
8	5	311	KC1	CHD-C4C	2.17	1.40	1.35
6	8	314	CLA	CMD-C2D	-2.17	1.46	1.50
5	7	305	A86	C13-C11	-2.17	1.45	1.49
5	5	301	A86	C13-C11	-2.16	1.45	1.49
9	7	319	LMT	O1'-C1'	-2.16	1.36	1.40
5	5	305	A86	O1-C20	-2.16	1.43	1.46
7	7	310	KC2	C1C-C2C	-2.16	1.40	1.44
6	5	312	CLA	CMD-C2D	-2.15	1.46	1.50
7	5	310	KC2	C1C-C2C	-2.15	1.40	1.44
9	5	317	LMT	O4'-C4B	-2.15	1.37	1.43
8	9	315	KC1	C4A-C3A	-2.15	1.40	1.44
6	8	312	CLA	CMD-C2D	-2.14	1.46	1.50
6	5	314	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	311	CLA	CMD-C2D	-2.14	1.46	1.50
6	6	306	CLA	CMD-C2D	-2.14	1.46	1.50
5	6	303	A86	O1-C20	-2.13	1.43	1.46
9	5	316	LMT	O4'-C4B	-2.13	1.38	1.43
9	8	316	LMT	O4'-C4B	-2.12	1.38	1.43
6	7	314	CLA	CMD-C2D	-2.12	1.46	1.50
7	9	310	KC2	C1B-NB	-2.12	1.35	1.37
8	6	312	KC1	C4A-C3A	-2.12	1.40	1.44
7	9	310	KC2	C1D-CHD	2.12	1.46	1.41
5	9	304	A86	O1-C20	-2.12	1.43	1.46
7	6	309	KC2	C1D-CHD	2.11	1.46	1.41
7	6	309	KC2	C1C-C2C	-2.11	1.40	1.44
5	9	302	A86	C32-C31	-2.11	1.51	1.54
6	9	314	CLA	CMC-C2C	-2.11	1.46	1.50
7	5	310	KC2	C1D-CHD	2.10	1.46	1.41
6	7	311	CLA	CMD-C2D	-2.10	1.46	1.50
9	8	316	LMT	O1'-C1'	-2.10	1.36	1.40
6	9	313	CLA	CMD-C2D	-2.10	1.46	1.50
6	5	309	CLA	CMD-C2D	-2.09	1.46	1.50
7	7	310	KC2	C1D-CHD	2.09	1.46	1.41
6	9	309	CLA	CMD-C2D	-2.09	1.46	1.50
6	9	312	CLA	CMD-C2D	-2.08	1.46	1.50
5	5	302	A86	C32-C31	-2.08	1.51	1.54
6	5	306	CLA	CMD-C2D	-2.08	1.46	1.50
7	8	310	KC2	C1D-CHD	2.08	1.46	1.41
6	9	308	CLA	CMD-C2D	-2.08	1.46	1.50
5	7	304	A86	C13-C11	-2.08	1.45	1.49
7	7	312	KC2	C1D-CHD	2.08	1.46	1.41
6	5	307	CLA	CMD-C2D	-2.08	1.46	1.50
7	6	307	KC2	C1B-NB	-2.07	1.35	1.37
7	7	312	KC2	C1C-C2C	-2.07	1.40	1.44
5	9	301	A86	C13-C11	-2.07	1.45	1.49
7	6	307	KC2	C1D-CHD	2.07	1.46	1.41
7	8	310	KC2	C1C-C2C	-2.07	1.40	1.44
8	5	313	KC1	C4A-C3A	-2.06	1.40	1.44
6	8	309	CLA	CMD-C2D	-2.06	1.46	1.50
5	8	302	A86	C13-C11	-2.06	1.45	1.49
5	9	305	A86	C32-C31	-2.06	1.51	1.54
6	6	305	CLA	CMD-C2D	-2.06	1.46	1.50
6	7	309	CLA	CMD-C2D	-2.06	1.46	1.50
7	5	308	KC2	C1D-CHD	2.05	1.46	1.41
6	8	307	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	8	308	KC2	C1D-CHD	2.05	1.46	1.41
6	6	314	CLA	CMD-C2D	-2.05	1.46	1.50
8	7	315	KC1	C4A-C3A	-2.05	1.40	1.44
7	9	310	KC2	C1C-C2C	-2.05	1.40	1.44
7	5	308	KC2	C1B-NB	-2.05	1.35	1.37
6	7	316	CLA	CMD-C2D	-2.04	1.46	1.50
5	7	301	A86	C13-C11	-2.04	1.45	1.49
6	9	311	CLA	CMC-C2C	-2.04	1.46	1.50
6	8	307	CLA	CMC-C2C	-2.04	1.46	1.50
5	8	301	A86	C13-C11	-2.04	1.45	1.49
5	6	304	A86	C32-C31	-2.04	1.51	1.54
5	6	303	A86	C13-C11	-2.04	1.45	1.49
5	8	306	A86	C32-C31	-2.03	1.51	1.54
6	6	308	CLA	CMC-C2C	-2.03	1.46	1.50
6	7	308	CLA	CMD-C2D	-2.03	1.46	1.50
6	9	311	CLA	CMD-C2D	-2.03	1.46	1.50
8	8	313	KC1	C4A-C3A	-2.02	1.40	1.44
9	7	318	LMT	O1'-C1'	-2.02	1.36	1.40
5	5	303	A86	C13-C11	-2.02	1.45	1.49
6	9	309	CLA	CMC-C2C	-2.02	1.46	1.50
6	6	308	CLA	CMD-C2D	-2.02	1.46	1.50
6	5	315	CLA	CMD-C2D	-2.02	1.46	1.50
6	6	313	CLA	CMD-C2D	-2.01	1.46	1.50
6	9	314	CLA	CMD-C2D	-2.01	1.46	1.50
7	7	310	KC2	C1B-NB	-2.01	1.35	1.37
5	7	307	A86	C32-C31	-2.01	1.51	1.54
5	9	303	A86	C13-C11	-2.01	1.45	1.49
6	9	316	CLA	CMD-C2D	-2.01	1.46	1.50

All (998) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	9	302	A86	C23-C16-C22	-71.14	2.43	107.37
5	8	303	A86	C23-C16-C22	-70.91	2.77	107.37
5	5	304	A86	C34-O4-C38	31.66	176.90	117.90
5	8	304	A86	C34-O4-C38	30.59	174.90	117.90
5	9	307	A86	C34-O4-C38	28.79	171.55	117.90
5	7	305	A86	C34-O4-C38	25.90	166.17	117.90
5	7	302	A86	C34-O4-C38	23.38	161.47	117.90
5	8	306	A86	O1-C20-C19	21.32	129.40	113.38
5	6	303	A86	C34-O4-C38	21.28	157.56	117.90
5	9	306	A86	C34-O4-C38	21.08	157.18	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	8	301	A86	C34-O4-C38	20.13	155.41	117.90
5	5	318	A86	O4-C34-C33	19.97	157.32	107.59
5	8	305	A86	O4-C34-C33	19.72	156.72	107.59
5	9	301	A86	O4-C34-C33	19.27	155.59	107.59
5	9	304	A86	O1-C15-C14	-19.13	74.82	113.21
5	7	306	A86	O4-C34-C33	18.96	154.81	107.59
5	5	305	A86	O1-C15-C14	-18.94	75.20	113.21
5	5	301	A86	O1-C15-C14	-17.86	77.37	113.21
5	5	305	A86	O4-C34-C33	17.12	150.22	107.59
5	9	303	A86	O1-C15-C14	-16.94	79.21	113.21
5	5	305	A86	C34-O4-C38	16.94	149.47	117.90
5	9	307	A86	O1-C15-C14	-16.80	79.49	113.21
5	7	307	A86	O1-C15-C14	16.74	146.81	113.21
5	6	303	A86	O1-C15-C14	-16.53	80.03	113.21
5	7	306	A86	C34-O4-C38	16.39	148.44	117.90
5	5	303	A86	O1-C15-C14	-16.31	80.47	113.21
5	7	307	A86	O4-C34-C33	16.24	148.03	107.59
5	5	302	A86	O1-C15-C14	-16.02	81.06	113.21
5	8	305	A86	C34-O4-C38	15.86	147.46	117.90
5	8	301	A86	O1-C15-C14	-15.77	81.56	113.21
5	5	318	A86	O1-C15-C14	15.56	144.43	113.21
5	8	306	A86	O1-C20-C21	-15.55	96.42	115.06
5	7	303	A86	O1-C15-C14	-13.79	85.53	113.21
5	8	303	A86	C34-O4-C38	13.46	142.98	117.90
5	6	301	A86	C34-O4-C38	12.73	141.62	117.90
5	8	302	A86	O1-C15-C14	-12.59	87.95	113.21
5	7	302	A86	C23-C16-C22	-12.55	88.86	107.37
5	8	304	A86	C23-C16-C22	-12.41	89.06	107.37
5	5	301	A86	C34-O4-C38	12.23	140.68	117.90
5	9	302	A86	C34-O4-C38	12.22	140.67	117.90
5	7	304	A86	C23-C16-C22	-12.22	89.35	107.37
5	9	305	A86	C23-C16-C22	-12.15	89.45	107.37
5	5	304	A86	C23-C16-C22	-11.80	89.96	107.37
5	6	302	A86	O1-C15-C14	-11.59	89.95	113.21
5	9	304	A86	C34-O4-C38	11.20	138.77	117.90
5	6	304	A86	C34-O4-C38	11.11	138.59	117.90
5	7	303	A86	C34-O4-C38	11.00	138.40	117.90
5	8	306	A86	O4-C34-C33	10.62	134.05	107.59
5	9	301	A86	C23-C16-C22	-10.37	92.07	107.37
5	7	305	A86	C23-C16-C22	-10.20	92.32	107.37
5	6	301	A86	C23-C16-C22	-10.09	92.48	107.37
5	9	306	A86	C23-C16-C22	-9.99	92.63	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	7	306	A86	C23-C16-C22	-9.65	93.14	107.37
5	7	304	A86	C34-O4-C38	9.40	135.41	117.90
5	7	301	A86	O4-C34-C33	-9.21	84.64	107.59
5	8	306	A86	O1-C15-C14	9.20	131.67	113.21
5	7	301	A86	C23-C16-C22	-9.19	93.82	107.37
5	8	305	A86	C23-C16-C22	-9.12	93.92	107.37
5	5	301	A86	C23-C16-C22	-9.04	94.04	107.37
5	7	303	A86	O4-C34-C33	8.83	129.59	107.59
5	8	306	A86	C33-C32-C31	8.80	117.76	109.21
5	6	304	A86	C23-C16-C22	-8.70	94.54	107.37
5	5	303	A86	O4-C34-C33	8.50	128.76	107.59
5	5	303	A86	C34-O4-C38	8.49	133.71	117.90
5	5	318	A86	O4-C34-C35	-7.99	87.69	107.59
5	6	304	A86	O4-C34-C33	-7.97	87.75	107.59
5	8	305	A86	O1-C15-C14	-7.88	97.40	113.21
5	8	304	A86	O1-C15-C14	-7.57	98.03	113.21
5	5	304	A86	O1-C15-C14	-7.49	98.19	113.21
7	9	310	KC2	CHB-C1B-NB	7.48	131.33	124.45
5	7	304	A86	O1-C15-C14	-7.44	98.28	113.21
5	8	305	A86	O4-C34-C35	-7.29	89.44	107.59
7	5	308	KC2	CHB-C1B-NB	7.28	131.14	124.45
5	9	306	A86	O1-C15-C14	-7.26	98.63	113.21
7	7	312	KC2	CHB-C1B-NB	7.26	131.12	124.45
6	6	314	CLA	C4A-NA-C1A	7.25	109.97	106.71
5	8	301	A86	O1-C20-C19	-7.25	107.94	113.38
7	6	309	KC2	CHB-C1B-NB	7.24	131.10	124.45
7	8	308	KC2	CHB-C1B-NB	7.23	131.10	124.45
7	6	307	KC2	CHB-C1B-NB	7.22	131.09	124.45
7	8	310	KC2	CHB-C1B-NB	7.17	131.04	124.45
7	7	310	KC2	CHB-C1B-NB	7.16	131.03	124.45
7	5	310	KC2	CHB-C1B-NB	7.15	131.03	124.45
5	9	305	A86	O1-C15-C14	-7.13	98.91	113.21
8	5	311	KC1	CHC-C4B-NB	7.09	130.97	124.45
8	6	310	KC1	CHC-C4B-NB	7.08	130.96	124.45
5	9	301	A86	O4-C34-C35	-7.07	89.97	107.59
5	8	306	A86	C23-C16-C22	-7.04	96.98	107.37
6	5	312	CLA	C4A-NA-C1A	7.03	109.87	106.71
6	7	314	CLA	C4A-NA-C1A	6.98	109.84	106.71
5	9	302	A86	O4-C34-C33	-6.95	90.28	107.59
5	6	301	A86	C17-C16-C15	6.94	116.24	109.16
5	7	306	A86	O4-C34-C35	-6.94	90.31	107.59
5	8	303	A86	C17-C16-C15	6.89	116.19	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	9	312	CLA	C4A-NA-C1A	6.88	109.80	106.71
5	7	302	A86	O1-C15-C14	-6.85	99.46	113.21
6	7	308	CLA	C4A-NA-C1A	6.82	109.77	106.71
6	8	307	CLA	C4A-NA-C1A	6.81	109.77	106.71
6	7	309	CLA	C4A-NA-C1A	6.80	109.76	106.71
6	8	309	CLA	C4A-NA-C1A	6.79	109.76	106.71
6	5	307	CLA	C4A-NA-C1A	6.78	109.75	106.71
7	7	310	KC2	CHC-C4B-NB	6.72	130.62	124.45
5	7	305	A86	C17-C16-C15	6.70	116.00	109.16
5	9	302	A86	C17-C16-C15	6.70	116.00	109.16
6	9	313	CLA	C4A-NA-C1A	6.69	109.71	106.71
8	5	313	KC1	CHC-C4B-NB	6.67	130.58	124.45
6	8	312	CLA	C4A-NA-C1A	6.64	109.69	106.71
8	7	315	KC1	CHC-C4B-NB	6.64	130.55	124.45
6	7	311	CLA	C4A-NA-C1A	6.63	109.69	106.71
7	5	310	KC2	CHC-C4B-NB	6.63	130.54	124.45
6	9	308	CLA	C4A-NA-C1A	6.61	109.68	106.71
6	5	306	CLA	C4A-NA-C1A	6.60	109.67	106.71
5	9	304	A86	O4-C34-C33	-6.60	91.16	107.59
8	8	313	KC1	CHC-C4B-NB	6.59	130.51	124.45
6	6	306	CLA	C4A-NA-C1A	6.58	109.67	106.71
6	9	316	CLA	C4A-NA-C1A	6.58	109.66	106.71
8	8	311	KC1	CHC-C4B-NB	6.58	130.50	124.45
6	6	308	CLA	C4A-NA-C1A	6.54	109.64	106.71
6	6	313	CLA	C4A-NA-C1A	6.54	109.64	106.71
6	8	314	CLA	C4A-NA-C1A	6.54	109.64	106.71
6	6	305	CLA	C4A-NA-C1A	6.52	109.64	106.71
8	6	312	KC1	CHB-C1B-NB	6.51	130.44	124.45
5	6	304	A86	C17-C16-C15	6.49	115.79	109.16
7	5	308	KC2	CHC-C4B-NB	6.48	130.41	124.45
7	8	310	KC2	CHC-C4B-NB	6.47	130.40	124.45
6	9	311	CLA	C4A-NA-C1A	6.47	109.61	106.71
6	7	316	CLA	C4A-NA-C1A	6.47	109.61	106.71
5	7	306	A86	O1-C15-C14	-6.45	100.26	113.21
6	6	311	CLA	C4A-NA-C1A	6.44	109.60	106.71
6	9	309	CLA	C4A-NA-C1A	6.44	109.60	106.71
6	8	315	CLA	C4A-NA-C1A	6.43	109.60	106.71
7	6	307	KC2	CHC-C4B-NB	6.41	130.34	124.45
5	6	303	A86	C23-C16-C22	-6.40	97.93	107.37
6	9	314	CLA	C4A-NA-C1A	6.40	109.58	106.71
6	5	314	CLA	C4A-NA-C1A	6.40	109.58	106.71
5	7	302	A86	C17-C16-C15	6.40	115.69	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	5	315	CLA	C4A-NA-C1A	6.38	109.58	106.71
7	8	308	KC2	CHC-C4B-NB	6.38	130.32	124.45
6	5	309	CLA	C4A-NA-C1A	6.37	109.57	106.71
5	7	302	A86	C4-C5-C6	-6.34	118.26	127.31
7	7	312	KC2	CHC-C4B-NB	6.34	130.28	124.45
7	9	310	KC2	CHC-C4B-NB	6.32	130.26	124.45
5	5	318	A86	C23-C16-C22	-6.32	98.05	107.37
5	7	307	A86	C23-C16-C22	-6.28	98.10	107.37
8	5	313	KC1	CHB-C1B-NB	6.28	130.22	124.45
8	7	313	KC1	CHC-C4B-NB	6.27	130.22	124.45
5	8	301	A86	C23-C16-C22	-6.26	98.14	107.37
7	6	309	KC2	CHC-C4B-NB	6.24	130.19	124.45
8	6	312	KC1	CHC-C4B-NB	6.20	130.16	124.45
8	8	313	KC1	CHB-C1B-NB	6.19	130.15	124.45
5	7	301	A86	C17-C16-C15	6.17	115.46	109.16
8	5	311	KC1	CHB-C1B-NB	6.14	130.09	124.45
5	8	301	A86	C4-C5-C6	-6.13	118.56	127.31
8	9	315	KC1	CHC-C4B-NB	6.10	130.06	124.45
5	5	301	A86	C4-C5-C6	-6.10	118.61	127.31
8	7	315	KC1	CHB-C1B-NB	6.07	130.03	124.45
8	9	315	KC1	CHB-C1B-NB	6.07	130.03	124.45
5	6	301	A86	O1-C15-C14	-6.06	101.06	113.21
5	8	304	A86	C17-C16-C15	6.04	115.32	109.16
5	9	305	A86	C34-O4-C38	6.02	129.11	117.90
5	5	304	A86	C17-C16-C15	6.01	115.30	109.16
8	8	311	KC1	CHB-C1B-NB	6.00	129.97	124.45
5	9	305	A86	C17-C16-C15	5.98	115.27	109.16
5	5	305	A86	C3-C2-C1	-5.92	118.86	127.31
5	8	303	A86	C4-C5-C6	-5.91	118.88	127.31
5	5	302	A86	C34-O4-C38	5.89	128.88	117.90
5	9	301	A86	O1-C15-C14	-5.85	101.48	113.21
8	7	313	KC1	CHB-C1B-NB	5.81	129.79	124.45
5	9	301	A86	C17-C16-C15	5.80	115.08	109.16
5	9	302	A86	O1-C15-C14	-5.79	101.59	113.21
5	9	304	A86	O1-C20-C19	-5.75	109.06	113.38
5	5	305	A86	O4-C34-C35	-5.72	93.34	107.59
5	9	301	A86	C4-C5-C6	-5.72	119.14	127.31
5	9	302	A86	C25-C26-C27	-5.70	119.18	127.31
8	6	310	KC1	CHB-C1B-NB	5.70	129.69	124.45
5	8	305	A86	C17-C16-C15	5.69	114.97	109.16
5	8	305	A86	C3-C2-C1	-5.68	119.20	127.31
5	8	304	A86	C25-C26-C27	-5.66	119.23	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	7	301	A86	O1-C15-C14	-5.60	101.98	113.21
5	9	304	A86	C33-C32-C31	-5.57	103.80	109.21
5	6	302	A86	C34-O4-C38	5.56	128.26	117.90
5	6	303	A86	O1-C20-C19	-5.54	109.22	113.38
5	9	302	A86	C4-C5-C6	-5.52	119.44	127.31
5	7	304	A86	O4-C34-C33	-5.48	93.93	107.59
5	7	307	A86	O1-C20-C21	-5.46	108.51	115.06
5	7	306	A86	C3-C2-C1	-5.45	119.53	127.31
5	5	303	A86	C3-C2-C1	-5.40	119.60	127.31
5	5	305	A86	C23-C16-C22	-5.38	99.44	107.37
5	7	306	A86	C17-C16-C15	5.37	114.65	109.16
5	5	303	A86	O4-C34-C35	-5.37	94.21	107.59
5	8	303	A86	O1-C15-C14	-5.36	102.46	113.21
5	5	305	A86	C25-C26-C27	-5.35	119.67	127.31
5	8	301	A86	O1-C20-C21	-5.33	108.67	115.06
5	9	303	A86	C25-C26-C27	-5.29	119.76	127.31
5	6	303	A86	C25-C26-C27	-5.27	119.78	127.31
5	5	301	A86	C25-C26-C27	-5.26	119.80	127.31
5	9	306	A86	C3-C4-C5	-5.25	112.72	123.47
5	6	303	A86	C3-C2-C1	-5.24	119.83	127.31
5	8	302	A86	C4-C5-C6	-5.22	119.86	127.31
5	9	307	A86	C25-C26-C27	-5.17	119.93	127.31
5	5	304	A86	C25-C26-C27	-5.15	119.96	127.31
5	9	306	A86	O1-C20-C21	-5.14	108.90	115.06
5	8	306	A86	C4-C5-C6	-5.14	119.98	127.31
5	7	303	A86	C25-C26-C27	-5.13	119.99	127.31
5	5	318	A86	O1-C20-C21	-5.11	108.93	115.06
5	8	305	A86	C25-C26-C27	-5.11	120.02	127.31
5	9	303	A86	C3-C2-C1	-5.08	120.06	127.31
8	5	313	KC1	O2D-CGD-CBD	5.08	120.29	111.27
5	5	302	A86	C23-C16-C22	-5.06	99.90	107.37
5	7	303	A86	C4-C5-C6	-5.05	120.11	127.31
5	9	307	A86	C4-C5-C6	-5.04	120.11	127.31
5	7	304	A86	O1-C20-C21	-5.03	109.03	115.06
5	7	305	A86	C25-C26-C27	-5.02	120.15	127.31
5	5	318	A86	C4-C5-C6	-5.01	120.16	127.31
5	9	303	A86	O1-C20-C19	-5.01	109.62	113.38
7	6	307	KC2	O2D-CGD-CBD	5.00	120.15	111.27
5	7	303	A86	O4-C34-C35	-4.97	95.21	107.59
5	8	301	A86	C25-C26-C27	-4.97	120.22	127.31
8	7	315	KC1	O2D-CGD-CBD	4.96	120.09	111.27
8	9	315	KC1	O2D-CGD-CBD	4.96	120.08	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	301	A86	O1-C20-C19	-4.96	109.66	113.38
5	9	301	A86	C25-C26-C27	-4.96	120.23	127.31
5	6	302	A86	C4-C5-C6	-4.93	120.27	127.31
5	5	301	A86	O1-C20-C21	-4.92	109.16	115.06
7	5	308	KC2	O2D-CGD-CBD	4.92	120.01	111.27
8	6	312	KC1	O2D-CGD-CBD	4.90	119.97	111.27
5	8	306	A86	C34-O4-C38	4.88	126.98	117.90
5	6	304	A86	C4-C5-C6	-4.88	120.35	127.31
5	8	302	A86	C25-C26-C27	-4.88	120.35	127.31
5	7	303	A86	O4-C38-C39	4.87	120.05	111.09
5	6	302	A86	C25-C26-C27	-4.86	120.37	127.31
5	7	307	A86	C25-C26-C27	-4.86	120.38	127.31
5	5	305	A86	O1-C20-C19	-4.86	109.73	113.38
5	9	301	A86	C3-C2-C1	-4.85	120.39	127.31
5	9	304	A86	C25-C26-C27	-4.85	120.39	127.31
5	7	307	A86	C3-C2-C1	-4.84	120.40	127.31
5	7	302	A86	C25-C26-C27	-4.84	120.41	127.31
5	5	302	A86	O4-C38-C39	4.82	119.96	111.09
7	7	310	KC2	O2D-CGD-CBD	4.82	119.83	111.27
5	9	302	A86	C3-C2-C1	-4.81	120.44	127.31
5	7	305	A86	C3-C2-C1	-4.80	120.46	127.31
5	7	306	A86	C25-C26-C27	-4.79	120.48	127.31
5	7	305	A86	C33-C32-C31	-4.79	104.56	109.21
5	9	304	A86	C23-C16-C22	-4.79	100.31	107.37
5	8	302	A86	O4-C38-C39	4.78	119.89	111.09
5	8	306	A86	C25-C26-C27	-4.77	120.51	127.31
5	9	304	A86	O4-C38-C39	4.75	119.84	111.09
5	9	305	A86	C3-C2-C1	-4.75	120.53	127.31
5	7	303	A86	C23-C16-C22	-4.74	100.38	107.37
7	8	310	KC2	O2D-CGD-CBD	4.72	119.66	111.27
5	6	301	A86	C25-C26-C27	-4.72	120.57	127.31
5	5	303	A86	C23-C16-C22	-4.72	100.41	107.37
5	5	303	A86	O1-C20-C19	-4.70	109.85	113.38
5	5	302	A86	C4-C5-C6	-4.69	120.61	127.31
5	7	306	A86	O4-C38-C39	4.67	119.68	111.09
5	9	307	A86	C3-C2-C1	-4.66	120.66	127.31
5	7	305	A86	O4-C38-C39	4.66	119.66	111.09
5	5	305	A86	O1-C20-C21	-4.65	109.48	115.06
5	8	303	A86	O4-C38-C39	4.65	119.65	111.09
5	7	301	A86	C4-C5-C6	-4.65	120.68	127.31
5	8	305	A86	O4-C38-C39	4.64	119.62	111.09
5	6	302	A86	O4-C38-C39	4.64	119.62	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	9	302	A86	O4-C38-C39	4.63	119.60	111.09
5	6	303	A86	O1-C20-C21	-4.62	109.52	115.06
5	5	318	A86	O4-C38-C39	4.60	119.56	111.09
5	5	303	A86	C25-C26-C27	-4.59	120.76	127.31
5	9	307	A86	O1-C20-C19	-4.58	109.94	113.38
5	9	302	A86	O1-C20-C21	-4.58	109.57	115.06
5	7	306	A86	O1-C20-C21	-4.57	109.58	115.06
5	7	307	A86	O4-C38-C39	4.56	119.48	111.09
5	8	306	A86	O4-C38-C39	4.56	119.47	111.09
5	7	307	A86	O4-C34-C35	-4.55	96.26	107.59
5	5	303	A86	C4-C5-C6	-4.55	120.82	127.31
5	5	305	A86	O4-C38-C39	4.54	119.44	111.09
7	7	312	KC2	O2D-CGD-CBD	4.54	119.33	111.27
6	8	312	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
5	7	301	A86	C25-C26-C27	-4.53	120.84	127.31
5	7	304	A86	O4-C38-C39	4.53	119.43	111.09
5	6	304	A86	C3-C2-C1	-4.52	120.86	127.31
5	9	301	A86	O4-C38-C39	4.52	119.41	111.09
5	6	301	A86	C4-C5-C6	-4.52	120.86	127.31
5	7	303	A86	C3-C2-C1	-4.52	120.86	127.31
5	7	301	A86	O4-C38-C39	4.52	119.40	111.09
5	5	304	A86	O4-C38-C39	4.51	119.38	111.09
5	7	302	A86	O4-C38-C39	4.50	119.36	111.09
5	8	304	A86	O4-C38-C39	4.50	119.36	111.09
5	5	303	A86	O4-C38-C39	4.49	119.35	111.09
5	5	301	A86	O4-C38-C39	4.49	119.35	111.09
5	9	307	A86	O4-C34-C33	-4.49	96.42	107.59
5	5	302	A86	C25-C26-C27	-4.49	120.91	127.31
5	9	306	A86	O4-C38-C39	4.48	119.33	111.09
5	9	303	A86	O4-C38-C39	4.48	119.33	111.09
7	9	310	KC2	O2D-CGD-CBD	4.47	119.22	111.27
5	8	301	A86	O4-C38-C39	4.47	119.32	111.09
5	9	305	A86	O1-C20-C21	-4.46	109.72	115.06
5	9	305	A86	O4-C38-C39	4.45	119.28	111.09
5	8	302	A86	O1-C20-C21	-4.45	109.73	115.06
5	6	301	A86	O4-C38-C39	4.45	119.27	111.09
5	8	302	A86	O1-C20-C19	-4.44	110.04	113.38
5	5	304	A86	C33-C32-C31	-4.43	104.90	109.21
8	8	313	KC1	O2D-CGD-CBD	4.43	119.13	111.27
5	7	305	A86	O1-C20-C21	-4.42	109.76	115.06
5	8	306	A86	C35-C34-C33	4.42	117.58	109.88
5	9	306	A86	C25-C26-C27	-4.40	121.03	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	304	A86	O4-C34-C33	-4.40	96.63	107.59
5	9	303	A86	C23-C16-C22	-4.39	100.89	107.37
5	5	318	A86	C25-C26-C27	-4.39	121.04	127.31
5	5	301	A86	C3-C2-C1	-4.39	121.04	127.31
7	5	310	KC2	O2D-CGD-CBD	4.39	119.06	111.27
5	6	303	A86	O4-C38-C39	4.39	119.16	111.09
5	6	304	A86	O4-C38-C39	4.38	119.15	111.09
5	9	307	A86	O4-C38-C39	4.37	119.13	111.09
8	5	311	KC1	O2D-CGD-CBD	4.37	119.03	111.27
5	5	302	A86	C3-C2-C1	-4.36	121.09	127.31
5	8	304	A86	C33-C32-C31	-4.35	104.98	109.21
5	7	304	A86	C17-C16-C15	4.35	113.60	109.16
5	7	304	A86	C3-C2-C1	-4.34	121.12	127.31
5	9	306	A86	C17-C16-C15	4.32	113.57	109.16
6	9	314	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
5	6	302	A86	O1-C20-C21	-4.31	109.89	115.06
5	6	304	A86	C25-C26-C27	-4.31	121.16	127.31
8	6	310	KC1	O2D-CGD-CBD	4.29	118.90	111.27
7	6	309	KC2	O2D-CGD-CBD	4.27	118.86	111.27
5	9	301	A86	O1-C20-C21	-4.27	109.94	115.06
5	9	303	A86	C4-C5-C6	-4.26	121.23	127.31
5	6	302	A86	C3-C2-C1	-4.25	121.24	127.31
5	9	305	A86	C25-C26-C27	-4.25	121.25	127.31
5	7	304	A86	C4-C5-C6	-4.25	121.25	127.31
5	8	303	A86	C25-C26-C27	-4.24	121.25	127.31
5	5	304	A86	O1-C20-C21	-4.24	109.98	115.06
5	7	301	A86	C3-C2-C1	-4.24	121.26	127.31
5	6	301	A86	C3-C2-C1	-4.23	121.27	127.31
5	7	306	A86	C4-C5-C6	-4.23	121.28	127.31
5	8	306	A86	O4-C34-C35	-4.22	97.07	107.59
5	9	304	A86	O1-C20-C21	-4.22	110.00	115.06
5	6	302	A86	O1-C20-C19	-4.21	110.22	113.38
5	5	303	A86	C33-C32-C31	-4.19	105.14	109.21
5	8	303	A86	O4-C34-C33	4.18	118.01	107.59
5	8	304	A86	O1-C20-C21	-4.18	110.05	115.06
5	7	304	A86	C25-C26-C27	-4.16	121.37	127.31
5	7	305	A86	O4-C34-C33	4.16	117.95	107.59
5	8	305	A86	O1-C20-C21	-4.14	110.10	115.06
5	8	301	A86	C3-C2-C1	-4.14	121.41	127.31
5	5	305	A86	C4-C5-C6	-4.13	121.41	127.31
5	5	318	A86	C3-C2-C1	-4.13	121.41	127.31
5	6	304	A86	O1-C15-C14	-4.13	104.92	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	7	303	A86	O1-C20-C21	-4.13	110.11	115.06
5	5	303	A86	O1-C20-C21	-4.12	110.12	115.06
5	8	302	A86	C3-C2-C1	-4.12	121.43	127.31
5	6	302	A86	C23-C16-C22	-4.11	101.31	107.37
5	5	302	A86	O1-C20-C19	-4.11	110.30	113.38
5	8	304	A86	C3-C2-C1	-4.10	121.46	127.31
6	7	311	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
6	8	309	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
8	8	311	KC1	O2D-CGD-CBD	4.07	118.50	111.27
5	6	303	A86	C4-C5-C6	-4.07	121.50	127.31
8	7	313	KC1	O2D-CGD-CBD	4.07	118.50	111.27
5	7	303	A86	O1-C20-C19	-4.06	110.33	113.38
5	6	304	A86	O1-C20-C21	-4.06	110.19	115.06
5	9	307	A86	O1-C20-C21	-4.06	110.19	115.06
7	8	308	KC2	O2D-CGD-CBD	4.05	118.46	111.27
6	9	311	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
5	9	303	A86	O1-C20-C21	-4.04	110.22	115.06
5	5	302	A86	O1-C20-C21	-4.03	110.23	115.06
6	6	308	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
6	7	309	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
6	9	309	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
6	9	313	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
5	8	305	A86	C4-C5-C6	-4.01	121.59	127.31
7	5	308	KC2	C4B-CHC-C1C	-3.99	117.44	126.06
5	7	307	A86	C4-C5-C6	-3.99	121.61	127.31
7	7	310	KC2	C4B-CHC-C1C	-3.96	117.51	126.06
6	6	313	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
5	7	305	A86	C4-C5-C6	-3.94	121.68	127.31
5	6	303	A86	O4-C34-C33	-3.94	97.78	107.59
7	6	307	KC2	C4B-CHC-C1C	-3.93	117.58	126.06
5	9	307	A86	C23-C16-C22	-3.91	101.60	107.37
5	9	306	A86	C33-C32-C31	-3.91	105.41	109.21
7	5	310	KC2	C4B-CHC-C1C	-3.91	117.63	126.06
6	6	306	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
6	7	308	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
7	8	308	KC2	C4B-CHC-C1C	-3.88	117.69	126.06
7	8	310	KC2	C4B-CHC-C1C	-3.88	117.70	126.06
6	6	314	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
7	9	310	KC2	C4B-CHC-C1C	-3.87	117.72	126.06
7	7	312	KC2	C4B-CHC-C1C	-3.84	117.77	126.06
6	5	312	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
6	9	316	CLA	CMB-C2B-C1B	-3.83	122.58	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	8	306	A86	C3-C2-C1	-3.81	121.88	127.31
7	6	309	KC2	C4B-CHC-C1C	-3.80	117.85	126.06
5	5	304	A86	C3-C2-C1	-3.79	121.90	127.31
6	5	306	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
5	7	302	A86	C3-C2-C1	-3.77	121.93	127.31
6	8	312	CLA	CMB-C2B-C3B	3.76	131.71	124.68
6	6	311	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
6	9	308	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
6	9	314	CLA	CMB-C2B-C3B	3.71	131.62	124.68
6	5	307	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
6	7	314	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
6	8	307	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
5	8	304	A86	C4-C5-C6	-3.61	122.16	127.31
6	6	305	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
7	9	310	KC2	CHB-C1B-C2B	-3.58	117.98	125.48
5	9	302	A86	C36-C31-C32	3.57	123.24	119.70
5	8	302	A86	C23-C16-C22	-3.56	102.12	107.37
6	8	315	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
6	7	316	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
5	7	301	A86	O1-C20-C21	-3.52	110.84	115.06
7	7	310	KC2	CHC-C4B-C3B	-3.52	119.24	125.26
5	7	307	A86	C34-O4-C38	3.52	124.45	117.90
5	7	307	A86	O1-C20-C19	-3.52	110.74	113.38
5	9	305	A86	C4-C5-C6	-3.51	122.30	127.31
5	5	318	A86	O1-C20-C19	-3.50	110.75	113.38
7	6	307	KC2	CHB-C1B-C2B	-3.48	118.19	125.48
6	5	309	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
7	5	308	KC2	CHC-C4B-C3B	-3.47	119.33	125.26
6	7	311	CLA	CMB-C2B-C3B	3.47	131.17	124.68
7	5	308	KC2	CHB-C1B-C2B	-3.46	118.21	125.48
5	7	305	A86	O1-C15-C14	-3.46	106.26	113.21
6	8	314	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
6	8	309	CLA	CMB-C2B-C3B	3.44	131.11	124.68
6	6	308	CLA	CMB-C2B-C3B	3.44	131.11	124.68
7	5	310	KC2	CHC-C4B-C3B	-3.43	119.39	125.26
5	7	306	A86	C36-C31-C32	3.42	123.09	119.70
5	7	302	A86	C33-C32-C31	-3.42	105.89	109.21
7	7	312	KC2	CHB-C1B-C2B	-3.42	118.32	125.48
5	6	301	A86	C12-C11-C13	3.41	121.76	116.02
5	9	306	A86	O1-C20-C19	-3.41	110.82	113.38
6	5	314	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
6	9	309	CLA	CMB-C2B-C3B	3.40	131.04	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	7	309	CLA	CMB-C2B-C3B	3.40	131.04	124.68
8	6	310	KC1	CHC-C4B-C3B	-3.40	119.44	125.26
5	6	302	A86	C17-C16-C15	3.40	112.63	109.16
7	8	310	KC2	CHB-C1B-C2B	-3.40	118.36	125.48
5	7	304	A86	C33-C32-C31	-3.38	105.92	109.21
7	6	309	KC2	CHB-C1B-C2B	-3.38	118.39	125.48
7	8	308	KC2	CHB-C1B-C2B	-3.38	118.39	125.48
5	5	302	A86	C17-C16-C15	3.38	112.61	109.16
6	9	312	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
7	5	310	KC2	CHB-C1B-C2B	-3.38	118.40	125.48
6	5	315	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
5	7	307	A86	C36-C31-C32	3.37	123.04	119.70
6	9	313	CLA	CMB-C2B-C3B	3.36	130.97	124.68
6	9	311	CLA	CMB-C2B-C3B	3.35	130.94	124.68
5	8	303	A86	C33-C32-C31	-3.34	105.97	109.21
5	8	304	A86	C12-C11-C13	3.34	121.63	116.02
5	5	318	A86	C36-C31-C32	3.33	123.00	119.70
7	8	308	KC2	CHC-C4B-C3B	-3.33	119.57	125.26
8	5	311	KC1	CHC-C4B-C3B	-3.33	119.57	125.26
6	6	313	CLA	CMB-C2B-C3B	3.32	130.89	124.68
5	8	305	A86	C36-C31-C32	3.32	122.99	119.70
7	6	307	KC2	CHC-C4B-C3B	-3.32	119.58	125.26
7	7	310	KC2	CHB-C1B-C2B	-3.31	118.54	125.48
7	8	310	KC2	CHC-C4B-C3B	-3.30	119.61	125.26
6	7	308	CLA	CMB-C2B-C3B	3.30	130.84	124.68
5	7	302	A86	O1-C20-C21	-3.29	111.11	115.06
5	8	303	A86	O1-C20-C21	-3.29	111.11	115.06
5	7	302	A86	C4-C3-C2	-3.29	116.73	123.47
5	9	302	A86	C40-C32-C31	-3.28	107.53	110.47
5	8	302	A86	C17-C16-C15	3.28	112.51	109.16
5	7	301	A86	C12-C11-C13	3.28	121.53	116.02
5	6	301	A86	O1-C20-C21	-3.26	111.15	115.06
5	5	305	A86	C36-C31-C32	3.26	122.93	119.70
7	9	310	KC2	CHC-C4B-C3B	-3.25	119.70	125.26
7	7	312	KC2	CHC-C4B-C3B	-3.25	119.71	125.26
5	5	302	A86	O4-C34-C33	3.24	115.67	107.59
6	5	306	CLA	CMB-C2B-C3B	3.24	130.75	124.68
6	6	306	CLA	CMB-C2B-C3B	3.24	130.74	124.68
6	6	314	CLA	CMB-C2B-C3B	3.23	130.72	124.68
6	9	316	CLA	CMB-C2B-C3B	3.22	130.71	124.68
5	7	303	A86	C40-C32-C31	-3.22	107.59	110.47
6	5	312	CLA	CMB-C2B-C3B	3.20	130.67	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	5	313	KC1	CHC-C4B-C3B	-3.20	119.78	125.26
5	5	304	A86	C12-C11-C13	3.20	121.40	116.02
5	9	301	A86	C36-C31-C32	3.20	122.87	119.70
5	7	305	A86	O1-C20-C19	-3.19	110.99	113.38
5	8	303	A86	O4-C34-C35	-3.19	99.66	107.59
7	6	309	KC2	CHC-C4B-C3B	-3.18	119.82	125.26
5	9	305	A86	C12-C11-C13	3.17	121.35	116.02
6	6	311	CLA	CMB-C2B-C3B	3.17	130.61	124.68
8	7	315	KC1	CHC-C4B-C3B	-3.17	119.83	125.26
5	9	302	A86	O1-C20-C19	-3.16	111.00	113.38
8	8	313	KC1	CHC-C4B-C3B	-3.16	119.86	125.26
5	5	302	A86	C40-C32-C31	-3.15	107.66	110.47
6	7	314	CLA	CMB-C2B-C3B	3.13	130.54	124.68
5	5	304	A86	C4-C5-C6	-3.13	122.85	127.31
5	7	305	A86	O4-C34-C35	-3.13	99.81	107.59
5	5	301	A86	C9-C8-C6	-3.11	117.68	126.42
5	7	302	A86	C12-C11-C13	3.10	121.24	116.02
6	9	308	CLA	CMB-C2B-C3B	3.10	130.48	124.68
6	5	307	CLA	CMB-C2B-C3B	3.10	130.48	124.68
7	6	309	KC2	C3D-CAD-CBD	-3.10	103.52	107.61
5	5	304	A86	O1-C20-C19	-3.10	111.06	113.38
6	8	307	CLA	CMB-C2B-C3B	3.09	130.46	124.68
8	8	311	KC1	CHC-C4B-C3B	-3.09	119.98	125.26
6	6	311	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
5	7	303	A86	C17-C16-C15	3.05	112.28	109.16
5	8	306	A86	C36-C31-C32	3.04	122.71	119.70
6	6	306	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
5	8	303	A86	C3-C2-C1	-3.03	122.98	127.31
6	9	309	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
5	8	301	A86	C9-C8-C6	-3.03	117.91	126.42
6	5	307	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
6	6	305	CLA	CMB-C2B-C3B	3.03	130.34	124.68
5	8	304	A86	O1-C20-C19	-3.02	111.11	113.38
7	5	310	KC2	C1A-NA-C4A	-3.00	105.36	106.71
5	7	306	A86	O1-C20-C19	-2.99	111.13	113.38
7	6	307	KC2	CBD-CHA-C1A	2.98	134.45	128.88
7	5	308	KC2	CBD-CHA-C1A	2.96	134.39	128.88
5	7	306	A86	C33-C32-C31	-2.95	106.34	109.21
6	9	311	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
6	9	316	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
6	8	315	CLA	CMB-C2B-C3B	2.93	130.16	124.68
8	8	311	KC1	O2D-CGD-O1D	-2.93	118.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	9	315	KC1	CHC-C4B-C3B	-2.93	120.25	125.26
5	8	303	A86	O1-C20-C19	-2.92	111.19	113.38
5	5	301	A86	C12-C11-C13	2.92	120.93	116.02
5	8	302	A86	C40-C32-C31	-2.92	107.86	110.47
6	8	309	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
6	9	313	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
5	6	304	A86	O1-C20-C19	-2.92	111.19	113.38
5	6	302	A86	C12-C11-C13	2.91	120.92	116.02
5	8	301	A86	C9-C10-C11	-2.91	118.05	126.61
7	8	310	KC2	C3D-CAD-CBD	-2.91	103.78	107.61
8	8	311	KC1	O1D-CGD-CBD	-2.90	118.55	124.48
6	9	308	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
5	7	301	A86	C33-C32-C31	-2.88	106.41	109.21
6	8	307	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
6	6	313	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
8	8	311	KC1	CBD-CHA-C1A	2.88	134.25	128.88
7	5	310	KC2	C3D-CAD-CBD	-2.88	103.81	107.61
5	9	305	A86	O1-C20-C19	-2.88	111.22	113.38
8	7	313	KC1	CHC-C4B-C3B	-2.87	120.34	125.26
6	5	314	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
6	5	312	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
9	5	316	LMT	C3'-C4'-C5'	-2.87	104.35	110.93
5	5	305	A86	C33-C32-C31	-2.87	106.42	109.21
6	7	316	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
5	6	302	A86	C40-C32-C31	-2.86	107.91	110.47
6	8	315	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
6	5	309	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
7	8	308	KC2	CBD-CHA-C1A	2.85	134.20	128.88
6	5	315	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
6	7	309	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
6	9	312	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
6	9	316	CLA	CAA-C2A-C3A	-2.84	109.47	116.10
6	8	314	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
6	9	312	CLA	CMB-C2B-C3B	2.84	129.99	124.68
8	6	312	KC1	CHC-C4B-C3B	-2.84	120.41	125.26
5	8	305	A86	O1-C20-C19	-2.84	111.25	113.38
7	7	312	KC2	CBD-CHA-C1A	2.83	134.17	128.88
6	5	309	CLA	CMB-C2B-C3B	2.83	129.97	124.68
6	7	314	CLA	CHB-C4A-NA	2.83	128.42	124.51
6	6	305	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
7	9	310	KC2	CBD-CHA-C1A	2.81	134.12	128.88
6	8	312	CLA	O2D-CGD-O1D	-2.80	118.35	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7	318	LMT	C1'-O5'-C5'	-2.80	108.18	113.69
7	7	312	KC2	C1A-NA-C4A	-2.80	105.45	106.71
7	6	307	KC2	CHD-C4C-NC	2.80	128.45	124.20
8	5	311	KC1	O1D-CGD-CBD	-2.80	118.76	124.48
8	6	312	KC1	CHB-C1B-C2B	-2.80	119.61	125.48
9	8	316	LMT	C1'-O5'-C5'	-2.79	108.22	113.69
6	5	314	CLA	CMB-C2B-C3B	2.79	129.89	124.68
6	6	314	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
7	5	308	KC2	CHD-C4C-NC	2.78	128.43	124.20
6	5	306	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
6	7	308	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
5	7	307	A86	C41-C32-C31	-2.78	107.98	110.47
8	8	313	KC1	O1D-CGD-CBD	-2.78	118.80	124.48
8	7	313	KC1	O1D-CGD-CBD	-2.78	118.80	124.48
6	8	314	CLA	CMB-C2B-C3B	2.77	129.87	124.68
6	7	311	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
6	6	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
6	5	315	CLA	CMB-C2B-C3B	2.76	129.85	124.68
6	7	316	CLA	CMB-C2B-C3B	2.76	129.84	124.68
5	8	302	A86	C4-C3-C2	-2.76	117.82	123.47
6	7	314	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
7	7	310	KC2	CHD-C4C-NC	2.75	128.38	124.20
7	7	310	KC2	CBD-CHA-C1A	2.75	134.01	128.88
5	8	305	A86	C33-C32-C31	-2.75	106.54	109.21
5	5	302	A86	C12-C11-C13	2.74	120.63	116.02
8	7	313	KC1	O2D-CGD-O1D	-2.74	118.47	123.84
6	5	312	CLA	CHB-C4A-NA	2.74	128.31	124.51
7	8	308	KC2	C1A-NA-C4A	-2.74	105.47	106.71
7	7	312	KC2	C3D-CAD-CBD	-2.74	104.00	107.61
6	9	312	CLA	CHB-C4A-NA	2.74	128.30	124.51
7	6	309	KC2	O1D-CGD-CBD	-2.74	118.88	124.48
5	6	303	A86	C40-C32-C31	-2.74	108.02	110.47
5	8	304	A86	C10-C9-C8	-2.73	114.68	123.22
5	9	305	A86	C10-C9-C8	-2.73	114.68	123.22
5	9	301	A86	O1-C20-C19	-2.73	111.33	113.38
7	8	308	KC2	O1D-CGD-CBD	-2.72	118.91	124.48
7	7	312	KC2	CHD-C4C-NC	2.72	128.33	124.20
5	5	301	A86	C17-C16-C15	2.71	111.93	109.16
7	9	310	KC2	O1D-CGD-CBD	-2.71	118.94	124.48
7	8	310	KC2	C1A-NA-C4A	-2.70	105.49	106.71
9	5	317	LMT	C1'-O5'-C5'	-2.70	108.38	113.69
6	6	314	CLA	CHB-C4A-NA	2.69	128.23	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	9	310	KC2	CHD-C4C-NC	2.68	128.27	124.20
5	6	303	A86	C3-C4-C5	-2.68	117.98	123.47
8	6	312	KC1	C3D-CAD-CBD	-2.68	104.08	107.61
6	8	312	CLA	CHB-C4A-NA	2.68	128.21	124.51
5	8	303	A86	C4-C3-C2	-2.67	118.01	123.47
8	5	311	KC1	CBD-CHA-C1A	2.67	133.85	128.88
8	5	311	KC1	O2D-CGD-O1D	-2.66	118.63	123.84
5	5	305	A86	C12-C11-C13	2.66	120.48	116.02
5	8	301	A86	C4-C3-C2	-2.66	118.03	123.47
9	7	319	LMT	C1'-O5'-C5'	-2.65	108.48	113.69
7	9	310	KC2	C1A-NA-C4A	-2.65	105.51	106.71
6	9	314	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
5	5	304	A86	C10-C9-C8	-2.64	114.97	123.22
5	7	304	A86	O1-C20-C19	-2.64	111.40	113.38
8	6	310	KC1	C4B-CHC-C1C	-2.64	120.36	126.06
8	6	310	KC1	CBD-CHA-C1A	2.64	133.80	128.88
5	5	302	A86	O4-C34-C35	-2.64	101.03	107.59
5	5	305	A86	C25-C24-C1	-2.63	119.02	126.42
7	5	310	KC2	CBD-CHA-C1A	2.62	133.78	128.88
5	7	305	A86	C3-C4-C5	-2.62	118.10	123.47
7	8	310	KC2	CHD-C4C-NC	2.62	128.18	124.20
7	6	309	KC2	C1A-NA-C4A	-2.62	105.53	106.71
7	8	310	KC2	CBD-CHA-C1A	2.61	133.74	128.88
5	8	301	A86	C17-C16-C15	2.60	111.82	109.16
6	5	307	CLA	CHB-C4A-NA	2.60	128.11	124.51
8	6	310	KC1	O1D-CGD-CBD	-2.60	119.17	124.48
5	9	301	A86	C9-C8-C6	-2.59	119.13	126.42
5	6	302	A86	O4-C34-C35	-2.59	101.14	107.59
5	6	304	A86	C36-C31-C32	2.59	122.27	119.70
8	9	315	KC1	CHB-C1B-C2B	-2.59	120.05	125.48
5	8	305	A86	C12-C11-C13	2.59	120.37	116.02
8	5	311	KC1	C4B-CHC-C1C	-2.58	120.49	126.06
8	7	313	KC1	C4B-CHC-C1C	-2.58	120.49	126.06
6	7	309	CLA	CHB-C4A-NA	2.58	128.07	124.51
5	5	302	A86	O4-C38-O5	-2.57	117.85	122.96
5	7	307	A86	C3-C4-C5	-2.57	118.20	123.47
6	9	316	CLA	CHB-C4A-NA	2.57	128.07	124.51
8	8	311	KC1	CHB-C1B-C2B	-2.57	120.09	125.48
8	5	311	KC1	CHB-C1B-C2B	-2.56	120.10	125.48
8	5	313	KC1	CHB-C1B-C2B	-2.56	120.11	125.48
7	7	310	KC2	C3D-CAD-CBD	-2.56	104.23	107.61
5	9	303	A86	C3-C4-C5	-2.56	118.23	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	301	A86	O4-C34-C35	-2.56	101.22	107.59
6	8	307	CLA	CHB-C4A-NA	2.56	128.05	124.51
6	8	315	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
7	9	310	KC2	C3D-CAD-CBD	-2.55	104.25	107.61
5	8	306	A86	O1-C15-C20	-2.55	56.91	59.40
6	5	315	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
8	7	315	KC1	CBD-CHA-C1A	2.54	133.62	128.88
7	6	307	KC2	C3D-CAD-CBD	-2.54	104.26	107.61
7	5	308	KC2	C1A-NA-C4A	-2.54	105.56	106.71
7	5	310	KC2	O1D-CGD-CBD	-2.54	119.29	124.48
8	8	313	KC1	CHB-C1B-C2B	-2.54	120.15	125.48
8	9	315	KC1	CBD-CHA-C1A	2.54	133.61	128.88
6	8	309	CLA	CHB-C4A-NA	2.54	128.02	124.51
7	8	308	KC2	O2D-CGD-O1D	-2.54	118.88	123.84
6	6	311	CLA	CHB-C4A-NA	2.53	128.02	124.51
5	7	303	A86	O4-C38-O5	-2.53	117.93	122.96
7	7	312	KC2	O1D-CGD-CBD	-2.53	119.30	124.48
7	6	309	KC2	CBD-CHA-C1A	2.53	133.60	128.88
8	6	310	KC1	O2D-CGD-O1D	-2.53	118.89	123.84
7	7	310	KC2	C1A-NA-C4A	-2.53	105.57	106.71
8	5	313	KC1	C4B-CHC-C1C	-2.53	120.60	126.06
6	7	308	CLA	CHB-C4A-NA	2.53	128.01	124.51
5	9	307	A86	C40-C32-C31	-2.52	108.22	110.47
5	9	306	A86	C24-C1-C2	-2.52	115.07	118.94
5	8	302	A86	C12-C11-C13	2.52	120.25	116.02
8	8	311	KC1	C4B-CHC-C1C	-2.51	120.64	126.06
7	8	308	KC2	C3D-CAD-CBD	-2.51	104.30	107.61
6	5	306	CLA	CHB-C4A-NA	2.51	127.98	124.51
5	6	304	A86	C9-C8-C6	-2.51	119.38	126.42
6	6	308	CLA	CHB-C4A-NA	2.50	127.97	124.51
5	9	307	A86	C12-C11-C13	2.50	120.23	116.02
5	8	302	A86	O4-C38-O5	-2.50	117.99	122.96
5	7	307	A86	C20-C19-C18	2.50	117.70	112.75
6	6	313	CLA	CHB-C4A-NA	2.50	127.97	124.51
8	7	315	KC1	C4B-CHC-C1C	-2.50	120.66	126.06
8	8	313	KC1	C4B-CHC-C1C	-2.50	120.67	126.06
5	9	302	A86	C9-C10-C11	-2.49	119.27	126.61
6	5	314	CLA	CHB-C4A-NA	2.49	127.96	124.51
5	5	301	A86	C33-C32-C31	-2.49	106.79	109.21
5	6	304	A86	C9-C10-C11	-2.49	119.30	126.61
7	6	309	KC2	O2D-CGD-O1D	-2.49	118.98	123.84
8	7	315	KC1	CHB-C1B-C2B	-2.48	120.27	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	9	302	A86	C9-C8-C6	-2.48	119.44	126.42
9	5	317	LMT	C3'-C4'-C5'	-2.48	105.23	110.93
5	8	305	A86	C25-C24-C1	-2.48	119.44	126.42
8	6	312	KC1	C4B-CHC-C1C	-2.48	120.70	126.06
6	9	308	CLA	CHB-C4A-NA	2.48	127.94	124.51
8	7	315	KC1	C3D-CAD-CBD	-2.48	104.34	107.61
6	9	314	CLA	C1-C2-C3	-2.48	121.75	126.04
5	9	305	A86	C3-C4-C5	-2.48	118.39	123.47
5	8	304	A86	C28-C27-C26	-2.48	119.45	122.92
5	9	306	A86	C12-C11-C13	2.48	120.19	116.02
8	9	315	KC1	C4B-CHC-C1C	-2.48	120.71	126.06
8	8	313	KC1	CBD-CHA-C1A	2.48	133.50	128.88
5	9	303	A86	O4-C34-C35	-2.48	101.42	107.59
5	9	307	A86	C17-C16-C15	2.47	111.69	109.16
6	9	313	CLA	CHB-C4A-NA	2.47	127.93	124.51
5	7	305	A86	C23-C16-C17	2.47	113.28	108.98
5	5	301	A86	C22-C16-C17	2.47	113.27	108.98
8	5	313	KC1	CBD-CHA-C1A	2.47	133.48	128.88
6	8	309	CLA	C1-C2-C3	-2.46	121.79	126.04
6	7	316	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
10	7	317	LMG	O7-C10-C11	2.46	116.80	111.50
5	9	302	A86	C28-C27-C26	-2.46	119.48	122.92
7	5	308	KC2	C3D-CAD-CBD	-2.46	104.37	107.61
5	7	305	A86	C9-C10-C11	-2.46	119.39	126.61
6	7	311	CLA	CHB-C4A-NA	2.45	127.91	124.51
5	8	305	A86	C3-C4-C5	-2.45	118.45	123.47
5	6	301	A86	C33-C32-C31	-2.45	106.83	109.21
6	8	314	CLA	CHB-C4A-NA	2.45	127.89	124.51
6	5	309	CLA	CHB-C4A-NA	2.44	127.89	124.51
6	6	311	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
7	6	307	KC2	C1A-NA-C4A	-2.44	105.61	106.71
6	6	305	CLA	CHB-C4A-NA	2.43	127.88	124.51
5	9	306	A86	C-C1-C24	2.43	121.91	118.08
5	6	302	A86	C4-C3-C2	-2.43	118.49	123.47
5	7	307	A86	O4-C38-O5	-2.43	118.13	122.96
9	5	316	LMT	C1'-O5'-C5'	-2.43	108.92	113.69
5	8	306	A86	C41-C32-C33	-2.43	98.16	109.05
5	6	302	A86	O4-C38-O5	-2.42	118.14	122.96
5	7	303	A86	C12-C11-C13	2.42	120.09	116.02
7	6	309	KC2	CHD-C4C-NC	2.42	127.88	124.20
8	5	311	KC1	CMD-C2D-C1D	-2.42	124.74	128.46
5	7	306	A86	C12-C11-C13	2.42	120.09	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	5	310	KC2	CHD-C4C-NC	2.42	127.88	124.20
5	5	318	A86	C20-C19-C18	2.42	117.53	112.75
5	8	303	A86	C9-C8-C6	-2.42	119.62	126.42
8	6	312	KC1	CBD-CHA-C1A	2.41	133.38	128.88
6	6	308	CLA	C1-C2-C3	-2.41	121.87	126.04
5	5	304	A86	C3-C4-C5	-2.41	118.53	123.47
5	7	301	A86	O1-C20-C19	-2.41	111.57	113.38
5	9	302	A86	C25-C24-C1	-2.41	119.64	126.42
7	9	310	KC2	O2D-CGD-O1D	-2.41	119.13	123.84
5	9	303	A86	C33-C32-C31	-2.41	106.87	109.21
6	8	315	CLA	CHB-C4A-NA	2.41	127.84	124.51
5	9	302	A86	O4-C38-O5	-2.40	118.19	122.96
5	7	302	A86	C9-C8-C6	-2.40	119.66	126.42
5	8	303	A86	O4-C38-O5	-2.40	118.19	122.96
5	7	305	A86	C12-C11-C13	2.40	120.06	116.02
5	8	304	A86	O4-C38-O5	-2.40	118.19	122.96
5	7	306	A86	O4-C38-O5	-2.40	118.20	122.96
6	9	309	CLA	CHB-C4A-NA	2.39	127.82	124.51
5	7	307	A86	C9-C10-C11	-2.39	119.58	126.61
5	5	318	A86	O4-C38-O5	-2.39	118.21	122.96
5	5	318	A86	C17-C16-C15	2.39	111.60	109.16
7	6	307	KC2	O1D-CGD-CBD	-2.38	119.61	124.48
5	8	305	A86	O4-C38-O5	-2.38	118.24	122.96
8	7	313	KC1	C3D-CAD-CBD	-2.38	104.48	107.61
5	7	301	A86	C4-C3-C2	-2.38	118.61	123.47
5	6	302	A86	O4-C34-C33	2.37	113.49	107.59
5	7	301	A86	O4-C38-O5	-2.37	118.26	122.96
5	7	302	A86	O4-C38-O5	-2.37	118.26	122.96
6	9	311	CLA	CHB-C4A-NA	2.36	127.78	124.51
5	9	301	A86	O4-C38-O5	-2.36	118.27	122.96
8	8	313	KC1	O2D-CGD-O1D	-2.36	119.23	123.84
7	8	308	KC2	CHD-C4C-NC	2.36	127.78	124.20
5	9	306	A86	O4-C38-O5	-2.36	118.28	122.96
5	5	301	A86	C4-C3-C2	-2.35	118.65	123.47
6	7	316	CLA	CHB-C4A-NA	2.35	127.77	124.51
5	5	301	A86	O4-C34-C33	2.35	113.44	107.59
6	5	314	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
6	9	313	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
6	9	314	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
5	7	305	A86	O4-C38-O5	-2.34	118.30	122.96
5	5	303	A86	O4-C38-O5	-2.34	118.31	122.96
6	5	306	CLA	C1B-CHB-C4A	-2.34	125.48	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	9	314	CLA	CHB-C4A-NA	2.34	127.75	124.51
7	5	308	KC2	O1D-CGD-CBD	-2.34	119.69	124.48
5	5	303	A86	C3-C4-C5	-2.34	118.68	123.47
6	8	314	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
5	5	305	A86	O4-C38-O5	-2.34	118.31	122.96
8	7	313	KC1	CHB-C1B-C2B	-2.34	120.58	125.48
6	7	308	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
7	7	312	KC2	O2D-CGD-O1D	-2.34	119.27	123.84
5	8	301	A86	O4-C38-O5	-2.33	118.33	122.96
6	5	315	CLA	CHB-C4A-NA	2.33	127.73	124.51
7	6	309	KC2	C1B-CHB-C4A	-2.33	121.04	126.06
5	9	307	A86	O4-C38-O5	-2.33	118.34	122.96
5	9	307	A86	C4-C3-C2	-2.33	118.71	123.47
6	6	308	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
6	6	306	CLA	CHB-C4A-NA	2.32	127.73	124.51
5	5	301	A86	O4-C38-O5	-2.32	118.36	122.96
6	9	311	CLA	C1-C2-C3	-2.32	122.03	126.04
5	9	304	A86	O4-C38-O5	-2.32	118.36	122.96
6	5	309	CLA	C1-C2-C3	-2.32	122.04	126.04
5	7	306	A86	C3-C4-C5	-2.31	118.74	123.47
6	9	309	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
7	5	310	KC2	O2D-CGD-O1D	-2.31	119.32	123.84
6	6	305	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
5	8	303	A86	C7-C6-C5	-2.31	119.69	122.92
5	9	301	A86	C7-C6-C5	-2.31	119.69	122.92
8	6	310	KC1	CHB-C1B-C2B	-2.31	120.64	125.48
7	8	310	KC2	O1D-CGD-CBD	-2.30	119.77	124.48
5	6	301	A86	O4-C38-O5	-2.30	118.39	122.96
8	5	313	KC1	O1D-CGD-CBD	-2.30	119.78	124.48
5	8	306	A86	O4-C38-O5	-2.30	118.39	122.96
5	7	303	A86	C4-C3-C2	-2.29	118.77	123.47
8	7	313	KC1	CBD-CHA-C1A	2.29	133.16	128.88
5	7	302	A86	O1-C20-C19	-2.29	111.66	113.38
5	7	301	A86	C10-C9-C8	-2.29	116.06	123.22
6	8	307	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
8	7	315	KC1	O1D-CGD-CBD	-2.29	119.80	124.48
5	5	304	A86	C25-C24-C1	-2.29	119.99	126.42
5	7	306	A86	C25-C24-C1	-2.28	120.00	126.42
6	8	307	CLA	C1-C2-C3	-2.28	122.09	126.04
8	8	313	KC1	C3D-CAD-CBD	-2.28	104.60	107.61
5	9	303	A86	O4-C38-O5	-2.27	118.44	122.96
6	6	313	CLA	C1B-CHB-C4A	-2.27	125.61	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	305	A86	C-C1-C2	-2.27	119.74	122.92
5	6	301	A86	C4-C3-C2	-2.27	118.82	123.47
7	8	310	KC2	C1B-CHB-C4A	-2.27	121.16	126.06
6	9	312	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
5	5	304	A86	O4-C38-O5	-2.27	118.46	122.96
6	6	314	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
7	7	310	KC2	O1D-CGD-CBD	-2.26	119.86	124.48
7	9	310	KC2	C1B-CHB-C4A	-2.26	121.18	126.06
6	5	307	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
5	7	304	A86	O4-C38-O5	-2.26	118.48	122.96
5	6	303	A86	C28-C27-C26	-2.26	119.76	122.92
6	7	311	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
7	5	310	KC2	C1B-CHB-C4A	-2.25	121.20	126.06
6	5	312	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
7	7	312	KC2	C1B-CHB-C4A	-2.25	121.20	126.06
6	9	311	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
5	9	306	A86	C26-C25-C24	-2.25	116.20	123.22
6	9	308	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
6	7	309	CLA	C1-C2-C3	-2.25	122.16	126.04
7	6	307	KC2	CHB-C4A-C3A	-2.24	121.47	124.98
6	7	309	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
8	6	312	KC1	O1D-CGD-CBD	-2.24	119.90	124.48
5	5	302	A86	C4-C3-C2	-2.24	118.88	123.47
6	5	309	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
6	9	316	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
5	6	303	A86	C12-C11-C13	2.24	119.78	116.02
8	5	313	KC1	C3D-CAD-CBD	-2.24	104.66	107.61
7	5	310	KC2	CHB-C4A-C3A	-2.24	121.48	124.98
6	7	314	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
5	6	303	A86	C23-C16-C17	2.24	112.87	108.98
5	6	304	A86	O4-C38-O5	-2.23	118.53	122.96
5	6	303	A86	O4-C38-O5	-2.23	118.53	122.96
6	6	306	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
7	7	312	KC2	CHB-C4A-C3A	-2.23	121.50	124.98
9	7	318	LMT	C3'-C4'-C5'	-2.23	105.82	110.93
5	7	307	A86	O1-C15-C20	-2.22	57.23	59.40
5	5	318	A86	O1-C15-C20	-2.22	57.23	59.40
7	6	307	KC2	C1B-CHB-C4A	-2.22	121.26	126.06
7	5	308	KC2	C1B-CHB-C4A	-2.22	121.27	126.06
5	7	303	A86	C9-C8-C6	-2.22	120.18	126.42
6	8	309	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
7	8	310	KC2	CHB-C4A-C3A	-2.22	121.51	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	9	304	A86	C12-C11-C13	2.21	119.74	116.02
5	7	304	A86	C3-C4-C5	-2.21	118.95	123.47
5	8	304	A86	C4-C3-C2	-2.21	118.95	123.47
5	9	306	A86	C9-C10-C11	-2.21	120.12	126.61
5	5	305	A86	C3-C4-C5	-2.21	118.96	123.47
5	6	304	A86	C4-C3-C2	-2.20	118.97	123.47
7	8	308	KC2	C1B-CHB-C4A	-2.20	121.31	126.06
5	5	301	A86	C25-C24-C1	-2.19	120.25	126.42
5	7	303	A86	C28-C27-C26	-2.19	119.85	122.92
7	7	310	KC2	C1B-CHB-C4A	-2.19	121.33	126.06
6	8	312	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
6	6	311	CLA	CHD-C1D-ND	-2.19	122.44	124.45
5	9	303	A86	C12-C11-C13	2.19	119.69	116.02
8	9	315	KC1	O2D-CGD-O1D	-2.18	119.58	123.84
6	9	311	CLA	CHD-C1D-ND	-2.18	122.45	124.45
8	5	311	KC1	C2A-C3A-C4A	2.18	108.10	106.49
5	8	306	A86	C41-C32-C31	-2.18	108.52	110.47
8	9	315	KC1	C2A-C3A-C4A	2.17	108.10	106.49
8	5	313	KC1	C1A-C2A-C3A	-2.17	105.39	107.11
5	6	304	A86	C3-C4-C5	-2.17	119.02	123.47
6	8	315	CLA	CHD-C1D-ND	-2.17	122.46	124.45
5	7	307	A86	C25-C24-C1	-2.17	120.32	126.42
5	6	303	A86	C9-C10-C11	-2.17	120.23	126.61
6	9	314	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
5	5	304	A86	C28-C27-C26	-2.17	119.88	122.92
5	7	304	A86	C25-C24-C1	-2.17	120.32	126.42
5	5	303	A86	C17-C16-C15	2.17	111.38	109.16
5	7	304	A86	O1-C15-C20	-2.17	57.28	59.40
5	6	301	A86	O1-C20-C19	-2.17	111.75	113.38
5	9	305	A86	O4-C38-O5	-2.16	118.66	122.96
8	8	313	KC1	C1A-C2A-C3A	-2.16	105.40	107.11
5	8	306	A86	C4-C3-C2	-2.16	119.06	123.47
8	6	310	KC1	C3D-CAD-CBD	-2.16	104.77	107.61
7	5	308	KC2	CHB-C4A-C3A	-2.15	121.61	124.98
5	8	301	A86	C40-C32-C31	-2.15	108.55	110.47
8	6	312	KC1	C1A-C2A-C3A	-2.15	105.41	107.11
6	6	306	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
8	8	311	KC1	C2A-C3A-C4A	2.15	108.08	106.49
8	9	315	KC1	C3D-CAD-CBD	-2.15	104.78	107.61
6	9	314	CLA	CHD-C1D-ND	-2.15	122.48	124.45
7	9	310	KC2	CHB-C4A-C3A	-2.15	121.63	124.98
6	5	307	CLA	O2A-CGA-O1A	-2.14	118.18	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	7	311	CLA	C1-C2-C3	-2.14	122.34	126.04
5	6	302	A86	C9-C8-C6	-2.14	120.40	126.42
8	5	313	KC1	O2D-CGD-O1D	-2.14	119.65	123.84
7	8	310	KC2	O2D-CGD-O1D	-2.14	119.65	123.84
5	9	303	A86	C40-C32-C31	-2.14	108.56	110.47
8	7	313	KC1	C2A-C3A-C4A	2.14	108.07	106.49
5	9	301	A86	C25-C24-C1	-2.13	120.42	126.42
5	8	304	A86	C25-C24-C1	-2.13	120.42	126.42
6	5	306	CLA	CHD-C1D-ND	-2.13	122.50	124.45
5	8	303	A86	C25-C24-C1	-2.13	120.43	126.42
5	5	303	A86	C9-C10-C11	-2.13	120.34	126.61
9	8	316	LMT	C3'-C4'-C5'	-2.13	106.05	110.93
5	6	304	A86	C12-C11-C13	2.13	119.60	116.02
5	6	303	A86	C25-C24-C1	-2.13	120.44	126.42
6	9	309	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
5	8	304	A86	C3-C4-C5	-2.13	119.12	123.47
5	8	305	A86	C-C1-C2	-2.12	119.95	122.92
5	9	303	A86	C9-C10-C11	-2.12	120.37	126.61
6	6	308	CLA	CHD-C1D-ND	-2.12	122.51	124.45
6	7	308	CLA	CHD-C1D-ND	-2.12	122.51	124.45
6	9	309	CLA	CHD-C1D-ND	-2.12	122.51	124.45
5	7	305	A86	C9-C8-C6	-2.12	120.47	126.42
7	6	309	KC2	CHB-C4A-C3A	-2.11	121.67	124.98
5	9	301	A86	C-C1-C2	-2.11	119.96	122.92
8	8	311	KC1	C3D-CAD-CBD	-2.11	104.82	107.61
5	9	302	A86	C4-C3-C2	-2.11	119.15	123.47
5	9	305	A86	O4-C34-C35	-2.11	102.34	107.59
5	7	307	A86	C21-C20-C19	-2.10	111.91	114.28
6	5	309	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
5	9	307	A86	C9-C8-C6	-2.10	120.51	126.42
5	6	303	A86	C17-C16-C15	2.10	111.31	109.16
8	7	315	KC1	C2A-C3A-C4A	2.10	108.05	106.49
5	9	305	A86	O4-C34-C33	2.10	112.82	107.59
6	5	309	CLA	CHD-C1D-ND	-2.10	122.53	124.45
5	8	306	A86	C7-C6-C5	-2.10	119.98	122.92
5	8	302	A86	C28-C27-C26	-2.10	119.98	122.92
5	9	307	A86	C28-C27-C26	-2.09	119.99	122.92
6	9	311	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
5	7	306	A86	O1-C15-C20	-2.09	57.35	59.40
5	9	303	A86	O4-C34-C33	2.09	112.80	107.59
7	7	310	KC2	O2D-CGD-O1D	-2.09	119.75	123.84
6	7	314	CLA	C2A-C1A-CHA	2.09	127.52	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	9	301	A86	O1-C15-C20	-2.09	57.36	59.40
6	6	305	CLA	CHD-C1D-ND	-2.09	122.53	124.45
5	5	318	A86	C7-C6-C5	-2.09	120.00	122.92
5	5	303	A86	C12-C11-C13	2.09	119.53	116.02
6	6	311	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
5	9	306	A86	O4-C34-C35	-2.09	102.40	107.59
5	5	305	A86	C28-C27-C26	-2.08	120.00	122.92
5	6	301	A86	C9-C8-C6	-2.08	120.57	126.42
5	9	307	A86	C25-C24-C1	-2.08	120.57	126.42
5	9	303	A86	C28-C27-C26	-2.08	120.01	122.92
5	5	304	A86	C4-C3-C2	-2.08	119.22	123.47
5	5	318	A86	C21-C20-C19	-2.07	111.95	114.28
6	6	313	CLA	CHD-C1D-ND	-2.07	122.56	124.45
5	9	306	A86	O1-C15-C20	-2.07	57.38	59.40
7	5	310	KC2	C1A-C2A-C3A	-2.07	105.47	107.11
6	8	309	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
8	5	313	KC1	C2A-C3A-C4A	2.06	108.02	106.49
8	7	315	KC1	C1A-C2A-C3A	-2.06	105.48	107.11
5	5	304	A86	O1-C15-C20	-2.06	57.39	59.40
5	9	304	A86	C28-C27-C26	-2.06	120.04	122.92
5	7	303	A86	C9-C10-C11	-2.06	120.56	126.61
8	6	310	KC1	C2A-C3A-C4A	2.06	108.01	106.49
7	8	308	KC2	CHB-C4A-C3A	-2.06	121.77	124.98
5	5	303	A86	C9-C8-C6	-2.06	120.64	126.42
5	8	304	A86	O1-C15-C20	-2.05	57.39	59.40
8	7	315	KC1	O2D-CGD-O1D	-2.05	119.83	123.84
5	9	305	A86	O1-C15-C20	-2.05	57.40	59.40
8	8	313	KC1	C2A-C3A-C4A	2.05	108.01	106.49
8	5	311	KC1	C3D-CAD-CBD	-2.05	104.91	107.61
5	9	307	A86	C9-C10-C11	-2.05	120.58	126.61
6	5	306	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
8	6	312	KC1	O2D-CGD-O1D	-2.05	119.84	123.84
6	6	308	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
6	7	316	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
5	9	305	A86	C41-C32-C31	-2.04	108.64	110.47
6	7	308	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
6	7	311	CLA	CHD-C1D-ND	-2.04	122.58	124.45
8	9	315	KC1	O1D-CGD-CBD	-2.04	120.31	124.48
6	8	312	CLA	C2A-C1A-CHA	2.04	127.42	123.86
5	5	302	A86	C9-C8-C6	-2.03	120.70	126.42
5	6	302	A86	C28-C27-C26	-2.03	120.07	122.92
6	8	309	CLA	CHD-C1D-ND	-2.03	122.58	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	6	307	KC2	O2D-CGD-O1D	-2.03	119.86	123.84
5	7	301	A86	O1-C15-C20	-2.03	57.41	59.40
5	7	306	A86	C-C1-C2	-2.03	120.08	122.92
6	5	312	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
5	7	305	A86	C4-C3-C2	-2.03	119.32	123.47
6	8	312	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
5	7	305	A86	O1-C15-C20	-2.02	57.42	59.40
6	5	312	CLA	C2A-C1A-CHA	2.02	127.40	123.86
5	7	301	A86	C3-C4-C5	-2.02	119.33	123.47
6	7	311	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
5	9	306	A86	C28-C27-C26	-2.02	120.09	122.92
5	5	318	A86	C4-C3-C2	-2.02	119.34	123.47
5	8	305	A86	O1-C15-C20	-2.02	57.43	59.40
5	6	303	A86	C33-C32-C31	-2.01	107.25	109.21
7	8	308	KC2	C2A-C3A-C4A	2.01	107.98	106.49
6	5	307	CLA	CHD-C1D-ND	-2.01	122.60	124.45
5	9	302	A86	C41-C32-C31	-2.01	108.67	110.47
5	5	303	A86	C25-C24-C1	-2.01	120.78	126.42
5	9	307	A86	C36-C31-C32	2.01	121.69	119.70
5	9	307	A86	C35-C34-C33	-2.01	106.38	109.88
6	6	305	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
5	8	301	A86	C7-C6-C5	-2.00	120.12	122.92

All (29) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	6	305	CLA	ND
6	6	306	CLA	ND
6	6	308	CLA	ND
6	6	311	CLA	ND
6	6	313	CLA	ND
6	6	314	CLA	ND
6	8	307	CLA	ND
6	8	309	CLA	ND
6	8	312	CLA	ND
6	8	314	CLA	ND
6	8	315	CLA	ND
6	9	308	CLA	ND
6	9	309	CLA	ND
6	9	311	CLA	ND
6	9	312	CLA	ND
6	9	313	CLA	ND

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Mol	Chain	Res	Type	Atom
6	9	314	CLA	ND
6	9	316	CLA	ND
6	5	306	CLA	ND
6	5	307	CLA	ND
6	5	309	CLA	ND
6	5	312	CLA	ND
6	5	314	CLA	ND
6	5	315	CLA	ND
6	7	308	CLA	ND
6	7	309	CLA	ND
6	7	311	CLA	ND
6	7	314	CLA	ND
6	7	316	CLA	ND

All (681) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	6	302	A86	C12-C11-C13-O
5	6	302	A86	C12-C11-C13-C14
5	6	302	A86	C13-C14-C15-O1
5	6	303	A86	C10-C11-C13-O
5	6	303	A86	C12-C11-C13-O
5	6	303	A86	C13-C14-C15-C16
5	6	303	A86	C13-C14-C15-O1
5	6	304	A86	C12-C11-C13-C14
5	6	304	A86	C13-C14-C15-O1
5	8	301	A86	C12-C11-C13-C14
5	8	301	A86	C13-C14-C15-C20
5	8	301	A86	C13-C14-C15-O1
5	8	302	A86	C12-C11-C13-O
5	8	302	A86	C12-C11-C13-C14
5	8	302	A86	C13-C14-C15-O1
5	8	303	A86	C11-C10-C9-C8
5	8	303	A86	C10-C11-C13-O
5	8	303	A86	C33-C34-O4-C38
5	8	303	A86	C5-C6-C8-C9
5	8	303	A86	C7-C6-C8-C9
5	8	304	A86	C10-C11-C13-O
5	8	304	A86	C12-C11-C13-O
5	8	304	A86	C33-C34-O4-C38
5	8	305	A86	C10-C11-C13-O
5	8	305	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
5	8	305	A86	C12-C11-C13-C14
5	8	306	A86	C11-C10-C9-C8
5	8	306	A86	C12-C11-C13-O
5	8	306	A86	C12-C11-C13-C14
5	8	306	A86	C13-C14-C15-C16
5	8	306	A86	C13-C14-C15-O1
5	8	306	A86	C33-C34-O4-C38
5	9	301	A86	C11-C10-C9-C8
5	9	301	A86	C12-C11-C13-O
5	9	301	A86	C13-C14-C15-O1
5	9	301	A86	C33-C34-O4-C38
5	9	302	A86	C12-C11-C13-C14
5	9	303	A86	C10-C11-C13-O
5	9	303	A86	C12-C11-C13-O
5	9	303	A86	C13-C14-C15-C16
5	9	304	A86	C12-C11-C13-O
5	9	304	A86	C12-C11-C13-C14
5	9	304	A86	C1-C2-C3-C4
5	9	304	A86	C39-C38-O4-C34
5	9	304	A86	C3-C4-C5-C6
5	9	305	A86	C10-C11-C13-O
5	9	305	A86	C12-C11-C13-O
5	9	306	A86	C12-C11-C13-O
5	9	306	A86	C1-C2-C3-C4
5	9	307	A86	C12-C11-C13-O
5	9	307	A86	C12-C11-C13-C14
5	9	307	A86	C13-C14-C15-C16
5	5	301	A86	C13-C14-C15-O1
5	5	302	A86	C10-C11-C13-O
5	5	302	A86	C12-C11-C13-O
5	5	302	A86	C13-C14-C15-O1
5	5	303	A86	C12-C11-C13-O
5	5	303	A86	C12-C11-C13-C14
5	5	303	A86	C13-C14-C15-C16
5	5	304	A86	C12-C11-C13-O
5	5	304	A86	C33-C34-O4-C38
5	5	305	A86	C12-C11-C13-O
5	5	305	A86	C12-C11-C13-C14
5	5	305	A86	C13-C14-C15-C16
5	5	318	A86	C11-C10-C9-C8
5	5	318	A86	C10-C11-C13-O
5	5	318	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
5	5	318	A86	C12-C11-C13-C14
5	5	318	A86	C13-C14-C15-C16
5	5	318	A86	C33-C34-O4-C38
5	7	301	A86	C10-C11-C13-O
5	7	301	A86	C12-C11-C13-O
5	7	301	A86	C13-C14-C15-C16
5	7	302	A86	C12-C11-C13-O
5	7	303	A86	C12-C11-C13-O
5	7	303	A86	C12-C11-C13-C14
5	7	303	A86	C13-C14-C15-O1
5	7	303	A86	C39-C38-O4-C34
5	7	304	A86	C10-C11-C13-O
5	7	305	A86	C10-C11-C13-O
5	7	305	A86	C12-C11-C13-O
5	7	305	A86	C12-C11-C13-C14
5	7	305	A86	C13-C14-C15-C16
5	7	305	A86	C13-C14-C15-C20
5	7	306	A86	C12-C11-C13-C14
5	7	307	A86	C10-C11-C13-O
5	7	307	A86	C12-C11-C13-O
5	7	307	A86	C13-C14-C15-C16
5	7	307	A86	C33-C34-O4-C38
6	6	311	CLA	C1A-C2A-CAA-CBA
6	6	311	CLA	C3A-C2A-CAA-CBA
6	6	313	CLA	CBD-CGD-O2D-CED
6	6	314	CLA	CHA-CBD-CGD-O1D
6	6	314	CLA	CHA-CBD-CGD-O2D
6	8	314	CLA	CBD-CGD-O2D-CED
6	8	315	CLA	C1A-C2A-CAA-CBA
6	9	308	CLA	CHA-CBD-CGD-O1D
6	9	308	CLA	CHA-CBD-CGD-O2D
6	9	312	CLA	C1A-C2A-CAA-CBA
6	9	314	CLA	C1A-C2A-CAA-CBA
6	9	316	CLA	CBD-CGD-O2D-CED
6	5	314	CLA	CBD-CGD-O2D-CED
6	5	315	CLA	C1A-C2A-CAA-CBA
6	5	315	CLA	CBA-CGA-O2A-C1
6	5	315	CLA	O1A-CGA-O2A-C1
6	7	309	CLA	C2-C3-C5-C6
6	7	309	CLA	C4-C3-C5-C6
7	6	307	KC2	C1A-C2A-CAA-CBA
7	6	307	KC2	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
7	6	307	KC2	C2B-C3B-CAB-CBB
7	6	307	KC2	C4B-C3B-CAB-CBB
7	6	309	KC2	C1A-C2A-CAA-CBA
7	6	309	KC2	C2B-C3B-CAB-CBB
7	6	309	KC2	C4B-C3B-CAB-CBB
7	8	308	KC2	C1A-C2A-CAA-CBA
7	8	308	KC2	C3A-C2A-CAA-CBA
7	8	308	KC2	C2B-C3B-CAB-CBB
7	8	310	KC2	C1A-C2A-CAA-CBA
7	8	310	KC2	C2B-C3B-CAB-CBB
7	8	310	KC2	C4B-C3B-CAB-CBB
7	8	310	KC2	C2C-C3C-CAC-CBC
7	8	310	KC2	C2A-CAA-CBA-CGA
7	9	310	KC2	C1A-C2A-CAA-CBA
7	9	310	KC2	C3A-C2A-CAA-CBA
7	9	310	KC2	C2B-C3B-CAB-CBB
7	9	310	KC2	C2C-C3C-CAC-CBC
7	9	310	KC2	C4C-C3C-CAC-CBC
7	5	308	KC2	C1A-C2A-CAA-CBA
7	5	308	KC2	C3A-C2A-CAA-CBA
7	5	308	KC2	C2B-C3B-CAB-CBB
7	5	308	KC2	C2C-C3C-CAC-CBC
7	5	310	KC2	C2B-C3B-CAB-CBB
7	5	310	KC2	C4B-C3B-CAB-CBB
7	5	310	KC2	CAA-CBA-CGA-O2A
7	7	310	KC2	C1A-C2A-CAA-CBA
7	7	310	KC2	C3A-C2A-CAA-CBA
7	7	310	KC2	C2B-C3B-CAB-CBB
7	7	310	KC2	C2C-C3C-CAC-CBC
7	7	312	KC2	C2B-C3B-CAB-CBB
7	7	312	KC2	C4B-C3B-CAB-CBB
7	7	312	KC2	C2C-C3C-CAC-CBC
8	6	310	KC1	C2B-C3B-CAB-CBB
8	8	311	KC1	C1A-C2A-CAA-CBA
8	8	311	KC1	C2B-C3B-CAB-CBB
8	8	311	KC1	C4B-C3B-CAB-CBB
8	5	311	KC1	C2B-C3B-CAB-CBB
8	5	313	KC1	C2B-C3B-CAB-CBB
8	7	313	KC1	C2B-C3B-CAB-CBB
8	7	315	KC1	C2B-C3B-CAB-CBB
9	5	317	LMT	C2'-C1'-O1'-C1
9	5	317	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
9	5	317	LMT	C2-C1-O1'-C1'
9	7	318	LMT	C2-C1-O1'-C1'
9	7	319	LMT	C2'-C1'-O1'-C1
9	7	319	LMT	O5'-C1'-O1'-C1
9	7	319	LMT	C2-C1-O1'-C1'
10	7	317	LMG	C2-C1-O1-C7
10	7	317	LMG	O6-C1-O1-C7
10	7	317	LMG	O9-C10-O7-C8
10	7	317	LMG	C11-C10-O7-C8
5	6	301	A86	C39-C38-O4-C34
5	6	302	A86	C39-C38-O4-C34
5	6	303	A86	C39-C38-O4-C34
5	6	304	A86	C39-C38-O4-C34
5	8	302	A86	C39-C38-O4-C34
5	8	303	A86	C39-C38-O4-C34
5	8	305	A86	C39-C38-O4-C34
5	8	306	A86	C39-C38-O4-C34
5	9	301	A86	C39-C38-O4-C34
5	9	302	A86	C39-C38-O4-C34
5	9	303	A86	C39-C38-O4-C34
5	9	305	A86	C39-C38-O4-C34
5	9	306	A86	C39-C38-O4-C34
5	9	307	A86	C39-C38-O4-C34
5	5	301	A86	C39-C38-O4-C34
5	5	302	A86	C39-C38-O4-C34
5	5	303	A86	C39-C38-O4-C34
5	5	304	A86	C39-C38-O4-C34
5	5	305	A86	C39-C38-O4-C34
5	5	318	A86	C39-C38-O4-C34
5	7	301	A86	C39-C38-O4-C34
5	7	304	A86	C39-C38-O4-C34
5	7	305	A86	C39-C38-O4-C34
5	7	306	A86	C39-C38-O4-C34
5	7	307	A86	C39-C38-O4-C34
6	6	313	CLA	O1D-CGD-O2D-CED
6	9	313	CLA	O1D-CGD-O2D-CED
6	9	316	CLA	O1D-CGD-O2D-CED
6	6	311	CLA	CBD-CGD-O2D-CED
6	9	313	CLA	CBD-CGD-O2D-CED
6	7	316	CLA	CBD-CGD-O2D-CED
6	9	309	CLA	O1A-CGA-O2A-C1
6	5	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
6	5	314	CLA	O1D-CGD-O2D-CED
5	7	305	A86	C33-C34-O4-C38
6	8	314	CLA	O1D-CGD-O2D-CED
6	7	316	CLA	O1D-CGD-O2D-CED
6	5	307	CLA	CBA-CGA-O2A-C1
6	8	315	CLA	CBD-CGD-O2D-CED
6	9	314	CLA	CBD-CGD-O2D-CED
6	5	315	CLA	CBD-CGD-O2D-CED
7	8	308	KC2	CBD-CGD-O2D-CED
5	9	304	A86	O5-C38-O4-C34
5	6	301	A86	O5-C38-O4-C34
5	6	302	A86	O5-C38-O4-C34
5	6	303	A86	O5-C38-O4-C34
5	6	304	A86	O5-C38-O4-C34
5	8	302	A86	O5-C38-O4-C34
5	8	303	A86	O5-C38-O4-C34
5	8	305	A86	O5-C38-O4-C34
5	8	306	A86	O5-C38-O4-C34
5	9	301	A86	O5-C38-O4-C34
5	9	302	A86	O5-C38-O4-C34
5	9	303	A86	O5-C38-O4-C34
5	9	305	A86	O5-C38-O4-C34
5	9	306	A86	O5-C38-O4-C34
5	9	307	A86	O5-C38-O4-C34
5	5	301	A86	O5-C38-O4-C34
5	5	302	A86	O5-C38-O4-C34
5	5	303	A86	O5-C38-O4-C34
5	5	304	A86	O5-C38-O4-C34
5	5	305	A86	O5-C38-O4-C34
5	5	318	A86	O5-C38-O4-C34
5	7	301	A86	O5-C38-O4-C34
5	7	303	A86	O5-C38-O4-C34
5	7	304	A86	O5-C38-O4-C34
5	7	305	A86	O5-C38-O4-C34
5	7	306	A86	O5-C38-O4-C34
5	7	307	A86	O5-C38-O4-C34
8	8	313	KC1	CBD-CGD-O2D-CED
6	8	315	CLA	CBA-CGA-O2A-C1
6	8	315	CLA	O1A-CGA-O2A-C1
6	7	316	CLA	C3-C5-C6-C7
6	8	312	CLA	CBA-CGA-O2A-C1
6	9	309	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
6	7	308	CLA	CBD-CGD-O2D-CED
7	6	309	KC2	CBD-CGD-O2D-CED
6	5	314	CLA	C2A-CAA-CBA-CGA
6	9	309	CLA	C3-C5-C6-C7
6	5	307	CLA	C3-C5-C6-C7
6	9	313	CLA	CBA-CGA-O2A-C1
6	5	312	CLA	CBA-CGA-O2A-C1
6	7	314	CLA	CBA-CGA-O2A-C1
6	9	314	CLA	O1A-CGA-O2A-C1
6	5	312	CLA	O1A-CGA-O2A-C1
6	7	314	CLA	O1A-CGA-O2A-C1
5	8	301	A86	C39-C38-O4-C34
5	8	304	A86	C39-C38-O4-C34
5	7	302	A86	C39-C38-O4-C34
6	5	307	CLA	CBD-CGD-O2D-CED
6	9	314	CLA	CBA-CGA-O2A-C1
5	8	301	A86	O5-C38-O4-C34
5	8	304	A86	O5-C38-O4-C34
5	7	302	A86	O5-C38-O4-C34
6	8	312	CLA	O1A-CGA-O2A-C1
9	7	318	LMT	O5'-C5'-C6'-O6'
6	5	314	CLA	CBA-CGA-O2A-C1
9	7	319	LMT	O5'-C5'-C6'-O6'
6	6	311	CLA	O1D-CGD-O2D-CED
7	9	310	KC2	CAA-CBA-CGA-O2A
6	9	313	CLA	O1A-CGA-O2A-C1
6	8	314	CLA	C2A-CAA-CBA-CGA
6	6	305	CLA	CBD-CGD-O2D-CED
8	8	311	KC1	CAA-CBA-CGA-O1A
5	6	301	A86	C35-C34-O4-C38
5	6	303	A86	C35-C34-O4-C38
5	8	306	A86	C35-C34-O4-C38
5	9	301	A86	C35-C34-O4-C38
5	9	302	A86	C35-C34-O4-C38
5	9	303	A86	C35-C34-O4-C38
5	9	305	A86	C35-C34-O4-C38
5	9	306	A86	C35-C34-O4-C38
5	9	307	A86	C35-C34-O4-C38
5	5	301	A86	C35-C34-O4-C38
5	5	303	A86	C35-C34-O4-C38
5	7	307	A86	C35-C34-O4-C38
7	5	310	KC2	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
6	5	315	CLA	O1D-CGD-O2D-CED
6	6	311	CLA	CBA-CGA-O2A-C1
6	8	307	CLA	CBA-CGA-O2A-C1
6	7	309	CLA	CBA-CGA-O2A-C1
8	8	311	KC1	CAA-CBA-CGA-O2A
8	5	313	KC1	CAA-CBA-CGA-O2A
6	6	305	CLA	C8-C10-C11-C12
6	6	311	CLA	O1A-CGA-O2A-C1
6	6	305	CLA	C11-C10-C8-C9
6	6	314	CLA	C11-C10-C8-C9
6	7	309	CLA	C6-C7-C8-C9
6	7	309	CLA	C11-C12-C13-C14
5	8	304	A86	C35-C34-O4-C38
5	5	318	A86	C35-C34-O4-C38
5	7	302	A86	C35-C34-O4-C38
5	7	305	A86	C35-C34-O4-C38
6	5	307	CLA	C2A-CAA-CBA-CGA
5	8	306	A86	C7-C6-C8-C9
8	8	313	KC1	CAA-CBA-CGA-O2A
8	9	315	KC1	CAA-CBA-CGA-O2A
6	6	305	CLA	C10-C11-C12-C13
6	6	314	CLA	C5-C6-C7-C8
6	9	314	CLA	C8-C10-C11-C12
6	5	307	CLA	C5-C6-C7-C8
6	7	309	CLA	C10-C11-C12-C13
6	9	314	CLA	O1D-CGD-O2D-CED
5	8	301	A86	C35-C34-O4-C38
5	8	305	A86	C35-C34-O4-C38
5	5	305	A86	C35-C34-O4-C38
5	7	306	A86	C35-C34-O4-C38
6	5	314	CLA	O1A-CGA-O2A-C1
6	8	315	CLA	O1D-CGD-O2D-CED
7	5	310	KC2	CAA-CBA-CGA-O1A
6	9	313	CLA	C11-C10-C8-C7
6	5	306	CLA	C6-C7-C8-C10
6	7	309	CLA	C11-C12-C13-C15
5	7	303	A86	C35-C34-O4-C38
6	5	306	CLA	C10-C11-C12-C13
6	8	307	CLA	O1A-CGA-O2A-C1
6	7	309	CLA	O1A-CGA-O2A-C1
6	6	308	CLA	CBD-CGD-O2D-CED
6	9	314	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	7	319	LMT	O1'-C1-C2-C3
5	6	302	A86	C35-C34-O4-C38
5	6	304	A86	C35-C34-O4-C38
5	9	304	A86	C35-C34-O4-C38
5	7	301	A86	C35-C34-O4-C38
5	7	304	A86	C35-C34-O4-C38
6	9	311	CLA	C8-C10-C11-C12
6	5	306	CLA	C5-C6-C7-C8
6	7	309	CLA	C5-C6-C7-C8
6	6	313	CLA	CBA-CGA-O2A-C1
6	6	311	CLA	C5-C6-C7-C8
9	7	318	LMT	C4'-C5'-C6'-O6'
6	7	308	CLA	C10-C11-C12-C13
5	8	303	A86	C35-C34-O4-C38
5	5	304	A86	C35-C34-O4-C38
6	7	308	CLA	O1D-CGD-O2D-CED
9	7	319	LMT	O5B-C5B-C6B-O6B
5	8	302	A86	C35-C34-O4-C38
5	5	302	A86	C35-C34-O4-C38
7	6	307	KC2	CAA-CBA-CGA-O2A
7	8	308	KC2	C2A-CAA-CBA-CGA
7	9	310	KC2	C2A-CAA-CBA-CGA
7	5	310	KC2	C2A-CAA-CBA-CGA
7	7	312	KC2	C2A-CAA-CBA-CGA
8	6	312	KC1	C2A-CAA-CBA-CGA
8	8	311	KC1	C2A-CAA-CBA-CGA
6	5	309	CLA	C6-C7-C8-C10
6	7	316	CLA	CBA-CGA-O2A-C1
8	5	311	KC1	CBD-CGD-O2D-CED
6	6	306	CLA	C11-C12-C13-C15
6	5	307	CLA	O1D-CGD-O2D-CED
6	8	309	CLA	C4-C3-C5-C6
6	9	313	CLA	C11-C10-C8-C9
6	9	314	CLA	C6-C7-C8-C9
6	7	308	CLA	C11-C10-C8-C9
5	7	303	A86	C33-C34-O4-C38
5	8	306	A86	C5-C6-C8-C9
5	5	318	A86	C5-C6-C8-C9
9	8	316	LMT	O5'-C1'-O1'-C1
6	9	308	CLA	CBD-CGD-O2D-CED
6	6	313	CLA	C3A-C2A-CAA-CBA
6	8	312	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	9	312	CLA	C3A-C2A-CAA-CBA
6	9	314	CLA	C3A-C2A-CAA-CBA
6	5	312	CLA	C3A-C2A-CAA-CBA
6	5	315	CLA	C3A-C2A-CAA-CBA
6	7	314	CLA	C3A-C2A-CAA-CBA
6	5	306	CLA	CBD-CGD-O2D-CED
6	6	308	CLA	C4-C3-C5-C6
6	6	314	CLA	CBA-CGA-O2A-C1
6	6	308	CLA	C2-C3-C5-C6
9	7	319	LMT	C6-C7-C8-C9
7	8	308	KC2	CAA-CBA-CGA-O2A
7	9	310	KC2	CAA-CBA-CGA-O1A
6	7	316	CLA	O1A-CGA-O2A-C1
9	7	319	LMT	C4'-C5'-C6'-O6'
6	5	306	CLA	C13-C15-C16-C17
8	6	312	KC1	CAA-CBA-CGA-O2A
9	5	317	LMT	O5'-C5'-C6'-O6'
6	6	314	CLA	C11-C10-C8-C7
6	8	309	CLA	C2-C3-C5-C6
6	5	309	CLA	C2-C3-C5-C6
6	7	308	CLA	C6-C7-C8-C10
6	7	316	CLA	C12-C13-C15-C16
6	6	314	CLA	O1A-CGA-O2A-C1
6	6	306	CLA	C11-C12-C13-C14
5	5	302	A86	C33-C34-O4-C38
7	6	307	KC2	C2C-C3C-CAC-CBC
7	6	309	KC2	C2C-C3C-CAC-CBC
7	5	310	KC2	C2C-C3C-CAC-CBC
8	6	312	KC1	C2B-C3B-CAB-CBB
8	8	313	KC1	C2B-C3B-CAB-CBB
9	5	317	LMT	C4'-C5'-C6'-O6'
7	6	309	KC2	C4C-C3C-CAC-CBC
7	8	308	KC2	C4B-C3B-CAB-CBB
7	8	310	KC2	C4C-C3C-CAC-CBC
7	9	310	KC2	C4B-C3B-CAB-CBB
7	5	308	KC2	C4B-C3B-CAB-CBB
7	5	308	KC2	C4C-C3C-CAC-CBC
7	5	310	KC2	C4C-C3C-CAC-CBC
7	7	310	KC2	C4B-C3B-CAB-CBB
7	7	310	KC2	C4C-C3C-CAC-CBC
7	7	312	KC2	C4C-C3C-CAC-CBC
8	6	310	KC1	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
8	8	313	KC1	C4B-C3B-CAB-CBB
8	5	311	KC1	C4B-C3B-CAB-CBB
8	5	313	KC1	C4B-C3B-CAB-CBB
8	7	313	KC1	C4B-C3B-CAB-CBB
8	7	315	KC1	C4B-C3B-CAB-CBB
6	8	307	CLA	C5-C6-C7-C8
6	6	314	CLA	C15-C16-C17-C18
6	7	308	CLA	C5-C6-C7-C8
6	5	309	CLA	C4-C3-C5-C6
6	6	311	CLA	C11-C12-C13-C14
6	5	306	CLA	C6-C7-C8-C9
6	7	309	CLA	C2A-CAA-CBA-CGA
9	7	318	LMT	O1'-C1-C2-C3
10	9	317	LMG	O6-C5-C6-O5
5	5	318	A86	C7-C6-C8-C9
6	6	313	CLA	C1A-C2A-CAA-CBA
6	8	312	CLA	C1A-C2A-CAA-CBA
6	9	309	CLA	C1A-C2A-CAA-CBA
6	5	312	CLA	C1A-C2A-CAA-CBA
6	5	314	CLA	C1A-C2A-CAA-CBA
6	7	314	CLA	C1A-C2A-CAA-CBA
6	5	309	CLA	C6-C7-C8-C9
8	7	313	KC1	CAA-CBA-CGA-O2A
8	7	315	KC1	CAA-CBA-CGA-O2A
10	9	317	LMG	C11-C10-O7-C8
6	6	305	CLA	O1D-CGD-O2D-CED
10	9	317	LMG	C30-C31-C32-C33
5	5	303	A86	C33-C34-O4-C38
9	5	316	LMT	O5'-C5'-C6'-O6'
6	9	312	CLA	CBA-CGA-O2A-C1
9	5	316	LMT	O5'-C1'-O1'-C1
6	6	313	CLA	O1A-CGA-O2A-C1
7	6	307	KC2	CBD-CGD-O2D-CED
9	5	317	LMT	C1-C2-C3-C4
9	7	318	LMT	O5B-C5B-C6B-O6B
7	5	308	KC2	CAA-CBA-CGA-O2A
6	7	308	CLA	C8-C10-C11-C12
6	6	305	CLA	C11-C10-C8-C7
6	6	306	CLA	C6-C7-C8-C10
6	6	311	CLA	C11-C12-C13-C15
6	6	314	CLA	C11-C12-C13-C15
6	9	314	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
6	6	306	CLA	C6-C7-C8-C9
6	6	314	CLA	C6-C7-C8-C9
6	6	314	CLA	C11-C12-C13-C14
6	9	314	CLA	C11-C10-C8-C9
6	5	306	CLA	C11-C12-C13-C14
6	7	308	CLA	C6-C7-C8-C9
6	7	309	CLA	C11-C10-C8-C9
6	7	316	CLA	C11-C12-C13-C14
6	7	316	CLA	C14-C13-C15-C16
6	6	308	CLA	O1D-CGD-O2D-CED
9	7	319	LMT	C7-C8-C9-C10
9	7	318	LMT	O5B-C1B-O1B-C4'
6	9	308	CLA	O1D-CGD-O2D-CED
9	7	318	LMT	C2B-C1B-O1B-C4'
10	9	317	LMG	C29-C28-O8-C9
6	8	315	CLA	C3A-C2A-CAA-CBA
6	5	314	CLA	C3A-C2A-CAA-CBA
6	9	309	CLA	CBD-CGD-O2D-CED
6	9	309	CLA	C11-C12-C13-C14
5	6	304	A86	C10-C11-C13-C14
5	8	301	A86	C10-C11-C13-C14
5	8	302	A86	C10-C11-C13-C14
5	9	301	A86	C10-C11-C13-C14
5	9	302	A86	C10-C11-C13-C14
5	5	305	A86	C10-C11-C13-C14
5	7	301	A86	C10-C11-C13-C14
5	7	302	A86	C10-C11-C13-C14
5	7	303	A86	C10-C11-C13-C14
5	7	306	A86	C10-C11-C13-C14
6	5	307	CLA	C2-C1-O2A-CGA
5	8	302	A86	C33-C34-O4-C38
7	7	312	KC2	C1A-C2A-CAA-CBA
8	9	315	KC1	C1A-C2A-CAA-CBA
8	5	311	KC1	C1A-C2A-CAA-CBA
8	7	313	KC1	C1A-C2A-CAA-CBA
6	9	309	CLA	C5-C6-C7-C8
6	5	306	CLA	O1D-CGD-O2D-CED
6	6	314	CLA	C6-C7-C8-C10
6	5	306	CLA	C11-C12-C13-C15
6	7	309	CLA	C11-C10-C8-C7
6	7	316	CLA	C6-C7-C8-C10
6	7	316	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
6	6	311	CLA	C8-C10-C11-C12
6	8	312	CLA	CAD-CBD-CGD-O2D
6	9	311	CLA	CAD-CBD-CGD-O2D
6	9	313	CLA	CAD-CBD-CGD-O2D
6	5	312	CLA	CAD-CBD-CGD-O2D
8	9	315	KC1	C2B-C3B-CAB-CBB
8	9	315	KC1	CAD-CBD-CGD-O2D
5	6	301	A86	C12-C11-C13-O
5	6	304	A86	C12-C11-C13-O
5	8	301	A86	C12-C11-C13-O
5	8	303	A86	C12-C11-C13-O
5	9	302	A86	C12-C11-C13-O
5	5	301	A86	C12-C11-C13-O
5	7	304	A86	C12-C11-C13-O
5	7	306	A86	C12-C11-C13-O
7	6	307	KC2	C4C-C3C-CAC-CBC
6	9	309	CLA	C2A-CAA-CBA-CGA
6	9	309	CLA	C11-C12-C13-C15
6	6	311	CLA	CHA-CBD-CGD-O1D
6	5	306	CLA	CHA-CBD-CGD-O1D
6	5	312	CLA	CHA-CBD-CGD-O1D
7	9	310	KC2	CHA-CBD-CGD-O2D
8	6	312	KC1	CHA-CBD-CGD-O2D
8	5	313	KC1	CHA-CBD-CGD-O2D
8	7	315	KC1	CHA-CBD-CGD-O1D
8	7	315	KC1	CHA-CBD-CGD-O2D
6	9	314	CLA	C3-C5-C6-C7
7	7	312	KC2	CBD-CGD-O2D-CED
5	6	301	A86	C10-C11-C13-O
5	6	302	A86	C10-C11-C13-O
5	6	304	A86	C10-C11-C13-O
5	8	301	A86	C10-C11-C13-O
5	8	302	A86	C10-C11-C13-O
5	8	306	A86	C10-C11-C13-O
5	9	301	A86	C10-C11-C13-O
5	9	302	A86	C10-C11-C13-O
5	9	304	A86	C10-C11-C13-O
5	9	304	A86	C13-C14-C15-O1
5	9	306	A86	C10-C11-C13-O
5	9	307	A86	C10-C11-C13-O
5	5	301	A86	C10-C11-C13-O
5	5	303	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
5	5	304	A86	C10-C11-C13-O
5	5	305	A86	C10-C11-C13-O
5	7	302	A86	C10-C11-C13-O
5	7	303	A86	C10-C11-C13-O
5	7	306	A86	C10-C11-C13-O
6	7	311	CLA	C4-C3-C5-C6
6	8	307	CLA	C6-C7-C8-C9
6	7	316	CLA	C6-C7-C8-C9
8	8	311	KC1	CBD-CGD-O2D-CED
6	6	313	CLA	C2A-CAA-CBA-CGA
6	9	311	CLA	C2A-CAA-CBA-CGA
5	6	302	A86	C33-C34-O4-C38
6	6	306	CLA	C3-C5-C6-C7
6	6	311	CLA	CAD-CBD-CGD-O1D
10	7	317	LMG	C29-C28-O8-C9
10	9	317	LMG	O9-C10-O7-C8
6	7	311	CLA	C6-C7-C8-C9
6	8	307	CLA	C6-C7-C8-C10
6	9	314	CLA	C12-C13-C15-C16
6	7	309	CLA	C6-C7-C8-C10
6	7	311	CLA	C2-C3-C5-C6
6	5	306	CLA	C8-C10-C11-C12
10	9	317	LMG	O10-C28-O8-C9
5	6	304	A86	C13-C14-C15-C20
5	8	305	A86	C13-C14-C15-C20
5	9	306	A86	C13-C14-C15-C20
5	7	304	A86	C13-C14-C15-C20
5	7	306	A86	C13-C14-C15-C20
5	5	301	A86	C33-C34-O4-C38
5	7	302	A86	C33-C34-O4-C38
5	9	305	A86	C33-C34-O4-C38
6	8	307	CLA	C2A-CAA-CBA-CGA
6	5	309	CLA	C2A-CAA-CBA-CGA
5	6	301	A86	C12-C11-C13-C14
5	6	303	A86	C12-C11-C13-C14
5	8	303	A86	C12-C11-C13-C14
5	8	304	A86	C12-C11-C13-C14
5	9	301	A86	C12-C11-C13-C14
5	9	303	A86	C12-C11-C13-C14
5	9	305	A86	C12-C11-C13-C14
5	9	306	A86	C12-C11-C13-C14
5	5	301	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
5	5	302	A86	C12-C11-C13-C14
5	5	304	A86	C12-C11-C13-C14
5	7	302	A86	C12-C11-C13-C14
5	7	304	A86	C12-C11-C13-C14
5	7	307	A86	C12-C11-C13-C14
6	9	309	CLA	O1D-CGD-O2D-CED
6	7	308	CLA	CBA-CGA-O2A-C1
6	7	308	CLA	O1A-CGA-O2A-C1
6	6	313	CLA	CAA-CBA-CGA-O2A
9	5	316	LMT	C2B-C1B-O1B-C4'
6	6	305	CLA	C13-C15-C16-C17
6	9	312	CLA	O1A-CGA-O2A-C1
6	7	308	CLA	C11-C10-C8-C7
6	6	314	CLA	C16-C17-C18-C19
5	9	306	A86	C33-C34-O4-C38
9	5	316	LMT	O5B-C1B-O1B-C4'
8	6	310	KC1	CAA-CBA-CGA-O2A
6	7	311	CLA	C6-C7-C8-C10
6	6	308	CLA	C2A-CAA-CBA-CGA
8	6	312	KC1	C4B-C3B-CAB-CBB
6	8	309	CLA	C2A-CAA-CBA-CGA
6	9	312	CLA	C2A-CAA-CBA-CGA
6	5	306	CLA	C11-C10-C8-C9
5	9	303	A86	C33-C34-O4-C38
6	6	306	CLA	C1A-C2A-CAA-CBA
6	6	311	CLA	C6-C7-C8-C10
6	9	311	CLA	C6-C7-C8-C10
6	5	307	CLA	C16-C17-C18-C20
6	6	305	CLA	C15-C16-C17-C18
6	6	311	CLA	C13-C15-C16-C17
9	5	316	LMT	O5B-C5B-C6B-O6B
5	8	303	A86	C13-C14-C15-C16
5	8	304	A86	C13-C14-C15-C16
5	9	305	A86	C13-C14-C15-C16
5	6	301	A86	C10-C11-C13-C14
5	6	302	A86	C10-C11-C13-C14
5	6	303	A86	C10-C11-C13-C14
5	8	303	A86	C10-C11-C13-C14
5	8	304	A86	C10-C11-C13-C14
5	8	305	A86	C10-C11-C13-C14
5	8	306	A86	C10-C11-C13-C14
5	9	303	A86	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
5	9	304	A86	C10-C11-C13-C14
5	9	305	A86	C10-C11-C13-C14
5	9	306	A86	C10-C11-C13-C14
5	9	307	A86	C10-C11-C13-C14
5	5	301	A86	C10-C11-C13-C14
5	5	302	A86	C10-C11-C13-C14
5	5	303	A86	C10-C11-C13-C14
5	5	304	A86	C10-C11-C13-C14
5	5	318	A86	C10-C11-C13-C14
5	7	304	A86	C10-C11-C13-C14
5	7	305	A86	C10-C11-C13-C14
5	7	307	A86	C10-C11-C13-C14
6	5	314	CLA	CAA-CBA-CGA-O2A
7	5	310	KC2	C1A-C2A-CAA-CBA
8	6	310	KC1	C1A-C2A-CAA-CBA
6	7	311	CLA	C2A-CAA-CBA-CGA
6	9	312	CLA	C4C-C3C-CAC-CBC
9	7	318	LMT	C4-C5-C6-C7
5	6	301	A86	C33-C34-O4-C38
8	8	313	KC1	C2A-CAA-CBA-CGA
6	9	311	CLA	C6-C7-C8-C9
6	9	311	CLA	C11-C10-C8-C9
6	9	314	CLA	C14-C13-C15-C16
6	9	312	CLA	C2C-C3C-CAC-CBC
6	8	309	CLA	CAD-CBD-CGD-O2D
6	9	309	CLA	CAD-CBD-CGD-O2D
9	7	319	LMT	C3-C4-C5-C6
10	7	317	LMG	O10-C28-O8-C9
6	6	311	CLA	O2A-C1-C2-C3
8	9	315	KC1	C4B-C3B-CAB-CBB
6	7	316	CLA	C10-C11-C12-C13
5	8	301	A86	C33-C34-O4-C38
6	6	311	CLA	CHA-CBD-CGD-O2D
6	8	307	CLA	CHA-CBD-CGD-O1D
6	8	307	CLA	CHA-CBD-CGD-O2D
6	5	306	CLA	CHA-CBD-CGD-O2D
6	7	314	CLA	CHA-CBD-CGD-O2D
7	6	307	KC2	CHA-CBD-CGD-O2D
7	6	309	KC2	CHA-CBD-CGD-O1D
7	8	308	KC2	CHA-CBD-CGD-O2D
8	6	312	KC1	CHA-CBD-CGD-O1D
8	8	311	KC1	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
8	8	313	KC1	CHA-CBD-CGD-O1D
8	5	313	KC1	CHA-CBD-CGD-O1D
6	8	312	CLA	CAA-CBA-CGA-O2A
6	7	314	CLA	CAA-CBA-CGA-O2A
5	5	303	A86	C13-C14-C15-O1
6	5	312	CLA	CAA-CBA-CGA-O2A
7	9	310	KC2	CBD-CGD-O2D-CED
9	5	316	LMT	C3-C4-C5-C6
8	8	313	KC1	CAA-CBA-CGA-O1A
6	6	311	CLA	C2A-CAA-CBA-CGA
6	5	312	CLA	CAA-CBA-CGA-O1A
6	8	307	CLA	CAD-CBD-CGD-O1D
7	6	309	KC2	CAD-CBD-CGD-O1D
8	8	313	KC1	CAD-CBD-CGD-O1D
6	8	314	CLA	CAA-CBA-CGA-O2A
6	8	314	CLA	CBA-CGA-O2A-C1
6	5	307	CLA	CAA-CBA-CGA-O2A
6	8	309	CLA	C3-C5-C6-C7
6	7	314	CLA	CAA-CBA-CGA-O1A
6	9	309	CLA	CAA-CBA-CGA-O2A
6	8	312	CLA	CAA-CBA-CGA-O1A
6	9	309	CLA	CAA-CBA-CGA-O1A
6	9	312	CLA	CAA-CBA-CGA-O2A
6	5	307	CLA	C16-C17-C18-C19
6	8	314	CLA	CAA-CBA-CGA-O1A
10	9	317	LMG	O8-C28-C29-C30

There are no ring outliers.

41 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	9	305	A86	1	0
6	6	311	CLA	5	0
6	7	309	CLA	5	0
6	5	306	CLA	4	0
6	9	314	CLA	6	0
5	7	305	A86	1	0
5	9	302	A86	1	0
9	8	316	LMT	1	0
5	6	301	A86	1	0
5	5	301	A86	1	0
5	7	304	A86	1	0

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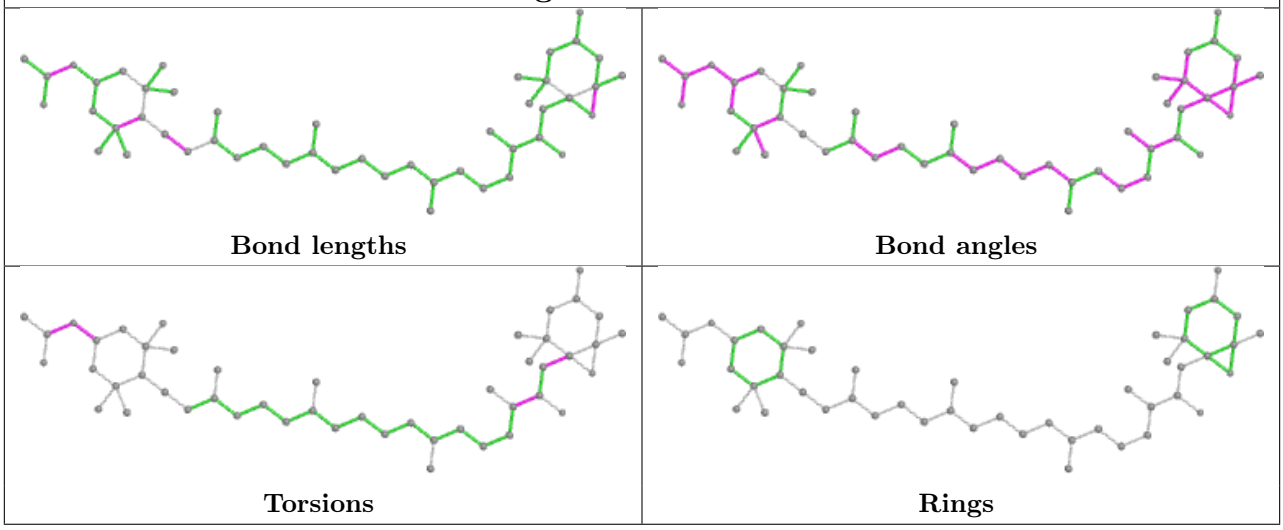
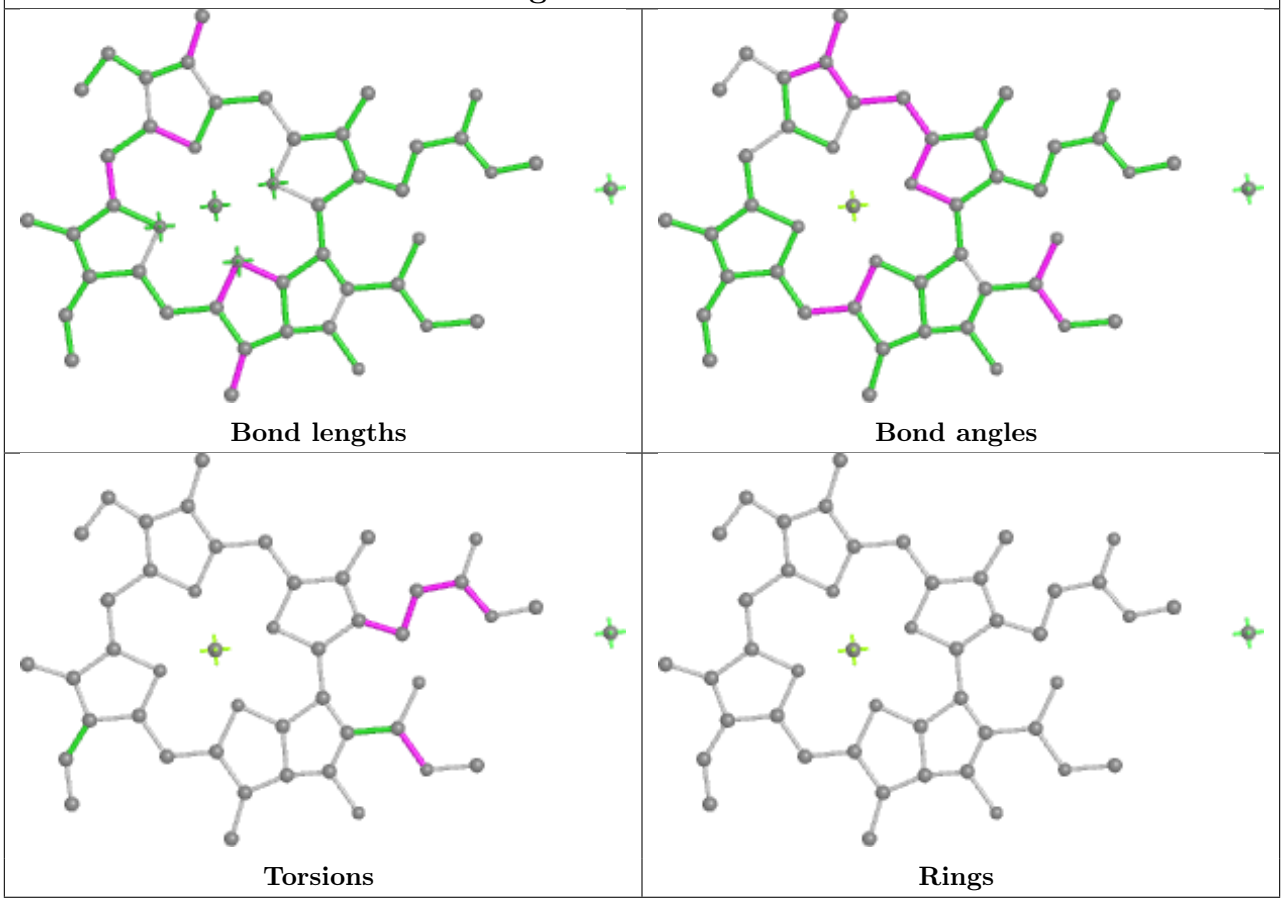
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	8	314	CLA	3	0
6	8	309	CLA	1	0
6	7	314	CLA	3	0
6	5	309	CLA	1	0
5	8	303	A86	1	0
6	8	312	CLA	3	0
6	9	313	CLA	4	0
5	5	304	A86	1	0
6	5	312	CLA	4	0
6	6	306	CLA	1	0
6	9	308	CLA	4	0
10	9	317	LMG	3	0
7	5	308	KC2	1	0
6	5	307	CLA	2	0
6	8	307	CLA	4	0
7	5	310	KC2	1	0
6	8	315	CLA	1	0
8	8	311	KC1	2	0
6	9	311	CLA	3	0
9	7	318	LMT	2	0
10	7	317	LMG	6	0
6	7	316	CLA	6	0
6	5	314	CLA	2	0
6	9	309	CLA	2	0
6	6	305	CLA	5	0
9	7	319	LMT	2	0
5	8	304	A86	1	0
6	7	308	CLA	3	0
5	9	303	A86	1	0
6	9	312	CLA	3	0

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

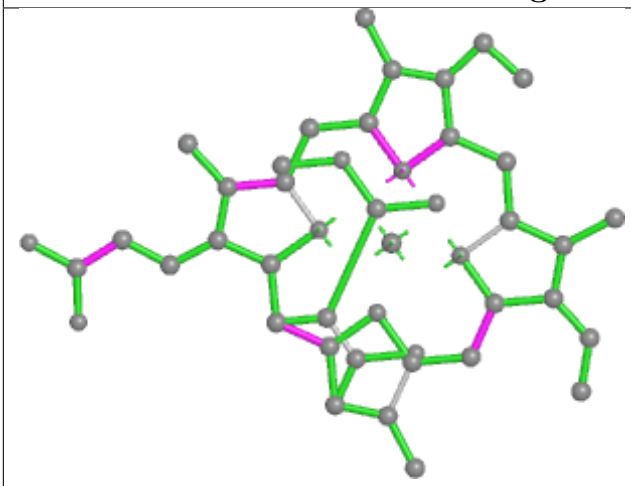
Ligand A86 9 305



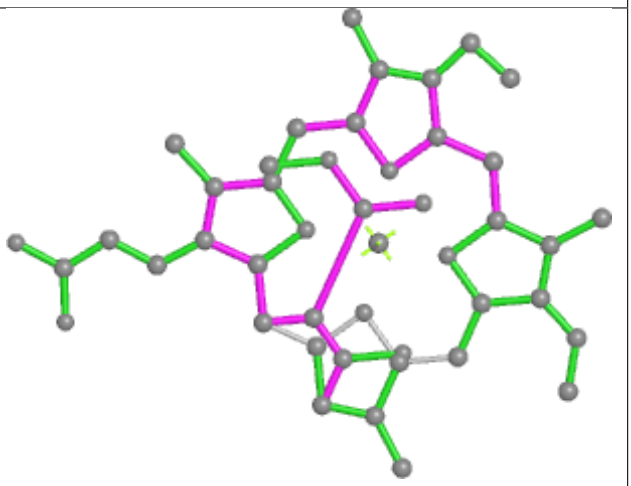
Ligand CLA 6 313



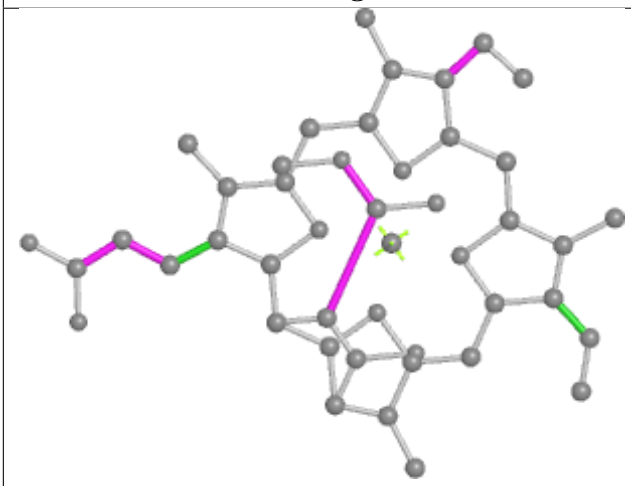
Ligand KC1 8 313



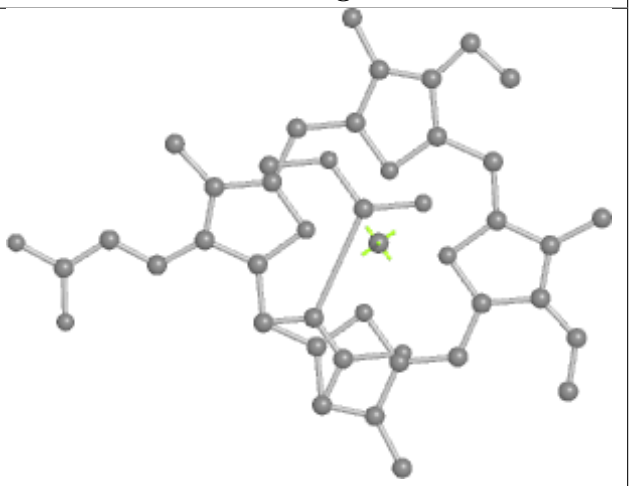
Bond lengths



Bond angles

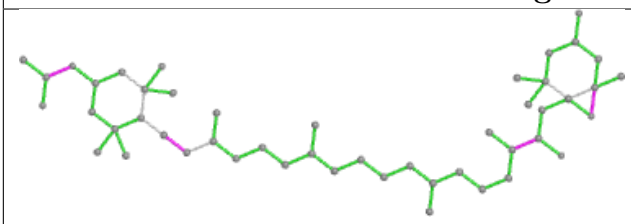


Torsions

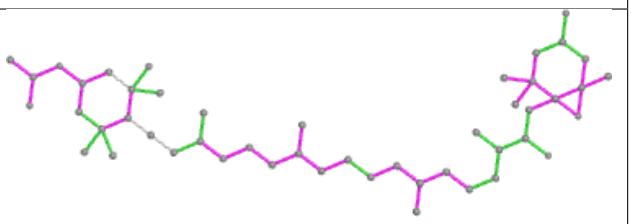


Rings

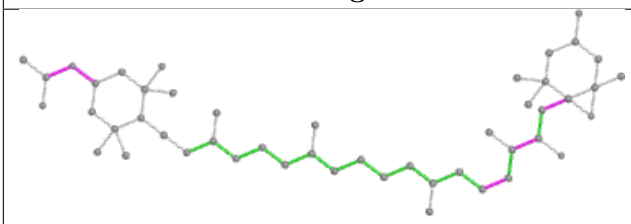
Ligand A86 9 301



Bond lengths



Bond angles



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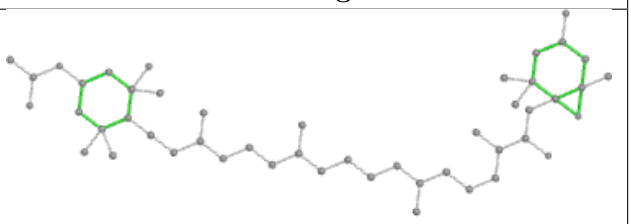
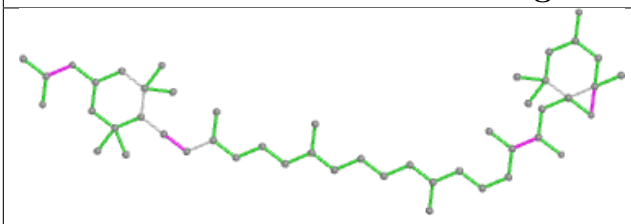
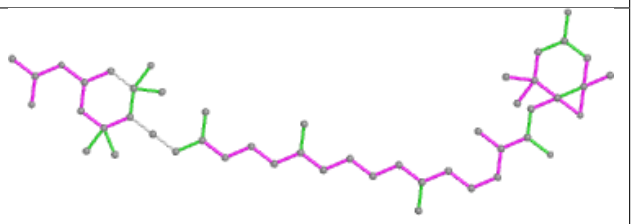


Rings

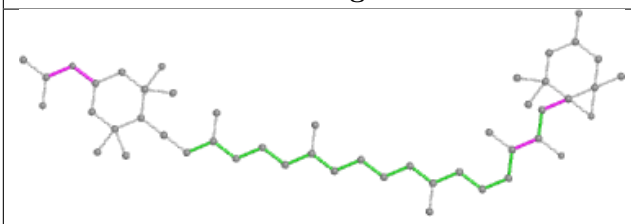
Ligand A86 5 303



Bond lengths



Bond angles



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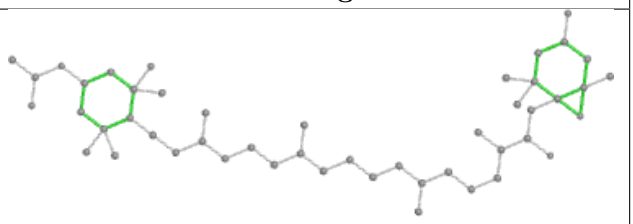
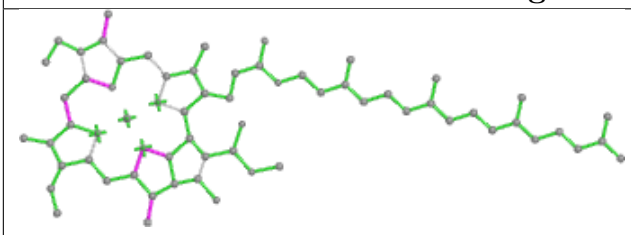
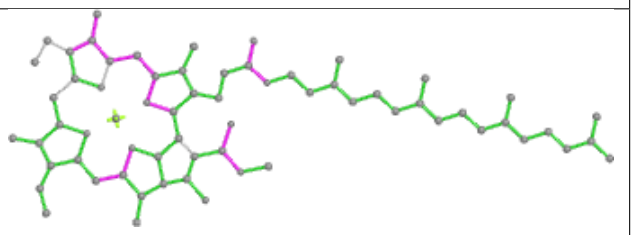


Rings

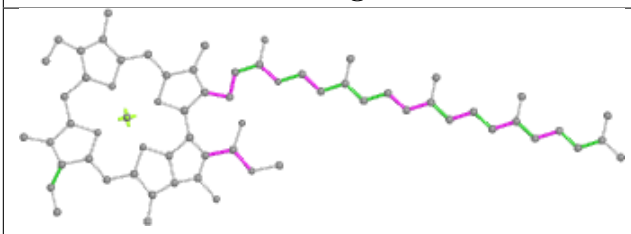
Ligand CLA 6 311



Bond lengths



Bond angles



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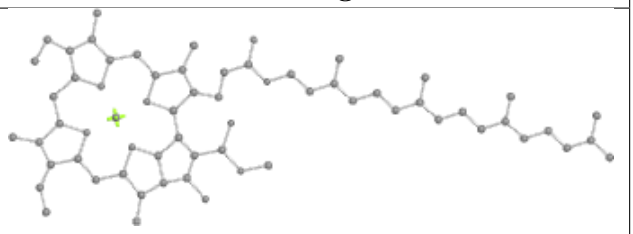
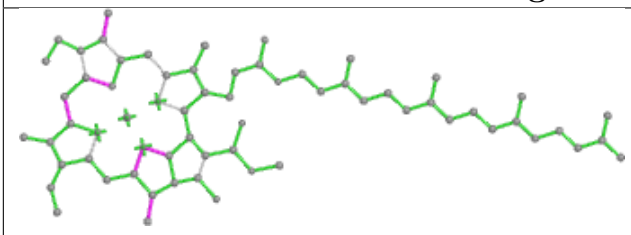


Rings

Ligand CLA 7 309



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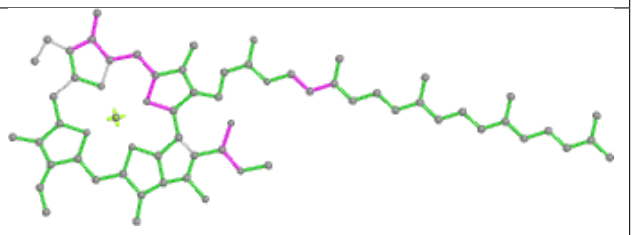

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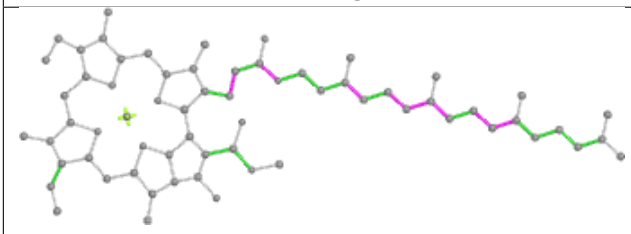

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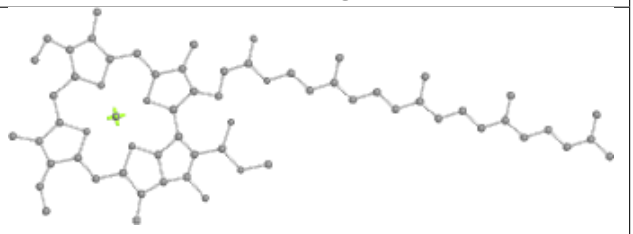

Rings

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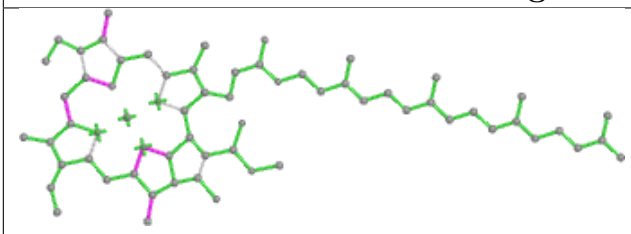

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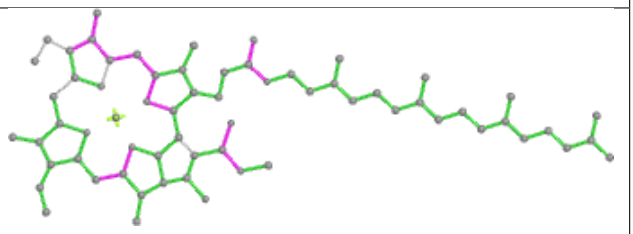

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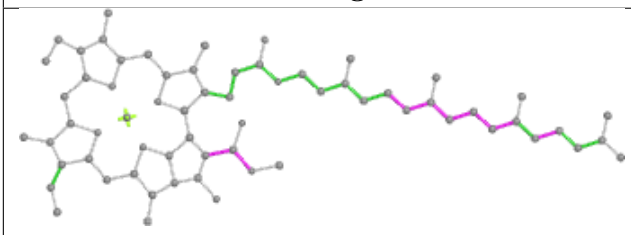

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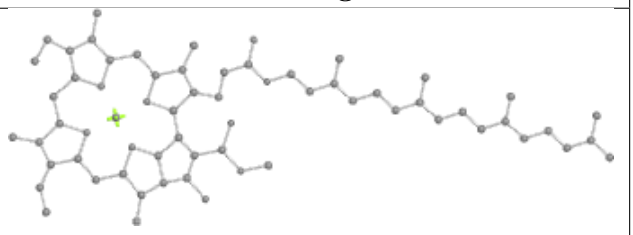
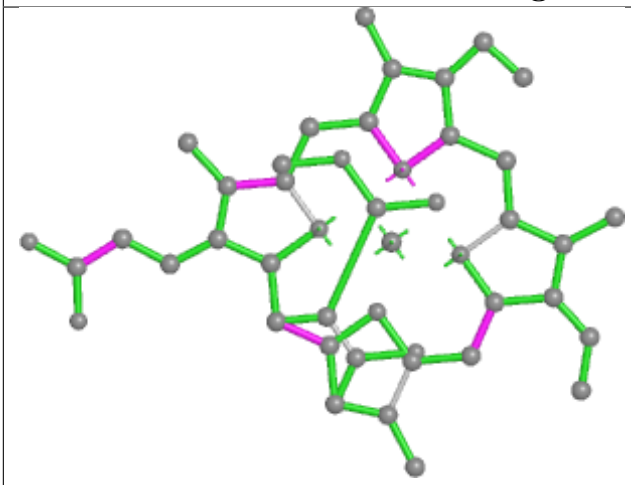


Rings

Ligand KC1 6 310



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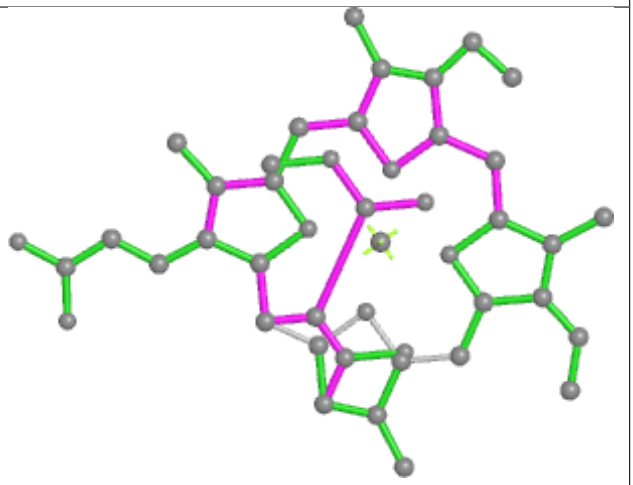

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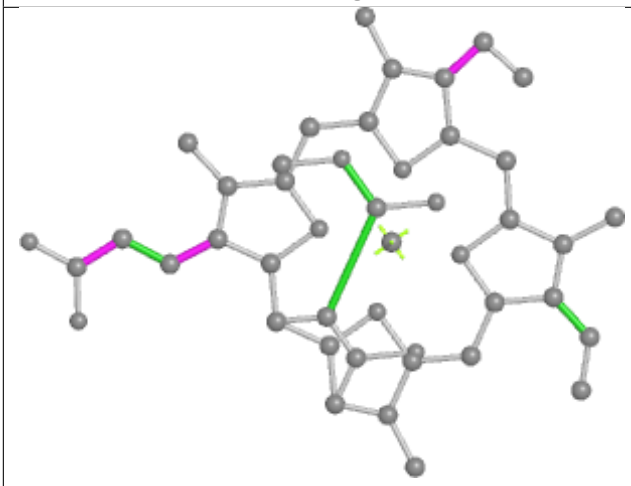

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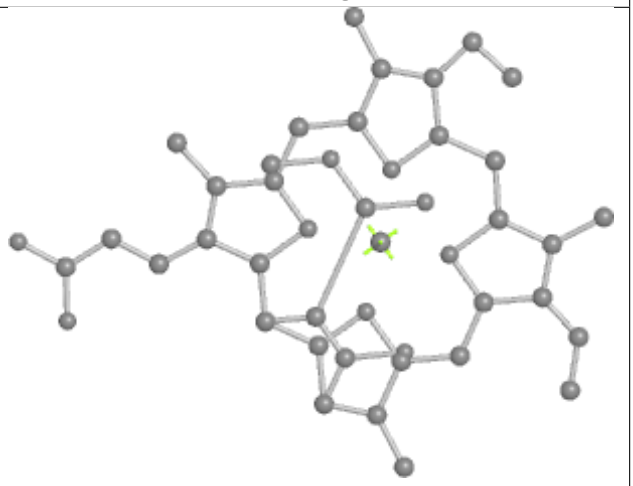
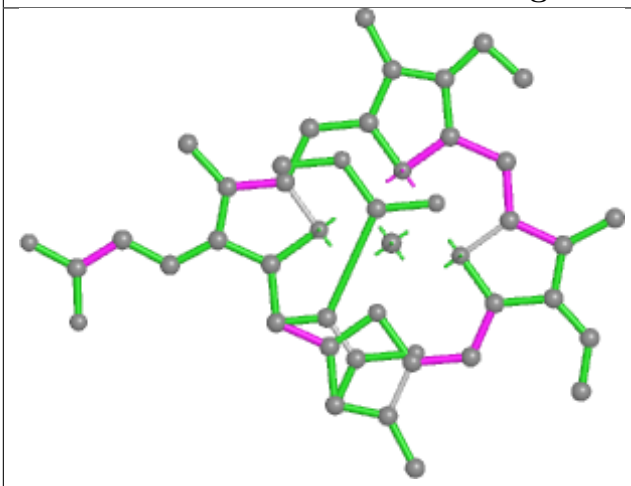


Rings

Ligand KC2 6 309



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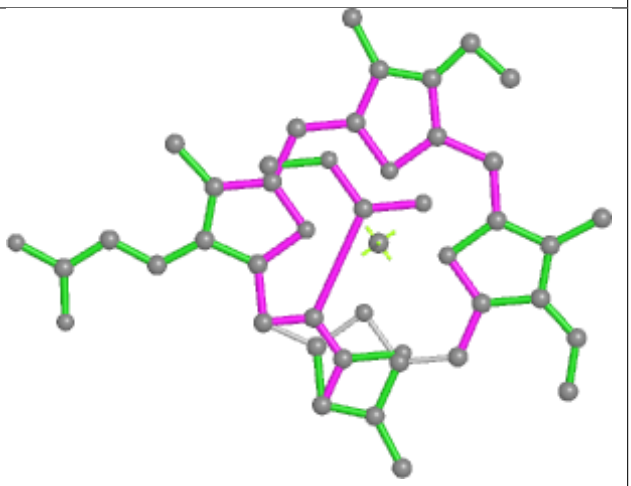
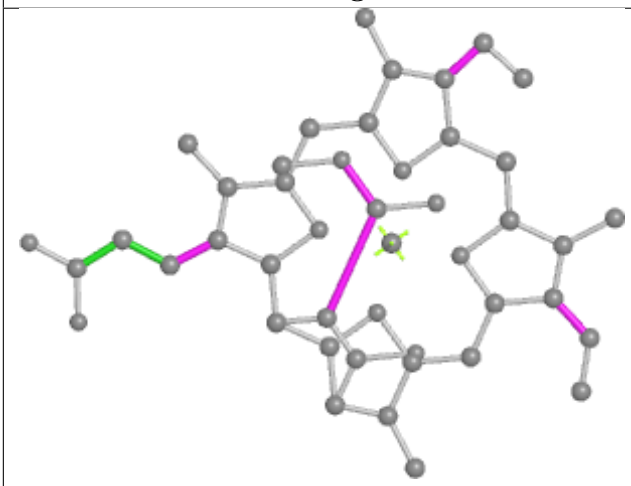


Bond angles



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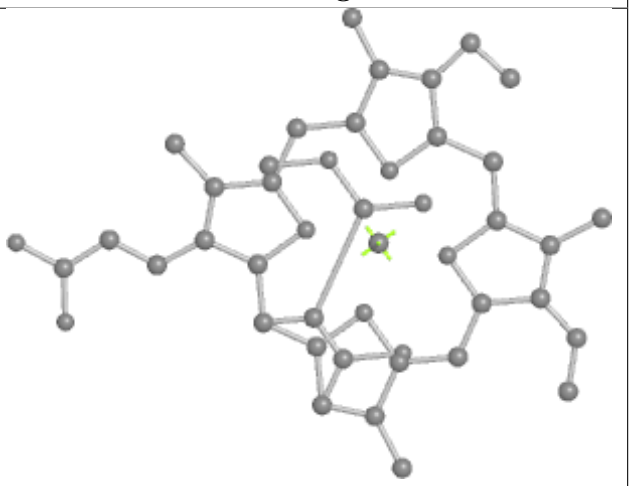
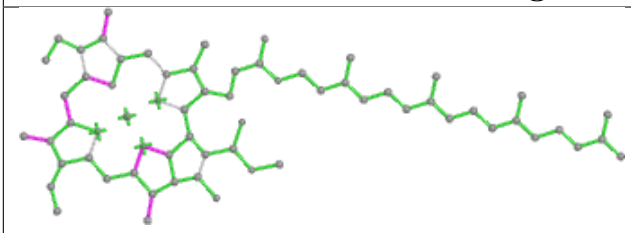
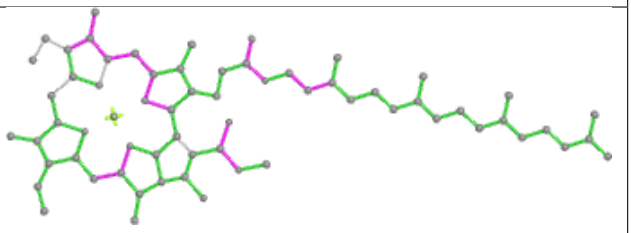


Rings

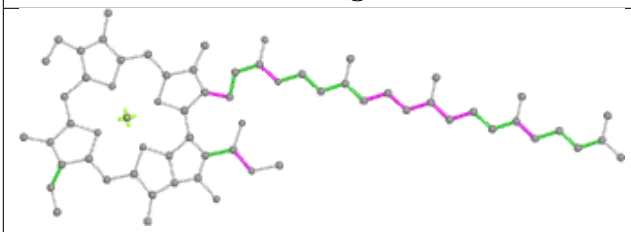
Ligand CLA 9 314



Bond lengths



Bond angles



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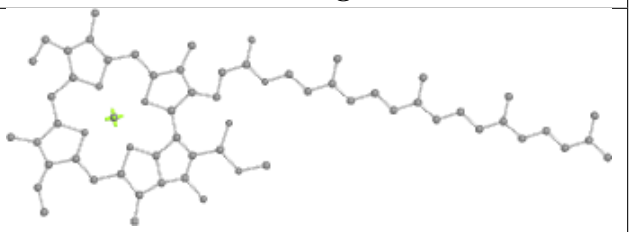
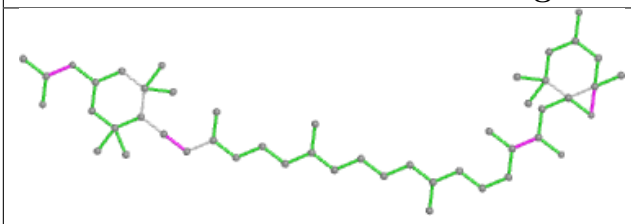


Rings

Ligand A86 7 305



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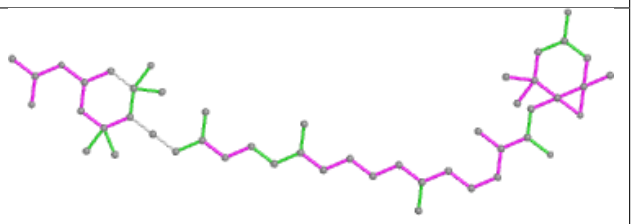

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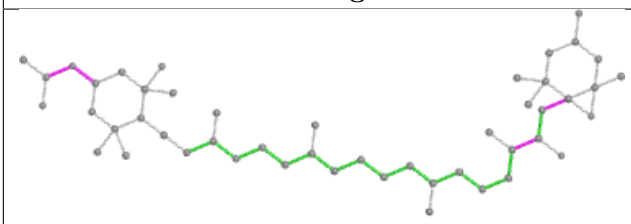
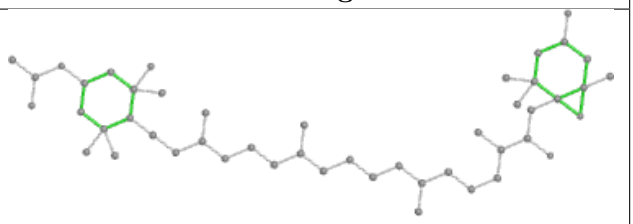
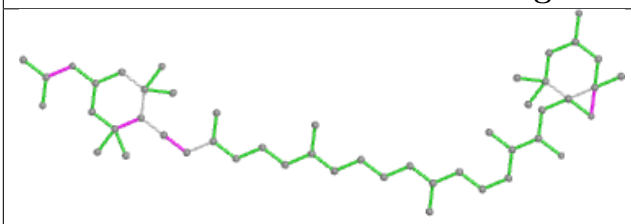


Torsions



Rings

Ligand A86 9 302



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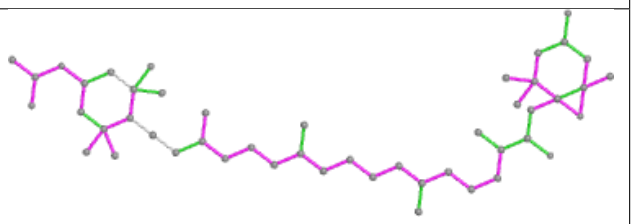

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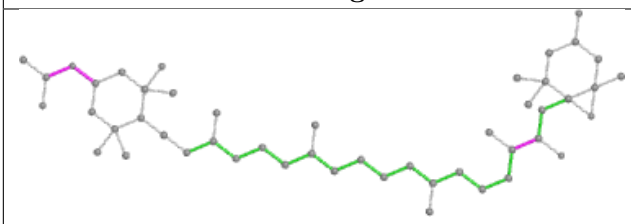

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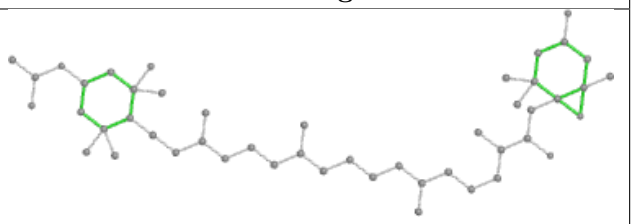

Rings

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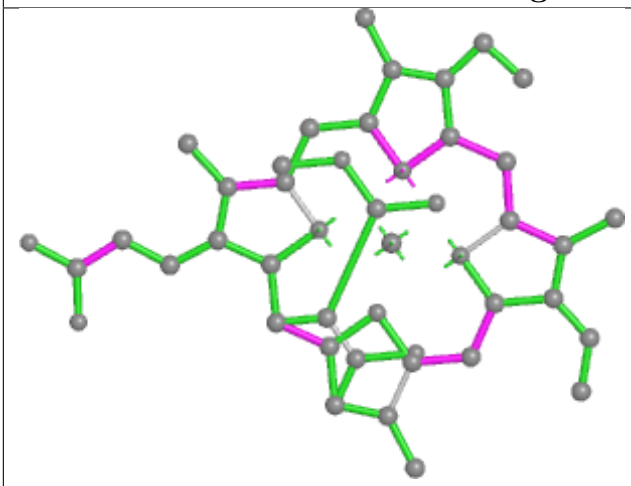

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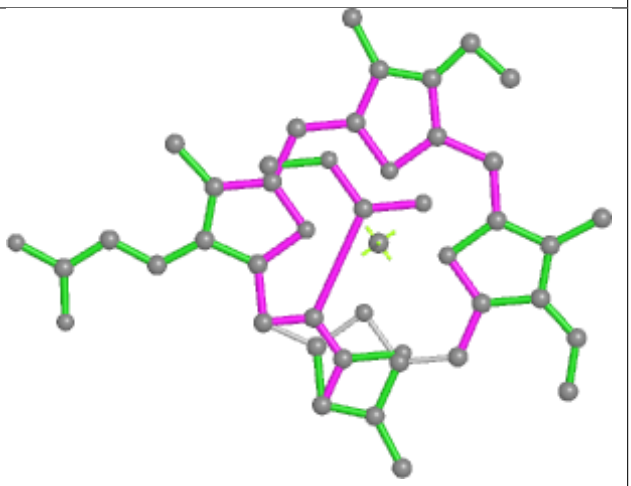

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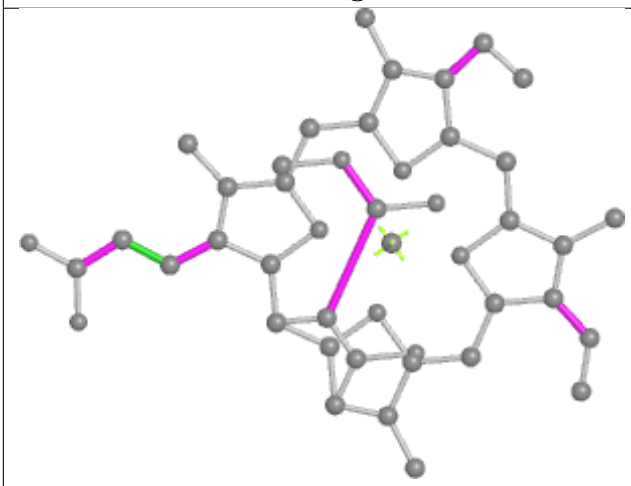

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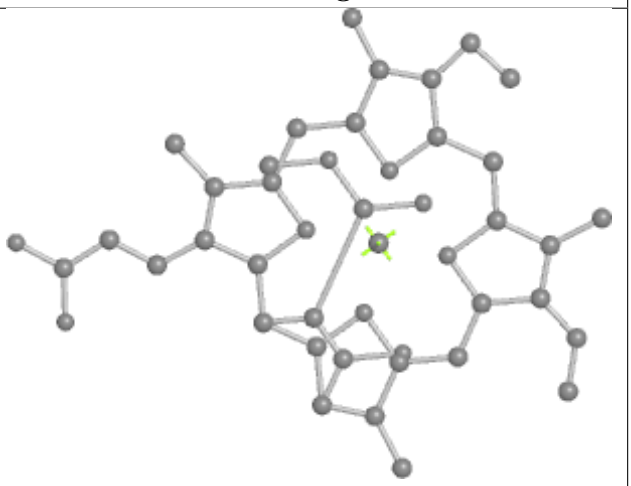

Rings

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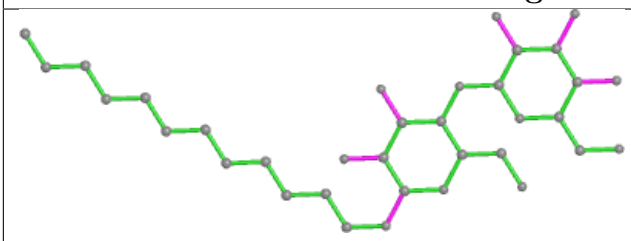

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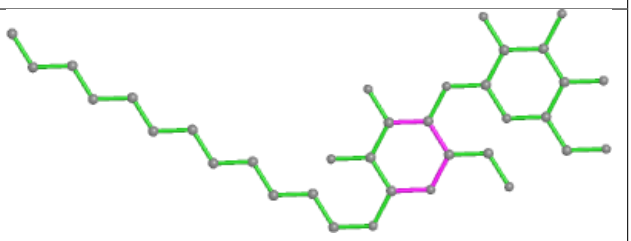

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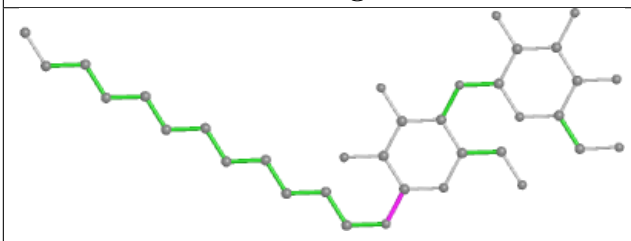

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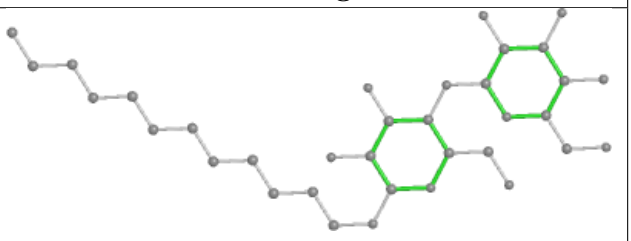

Rings

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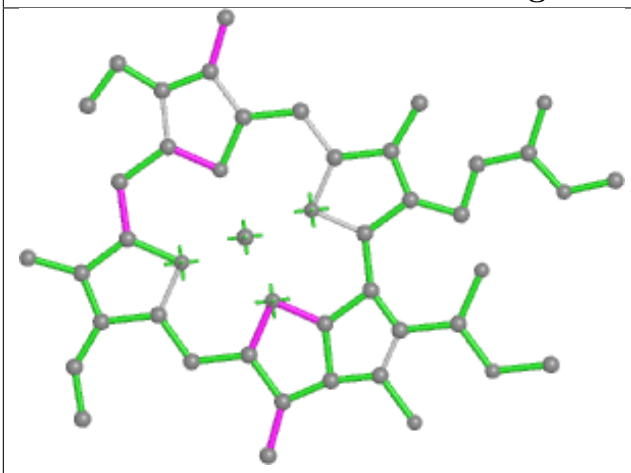

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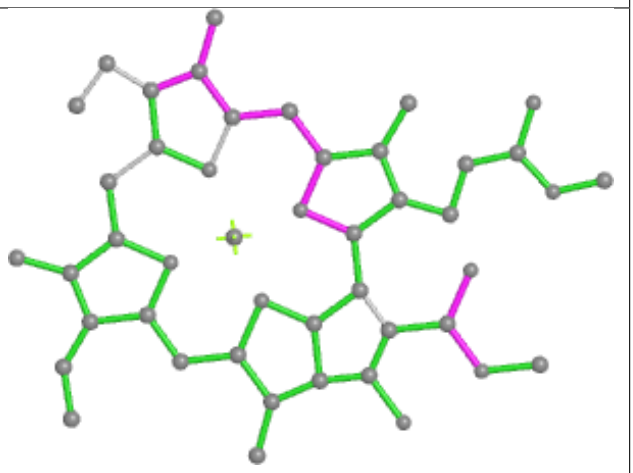

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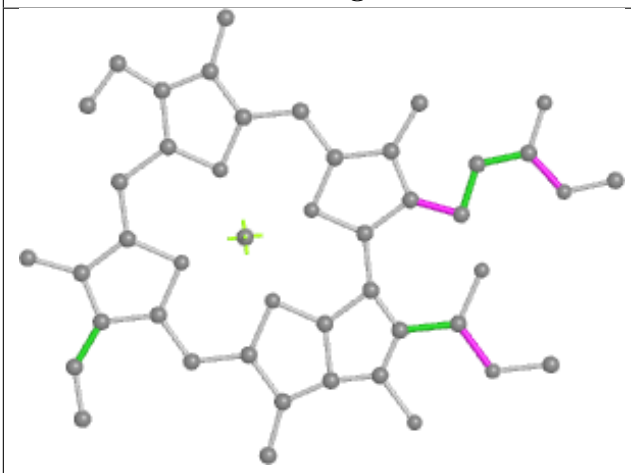

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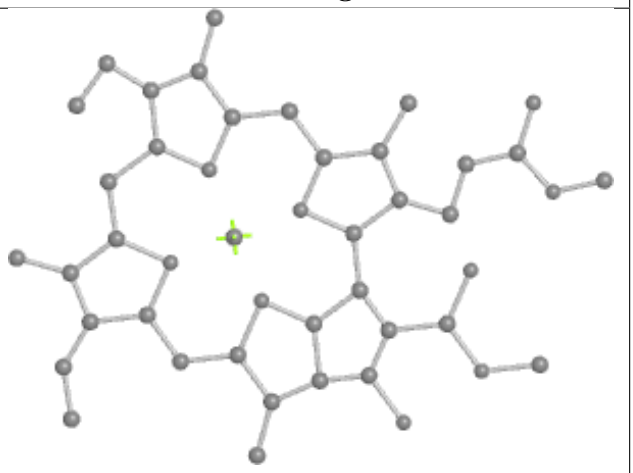
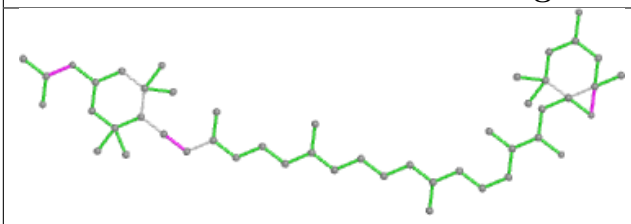


Rings

Ligand A86 6 301



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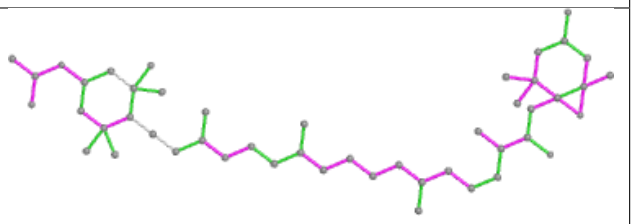

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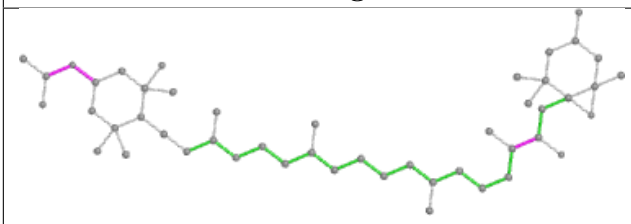

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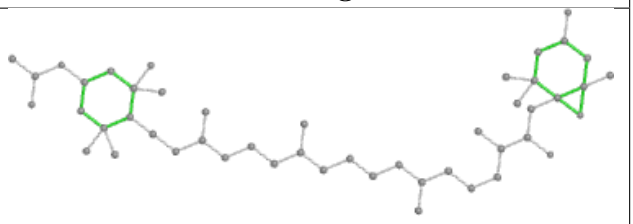

Rings

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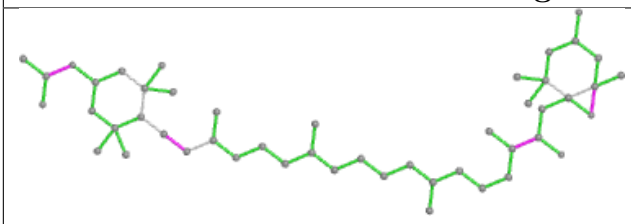

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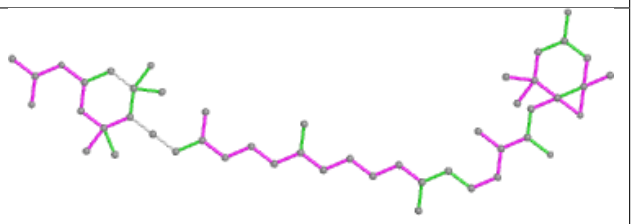

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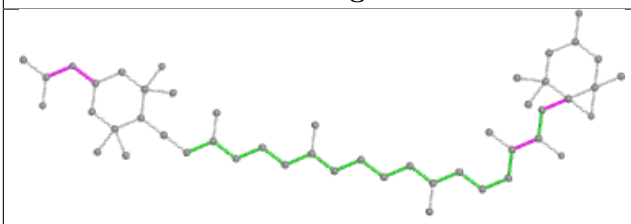

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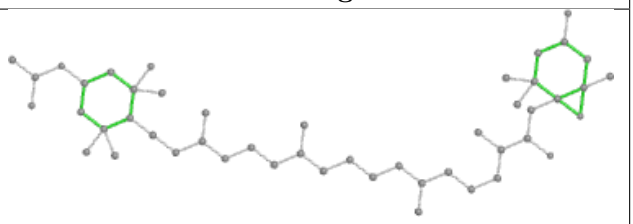

Rings

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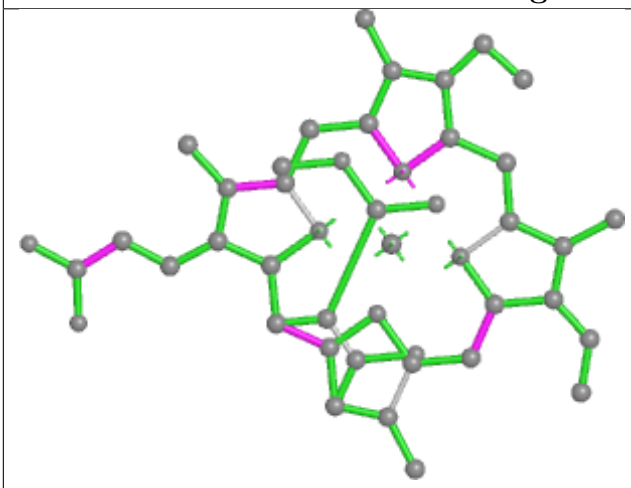

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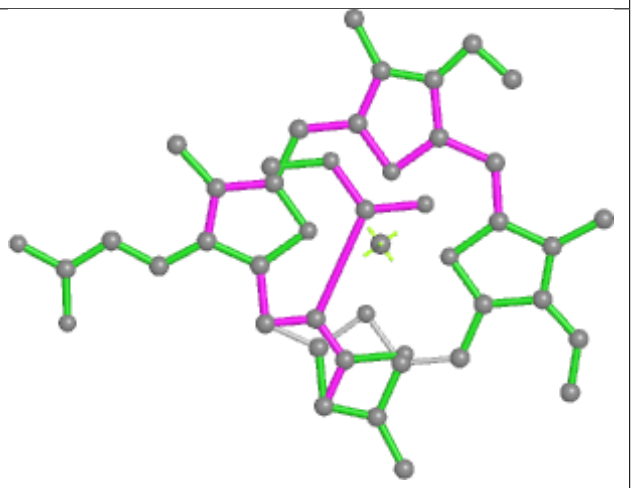

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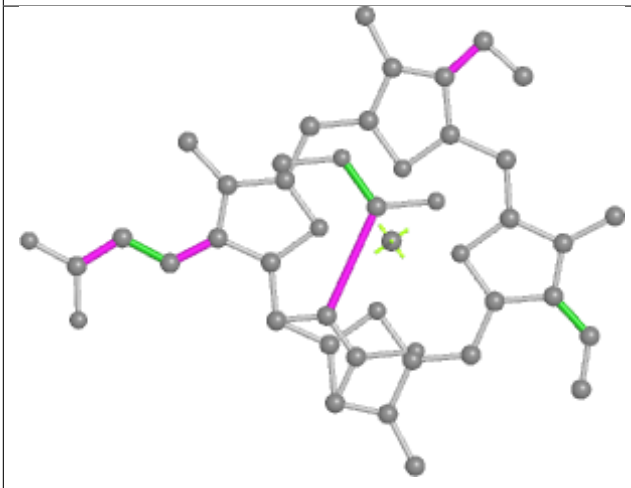

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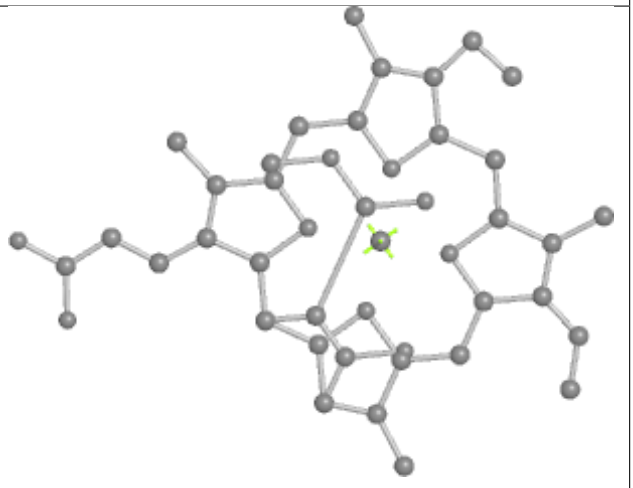

Rings

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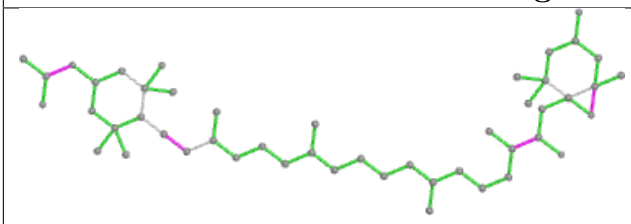

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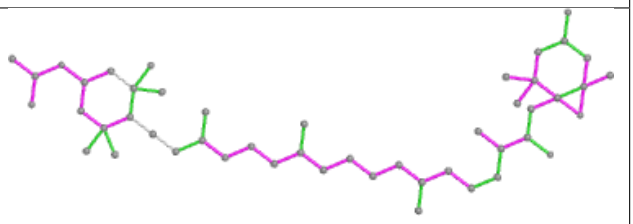

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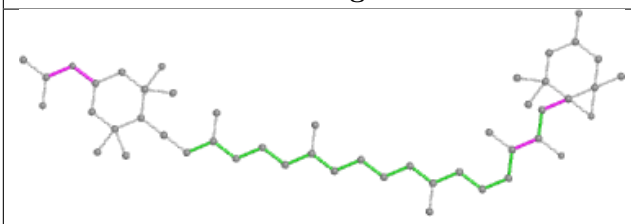

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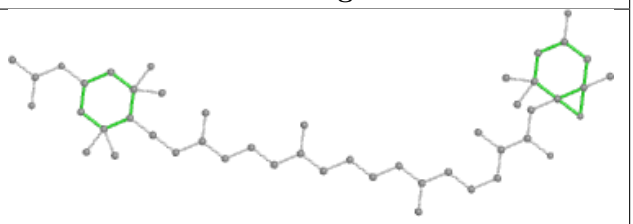

Rings

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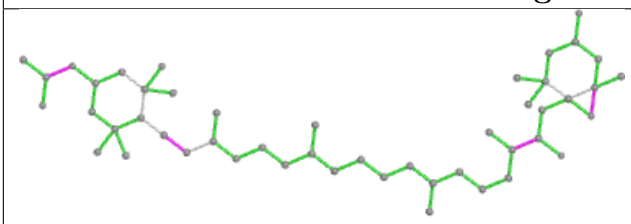

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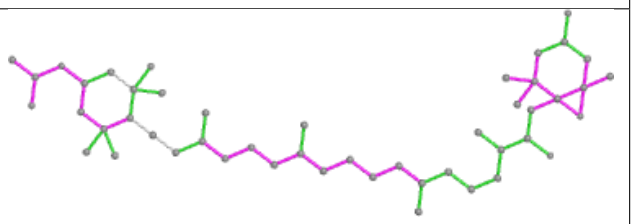

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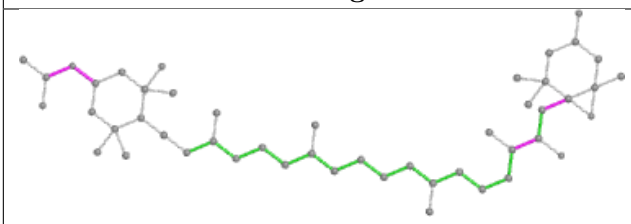

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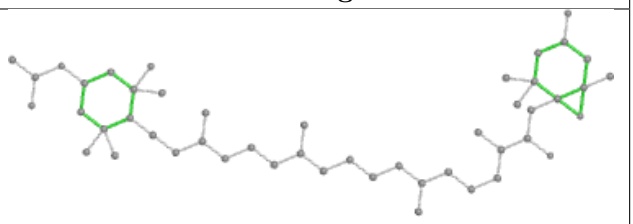

Rings

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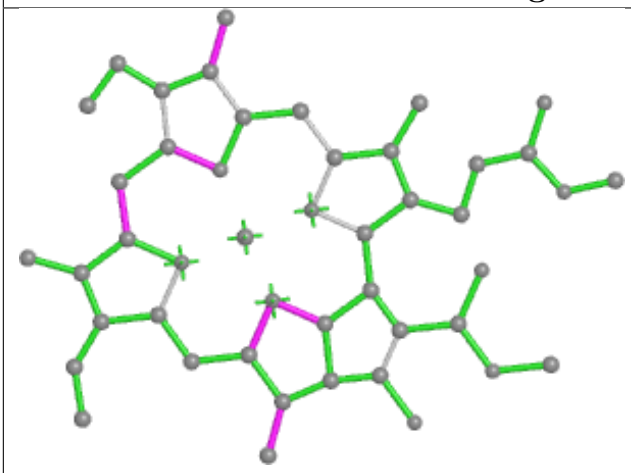

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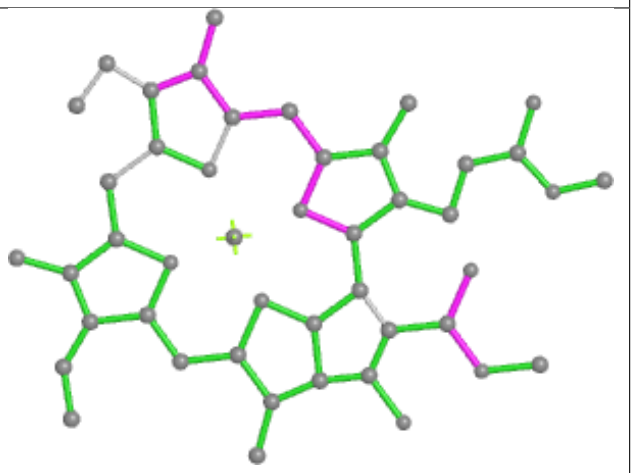

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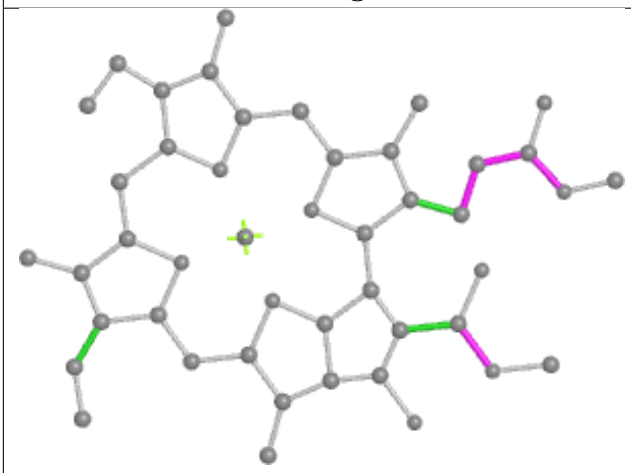

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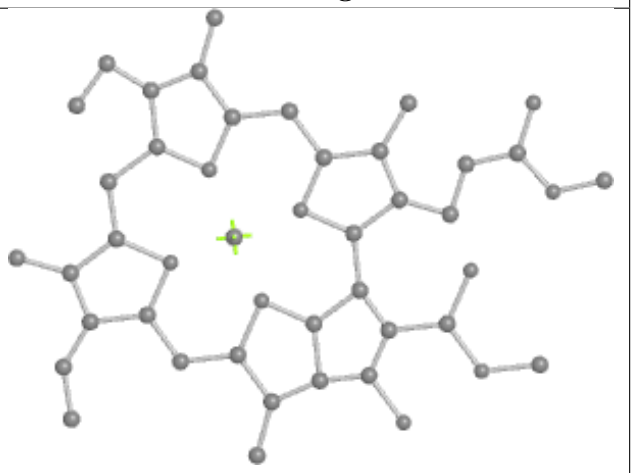

Rings

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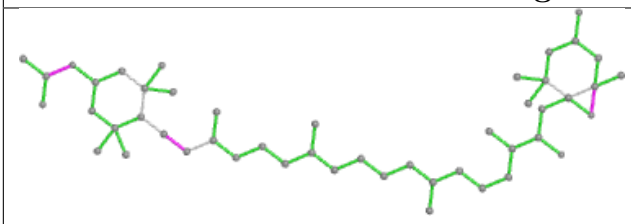

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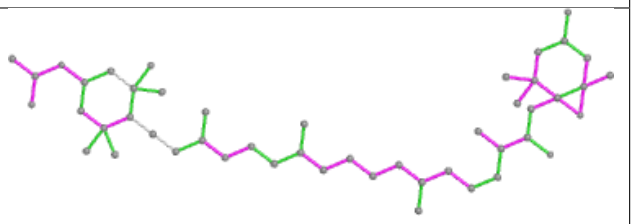

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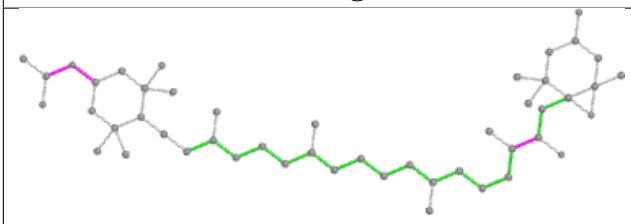

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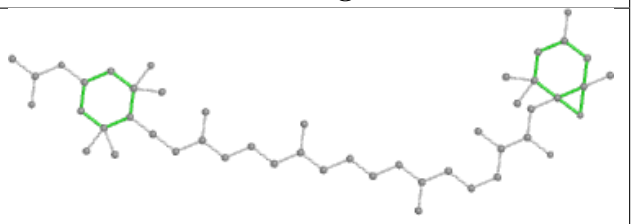

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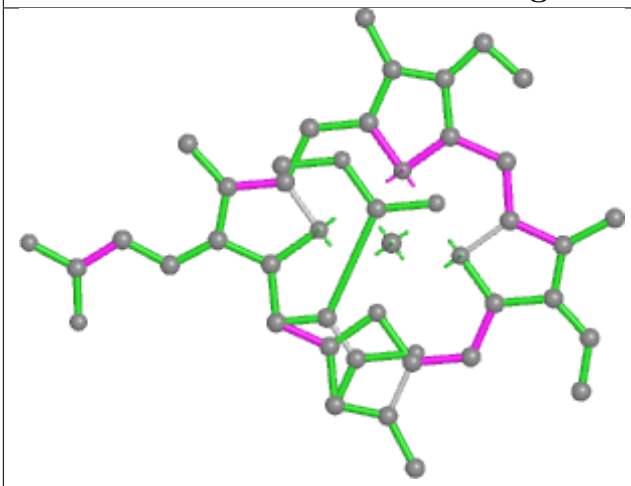

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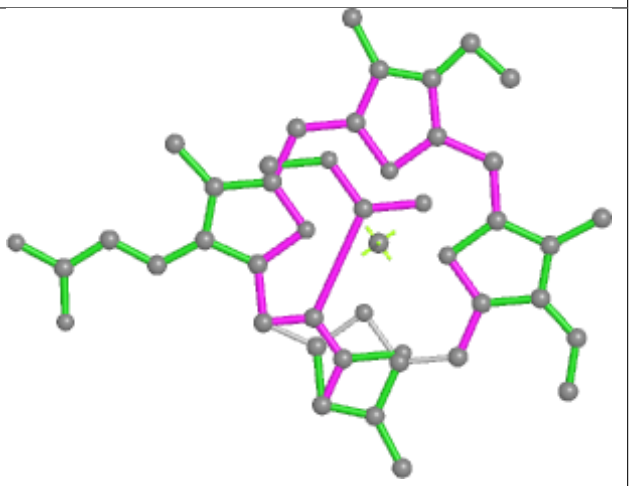

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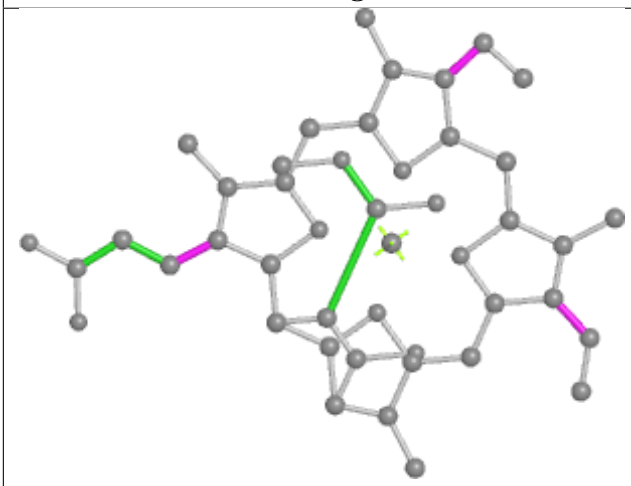

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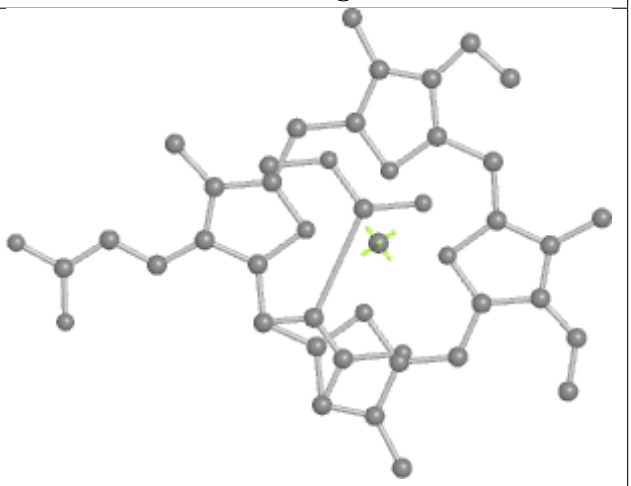

Rings

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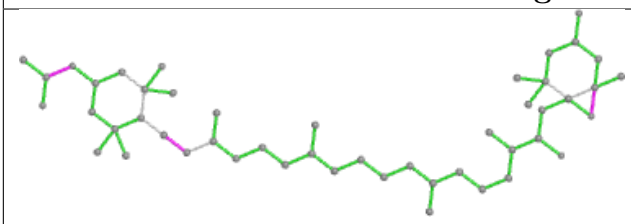

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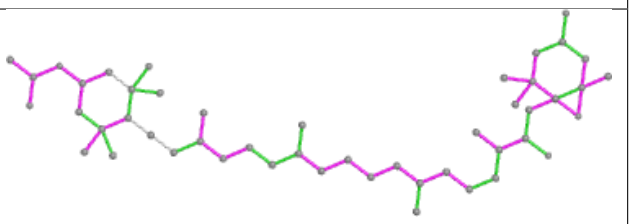

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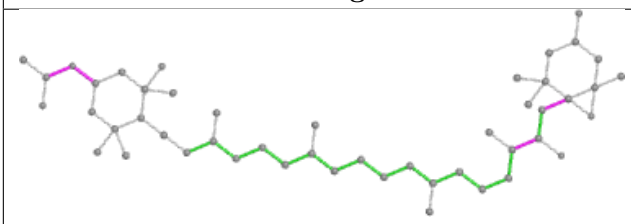

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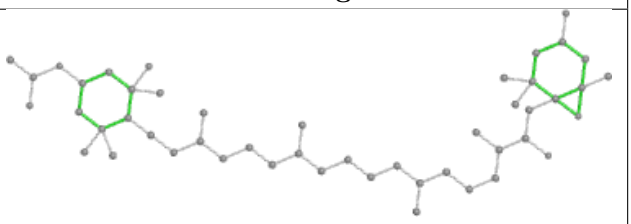
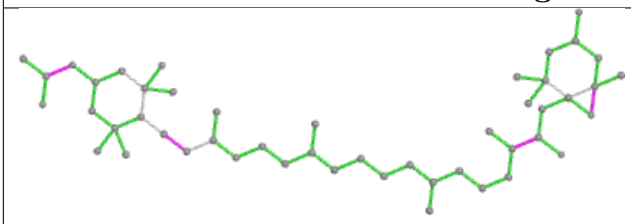


Rings

Ligand A86 8 302



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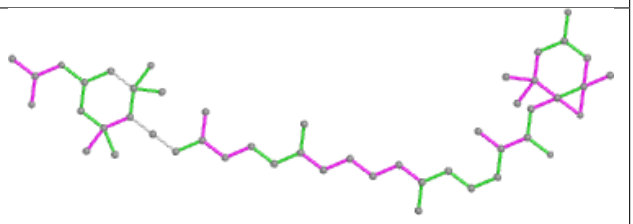
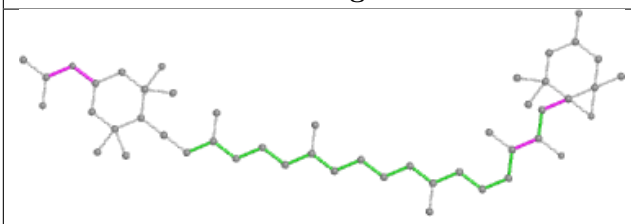


Bond angles



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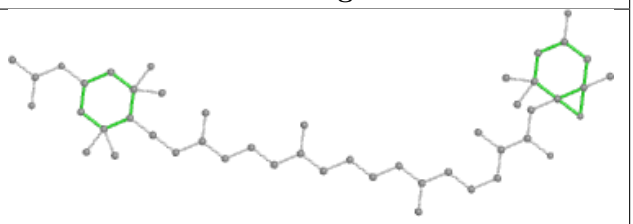
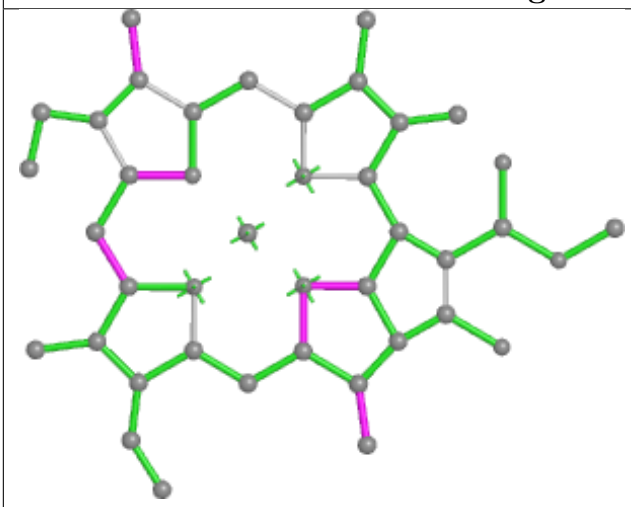
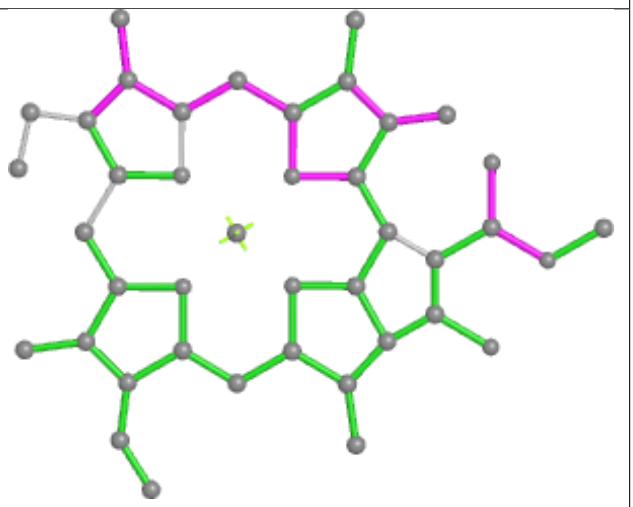


Rings

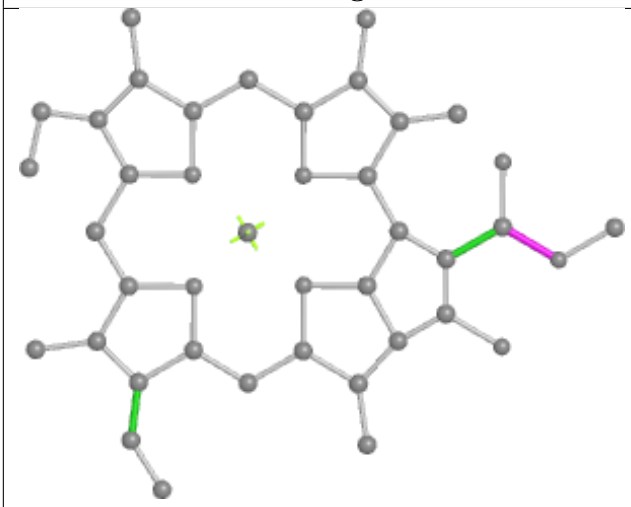
Ligand CLA 9 316



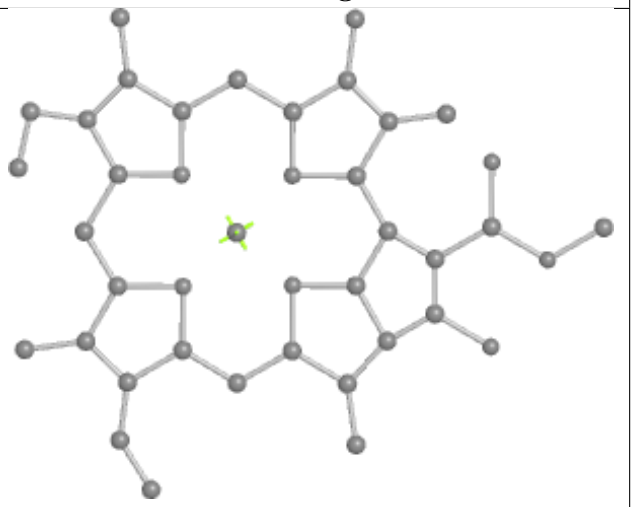
Bond lengths



Bond angles

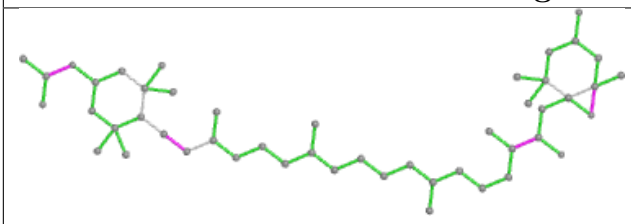


Torsions



Rings

Ligand A86 7 301



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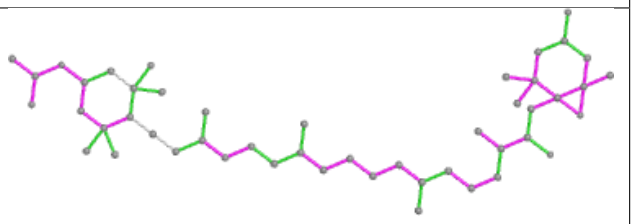

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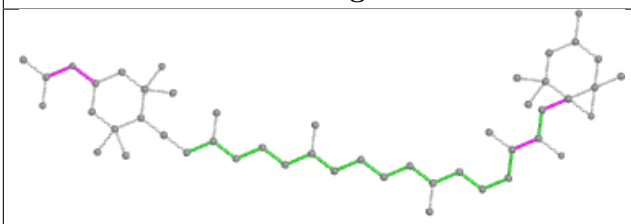

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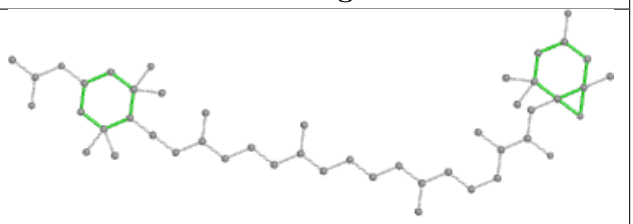
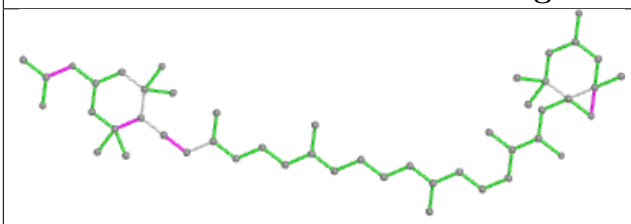


Rings

Ligand A86 7 307



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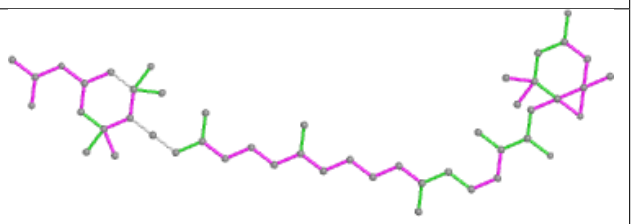

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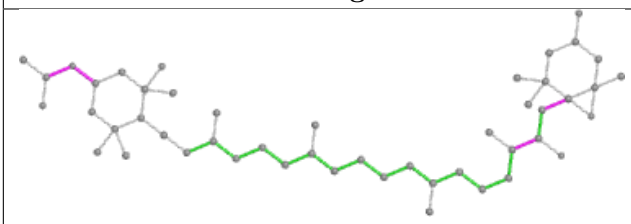

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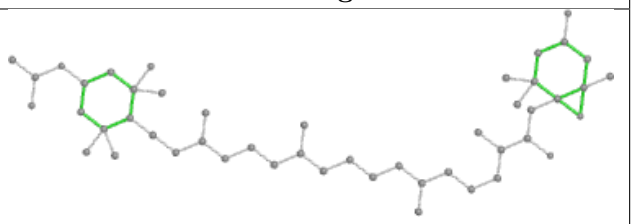
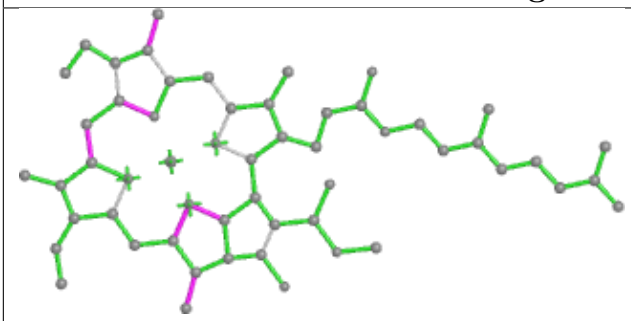


Rings

Ligand CLA 7 311



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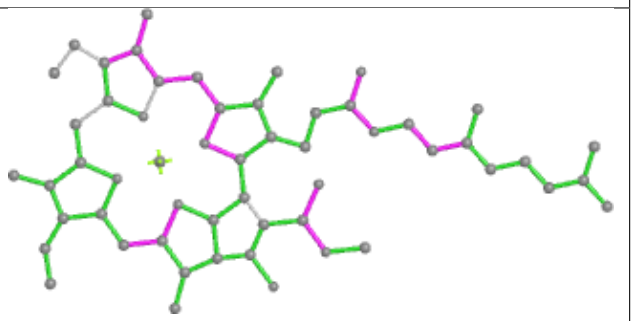

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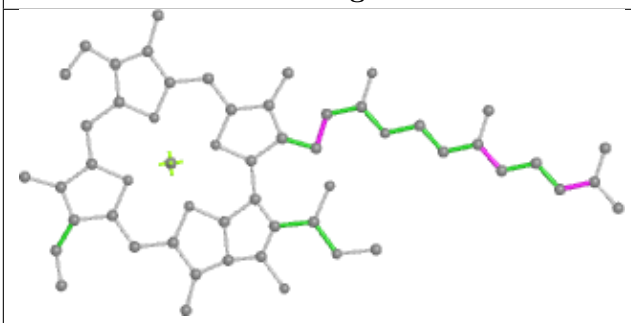

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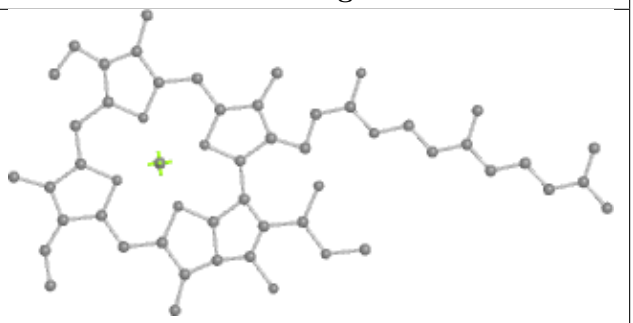
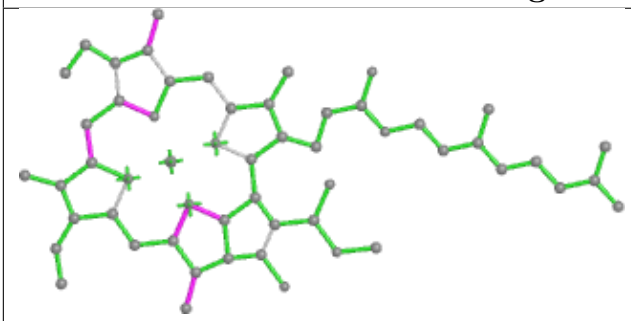


Rings

Ligand CLA 8 309



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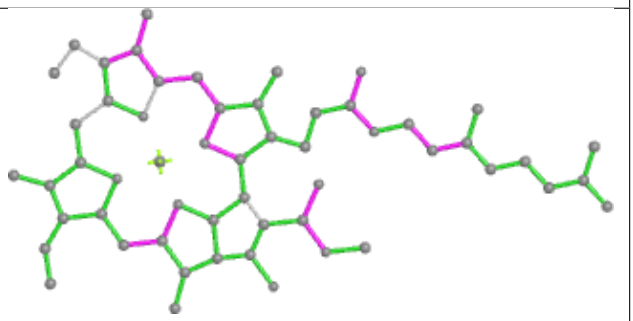
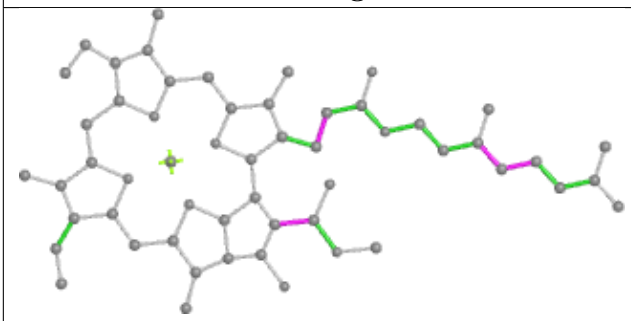


Bond angles



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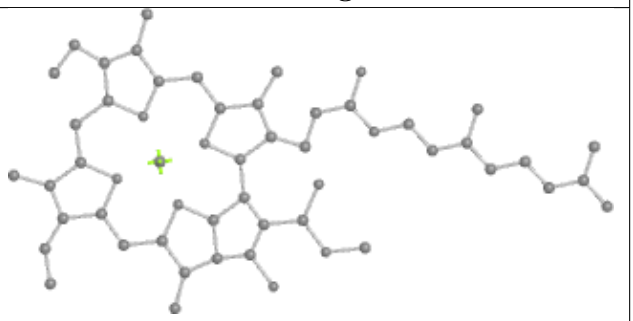
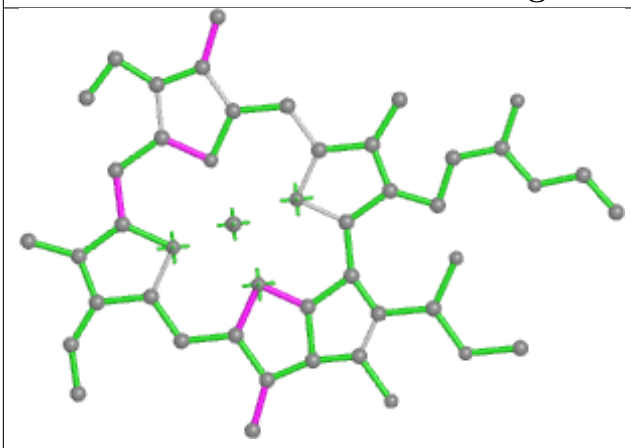


Rings

Ligand CLA 7 314



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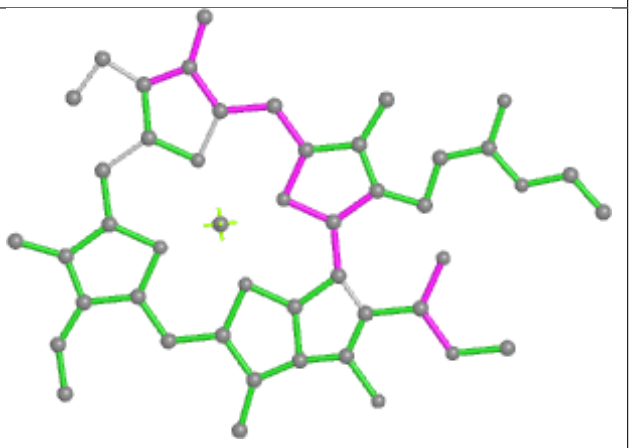
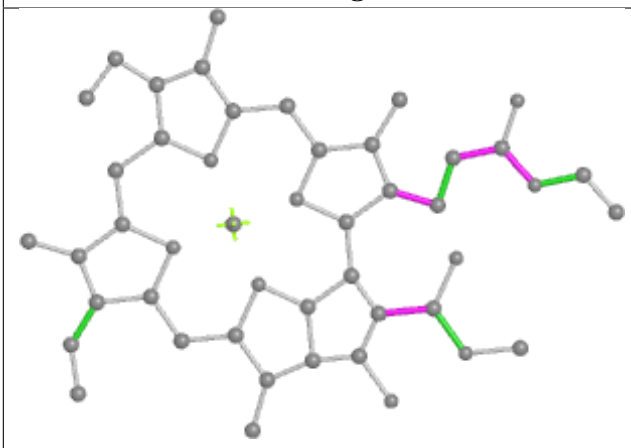


Bond angles



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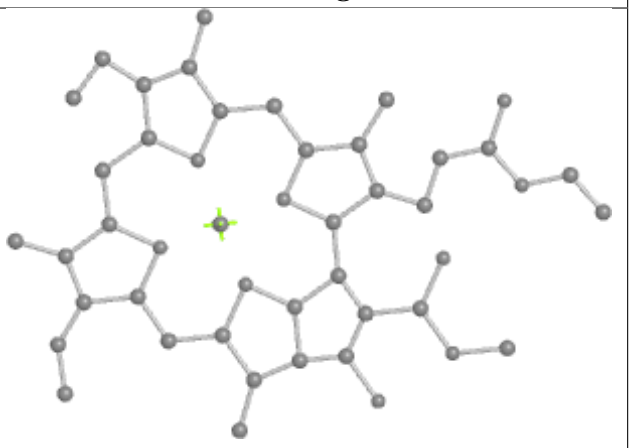
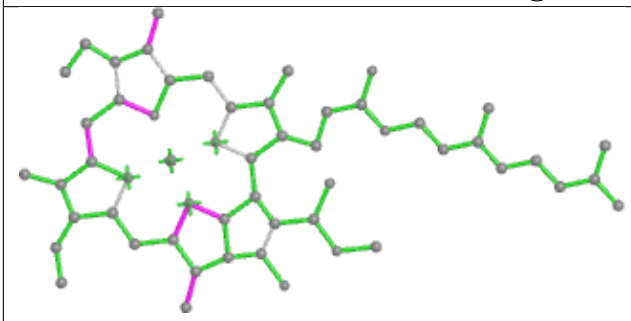


Rings

Ligand CLA 5 309



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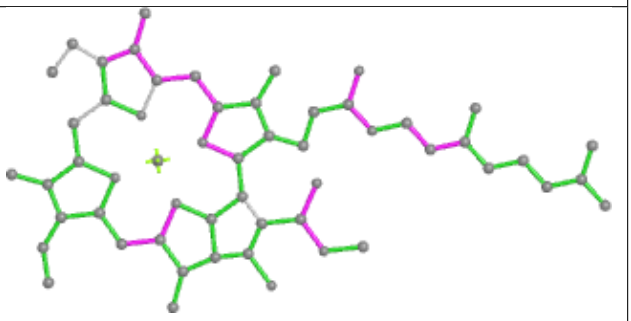

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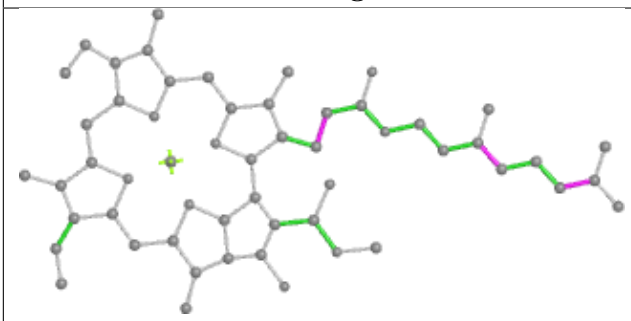

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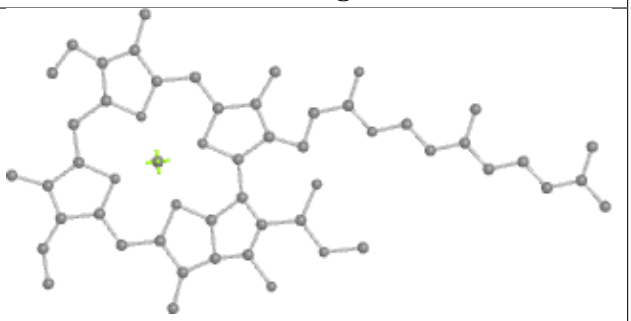
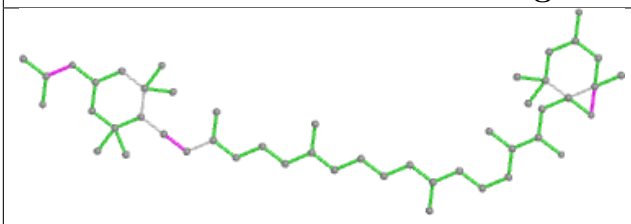


Rings

Ligand A86 8 303



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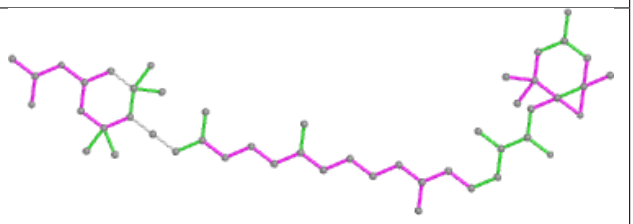

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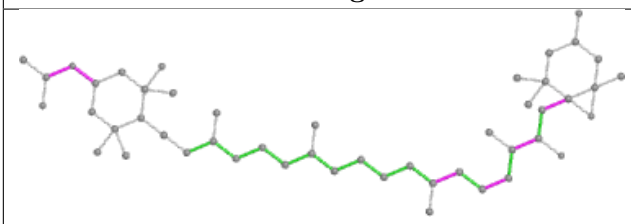

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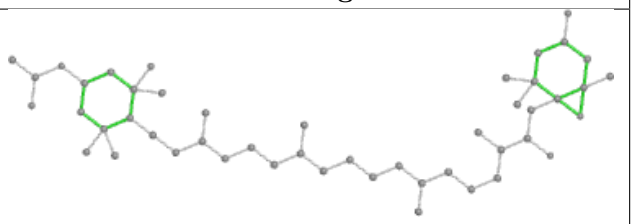
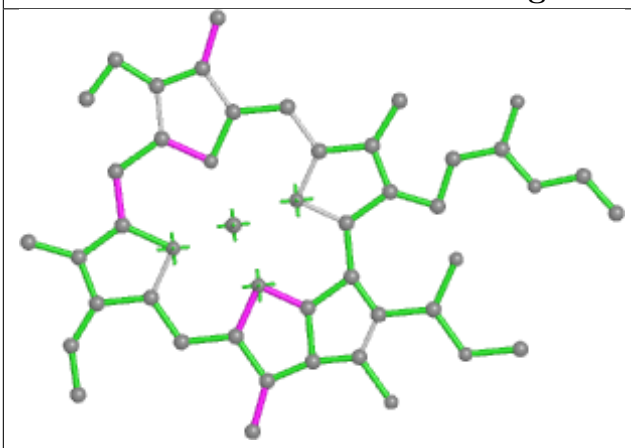


Rings

Ligand CLA 8 312



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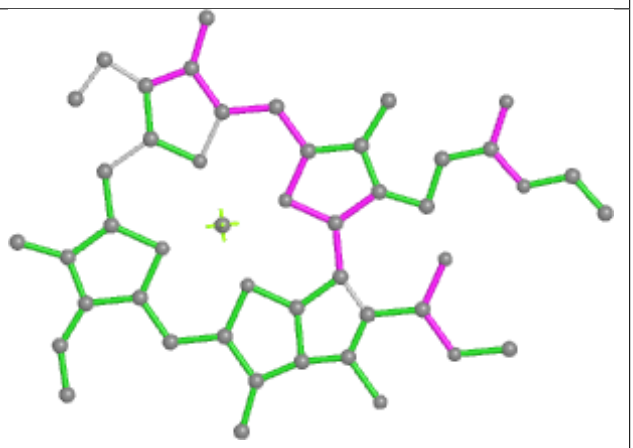
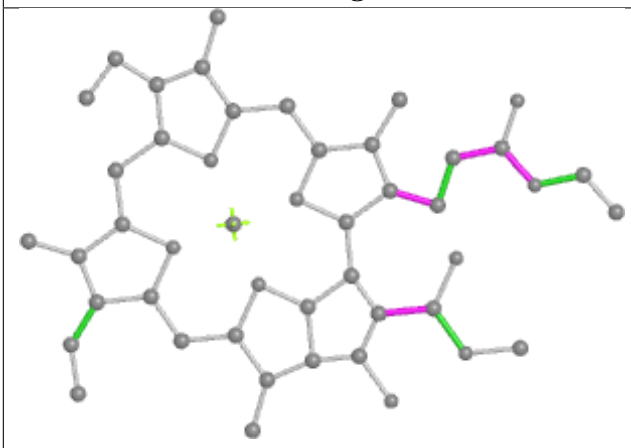


Bond angles



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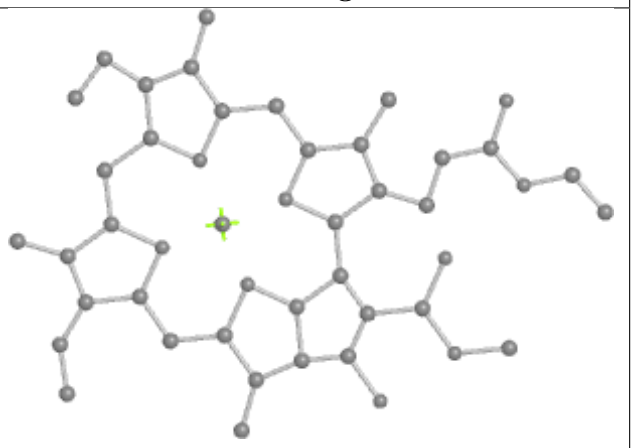
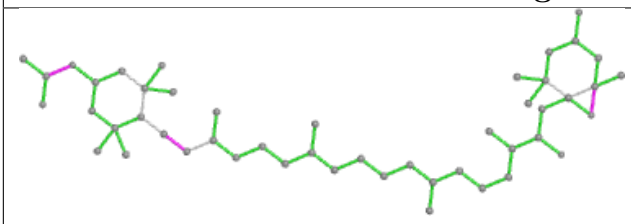


Rings

Ligand A86 7 306



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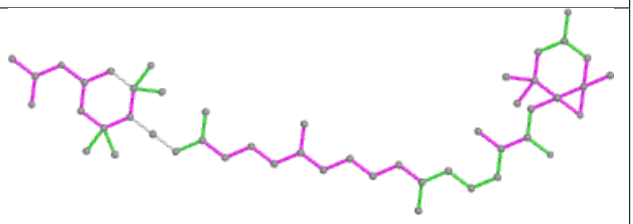

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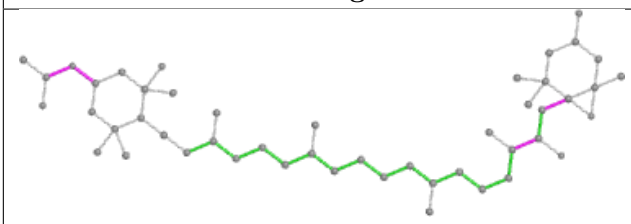
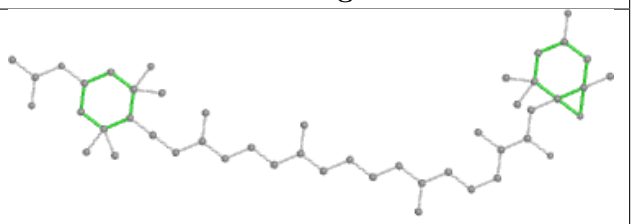
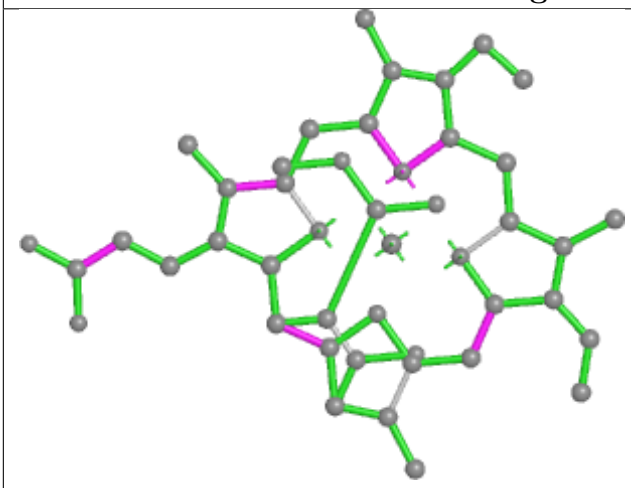


Torsions

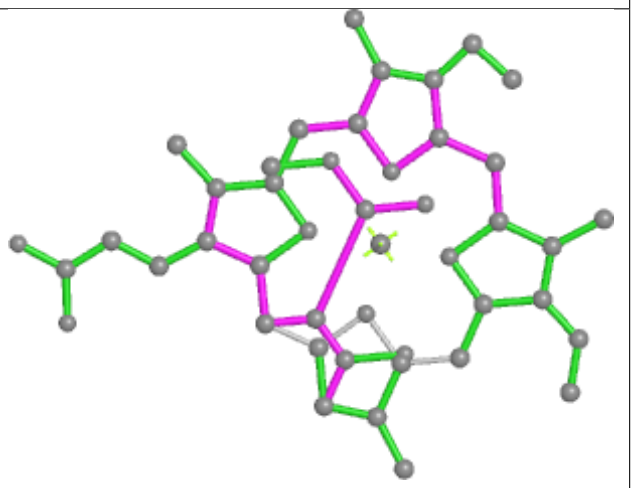


Rings

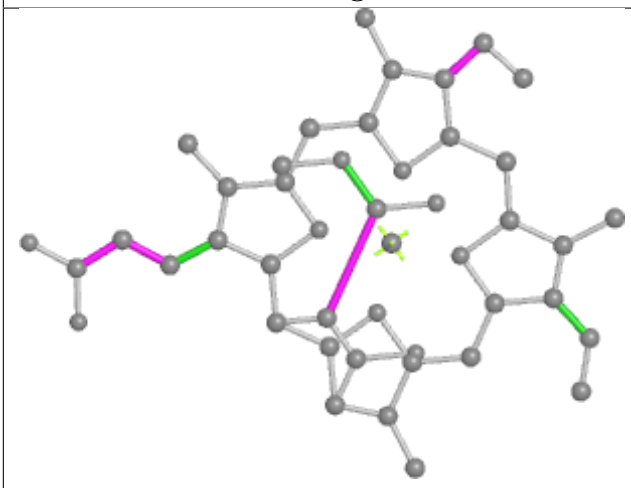
Ligand KC1 6 312



Bond lengths



Bond angles



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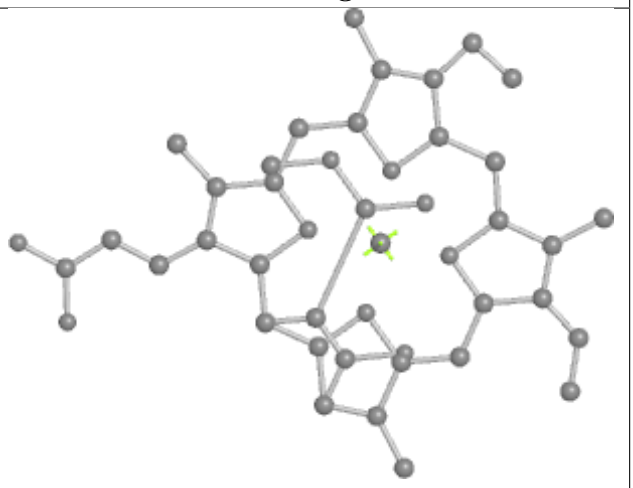
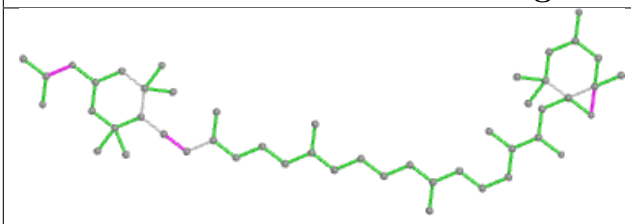


Rings

Ligand A86 5 318



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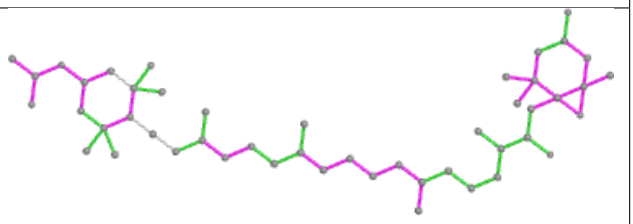
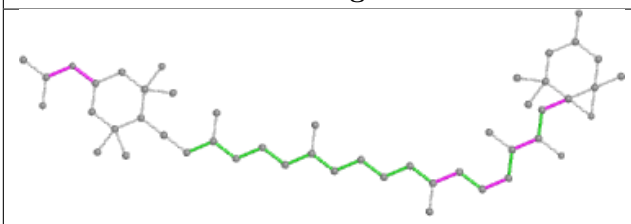


Bond angles



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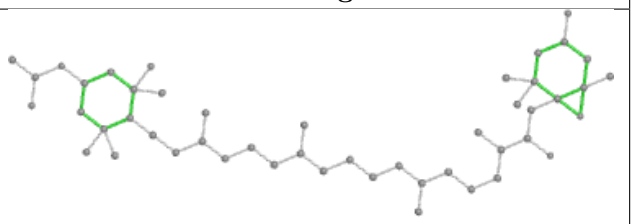
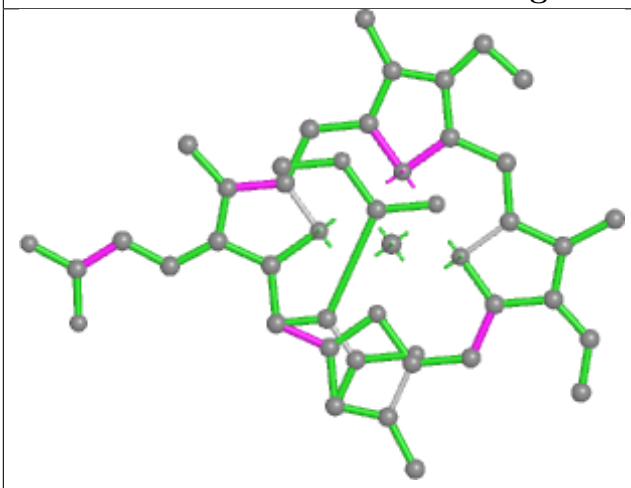


Rings

Ligand KC1 7 315



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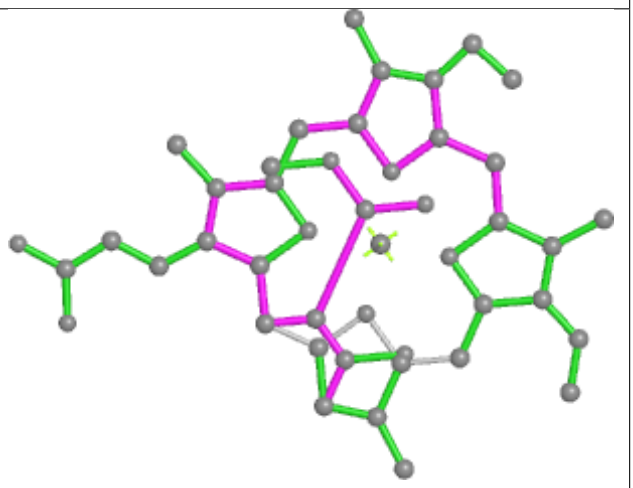

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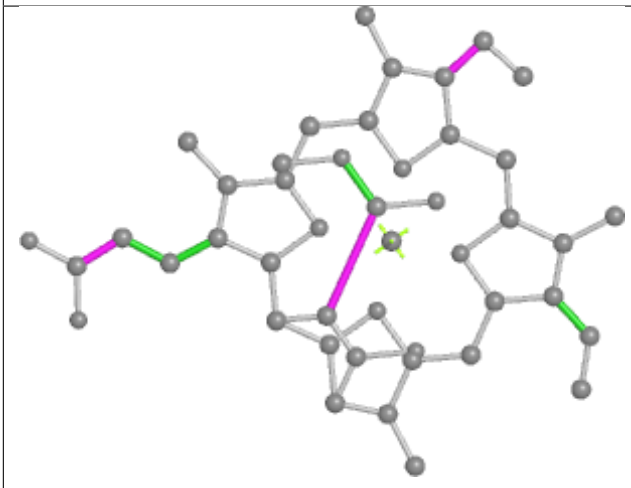

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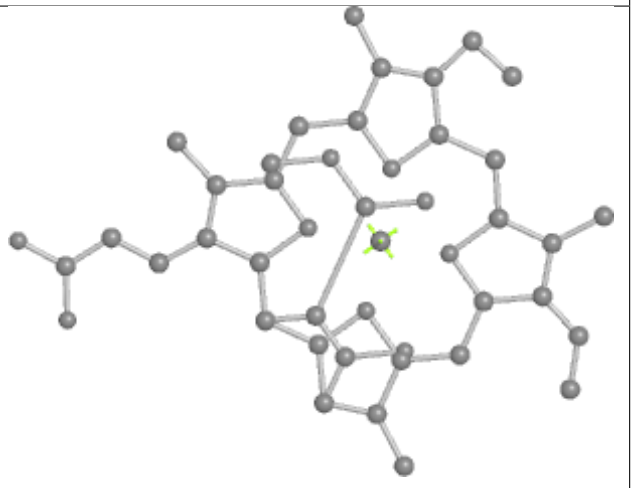
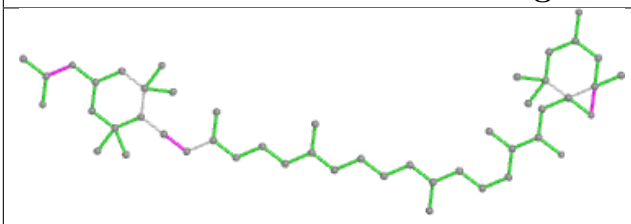
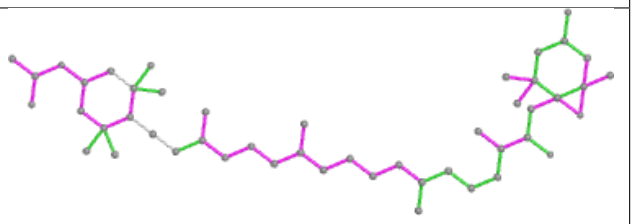


Rings

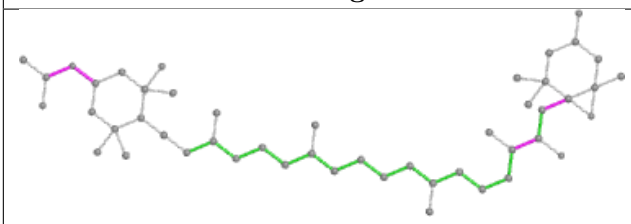
Ligand A86 5 305



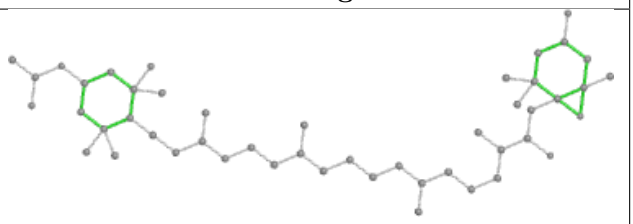
Bond lengths



Bond angles

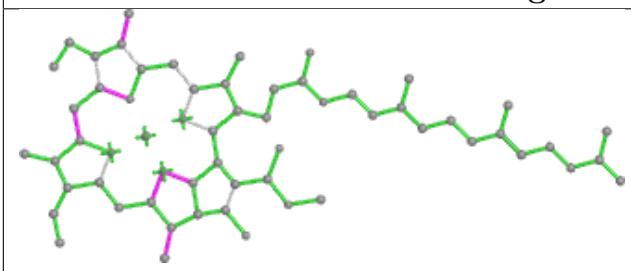


Torsions



Rings

Ligand CLA 9 313



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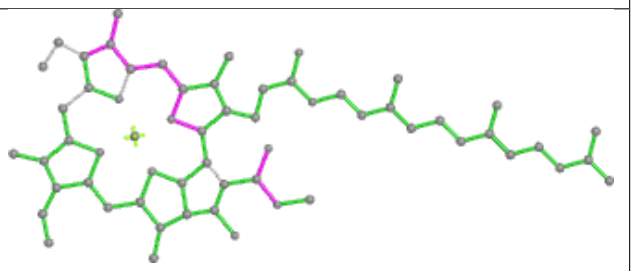
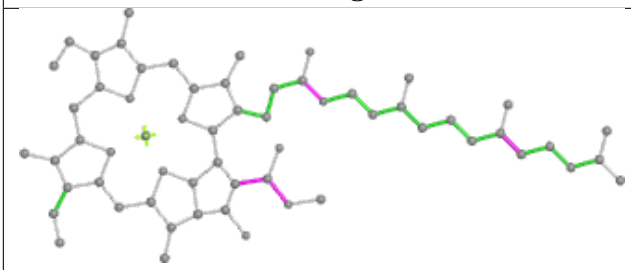
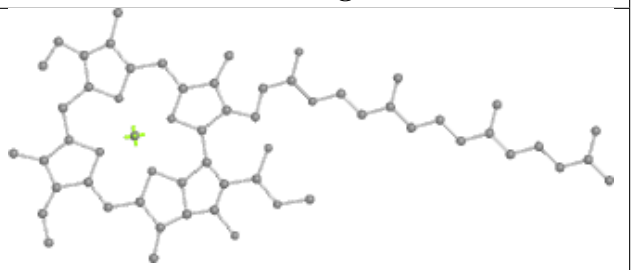


Bond angles

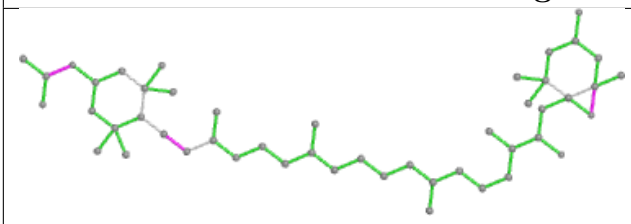


Torsions



Rings

Ligand A86 5 304



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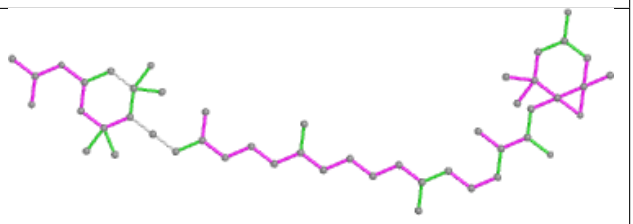

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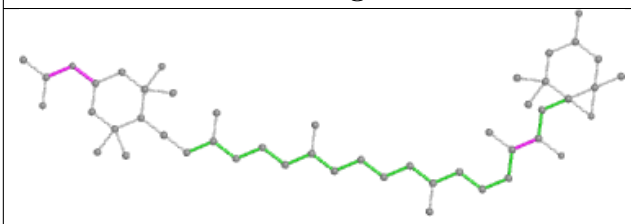

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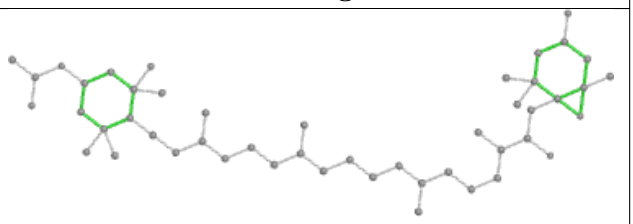
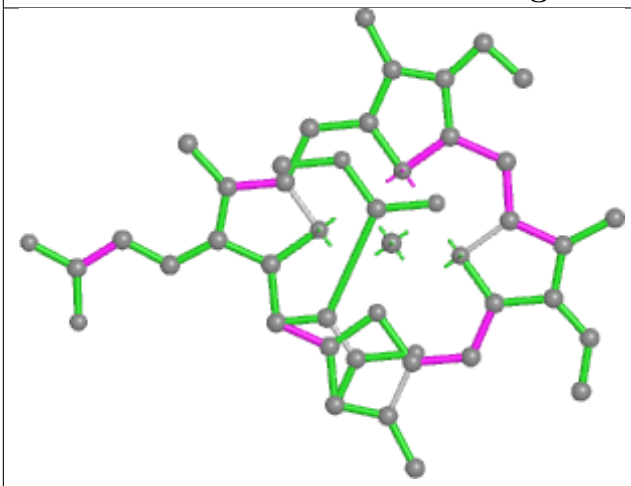


Rings

Ligand KC2 8 308



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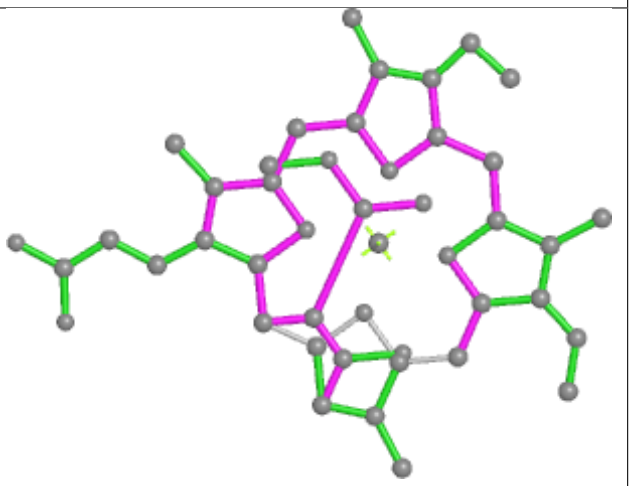

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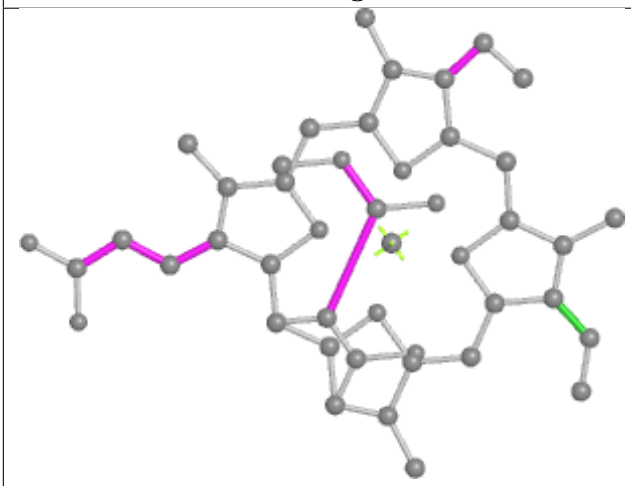

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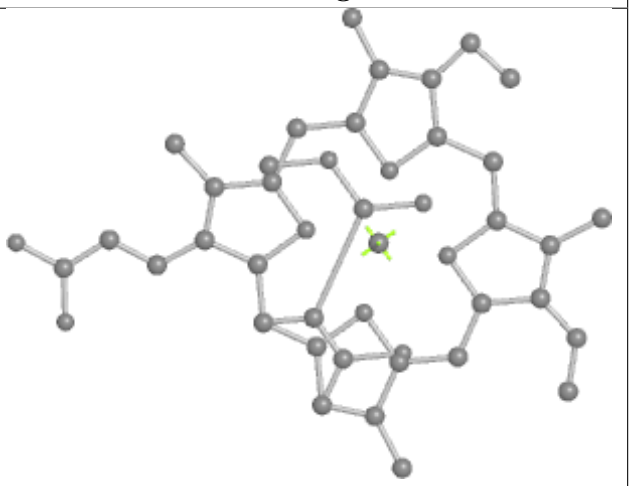
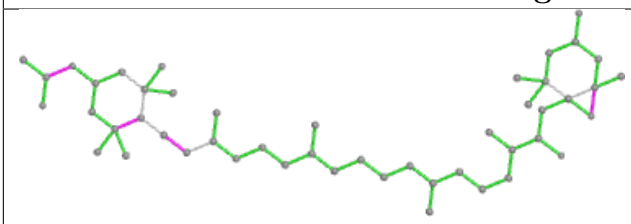


Rings

Ligand A86 6 304



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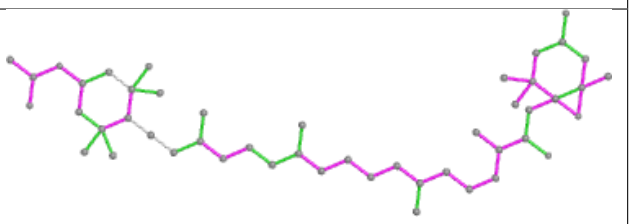
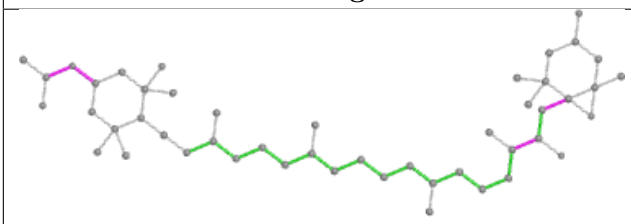


Bond angles



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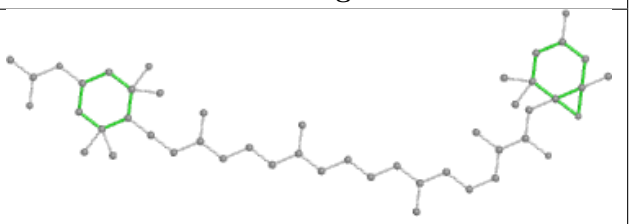
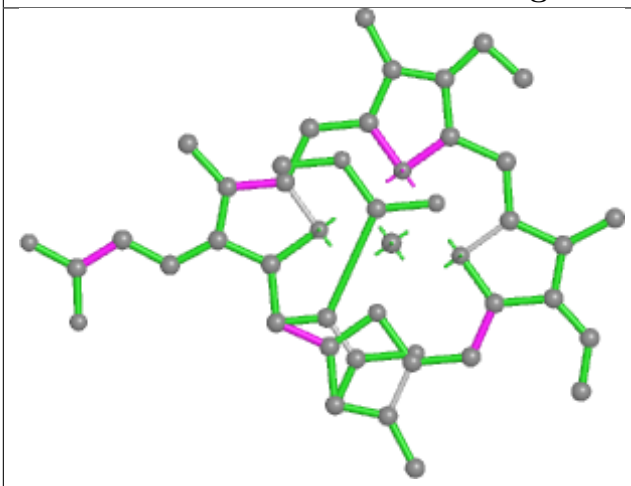


Rings

Ligand KC1 5 313



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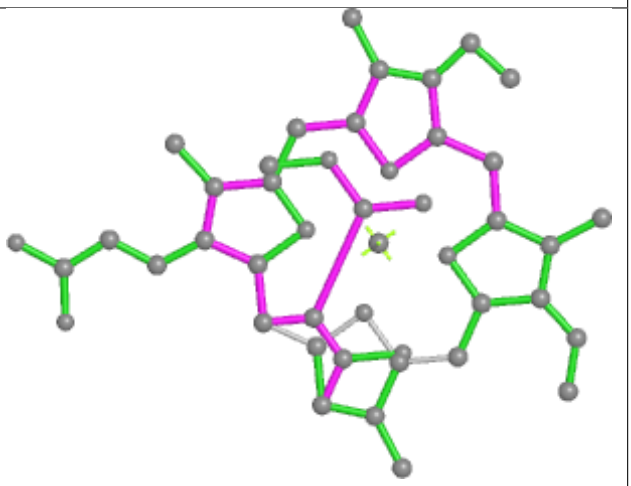

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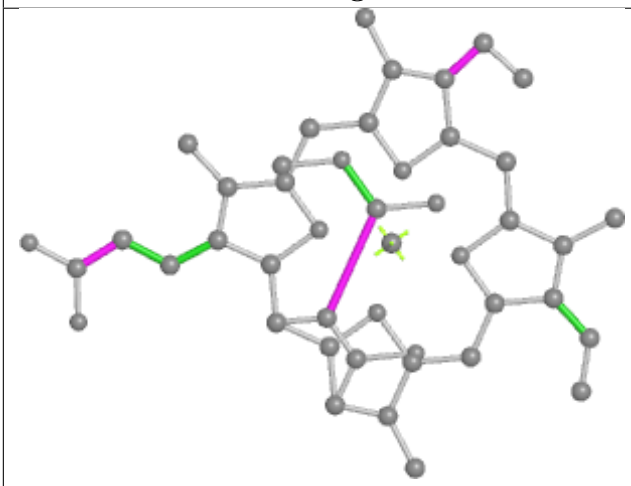

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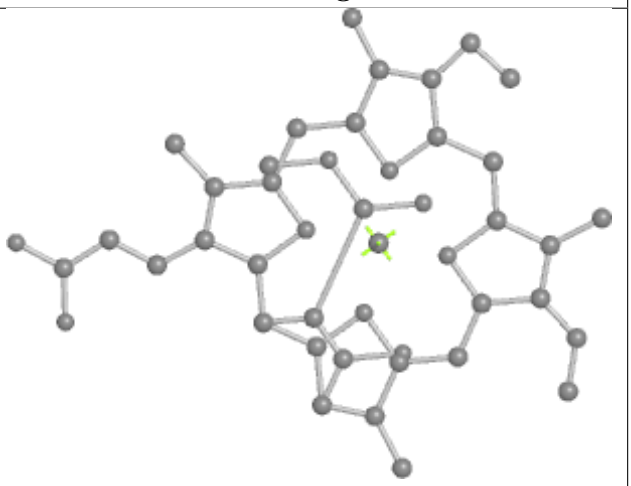
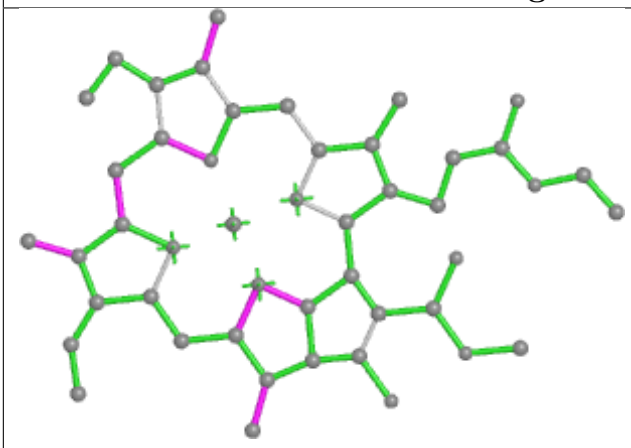


Rings

Ligand CLA 5 312



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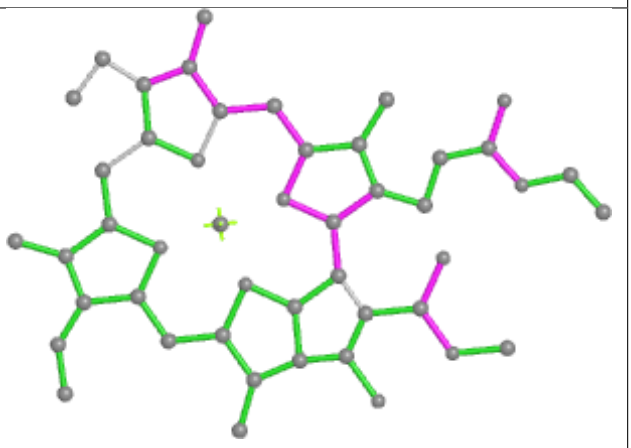

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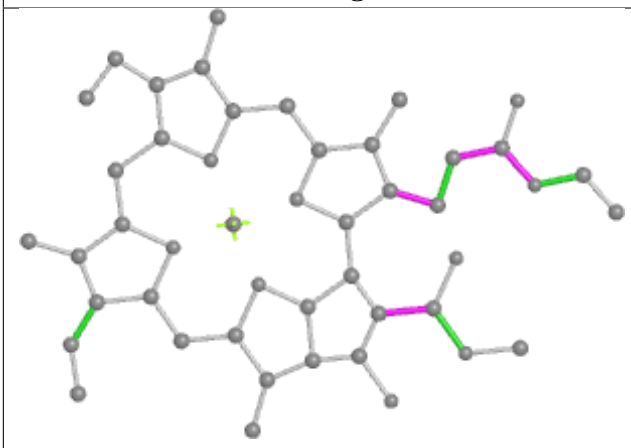

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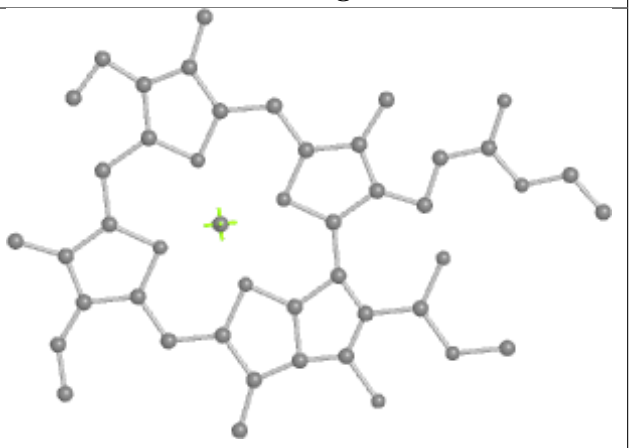
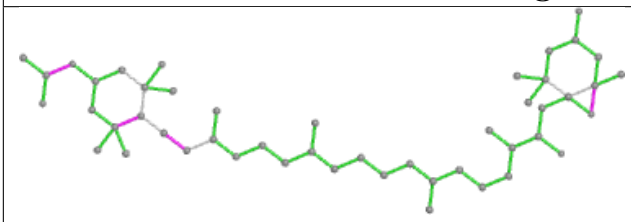


Rings

Ligand A86 8 306



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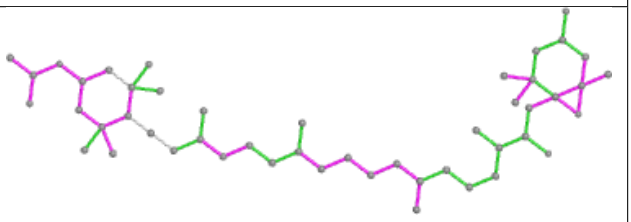

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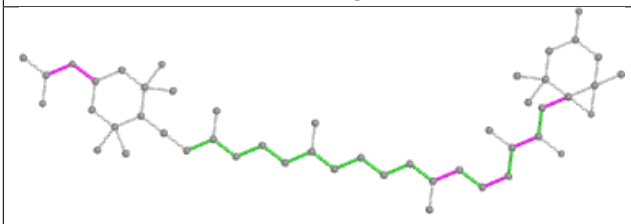

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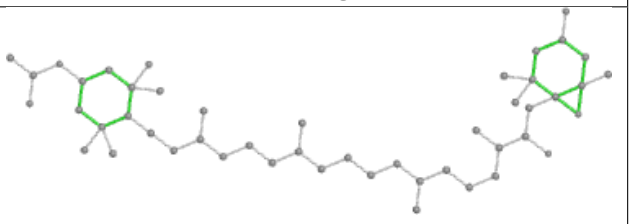
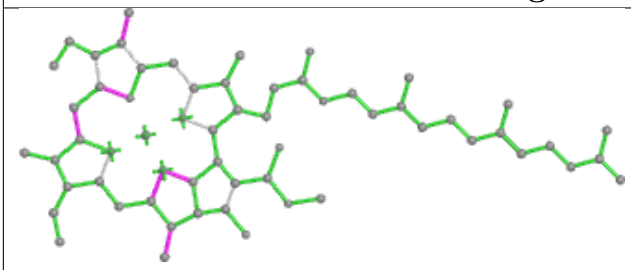


Rings

Ligand CLA 6 306



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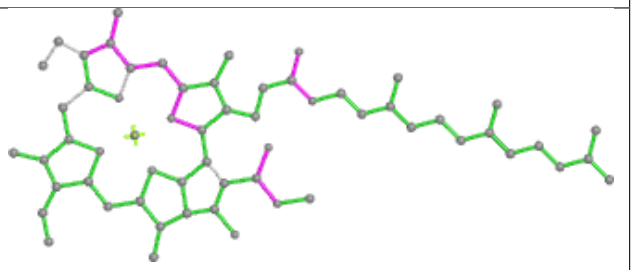

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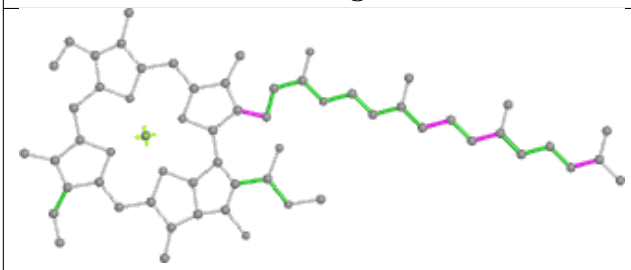

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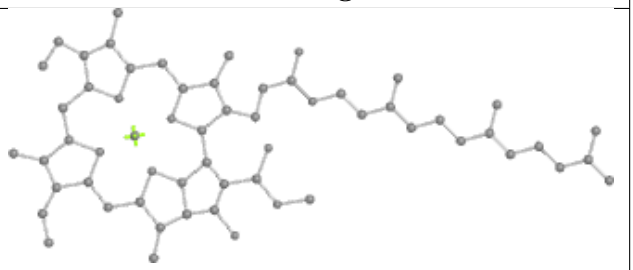
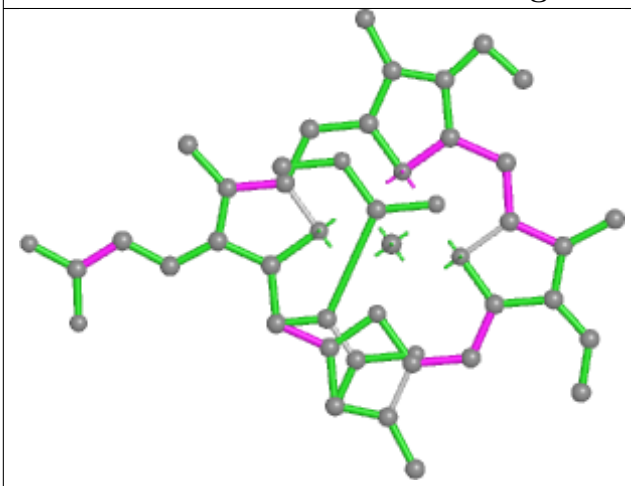


Rings

Ligand KC2 8 310



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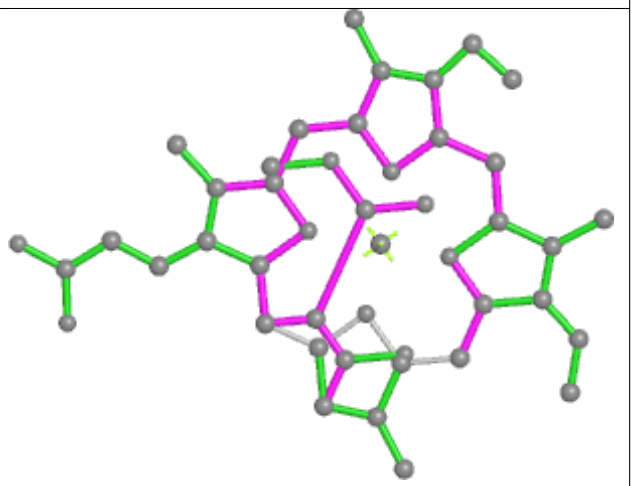

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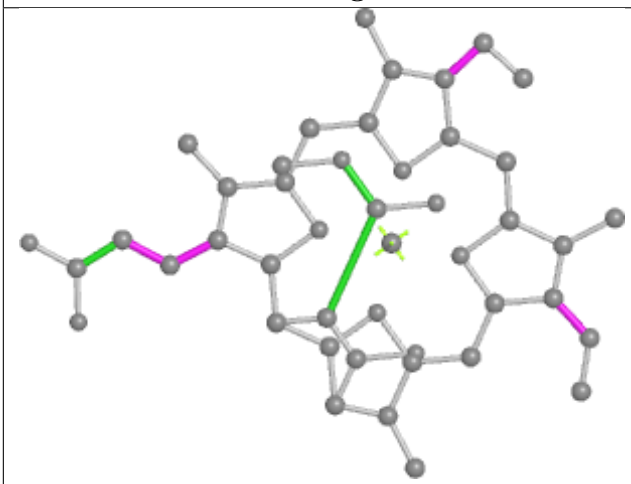

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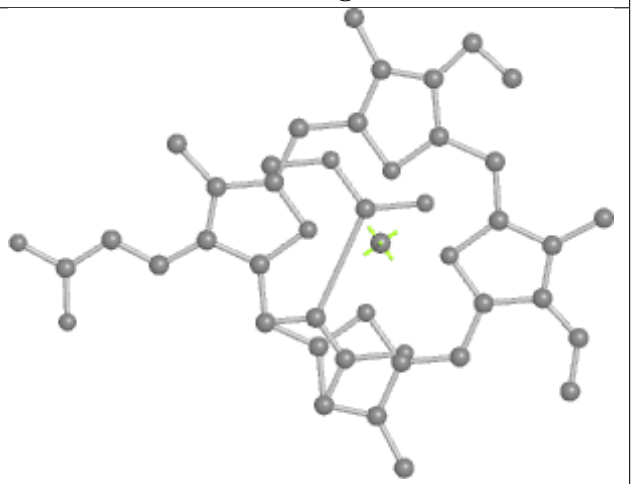
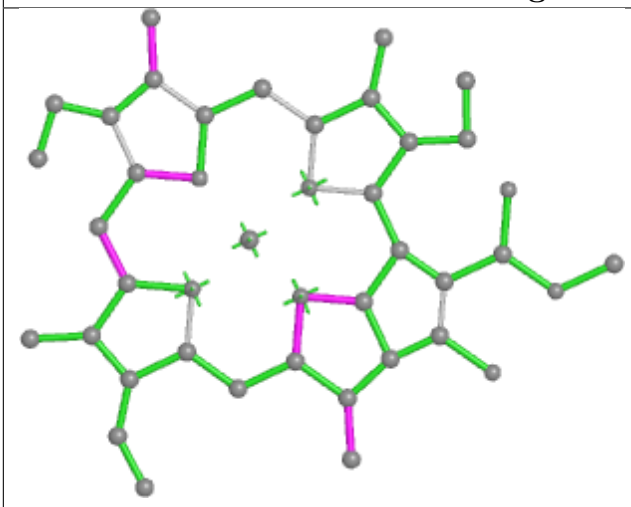


Rings

Ligand CLA 9 308



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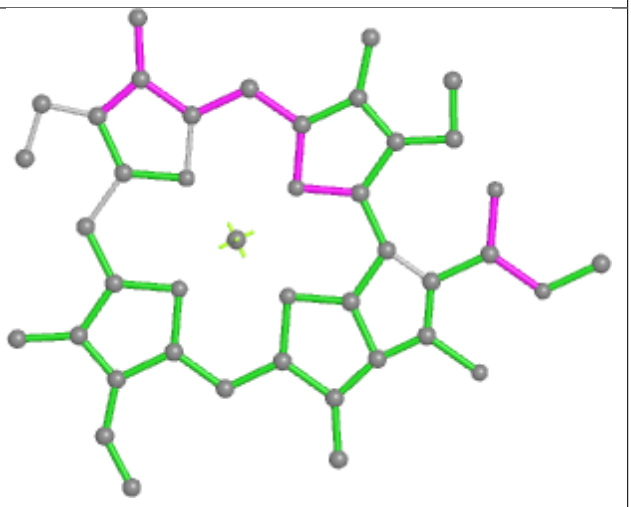

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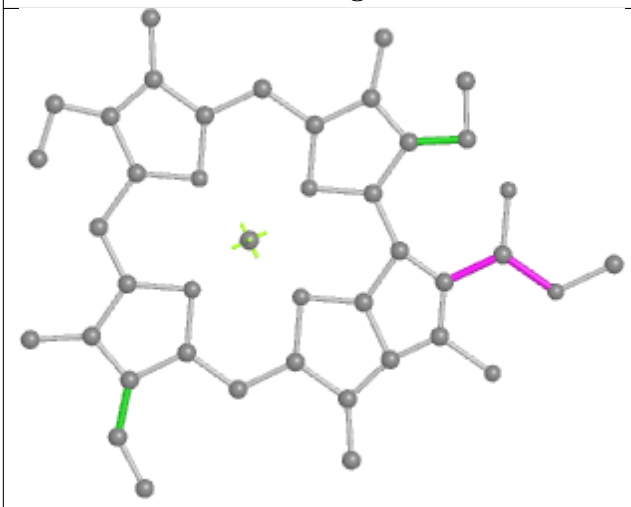

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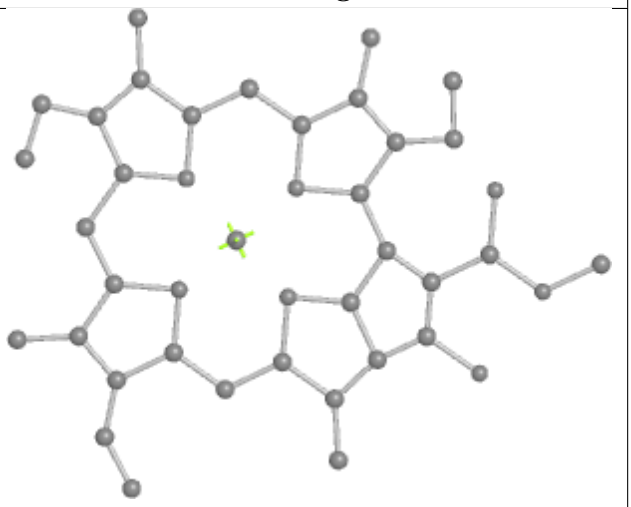
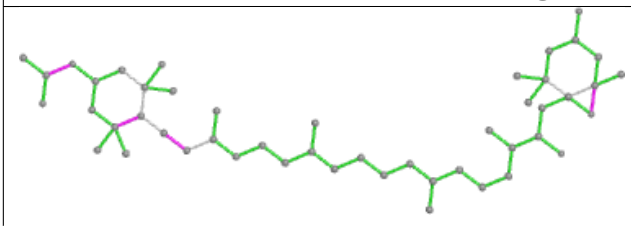


Rings

Ligand A86 5 302



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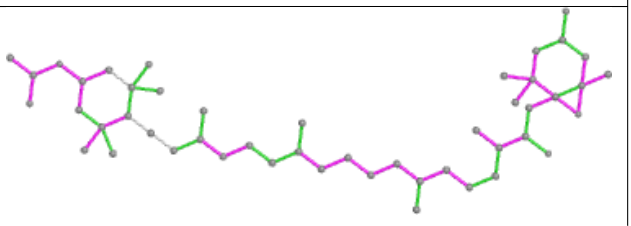

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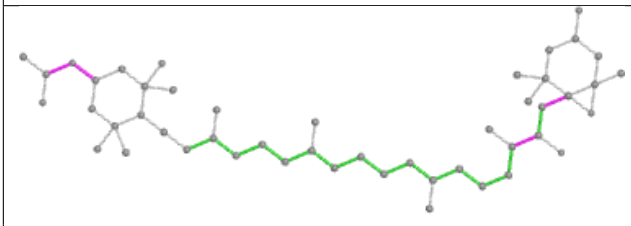

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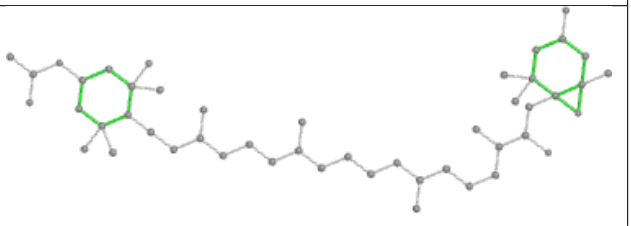
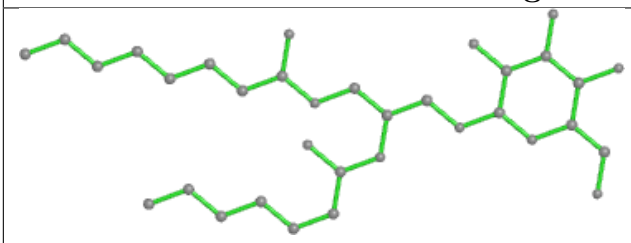


Rings

Ligand LMG 9 317



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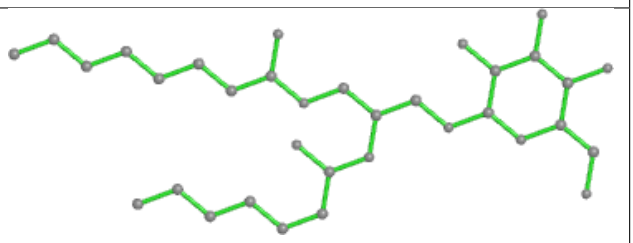

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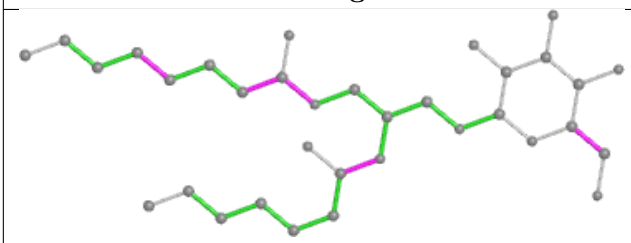

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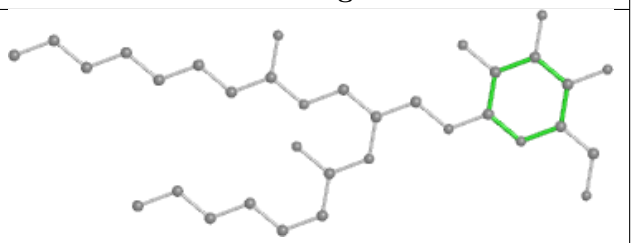
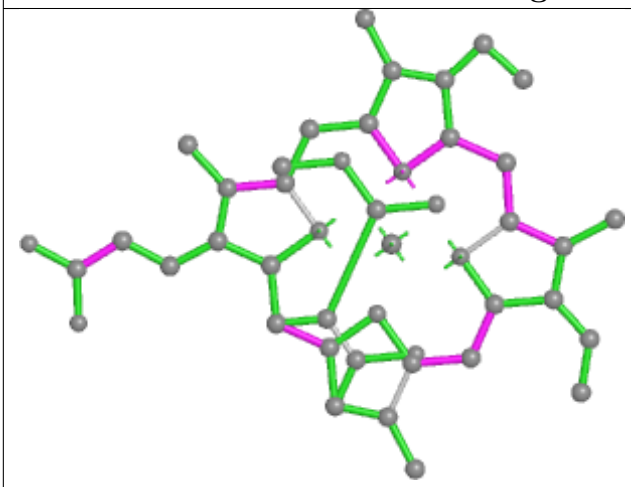


Rings

Ligand KC2 5 308



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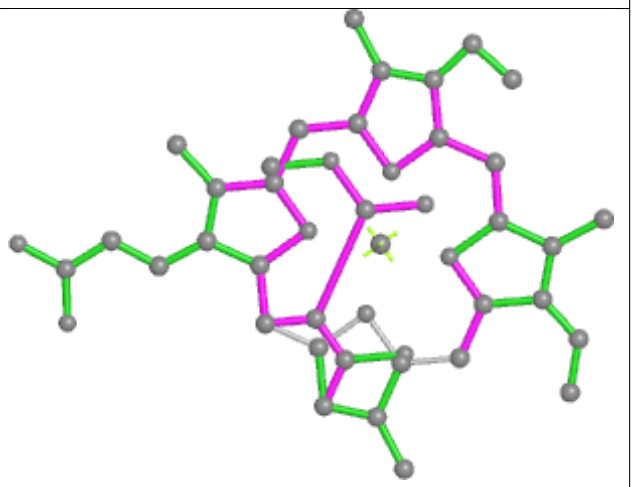

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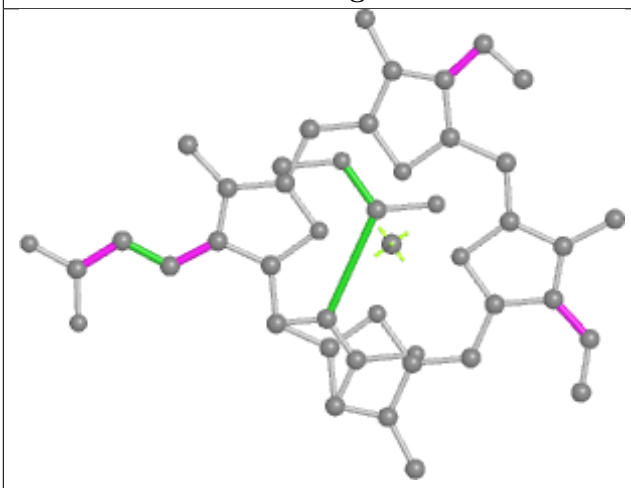

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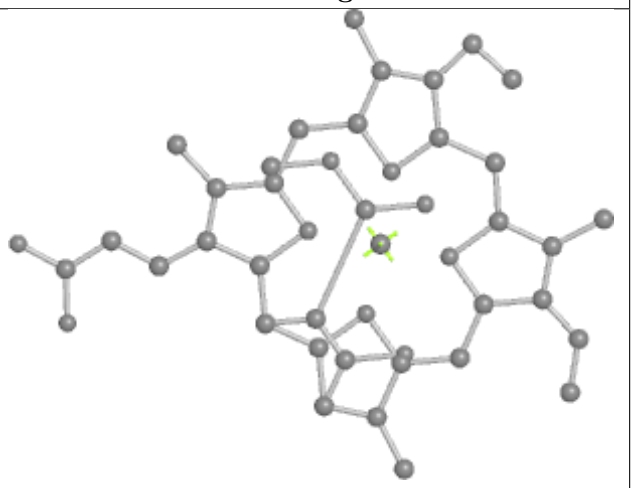
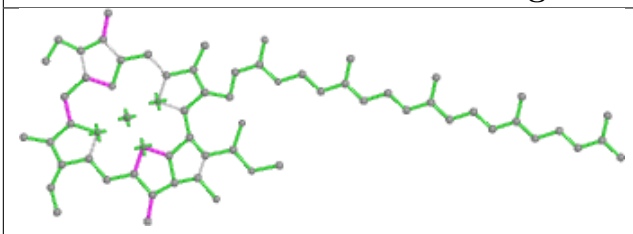


Rings

Ligand CLA 5 307



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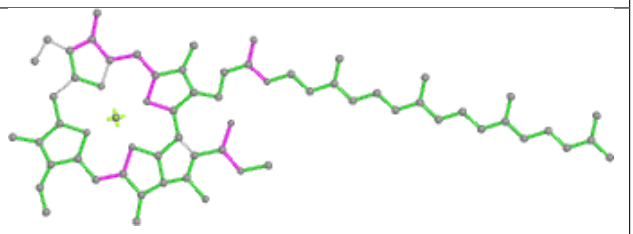
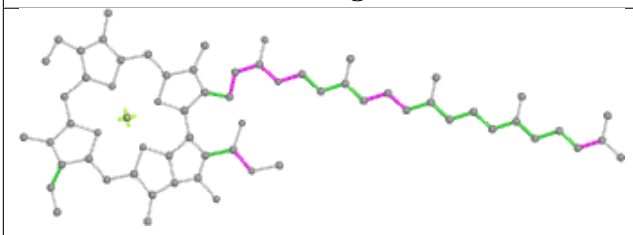


Bond angles



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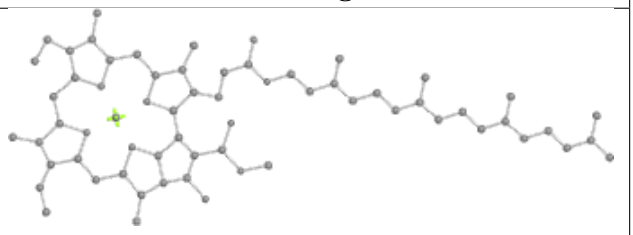
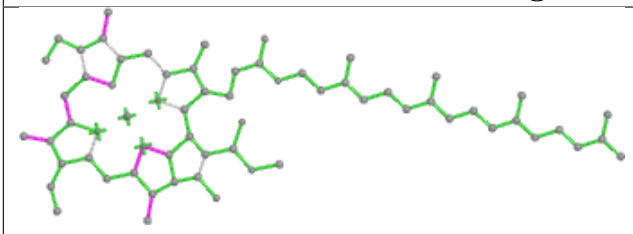


Rings

Ligand CLA 8 307



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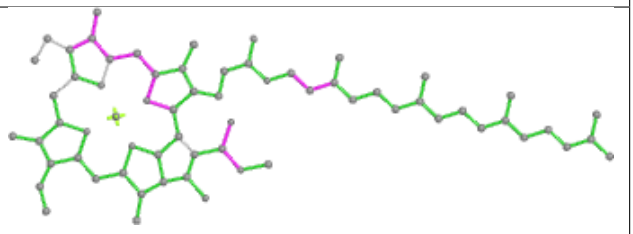
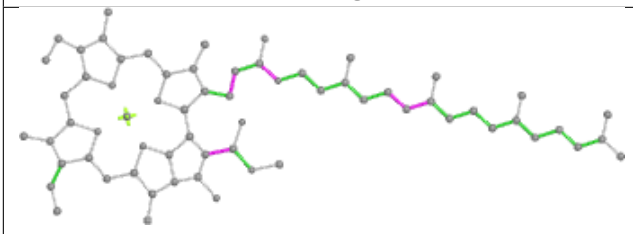


Bond angles



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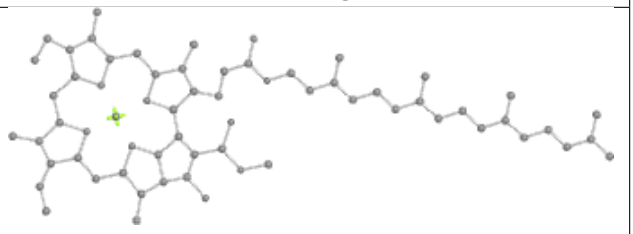
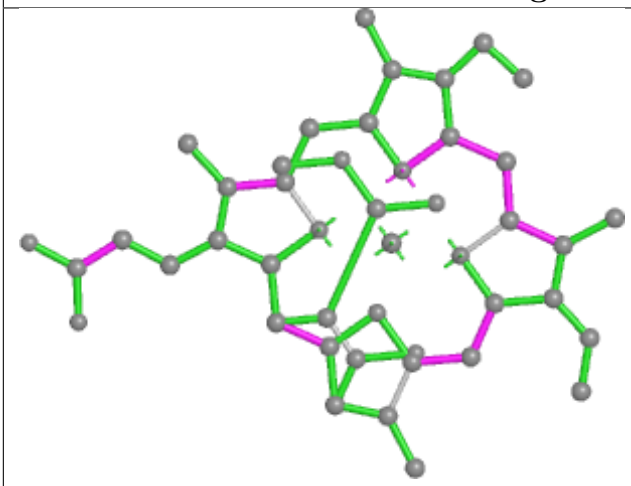
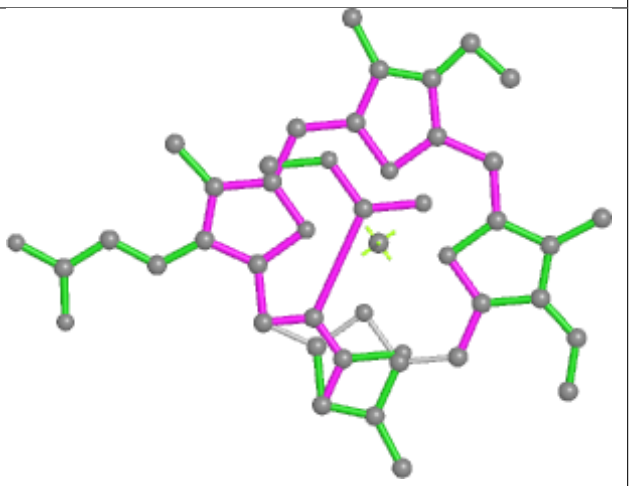


Rings

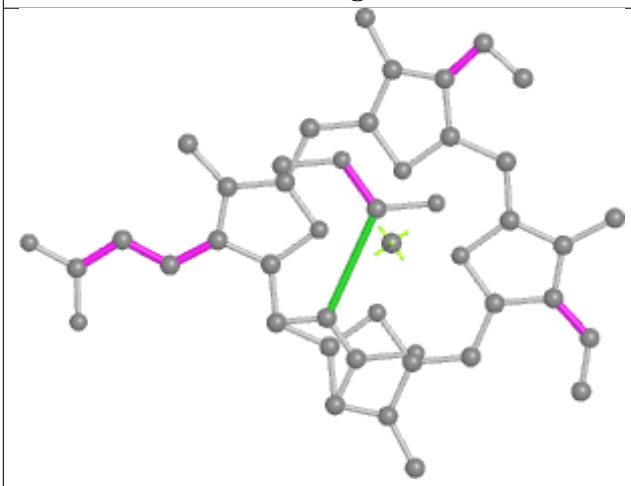
Ligand KC2 5 310



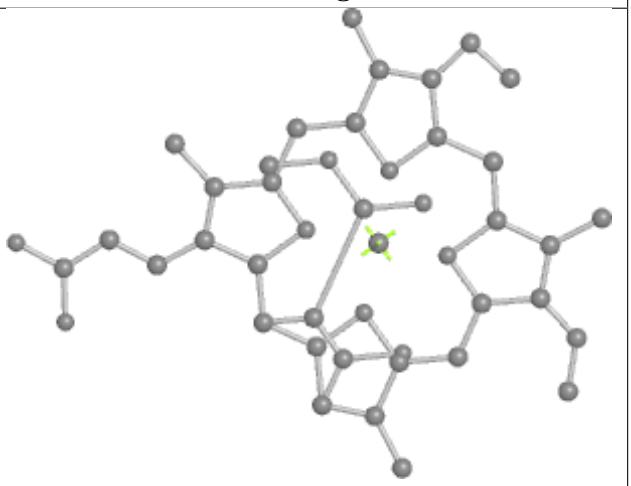
Bond lengths



Bond angles

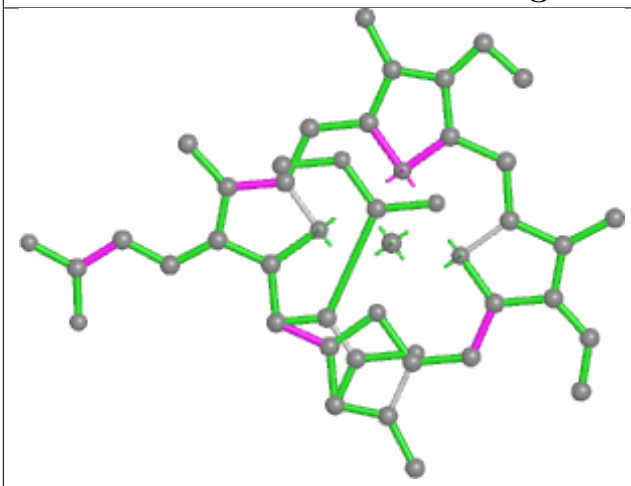


Torsions



Rings

Ligand KC1 7 313



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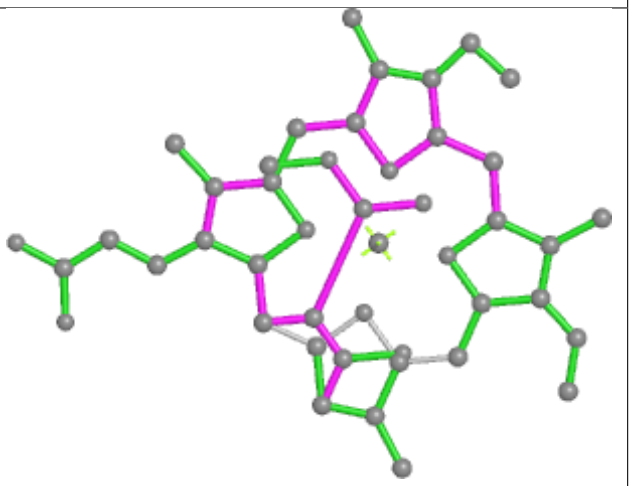
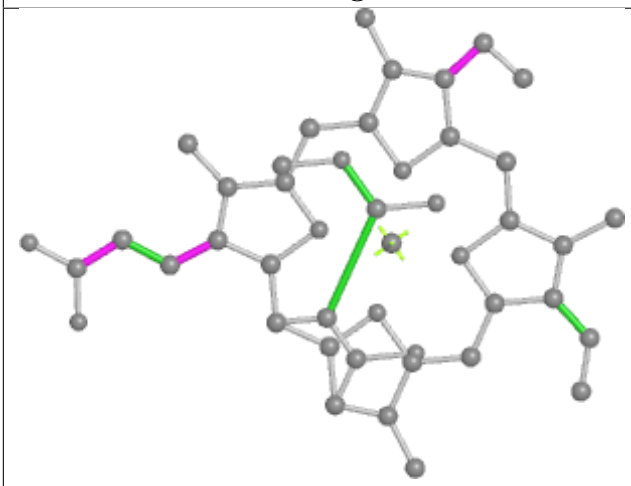
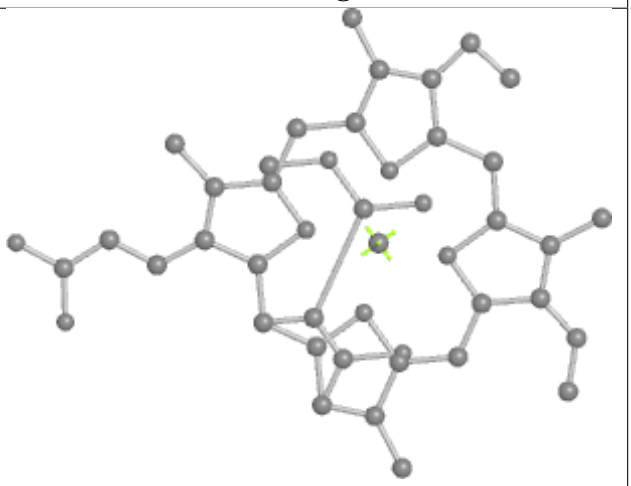


Bond angles

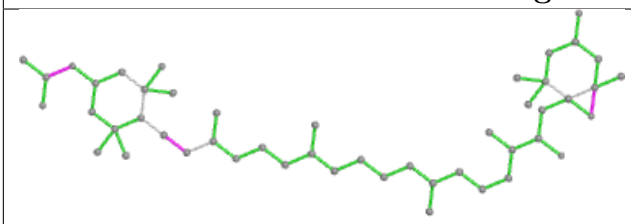


Torsions



Rings

Ligand A86 9 304



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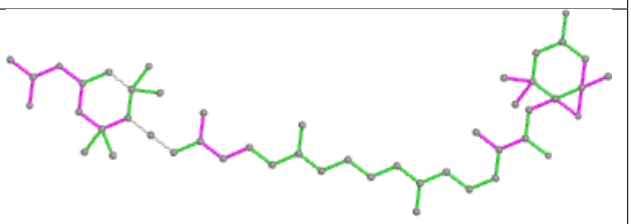
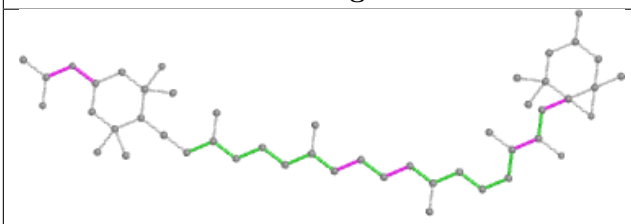


Bond angles



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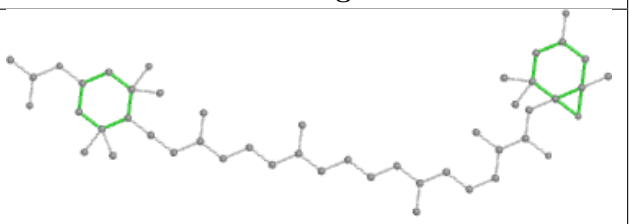
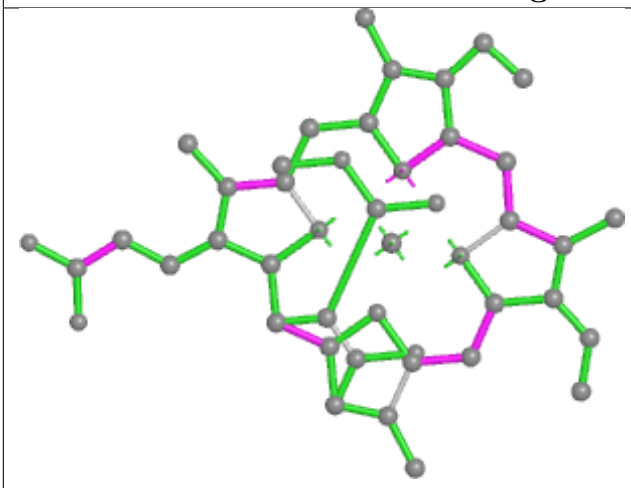


Rings

Ligand KC2 7 312



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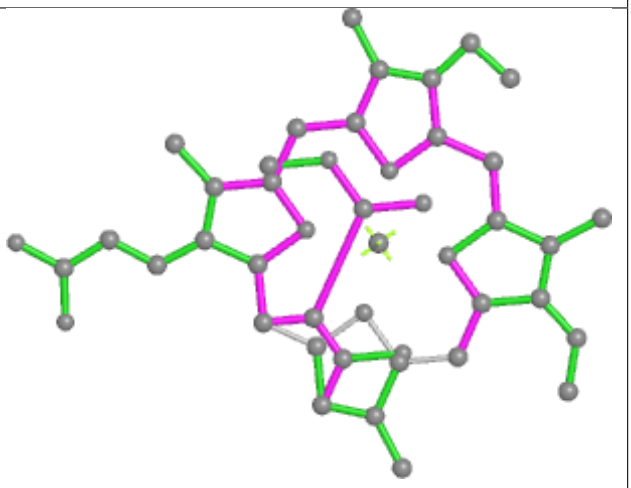

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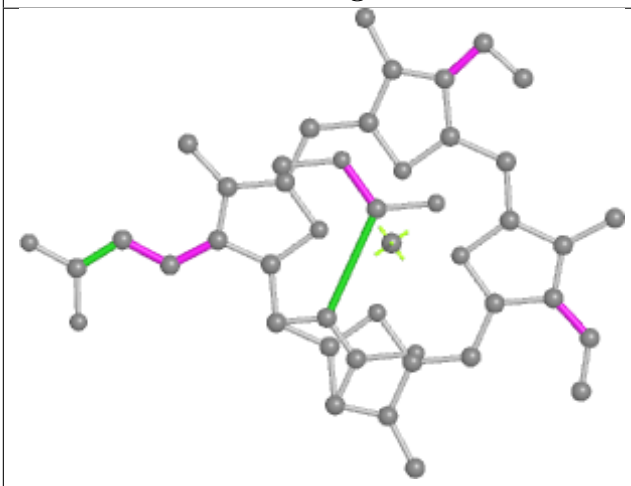

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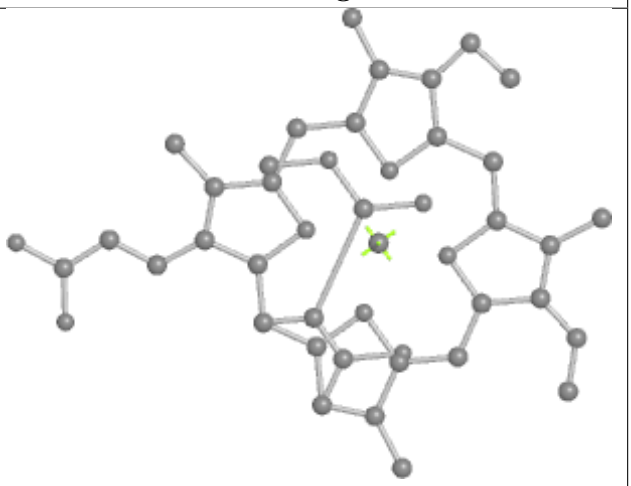
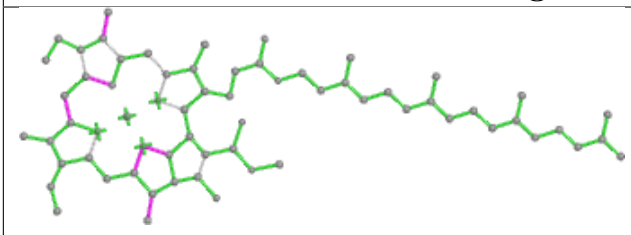


Rings

Ligand CLA 6 314



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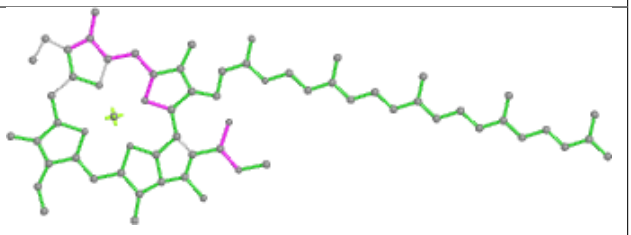
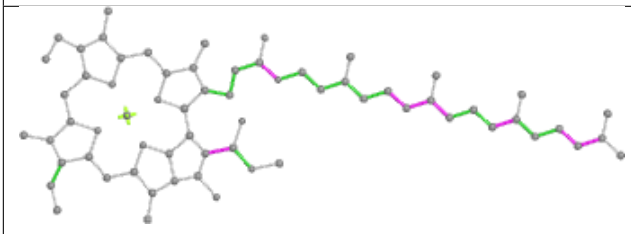


Bond angles



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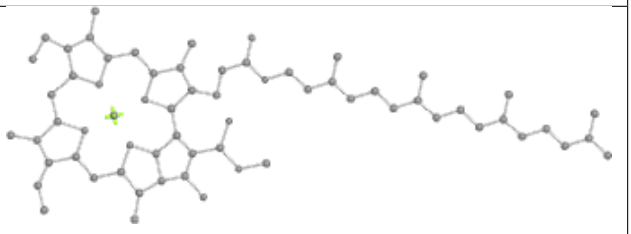
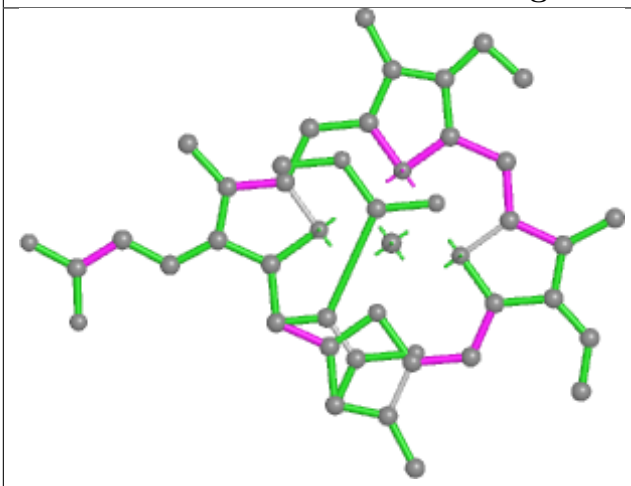


Rings

Ligand KC2 9 310



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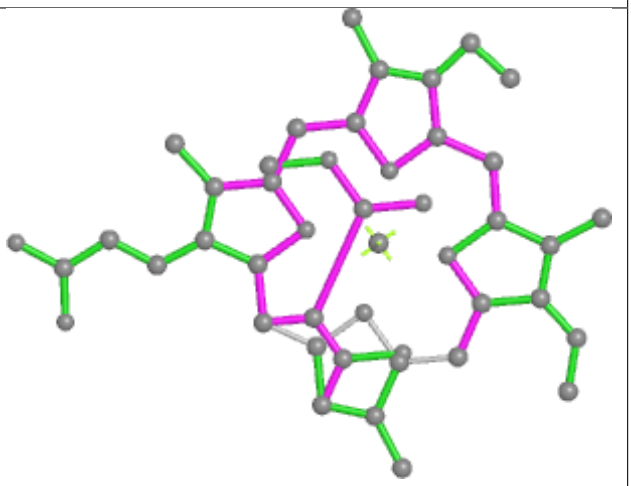

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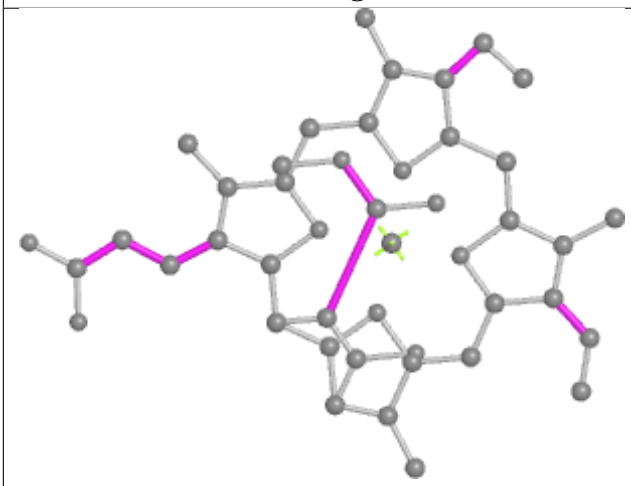

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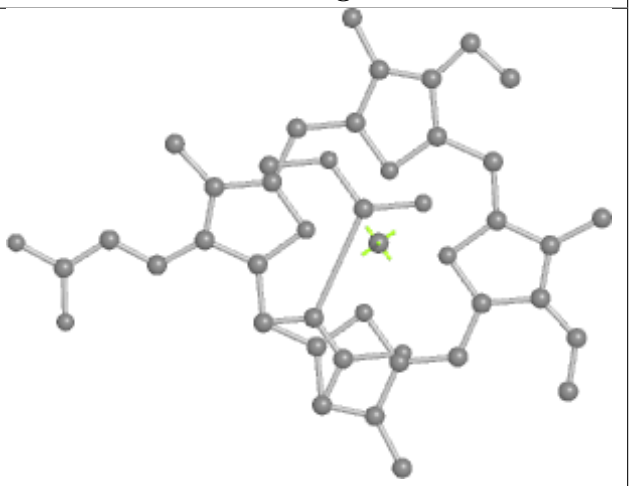
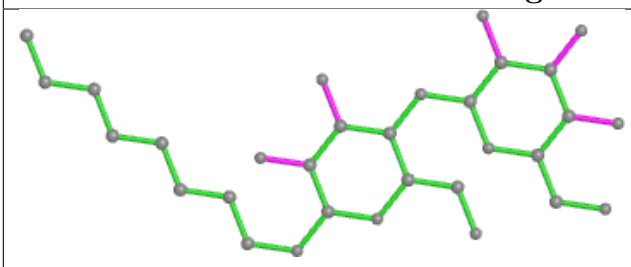


Rings

Ligand LMT 5 316



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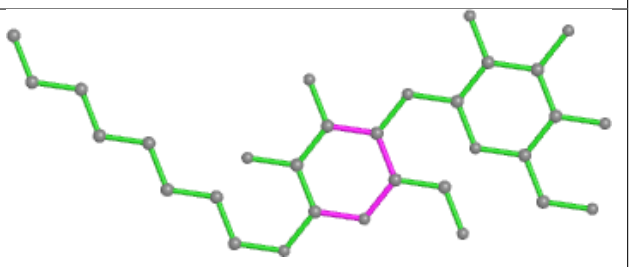

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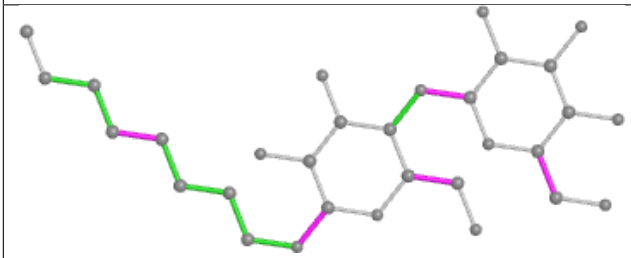

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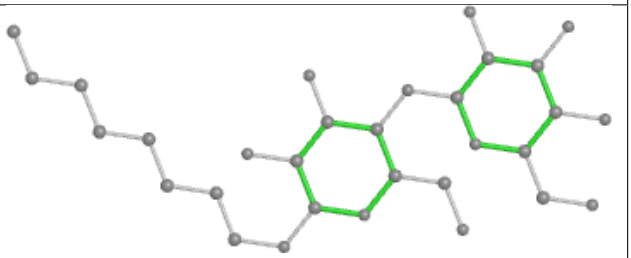
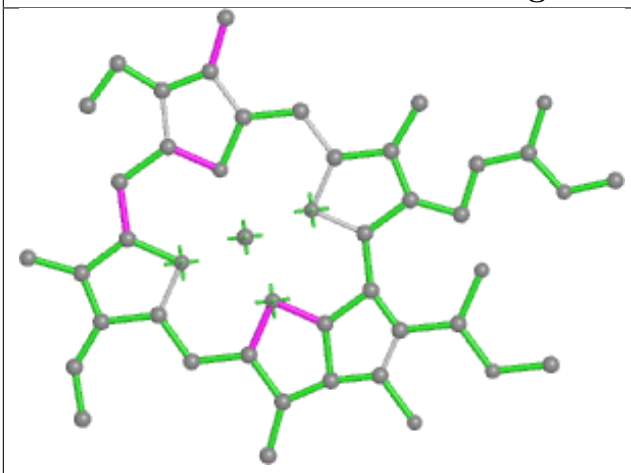


Rings

Ligand CLA 8 315



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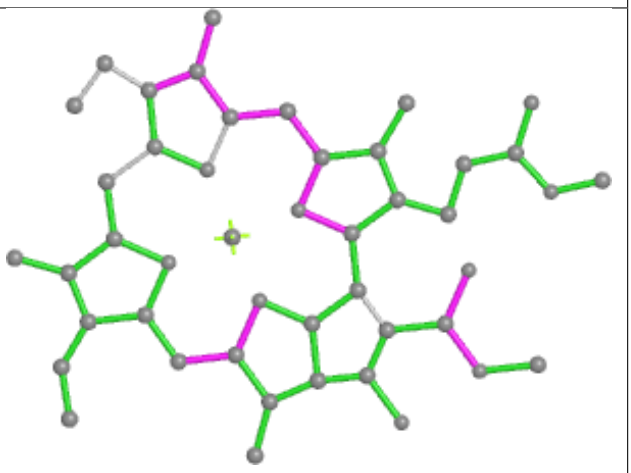

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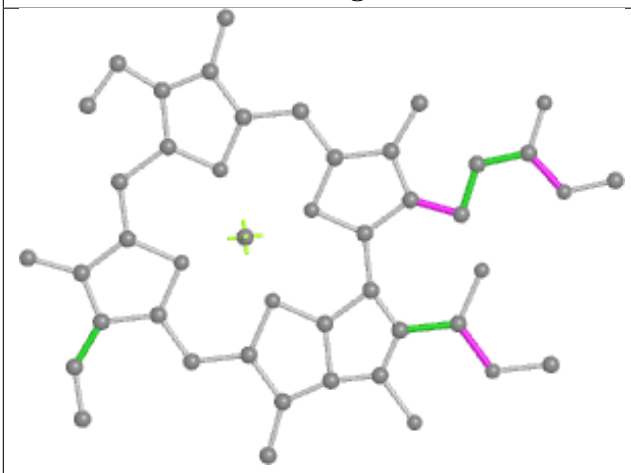

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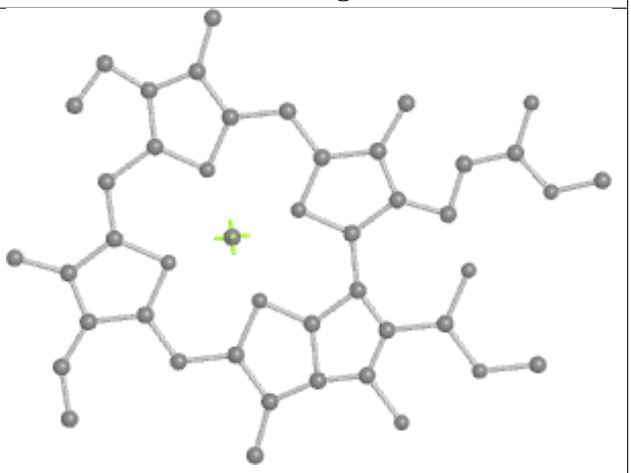
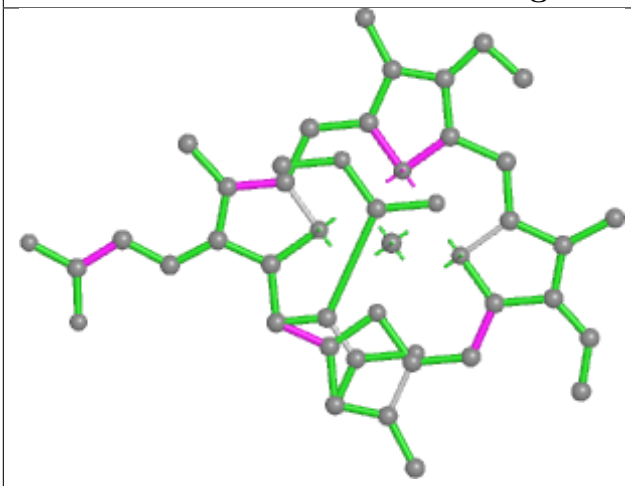


Rings

Ligand KC1 8 311



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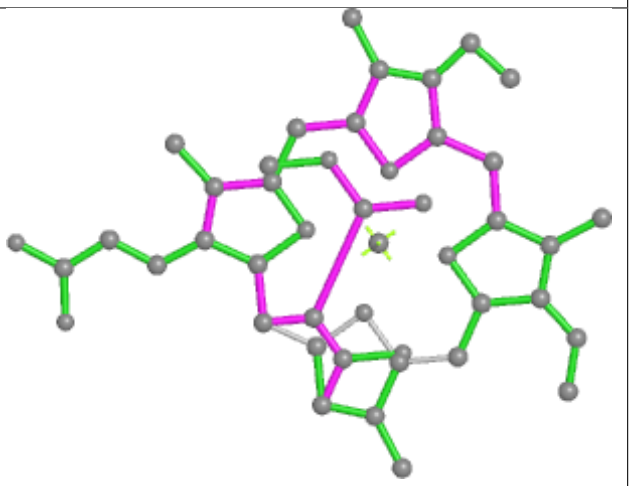
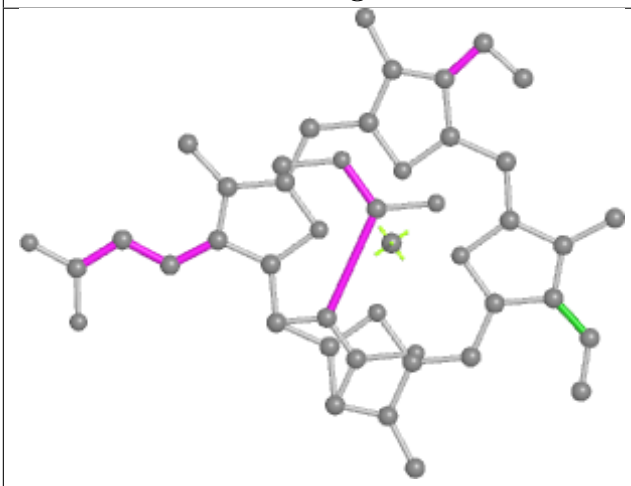


Bond angles



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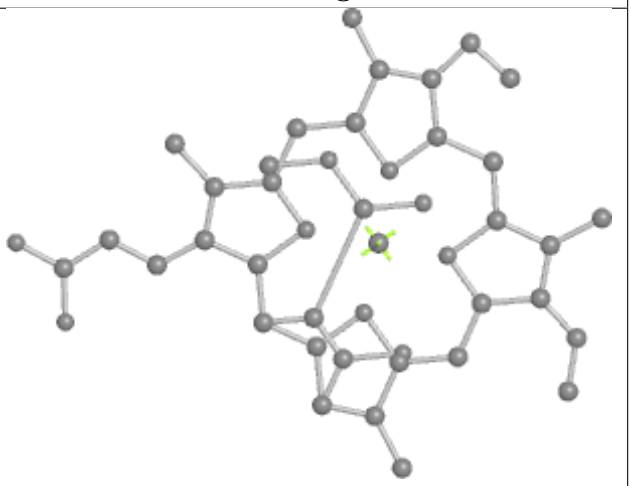
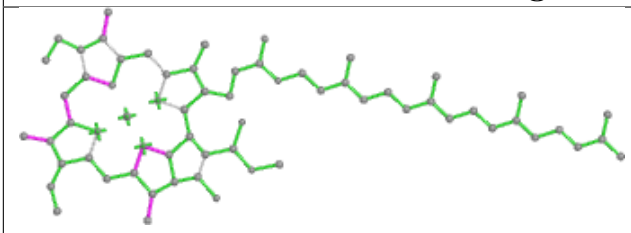


Rings

Ligand CLA 9 311



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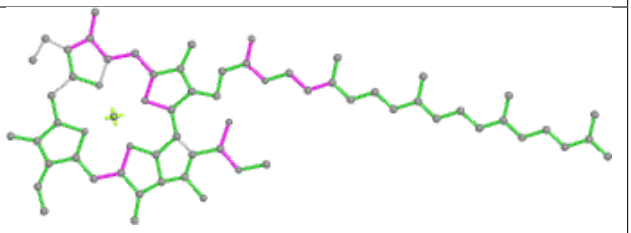
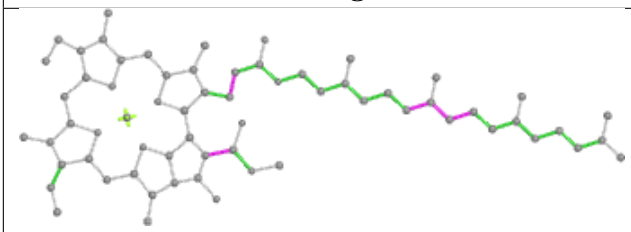


Bond angles



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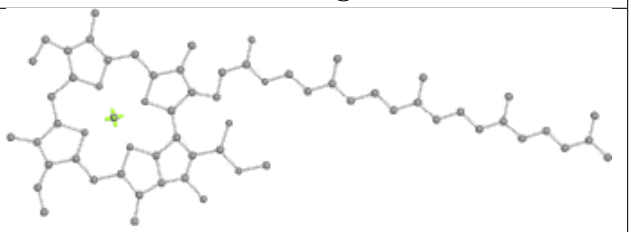
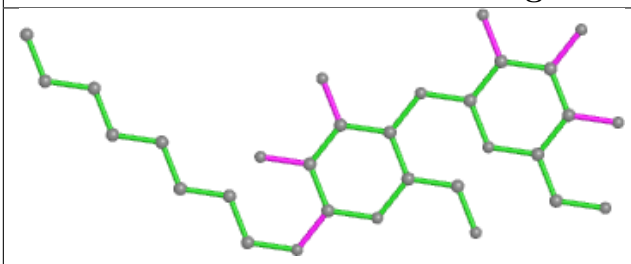


Rings

Ligand LMT 7 318



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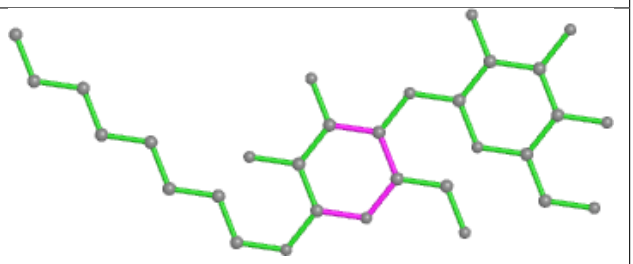
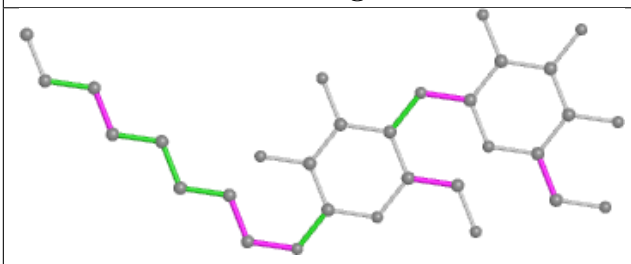


Bond angles



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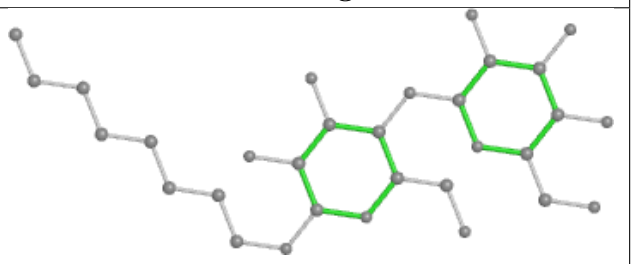
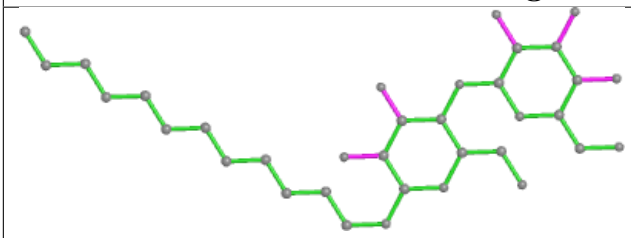


Rings

Ligand LMT 5 317



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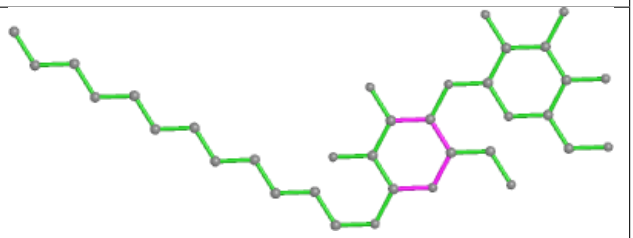
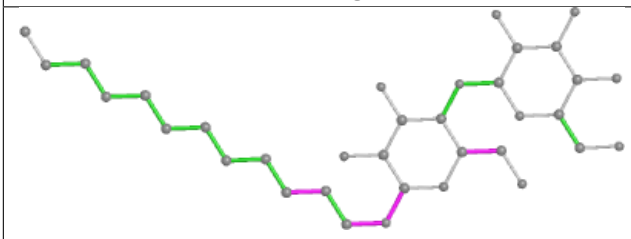


Bond angles



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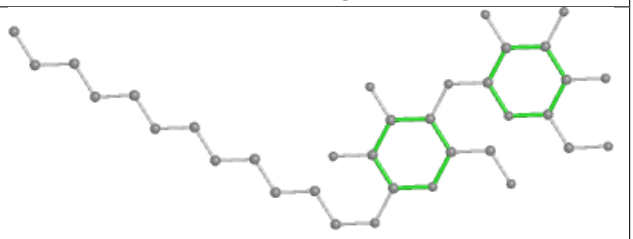
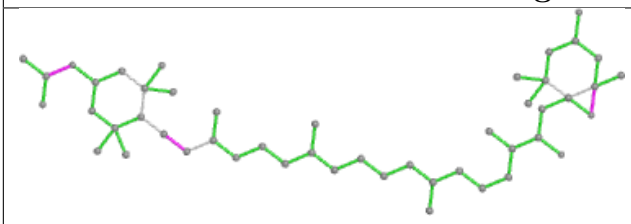


Rings

Ligand A86 8 305



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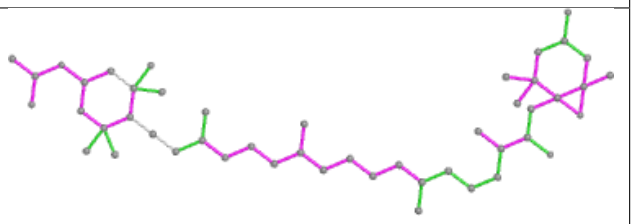
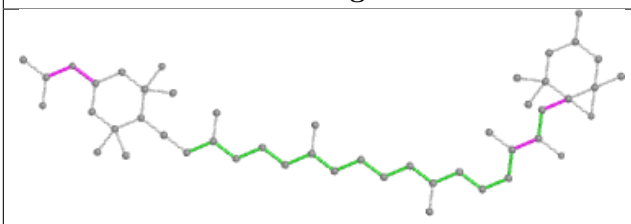
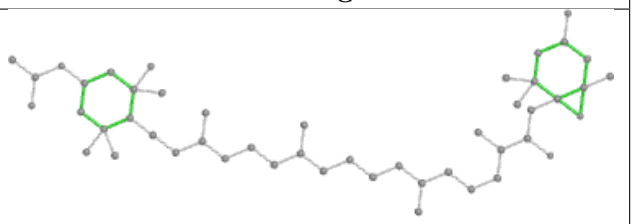


Bond angles

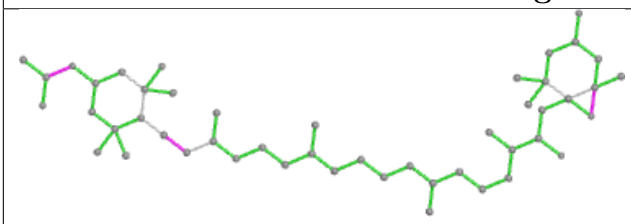


Torsions

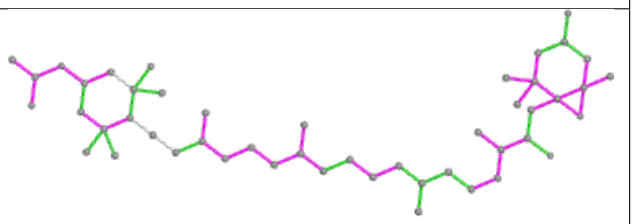


Rings

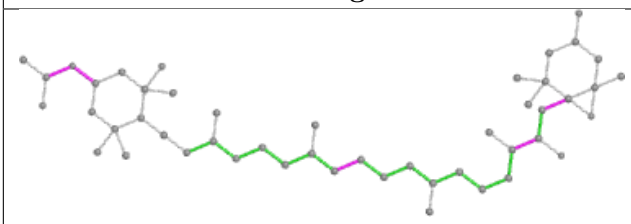
Ligand A86 9 306



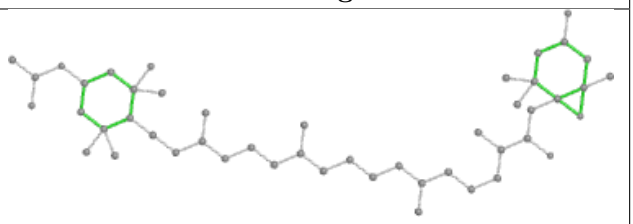
Bond lengths



Bond angles

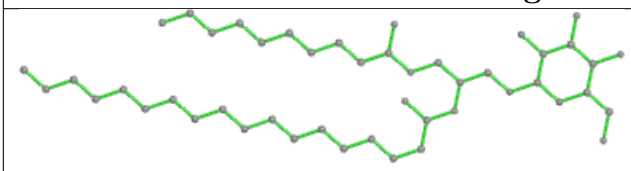


Torsions

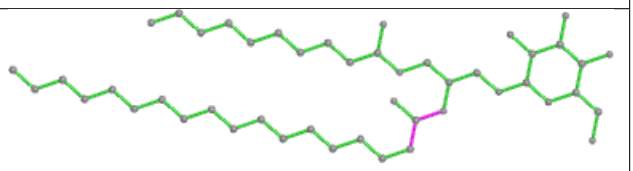


Rings

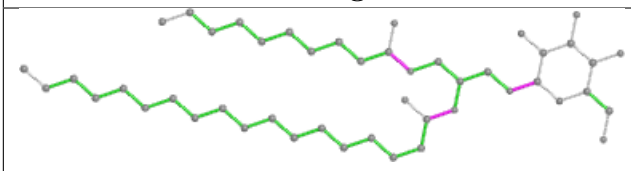
Ligand LMG 7 317



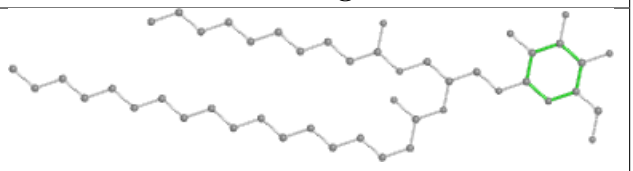
Bond lengths



Bond angles

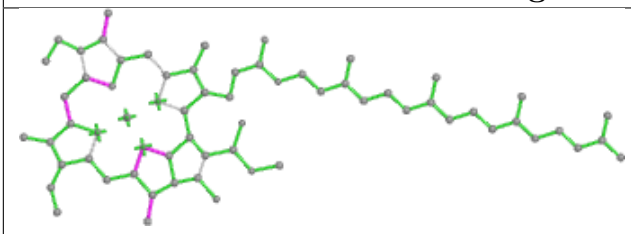


Torsions



Rings

Ligand CLA 7 316



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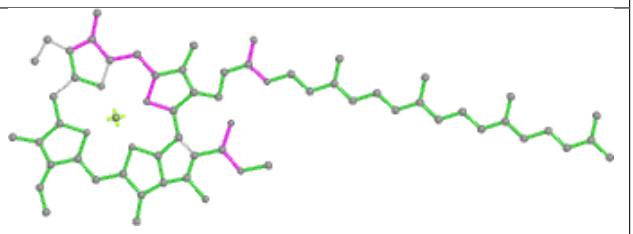

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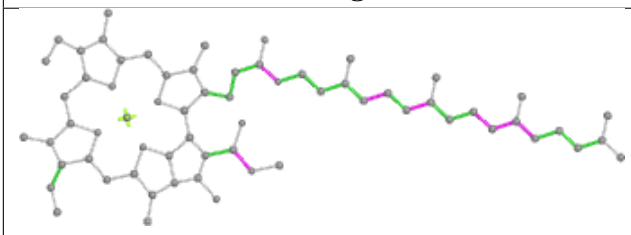

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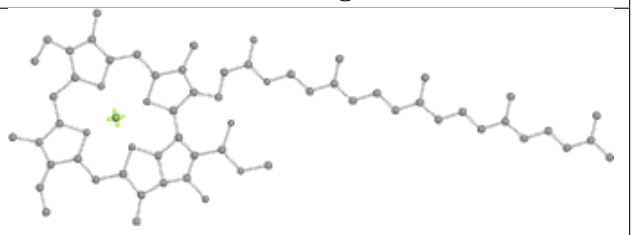
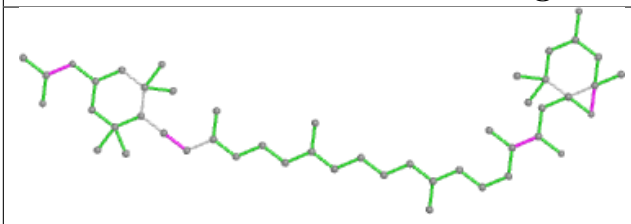


Rings

Ligand A86 8 301



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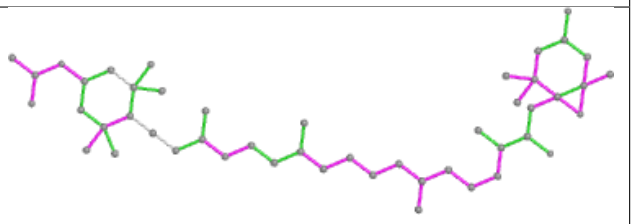

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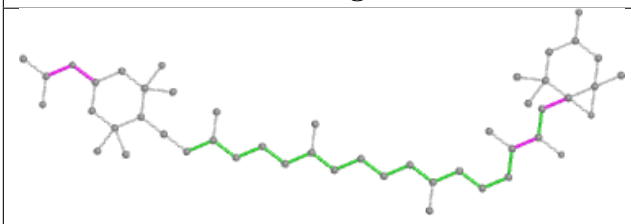

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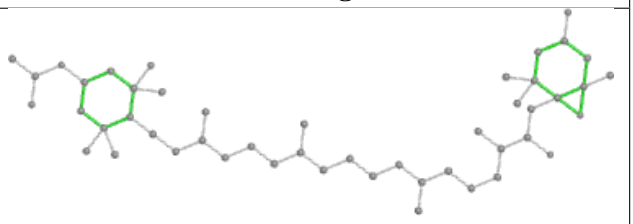
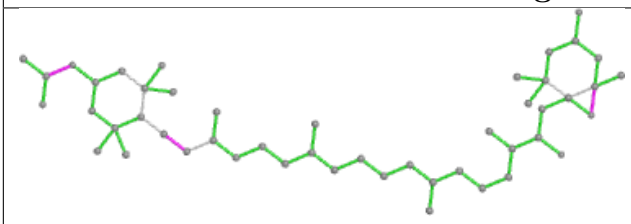


Rings

Ligand A86 9 307



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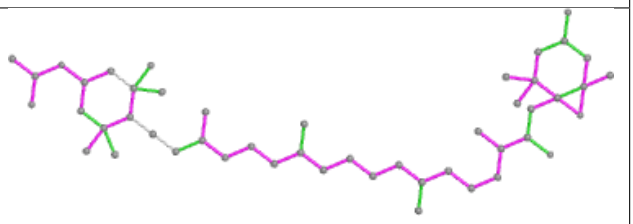
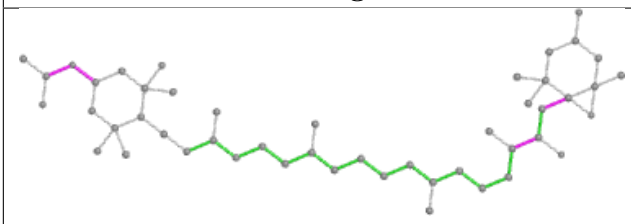


Bond angles



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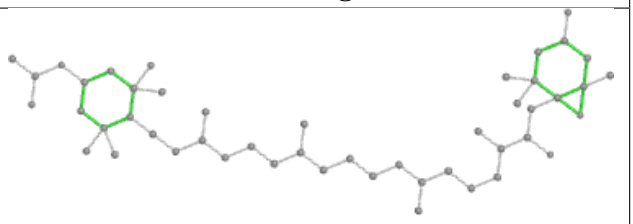
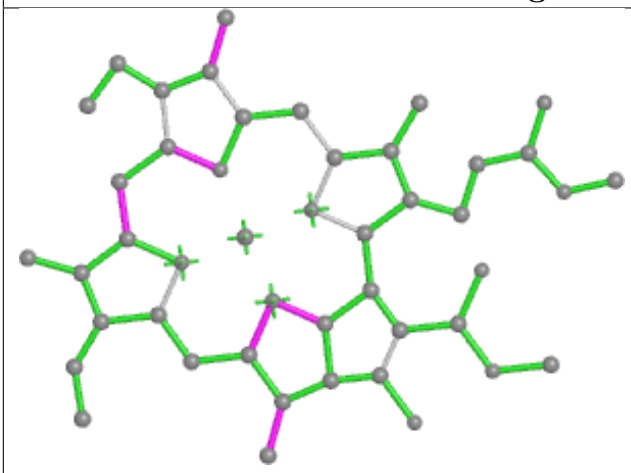


Rings

Ligand CLA 5 314



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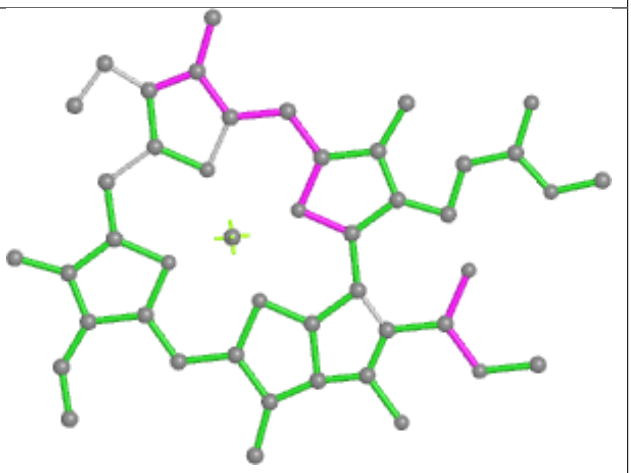
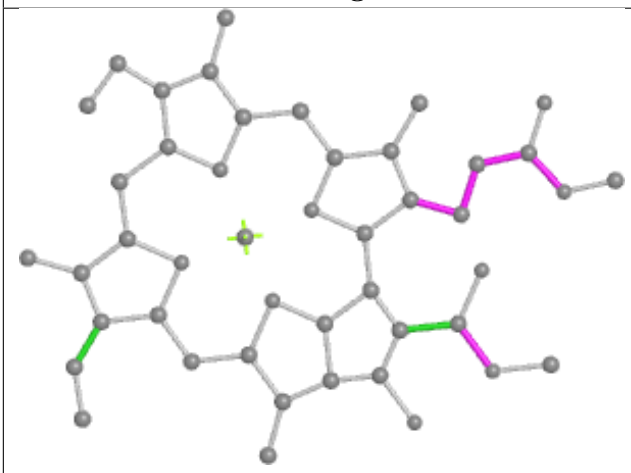


Bond angles



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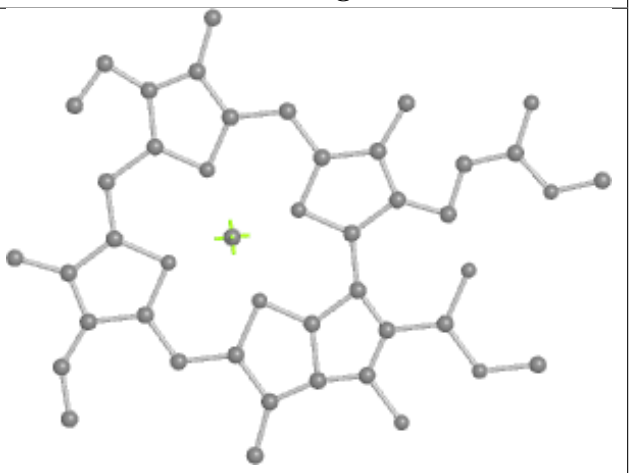
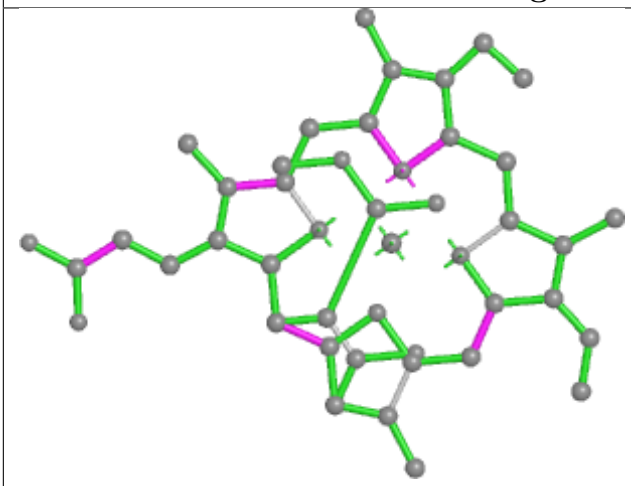


Rings

Ligand KC1 5 311



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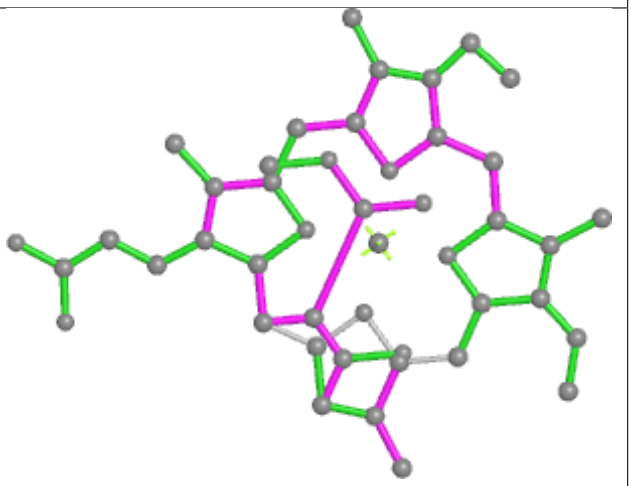

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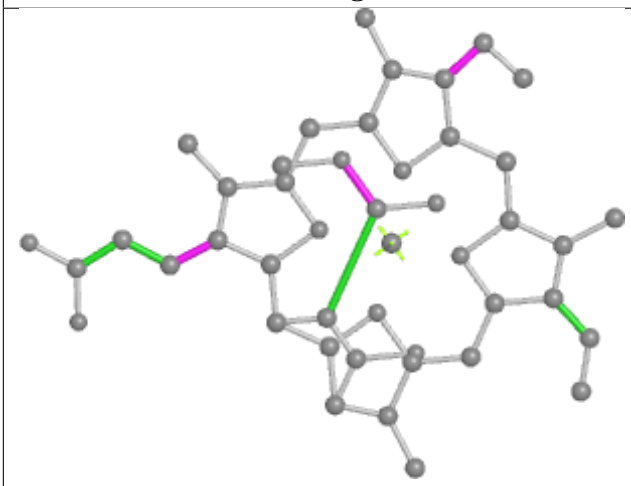

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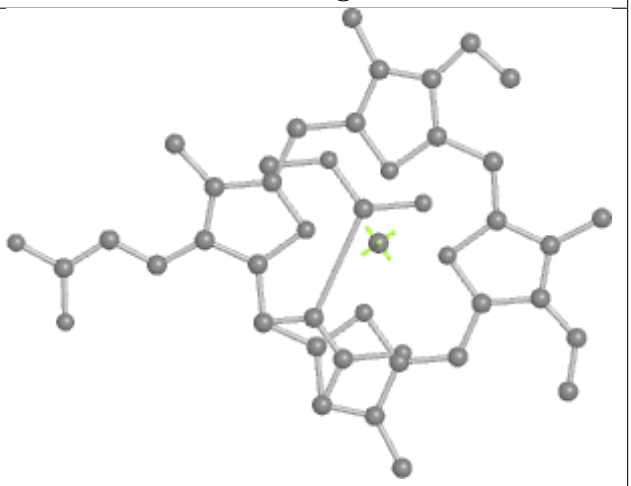
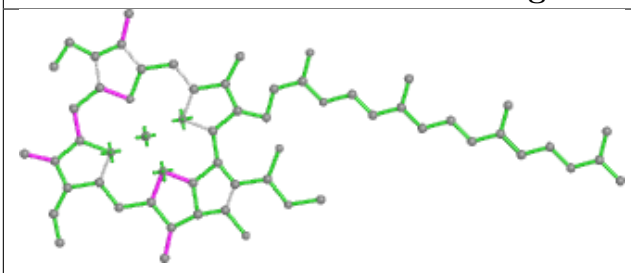


Rings

Ligand CLA 9 309



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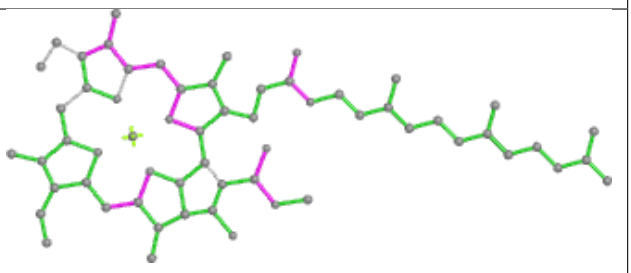

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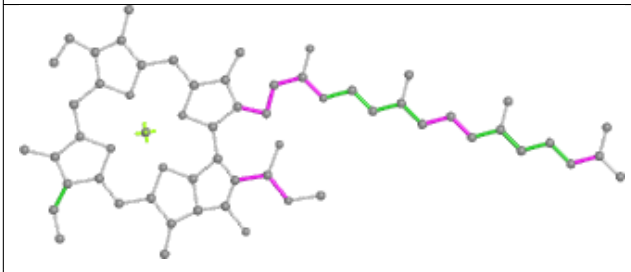

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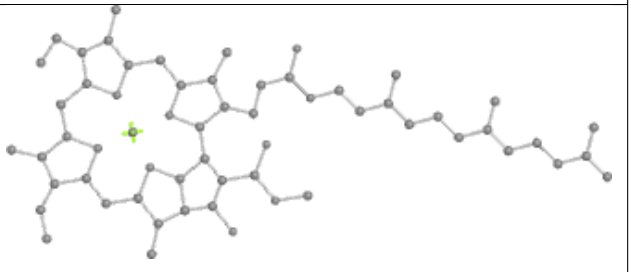
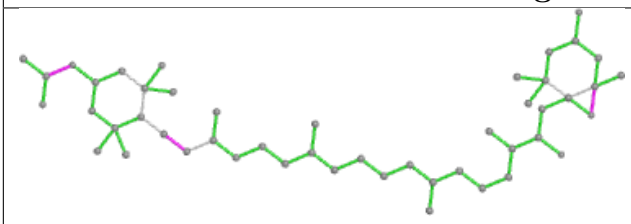


Rings

Ligand A86 7 303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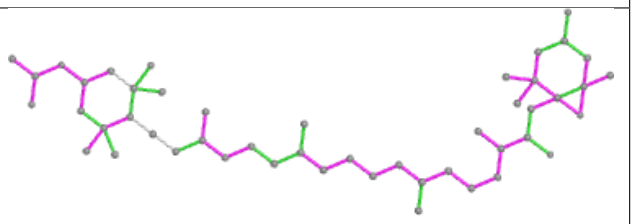
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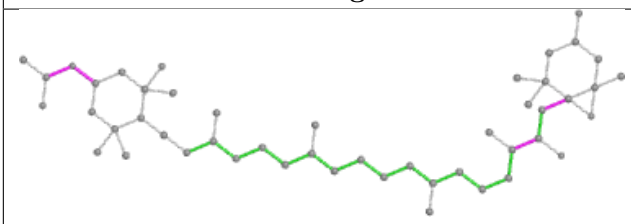
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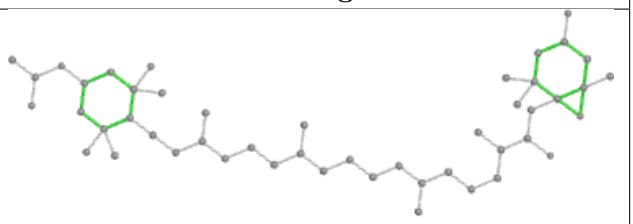
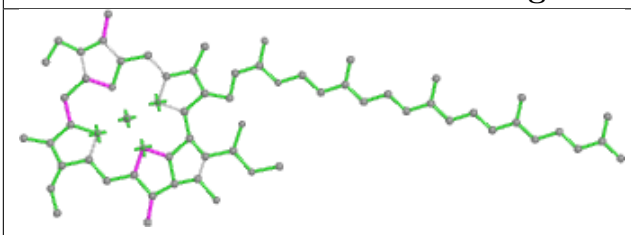

Rings

Ligand CLA 6 305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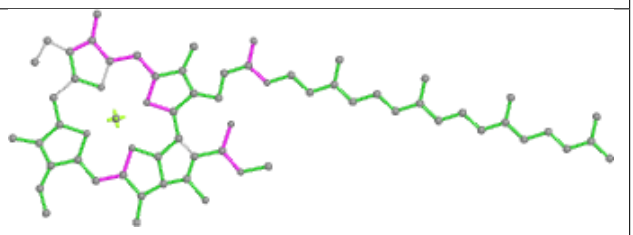
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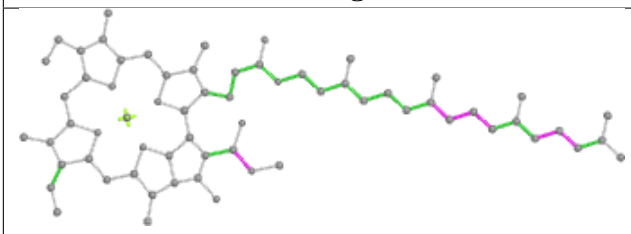
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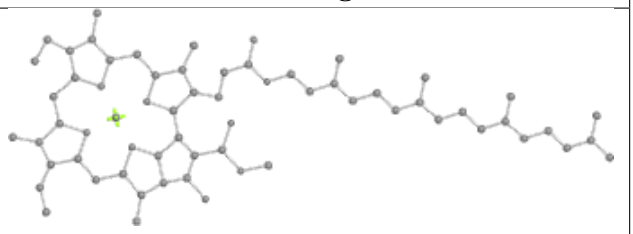
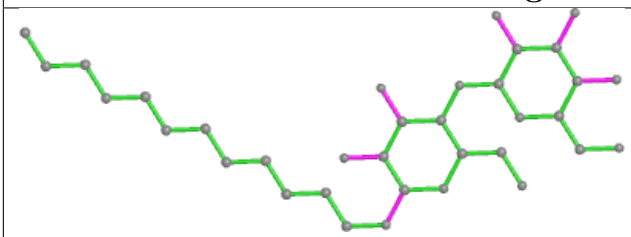

Rings

Ligand LMT 7 319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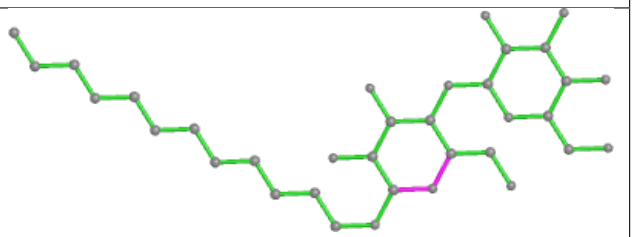
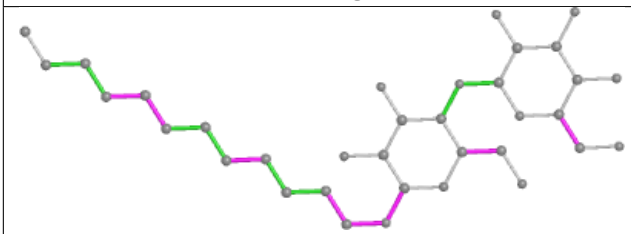

Bond angles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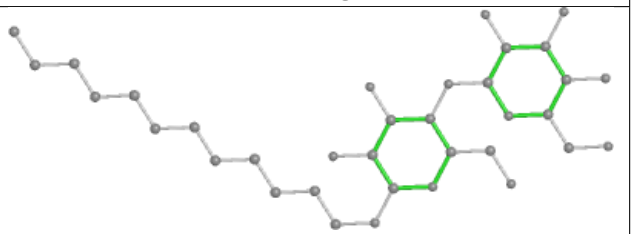
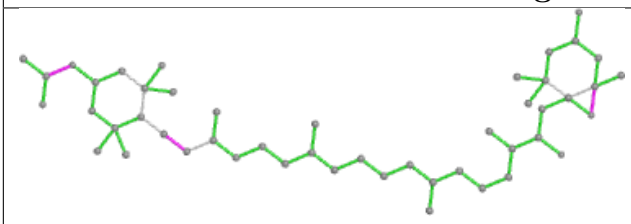

Rings

Ligand A86 8 304



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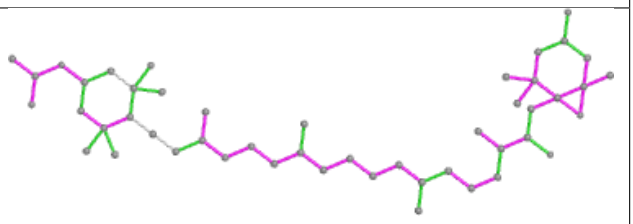

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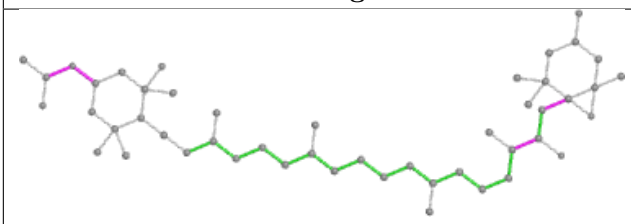

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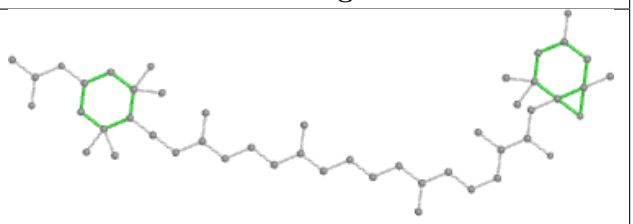
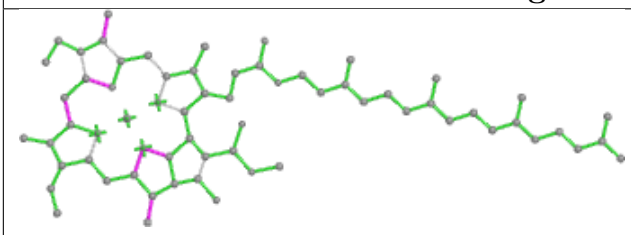


Rings

Ligand CLA 7 308



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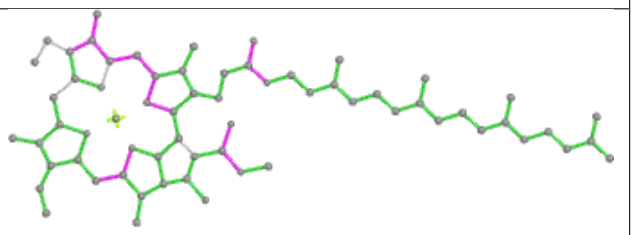
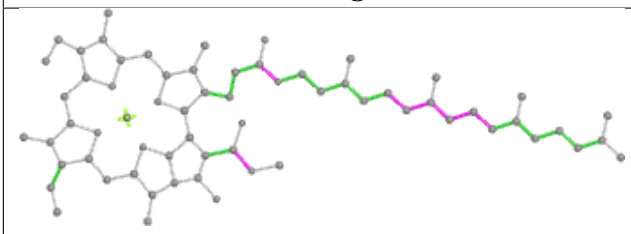


Bond angles



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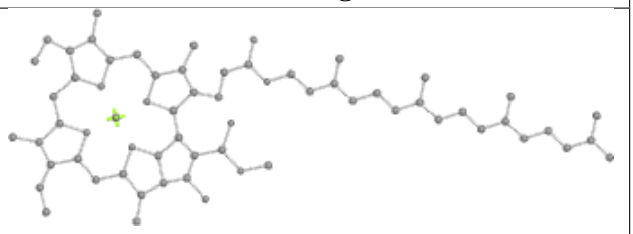
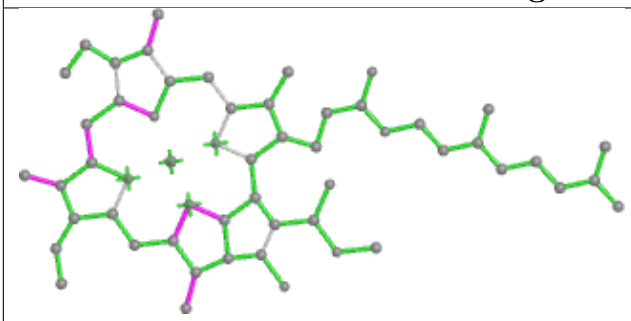


Rings

Ligand CLA 6 308



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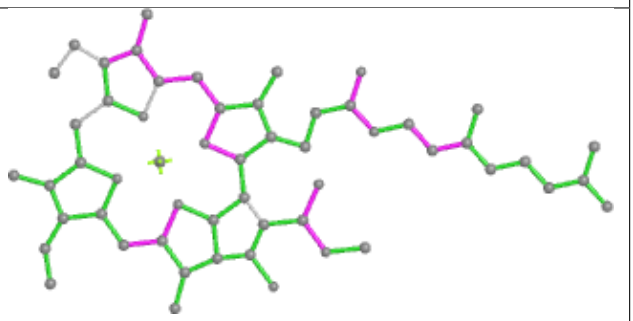
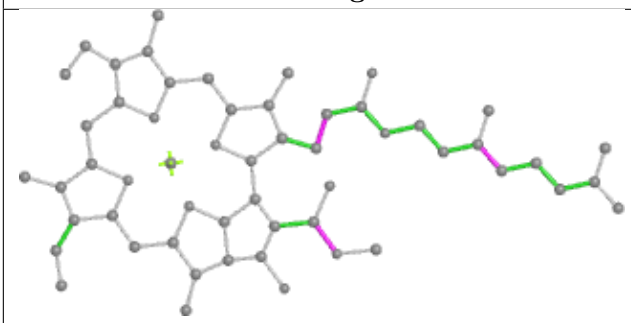
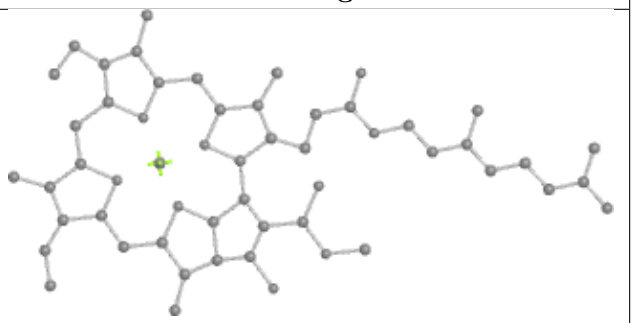


Bond angles

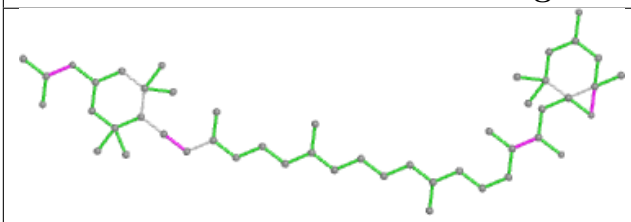


Torsions



Rings

Ligand A86 9 303



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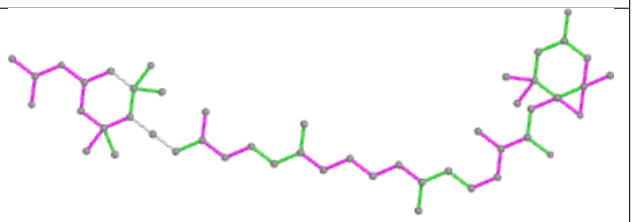
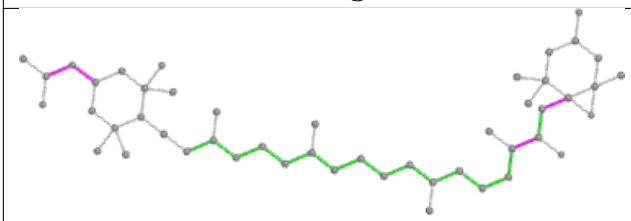


Bond angles



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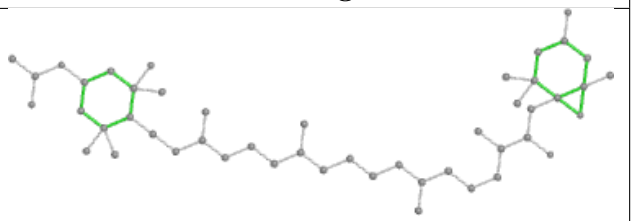
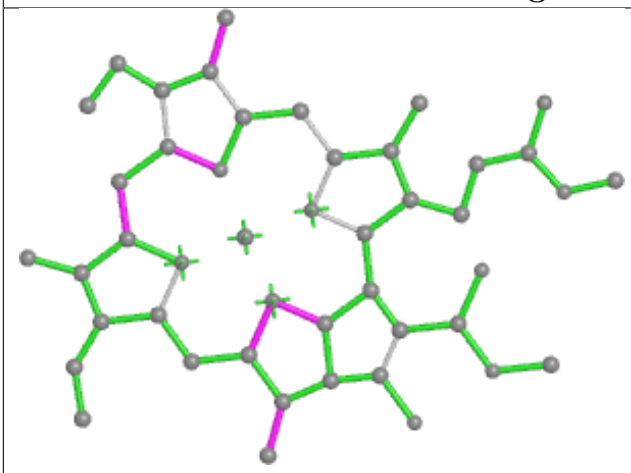


Rings

Ligand CLA 9 312



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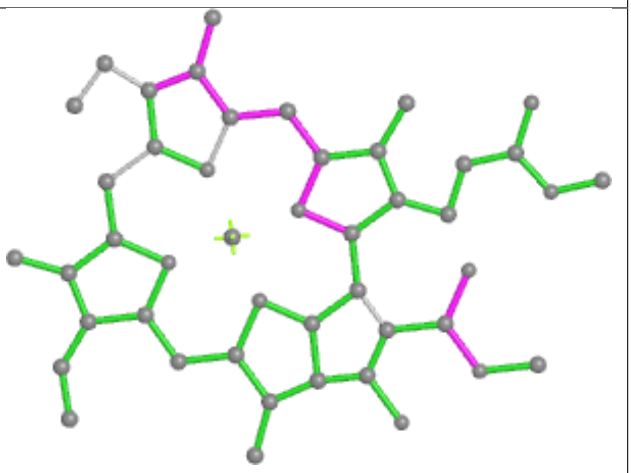

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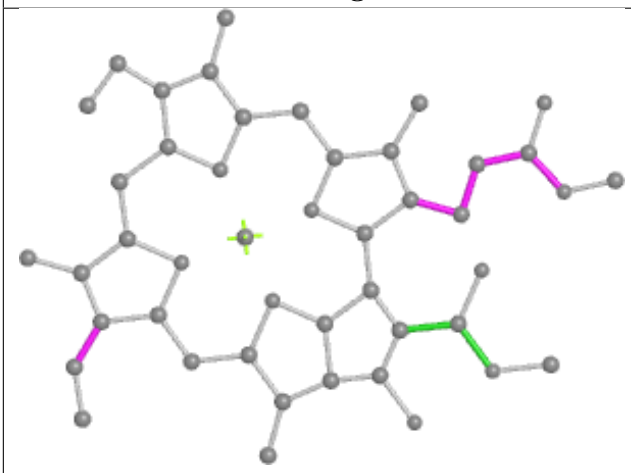
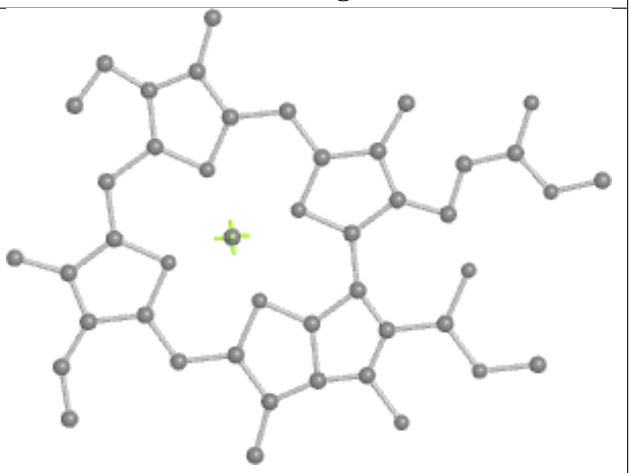


Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

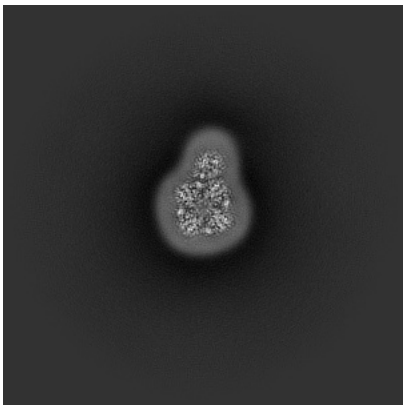
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37442. These allow visual inspection of the internal detail of the map and identification of artifacts.

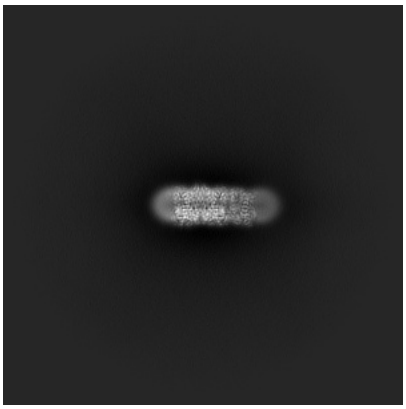
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

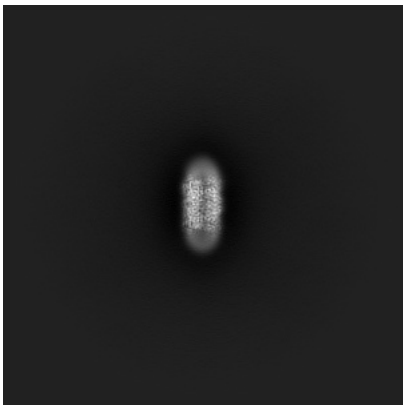
6.1.1 Primary map



X

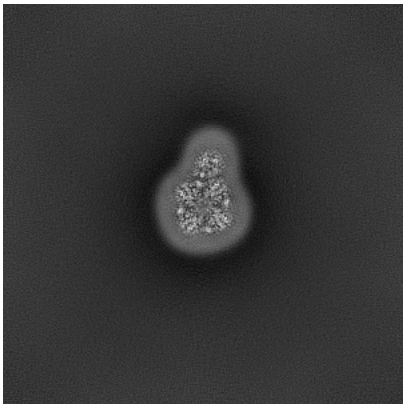


Y

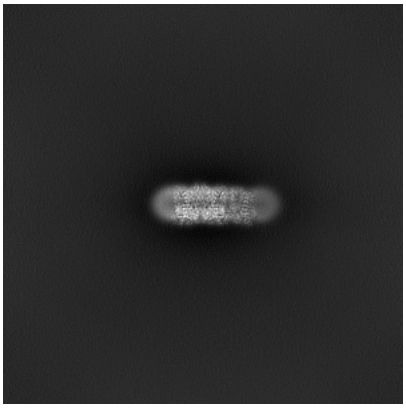


Z

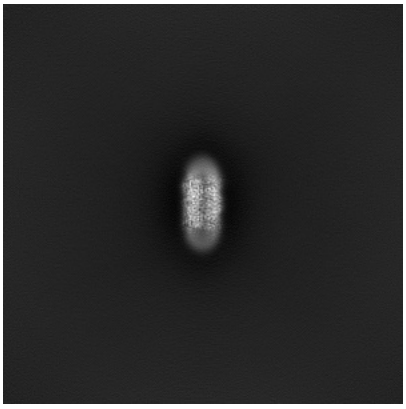
6.1.2 Raw map



X



Y

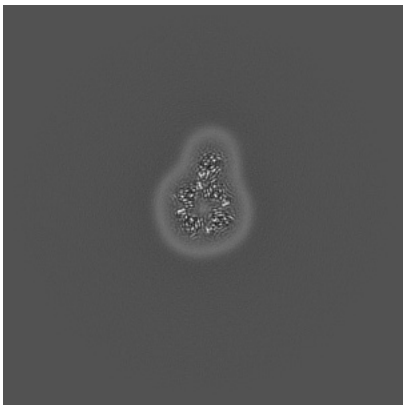


Z

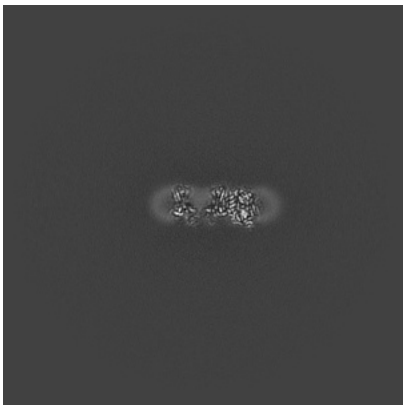
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

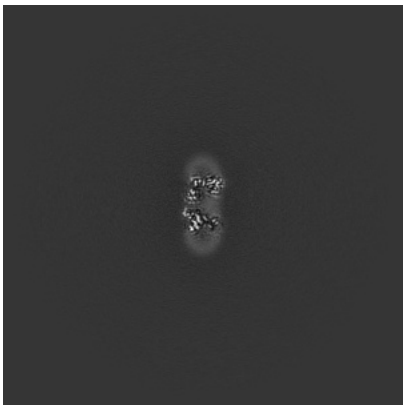
6.2.1 Primary map



X Index: 240

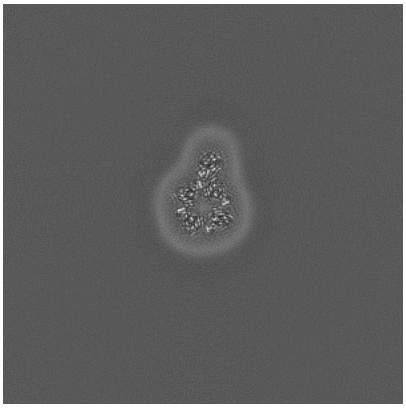


Y Index: 240

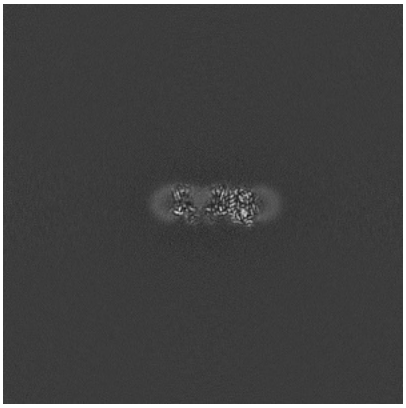


Z Index: 240

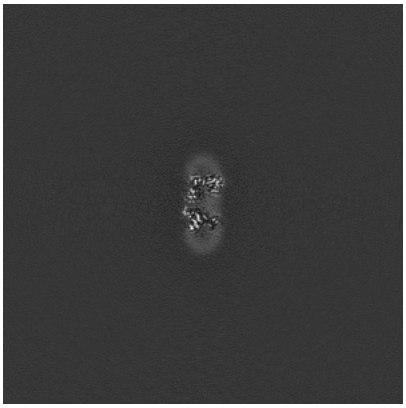
6.2.2 Raw map



X Index: 240



Y Index: 240

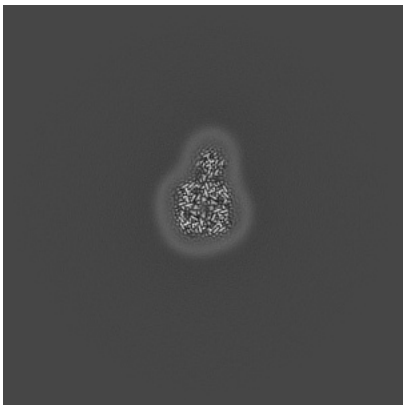


Z Index: 240

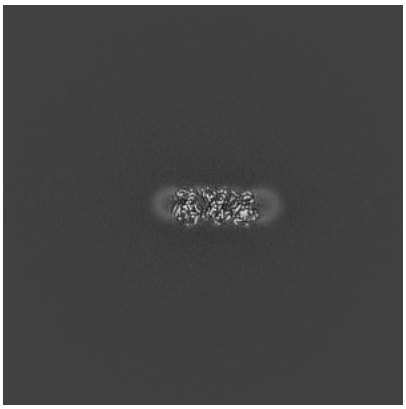
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

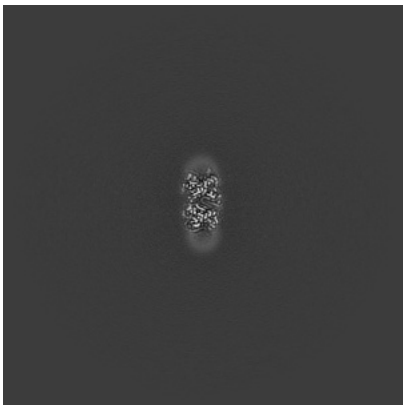
6.3.1 Primary map



X Index: 233

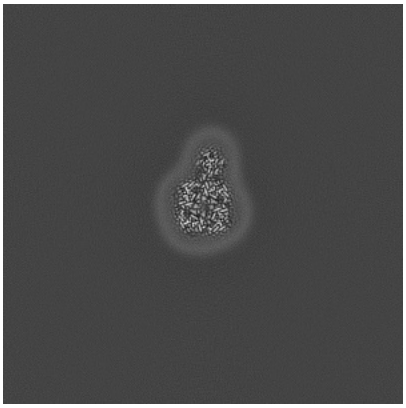


Y Index: 256

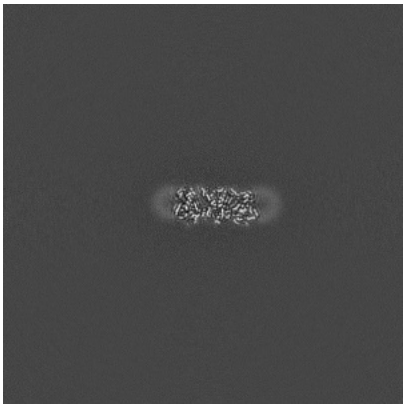


Z Index: 220

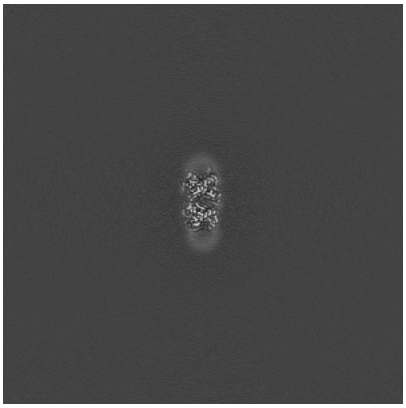
6.3.2 Raw map



X Index: 233



Y Index: 255

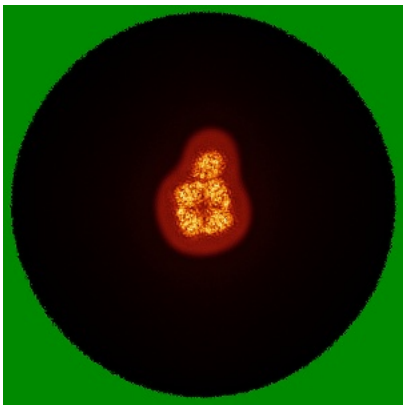


Z Index: 220

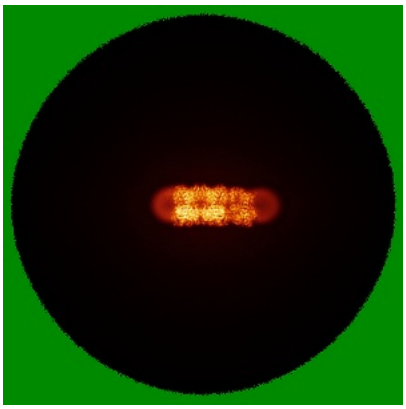
The images above show the largest variance slices of the map in three orthogonal directions.

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

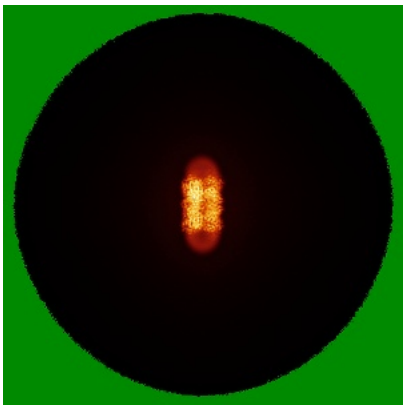
6.4.1 Primary map



X

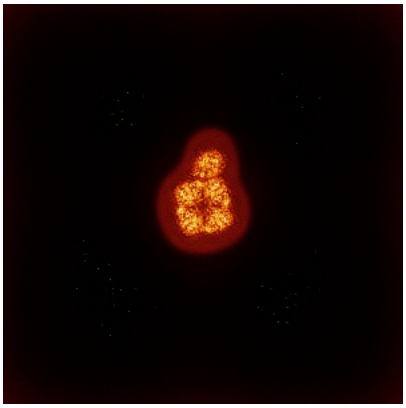


Y

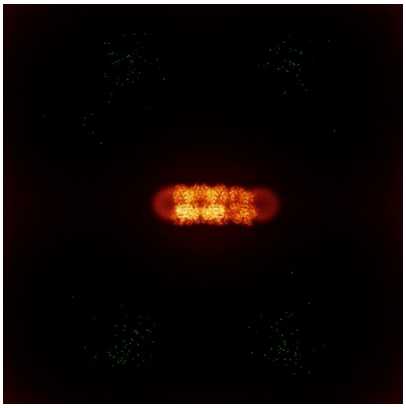


Z

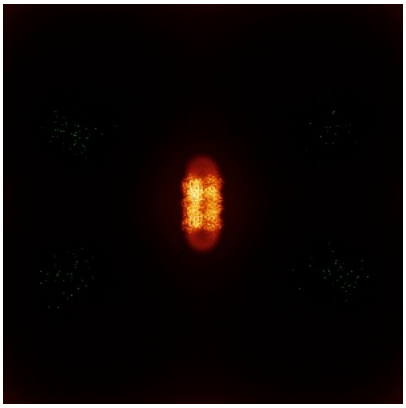
6.4.2 Raw map



X



Y

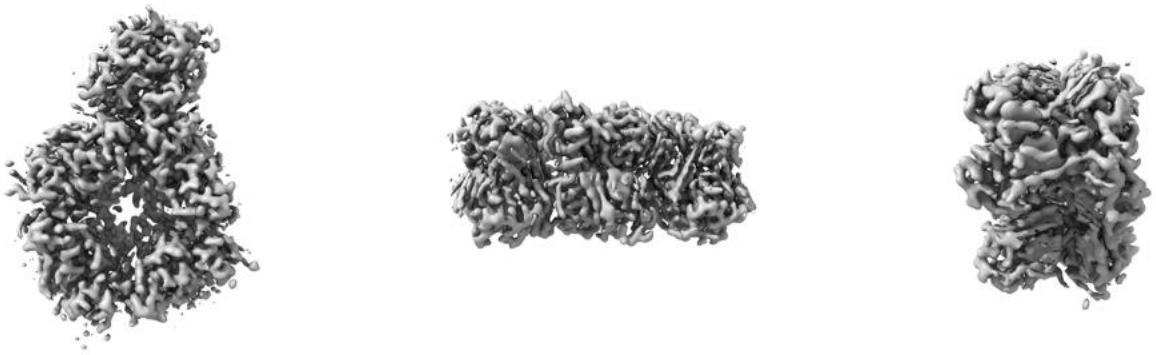


Z

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)

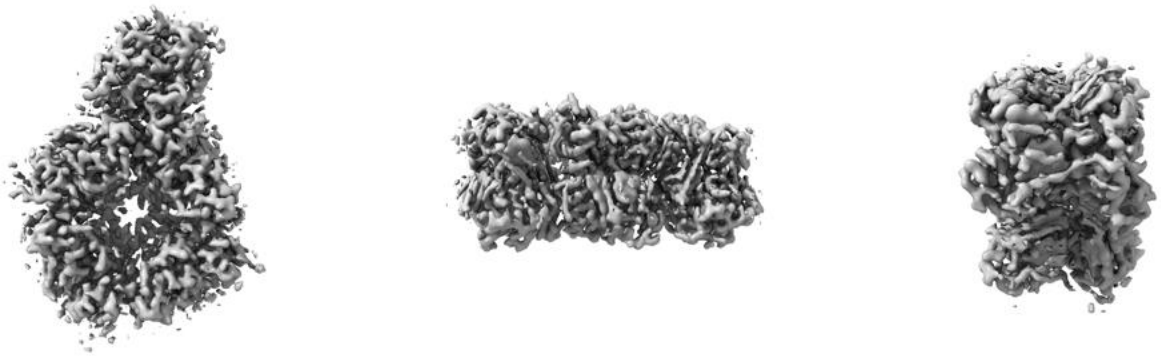
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.27. 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.

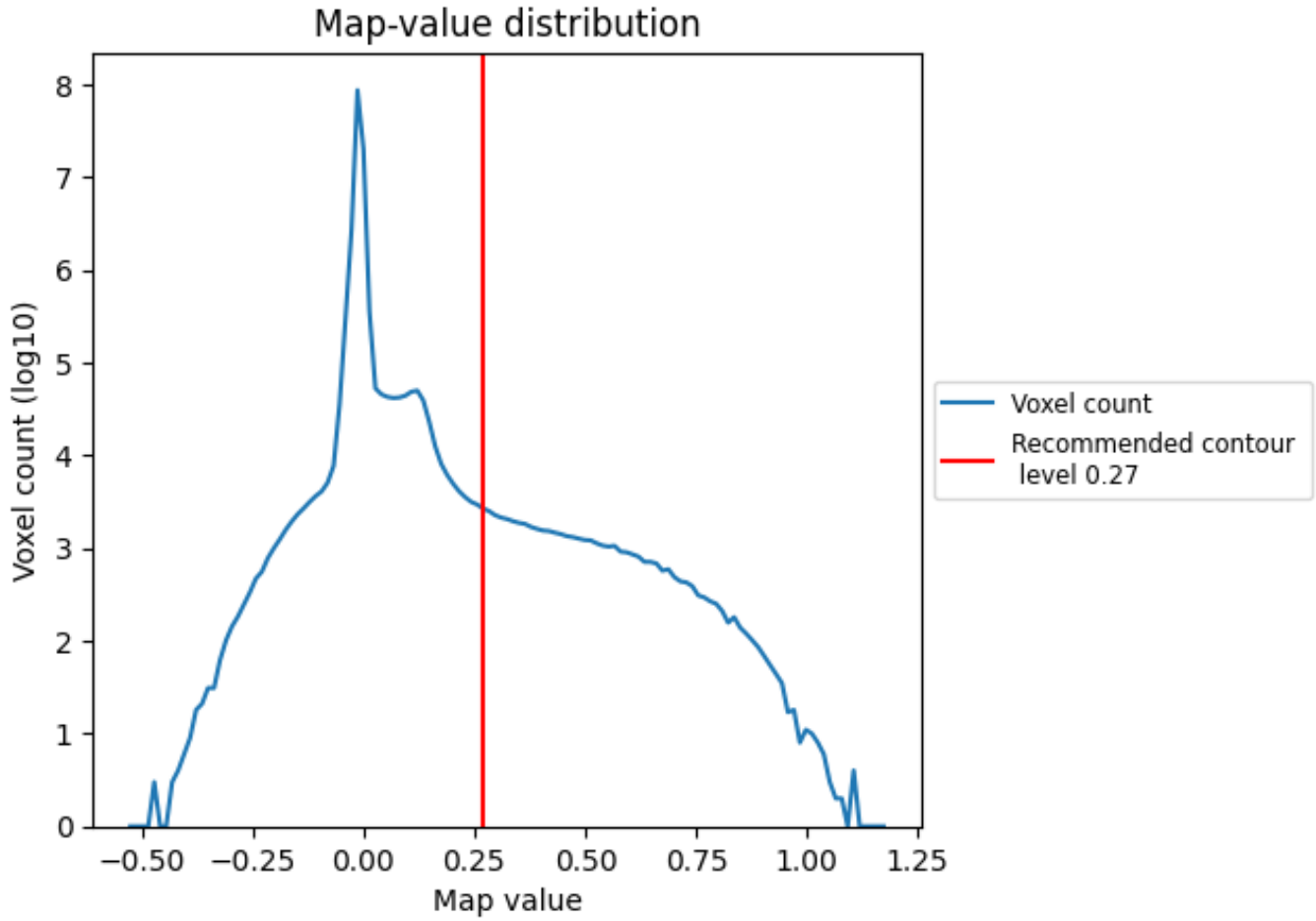
6.6 Mask visualisation (i)

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

7 Map analysis

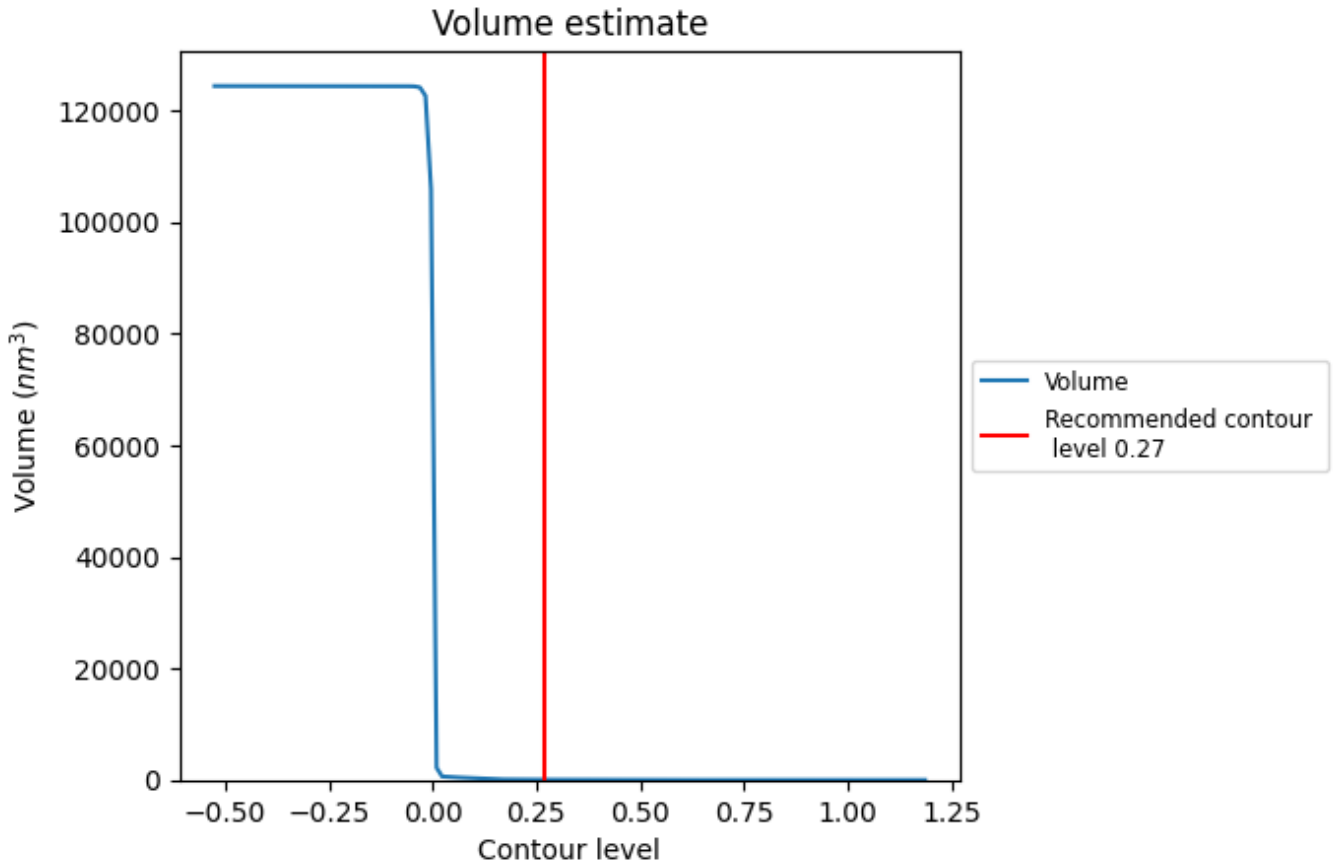
This section contains the results of statistical analysis of the map.

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.

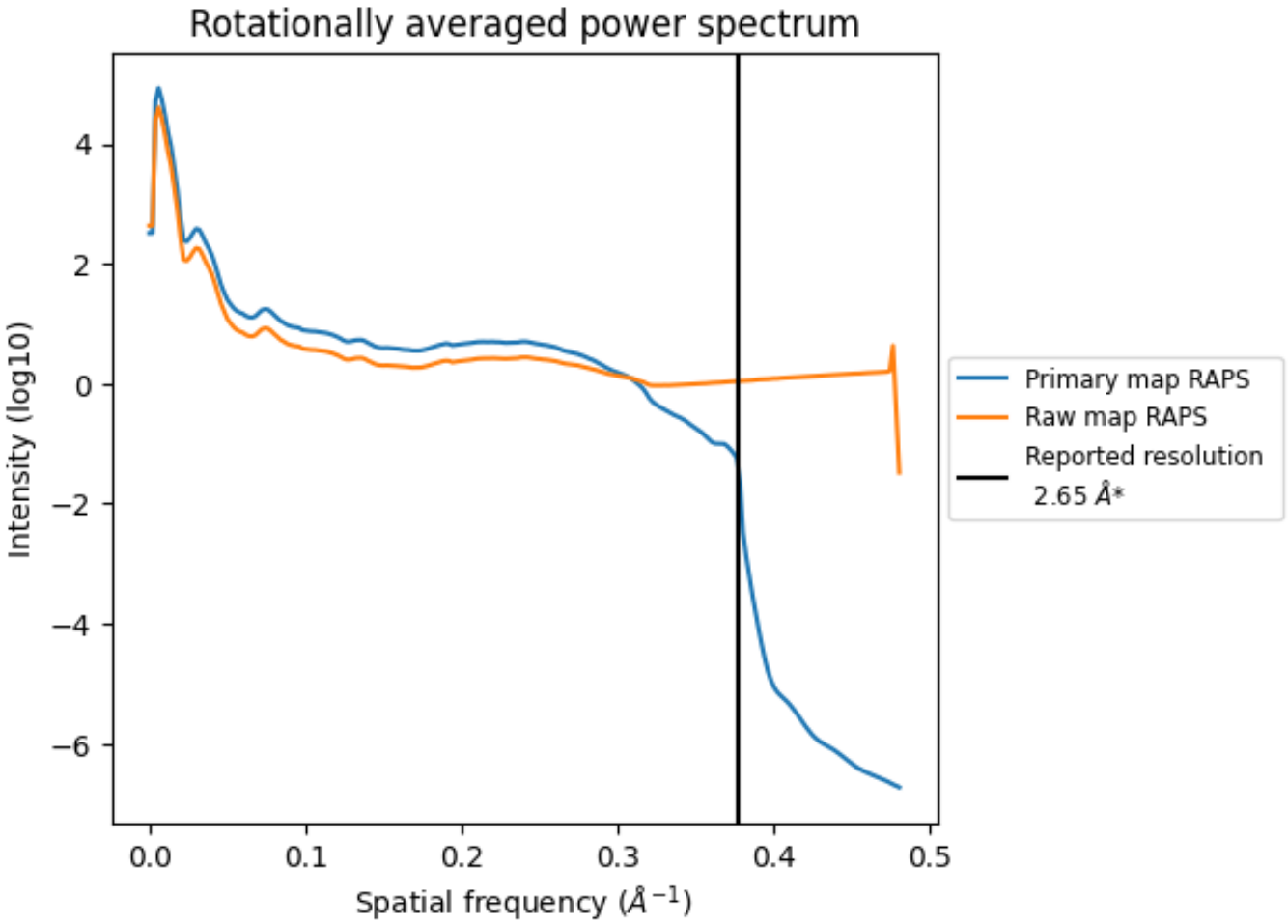
7.2 Volume estimate



The volume at the recommended contour level is 54 nm^3; this corresponds to an approximate mass of 49 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)

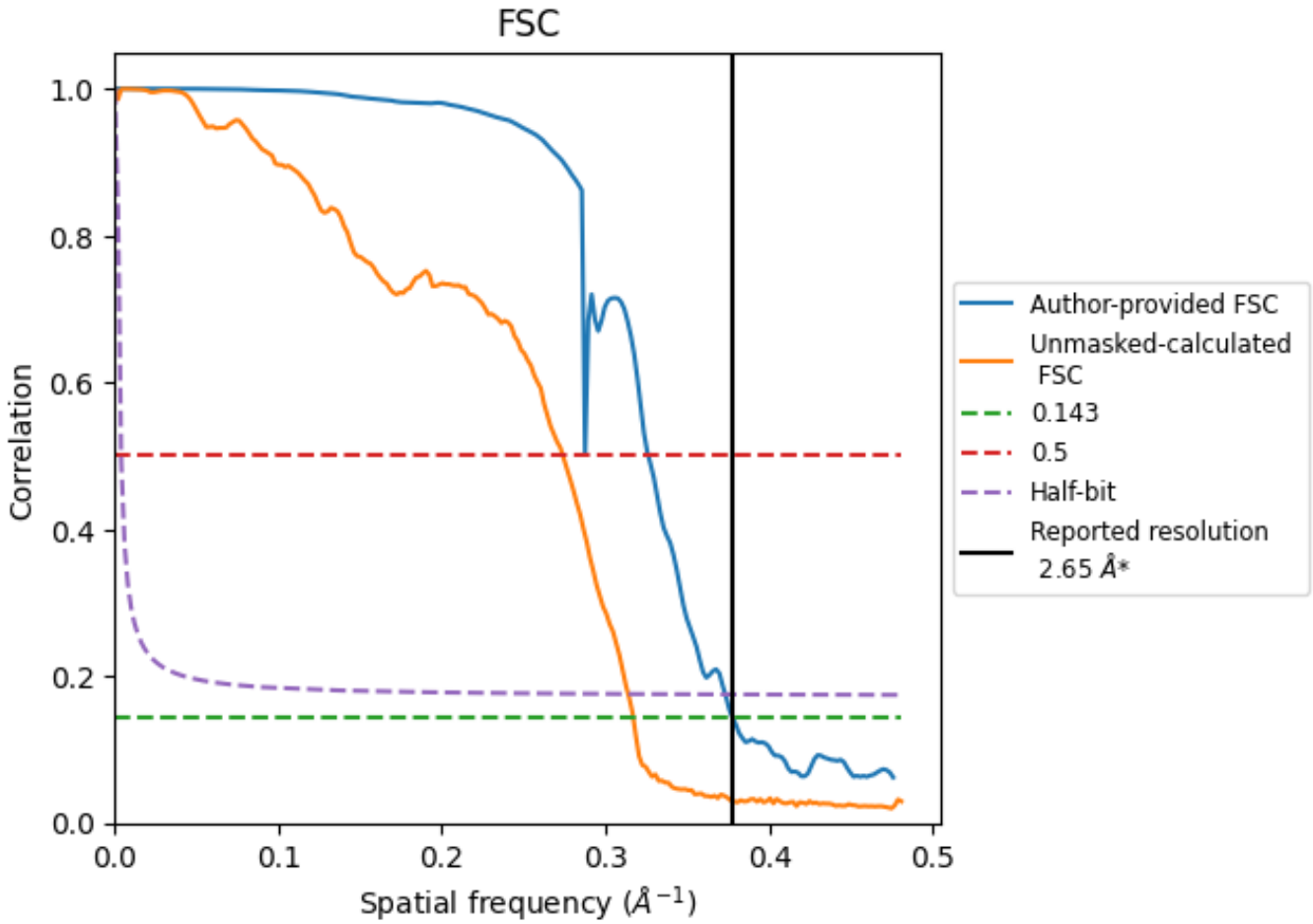


*Reported resolution corresponds to spatial frequency of 0.377 Å^{-1}

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 0.377 Å^{-1}

8.2 Resolution estimates (i)

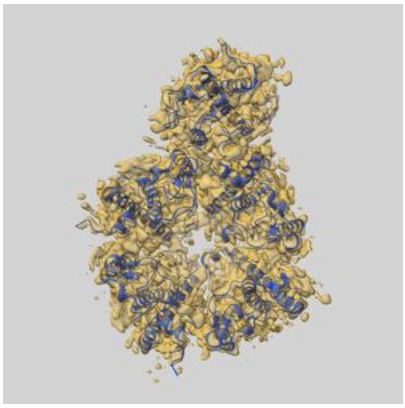
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.65	3.07	2.68
Unmasked-calculated*	3.16	3.65	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.16 differs from the reported value 2.65 by more than 10 %

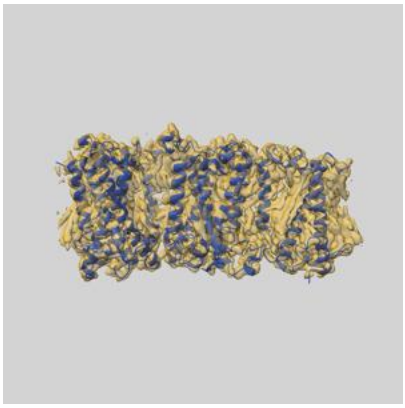
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37442 and PDB model 8WCL. Per-residue inclusion information can be found in section 3 on page 13.

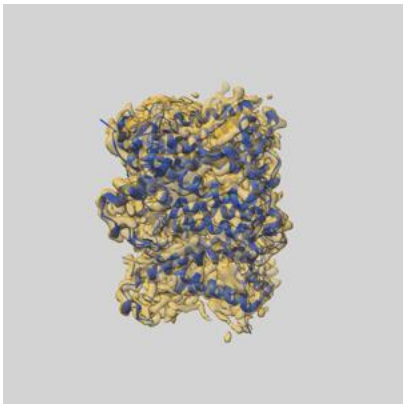
9.1 Map-model overlay



X



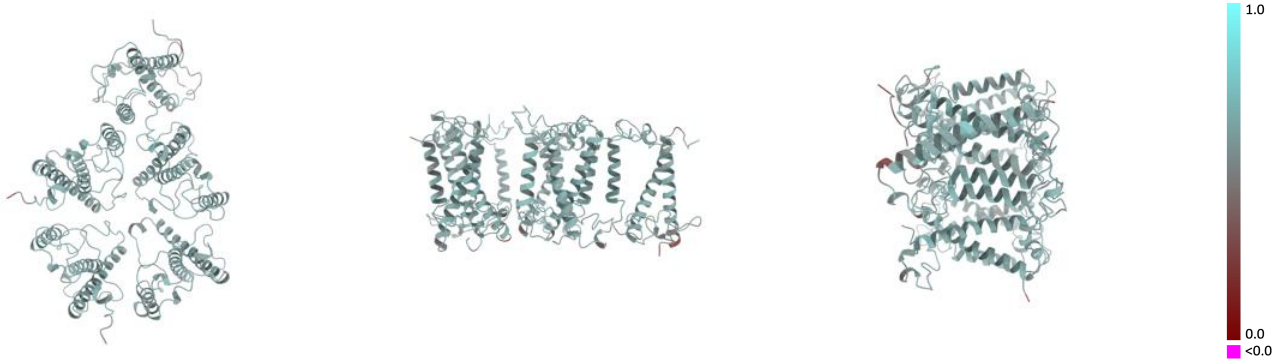
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

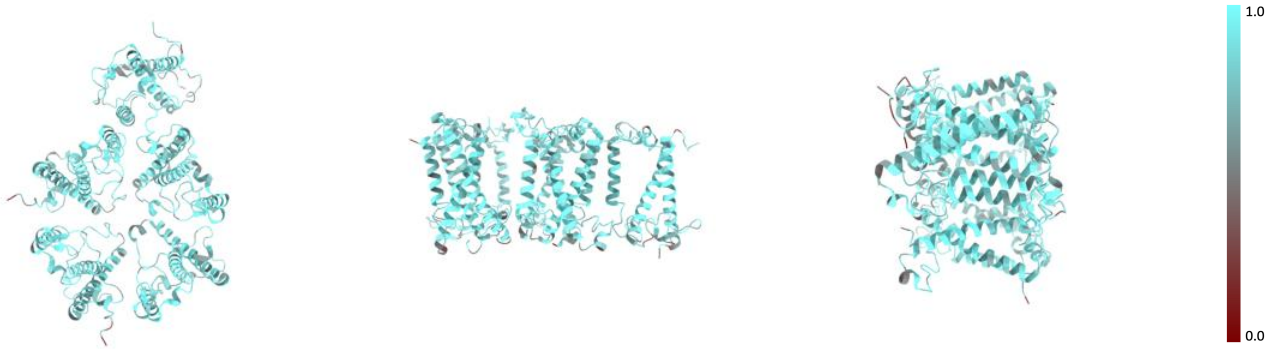
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

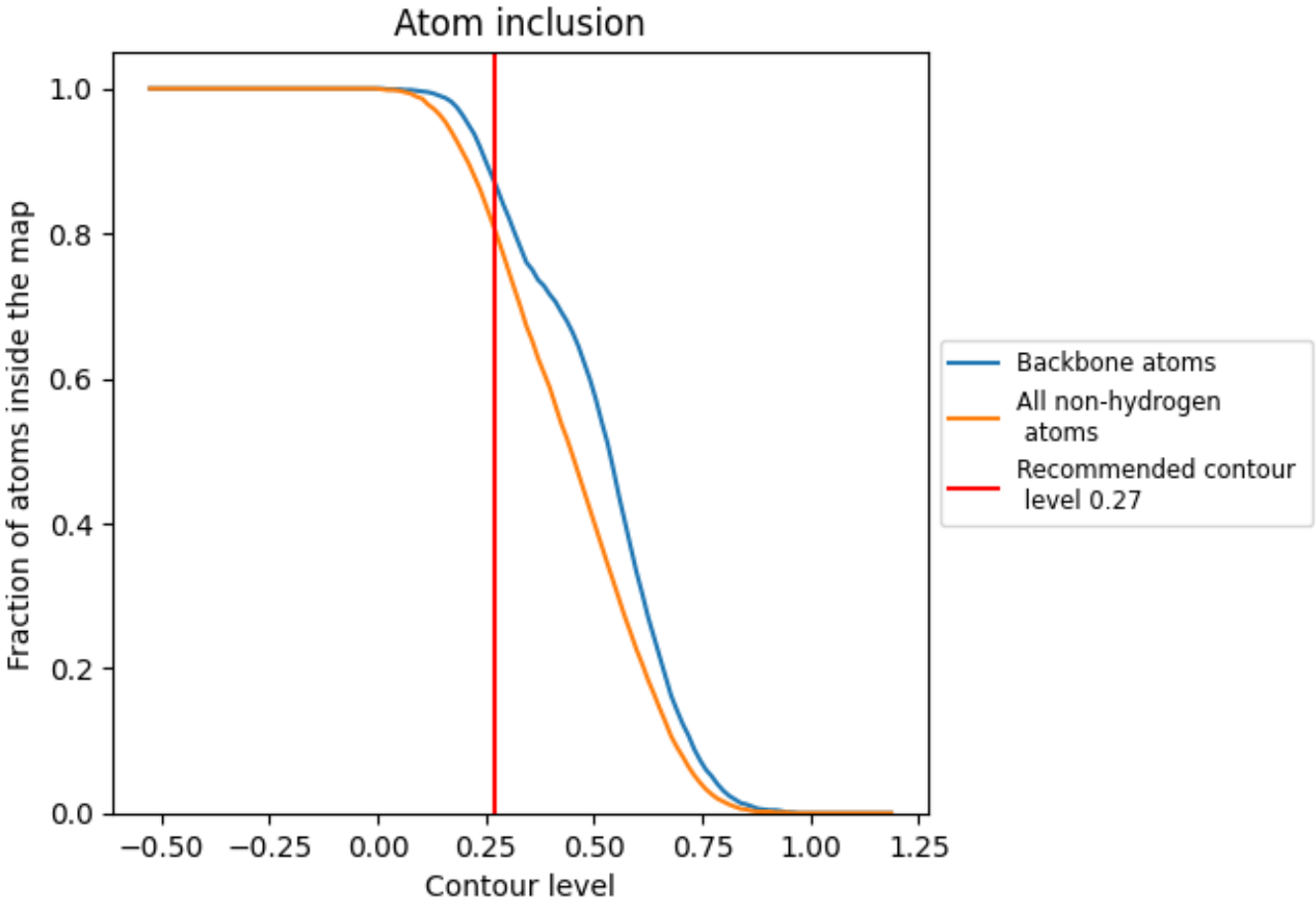
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.27).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 81% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.5850
5	0.8050	0.5850
6	0.8220	0.5840
7	0.8110	0.5930
8	0.8110	0.5900
9	0.7850	0.5720